

# wwPDB EM Map/Model Validation Report (i)

#### Aug 31, 2016 – 03:32 PM BST

PDB ID : 1gr5

EMDB ID: : EMD-1042

Title: Solution Structure of apo GroEL by Cryo-Electron microscopy

Authors: Ranson, N.A.; Farr, G.W.; Roseman, A.M.; Gowen, B.; Fenton, W.A.; Hor-

wich, A.L.; Saibil, H.R.

Deposited on : 2001-12-14

Resolution: 7.90 Å(reported)

Based on PDB ID : 1DER

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry. For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

http://wwpdb.org/validation/2016/EMValidationReportHelp

MolProbity: 4.02b-467

Mogul: NOT EXECUTED

Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)

EM map analysis : Beta 0.1

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)

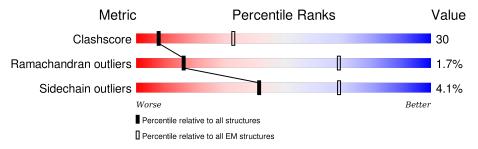
Validation Pipeline (wwPDB-VP) : trunk27980

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 7.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of ch	ain	
1	A	547	59%	33%	• 5%
1	В	547	60%	33%	• 5%
1	С	547	61%	32%	• 5%
1	D	547	60%	33%	• 5%
1	Е	547	60%	33%	• 5%
1	F	547	60%	33%	• 5%
1	G	547	60%	33%	• 5%
1	Н	547	59%	34%	• 5%
1	I	547	58%	34%	• 5%



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Mol	Chain	Length	Quality of cl	hain	
1	ī	547			
1	J	347	58%	35%	• 5%
1	K	547	58%	34%	• 5%
1	${ m L}$	547			
1	Ъ	347	58%	35%	• 5%
1	Μ	547	58%	35%	• 5%
-	NT	F 4 F			
1	N	547	58%	35%	• 5%



### 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 52668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called 60 KDA CHAPERONIN.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	۸	F 1 77	Total	С	N	О	S	0	0
1	A	517	3762	2372	614	757	19	0	0
1	В	517	Total	С	N	О	S	0	0
1	Б	917	3762	2372	614	757	19	0	0
1	С	517	Total	С	Ν	О	S	0	0
1		911	3762	2372	614	757	19	U	U
1	D	517	Total	С	N	О	S	0	0
1	D	911	3762	2372	614	757	19	U	U
1	Е	517	Total	С	N	О	S	0	0
1	Ľ	911	3762	2372	614	757	19	U	U
1	F	517	Total	С	N	О	S	0	0
1	I.	917	3762	2372	614	757	19		0
1	G	517	Total	С	Ν	О	S	0	0
1	G	917	3762	2372	614	757	19	U	U
1	Н	517	Total	С	Ν	О	S	0	0
1	11	917	3762	2372	614	757	19	U	0
1	I	517	Total	$^{\mathrm{C}}$	N	Ο	$\mathbf{S}$	0	0
1	1	917	3762	2372	614	757	19	U	U
1	J	517	Total	С	Ν	О	S	0	0
1	9	917	3762	2372	614	757	19	U	U
1	K	517	Total	С	N	О	S	0	0
1	11	917	3762	2372	614	757	19	U	U
1	L	517	Total	С	N	Ο	S	0	0
1	П	917	3762	2372	614	757	19	U	U
1	M	517	Total	С	N	О	S	0	0
1	111	011	3762	2372	614	757	19	U	U
1	N	517	Total	С	Ν	О	S	0	0
1	1 1	011	3762	2372	614	757	19	U	

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
A	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6



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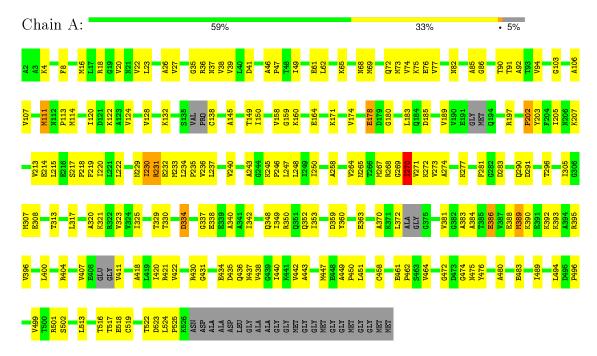
Chain	Residue	Modelled	Actual	Comment	Reference
В	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
В	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
С	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
С	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
D	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
D	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
Е	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
Е	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
F	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
F	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
G	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
G	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
Н	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
Н	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
I	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
I	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
J	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
J	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
K	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
K	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
L	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
L	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
M	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
M	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6
N	13	GLY	ARG	ENGINEERED MUTATION	UNP P0A6F6
N	126	VAL	ALA	ENGINEERED MUTATION	UNP P0A6F6

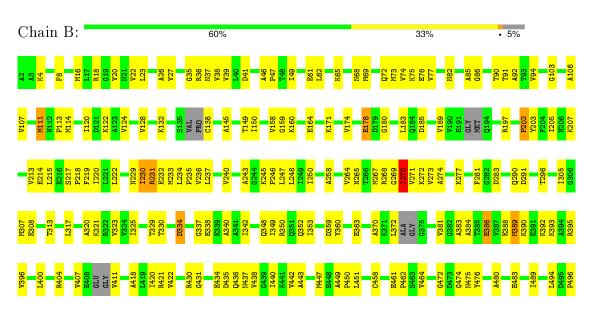


#### 3 Residue-property plots (i)

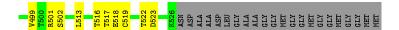
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

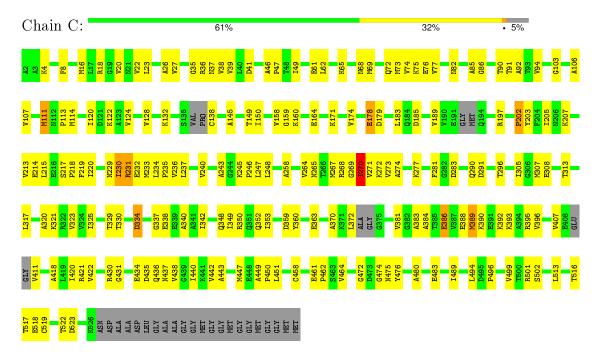
• Molecule 1: 60 KDA CHAPERONIN



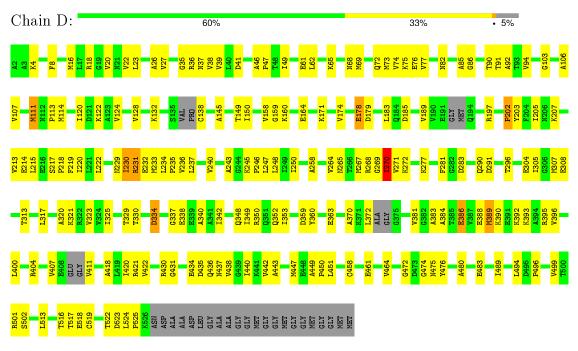








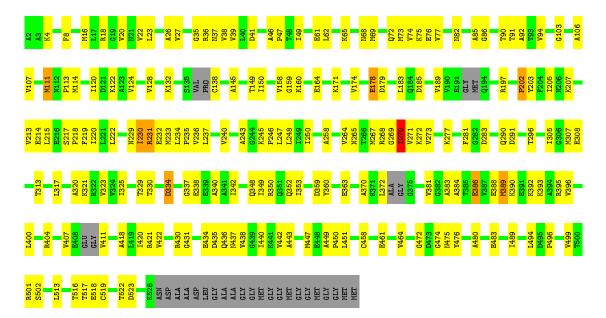
• Molecule 1: 60 KDA CHAPERONIN

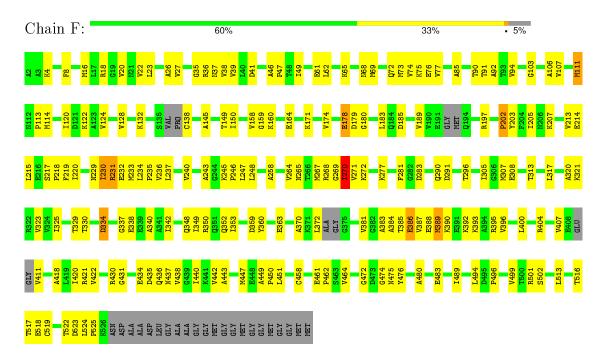


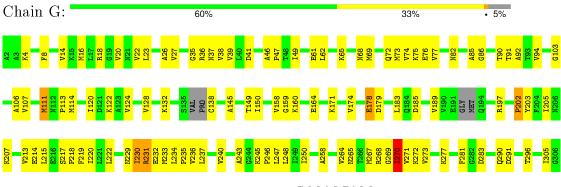
• Molecule 1: 60 KDA CHAPERONIN

Chain E: 60% 33% • 5%

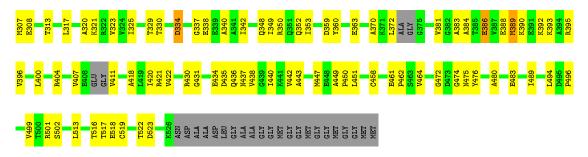


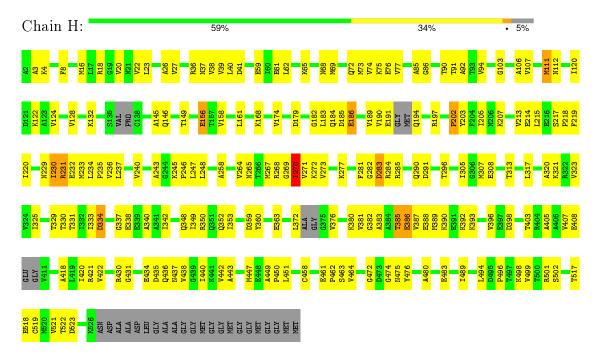


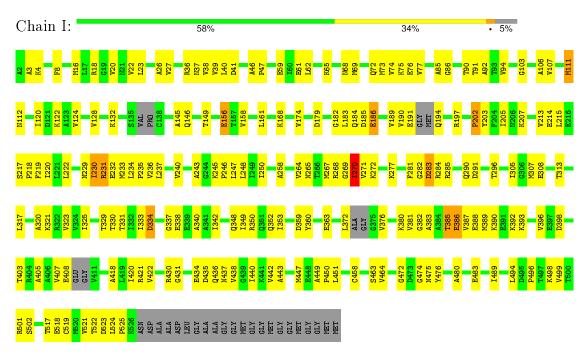




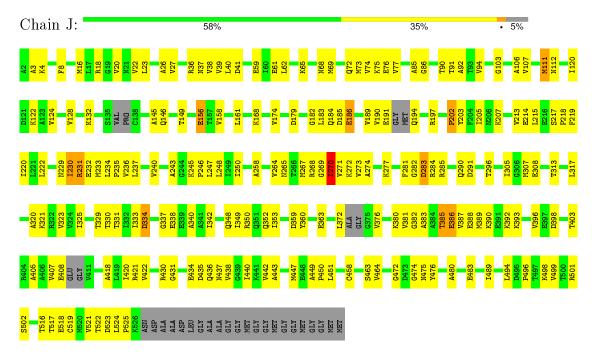




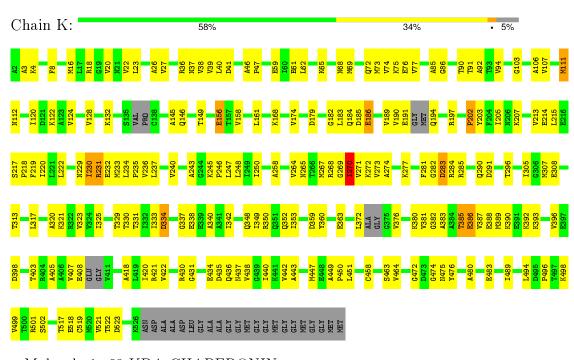


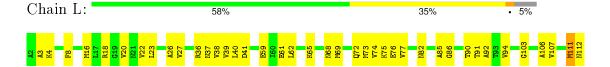




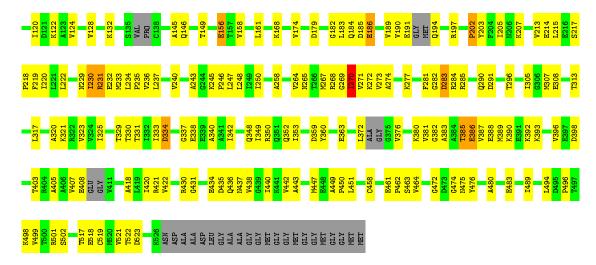


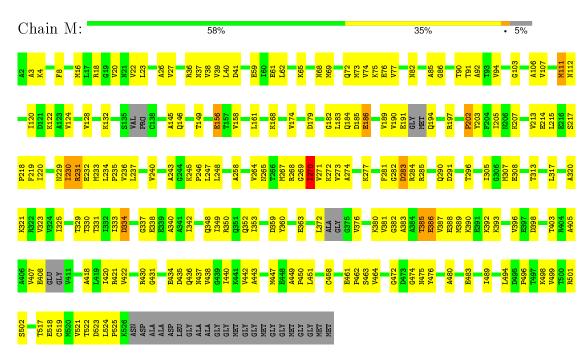
• Molecule 1: 60 KDA CHAPERONIN

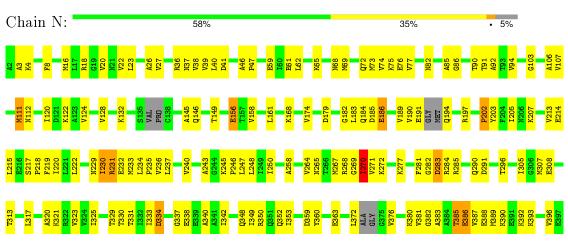




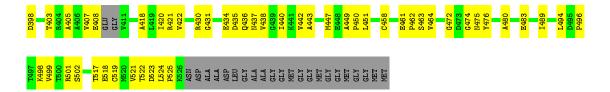














# 4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CLASS AVERAGES	Depositor
Microscope	FEI CM200	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	40200	Depositor
Image detector	KODAK SO-163 FILM	Depositor

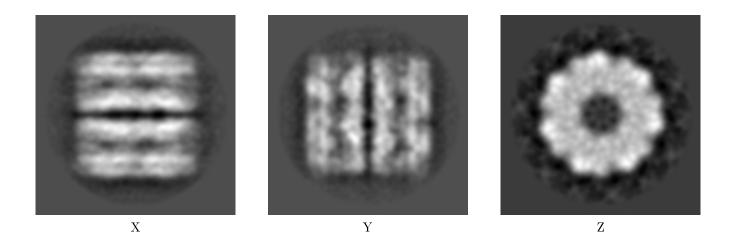


# 5 Visual analysis (i)

### 5.1 Map parameters (i)

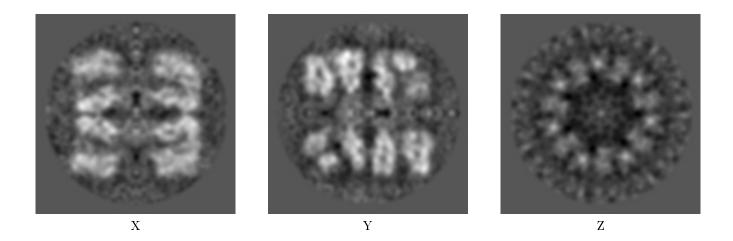
Property	Value
Endianness	big-endian
Voxel size (Å)	1.74
Axis order	XYZ
Grid points in X	128
Grid points in Y	128
Grid points in Z	128
Minimum density	-0.319
Maximum density	0.646
Average density	0.0243
Standard deviation of density	0.102
Range of density values	0.965
Recommended contour level	0.285

## 5.2 Orthogonal projections (i)

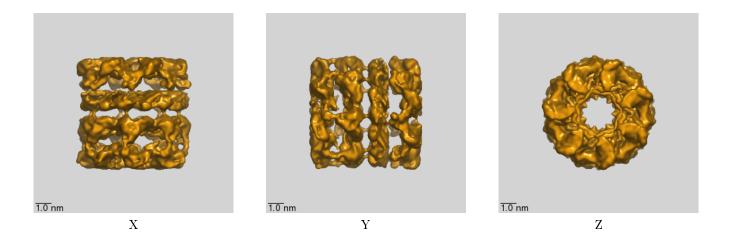




## 5.3 Central slices (i)

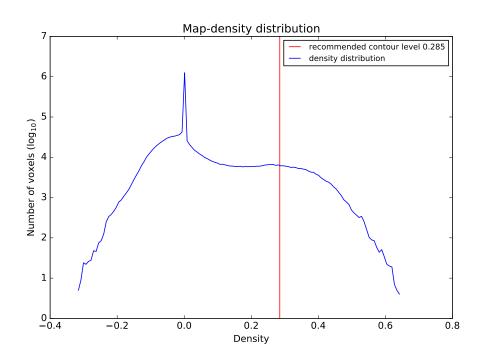


# 5.4 Orthogonal surface views (i)

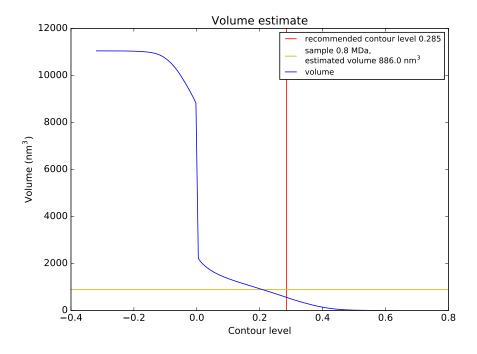




#### 5.5 Map-density distribution (i)

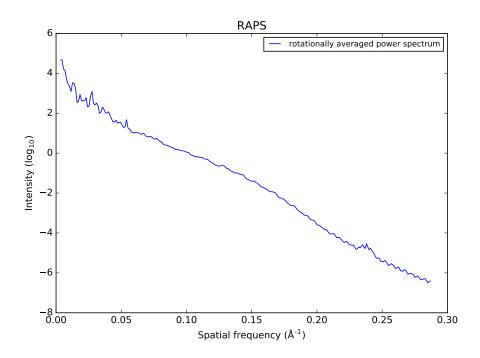


### 5.6 Volume estimate versus contour level 🥦

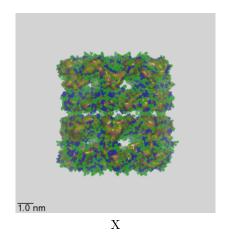


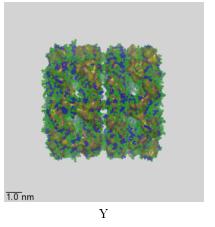


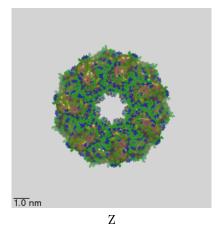
### 5.7 Rotationally-averaged power spectrum (i)



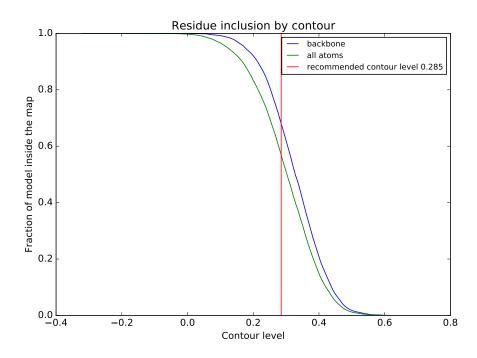
### 5.8 Model-to-map fit (i)



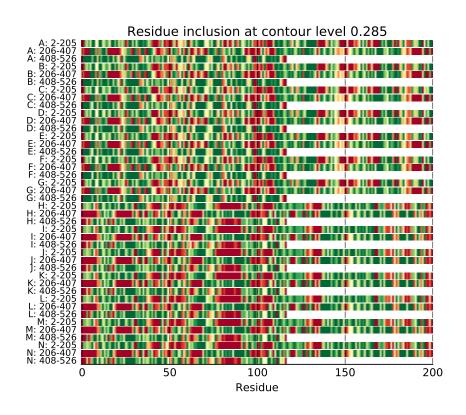




#### 5.9 Residue inclusion versus contour level (i)



#### 5.10 Residue inclusion at recommended contour level (i)





## 6 Model quality (i)

#### 6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Chain		ond lengths	Bond angles		
IVIOI			# Z >2	RMSZ	# Z >2	
1	A	1.43	$2/7570 \ (0.0\%)$	0.56	$2/10186 \; (0.0\%)$	
1	В	1.43	$2/7570 \ (0.0\%)$	0.56	$2/10186 \ (0.0\%)$	
1	С	1.43	$2/7570 \ (0.0\%)$	0.56	$2/10186 \ (0.0\%)$	
1	D	1.43	2/7570~(0.0%)	0.56	$2/10186 \ (0.0\%)$	
1	E	1.43	2/7570~(0.0%)	0.56	$2/10186 \ (0.0\%)$	
1	F	1.43	2/7570~(0.0%)	0.56	$2/10186 \ (0.0\%)$	
1	G	1.43	2/7570~(0.0%)	0.56	$2/10186 \ (0.0\%)$	
1	Н	0.27	0/7570	0.55	0/10186	
1	I	0.27	0/7570	0.55	0/10186	
1	J	0.27	0/7570	0.55	0/10186	
1	K	0.27	0/7570	0.55	0/10186	
1	L	0.27	0/7570	0.55	0/10186	
1	М	0.27	0/7570	0.55	0/10186	
1	N	0.27	0/7570	0.55	0/10186	
All	All	1.03	$14/105980 \ (0.0\%)$	0.55	$14/142604 \ (0.0\%)$	

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	E	386	GLU	CB-CG	86.48	3.16	1.52
1	Е	386	GLU	CB-CG	86.48	3.16	1.52
1	G	386	GLU	CB-CG	86.47	3.16	1.52
1	G	386	GLU	CB-CG	86.47	3.16	1.52
1	A	386	GLU	CB-CG	86.47	3.16	1.52
1	A	386	GLU	CB-CG	86.47	3.16	1.52
1	С	386	GLU	CB-CG	86.46	3.16	1.52
1	С	386	GLU	CB-CG	86.46	3.16	1.52
1	D	386	GLU	CB-CG	86.46	3.16	1.52
1	D	386	GLU	CB-CG	86.46	3.16	1.52
1	В	386	GLU	CB-CG	86.45	3.16	1.52
1	В	386	GLU	CB-CG	86.45	3.16	1.52
1	F	386	GLU	CB-CG	86.45	3.16	1.52
1	F	386	GLU	CB-CG	86.45	3.16	1.52



All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	D	386	GLU	CA-CB-CG	7.43	129.74	113.40
1	D	386	GLU	CA-CB-CG	7.43	129.74	113.40
1	F	386	GLU	CA-CB-CG	7.43	129.74	113.40
1	F	386	GLU	CA-CB-CG	7.43	129.74	113.40
1	В	386	GLU	CA-CB-CG	7.42	129.73	113.40
1	В	386	GLU	CA-CB-CG	7.42	129.73	113.40
1	A	386	GLU	CA-CB-CG	7.42	129.73	113.40
1	A	386	GLU	CA-CB-CG	7.42	129.73	113.40
1	С	386	GLU	CA-CB-CG	7.42	129.72	113.40
1	С	386	GLU	CA-CB-CG	7.42	129.72	113.40
1	G	386	GLU	CA-CB-CG	7.42	129.72	113.40
1	G	386	GLU	CA-CB-CG	7.42	129.72	113.40
1	E	386	GLU	CA-CB-CG	7.41	129.70	113.40
1	Е	386	GLU	CA-CB-CG	7.41	129.70	113.40

There are no chirality outliers.

There are no planarity outliers.

#### 6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3762	0	3841	341	0
1	В	3762	0	3841	339	0
1	С	3762	0	3841	342	0
1	D	3762	0	3841	338	0
1	E	3762	0	3841	339	0
1	F	3762	0	3841	338	0
1	G	3762	0	3841	340	0
1	Н	3762	0	3837	317	0
1	I	3762	0	3837	318	0
1	J	3762	0	3837	318	0
1	K	3762	0	3837	314	0
1	L	3762	0	3837	319	0
1	M	3762	0	3837	326	0
1	N	3762	0	3837	321	0
All	All	52668	0	53746	3163	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (3163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \textbf{Interatomic} \\ \textbf{distance (Å)} \end{array}$	Clash overlap (Å)
1:C:47:PRO:CD	1:D:73:MET:HG2	1.20	1.64
1:D:47:PRO:CD	1:E:73:MET:HG2	1.20	1.63
1:A:150:ILE:CD1	1:A:411:VAL:HG11	1.15	1.62
1:B:150:ILE:CD1	1:B:411:VAL:HG11	1.15	1.62
1:B:47:PRO:CD	1:C:73:MET:HG2	1.20	1.62
1:E:47:PRO:CD	1:F:73:MET:HG2	1.20	1.59
1:G:150:ILE:CD1	1:G:411:VAL:HG11	1.16	1.59
1:C:150:ILE:CD1	1:C:411:VAL:HG11	1.15	1.59
1:A:47:PRO:CD	1:B:73:MET:HG2	1.20	1.58
1:A:73:MET:CG	1:G:47:PRO:HD2	1.33	1.58
1:F:47:PRO:HD2	1:G:73:MET:CG	1.33	1.58
1:F:47:PRO:CD	1:G:73:MET:HG2	1.20	1.57
1:A:73:MET:HG2	1:G:47:PRO:CD	1.20	1.56
1:F:150:ILE:CD1	1:F:411:VAL:HG11	1.15	1.56
1:D:150:ILE:CD1	1:D:411:VAL:HG11	1.15	1.55
1:A:47:PRO:HD2	1:B:73:MET:CG	1.33	1.55
1:E:47:PRO:HD2	1:F:73:MET:CG	1.33	1.55
1:E:150:ILE:CD1	1:E:411:VAL:HG11	1.15	1.55
1:D:47:PRO:HD2	1:E:73:MET:CG	1.33	1.54
1:B:47:PRO:HD2	1:C:73:MET:CG	1.33	1.54
1:C:46:ALA:HB2	1:D:76:GLU:CG	1.39	1.53
1:A:46:ALA:HB2	1:B:76:GLU:CG	1.39	1.53
1:A:37:ASN:HB2	1:B:516:THR:C	1.29	1.53
1:F:37:ASN:HB2	1:G:516:THR:C	1.29	1.52
1:C:47:PRO:HD2	1:D:73:MET:CG	1.33	1.52
1:E:46:ALA:HB2	1:F:76:GLU:CG	1.39	1.51
1:C:37:ASN:HB2	1:D:516:THR:C	1.29	1.50
1:D:37:ASN:HB2	1:E:516:THR:C	1.29	1.50
1:B:46:ALA:HB2	1:C:76:GLU:CG	1.39	1.49
1:A:76:GLU:CG	1:G:46:ALA:HB2	1.39	1.49
1:F:46:ALA:HB2	1:G:76:GLU:CG	1.39	1.49
1:D:46:ALA:HB2	1:E:76:GLU:CG	1.39	1.48
1:B:46:ALA:CB	1:C:76:GLU:HG3	1.43	1.48
1:A:516:THR:C	1:G:37:ASN:HB2	1.29	1.48
1:A:46:ALA:CB	1:B:76:GLU:HG3	1.43	1.48
1:C:46:ALA:CB	1:D:76:GLU:HG3	1.43	1.47
1:B:37:ASN:HB2	1:C:516:THR:C	1.29	1.47



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:L:386:GLU:CB	1:M:284:ARG:HE	1.05	1.46
1:D:46:ALA:CB	1:E:76:GLU:HG3	1.43	1.46
1:E:37:ASN:HB2	1:F:516:THR:C	1.29	1.46
1:A:76:GLU:HG3	1:G:46:ALA:CB	1.43	1.46
1:F:46:ALA:CB	1:G:76:GLU:HG3	1.43	1.46
1:J:386:GLU:CB	1:K:284:ARG:HE	1.05	1.45
1:E:46:ALA:CB	1:F:76:GLU:HG3	1.43	1.44
1:H:284:ARG:HE	1:N:386:GLU:CB	1.05	1.43
1:H:386:GLU:CB	1:I:284:ARG:HE	1.05	1.43
1:B:47:PRO:CD	1:C:73:MET:CG	1.89	1.43
1:D:386:GLU:CG	1:E:281:PHE:CE2	2.03	1.42
1:C:386:GLU:CG	1:D:281:PHE:CE2	2.03	1.42
1:E:386:GLU:CG	1:F:281:PHE:CE2	2.03	1.42
1:C:47:PRO:CD	1:D:73:MET:CG	1.89	1.42
1:B:386:GLU:CG	1:C:281:PHE:CE2	2.03	1.42
1:D:47:PRO:CD	1:E:73:MET:CG	1.89	1.41
1:A:386:GLU:CG	1:B:281:PHE:CE2	2.03	1.41
1:A:47:PRO:CD	1:B:73:MET:CG	1.89	1.40
1:A:281:PHE:CE2	1:G:386:GLU:CG	2.03	1.40
1:F:386:GLU:CG	1:G:281:PHE:CE2	2.03	1.39
1:M:386:GLU:CB	1:N:284:ARG:HE	1.05	1.38
1:E:47:PRO:CD	1:F:73:MET:CG	1.89	1.38
1:A:69:MET:HG2	1:G:41:ASP:OD1	1.20	1.36
1:I:386:GLU:CB	1:J:284:ARG:HE	1.05	1.36
1:K:386:GLU:CB	1:L:284:ARG:HE	1.05	1.36
1:A:41:ASP:CG	1:B:69:MET:HG2	1.46	1.35
1:F:47:PRO:CD	1:G:73:MET:CG	1.89	1.35
1:A:73:MET:CG	1:G:47:PRO:CD	1.89	1.35
1:A:69:MET:HG2	1:G:41:ASP:CG	1.46	1.35
1:E:41:ASP:OD1	1:F:69:MET:HG2	1.20	1.34
1:I:270:ILE:CG2	1:J:229:ASN:O	1.76	1.34
1:B:41:ASP:OD1	1:C:69:MET:HG2	1.20	1.33
1:J:270:ILE:CG2	1:K:229:ASN:O	1.76	1.33
1:B:41:ASP:CG	1:C:69:MET:HG2	1.46	1.33
1:H:270:ILE:CG2	1:I:229:ASN:O	1.76	1.33
1:K:270:ILE:CG2	1:L:229:ASN:O	1.76	1.32
1:H:229:ASN:O	1:N:270:ILE:CG2	1.76	1.32
1:C:41:ASP:CG	1:D:69:MET:HG2	1.46	1.32
1:F:41:ASP:CG	1:G:69:MET:HG2	1.46	1.32
1:L:270:ILE:CG2	1:M:229:ASN:O	1.76	1.32
1:A:516:THR:O	1:G:37:ASN:HB2	1.30	1.31



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance}\;({ m \AA})$	overlap (Å)
1:K:270:ILE:HG23	1:L:229:ASN:O	1.23	1.31
1:L:270:ILE:HG23	1:M:229:ASN:O	1.23	1.31
1:M:270:ILE:CG2	1:N:229:ASN:O	1.76	1.31
1:D:41:ASP:CG	1:E:69:MET:HG2	1.46	1.31
1:D:37:ASN:HB2	1:E:516:THR:O	1.30	1.31
1:H:284:ARG:NE	1:N:386:GLU:CB	1.80	1.31
1:H:270:ILE:HG23	1:I:229:ASN:O	1.23	1.31
1:E:41:ASP:CG	1:F:69:MET:HG2	1.46	1.30
1:A:37:ASN:HB2	1:B:516:THR:O	1.30	1.30
1:A:41:ASP:OD1	1:B:69:MET:HG2	1.20	1.30
1:I:270:ILE:HG23	1:J:229:ASN:O	1.23	1.30
1:C:37:ASN:HB2	1:D:516:THR:O	1.30	1.29
1:E:47:PRO:CG	1:F:73:MET:CG	2.11	1.29
1:A:73:MET:CG	1:G:47:PRO:CG	2.11	1.29
1:L:386:GLU:CB	1:M:284:ARG:NE	1.80	1.29
1:F:150:ILE:CD1	1:F:411:VAL:CG1	2.11	1.28
1:D:41:ASP:OD1	1:E:69:MET:HG2	1.20	1.28
1:B:37:ASN:HB2	1:C:516:THR:O	1.30	1.28
1:E:150:ILE:CD1	1:E:411:VAL:CG1	2.11	1.28
1:K:386:GLU:CB	1:L:284:ARG:NE	1.80	1.28
1:H:229:ASN:O	1:N:270:ILE:HG23	1.23	1.28
1:F:47:PRO:CG	1:G:73:MET:CG	2.11	1.28
1:E:37:ASN:HB2	1:F:516:THR:O	1.30	1.28
1:M:39:VAL:HG12	1:N:69:MET:CE	1.63	1.28
1:G:150:ILE:CD1	1:G:411:VAL:CG1	2.12	1.28
1:H:69:MET:CE	1:N:39:VAL:HG12	1.63	1.28
1:F:37:ASN:HB2	1:G:516:THR:O	1.29	1.27
1:F:41:ASP:OD1	1:G:69:MET:HG2	1.20	1.27
1:L:39:VAL:HG12	1:M:69:MET:CE	1.63	1.27
1:B:47:PRO:CG	1:C:73:MET:CG	2.11	1.27
1:D:47:PRO:CG	1:E:73:MET:CG	2.11	1.27
1:H:386:GLU:CB	1:I:284:ARG:NE	1.80	1.27
1:J:270:ILE:HG23	1:K:229:ASN:O	1.23	1.27
1:A:47:PRO:CG	1:B:73:MET:CG	2.11	1.27
1:M:270:ILE:HG23	1:N:229:ASN:O	1.22	1.27
1:C:47:PRO:CG	1:D:73:MET:CG	2.11	1.27
1:D:150:ILE:CD1	1:D:411:VAL:CG1	2.11	1.27
1:K:39:VAL:HG12	1:L:69:MET:CE	1.63	1.26
1:H:39:VAL:HG12	1:I:69:MET:CE	1.63	1.26
1:J:39:VAL:HG12	1:K:69:MET:CE	1.63	1.26
1:C:41:ASP:OD1	1:D:69:MET:HG2	1.20	1.25



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; ({\rm \AA})$	$overlap (\AA)$
1:A:150:ILE:CD1	1:A:411:VAL:CG1	2.11	1.25
1:C:150:ILE:CD1	1:C:411:VAL:CG1	2.11	1.25
1:B:150:ILE:CD1	1:B:411:VAL:CG1	2.11	1.25
1:I:39:VAL:HG12	1:J:69:MET:CE	1.63	1.25
1:M:386:GLU:CB	1:N:284:ARG:NE	1.80	1.25
1:E:37:ASN:CB	1:F:516:THR:O	1.85	1.24
1:I:85:ALA:O	1:I:405:ALA:HB1	1.36	1.24
1:L:85:ALA:C	1:L:405:ALA:HB1	1.57	1.24
1:F:37:ASN:CB	1:G:516:THR:O	1.85	1.24
1:A:49:ILE:CG1	1:B:513:LEU:HB3	1.68	1.24
1:A:513:LEU:HB3	1:G:49:ILE:CG1	1.68	1.24
1:D:37:ASN:CB	1:E:516:THR:O	1.85	1.24
1:H:85:ALA:O	1:H:405:ALA:HB1	1.36	1.24
1:E:49:ILE:CG1	1:F:513:LEU:HB3	1.68	1.24
1:F:49:ILE:CG1	1:G:513:LEU:HB3	1.68	1.24
1:D:49:ILE:CG1	1:E:513:LEU:HB3	1.68	1.23
1:B:37:ASN:CB	1:C:516:THR:O	1.85	1.23
1:A:37:ASN:CB	1:B:516:THR:O	1.85	1.23
1:M:85:ALA:C	1:M:405:ALA:HB1	1.57	1.23
1:A:516:THR:O	1:G:37:ASN:CB	1.85	1.23
1:H:85:ALA:C	1:H:405:ALA:HB1	1.57	1.23
1:J:85:ALA:C	1:J:405:ALA:HB1	1.57	1.23
1:K:85:ALA:C	1:K:405:ALA:HB1	1.57	1.23
1:B:49:ILE:CG1	1:C:513:LEU:HB3	1.68	1.23
1:I:85:ALA:C	1:I:405:ALA:HB1	1.57	1.23
1:A:270:ILE:CG2	1:B:229:ASN:O	1.87	1.22
1:C:270:ILE:CG2	1:D:229:ASN:O	1.88	1.22
1:B:270:ILE:CG2	1:C:229:ASN:O	1.88	1.22
1:A:229:ASN:O	1:G:270:ILE:CG2	1.88	1.22
1:C:49:ILE:CG1	1:D:513:LEU:HB3	1.68	1.22
1:C:37:ASN:CB	1:D:516:THR:O	1.85	1.22
1:I:386:GLU:CB	1:J:284:ARG:NE	1.80	1.21
1:N:85:ALA:C	1:N:405:ALA:HB1	1.57	1.21
1:M:85:ALA:O	1:M:405:ALA:HB1	1.36	1.21
1:E:270:ILE:CG2	1:F:229:ASN:O	1.88	1.21
1:F:270:ILE:CG2	1:G:229:ASN:O	1.88	1.20
1:K:85:ALA:O	1:K:405:ALA:HB1	1.36	1.20
1:J:85:ALA:O	1:J:405:ALA:HB1	1.36	1.20
1:D:270:ILE:CG2	1:E:229:ASN:O	1.87	1.20
1:N:85:ALA:O	1:N:405:ALA:HB1	1.36	1.19
1:L:85:ALA:O	1:L:405:ALA:HB1	1.36	1.19



Continued from previous page...

A	ous page	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:F:150:ILE:HD13	1:F:411:VAL:CG1	1.73	1.18
1:E:150:ILE:HD13	1:E:411:VAL:CG1	1.73	1.18
1:J:386:GLU:CB	1:K:284:ARG:NE	1.80	1.18
1:G:150:ILE:HD13	1:G:411:VAL:CG1	1.73	1.17
1:D:150:ILE:HD13	1:D:411:VAL:CG1	1.73	1.17
1:I:39:VAL:CG1	1:J:69:MET:HE2	1.75	1.17
1:J:36:ARG:HG3	1:K:518:GLU:HG3	1.21	1.17
1:E:47:PRO:HG2	1:F:73:MET:CG	1.74	1.16
1:A:150:ILE:HD13	1:A:411:VAL:CG1	1.73	1.16
1:E:47:PRO:CG	1:F:73:MET:HG3	1.75	1.16
1:C:150:ILE:HD13	1:C:411:VAL:CG1	1.73	1.16
1:A:73:MET:HG3	1:G:47:PRO:CG	1.75	1.15
1:H:281:PHE:CD2	1:N:390:LYS:N	2.03	1.15
1:C:47:PRO:CG	1:D:73:MET:HG3	1.75	1.15
1:B:150:ILE:HD13	1:B:411:VAL:CG1	1.73	1.15
1:B:47:PRO:HG2	1:C:73:MET:HG3	1.23	1.15
1:I:390:LYS:HG2	1:J:281:PHE:CB	1.77	1.15
1:C:37:ASN:CA	1:D:516:THR:O	1.95	1.15
1:E:37:ASN:CA	1:F:516:THR:O	1.95	1.15
1:A:47:PRO:HG2	1:B:73:MET:HG3	1.23	1.15
1:D:37:ASN:CA	1:E:516:THR:O	1.95	1.15
1:M:390:LYS:HG2	1:N:281:PHE:CB	1.77	1.15
1:L:85:ALA:O	1:L:405:ALA:CB	1.95	1.15
1:H:85:ALA:O	1:H:405:ALA:CB	1.95	1.15
1:M:85:ALA:O	1:M:405:ALA:CB	1.95	1.15
1:C:49:ILE:HG13	1:D:513:LEU:HB3	1.15	1.15
1:N:85:ALA:O	1:N:405:ALA:CB	1.95	1.15
1:J:390:LYS:HG2	1:K:281:PHE:CB	1.77	1.14
1:C:47:PRO:HG2	1:D:73:MET:CG	1.74	1.14
1:B:49:ILE:HG13	1:C:513:LEU:HB3	1.15	1.14
1:H:281:PHE:CB	1:N:390:LYS:HG2	1.77	1.14
1:A:516:THR:O	1:G:37:ASN:CA	1.95	1.14
1:F:49:ILE:HG13	1:G:513:LEU:CB	1.78	1.14
1:I:36:ARG:HG3	1:J:518:GLU:HG3	1.21	1.14
1:B:47:PRO:HG2	1:C:73:MET:CG	1.74	1.14
1:L:390:LYS:HG2	1:M:281:PHE:CB	1.77	1.14
1:A:513:LEU:CB	1:G:49:ILE:HG13	1.78	1.14
1:K:85:ALA:O	1:K:405:ALA:CB	1.95	1.14
1:D:47:PRO:HG2	1:E:73:MET:CG	1.74	1.13
1:I:85:ALA:O	1:I:405:ALA:CB	1.95	1.13
1:A:49:ILE:HG13	1:B:513:LEU:HB3	1.15	1.13



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A , 4	A. 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:E:49:ILE:HG13	1:F:513:LEU:CB	1.78	1.13
1:B:37:ASN:CA	1:C:516:THR:O	1.95	1.13
1:A:37:ASN:CA	1:B:516:THR:O	1.95	1.13
1:M:390:LYS:CE	1:N:281:PHE:HB2	1.78	1.13
1:A:49:ILE:HG13	1:B:513:LEU:CB	1.78	1.13
1:A:47:PRO:HG2	1:B:73:MET:CG	1.74	1.13
1:F:37:ASN:CA	1:G:516:THR:O	1.95	1.13
1:F:47:PRO:HG2	1:G:73:MET:CG	1.74	1.13
1:L:390:LYS:CE	1:M:281:PHE:HB2	1.78	1.13
1:H:390:LYS:HG2	1:I:281:PHE:CB	1.77	1.13
1:H:281:PHE:HB2	1:N:390:LYS:CE	1.78	1.13
1:K:390:LYS:CE	1:L:281:PHE:HB2	1.78	1.13
1:D:49:ILE:HG13	1:E:513:LEU:HB3	1.15	1.13
1:E:47:PRO:HG2	1:F:73:MET:HG3	1.23	1.13
1:J:390:LYS:CE	1:K:281:PHE:HB2	1.78	1.13
1:K:390:LYS:HG2	1:L:281:PHE:CB	1.77	1.12
1:D:49:ILE:HG13	1:E:513:LEU:CB	1.78	1.12
1:B:49:ILE:HG13	1:C:513:LEU:CB	1.78	1.12
1:H:390:LYS:CE	1:I:281:PHE:HB2	1.78	1.12
1:B:47:PRO:CG	1:C:73:MET:HG3	1.75	1.12
1:A:73:MET:CG	1:G:47:PRO:HG2	1.74	1.12
1:K:36:ARG:HG3	1:L:518:GLU:HG3	1.21	1.12
1:B:150:ILE:HD12	1:B:411:VAL:CG1	1.76	1.11
1:E:41:ASP:CG	1:F:69:MET:CG	2.18	1.11
1:F:46:ALA:CB	1:G:76:GLU:CG	2.13	1.11
1:L:390:LYS:N	1:M:281:PHE:CD2	2.03	1.11
1:I:390:LYS:CE	1:J:281:PHE:HB2	1.78	1.11
1:M:36:ARG:HG3	1:N:518:GLU:HG3	1.21	1.11
1:F:41:ASP:CG	1:G:69:MET:CG	2.18	1.11
1:C:49:ILE:HG13	1:D:513:LEU:CB	1.78	1.11
1:A:76:GLU:HG2	1:G:46:ALA:HB2	1.14	1.11
1:M:390:LYS:N	1:N:281:PHE:CD2	2.03	1.11
1:J:85:ALA:O	1:J:405:ALA:CB	1.95	1.11
1:C:47:PRO:HG2	1:D:73:MET:HG3	1.23	1.11
1:D:41:ASP:CG	1:E:69:MET:CG	2.18	1.11
1:C:150:ILE:HD12	1:C:411:VAL:CG1	1.76	1.11
1:F:47:PRO:CG	1:G:73:MET:HG3	1.75	1.11
1:F:46:ALA:HB2	1:G:76:GLU:HG2	1.15	1.11
1:D:47:PRO:CG	1:E:73:MET:HG3	1.75	1.11
1:A:150:ILE:HD12	1:A:411:VAL:CG1	1.76	1.11
1:F:47:PRO:HG2	1:G:73:MET:HG3	1.23	1.11



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	$overlap(\AA)$
1:H:69:MET:HE2	1:N:39:VAL:CG1	1.80	1.11
1:H:518:GLU:HG3	1:N:36:ARG:HG3	1.21	1.10
1:A:46:ALA:HB2	1:B:76:GLU:HG2	1.15	1.10
1:B:37:ASN:CB	1:C:516:THR:C	2.20	1.10
1:A:73:MET:HG3	1:G:47:PRO:HG2	1.23	1.10
1:A:69:MET:CG	1:G:41:ASP:CG	2.18	1.10
1:J:390:LYS:N	1:K:281:PHE:CD2	2.03	1.10
1:A:513:LEU:HB3	1:G:49:ILE:HG13	1.15	1.10
1:D:150:ILE:HD12	1:D:411:VAL:CG1	1.76	1.09
1:L:36:ARG:HG3	1:M:518:GLU:HG3	1.21	1.09
1:D:47:PRO:HG2	1:E:73:MET:HG3	1.23	1.09
1:H:39:VAL:CG1	1:I:69:MET:HE2	1.81	1.09
1:F:37:ASN:CB	1:G:516:THR:C	2.20	1.09
1:I:386:GLU:HB2	1:J:284:ARG:NE	1.51	1.09
1:C:46:ALA:HB2	1:D:76:GLU:HG2	1.15	1.09
1:B:46:ALA:HB2	1:C:76:GLU:HG2	1.15	1.09
1:E:46:ALA:HB2	1:F:76:GLU:HG2	1.14	1.09
1:A:516:THR:C	1:G:37:ASN:CB	2.20	1.09
1:H:284:ARG:CZ	1:N:386:GLU:HB3	1.83	1.09
1:H:390:LYS:HE2	1:I:281:PHE:CB	1.83	1.09
1:I:390:LYS:HE2	1:J:281:PHE:CB	1.83	1.09
1:I:390:LYS:HG2	1:J:281:PHE:CG	1.88	1.09
1:C:41:ASP:CG	1:D:69:MET:CG	2.18	1.09
1:H:281:PHE:CB	1:N:390:LYS:HE2	1.83	1.09
1:H:386:GLU:HB3	1:I:284:ARG:CZ	1.83	1.09
1:I:386:GLU:HB3	1:J:284:ARG:CZ	1.83	1.09
1:D:46:ALA:HB2	1:E:76:GLU:HG2	1.15	1.08
1:G:150:ILE:HD12	1:G:411:VAL:CG1	1.76	1.08
1:J:390:LYS:HE2	1:K:281:PHE:CB	1.83	1.08
1:M:386:GLU:HB3	1:N:284:ARG:CZ	1.83	1.08
1:I:388:GLU:N	1:J:281:PHE:CE1	2.21	1.08
1:C:46:ALA:CB	1:D:76:GLU:CG	2.13	1.08
1:B:41:ASP:CG	1:C:69:MET:CG	2.18	1.08
1:J:386:GLU:HB2	1:K:284:ARG:NE	1.51	1.08
1:A:183:LEU:HA	1:A:383:ALA:HB3	1.36	1.08
1:A:47:PRO:CG	1:B:73:MET:HG3	1.75	1.08
1:L:388:GLU:N	1:M:281:PHE:CE1	2.21	1.08
1:H:386:GLU:HB2	1:I:284:ARG:NE	1.51	1.08
1:A:46:ALA:CB	1:B:76:GLU:CG	2.13	1.08
1:J:386:GLU:HB3	1:K:284:ARG:CZ	1.83	1.08
1:H:281:PHE:CG	1:N:390:LYS:HG2	1.88	1.08



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Continued from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap (Å)
1:M:388:GLU:N	1:N:281:PHE:CE1	2.21	1.08
1:M:390:LYS:HE2	1:N:281:PHE:CB	1.83	1.08
1:J:39:VAL:CG1	1:K:69:MET:HE2	1.82	1.08
1:F:183:LEU:HA	1:F:383:ALA:HB3	1.36	1.08
1:G:183:LEU:HA	1:G:383:ALA:HB3	1.36	1.08
1:L:386:GLU:HB3	1:M:284:ARG:CZ	1.83	1.08
1:J:390:LYS:HG2	1:K:281:PHE:CG	1.88	1.08
1:K:39:VAL:CG1	1:L:69:MET:HE2	1.81	1.08
1:H:281:PHE:CE1	1:N:388:GLU:N	2.21	1.07
1:H:390:LYS:HG2	1:I:281:PHE:CG	1.88	1.07
1:K:390:LYS:HE2	1:L:281:PHE:CB	1.83	1.07
1:E:49:ILE:HG13	1:F:513:LEU:HB3	1.15	1.07
1:E:183:LEU:HA	1:E:383:ALA:HB3	1.36	1.07
1:A:37:ASN:CB	1:B:516:THR:C	2.20	1.07
1:E:150:ILE:HD12	1:E:411:VAL:CG1	1.76	1.07
1:L:390:LYS:HE2	1:M:281:PHE:CB	1.83	1.07
1:H:388:GLU:N	1:I:281:PHE:CE1	2.21	1.07
1:J:388:GLU:N	1:K:281:PHE:CE1	2.21	1.07
1:H:36:ARG:HG3	1:I:518:GLU:HG3	1.21	1.07
1:C:37:ASN:CB	1:D:516:THR:C	2.20	1.07
1:D:37:ASN:CB	1:E:516:THR:C	2.20	1.07
1:A:41:ASP:CG	1:B:69:MET:CG	2.18	1.07
1:K:386:GLU:HB3	1:L:284:ARG:CZ	1.83	1.07
1:K:388:GLU:N	1:L:281:PHE:CE1	2.21	1.07
1:K:390:LYS:HG2	1:L:281:PHE:CG	1.88	1.07
1:K:36:ARG:CB	1:L:518:GLU:HB2	1.84	1.07
1:B:183:LEU:HA	1:B:383:ALA:HB3	1.36	1.07
1:F:150:ILE:HD12	1:F:411:VAL:CG1	1.76	1.07
1:H:36:ARG:CB	1:I:518:GLU:HB2	1.84	1.07
1:L:390:LYS:HG2	1:M:281:PHE:CG	1.88	1.06
1:M:390:LYS:HG2	1:N:281:PHE:CG	1.88	1.06
1:D:183:LEU:HA	1:D:383:ALA:HB3	1.36	1.06
1:E:37:ASN:CB	1:F:516:THR:C	2.20	1.06
1:I:390:LYS:HE2	1:J:281:PHE:HB2	1.08	1.06
1:M:36:ARG:CB	1:N:518:GLU:HB2	1.85	1.06
1:H:390:LYS:HE2	1:I:281:PHE:HB2	1.08	1.06
1:H:69:MET:CE	1:N:39:VAL:CG1	2.33	1.06
1:L:39:VAL:CG1	1:M:69:MET:HE2	1.84	1.06
1:H:390:LYS:N	1:I:281:PHE:CD2	2.03	1.06
1:H:518:GLU:HB2	1:N:36:ARG:CB	1.85	1.06
1:J:390:LYS:HE2	1:K:281:PHE:HB2	1.08	1.06



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:J:36:ARG:CB	1:K:518:GLU:HB2	1.84	1.06
1:D:39:VAL:H	1:E:517:THR:HG23	1.18	1.05
1:H:39:VAL:CG1	1:I:69:MET:CE	2.34	1.05
1:J:39:VAL:CG1	1:K:69:MET:CE	2.34	1.05
1:F:49:ILE:HG13	1:G:513:LEU:HB3	1.15	1.05
1:E:39:VAL:H	1:F:517:THR:HG23	1.18	1.05
1:K:386:GLU:HB2	1:L:284:ARG:NE	1.51	1.05
1:M:39:VAL:CG1	1:N:69:MET:CE	2.34	1.05
1:M:39:VAL:CG1	1:N:69:MET:HE2	1.86	1.05
1:L:36:ARG:CB	1:M:518:GLU:HB2	1.85	1.05
1:L:386:GLU:HB2	1:M:284:ARG:HE	0.88	1.05
1:C:183:LEU:HA	1:C:383:ALA:HB3	1.36	1.05
1:E:46:ALA:CB	1:F:76:GLU:CG	2.13	1.05
1:H:284:ARG:NE	1:N:386:GLU:HB2	1.51	1.05
1:M:39:VAL:HG12	1:N:69:MET:HE2	1.36	1.05
1:A:39:VAL:H	1:B:517:THR:HG23	1.18	1.05
1:H:281:PHE:HB2	1:N:390:LYS:HE2	1.08	1.05
1:K:386:GLU:HB2	1:L:284:ARG:HE	0.88	1.05
1:I:36:ARG:CB	1:J:518:GLU:HB2	1.85	1.05
1:F:46:ALA:HB3	1:G:76:GLU:HG3	1.38	1.04
1:M:386:GLU:HB2	1:N:284:ARG:HE	0.88	1.04
1:A:76:GLU:CG	1:G:46:ALA:CB	2.13	1.04
1:L:39:VAL:CG1	1:M:69:MET:CE	2.33	1.04
1:I:390:LYS:N	1:J:281:PHE:CD2	2.03	1.04
1:L:390:LYS:HE2	1:M:281:PHE:HB2	1.08	1.04
1:J:386:GLU:HB2	1:K:284:ARG:HE	0.88	1.04
1:H:284:ARG:HE	1:N:386:GLU:HB2	0.88	1.04
1:M:390:LYS:HE2	1:N:281:PHE:HB2	1.08	1.04
1:E:46:ALA:HB3	1:F:76:GLU:HG3	1.38	1.04
1:C:39:VAL:H	1:D:517:THR:HG23	1.18	1.03
1:H:386:GLU:HB2	1:I:284:ARG:HE	0.88	1.03
1:I:386:GLU:HB2	1:J:284:ARG:HE	0.89	1.03
1:K:390:LYS:HE2	1:L:281:PHE:HB2	1.08	1.03
1:I:174:VAL:HG11	1:I:331:THR:OG1	1.59	1.03
1:F:39:VAL:H	1:G:517:THR:HG23	1.18	1.03
1:C:270:ILE:HG22	1:D:229:ASN:HA	1.37	1.03
1:E:270:ILE:HG23	1:F:229:ASN:O	1.58	1.03
1:J:174:VAL:HG11	1:J:331:THR:OG1	1.58	1.03
1:H:174:VAL:HG11	1:H:331:THR:OG1	1.58	1.03
1:B:150:ILE:HD13	1:B:411:VAL:HG11	1.03	1.03
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.39	1.03



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:A:76:GLU:HG3	1:G:46:ALA:HB3	1.38	1.03
1:K:39:VAL:CG1	1:L:69:MET:CE	2.34	1.03
1:L:386:GLU:HB2	1:M:284:ARG:NE	1.51	1.02
1:A:41:ASP:OD1	1:B:69:MET:CG	2.07	1.02
1:M:386:GLU:HB2	1:N:284:ARG:NE	1.51	1.02
1:K:386:GLU:CB	1:L:284:ARG:CZ	2.38	1.02
1:B:270:ILE:HG22	1:C:229:ASN:HA	1.37	1.02
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.39	1.02
1:B:41:ASP:OD1	1:C:69:MET:CG	2.07	1.02
1:M:386:GLU:CB	1:N:284:ARG:CZ	2.38	1.02
1:D:270:ILE:HG22	1:E:229:ASN:HA	1.37	1.02
1:M:36:ARG:HB3	1:N:518:GLU:HB2	1.42	1.02
1:L:36:ARG:HB3	1:M:518:GLU:HB2	1.42	1.02
1:J:386:GLU:CB	1:K:284:ARG:CZ	2.38	1.02
1:A:229:ASN:O	1:G:270:ILE:HG23	1.58	1.02
1:K:174:VAL:HG11	1:K:331:THR:OG1	1.58	1.02
1:D:41:ASP:OD1	1:E:69:MET:CG	2.07	1.02
1:E:41:ASP:OD1	1:F:69:MET:CG	2.07	1.02
1:G:150:ILE:HD13	1:G:411:VAL:HG11	1.03	1.02
1:A:69:MET:CG	1:G:41:ASP:OD1	2.07	1.02
1:L:39:VAL:HG12	1:M:69:MET:HE2	1.35	1.02
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.39	1.02
1:B:39:VAL:H	1:C:517:THR:HG23	1.18	1.01
1:K:39:VAL:HG12	1:L:69:MET:HE2	1.33	1.01
1:A:49:ILE:HB	1:B:513:LEU:HD22	1.39	1.01
1:A:229:ASN:HA	1:G:270:ILE:HG22	1.37	1.01
1:K:36:ARG:HB3	1:L:518:GLU:HB2	1.42	1.01
1:N:174:VAL:HG11	1:N:331:THR:OG1	1.58	1.01
1:H:386:GLU:CB	1:I:284:ARG:CZ	2.38	1.01
1:K:390:LYS:N	1:L:281:PHE:CD2	2.03	1.01
1:H:519:CYS:HB3	1:N:38:VAL:HG22	1.39	1.01
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.39	1.01
1:B:46:ALA:CB	1:C:76:GLU:CG	2.13	1.01
1:F:41:ASP:OD1	1:G:69:MET:CG	2.07	1.01
1:D:49:ILE:HB	1:E:513:LEU:HD22	1.39	1.01
1:B:49:ILE:HB	1:C:513:LEU:HD22	1.39	1.01
1:F:270:ILE:HG22	1:G:229:ASN:HA	1.37	1.01
1:L:38:VAL:HG22	1:M:519:CYS:HB3	1.39	1.01
1:D:46:ALA:HB3	1:E:76:GLU:HG3	1.38	1.01
1:A:150:ILE:HD13	1:A:411:VAL:HG11	1.03	1.01
1:A:517:THR:HG23	1:G:39:VAL:H	1.18	1.01



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$overlap(\AA)$
1:D:150:ILE:HD13	1:D:411:VAL:HG11	1.03	1.01
1:H:69:MET:HE2	1:N:39:VAL:HG12	1.33	1.01
1:C:49:ILE:HB	1:D:513:LEU:HD22	1.39	1.01
1:J:39:VAL:HG12	1:K:69:MET:HE2	1.34	1.01
1:E:49:ILE:CD1	1:F:513:LEU:HB3	1.91	1.01
1:H:518:GLU:HB2	1:N:36:ARG:HB3	1.42	1.01
1:L:386:GLU:CB	1:M:284:ARG:CZ	2.38	1.00
1:A:513:LEU:HD22	1:G:49:ILE:HB	1.39	1.00
1:F:49:ILE:CD1	1:G:513:LEU:HB3	1.91	1.00
1:M:174:VAL:HG11	1:M:331:THR:OG1	1.58	1.00
1:D:49:ILE:CD1	1:E:513:LEU:HB3	1.91	1.00
1:B:270:ILE:HG23	1:C:229:ASN:O	1.58	1.00
1:F:270:ILE:HG23	1:G:229:ASN:O	1.58	1.00
1:A:270:ILE:HG22	1:B:229:ASN:HA	1.37	1.00
1:A:270:ILE:HG23	1:B:229:ASN:O	1.58	1.00
1:L:270:ILE:HG22	1:M:229:ASN:HA	1.43	1.00
1:C:150:ILE:HD13	1:C:411:VAL:HG11	1.03	1.00
1:A:513:LEU:HB3	1:G:49:ILE:CD1	1.91	1.00
1:C:41:ASP:OD1	1:D:69:MET:CG	2.07	1.00
1:L:174:VAL:HG11	1:L:331:THR:OG1	1.58	1.00
1:M:270:ILE:HG22	1:N:229:ASN:HA	1.43	0.99
1:E:49:ILE:HB	1:F:513:LEU:HD22	1.39	0.99
1:E:270:ILE:HG22	1:F:229:ASN:HA	1.37	0.99
1:J:36:ARG:HB3	1:K:518:GLU:HB2	1.42	0.99
1:A:8:PHE:CE2	1:G:26:ALA:HB2	1.97	0.99
1:E:150:ILE:HD13	1:E:411:VAL:HG11	1.03	0.99
1:K:388:GLU:N	1:L:281:PHE:CZ	2.29	0.99
1:B:49:ILE:CB	1:C:513:LEU:HD22	1.92	0.99
1:B:46:ALA:HB3	1:C:76:GLU:HG3	1.38	0.99
1:A:49:ILE:CB	1:B:513:LEU:HD22	1.92	0.99
1:A:26:ALA:HB2	1:B:8:PHE:CE2	1.97	0.99
1:A:46:ALA:HB3	1:B:76:GLU:HG3	1.38	0.99
1:C:270:ILE:HG23	1:D:229:ASN:O	1.58	0.99
1:C:49:ILE:CD1	1:D:513:LEU:HB3	1.91	0.99
1:D:270:ILE:HG23	1:E:229:ASN:O	1.58	0.99
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.39	0.99
1:F:26:ALA:HB2	1:G:8:PHE:CE2	1.97	0.99
1:C:49:ILE:CB	1:D:513:LEU:HD22	1.92	0.99
1:H:36:ARG:HB3	1:I:518:GLU:HB2	1.42	0.99
1:D:26:ALA:HB2	1:E:8:PHE:CE2	1.97	0.99
1:B:49:ILE:CD1	1:C:513:LEU:HB3	1.91	0.99



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$ \text{overlap } (\mathring{\mathbf{A}})$
1:B:26:ALA:HB2	1:C:8:PHE:CE2	1.97	0.99
1:C:46:ALA:HB3	1:D:76:GLU:HG3	1.38	0.99
1:H:284:ARG:CZ	1:N:386:GLU:CB	2.38	0.99
1:A:49:ILE:CD1	1:B:513:LEU:HB3	1.91	0.99
1:F:49:ILE:HB	1:G:513:LEU:HD22	1.39	0.99
1:J:388:GLU:N	1:K:281:PHE:CZ	2.29	0.98
1:F:150:ILE:HD13	1:F:411:VAL:HG11	1.03	0.98
1:A:513:LEU:HD22	1:G:49:ILE:CB	1.92	0.98
1:D:47:PRO:CD	1:E:73:MET:HG3	1.87	0.98
1:K:270:ILE:HG22	1:L:229:ASN:HA	1.43	0.98
1:I:39:VAL:CG1	1:J:69:MET:CE	2.34	0.98
1:H:39:VAL:HG12	1:I:69:MET:HE2	1.33	0.98
1:I:386:GLU:CB	1:J:284:ARG:CZ	2.38	0.98
1:I:39:VAL:HG12	1:J:69:MET:HE2	1.31	0.98
1:I:36:ARG:HB3	1:J:518:GLU:HB2	1.42	0.98
1:B:47:PRO:CD	1:C:73:MET:HG3	1.87	0.98
1:D:49:ILE:CB	1:E:513:LEU:HD22	1.92	0.98
1:C:26:ALA:HB2	1:D:8:PHE:CE2	1.97	0.98
1:F:49:ILE:CB	1:G:513:LEU:HD22	1.92	0.98
1:E:270:ILE:HG21	1:F:229:ASN:O	1.64	0.98
1:H:281:PHE:CZ	1:N:388:GLU:N	2.29	0.98
1:E:49:ILE:CB	1:F:513:LEU:HD22	1.92	0.98
1:L:388:GLU:N	1:M:281:PHE:CZ	2.29	0.98
1:E:26:ALA:HB2	1:F:8:PHE:CE2	1.97	0.98
1:D:270:ILE:HG21	1:E:229:ASN:O	1.64	0.98
1:F:47:PRO:CD	1:G:73:MET:HG3	1.87	0.97
1:H:229:ASN:HA	1:N:270:ILE:HG22	1.43	0.97
1:D:46:ALA:CB	1:E:76:GLU:CG	2.13	0.97
1:F:270:ILE:HG21	1:G:229:ASN:O	1.64	0.97
1:H:388:GLU:N	1:I:281:PHE:CZ	2.29	0.97
1:H:270:ILE:HG22	1:I:229:ASN:HA	1.43	0.97
1:A:73:MET:HG3	1:G:47:PRO:CD	1.87	0.97
1:A:114:MET:CE	1:G:35:GLY:O	2.13	0.97
1:D:35:GLY:O	1:E:114:MET:CE	2.13	0.96
1:B:35:GLY:O	1:C:114:MET:CE	2.13	0.96
1:E:26:ALA:HB2	1:F:8:PHE:HE2	1.30	0.96
1:I:270:ILE:HG22	1:J:229:ASN:HA	1.43	0.96
1:C:35:GLY:O	1:D:114:MET:CE	2.13	0.96
1:I:388:GLU:N	1:J:281:PHE:CZ	2.29	0.96
1:J:270:ILE:HG22	1:K:229:ASN:HA	1.43	0.96
1:A:26:ALA:HB2	1:B:8:PHE:HE2	1.30	0.96



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap (\AA)$
1:A:35:GLY:O	1:B:114:MET:CE	2.13	0.96
1:B:37:ASN:HB2	1:C:516:THR:CA	1.87	0.96
1:A:517:THR:HG23	1:G:39:VAL:N	1.80	0.96
1:M:388:GLU:N	1:N:281:PHE:CZ	2.29	0.96
1:F:35:GLY:O	1:G:114:MET:CE	2.13	0.96
1:E:35:GLY:O	1:F:114:MET:CE	2.13	0.96
1:E:39:VAL:N	1:F:517:THR:HG23	1.80	0.96
1:C:39:VAL:N	1:D:517:THR:HG23	1.80	0.95
1:A:39:VAL:N	1:B:517:THR:HG23	1.80	0.95
1:F:39:VAL:N	1:G:517:THR:HG23	1.80	0.95
1:C:270:ILE:HG21	1:D:229:ASN:O	1.64	0.95
1:A:47:PRO:CD	1:B:73:MET:HG3	1.87	0.95
1:K:405:ALA:O	1:K:498:LYS:CE	2.15	0.95
1:B:39:VAL:N	1:C:517:THR:HG23	1.80	0.95
1:D:39:VAL:N	1:E:517:THR:HG23	1.80	0.94
1:H:387:VAL:C	1:I:281:PHE:CE1	2.41	0.94
1:B:26:ALA:HB2	1:C:8:PHE:HE2	1.30	0.94
1:L:405:ALA:O	1:L:498:LYS:CE	2.15	0.94
1:N:405:ALA:O	1:N:498:LYS:CE	2.15	0.94
1:J:387:VAL:C	1:K:281:PHE:CE1	2.41	0.94
1:I:387:VAL:C	1:J:281:PHE:CE1	2.41	0.94
1:J:405:ALA:O	1:J:498:LYS:CE	2.15	0.94
1:A:229:ASN:O	1:G:270:ILE:HG21	1.64	0.94
1:H:405:ALA:O	1:H:498:LYS:CE	2.15	0.94
1:H:281:PHE:CE1	1:N:387:VAL:C	2.41	0.94
1:F:47:PRO:CG	1:G:73:MET:HG2	1.88	0.94
1:L:387:VAL:C	1:M:281:PHE:CE1	2.41	0.94
1:M:405:ALA:O	1:M:498:LYS:CE	2.15	0.94
1:E:37:ASN:HB2	1:F:516:THR:CA	1.87	0.94
1:E:39:VAL:HB	1:F:517:THR:HG21	1.51	0.93
1:A:517:THR:HG21	1:G:39:VAL:HB	1.50	0.93
1:A:39:VAL:HB	1:B:517:THR:HG21	1.50	0.93
1:C:26:ALA:HB2	1:D:8:PHE:HE2	1.30	0.93
1:B:150:ILE:HD12	1:B:411:VAL:HG11	0.95	0.93
1:G:150:ILE:HD12	1:G:411:VAL:HG11	0.95	0.93
1:A:516:THR:CA	1:G:37:ASN:HB2	1.87	0.93
1:B:270:ILE:HG21	1:C:229:ASN:O	1.64	0.93
1:C:150:ILE:HD12	1:C:411:VAL:HG11	0.95	0.93
1:K:387:VAL:C	1:L:281:PHE:CE1	2.41	0.93
1:B:49:ILE:HG13	1:C:513:LEU:HD13	1.51	0.93
1:F:150:ILE:HD12	1:F:411:VAL:HG11	0.95	0.93



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	overlap $( ext{Å})$
1:M:387:VAL:C	1:N:281:PHE:CE1	2.41	0.93
1:F:26:ALA:HB2	1:G:8:PHE:HE2	1.30	0.93
1:A:49:ILE:HG13	1:B:513:LEU:HD13	1.51	0.93
1:C:49:ILE:HG13	1:D:513:LEU:HD13	1.51	0.93
1:A:150:ILE:HD12	1:A:411:VAL:HG11	0.95	0.93
1:D:386:GLU:CG	1:E:281:PHE:CD2	2.52	0.93
1:I:405:ALA:O	1:I:498:LYS:CE	2.15	0.93
1:E:47:PRO:CG	1:F:73:MET:HG2	1.88	0.93
1:A:513:LEU:HD13	1:G:49:ILE:HG13	1.51	0.93
1:F:39:VAL:HB	1:G:517:THR:HG21	1.50	0.93
1:B:386:GLU:CG	1:C:281:PHE:CD2	2.52	0.93
1:F:49:ILE:HG13	1:G:513:LEU:CG	1.99	0.92
1:E:150:ILE:HD12	1:E:411:VAL:HG11	0.95	0.92
1:C:386:GLU:CG	1:D:281:PHE:CD2	2.52	0.92
1:D:150:ILE:HD12	1:D:411:VAL:HG11	0.95	0.92
1:D:37:ASN:HB2	1:E:516:THR:CA	1.87	0.92
1:D:47:PRO:CG	1:E:73:MET:HG2	1.88	0.92
1:E:49:ILE:HG13	1:F:513:LEU:CG	1.99	0.92
1:A:8:PHE:HE2	1:G:26:ALA:HB2	1.30	0.92
1:C:39:VAL:HB	1:D:517:THR:HG21	1.50	0.92
1:E:386:GLU:CG	1:F:281:PHE:CD2	2.52	0.92
1:A:513:LEU:CG	1:G:49:ILE:HG13	1.99	0.92
1:A:270:ILE:HG21	1:B:229:ASN:O	1.64	0.92
1:A:281:PHE:CD2	1:G:386:GLU:CG	2.52	0.92
1:F:386:GLU:CG	1:G:281:PHE:CD2	2.52	0.91
1:A:386:GLU:CG	1:B:281:PHE:CD2	2.52	0.91
1:D:49:ILE:HG13	1:E:513:LEU:HD13	1.51	0.91
1:F:49:ILE:HG13	1:G:513:LEU:HD13	1.51	0.91
1:C:49:ILE:HG13	1:D:513:LEU:CG	1.99	0.91
1:D:49:ILE:HG13	1:E:513:LEU:CG	1.99	0.91
1:L:408:GLU:CG	1:L:498:LYS:HE2	2.01	0.91
1:B:39:VAL:HB	1:C:517:THR:HG21	1.50	0.91
1:H:408:GLU:CG	1:H:498:LYS:HE2	2.01	0.91
1:D:26:ALA:HB2	1:E:8:PHE:HE2	1.30	0.91
1:I:408:GLU:CG	1:I:498:LYS:HE2	2.01	0.90
1:E:49:ILE:HG13	1:F:513:LEU:HD13	1.51	0.90
1:B:49:ILE:HG13	1:C:513:LEU:CG	1.99	0.90
1:A:49:ILE:HG13	1:B:513:LEU:CG	1.99	0.90
1:N:408:GLU:CG	1:N:498:LYS:HE2	2.01	0.90
1:B:49:ILE:HG13	1:C:513:LEU:CD1	2.02	0.90
1:M:39:VAL:HG12	1:N:69:MET:HE1	1.52	0.90



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:J:408:GLU:CG	1:J:498:LYS:HE2	2.01	0.90
1:C:47:PRO:CG	1:D:73:MET:HG2	1.88	0.90
1:D:39:VAL:HB	1:E:517:THR:HG21	1.51	0.90
1:B:47:PRO:CG	1:C:73:MET:HG2	1.88	0.90
1:H:232:GLU:HG3	1:N:245:LYS:HE2	1.54	0.90
1:M:408:GLU:CG	1:M:498:LYS:HE2	2.01	0.90
1:B:37:ASN:C	1:C:516:THR:O	2.11	0.89
1:L:39:VAL:HG12	1:M:69:MET:HE1	1.53	0.89
1:A:513:LEU:CD1	1:G:49:ILE:HG13	2.02	0.89
1:D:49:ILE:HG13	1:E:513:LEU:CD1	2.02	0.89
1:C:39:VAL:CB	1:D:517:THR:HG21	1.94	0.89
1:A:37:ASN:C	1:B:516:THR:O	2.11	0.89
1:C:37:ASN:C	1:D:516:THR:O	2.11	0.89
1:H:245:LYS:HE2	1:I:232:GLU:HG3	1.54	0.89
1:A:49:ILE:HG13	1:B:513:LEU:CD1	2.02	0.89
1:C:49:ILE:HG13	1:D:513:LEU:CD1	2.02	0.89
1:I:245:LYS:HE2	1:J:232:GLU:HG3	1.54	0.89
1:F:49:ILE:HG13	1:G:513:LEU:CD1	2.02	0.89
1:K:408:GLU:CG	1:K:498:LYS:HE2	2.01	0.89
1:M:36:ARG:HG3	1:N:518:GLU:CG	2.03	0.89
1:A:516:THR:O	1:G:37:ASN:C	2.11	0.89
1:M:245:LYS:HE2	1:N:232:GLU:HG3	1.54	0.89
1:H:518:GLU:CG	1:N:36:ARG:HG3	2.03	0.89
1:L:36:ARG:HG3	1:M:518:GLU:CG	2.03	0.88
1:H:284:ARG:CZ	1:N:385:THR:HB	2.04	0.88
1:L:270:ILE:HG22	1:M:229:ASN:CA	2.04	0.88
1:J:39:VAL:HG12	1:K:69:MET:HE1	1.54	0.88
1:E:49:ILE:HG13	1:F:513:LEU:CD1	2.02	0.88
1:D:37:ASN:C	1:E:516:THR:O	2.11	0.88
1:M:270:ILE:HG22	1:N:229:ASN:CA	2.04	0.88
1:F:39:VAL:CB	1:G:517:THR:HG21	1.94	0.88
1:K:270:ILE:HG22	1:L:229:ASN:CA	2.04	0.88
1:K:245:LYS:HE2	1:L:232:GLU:HG3	1.54	0.88
1:F:150:ILE:HG12	1:F:494:LEU:HD12	1.56	0.88
1:H:36:ARG:HG3	1:I:518:GLU:CG	2.03	0.88
1:I:174:VAL:HG22	1:I:194:GLN:CB	2.04	0.88
1:J:174:VAL:HG22	1:J:194:GLN:CB	2.04	0.88
1:G:150:ILE:HG12	1:G:494:LEU:HD12	1.56	0.88
1:H:390:LYS:CG	1:I:281:PHE:CB	2.52	0.88
1:N:174:VAL:HG22	1:N:194:GLN:CB	2.04	0.88
1:K:385:THR:HB	1:L:284:ARG:CZ	2.04	0.88



Continued from previous page...

Continued from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:K:36:ARG:HG3	1:L:518:GLU:CG	2.03	0.88
1:C:37:ASN:HB2	1:D:516:THR:CA	1.87	0.88
1:A:150:ILE:HG12	1:A:494:LEU:HD12	1.56	0.88
1:H:385:THR:HB	1:I:284:ARG:CZ	2.04	0.88
1:E:37:ASN:C	1:F:516:THR:O	2.11	0.87
1:E:150:ILE:HG12	1:E:494:LEU:HD12	1.56	0.87
1:I:385:THR:HB	1:J:284:ARG:CZ	2.04	0.87
1:J:245:LYS:HE2	1:K:232:GLU:HG3	1.54	0.87
1:L:245:LYS:HE2	1:M:232:GLU:HG3	1.54	0.87
1:H:174:VAL:HG22	1:H:194:GLN:CB	2.04	0.87
1:F:37:ASN:C	1:G:516:THR:O	2.11	0.87
1:K:39:VAL:HG12	1:L:69:MET:HE1	1.55	0.87
1:A:37:ASN:HB2	1:B:516:THR:CA	1.87	0.87
1:H:39:VAL:HG12	1:I:69:MET:HE1	1.55	0.87
1:B:39:VAL:CB	1:C:517:THR:CG2	2.43	0.87
1:L:385:THR:HB	1:M:284:ARG:CZ	2.04	0.87
1:I:36:ARG:HG3	1:J:518:GLU:CG	2.03	0.87
1:K:174:VAL:HG22	1:K:194:GLN:CB	2.04	0.87
1:E:47:PRO:CD	1:F:73:MET:HG3	1.87	0.87
1:J:270:ILE:HG22	1:K:229:ASN:CA	2.04	0.87
1:H:229:ASN:CA	1:N:270:ILE:HG22	2.04	0.87
1:J:36:ARG:HG3	1:K:518:GLU:CG	2.03	0.87
1:J:385:THR:HB	1:K:284:ARG:CZ	2.04	0.87
1:J:390:LYS:CG	1:K:281:PHE:CB	2.52	0.87
1:L:390:LYS:CG	1:M:281:PHE:CB	2.52	0.87
1:N:408:GLU:HG3	1:N:498:LYS:CE	2.05	0.87
1:I:408:GLU:HG3	1:I:498:LYS:CE	2.05	0.87
1:H:408:GLU:HG3	1:H:498:LYS:CE	2.05	0.87
1:M:408:GLU:HG3	1:M:498:LYS:CE	2.05	0.87
1:H:281:PHE:CB	1:N:390:LYS:CG	2.52	0.86
1:J:408:GLU:HG3	1:J:498:LYS:CE	2.05	0.86
1:M:385:THR:HB	1:N:284:ARG:CZ	2.04	0.86
1:M:174:VAL:HG22	1:M:194:GLN:CB	2.04	0.86
1:H:69:MET:HE1	1:N:39:VAL:HG12	1.55	0.86
1:I:390:LYS:CG	1:J:281:PHE:CB	2.52	0.86
1:K:390:LYS:CG	1:L:281:PHE:CB	2.52	0.86
1:D:150:ILE:HG12	1:D:494:LEU:HD12	1.56	0.86
1:M:390:LYS:CG	1:N:281:PHE:CB	2.52	0.86
1:L:174:VAL:HG22	1:L:194:GLN:CB	2.04	0.86
1:B:150:ILE:HG12	1:B:494:LEU:HD12	1.56	0.86
1:E:39:VAL:CB	1:F:517:THR:CG2	2.43	0.86



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:H:270:ILE:HG22	1:I:229:ASN:CA	2.04	0.86
1:I:270:ILE:HG22	1:J:229:ASN:CA	2.04	0.86
1:K:408:GLU:HG3	1:K:498:LYS:CE	2.05	0.86
1:D:39:VAL:CB	1:E:517:THR:HG21	1.94	0.85
1:L:408:GLU:HG3	1:L:498:LYS:CE	2.05	0.85
1:I:39:VAL:HG11	1:J:69:MET:HE2	1.56	0.85
1:A:281:PHE:CZ	1:G:386:GLU:CG	2.60	0.85
1:C:386:GLU:CG	1:D:281:PHE:CZ	2.60	0.85
1:B:386:GLU:CG	1:C:281:PHE:CZ	2.60	0.85
1:I:39:VAL:HG12	1:J:69:MET:HE1	1.58	0.85
1:A:47:PRO:CG	1:B:73:MET:HG2	1.88	0.85
1:F:386:GLU:CG	1:G:281:PHE:CZ	2.60	0.85
1:E:39:VAL:CB	1:F:517:THR:HG21	1.94	0.84
1:D:386:GLU:CG	1:E:281:PHE:CZ	2.60	0.84
1:A:386:GLU:CG	1:B:281:PHE:CZ	2.60	0.84
1:H:232:GLU:CG	1:N:245:LYS:HE2	2.08	0.84
1:F:39:VAL:CB	1:G:517:THR:CG2	2.43	0.84
1:E:386:GLU:CG	1:F:281:PHE:CZ	2.60	0.83
1:C:150:ILE:HG12	1:C:494:LEU:HD12	1.56	0.83
1:I:245:LYS:HE2	1:J:232:GLU:CG	2.08	0.83
1:A:517:THR:CG2	1:G:39:VAL:CB	2.43	0.83
1:H:245:LYS:HE2	1:I:232:GLU:CG	2.08	0.83
1:M:39:VAL:CG1	1:N:69:MET:HE1	2.07	0.83
1:E:270:ILE:CG2	1:F:229:ASN:C	2.47	0.83
1:J:245:LYS:HE2	1:K:232:GLU:CG	2.08	0.83
1:K:245:LYS:HE2	1:L:232:GLU:CG	2.08	0.83
1:M:38:VAL:HA	1:N:519:CYS:O	1.79	0.83
1:C:47:PRO:CD	1:D:73:MET:HG3	1.87	0.83
1:I:405:ALA:O	1:I:498:LYS:HE2	1.79	0.83
1:M:405:ALA:O	1:M:498:LYS:HE2	1.79	0.83
1:F:270:ILE:CG2	1:G:229:ASN:C	2.47	0.83
1:D:39:VAL:CB	1:E:517:THR:CG2	2.43	0.82
1:L:245:LYS:HE2	1:M:232:GLU:CG	2.08	0.82
1:D:270:ILE:CG2	1:E:229:ASN:C	2.47	0.82
1:C:39:VAL:CB	1:D:517:THR:CG2	2.43	0.82
1:M:245:LYS:HE2	1:N:232:GLU:CG	2.08	0.82
1:K:405:ALA:O	1:K:498:LYS:HE2	1.79	0.82
1:M:405:ALA:O	1:M:498:LYS:HD3	1.80	0.82
1:A:270:ILE:CG2	1:B:229:ASN:C	2.47	0.82
1:H:38:VAL:HA	1:I:519:CYS:O	1.79	0.82
1:E:26:ALA:CB	1:F:8:PHE:HE2	1.93	0.82



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:C:38:VAL:HG13	1:D:519:CYS:HB3	1.62	0.82
1:B:38:VAL:HG13	1:C:519:CYS:HB3	1.62	0.82
1:H:405:ALA:O	1:H:498:LYS:HE2	1.79	0.82
1:N:405:ALA:O	1:N:498:LYS:HD3	1.80	0.82
1:H:65:LYS:HB3	1:H:522:THR:HG21	1.62	0.81
1:L:405:ALA:O	1:L:498:LYS:HD3	1.80	0.81
1:B:270:ILE:CG2	1:C:229:ASN:C	2.47	0.81
1:N:65:LYS:HB3	1:N:522:THR:HG21	1.62	0.81
1:M:65:LYS:HB3	1:M:522:THR:HG21	1.62	0.81
1:E:65:LYS:HB3	1:E:522:THR:HG21	1.62	0.81
1:H:69:MET:HE2	1:N:39:VAL:HG11	1.61	0.81
1:L:39:VAL:CG1	1:M:69:MET:HE1	2.09	0.81
1:I:65:LYS:HB3	1:I:522:THR:HG21	1.62	0.81
1:I:405:ALA:O	1:I:498:LYS:HD3	1.80	0.81
1:K:405:ALA:O	1:K:498:LYS:HD3	1.80	0.81
1:A:229:ASN:C	1:G:270:ILE:CG2	2.47	0.81
1:L:38:VAL:HA	1:M:519:CYS:O	1.79	0.81
1:K:38:VAL:HA	1:L:519:CYS:O	1.79	0.81
1:C:26:ALA:CB	1:D:8:PHE:HE2	1.93	0.81
1:F:65:LYS:HB3	1:F:522:THR:HG21	1.62	0.81
1:I:38:VAL:HA	1:J:519:CYS:O	1.79	0.81
1:H:405:ALA:O	1:H:498:LYS:HD3	1.80	0.81
1:C:270:ILE:CG2	1:D:229:ASN:C	2.47	0.81
1:H:519:CYS:O	1:N:38:VAL:HA	1.79	0.81
1:D:35:GLY:O	1:E:114:MET:HE2	1.81	0.81
1:D:38:VAL:HG13	1:E:519:CYS:HB3	1.62	0.81
1:A:38:VAL:HG13	1:B:519:CYS:HB3	1.61	0.81
1:A:73:MET:HG2	1:G:47:PRO:CG	1.88	0.81
1:F:37:ASN:N	1:G:516:THR:HG22	1.84	0.81
1:J:38:VAL:HA	1:K:519:CYS:O	1.79	0.81
1:D:26:ALA:CB	1:E:8:PHE:HE2	1.93	0.81
1:D:65:LYS:HB3	1:D:522:THR:HG21	1.62	0.81
1:L:405:ALA:O	1:L:498:LYS:HE2	1.79	0.81
1:J:405:ALA:O	1:J:498:LYS:HD3	1.80	0.81
1:N:405:ALA:O	1:N:498:LYS:HE2	1.79	0.81
1:M:174:VAL:CG2	1:M:194:GLN:HB2	2.11	0.81
1:B:26:ALA:CB	1:C:8:PHE:HE2	1.93	0.81
1:G:65:LYS:HB3	1:G:522:THR:HG21	1.62	0.81
1:B:35:GLY:O	1:C:114:MET:HE2	1.81	0.81
1:L:65:LYS:HB3	1:L:522:THR:HG21	1.62	0.80
1:J:405:ALA:O	1:J:498:LYS:HE2	1.79	0.80



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	overlap (Å)
1:F:26:ALA:CB	1:G:8:PHE:HE2	1.93	0.80
1:A:519:CYS:HB3	1:G:38:VAL:HG13	1.62	0.80
1:H:174:VAL:CG2	1:H:194:GLN:HB2	2.11	0.80
1:J:65:LYS:HB3	1:J:522:THR:HG21	1.62	0.80
1:I:174:VAL:CG2	1:I:194:GLN:HB2	2.11	0.80
1:L:174:VAL:CG2	1:L:194:GLN:HB2	2.11	0.80
1:A:8:PHE:HE2	1:G:26:ALA:CB	1.93	0.80
1:A:26:ALA:CB	1:B:8:PHE:HE2	1.93	0.80
1:H:182:GLY:N	1:I:283:ASP:CB	2.29	0.80
1:F:38:VAL:HG13	1:G:519:CYS:HB3	1.62	0.80
1:L:385:THR:CB	1:M:284:ARG:CZ	2.60	0.80
1:J:174:VAL:CG2	1:J:194:GLN:HB2	2.11	0.80
1:F:35:GLY:O	1:G:114:MET:HE2	1.79	0.80
1:E:37:ASN:N	1:F:516:THR:HG22	1.84	0.80
1:H:39:VAL:HG11	1:I:69:MET:HE2	1.63	0.80
1:N:174:VAL:CG2	1:N:194:GLN:HB2	2.11	0.80
1:J:59:GLU:O	1:K:4:LYS:HG3	1.83	0.79
1:B:65:LYS:HB3	1:B:522:THR:HG21	1.62	0.79
1:M:385:THR:CB	1:N:284:ARG:CZ	2.60	0.79
1:K:174:VAL:CG2	1:K:194:GLN:HB2	2.11	0.79
1:H:59:GLU:O	1:I:4:LYS:HG3	1.83	0.79
1:H:4:LYS:HG3	1:N:59:GLU:O	1.83	0.79
1:L:36:ARG:HB2	1:M:518:GLU:HB2	1.65	0.79
1:M:182:GLY:N	1:N:283:ASP:CB	2.29	0.79
1:F:47:PRO:HD2	1:G:73:MET:CB	2.11	0.79
1:K:385:THR:CB	1:L:284:ARG:CZ	2.60	0.79
1:N:408:GLU:CG	1:N:498:LYS:CE	2.61	0.79
1:H:518:GLU:HB2	1:N:36:ARG:HB2	1.65	0.79
1:C:65:LYS:HB3	1:C:522:THR:HG21	1.62	0.79
1:E:47:PRO:HD2	1:F:73:MET:CB	2.11	0.79
1:E:49:ILE:CG1	1:F:513:LEU:HD13	2.12	0.79
1:D:37:ASN:N	1:E:516:THR:HG22	1.84	0.79
1:D:47:PRO:HD2	1:E:73:MET:CB	2.11	0.79
1:E:38:VAL:HG13	1:F:519:CYS:HB3	1.62	0.79
1:A:73:MET:CB	1:G:47:PRO:HD2	2.11	0.79
1:I:390:LYS:HG2	1:J:281:PHE:HB2	1.64	0.79
1:I:36:ARG:HB2	1:J:518:GLU:HB2	1.65	0.79
1:C:291:ASP:HB3	1:C:372:LEU:HD11	1.65	0.79
1:C:178:GLU:HA	1:C:393:LYS:HE2	1.65	0.79
1:F:49:ILE:CG1	1:G:513:LEU:HD13	2.12	0.79
1:M:408:GLU:CG	1:M:498:LYS:CE	2.61	0.79



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Continued from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:B:49:ILE:CG1	1:C:513:LEU:HD13	2.12	0.79
1:L:182:GLY:N	1:M:283:ASP:CB	2.29	0.79
1:L:59:GLU:O	1:M:4:LYS:HG3	1.83	0.79
1:H:291:ASP:HB3	1:H:372:LEU:HD11	1.65	0.79
1:I:291:ASP:HB3	1:I:372:LEU:HD11	1.65	0.79
1:K:39:VAL:HG11	1:L:69:MET:HE2	1.63	0.79
1:M:59:GLU:O	1:N:4:LYS:HG3	1.83	0.79
1:C:47:PRO:HD2	1:D:73:MET:CB	2.11	0.79
1:A:47:PRO:HD2	1:B:73:MET:CB	2.11	0.79
1:A:65:LYS:HB3	1:A:522:THR:HG21	1.62	0.79
1:I:385:THR:CB	1:J:284:ARG:CZ	2.60	0.79
1:K:65:LYS:HB3	1:K:522:THR:HG21	1.62	0.79
1:L:408:GLU:CG	1:L:498:LYS:CE	2.61	0.79
1:K:408:GLU:CG	1:K:498:LYS:CE	2.61	0.79
1:D:178:GLU:HA	1:D:393:LYS:HE2	1.65	0.79
1:B:291:ASP:HB3	1:B:372:LEU:HD11	1.65	0.79
1:D:47:PRO:HG2	1:E:73:MET:SD	2.23	0.78
1:B:47:PRO:HD2	1:C:73:MET:CB	2.11	0.78
1:H:385:THR:CB	1:I:284:ARG:CZ	2.60	0.78
1:C:49:ILE:CG1	1:D:513:LEU:HD13	2.12	0.78
1:K:36:ARG:HB2	1:L:518:GLU:HB2	1.65	0.78
1:E:178:GLU:HA	1:E:393:LYS:HE2	1.65	0.78
1:C:47:PRO:HG2	1:D:73:MET:SD	2.23	0.78
1:H:281:PHE:HB2	1:N:390:LYS:HG2	1.64	0.78
1:D:270:ILE:CG2	1:E:229:ASN:HA	2.13	0.78
1:D:291:ASP:HB3	1:D:372:LEU:HD11	1.65	0.78
1:A:39:VAL:CB	1:B:517:THR:CG2	2.43	0.78
1:A:49:ILE:CG1	1:B:513:LEU:HD13	2.12	0.78
1:H:36:ARG:HB2	1:I:518:GLU:HB2	1.65	0.78
1:B:178:GLU:HA	1:B:393:LYS:HE2	1.65	0.78
1:A:47:PRO:HG2	1:B:73:MET:SD	2.24	0.78
1:F:47:PRO:HG2	1:G:73:MET:SD	2.23	0.78
1:A:270:ILE:CG2	1:B:229:ASN:HA	2.13	0.78
1:E:270:ILE:CG2	1:F:229:ASN:HA	2.13	0.78
1:M:36:ARG:HB2	1:N:518:GLU:HB2	1.65	0.78
1:I:174:VAL:HG22	1:I:194:GLN:HB2	1.66	0.78
1:J:174:VAL:HG22	1:J:194:GLN:HB2	1.66	0.78
1:K:182:GLY:N	1:L:283:ASP:CB	2.29	0.78
1:J:385:THR:CB	1:K:284:ARG:CZ	2.60	0.78
1:D:49:ILE:CG1	1:E:513:LEU:HD13	2.12	0.78
1:H:390:LYS:HG2	1:I:281:PHE:HB2	1.64	0.78



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:J:39:VAL:HG11	1:K:69:MET:HE2	1.64	0.78
1:M:86:GLY:HA3	1:M:405:ALA:CB	2.14	0.78
1:J:291:ASP:HB3	1:J:372:LEU:HD11	1.65	0.78
1:F:270:ILE:CG2	1:G:229:ASN:HA	2.13	0.78
1:I:59:GLU:O	1:J:4:LYS:HG3	1.83	0.78
1:I:191:GLU:O	1:I:334:ASP:HA	1.84	0.78
1:A:291:ASP:HB3	1:A:372:LEU:HD11	1.65	0.78
1:J:86:GLY:HA3	1:J:405:ALA:CB	2.14	0.77
1:A:229:ASN:HA	1:G:270:ILE:CG2	2.13	0.77
1:B:47:PRO:HG2	1:C:73:MET:SD	2.23	0.77
1:J:390:LYS:HG2	1:K:281:PHE:HB2	1.64	0.77
1:A:513:LEU:HD13	1:G:49:ILE:CG1	2.13	0.77
1:K:59:GLU:O	1:L:4:LYS:HG3	1.83	0.77
1:L:191:GLU:O	1:L:334:ASP:HA	1.84	0.77
1:N:291:ASP:HB3	1:N:372:LEU:HD11	1.65	0.77
1:I:182:GLY:N	1:J:283:ASP:CB	2.29	0.77
1:M:390:LYS:HG2	1:N:281:PHE:HB2	1.64	0.77
1:H:174:VAL:HG22	1:H:194:GLN:HB2	1.66	0.77
1:E:47:PRO:HG2	1:F:73:MET:SD	2.23	0.77
1:H:284:ARG:CZ	1:N:385:THR:CB	2.60	0.77
1:H:408:GLU:CG	1:H:498:LYS:CE	2.61	0.77
1:B:270:ILE:CD1	1:C:231:ARG:HG3	2.15	0.77
1:L:291:ASP:HB3	1:L:372:LEU:HD11	1.65	0.77
1:N:86:GLY:HA3	1:N:405:ALA:CB	2.14	0.77
1:G:178:GLU:HA	1:G:393:LYS:HE2	1.65	0.77
1:F:291:ASP:HB3	1:F:372:LEU:HD11	1.65	0.77
1:I:405:ALA:O	1:I:498:LYS:CD	2.33	0.77
1:H:86:GLY:HA3	1:H:405:ALA:CB	2.14	0.77
1:I:174:VAL:HG22	1:I:194:GLN:HB3	1.66	0.77
1:H:174:VAL:HG22	1:H:194:GLN:HB3	1.66	0.77
1:K:174:VAL:HG22	1:K:194:GLN:HB2	1.66	0.77
1:F:178:GLU:HA	1:F:393:LYS:HE2	1.65	0.77
1:E:291:ASP:HB3	1:E:372:LEU:HD11	1.65	0.77
1:G:291:ASP:HB3	1:G:372:LEU:HD11	1.65	0.77
1:D:39:VAL:O	1:E:519:CYS:O	2.03	0.77
1:I:408:GLU:CG	1:I:498:LYS:CE	2.61	0.77
1:F:270:ILE:CD1	1:G:231:ARG:HG3	2.15	0.77
1:M:191:GLU:O	1:M:334:ASP:HA	1.84	0.77
1:B:37:ASN:N	1:C:516:THR:O	2.17	0.77
1:A:37:ASN:N	1:B:516:THR:O	2.17	0.77
1:K:191:GLU:O	1:K:334:ASP:HA	1.84	0.77



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:A:178:GLU:HA	1:A:393:LYS:HE2	1.65	0.77
1:M:291:ASP:HB3	1:M:372:LEU:HD11	1.65	0.77
1:M:390:LYS:CD	1:N:281:PHE:HB2	2.15	0.77
1:K:390:LYS:CD	1:L:281:PHE:HB2	2.15	0.77
1:D:270:ILE:CD1	1:E:231:ARG:HG3	2.15	0.77
1:K:291:ASP:HB3	1:K:372:LEU:HD11	1.65	0.77
1:H:191:GLU:O	1:H:334:ASP:HA	1.84	0.77
1:A:231:ARG:HG3	1:G:270:ILE:CD1	2.15	0.76
1:J:191:GLU:O	1:J:334:ASP:HA	1.84	0.76
1:N:191:GLU:O	1:N:334:ASP:HA	1.84	0.76
1:C:37:ASN:N	1:D:516:THR:O	2.17	0.76
1:D:37:ASN:N	1:E:516:THR:O	2.17	0.76
1:I:86:GLY:HA3	1:I:405:ALA:CB	2.14	0.76
1:L:86:GLY:HA3	1:L:405:ALA:CB	2.14	0.76
1:J:408:GLU:CG	1:J:498:LYS:CE	2.61	0.76
1:J:405:ALA:O	1:J:498:LYS:CD	2.33	0.76
1:E:270:ILE:CD1	1:F:231:ARG:HG3	2.15	0.76
1:J:174:VAL:HG22	1:J:194:GLN:HB3	1.66	0.76
1:C:270:ILE:CD1	1:D:231:ARG:HG3	2.15	0.76
1:N:405:ALA:O	1:N:498:LYS:CD	2.33	0.76
1:N:174:VAL:HG22	1:N:194:GLN:HB3	1.66	0.76
1:A:73:MET:SD	1:G:47:PRO:HG2	2.23	0.76
1:M:36:ARG:CG	1:N:518:GLU:HG3	2.12	0.76
1:F:37:ASN:N	1:G:516:THR:O	2.17	0.76
1:K:39:VAL:CG1	1:L:69:MET:HE1	2.12	0.76
1:M:405:ALA:O	1:M:498:LYS:CD	2.33	0.76
1:K:86:GLY:HA3	1:K:405:ALA:CB	2.14	0.76
1:H:283:ASP:CB	1:N:182:GLY:N	2.29	0.76
1:C:39:VAL:O	1:D:519:CYS:O	2.03	0.76
1:E:39:VAL:O	1:F:519:CYS:O	2.03	0.76
1:A:516:THR:O	1:G:37:ASN:N	2.17	0.76
1:H:405:ALA:O	1:H:498:LYS:CD	2.33	0.76
1:L:36:ARG:CG	1:M:518:GLU:HG3	2.12	0.76
1:C:150:ILE:HD11	1:C:494:LEU:HD13	1.67	0.76
1:E:150:ILE:HD11	1:E:494:LEU:HD13	1.67	0.76
1:L:408:GLU:HG2	1:L:498:LYS:HE2	1.67	0.76
1:C:37:ASN:N	1:D:516:THR:HG22	1.84	0.76
1:F:39:VAL:O	1:G:519:CYS:O	2.03	0.76
1:C:270:ILE:HG22	1:D:229:ASN:CA	2.16	0.76
1:B:150:ILE:HD11	1:B:494:LEU:HD13	1.67	0.76
1:I:390:LYS:CD	1:J:281:PHE:HB2	2.15	0.76



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	overlap(Å)
1:H:408:GLU:HG2	1:H:498:LYS:HE2	1.67	0.76
1:J:408:GLU:HG2	1:J:498:LYS:HE2	1.67	0.76
1:A:270:ILE:CD1	1:B:231:ARG:HG3	2.15	0.76
1:A:519:CYS:O	1:G:39:VAL:O	2.03	0.76
1:L:390:LYS:HG2	1:M:281:PHE:HB2	1.64	0.76
1:D:270:ILE:HG22	1:E:229:ASN:CA	2.16	0.76
1:M:174:VAL:HG22	1:M:194:GLN:HB2	1.66	0.76
1:L:174:VAL:HG22	1:L:194:GLN:HB2	1.66	0.76
1:K:390:LYS:HG2	1:L:281:PHE:HB2	1.64	0.75
1:H:232:GLU:OE2	1:N:245:LYS:HD3	1.87	0.75
1:C:270:ILE:CG2	1:D:229:ASN:HA	2.13	0.75
1:B:37:ASN:N	1:C:516:THR:HG22	1.84	0.75
1:E:37:ASN:N	1:F:516:THR:O	2.17	0.75
1:A:37:ASN:N	1:B:516:THR:HG22	1.84	0.75
1:F:150:ILE:HD11	1:F:494:LEU:HD13	1.67	0.75
1:J:245:LYS:HD3	1:K:232:GLU:OE2	1.86	0.75
1:K:245:LYS:HD3	1:L:232:GLU:OE2	1.86	0.75
1:K:408:GLU:HG2	1:K:498:LYS:HE2	1.67	0.75
1:H:36:ARG:CG	1:I:518:GLU:HG3	2.12	0.75
1:N:174:VAL:HG22	1:N:194:GLN:HB2	1.66	0.75
1:H:390:LYS:CD	1:I:281:PHE:HB2	2.15	0.75
1:L:405:ALA:O	1:L:498:LYS:CD	2.33	0.75
1:K:405:ALA:O	1:K:498:LYS:CD	2.33	0.75
1:N:408:GLU:HG2	1:N:498:LYS:HE2	1.67	0.75
1:J:36:ARG:HB2	1:K:518:GLU:HB2	1.65	0.75
1:J:182:GLY:N	1:K:283:ASP:CB	2.29	0.75
1:L:245:LYS:HD3	1:M:232:GLU:OE2	1.86	0.75
1:K:36:ARG:CG	1:L:518:GLU:HG3	2.12	0.75
1:K:174:VAL:HG22	1:K:194:GLN:HB3	1.66	0.75
1:B:39:VAL:O	1:C:519:CYS:O	2.03	0.75
1:L:390:LYS:CD	1:M:281:PHE:HB2	2.16	0.75
1:M:408:GLU:HG2	1:M:498:LYS:HE2	1.67	0.75
1:M:174:VAL:HG22	1:M:194:GLN:HB3	1.66	0.75
1:A:39:VAL:O	1:B:519:CYS:O	2.03	0.75
1:H:281:PHE:HB2	1:N:390:LYS:CD	2.16	0.75
1:I:245:LYS:HD3	1:J:232:GLU:OE2	1.86	0.75
1:M:245:LYS:HD3	1:N:232:GLU:OE2	1.86	0.75
1:B:270:ILE:CG2	1:C:229:ASN:HA	2.13	0.75
1:J:390:LYS:CD	1:K:281:PHE:HB2	2.15	0.75
1:D:150:ILE:HD11	1:D:494:LEU:HD13	1.67	0.74
1:H:245:LYS:HD3	1:I:232:GLU:OE2	1.87	0.74



Continued from previous page...

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:G:150:ILE:HD11	1:G:494:LEU:HD13	1.67	0.74
1:F:38:VAL:HA	1:G:518:GLU:H	1.51	0.74
1:L:39:VAL:HG11	1:M:69:MET:HE2	1.66	0.74
1:I:408:GLU:HG2	1:I:498:LYS:HE2	1.66	0.74
1:A:245:LYS:HE2	1:B:232:GLU:HG3	1.69	0.74
1:C:245:LYS:HE2	1:D:232:GLU:HG3	1.69	0.74
1:B:245:LYS:HE2	1:C:232:GLU:HG3	1.69	0.74
1:L:174:VAL:HG22	1:L:194:GLN:HB3	1.66	0.74
1:A:150:ILE:HD11	1:A:494:LEU:HD13	1.67	0.74
1:A:518:GLU:H	1:G:38:VAL:HA	1.51	0.74
1:E:38:VAL:HA	1:F:518:GLU:H	1.51	0.74
1:C:39:VAL:HB	1:D:517:THR:CG2	2.15	0.74
1:B:38:VAL:HA	1:C:518:GLU:H	1.51	0.74
1:M:146:GLN:NE2	1:M:494:LEU:HD12	2.03	0.74
1:A:38:VAL:HA	1:B:518:GLU:H	1.51	0.74
1:A:232:GLU:HG3	1:G:245:LYS:HE2	1.69	0.74
1:F:270:ILE:HG22	1:G:229:ASN:CA	2.16	0.73
1:A:516:THR:HG22	1:G:37:ASN:N	1.84	0.73
1:E:270:ILE:HG22	1:F:229:ASN:CA	2.16	0.73
1:K:390:LYS:CG	1:L:281:PHE:HB2	2.18	0.73
1:K:146:GLN:NE2	1:K:494:LEU:HD12	2.03	0.73
1:C:38:VAL:HA	1:D:518:GLU:H	1.51	0.73
1:D:38:VAL:HA	1:E:518:GLU:H	1.51	0.73
1:H:231:ARG:HG3	1:N:270:ILE:HG12	1.70	0.73
1:D:47:PRO:HB2	1:E:73:MET:SD	2.29	0.73
1:B:47:PRO:HB2	1:C:73:MET:SD	2.29	0.73
1:J:390:LYS:CG	1:K:281:PHE:HB2	2.18	0.73
1:H:270:ILE:HG12	1:I:231:ARG:HG3	1.70	0.73
1:I:146:GLN:NE2	1:I:494:LEU:HD12	2.03	0.73
1:D:245:LYS:HE2	1:E:232:GLU:HG3	1.69	0.73
1:H:146:GLN:NE2	1:H:494:LEU:HD12	2.03	0.73
1:A:73:MET:SD	1:G:47:PRO:HB2	2.29	0.73
1:K:270:ILE:CG2	1:L:229:ASN:C	2.57	0.73
1:F:245:LYS:HE2	1:G:232:GLU:HG3	1.69	0.73
1:E:47:PRO:HB2	1:F:73:MET:SD	2.29	0.73
1:L:390:LYS:CG	1:M:281:PHE:HB2	2.18	0.73
1:N:146:GLN:NE2	1:N:494:LEU:HD12	2.03	0.73
1:H:281:PHE:HB2	1:N:390:LYS:CG	2.18	0.73
1:J:36:ARG:CG	1:K:518:GLU:HG3	2.12	0.73
1:E:245:LYS:HE2	1:F:232:GLU:HG3	1.69	0.72
1:J:146:GLN:NE2	1:J:494:LEU:HD12	2.03	0.72



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:D:39:VAL:HB	1:E:517:THR:CG2	2.15	0.72
1:E:39:VAL:HB	1:F:517:THR:CG2	2.15	0.72
1:A:47:PRO:HB2	1:B:73:MET:SD	2.29	0.72
1:I:390:LYS:CG	1:J:281:PHE:HB2	2.18	0.72
1:I:270:ILE:CG2	1:J:229:ASN:C	2.57	0.72
1:I:270:ILE:HG12	1:J:231:ARG:HG3	1.70	0.72
1:M:270:ILE:HG12	1:N:231:ARG:HG3	1.70	0.72
1:J:270:ILE:CG2	1:K:229:ASN:C	2.57	0.72
1:C:47:PRO:HB2	1:D:73:MET:SD	2.29	0.72
1:C:150:ILE:HD13	1:C:411:VAL:CB	2.20	0.72
1:D:150:ILE:HD13	1:D:411:VAL:CB	2.20	0.72
1:H:390:LYS:CG	1:I:281:PHE:HB2	2.18	0.72
1:L:270:ILE:CG2	1:M:229:ASN:C	2.57	0.72
1:M:39:VAL:HG11	1:N:69:MET:HE2	1.69	0.72
1:A:270:ILE:HG22	1:B:229:ASN:CA	2.16	0.72
1:M:168:LYS:HD3	1:M:189:VAL:HG23	1.70	0.72
1:I:168:LYS:HD3	1:I:189:VAL:HG23	1.70	0.72
1:E:150:ILE:HD13	1:E:411:VAL:CB	2.20	0.72
1:K:270:ILE:HG12	1:L:231:ARG:HG3	1.71	0.72
1:L:168:LYS:HD3	1:L:189:VAL:HG23	1.70	0.72
1:N:168:LYS:HD3	1:N:189:VAL:HG23	1.70	0.72
1:G:150:ILE:HD13	1:G:411:VAL:CB	2.20	0.72
1:F:47:PRO:HB2	1:G:73:MET:SD	2.29	0.72
1:F:150:ILE:HD13	1:F:411:VAL:CB	2.20	0.72
1:H:270:ILE:CG2	1:I:229:ASN:C	2.57	0.72
1:L:146:GLN:NE2	1:L:494:LEU:HD12	2.03	0.72
1:A:150:ILE:HD13	1:A:411:VAL:CB	2.20	0.72
1:B:150:ILE:HD13	1:B:411:VAL:CB	2.20	0.72
1:J:168:LYS:HD3	1:J:189:VAL:HG23	1.70	0.72
1:J:270:ILE:HG12	1:K:231:ARG:HG3	1.70	0.71
1:L:270:ILE:HG12	1:M:231:ARG:HG3	1.70	0.71
1:H:39:VAL:CG1	1:I:69:MET:HE1	2.12	0.71
1:I:36:ARG:CG	1:J:518:GLU:HG3	2.12	0.71
1:K:37:ASN:HB2	1:L:517:THR:HA	1.72	0.71
1:H:37:ASN:HB2	1:I:517:THR:HA	1.72	0.71
1:H:168:LYS:HD3	1:H:189:VAL:HG23	1.70	0.71
1:K:168:LYS:HD3	1:K:189:VAL:HG23	1.70	0.71
1:I:37:ASN:HB2	1:J:517:THR:HA	1.72	0.71
1:J:37:ASN:HB2	1:K:517:THR:HA	1.72	0.71
1:B:39:VAL:HB	1:C:517:THR:CG2	2.15	0.71
1:M:270:ILE:CG2	1:N:229:ASN:C	2.57	0.71



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$\text{overlap } (\mathring{\mathbf{A}})$
1:B:150:ILE:CD1	1:B:494:LEU:HD13	2.21	0.71
1:M:218:PRO:HB3	1:M:246:PRO:HB2	1.73	0.71
1:J:174:VAL:CG2	1:J:194:GLN:CB	2.69	0.71
1:N:174:VAL:CG2	1:N:194:GLN:CB	2.69	0.71
1:L:37:ASN:HB2	1:M:517:THR:HA	1.72	0.71
1:N:218:PRO:HB3	1:N:246:PRO:HB2	1.73	0.71
1:C:150:ILE:CD1	1:C:494:LEU:HD13	2.21	0.71
1:L:390:LYS:CE	1:M:281:PHE:CB	2.56	0.71
1:B:49:ILE:HD12	1:C:513:LEU:HB3	1.73	0.71
1:E:218:PRO:HB3	1:E:246:PRO:HB2	1.73	0.71
1:D:150:ILE:CD1	1:D:494:LEU:HD13	2.21	0.71
1:J:39:VAL:CG1	1:K:69:MET:HE1	2.11	0.71
1:D:49:ILE:HD12	1:E:513:LEU:HB3	1.73	0.71
1:H:218:PRO:HB3	1:H:246:PRO:HB2	1.73	0.70
1:H:229:ASN:C	1:N:270:ILE:CG2	2.57	0.70
1:L:218:PRO:HB3	1:L:246:PRO:HB2	1.73	0.70
1:C:218:PRO:HB3	1:C:246:PRO:HB2	1.73	0.70
1:A:229:ASN:CA	1:G:270:ILE:HG22	2.16	0.70
1:D:218:PRO:HB3	1:D:246:PRO:HB2	1.73	0.70
1:L:174:VAL:CG2	1:L:194:GLN:CB	2.69	0.70
1:C:35:GLY:O	1:D:114:MET:HE2	1.91	0.70
1:F:150:ILE:CD1	1:F:494:LEU:HD13	2.21	0.70
1:A:513:LEU:HB3	1:G:49:ILE:HD12	1.73	0.70
1:K:390:LYS:CE	1:L:281:PHE:CB	2.56	0.70
1:F:218:PRO:HB3	1:F:246:PRO:HB2	1.73	0.70
1:H:517:THR:HA	1:N:37:ASN:HB2	1.72	0.70
1:A:150:ILE:CD1	1:A:494:LEU:HD13	2.21	0.70
1:C:381:VAL:HG11	1:C:393:LYS:HA	1.73	0.70
1:G:150:ILE:CD1	1:G:494:LEU:HD13	2.21	0.70
1:M:390:LYS:HG2	1:N:281:PHE:CD2	2.26	0.70
1:I:390:LYS:HG2	1:J:281:PHE:CD2	2.26	0.70
1:I:174:VAL:CG2	1:I:194:GLN:CB	2.69	0.70
1:F:381:VAL:HG11	1:F:393:LYS:HA	1.73	0.70
1:F:39:VAL:HB	1:G:517:THR:CG2	2.15	0.70
1:B:381:VAL:HG11	1:B:393:LYS:HA	1.73	0.70
1:J:390:LYS:HG2	1:K:281:PHE:CD2	2.26	0.70
1:H:281:PHE:CD2	1:N:390:LYS:HG2	2.26	0.70
1:H:390:LYS:HG2	1:I:281:PHE:CD2	2.26	0.70
1:I:218:PRO:HB3	1:I:246:PRO:HB2	1.73	0.70
1:G:381:VAL:HG11	1:G:393:LYS:HA	1.73	0.70
1:M:390:LYS:CE	1:N:281:PHE:CB	2.56	0.70



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	$overlap(\AA)$
1:D:381:VAL:HG11	1:D:393:LYS:HA	1.73	0.70
1:E:150:ILE:CD1	1:E:494:LEU:HD13	2.21	0.69
1:H:390:LYS:CE	1:I:281:PHE:CB	2.56	0.69
1:M:390:LYS:CG	1:N:281:PHE:HB2	2.18	0.69
1:B:218:PRO:HB3	1:B:246:PRO:HB2	1.73	0.69
1:A:35:GLY:O	1:B:114:MET:HE2	1.91	0.69
1:H:518:GLU:HG3	1:N:36:ARG:CG	2.12	0.69
1:J:458:CYS:O	1:K:112:ASN:ND2	2.25	0.69
1:L:390:LYS:HG2	1:M:281:PHE:CD2	2.26	0.69
1:A:41:ASP:OD2	1:B:69:MET:HG2	1.93	0.69
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.73	0.69
1:M:37:ASN:HB2	1:N:517:THR:HA	1.72	0.69
1:K:458:CYS:O	1:L:112:ASN:ND2	2.24	0.69
1:K:390:LYS:HG2	1:L:281:PHE:CD2	2.26	0.69
1:C:183:LEU:HA	1:C:383:ALA:CB	2.20	0.69
1:L:458:CYS:O	1:M:112:ASN:ND2	2.24	0.69
1:C:41:ASP:OD2	1:D:69:MET:HG2	1.93	0.69
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.73	0.69
1:A:270:ILE:HD13	1:B:231:ARG:HG3	1.75	0.69
1:B:270:ILE:HG22	1:C:229:ASN:CA	2.16	0.69
1:A:231:ARG:HG3	1:G:270:ILE:HD13	1.75	0.69
1:F:270:ILE:HD13	1:G:231:ARG:HG3	1.75	0.69
1:K:174:VAL:CG2	1:K:194:GLN:CB	2.69	0.69
1:C:37:ASN:O	1:D:516:THR:O	2.11	0.69
1:A:69:MET:HG2	1:G:41:ASP:OD2	1.93	0.69
1:E:49:ILE:HD12	1:F:513:LEU:HB3	1.73	0.69
1:A:218:PRO:HB3	1:A:246:PRO:HB2	1.73	0.69
1:E:41:ASP:OD2	1:F:69:MET:HG2	1.93	0.69
1:G:218:PRO:HB3	1:G:246:PRO:HB2	1.73	0.69
1:J:174:VAL:CG1	1:J:331:THR:OG1	2.40	0.69
1:M:174:VAL:CG2	1:M:194:GLN:CB	2.69	0.69
1:E:37:ASN:O	1:F:516:THR:O	2.10	0.69
1:B:270:ILE:HD13	1:C:231:ARG:HG3	1.75	0.69
1:C:49:ILE:HD12	1:D:513:LEU:HB3	1.73	0.69
1:B:37:ASN:O	1:C:516:THR:O	2.11	0.68
1:E:381:VAL:HG11	1:E:393:LYS:HA	1.73	0.68
1:F:37:ASN:O	1:G:516:THR:O	2.11	0.68
1:A:49:ILE:HD12	1:B:513:LEU:HB3	1.73	0.68
1:H:85:ALA:O	1:H:405:ALA:HB3	1.91	0.68
1:A:381:VAL:HG11	1:A:393:LYS:HA	1.73	0.68
1:M:270:ILE:HG22	1:N:229:ASN:O	1.91	0.68



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:D:37:ASN:O	1:E:516:THR:O	2.11	0.68
1:H:174:VAL:CG2	1:H:194:GLN:CB	2.69	0.68
1:A:114:MET:HE2	1:G:35:GLY:O	1.91	0.68
1:H:270:ILE:HG22	1:I:229:ASN:O	1.91	0.68
1:E:270:ILE:HD13	1:F:231:ARG:HG3	1.75	0.68
1:I:458:CYS:O	1:J:112:ASN:ND2	2.24	0.68
1:M:383:ALA:HB1	1:N:283:ASP:HB2	1.76	0.68
1:K:383:ALA:HB1	1:L:283:ASP:HB2	1.76	0.68
1:E:183:LEU:HA	1:E:383:ALA:CB	2.20	0.68
1:E:35:GLY:O	1:F:114:MET:HE2	1.94	0.68
1:L:383:ALA:HB1	1:M:283:ASP:HB2	1.76	0.68
1:K:390:LYS:HG2	1:L:281:PHE:HB3	1.74	0.68
1:K:387:VAL:CA	1:L:281:PHE:CD1	2.52	0.68
1:K:85:ALA:O	1:K:405:ALA:HB3	1.91	0.68
1:A:183:LEU:HA	1:A:383:ALA:CB	2.20	0.68
1:F:183:LEU:HA	1:F:383:ALA:CB	2.20	0.68
1:H:283:ASP:HB2	1:N:383:ALA:HB1	1.76	0.68
1:J:383:ALA:HB1	1:K:283:ASP:HB2	1.76	0.68
1:B:41:ASP:OD2	1:C:69:MET:HG2	1.93	0.67
1:F:35:GLY:O	1:G:114:MET:SD	2.53	0.67
1:G:183:LEU:HA	1:G:383:ALA:CB	2.20	0.67
1:A:37:ASN:O	1:B:516:THR:O	2.11	0.67
1:D:35:GLY:O	1:E:114:MET:SD	2.52	0.67
1:F:37:ASN:HB2	1:G:516:THR:CA	1.87	0.67
1:J:85:ALA:O	1:J:405:ALA:HB3	1.91	0.67
1:A:516:THR:O	1:G:37:ASN:O	2.11	0.67
1:C:270:ILE:HD13	1:D:231:ARG:HG3	1.75	0.67
1:I:174:VAL:CG1	1:I:331:THR:OG1	2.40	0.67
1:C:35:GLY:O	1:D:114:MET:SD	2.52	0.67
1:A:114:MET:SD	1:G:35:GLY:O	2.53	0.67
1:E:35:GLY:O	1:F:114:MET:SD	2.53	0.67
1:B:39:VAL:CB	1:C:517:THR:HG23	2.25	0.67
1:H:69:MET:HE1	1:N:39:VAL:CG1	2.13	0.67
1:N:174:VAL:HG11	1:N:331:THR:HG1	1.60	0.67
1:M:458:CYS:O	1:N:112:ASN:ND2	2.25	0.67
1:A:517:THR:HG23	1:G:39:VAL:CB	2.25	0.67
1:I:390:LYS:CE	1:J:281:PHE:CB	2.56	0.67
1:H:112:ASN:ND2	1:N:458:CYS:O	2.24	0.67
1:C:47:PRO:CG	1:D:73:MET:SD	2.83	0.66
1:J:390:LYS:HG2	1:K:281:PHE:HB3	1.74	0.66
1:H:281:PHE:HB3	1:N:390:LYS:HG2	1.74	0.66



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:D:270:ILE:HD13	1:E:231:ARG:HG3	1.75	0.66
1:A:39:VAL:CB	1:B:517:THR:HG23	2.25	0.66
1:A:517:THR:CG2	1:G:39:VAL:HB	2.15	0.66
1:L:85:ALA:O	1:L:405:ALA:HB3	1.91	0.66
1:I:383:ALA:HB1	1:J:283:ASP:HB2	1.76	0.66
1:J:390:LYS:CE	1:K:281:PHE:CB	2.56	0.66
1:M:174:VAL:CG1	1:M:331:THR:OG1	2.40	0.66
1:H:458:CYS:O	1:I:112:ASN:ND2	2.25	0.66
1:I:390:LYS:HG2	1:J:281:PHE:HB3	1.74	0.66
1:I:387:VAL:CA	1:J:281:PHE:CD1	2.52	0.66
1:K:270:ILE:HG22	1:L:229:ASN:O	1.91	0.66
1:H:270:ILE:CD1	1:I:231:ARG:HG3	2.26	0.66
1:A:245:LYS:HD3	1:B:232:GLU:CD	2.16	0.66
1:C:245:LYS:HD3	1:D:232:GLU:CD	2.16	0.66
1:B:245:LYS:HD3	1:C:232:GLU:CD	2.16	0.66
1:I:270:ILE:CD1	1:J:231:ARG:HG3	2.26	0.66
1:A:232:GLU:CD	1:G:245:LYS:HD3	2.16	0.66
1:K:174:VAL:CG1	1:K:331:THR:OG1	2.40	0.66
1:B:35:GLY:O	1:C:114:MET:SD	2.53	0.66
1:F:47:PRO:CG	1:G:73:MET:SD	2.83	0.66
1:B:49:ILE:CG2	1:C:513:LEU:HD22	2.26	0.66
1:H:383:ALA:HB1	1:I:283:ASP:HB2	1.76	0.66
1:D:47:PRO:CG	1:E:73:MET:SD	2.83	0.66
1:D:245:LYS:HD3	1:E:232:GLU:CD	2.16	0.66
1:A:35:GLY:O	1:B:114:MET:SD	2.53	0.66
1:H:231:ARG:HG3	1:N:270:ILE:CD1	2.26	0.66
1:A:49:ILE:CG2	1:B:513:LEU:HD22	2.26	0.66
1:C:49:ILE:CG2	1:D:513:LEU:HD22	2.26	0.66
1:D:270:ILE:CG2	1:E:229:ASN:CA	2.74	0.66
1:L:390:LYS:HG2	1:M:281:PHE:HB3	1.74	0.65
1:F:245:LYS:HD3	1:G:232:GLU:CD	2.16	0.65
1:A:39:VAL:CB	1:B:517:THR:HG21	1.94	0.65
1:L:270:ILE:CD1	1:M:231:ARG:HG3	2.26	0.65
1:I:85:ALA:O	1:I:405:ALA:HB3	1.91	0.65
1:A:513:LEU:HD22	1:G:49:ILE:CG2	2.26	0.65
1:N:85:ALA:O	1:N:405:ALA:HB3	1.91	0.65
1:D:41:ASP:OD2	1:E:69:MET:HG2	1.93	0.65
1:J:270:ILE:CD1	1:K:231:ARG:HG3	2.26	0.65
1:M:270:ILE:CD1	1:N:231:ARG:HG3	2.26	0.65
1:M:85:ALA:O	1:M:405:ALA:HB3	1.91	0.65
1:E:245:LYS:HD3	1:F:232:GLU:CD	2.16	0.65



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:A:47:PRO:CG	1:B:73:MET:SD	2.83	0.65
1:H:281:PHE:CD1	1:N:387:VAL:CA	2.52	0.65
1:C:270:ILE:CG2	1:D:229:ASN:CA	2.74	0.65
1:D:39:VAL:CB	1:E:517:THR:HG23	2.25	0.65
1:A:73:MET:SD	1:G:47:PRO:CG	2.83	0.65
1:F:39:VAL:CB	1:G:517:THR:HG23	2.24	0.65
1:M:146:GLN:HE22	1:M:494:LEU:CD1	2.10	0.65
1:A:37:ASN:O	1:B:518:GLU:N	2.30	0.65
1:F:37:ASN:O	1:G:518:GLU:N	2.30	0.65
1:F:270:ILE:CG2	1:G:229:ASN:CA	2.74	0.65
1:C:36:ARG:HD3	1:D:114:MET:HG2	1.78	0.65
1:C:39:VAL:CB	1:D:517:THR:HG23	2.25	0.65
1:D:37:ASN:O	1:E:518:GLU:N	2.30	0.65
1:K:270:ILE:CD1	1:L:231:ARG:HG3	2.26	0.65
1:B:270:ILE:CG2	1:C:229:ASN:CA	2.74	0.65
1:N:146:GLN:HE22	1:N:494:LEU:CD1	2.10	0.65
1:B:37:ASN:O	1:C:518:GLU:N	2.30	0.65
1:I:408:GLU:HG3	1:I:498:LYS:NZ	2.12	0.65
1:F:49:ILE:HD12	1:G:513:LEU:HB3	1.73	0.65
1:D:49:ILE:CG2	1:E:513:LEU:HD22	2.26	0.65
1:K:408:GLU:HG3	1:K:498:LYS:NZ	2.12	0.65
1:E:270:ILE:CG2	1:F:229:ASN:CA	2.74	0.65
1:H:174:VAL:CG1	1:H:331:THR:OG1	2.40	0.65
1:E:37:ASN:O	1:F:518:GLU:N	2.30	0.65
1:F:49:ILE:CG2	1:G:513:LEU:HD22	2.26	0.65
1:B:183:LEU:HA	1:B:383:ALA:CB	2.20	0.65
1:B:36:ARG:HD3	1:C:114:MET:HG2	1.78	0.65
1:H:86:GLY:N	1:H:405:ALA:HB1	2.12	0.65
1:D:36:ARG:HD3	1:E:114:MET:HG2	1.78	0.65
1:J:146:GLN:HE22	1:J:494:LEU:CD1	2.10	0.65
1:C:37:ASN:O	1:D:518:GLU:N	2.30	0.64
1:F:41:ASP:OD2	1:G:69:MET:HG2	1.93	0.64
1:J:387:VAL:C	1:K:281:PHE:CZ	2.69	0.64
1:H:281:PHE:CB	1:N:390:LYS:CE	2.56	0.64
1:N:408:GLU:HG3	1:N:498:LYS:NZ	2.12	0.64
1:I:146:GLN:HE22	1:I:494:LEU:CD1	2.10	0.64
1:H:146:GLN:HE22	1:H:494:LEU:CD1	2.10	0.64
1:A:518:GLU:N	1:G:37:ASN:O	2.30	0.64
1:L:146:GLN:HE22	1:L:494:LEU:CD1	2.10	0.64
1:E:47:PRO:CG	1:F:73:MET:SD	2.83	0.64
1:A:39:VAL:HB	1:B:517:THR:CG2	2.15	0.64



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:E:49:ILE:CG2	1:F:513:LEU:HD22	2.26	0.64
1:M:408:GLU:HG3	1:M:498:LYS:NZ	2.12	0.64
1:B:305:ILE:HG22	1:B:308:GLU:HB2	1.80	0.64
1:G:305:ILE:HG22	1:G:308:GLU:HB2	1.79	0.64
1:A:305:ILE:HG22	1:A:308:GLU:HB2	1.80	0.64
1:H:387:VAL:CA	1:I:281:PHE:CD1	2.52	0.64
1:M:390:LYS:HG2	1:N:281:PHE:HB3	1.74	0.64
1:H:408:GLU:HG3	1:H:498:LYS:NZ	2.12	0.64
1:A:270:ILE:CG2	1:B:229:ASN:CA	2.74	0.64
1:M:36:ARG:CB	1:N:518:GLU:CB	2.71	0.64
1:D:183:LEU:HA	1:D:383:ALA:CB	2.20	0.64
1:A:36:ARG:HD3	1:B:114:MET:HG2	1.78	0.64
1:K:146:GLN:HE22	1:K:494:LEU:CD1	2.10	0.64
1:I:245:LYS:HD3	1:J:232:GLU:CD	2.18	0.64
1:F:36:ARG:HD3	1:G:114:MET:HG2	1.78	0.64
1:F:305:ILE:HG22	1:F:308:GLU:HB2	1.80	0.64
1:H:386:GLU:OE2	1:I:285:ARG:HA	1.98	0.64
1:I:386:GLU:OE2	1:J:285:ARG:HA	1.98	0.64
1:H:245:LYS:HD3	1:I:232:GLU:CD	2.18	0.64
1:I:86:GLY:N	1:I:405:ALA:HB1	2.12	0.64
1:K:245:LYS:HD3	1:L:232:GLU:CD	2.18	0.64
1:L:408:GLU:HG3	1:L:498:LYS:NZ	2.12	0.64
1:L:387:VAL:C	1:M:281:PHE:CZ	2.69	0.64
1:I:387:VAL:C	1:J:281:PHE:CZ	2.69	0.64
1:K:387:VAL:C	1:L:281:PHE:CZ	2.69	0.64
1:J:245:LYS:HD3	1:K:232:GLU:CD	2.18	0.64
1:H:232:GLU:CD	1:N:245:LYS:HD3	2.18	0.64
1:M:245:LYS:HD3	1:N:232:GLU:CD	2.18	0.64
1:E:36:ARG:HD3	1:F:114:MET:HG2	1.78	0.64
1:E:39:VAL:CB	1:F:517:THR:HG23	2.25	0.63
1:H:285:ARG:HA	1:N:386:GLU:OE2	1.98	0.63
1:G:383:ALA:HA	1:G:389:MET:HG2	1.80	0.63
1:C:305:ILE:HG22	1:C:308:GLU:HB2	1.80	0.63
1:L:390:LYS:CG	1:M:281:PHE:HB3	2.28	0.63
1:J:386:GLU:OE2	1:K:285:ARG:HA	1.98	0.63
1:H:305:ILE:HG22	1:H:308:GLU:HB2	1.80	0.63
1:E:305:ILE:HG22	1:E:308:GLU:HB2	1.80	0.63
1:J:390:LYS:CG	1:K:281:PHE:HB3	2.28	0.63
1:H:390:LYS:HG2	1:I:281:PHE:HB3	1.74	0.63
1:J:270:ILE:HG22	1:K:229:ASN:O	1.91	0.63
1:J:408:GLU:HG3	1:J:498:LYS:NZ	2.12	0.63



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	$overlap(\AA)$
1:F:383:ALA:HA	1:F:389:MET:HG2	1.80	0.63
1:H:229:ASN:O	1:N:270:ILE:HG22	1.91	0.63
1:L:174:VAL:CG1	1:L:331:THR:OG1	2.40	0.63
1:A:114:MET:HG2	1:G:36:ARG:HD3	1.78	0.63
1:A:383:ALA:HA	1:A:389:MET:HG2	1.80	0.63
1:I:305:ILE:HG22	1:I:308:GLU:HB2	1.80	0.63
1:D:305:ILE:HG22	1:D:308:GLU:HB2	1.80	0.63
1:K:231:ARG:CZ	1:K:231:ARG:HB3	2.29	0.63
1:H:518:GLU:CB	1:N:36:ARG:CB	2.71	0.63
1:I:231:ARG:HB3	1:I:231:ARG:CZ	2.29	0.63
1:L:245:LYS:HD3	1:M:232:GLU:CD	2.18	0.63
1:N:174:VAL:CG1	1:N:331:THR:OG1	2.40	0.63
1:E:37:ASN:N	1:F:516:THR:CG2	2.62	0.63
1:L:36:ARG:CB	1:M:518:GLU:CB	2.71	0.63
1:E:383:ALA:HA	1:E:389:MET:HG2	1.80	0.63
1:N:305:ILE:HG22	1:N:308:GLU:HB2	1.80	0.63
1:L:386:GLU:OE2	1:M:285:ARG:HA	1.98	0.63
1:G:231:ARG:CZ	1:G:231:ARG:HB3	2.29	0.63
1:J:305:ILE:HG22	1:J:308:GLU:HB2	1.80	0.63
1:B:47:PRO:CG	1:C:73:MET:SD	2.83	0.62
1:M:386:GLU:OE2	1:N:285:ARG:HA	1.98	0.62
1:K:305:ILE:HG22	1:K:308:GLU:HB2	1.80	0.62
1:I:431:GLY:H	1:I:437:ASN:HD21	1.47	0.62
1:I:270:ILE:HG22	1:J:229:ASN:O	1.91	0.62
1:A:231:ARG:CZ	1:A:231:ARG:HB3	2.29	0.62
1:C:383:ALA:HA	1:C:389:MET:HG2	1.80	0.62
1:F:431:GLY:H	1:F:437:ASN:HD21	1.48	0.62
1:N:431:GLY:H	1:N:437:ASN:HD21	1.47	0.62
1:H:26:ALA:HA	1:I:8:PHE:CE2	2.34	0.62
1:J:270:ILE:CG1	1:K:231:ARG:HG3	2.30	0.62
1:L:270:ILE:CG1	1:M:231:ARG:HG3	2.30	0.62
1:M:26:ALA:HA	1:N:8:PHE:CE2	2.35	0.62
1:J:431:GLY:H	1:J:437:ASN:HD21	1.47	0.62
1:A:229:ASN:CA	1:G:270:ILE:CG2	2.74	0.62
1:G:150:ILE:HG12	1:G:494:LEU:CD1	2.29	0.62
1:J:86:GLY:N	1:J:405:ALA:HB1	2.13	0.62
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.81	0.62
1:M:305:ILE:HG22	1:M:308:GLU:HB2	1.80	0.62
1:L:305:ILE:HG22	1:L:308:GLU:HB2	1.80	0.62
1:D:150:ILE:HG12	1:D:494:LEU:CD1	2.28	0.62
1:J:387:VAL:CA	1:K:281:PHE:CD1	2.52	0.62



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:M:387:VAL:C	1:N:281:PHE:CZ	2.69	0.62
1:L:270:ILE:HG22	1:M:229:ASN:O	1.91	0.62
1:B:383:ALA:HA	1:B:389:MET:HG2	1.80	0.62
1:A:150:ILE:HG12	1:A:494:LEU:CD1	2.29	0.62
1:F:37:ASN:N	1:G:516:THR:CG2	2.62	0.62
1:F:150:ILE:HG12	1:F:494:LEU:CD1	2.29	0.62
1:H:270:ILE:CG1	1:I:231:ARG:HG3	2.30	0.62
1:H:41:ASP:CB	1:I:522:THR:HG23	2.30	0.62
1:B:231:ARG:CZ	1:B:231:ARG:HB3	2.29	0.62
1:M:431:GLY:H	1:M:437:ASN:HD21	1.47	0.62
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.81	0.62
1:F:231:ARG:CZ	1:F:231:ARG:HB3	2.29	0.62
1:C:35:GLY:O	1:D:114:MET:HE1	2.00	0.62
1:D:431:GLY:H	1:D:437:ASN:HD21	1.48	0.62
1:H:281:PHE:CZ	1:N:387:VAL:C	2.69	0.62
1:K:386:GLU:OE2	1:L:285:ARG:HA	1.98	0.62
1:D:383:ALA:HA	1:D:389:MET:HG2	1.80	0.62
1:I:41:ASP:CB	1:J:522:THR:HG23	2.30	0.62
1:I:26:ALA:HA	1:J:8:PHE:CE2	2.34	0.62
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.81	0.62
1:E:35:GLY:O	1:F:114:MET:HE1	1.97	0.61
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.81	0.61
1:L:26:ALA:HA	1:M:8:PHE:CE2	2.34	0.61
1:B:160:LYS:O	1:B:164:GLU:HG2	2.00	0.61
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.81	0.61
1:B:150:ILE:HG12	1:B:494:LEU:CD1	2.29	0.61
1:E:150:ILE:HG12	1:E:494:LEU:CD1	2.29	0.61
1:N:231:ARG:HB3	1:N:231:ARG:CZ	2.29	0.61
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.81	0.61
1:K:26:ALA:HA	1:L:8:PHE:CE2	2.34	0.61
1:H:8:PHE:CE2	1:N:26:ALA:HA	2.34	0.61
1:C:431:GLY:H	1:C:437:ASN:HD21	1.48	0.61
1:A:516:THR:CG2	1:G:37:ASN:N	2.62	0.61
1:H:387:VAL:C	1:I:281:PHE:CZ	2.69	0.61
1:H:231:ARG:HG3	1:N:270:ILE:CG1	2.30	0.61
1:M:41:ASP:CB	1:N:522:THR:HG23	2.30	0.61
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.81	0.61
1:H:231:ARG:HB3	1:H:231:ARG:CZ	2.29	0.61
1:I:39:VAL:CG1	1:J:69:MET:HE1	2.19	0.61
1:D:49:ILE:HG21	1:E:513:LEU:CD2	2.31	0.61
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.82	0.61



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.82	0.61
1:B:49:ILE:HG21	1:C:513:LEU:CD2	2.31	0.61
1:C:160:LYS:O	1:C:164:GLU:HG2	2.00	0.61
1:K:41:ASP:CB	1:L:522:THR:HG23	2.30	0.61
1:C:231:ARG:CZ	1:C:231:ARG:HB3	2.29	0.61
1:E:231:ARG:CZ	1:E:231:ARG:HB3	2.29	0.61
1:K:431:GLY:H	1:K:437:ASN:HD21	1.47	0.61
1:H:390:LYS:CG	1:I:281:PHE:HB3	2.28	0.61
1:J:231:ARG:CZ	1:J:231:ARG:HB3	2.29	0.61
1:M:231:ARG:CZ	1:M:231:ARG:HB3	2.29	0.61
1:M:86:GLY:N	1:M:405:ALA:HB1	2.12	0.61
1:D:231:ARG:HB3	1:D:231:ARG:CZ	2.29	0.61
1:E:431:GLY:H	1:E:437:ASN:HD21	1.48	0.61
1:H:281:PHE:HB3	1:N:390:LYS:CG	2.28	0.61
1:K:390:LYS:CG	1:L:281:PHE:HB3	2.28	0.61
1:I:270:ILE:CG1	1:J:231:ARG:HG3	2.30	0.61
1:K:270:ILE:CG1	1:L:231:ARG:HG3	2.30	0.61
1:M:270:ILE:CG1	1:N:231:ARG:HG3	2.30	0.61
1:C:49:ILE:HG21	1:D:513:LEU:CD2	2.31	0.61
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.81	0.61
1:A:49:ILE:HG21	1:B:513:LEU:CD2	2.31	0.61
1:E:49:ILE:HG21	1:F:513:LEU:CD2	2.31	0.61
1:D:160:LYS:O	1:D:164:GLU:HG2	2.00	0.61
1:L:41:ASP:CB	1:M:522:THR:HG23	2.30	0.61
1:J:26:ALA:HA	1:K:8:PHE:CE2	2.35	0.61
1:I:390:LYS:CG	1:J:281:PHE:HB3	2.28	0.60
1:L:231:ARG:CZ	1:L:231:ARG:HB3	2.29	0.60
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.81	0.60
1:L:86:GLY:N	1:L:405:ALA:HB1	2.12	0.60
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.82	0.60
1:H:36:ARG:CB	1:I:518:GLU:CB	2.71	0.60
1:G:431:GLY:H	1:G:437:ASN:HD21	1.48	0.60
1:E:160:LYS:O	1:E:164:GLU:HG2	2.00	0.60
1:H:522:THR:HG23	1:N:41:ASP:CB	2.30	0.60
1:K:86:GLY:N	1:K:405:ALA:HB1	2.12	0.60
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.81	0.60
1:A:8:PHE:HE2	1:G:26:ALA:CA	2.14	0.60
1:L:230:ILE:HG12	1:L:258:ALA:HA	1.83	0.60
1:N:230:ILE:HG12	1:N:258:ALA:HA	1.83	0.60
1:M:230:ILE:HG12	1:M:258:ALA:HA	1.83	0.60
1:B:230:ILE:HG12	1:B:258:ALA:HA	1.83	0.60



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Atom 1		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; ({\rm \AA})$	overlap (Å)
1:A:160:LYS:O	1:A:164:GLU:HG2	2.00	0.60
1:B:431:GLY:H	1:B:437:ASN:HD21	1.48	0.60
1:A:37:ASN:N	1:B:516:THR:CG2	2.62	0.60
1:A:26:ALA:CA	1:B:8:PHE:HE2	2.14	0.60
1:F:160:LYS:O	1:F:164:GLU:HG2	2.00	0.60
1:G:438:VAL:O	1:G:442:VAL:HG23	2.02	0.60
1:A:438:VAL:O	1:A:442:VAL:HG23	2.02	0.60
1:A:230:ILE:HG12	1:A:258:ALA:HA	1.83	0.60
1:B:37:ASN:N	1:C:516:THR:CG2	2.62	0.60
1:J:41:ASP:CB	1:K:522:THR:HG23	2.30	0.60
1:D:26:ALA:CA	1:E:8:PHE:HE2	2.14	0.60
1:L:431:GLY:H	1:L:437:ASN:HD21	1.47	0.60
1:A:431:GLY:H	1:A:437:ASN:HD21	1.48	0.60
1:B:438:VAL:O	1:B:442:VAL:HG23	2.02	0.60
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.81	0.60
1:G:230:ILE:HG12	1:G:258:ALA:HA	1.83	0.60
1:A:513:LEU:CD2	1:G:49:ILE:HG21	2.31	0.60
1:E:26:ALA:CA	1:F:8:PHE:HE2	2.14	0.60
1:H:230:ILE:HG12	1:H:258:ALA:HA	1.83	0.60
1:G:160:LYS:O	1:G:164:GLU:HG2	2.00	0.60
1:H:431:GLY:H	1:H:437:ASN:HD21	1.47	0.60
1:C:230:ILE:HG12	1:C:258:ALA:HA	1.83	0.60
1:F:230:ILE:HG12	1:F:258:ALA:HA	1.83	0.60
1:N:86:GLY:N	1:N:405:ALA:HB1	2.12	0.60
1:F:26:ALA:CA	1:G:8:PHE:HE2	2.14	0.60
1:L:387:VAL:CA	1:M:281:PHE:CD1	2.52	0.60
1:F:49:ILE:HG21	1:G:513:LEU:CD2	2.31	0.60
1:K:36:ARG:CB	1:L:518:GLU:CB	2.71	0.60
1:A:114:MET:HE1	1:G:35:GLY:O	2.00	0.60
1:F:438:VAL:O	1:F:442:VAL:HG23	2.02	0.60
1:K:438:VAL:O	1:K:442:VAL:HG23	2.02	0.60
1:B:26:ALA:CA	1:C:8:PHE:HE2	2.14	0.60
1:D:230:ILE:HG12	1:D:258:ALA:HA	1.83	0.60
1:K:230:ILE:HG12	1:K:258:ALA:HA	1.83	0.60
1:C:438:VAL:O	1:C:442:VAL:HG23	2.02	0.59
1:C:26:ALA:CA	1:D:8:PHE:HE2	2.14	0.59
1:N:438:VAL:O	1:N:442:VAL:HG23	2.02	0.59
1:I:230:ILE:HG12	1:I:258:ALA:HA	1.83	0.59
1:J:438:VAL:O	1:J:442:VAL:HG23	2.02	0.59
1:J:386:GLU:CA	1:K:281:PHE:N	2.65	0.59
1:L:438:VAL:O	1:L:442:VAL:HG23	2.02	0.59



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:M:390:LYS:CG	1:N:281:PHE:HB3	2.28	0.59
1:J:230:ILE:HG12	1:J:258:ALA:HA	1.83	0.59
1:A:49:ILE:HG21	1:B:513:LEU:HA	1.84	0.59
1:E:41:ASP:OD2	1:F:69:MET:CG	2.51	0.59
1:M:387:VAL:CA	1:N:281:PHE:CD1	2.52	0.59
1:M:270:ILE:HG22	1:N:229:ASN:C	2.22	0.59
1:M:438:VAL:O	1:M:442:VAL:HG23	2.02	0.59
1:E:230:ILE:HG12	1:E:258:ALA:HA	1.83	0.59
1:C:37:ASN:N	1:D:516:THR:CG2	2.62	0.59
1:H:386:GLU:CA	1:I:281:PHE:N	2.65	0.59
1:G:349:ILE:HA	1:G:352:GLN:CG	2.33	0.59
1:H:281:PHE:N	1:N:386:GLU:CA	2.65	0.59
1:I:36:ARG:CB	1:J:518:GLU:CB	2.71	0.59
1:K:349:ILE:HA	1:K:352:GLN:CG	2.33	0.59
1:F:47:PRO:CB	1:G:73:MET:SD	2.91	0.59
1:I:386:GLU:CA	1:J:281:PHE:N	2.65	0.59
1:L:349:ILE:HA	1:L:352:GLN:CG	2.33	0.59
1:C:349:ILE:HA	1:C:352:GLN:CG	2.33	0.59
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.85	0.59
1:D:349:ILE:HA	1:D:352:GLN:CG	2.33	0.59
1:E:47:PRO:CB	1:F:73:MET:SD	2.91	0.59
1:J:36:ARG:CB	1:K:518:GLU:CB	2.71	0.59
1:F:349:ILE:HA	1:F:352:GLN:CG	2.33	0.59
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.85	0.59
1:M:349:ILE:HA	1:M:352:GLN:CG	2.33	0.58
1:B:349:ILE:HA	1:B:352:GLN:CG	2.33	0.58
1:E:438:VAL:O	1:E:442:VAL:HG23	2.02	0.58
1:C:150:ILE:HG12	1:C:494:LEU:CD1	2.29	0.58
1:A:73:MET:SD	1:G:47:PRO:CB	2.91	0.58
1:H:36:ARG:CG	1:I:518:GLU:CG	2.79	0.58
1:I:438:VAL:O	1:I:442:VAL:HG23	2.02	0.58
1:D:438:VAL:O	1:D:442:VAL:HG23	2.02	0.58
1:J:349:ILE:HA	1:J:352:GLN:CG	2.33	0.58
1:D:41:ASP:OD2	1:E:69:MET:CG	2.51	0.58
1:B:47:PRO:CB	1:C:73:MET:SD	2.91	0.58
1:E:49:ILE:HG21	1:F:513:LEU:HA	1.84	0.58
1:F:49:ILE:HG21	1:G:513:LEU:HA	1.84	0.58
1:B:49:ILE:HG21	1:C:513:LEU:HA	1.84	0.58
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.85	0.58
1:A:513:LEU:HA	1:G:49:ILE:HG21	1.84	0.58
1:C:49:ILE:HG21	1:D:513:LEU:HA	1.84	0.58



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:N:161:LEU:HD21	1:N:185:ASP:HB3	1.84	0.58
1:L:386:GLU:OE2	1:M:285:ARG:HB2	2.04	0.58
1:H:229:ASN:C	1:N:270:ILE:HG22	2.22	0.58
1:D:47:PRO:CB	1:E:73:MET:SD	2.91	0.58
1:H:386:GLU:OE2	1:I:285:ARG:HB2	2.04	0.58
1:D:49:ILE:HG21	1:E:513:LEU:HA	1.84	0.58
1:A:35:GLY:O	1:B:114:MET:HE1	2.00	0.58
1:A:349:ILE:HA	1:A:352:GLN:CG	2.33	0.58
1:H:438:VAL:O	1:H:442:VAL:HG23	2.02	0.58
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.84	0.58
1:E:349:ILE:HA	1:E:352:GLN:CG	2.33	0.58
1:I:36:ARG:CG	1:J:518:GLU:CG	2.79	0.58
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.84	0.58
1:I:386:GLU:OE2	1:J:285:ARG:HB2	2.04	0.58
1:H:285:ARG:HB2	1:N:386:GLU:OE2	2.04	0.58
1:A:69:MET:CG	1:G:41:ASP:OD2	2.51	0.58
1:J:386:GLU:OE2	1:K:285:ARG:HB2	2.04	0.58
1:I:349:ILE:HA	1:I:352:GLN:CG	2.33	0.57
1:D:37:ASN:N	1:E:516:THR:CG2	2.62	0.57
1:A:47:PRO:CB	1:B:73:MET:SD	2.91	0.57
1:M:386:GLU:CA	1:N:281:PHE:N	2.65	0.57
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.84	0.57
1:C:47:PRO:CB	1:D:73:MET:SD	2.91	0.57
1:C:392:LYS:O	1:C:396:VAL:HG23	2.05	0.57
1:D:392:LYS:O	1:D:396:VAL:HG23	2.05	0.57
1:N:349:ILE:HA	1:N:352:GLN:CG	2.33	0.57
1:K:270:ILE:HG22	1:L:229:ASN:C	2.22	0.57
1:H:174:VAL:HG11	1:H:331:THR:HG1	1.67	0.57
1:K:431:GLY:H	1:K:437:ASN:ND2	2.03	0.57
1:B:392:LYS:O	1:B:396:VAL:HG23	2.05	0.57
1:M:386:GLU:OE2	1:N:285:ARG:HB2	2.04	0.57
1:E:392:LYS:O	1:E:396:VAL:HG23	2.05	0.57
1:H:174:VAL:HG21	1:H:194:GLN:HB2	1.86	0.57
1:H:59:GLU:O	1:I:4:LYS:CG	2.53	0.57
1:C:41:ASP:OD2	1:D:69:MET:CG	2.51	0.57
1:K:386:GLU:OE2	1:L:285:ARG:HB2	2.04	0.57
1:I:431:GLY:H	1:I:437:ASN:ND2	2.03	0.57
1:E:431:GLY:H	1:E:437:ASN:ND2	2.03	0.57
1:A:431:GLY:H	1:A:437:ASN:ND2	2.03	0.57
1:A:41:ASP:OD2	1:B:69:MET:CG	2.51	0.57
1:F:41:ASP:OD2	1:G:69:MET:CG	2.51	0.57



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Continuea from preva		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:H:270:ILE:HG22	1:I:229:ASN:C	2.22	0.57
1:D:26:ALA:HB2	1:E:8:PHE:CZ	2.40	0.57
1:C:26:ALA:HB2	1:D:8:PHE:CZ	2.40	0.57
1:L:59:GLU:O	1:M:4:LYS:CG	2.53	0.57
1:B:431:GLY:H	1:B:437:ASN:ND2	2.03	0.57
1:A:392:LYS:O	1:A:396:VAL:HG23	2.05	0.57
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.87	0.57
1:J:270:ILE:HG22	1:K:229:ASN:C	2.22	0.57
1:H:408:GLU:CG	1:H:498:LYS:NZ	2.68	0.57
1:G:431:GLY:H	1:G:437:ASN:ND2	2.03	0.57
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.87	0.57
1:I:59:GLU:O	1:J:4:LYS:CG	2.53	0.56
1:K:59:GLU:O	1:L:4:LYS:CG	2.53	0.56
1:J:383:ALA:CB	1:K:283:ASP:HB2	2.35	0.56
1:M:431:GLY:H	1:M:437:ASN:ND2	2.03	0.56
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.87	0.56
1:M:220:ILE:HD12	1:M:296:THR:HG21	1.87	0.56
1:H:220:ILE:HD12	1:H:296:THR:HG21	1.87	0.56
1:N:174:VAL:HG21	1:N:194:GLN:HB2	1.86	0.56
1:K:383:ALA:CB	1:L:283:ASP:HB2	2.35	0.56
1:C:431:GLY:H	1:C:437:ASN:ND2	2.03	0.56
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.87	0.56
1:H:349:ILE:HA	1:H:352:GLN:CG	2.33	0.56
1:L:270:ILE:HG22	1:M:229:ASN:C	2.22	0.56
1:N:408:GLU:CG	1:N:498:LYS:NZ	2.68	0.56
1:B:26:ALA:HB2	1:C:8:PHE:CZ	2.40	0.56
1:E:26:ALA:HB2	1:F:8:PHE:CZ	2.40	0.56
1:J:59:GLU:O	1:K:4:LYS:CG	2.53	0.56
1:I:183:LEU:H	1:I:383:ALA:HB3	1.70	0.56
1:D:431:GLY:H	1:D:437:ASN:ND2	2.03	0.56
1:G:392:LYS:O	1:G:396:VAL:HG23	2.05	0.56
1:J:390:LYS:HE2	1:K:281:PHE:CA	2.35	0.56
1:K:388:GLU:H	1:L:281:PHE:HE1	1.53	0.56
1:K:174:VAL:HG21	1:K:194:GLN:HB2	1.86	0.56
1:C:68:ASN:O	1:C:72:GLN:HG2	2.05	0.56
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.87	0.56
1:B:68:ASN:O	1:B:72:GLN:HG2	2.05	0.56
1:A:68:ASN:O	1:A:72:GLN:HG2	2.05	0.56
1:L:408:GLU:CG	1:L:498:LYS:NZ	2.68	0.56
1:M:408:GLU:CG	1:M:498:LYS:NZ	2.68	0.56
1:K:408:GLU:CG	1:K:498:LYS:NZ	2.68	0.56



Continued from previous page...

A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap(Å)
1:F:431:GLY:H	1:F:437:ASN:ND2	2.03	0.56
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.87	0.56
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.87	0.56
1:E:68:ASN:O	1:E:72:GLN:HG2	2.05	0.56
1:F:392:LYS:O	1:F:396:VAL:HG23	2.05	0.56
1:F:68:ASN:O	1:F:72:GLN:HG2	2.05	0.56
1:B:41:ASP:OD2	1:C:69:MET:CG	2.51	0.56
1:A:37:ASN:H	1:B:516:THR:HG22	1.70	0.56
1:K:390:LYS:HE2	1:L:281:PHE:CA	2.35	0.56
1:M:174:VAL:HG21	1:M:194:GLN:HB2	1.86	0.56
1:M:59:GLU:O	1:N:4:LYS:CG	2.53	0.56
1:H:283:ASP:HB2	1:N:383:ALA:CB	2.35	0.56
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.87	0.56
1:I:390:LYS:HE2	1:J:281:PHE:CA	2.35	0.56
1:F:383:ALA:HA	1:F:389:MET:CG	2.36	0.56
1:G:383:ALA:HA	1:G:389:MET:CG	2.36	0.56
1:J:431:GLY:H	1:J:437:ASN:ND2	2.03	0.56
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.87	0.56
1:M:36:ARG:CG	1:N:518:GLU:CG	2.79	0.56
1:H:183:LEU:H	1:H:383:ALA:HB3	1.70	0.56
1:H:383:ALA:CB	1:I:283:ASP:HB2	2.35	0.56
1:M:383:ALA:CB	1:N:283:ASP:HB2	2.35	0.56
1:N:431:GLY:H	1:N:437:ASN:ND2	2.03	0.56
1:H:68:ASN:O	1:H:72:GLN:HG2	2.05	0.56
1:D:68:ASN:O	1:D:72:GLN:HG2	2.05	0.56
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.87	0.56
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.87	0.56
1:L:390:LYS:HE2	1:M:281:PHE:CA	2.35	0.56
1:B:386:GLU:HG2	1:C:281:PHE:CD2	2.41	0.56
1:M:390:LYS:HE2	1:N:281:PHE:CA	2.35	0.56
1:M:270:ILE:CG2	1:N:229:ASN:CA	2.82	0.56
1:J:36:ARG:CG	1:K:518:GLU:CG	2.79	0.56
1:L:174:VAL:HG21	1:L:194:GLN:HB2	1.86	0.56
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.87	0.56
1:J:68:ASN:O	1:J:72:GLN:HG2	2.05	0.56
1:K:68:ASN:O	1:K:72:GLN:HG2	2.05	0.56
1:A:383:ALA:HA	1:A:389:MET:CG	2.36	0.56
1:I:68:ASN:O	1:I:72:GLN:HG2	2.05	0.56
1:H:281:PHE:CA	1:N:390:LYS:HE2	2.35	0.55
1:H:390:LYS:HE2	1:I:281:PHE:CA	2.35	0.55
1:E:386:GLU:HG2	1:F:281:PHE:CD2	2.41	0.55



Continued from previous page...

	ous page	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:L:183:LEU:H	1:L:383:ALA:HB3	1.70	0.55
1:I:383:ALA:CB	1:J:283:ASP:HB2	2.35	0.55
1:N:183:LEU:H	1:N:383:ALA:HB3	1.70	0.55
1:L:431:GLY:H	1:L:437:ASN:ND2	2.03	0.55
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.87	0.55
1:M:359:ASP:O	1:M:363:GLU:HG2	2.07	0.55
1:N:359:ASP:O	1:N:363:GLU:HG2	2.07	0.55
1:C:359:ASP:O	1:C:363:GLU:HG2	2.07	0.55
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.87	0.55
1:B:37:ASN:H	1:C:516:THR:HG22	1.70	0.55
1:I:270:ILE:HG22	1:J:229:ASN:C	2.22	0.55
1:B:383:ALA:HA	1:B:389:MET:CG	2.36	0.55
1:A:26:ALA:HB2	1:B:8:PHE:CZ	2.40	0.55
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.87	0.55
1:E:359:ASP:O	1:E:363:GLU:HG2	2.07	0.55
1:N:68:ASN:O	1:N:72:GLN:HG2	2.05	0.55
1:H:240:VAL:HG11	1:H:247:LEU:HB2	1.87	0.55
1:G:359:ASP:O	1:G:363:GLU:HG2	2.07	0.55
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.87	0.55
1:J:359:ASP:O	1:J:363:GLU:HG2	2.07	0.55
1:E:69:MET:O	1:E:73:MET:HG3	2.07	0.55
1:H:431:GLY:H	1:H:437:ASN:ND2	2.03	0.55
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.87	0.55
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.87	0.55
1:G:68:ASN:O	1:G:72:GLN:HG2	2.05	0.55
1:F:386:GLU:HG2	1:G:281:PHE:CD2	2.41	0.55
1:L:69:MET:O	1:L:73:MET:HG3	2.07	0.55
1:I:69:MET:O	1:I:73:MET:HG3	2.07	0.55
1:E:383:ALA:HA	1:E:389:MET:CG	2.36	0.55
1:J:183:LEU:H	1:J:383:ALA:HB3	1.70	0.55
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.87	0.55
1:N:338:GLU:HA	1:N:342:ILE:HD12	1.88	0.55
1:B:338:GLU:HA	1:B:342:ILE:HD12	1.89	0.55
1:H:338:GLU:HA	1:H:342:ILE:HD12	1.88	0.55
1:F:386:GLU:CG	1:G:281:PHE:HE2	2.07	0.55
1:K:183:LEU:H	1:K:383:ALA:HB3	1.70	0.55
1:L:146:GLN:HE22	1:L:494:LEU:HD12	1.70	0.55
1:K:359:ASP:O	1:K:363:GLU:HG2	2.07	0.55
1:H:359:ASP:O	1:H:363:GLU:HG2	2.07	0.55
1:L:386:GLU:CA	1:M:281:PHE:N	2.65	0.55
1:J:69:MET:O	1:J:73:MET:HG3	2.07	0.55



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:F:26:ALA:HB2	1:G:8:PHE:CZ	2.40	0.55
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.87	0.55
1:A:338:GLU:HA	1:A:342:ILE:HD12	1.89	0.55
1:H:420:ILE:HD12	1:H:451:LEU:HD13	1.89	0.55
1:I:240:VAL:HG11	1:I:247:LEU:HB2	1.87	0.55
1:N:420:ILE:HD12	1:N:451:LEU:HD13	1.89	0.55
1:I:359:ASP:O	1:I:363:GLU:HG2	2.07	0.55
1:M:68:ASN:O	1:M:72:GLN:HG2	2.05	0.55
1:M:69:MET:O	1:M:73:MET:HG3	2.07	0.55
1:K:69:MET:O	1:K:73:MET:HG3	2.07	0.55
1:B:420:ILE:HD12	1:B:451:LEU:HD13	1.89	0.55
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.87	0.55
1:J:388:GLU:H	1:K:281:PHE:HE1	1.53	0.55
1:I:229:ASN:ND2	1:I:232:GLU:HB2	2.22	0.55
1:N:229:ASN:ND2	1:N:232:GLU:HB2	2.22	0.55
1:H:69:MET:O	1:H:73:MET:HG3	2.07	0.55
1:H:145:ALA:O	1:H:149:THR:HG23	2.07	0.55
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.87	0.55
1:C:338:GLU:HA	1:C:342:ILE:HD12	1.89	0.55
1:I:338:GLU:HA	1:I:342:ILE:HD12	1.88	0.55
1:D:386:GLU:HG2	1:E:281:PHE:CD2	2.41	0.55
1:A:420:ILE:HD12	1:A:451:LEU:HD13	1.89	0.55
1:L:68:ASN:O	1:L:72:GLN:HG2	2.05	0.55
1:C:386:GLU:HG2	1:D:281:PHE:CD2	2.41	0.55
1:B:229:ASN:ND2	1:B:232:GLU:HB2	2.22	0.55
1:F:229:ASN:ND2	1:F:232:GLU:HB2	2.22	0.55
1:M:183:LEU:N	1:M:383:ALA:HB3	2.22	0.55
1:L:183:LEU:N	1:L:383:ALA:HB3	2.22	0.55
1:L:383:ALA:CB	1:M:283:ASP:HB2	2.35	0.55
1:A:38:VAL:CG1	1:B:519:CYS:HB3	2.37	0.54
1:M:229:ASN:ND2	1:M:232:GLU:HB2	2.22	0.54
1:C:383:ALA:HA	1:C:389:MET:CG	2.36	0.54
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.87	0.54
1:A:359:ASP:O	1:A:363:GLU:HG2	2.07	0.54
1:I:420:ILE:HD12	1:I:451:LEU:HD13	1.89	0.54
1:E:338:GLU:HA	1:E:342:ILE:HD12	1.88	0.54
1:N:392:LYS:O	1:N:396:VAL:HG23	2.07	0.54
1:K:338:GLU:HA	1:K:342:ILE:HD12	1.88	0.54
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.87	0.54
1:D:69:MET:O	1:D:73:MET:HG3	2.07	0.54
1:F:69:MET:O	1:F:73:MET:HG3	2.07	0.54



Continued from previous page...

Atom 1		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:H:229:ASN:ND2	1:H:232:GLU:HB2	2.22	0.54
1:H:4:LYS:CG	1:N:59:GLU:O	2.53	0.54
1:C:348:GLN:O	1:C:352:GLN:HG2	2.08	0.54
1:B:348:GLN:O	1:B:352:GLN:HG2	2.08	0.54
1:L:338:GLU:HA	1:L:342:ILE:HD12	1.88	0.54
1:I:145:ALA:O	1:I:149:THR:HG23	2.07	0.54
1:H:269:GLY:O	1:H:272:LYS:HG2	2.08	0.54
1:I:269:GLY:O	1:I:272:LYS:HG2	2.08	0.54
1:D:269:GLY:O	1:D:272:LYS:HG2	2.08	0.54
1:C:69:MET:O	1:C:73:MET:HG3	2.07	0.54
1:L:36:ARG:CG	1:M:518:GLU:CG	2.79	0.54
1:D:383:ALA:HA	1:D:389:MET:CG	2.36	0.54
1:D:348:GLN:O	1:D:352:GLN:HG2	2.08	0.54
1:J:348:GLN:O	1:J:352:GLN:HG2	2.08	0.54
1:F:359:ASP:O	1:F:363:GLU:HG2	2.07	0.54
1:M:338:GLU:HA	1:M:342:ILE:HD12	1.88	0.54
1:H:392:LYS:O	1:H:396:VAL:HG23	2.07	0.54
1:L:359:ASP:O	1:L:363:GLU:HG2	2.07	0.54
1:N:145:ALA:O	1:N:149:THR:HG23	2.07	0.54
1:M:269:GLY:O	1:M:272:LYS:HG2	2.08	0.54
1:M:392:LYS:O	1:M:396:VAL:HG23	2.07	0.54
1:C:420:ILE:HD12	1:C:451:LEU:HD13	1.89	0.54
1:A:229:ASN:ND2	1:A:232:GLU:HB2	2.22	0.54
1:E:229:ASN:ND2	1:E:232:GLU:HB2	2.22	0.54
1:A:8:PHE:CZ	1:G:26:ALA:HB2	2.40	0.54
1:I:183:LEU:N	1:I:383:ALA:HB3	2.22	0.54
1:F:305:ILE:O	1:F:308:GLU:HB2	2.08	0.54
1:M:305:ILE:O	1:M:308:GLU:HB2	2.08	0.54
1:G:348:GLN:O	1:G:352:GLN:HG2	2.08	0.54
1:E:269:GLY:O	1:E:272:LYS:HG2	2.08	0.54
1:M:145:ALA:O	1:M:149:THR:HG23	2.07	0.54
1:G:338:GLU:HA	1:G:342:ILE:HD12	1.89	0.54
1:M:420:ILE:HD12	1:M:451:LEU:HD13	1.89	0.54
1:N:269:GLY:O	1:N:272:LYS:HG2	2.08	0.54
1:C:18:ARG:O	1:C:22:VAL:HG23	2.08	0.54
1:D:18:ARG:O	1:D:22:VAL:HG23	2.08	0.54
1:C:269:GLY:O	1:C:272:LYS:HG2	2.08	0.54
1:D:359:ASP:O	1:D:363:GLU:HG2	2.07	0.54
1:C:37:ASN:H	1:D:516:THR:HG22	1.70	0.54
1:D:38:VAL:CG1	1:E:519:CYS:HB3	2.37	0.54
1:B:69:MET:O	1:B:73:MET:HG3	2.07	0.54



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:K:386:GLU:CA	1:L:281:PHE:N	2.65	0.54
1:D:229:ASN:ND2	1:D:232:GLU:HB2	2.22	0.54
1:M:183:LEU:H	1:M:383:ALA:HB3	1.70	0.54
1:N:183:LEU:N	1:N:383:ALA:HB3	2.23	0.54
1:H:305:ILE:O	1:H:308:GLU:HB2	2.08	0.54
1:J:305:ILE:O	1:J:308:GLU:HB2	2.08	0.54
1:A:348:GLN:O	1:A:352:GLN:HG2	2.08	0.54
1:N:348:GLN:O	1:N:352:GLN:HG2	2.08	0.54
1:H:348:GLN:O	1:H:352:GLN:HG2	2.08	0.54
1:F:338:GLU:HA	1:F:342:ILE:HD12	1.89	0.54
1:F:269:GLY:O	1:F:272:LYS:HG2	2.08	0.54
1:M:18:ARG:O	1:M:22:VAL:HG23	2.08	0.54
1:L:269:GLY:O	1:L:272:LYS:HG2	2.08	0.54
1:B:359:ASP:O	1:B:363:GLU:HG2	2.07	0.54
1:J:269:GLY:O	1:J:272:LYS:HG2	2.08	0.54
1:H:518:GLU:CG	1:N:36:ARG:CG	2.79	0.54
1:K:183:LEU:N	1:K:383:ALA:HB3	2.22	0.54
1:D:305:ILE:O	1:D:308:GLU:HB2	2.08	0.54
1:L:18:ARG:O	1:L:22:VAL:HG23	2.08	0.54
1:N:18:ARG:O	1:N:22:VAL:HG23	2.08	0.54
1:N:69:MET:O	1:N:73:MET:HG3	2.07	0.54
1:N:146:GLN:NE2	1:N:494:LEU:CD1	2.70	0.54
1:K:305:ILE:O	1:K:308:GLU:HB2	2.08	0.54
1:M:158:VAL:HG22	1:M:396:VAL:HG22	1.89	0.54
1:K:269:GLY:O	1:K:272:LYS:HG2	2.08	0.54
1:H:18:ARG:O	1:H:22:VAL:HG23	2.08	0.54
1:J:338:GLU:HA	1:J:342:ILE:HD12	1.88	0.54
1:I:18:ARG:O	1:I:22:VAL:HG23	2.08	0.54
1:A:386:GLU:CG	1:B:281:PHE:HE2	2.07	0.54
1:K:229:ASN:ND2	1:K:232:GLU:HB2	2.22	0.54
1:A:305:ILE:O	1:A:308:GLU:HB2	2.08	0.54
1:E:18:ARG:O	1:E:22:VAL:HG23	2.08	0.54
1:G:69:MET:O	1:G:73:MET:HG3	2.07	0.54
1:J:270:ILE:CG2	1:K:229:ASN:CA	2.82	0.54
1:J:183:LEU:N	1:J:383:ALA:HB3	2.23	0.54
1:B:305:ILE:O	1:B:308:GLU:HB2	2.08	0.54
1:E:348:GLN:O	1:E:352:GLN:HG2	2.08	0.54
1:A:18:ARG:O	1:A:22:VAL:HG23	2.08	0.54
1:G:420:ILE:HD12	1:G:451:LEU:HD13	1.89	0.54
1:G:269:GLY:O	1:G:272:LYS:HG2	2.08	0.54
1:L:158:VAL:HG22	1:L:396:VAL:HG22	1.89	0.54



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:B:18:ARG:O	1:B:22:VAL:HG23	2.08	0.54
1:I:305:ILE:O	1:I:308:GLU:HB2	2.08	0.54
1:G:18:ARG:O	1:G:22:VAL:HG23	2.08	0.54
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.89	0.54
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.89	0.54
1:A:69:MET:O	1:A:73:MET:HG3	2.07	0.53
1:K:348:GLN:O	1:K:352:GLN:HG2	2.08	0.53
1:F:348:GLN:O	1:F:352:GLN:HG2	2.08	0.53
1:L:145:ALA:O	1:L:149:THR:HG23	2.07	0.53
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.89	0.53
1:B:269:GLY:O	1:B:272:LYS:HG2	2.08	0.53
1:K:145:ALA:O	1:K:149:THR:HG23	2.07	0.53
1:D:338:GLU:HA	1:D:342:ILE:HD12	1.89	0.53
1:L:420:ILE:HD12	1:L:451:LEU:HD13	1.89	0.53
1:J:229:ASN:ND2	1:J:232:GLU:HB2	2.22	0.53
1:L:229:ASN:ND2	1:L:232:GLU:HB2	2.22	0.53
1:J:174:VAL:HG21	1:J:194:GLN:HB2	1.86	0.53
1:N:305:ILE:O	1:N:308:GLU:HB2	2.08	0.53
1:I:348:GLN:O	1:I:352:GLN:HG2	2.08	0.53
1:L:392:LYS:O	1:L:396:VAL:HG23	2.07	0.53
1:I:392:LYS:O	1:I:396:VAL:HG23	2.07	0.53
1:E:420:ILE:HD12	1:E:451:LEU:HD13	1.89	0.53
1:M:85:ALA:C	1:M:405:ALA:CB	2.50	0.53
1:G:229:ASN:ND2	1:G:232:GLU:HB2	2.22	0.53
1:H:183:LEU:N	1:H:383:ALA:HB3	2.22	0.53
1:E:305:ILE:O	1:E:308:GLU:HB2	2.08	0.53
1:J:392:LYS:O	1:J:396:VAL:HG23	2.08	0.53
1:A:269:GLY:O	1:A:272:LYS:HG2	2.08	0.53
1:J:18:ARG:O	1:J:22:VAL:HG23	2.08	0.53
1:H:158:VAL:HG22	1:H:396:VAL:HG22	1.89	0.53
1:K:18:ARG:O	1:K:22:VAL:HG23	2.08	0.53
1:C:229:ASN:ND2	1:C:232:GLU:HB2	2.22	0.53
1:L:305:ILE:O	1:L:308:GLU:HB2	2.08	0.53
1:L:348:GLN:O	1:L:352:GLN:HG2	2.08	0.53
1:M:348:GLN:O	1:M:352:GLN:HG2	2.08	0.53
1:I:158:VAL:HG22	1:I:396:VAL:HG22	1.90	0.53
1:F:420:ILE:HD12	1:F:451:LEU:HD13	1.89	0.53
1:F:18:ARG:O	1:F:22:VAL:HG23	2.08	0.53
1:J:145:ALA:O	1:J:149:THR:HG23	2.07	0.53
1:G:305:ILE:O	1:G:308:GLU:HB2	2.08	0.53
1:N:158:VAL:HG22	1:N:396:VAL:HG22	1.89	0.53



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$overlap(\AA)$
1:I:388:GLU:H	1:J:281:PHE:HE1	1.53	0.53
1:A:281:PHE:CD2	1:G:386:GLU:HG2	2.41	0.53
1:B:215:LEU:HD22	1:B:246:PRO:HB3	1.91	0.53
1:C:305:ILE:O	1:C:308:GLU:HB2	2.08	0.53
1:A:4:LYS:HB2	1:G:61:GLU:O	2.09	0.53
1:A:61:GLU:O	1:B:4:LYS:HB2	2.09	0.53
1:G:215:LEU:HD22	1:G:246:PRO:HB3	1.91	0.53
1:L:215:LEU:HD22	1:L:246:PRO:HB3	1.91	0.53
1:C:215:LEU:HD22	1:C:246:PRO:HB3	1.91	0.53
1:F:160:LYS:HB3	1:F:160:LYS:NZ	2.24	0.53
1:L:184:GLN:O	1:L:382:GLY:HA2	2.09	0.53
1:K:392:LYS:O	1:K:396:VAL:HG23	2.07	0.53
1:M:184:GLN:O	1:M:382:GLY:HA2	2.09	0.53
1:N:184:GLN:O	1:N:382:GLY:HA2	2.09	0.53
1:H:184:GLN:O	1:H:382:GLY:HA2	2.09	0.53
1:K:333:ILE:HA	1:K:376:VAL:HG21	1.91	0.53
1:E:38:VAL:CG1	1:F:519:CYS:HB3	2.37	0.52
1:J:158:VAL:HG22	1:J:396:VAL:HG22	1.89	0.52
1:K:158:VAL:HG22	1:K:396:VAL:HG22	1.89	0.52
1:J:215:LEU:HD22	1:J:246:PRO:HB3	1.91	0.52
1:I:174:VAL:HG21	1:I:194:GLN:HB2	1.86	0.52
1:J:333:ILE:HA	1:J:376:VAL:HG21	1.91	0.52
1:I:333:ILE:HA	1:I:376:VAL:HG21	1.91	0.52
1:L:333:ILE:HA	1:L:376:VAL:HG21	1.91	0.52
1:E:160:LYS:HB3	1:E:160:LYS:NZ	2.24	0.52
1:N:23:LEU:HD22	1:N:74:VAL:HG23	1.92	0.52
1:B:61:GLU:O	1:C:4:LYS:HB2	2.09	0.52
1:F:61:GLU:O	1:G:4:LYS:HB2	2.09	0.52
1:I:23:LEU:HD22	1:I:74:VAL:HG23	1.92	0.52
1:H:229:ASN:CA	1:N:270:ILE:CG2	2.82	0.52
1:L:85:ALA:C	1:L:405:ALA:CB	2.50	0.52
1:A:215:LEU:HD22	1:A:246:PRO:HB3	1.91	0.52
1:C:160:LYS:HB3	1:C:160:LYS:NZ	2.24	0.52
1:D:160:LYS:NZ	1:D:160:LYS:HB3	2.24	0.52
1:H:23:LEU:HD22	1:H:74:VAL:HG23	1.92	0.52
1:A:519:CYS:HB3	1:G:38:VAL:CG1	2.37	0.52
1:F:23:LEU:HD22	1:F:74:VAL:HG23	1.92	0.52
1:K:184:GLN:O	1:K:382:GLY:HA2	2.09	0.52
1:M:23:LEU:HD22	1:M:74:VAL:HG23	1.92	0.52
1:J:184:GLN:O	1:J:382:GLY:HA2	2.09	0.52
1:B:38:VAL:CG1	1:C:519:CYS:HB3	2.37	0.52



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$ ext{overlap }( ext{\AA})$
1:H:36:ARG:HB3	1:I:518:GLU:CB	2.28	0.52
1:E:23:LEU:HD22	1:E:74:VAL:HG23	1.92	0.52
1:J:23:LEU:HD22	1:J:74:VAL:HG23	1.92	0.52
1:I:184:GLN:O	1:I:382:GLY:HA2	2.09	0.52
1:K:36:ARG:CG	1:L:518:GLU:CG	2.79	0.52
1:B:160:LYS:NZ	1:B:160:LYS:HB3	2.24	0.52
1:H:270:ILE:CG2	1:I:229:ASN:CA	2.82	0.52
1:K:215:LEU:HD22	1:K:246:PRO:HB3	1.91	0.52
1:M:215:LEU:HD22	1:M:246:PRO:HB3	1.91	0.52
1:I:408:GLU:CG	1:I:498:LYS:NZ	2.68	0.52
1:F:215:LEU:HD22	1:F:246:PRO:HB3	1.91	0.52
1:A:114:MET:SD	1:G:36:ARG:HA	2.50	0.52
1:A:36:ARG:HA	1:B:114:MET:SD	2.50	0.52
1:A:160:LYS:NZ	1:A:160:LYS:HB3	2.24	0.52
1:M:333:ILE:HA	1:M:376:VAL:HG21	1.91	0.52
1:H:281:PHE:HE1	1:N:388:GLU:H	1.53	0.52
1:F:36:ARG:HA	1:G:114:MET:SD	2.50	0.52
1:E:36:ARG:HA	1:F:114:MET:SD	2.50	0.52
1:C:61:GLU:O	1:D:4:LYS:HB2	2.09	0.52
1:E:61:GLU:O	1:F:4:LYS:HB2	2.09	0.52
1:H:333:ILE:HA	1:H:376:VAL:HG21	1.91	0.52
1:E:234:LEU:N	1:E:235:PRO:HD2	2.25	0.52
1:D:36:ARG:HA	1:E:114:MET:SD	2.50	0.51
1:B:36:ARG:HA	1:C:114:MET:SD	2.50	0.51
1:B:171:LYS:HB2	1:B:407:VAL:HG11	1.92	0.51
1:G:23:LEU:HD22	1:G:74:VAL:HG23	1.92	0.51
1:E:215:LEU:HD22	1:E:246:PRO:HB3	1.91	0.51
1:D:215:LEU:HD22	1:D:246:PRO:HB3	1.91	0.51
1:G:234:LEU:N	1:G:235:PRO:HD2	2.25	0.51
1:C:171:LYS:HB2	1:C:407:VAL:HG11	1.92	0.51
1:C:36:ARG:HA	1:D:114:MET:SD	2.50	0.51
1:J:59:GLU:O	1:K:4:LYS:HE3	2.11	0.51
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.92	0.51
1:A:234:LEU:N	1:A:235:PRO:HD2	2.25	0.51
1:M:174:VAL:HG11	1:M:331:THR:HG1	1.71	0.51
1:M:59:GLU:O	1:N:4:LYS:HE3	2.11	0.51
1:G:171:LYS:HB2	1:G:407:VAL:HG11	1.92	0.51
1:N:234:LEU:N	1:N:235:PRO:HD2	2.26	0.51
1:D:171:LYS:HB2	1:D:407:VAL:HG11	1.92	0.51
1:H:86:GLY:CA	1:H:405:ALA:CB	2.88	0.51
1:J:36:ARG:HB3	1:K:518:GLU:CB	2.28	0.51



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Continued from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:H:59:GLU:O	1:I:4:LYS:HE3	2.11	0.51
1:G:160:LYS:HB3	1:G:160:LYS:NZ	2.24	0.51
1:K:23:LEU:HD22	1:K:74:VAL:HG23	1.92	0.51
1:D:61:GLU:O	1:E:4:LYS:HB2	2.09	0.51
1:I:234:LEU:N	1:I:235:PRO:HD2	2.26	0.51
1:J:234:LEU:N	1:J:235:PRO:HD2	2.26	0.51
1:B:384:ALA:HB3	1:B:388:GLU:HB2	1.93	0.51
1:L:23:LEU:HD22	1:L:74:VAL:HG23	1.92	0.51
1:H:388:GLU:H	1:I:281:PHE:HE1	1.53	0.51
1:C:384:ALA:HB3	1:C:388:GLU:HB2	1.93	0.51
1:D:384:ALA:HB3	1:D:388:GLU:HB2	1.93	0.51
1:L:234:LEU:N	1:L:235:PRO:HD2	2.26	0.51
1:E:384:ALA:HB3	1:E:388:GLU:HB2	1.93	0.51
1:D:234:LEU:N	1:D:235:PRO:HD2	2.25	0.51
1:E:171:LYS:HB2	1:E:407:VAL:HG11	1.93	0.51
1:A:384:ALA:HB3	1:A:388:GLU:HB2	1.93	0.51
1:H:215:LEU:HD22	1:H:246:PRO:HB3	1.91	0.51
1:K:59:GLU:O	1:L:4:LYS:HE3	2.11	0.51
1:F:384:ALA:HB3	1:F:388:GLU:HB2	1.93	0.51
1:B:23:LEU:HD22	1:B:74:VAL:HG23	1.92	0.51
1:K:234:LEU:N	1:K:235:PRO:HD2	2.26	0.51
1:I:215:LEU:HD22	1:I:246:PRO:HB3	1.91	0.51
1:N:215:LEU:HD22	1:N:246:PRO:HB3	1.91	0.51
1:I:86:GLY:CA	1:I:405:ALA:CB	2.88	0.51
1:B:234:LEU:N	1:B:235:PRO:HD2	2.25	0.51
1:D:23:LEU:HD22	1:D:74:VAL:HG23	1.92	0.51
1:N:333:ILE:HA	1:N:376:VAL:HG21	1.91	0.51
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.92	0.51
1:A:281:PHE:HE2	1:G:386:GLU:CG	2.07	0.51
1:L:59:GLU:O	1:M:4:LYS:HE3	2.11	0.51
1:C:234:LEU:N	1:C:235:PRO:HD2	2.25	0.51
1:G:384:ALA:HB3	1:G:388:GLU:HB2	1.93	0.51
1:H:285:ARG:CA	1:N:386:GLU:OE2	2.59	0.51
1:I:59:GLU:O	1:J:4:LYS:HE3	2.11	0.51
1:J:75:LYS:O	1:J:75:LYS:HD3	2.11	0.51
1:F:75:LYS:O	1:F:75:LYS:HD3	2.11	0.51
1:G:75:LYS:HD3	1:G:75:LYS:O	2.11	0.51
1:D:47:PRO:CB	1:E:73:MET:HG2	2.41	0.50
1:I:270:ILE:CG2	1:J:229:ASN:CA	2.82	0.50
1:M:39:VAL:CB	1:N:69:MET:HE1	2.41	0.50
1:C:23:LEU:HD22	1:C:74:VAL:HG23	1.92	0.50



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:A:75:LYS:O	1:A:75:LYS:HD3	2.11	0.50
1:K:75:LYS:HD3	1:K:75:LYS:O	2.11	0.50
1:I:386:GLU:CA	1:J:284:ARG:CZ	2.62	0.50
1:H:41:ASP:OD2	1:I:522:THR:HG23	2.12	0.50
1:F:26:ALA:CB	1:G:8:PHE:CE2	2.77	0.50
1:B:75:LYS:HD3	1:B:75:LYS:O	2.11	0.50
1:L:75:LYS:O	1:L:75:LYS:HD3	2.11	0.50
1:L:386:GLU:OE2	1:M:285:ARG:CA	2.59	0.50
1:M:386:GLU:OE2	1:N:285:ARG:CA	2.59	0.50
1:K:86:GLY:HA3	1:K:405:ALA:HB2	1.93	0.50
1:H:234:LEU:N	1:H:235:PRO:HD2	2.26	0.50
1:A:23:LEU:HD22	1:A:74:VAL:HG23	1.92	0.50
1:F:234:LEU:N	1:F:235:PRO:HD2	2.25	0.50
1:M:388:GLU:H	1:N:281:PHE:HE1	1.53	0.50
1:M:41:ASP:OD2	1:N:522:THR:HG23	2.11	0.50
1:L:381:VAL:HB	1:L:392:LYS:HG2	1.93	0.50
1:K:381:VAL:HB	1:K:392:LYS:HG2	1.93	0.50
1:C:75:LYS:HD3	1:C:75:LYS:O	2.11	0.50
1:C:47:PRO:CB	1:D:73:MET:HG2	2.42	0.50
1:H:4:LYS:HE3	1:N:59:GLU:O	2.11	0.50
1:D:248:LEU:HD22	1:D:323:VAL:HG11	1.94	0.50
1:J:41:ASP:OD2	1:K:522:THR:HG23	2.12	0.50
1:F:349:ILE:HA	1:F:352:GLN:HG2	1.93	0.50
1:E:349:ILE:HA	1:E:352:GLN:HG2	1.93	0.50
1:I:381:VAL:HB	1:I:392:LYS:HG2	1.93	0.50
1:D:75:LYS:HD3	1:D:75:LYS:O	2.11	0.50
1:E:75:LYS:HD3	1:E:75:LYS:O	2.11	0.50
1:K:386:GLU:OE2	1:L:285:ARG:CA	2.59	0.50
1:H:522:THR:HG23	1:N:41:ASP:OD2	2.12	0.50
1:I:86:GLY:HA3	1:I:405:ALA:HB2	1.93	0.50
1:F:229:ASN:O	1:F:231:ARG:N	2.45	0.50
1:E:229:ASN:O	1:E:231:ARG:N	2.45	0.50
1:I:36:ARG:HB3	1:J:518:GLU:CB	2.28	0.50
1:H:381:VAL:HB	1:H:392:LYS:HG2	1.93	0.50
1:M:234:LEU:N	1:M:235:PRO:HD2	2.26	0.50
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.94	0.50
1:K:41:ASP:OD2	1:L:522:THR:HG23	2.12	0.50
1:M:86:GLY:CA	1:M:405:ALA:CB	2.88	0.50
1:J:408:GLU:CG	1:J:498:LYS:NZ	2.68	0.50
1:C:49:ILE:HG21	1:D:513:LEU:HD22	1.94	0.50
1:K:62:LEU:HD12	1:K:62:LEU:N	2.27	0.50



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:M:75:LYS:HD3	1:M:75:LYS:O	2.11	0.50
1:D:47:PRO:HD2	1:E:73:MET:HG2	0.51	0.50
1:L:388:GLU:H	1:M:281:PHE:HE1	1.53	0.50
1:H:386:GLU:OE2	1:I:285:ARG:CA	2.59	0.50
1:I:386:GLU:OE2	1:J:285:ARG:CA	2.59	0.50
1:C:49:ILE:CG1	1:D:513:LEU:HD22	2.42	0.50
1:D:349:ILE:HA	1:D:352:GLN:HG2	1.93	0.50
1:I:75:LYS:O	1:I:75:LYS:HD3	2.11	0.50
1:I:229:ASN:O	1:I:231:ARG:N	2.45	0.49
1:B:49:ILE:HG21	1:C:513:LEU:HD22	1.94	0.49
1:I:41:ASP:OD2	1:J:522:THR:HG23	2.12	0.49
1:A:349:ILE:HA	1:A:352:GLN:HG2	1.93	0.49
1:E:62:LEU:N	1:E:62:LEU:HD12	2.27	0.49
1:L:62:LEU:HD12	1:L:62:LEU:N	2.27	0.49
1:A:47:PRO:CB	1:B:73:MET:CG	2.88	0.49
1:L:41:ASP:OD2	1:M:522:THR:HG23	2.11	0.49
1:J:86:GLY:HA3	1:J:405:ALA:HB2	1.93	0.49
1:I:248:LEU:HD22	1:I:323:VAL:HG11	1.94	0.49
1:K:248:LEU:HD22	1:K:323:VAL:HG11	1.94	0.49
1:J:386:GLU:CA	1:K:284:ARG:CZ	2.62	0.49
1:J:386:GLU:OE2	1:K:285:ARG:CA	2.59	0.49
1:M:386:GLU:OE2	1:N:285:ARG:CB	2.61	0.49
1:L:86:GLY:CA	1:L:405:ALA:CB	2.88	0.49
1:B:49:ILE:CG1	1:C:513:LEU:HD22	2.41	0.49
1:D:229:ASN:O	1:D:231:ARG:N	2.45	0.49
1:C:229:ASN:O	1:C:231:ARG:N	2.45	0.49
1:A:248:LEU:HD22	1:A:323:VAL:HG11	1.94	0.49
1:H:248:LEU:HD22	1:H:323:VAL:HG11	1.94	0.49
1:E:248:LEU:HD22	1:E:323:VAL:HG11	1.94	0.49
1:F:62:LEU:N	1:F:62:LEU:HD12	2.27	0.49
1:C:39:VAL:CA	1:D:517:THR:HG23	2.43	0.49
1:D:39:VAL:CA	1:E:517:THR:HG23	2.43	0.49
1:B:39:VAL:CA	1:C:517:THR:HG23	2.43	0.49
1:B:47:PRO:CB	1:C:73:MET:HG2	2.42	0.49
1:E:39:VAL:CA	1:F:517:THR:HG23	2.43	0.49
1:H:285:ARG:CB	1:N:386:GLU:OE2	2.61	0.49
1:D:49:ILE:CG1	1:E:513:LEU:HD22	2.42	0.49
1:J:86:GLY:CA	1:J:405:ALA:CB	2.88	0.49
1:K:36:ARG:HB3	1:L:518:GLU:CB	2.28	0.49
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.93	0.49
1:H:349:ILE:HA	1:H:352:GLN:HG2	1.93	0.49



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:A:475:ASN:ND2	1:A:489:ILE:HD12	2.28	0.49
1:M:62:LEU:HD12	1:M:62:LEU:N	2.27	0.49
1:D:47:PRO:CB	1:E:73:MET:CG	2.88	0.49
1:F:47:PRO:HD2	1:G:73:MET:HG2	0.51	0.49
1:H:281:PHE:HD2	1:N:389:MET:SD	2.36	0.49
1:H:389:MET:SD	1:I:281:PHE:HD2	2.36	0.49
1:A:386:GLU:HG2	1:B:281:PHE:CD2	2.41	0.49
1:G:229:ASN:O	1:G:231:ARG:N	2.45	0.49
1:G:349:ILE:HA	1:G:352:GLN:HG2	1.93	0.49
1:M:381:VAL:HB	1:M:392:LYS:HG2	1.93	0.49
1:J:381:VAL:HB	1:J:392:LYS:HG2	1.93	0.49
1:N:62:LEU:N	1:N:62:LEU:HD12	2.27	0.49
1:J:62:LEU:HD12	1:J:62:LEU:N	2.27	0.49
1:D:62:LEU:N	1:D:62:LEU:HD12	2.27	0.49
1:B:47:PRO:HD2	1:C:73:MET:HG2	0.51	0.49
1:A:47:PRO:HD2	1:B:73:MET:HG2	0.51	0.49
1:H:386:GLU:OE2	1:I:285:ARG:CB	2.61	0.49
1:M:389:MET:SD	1:N:281:PHE:HD2	2.36	0.49
1:J:229:ASN:O	1:J:231:ARG:N	2.45	0.49
1:K:229:ASN:O	1:K:231:ARG:N	2.45	0.49
1:H:229:ASN:O	1:H:231:ARG:N	2.45	0.49
1:M:229:ASN:O	1:M:231:ARG:N	2.45	0.49
1:A:229:ASN:O	1:A:231:ARG:N	2.45	0.49
1:I:349:ILE:HA	1:I:352:GLN:HG2	1.94	0.49
1:N:381:VAL:HB	1:N:392:LYS:HG2	1.93	0.49
1:N:75:LYS:O	1:N:75:LYS:HD3	2.11	0.49
1:A:73:MET:HG2	1:G:47:PRO:HD2	0.51	0.49
1:I:389:MET:SD	1:J:281:PHE:HD2	2.36	0.49
1:L:229:ASN:O	1:L:231:ARG:N	2.45	0.49
1:N:229:ASN:O	1:N:231:ARG:N	2.45	0.49
1:N:349:ILE:HA	1:N:352:GLN:HG2	1.93	0.49
1:L:248:LEU:HD22	1:L:323:VAL:HG11	1.94	0.49
1:G:248:LEU:HD22	1:G:323:VAL:HG11	1.94	0.49
1:F:475:ASN:ND2	1:F:489:ILE:HD12	2.28	0.49
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.95	0.49
1:I:62:LEU:HD12	1:I:62:LEU:N	2.27	0.49
1:A:517:THR:HG21	1:G:39:VAL:CB	1.94	0.49
1:F:47:PRO:CB	1:G:73:MET:CG	2.88	0.49
1:L:389:MET:SD	1:M:281:PHE:HD2	2.36	0.49
1:I:475:ASN:ND2	1:I:489:ILE:HD12	2.28	0.49
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.95	0.49



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:C:62:LEU:HD12	1:C:62:LEU:N	2.27	0.49
1:C:38:VAL:CG1	1:D:519:CYS:HB3	2.37	0.49
1:L:386:GLU:OE2	1:M:285:ARG:CB	2.61	0.49
1:J:386:GLU:OE2	1:K:285:ARG:CB	2.61	0.49
1:J:389:MET:SD	1:K:281:PHE:HD2	2.36	0.49
1:I:386:GLU:OE2	1:J:285:ARG:CB	2.61	0.49
1:K:386:GLU:OE2	1:L:285:ARG:CB	2.61	0.49
1:B:248:LEU:HD22	1:B:323:VAL:HG11	1.94	0.49
1:F:248:LEU:HD22	1:F:323:VAL:HG11	1.94	0.49
1:H:62:LEU:N	1:H:62:LEU:HD12	2.27	0.49
1:H:75:LYS:O	1:H:75:LYS:HD3	2.11	0.49
1:G:62:LEU:N	1:G:62:LEU:HD12	2.27	0.49
1:E:47:PRO:HD2	1:F:73:MET:HG2	0.51	0.49
1:K:389:MET:SD	1:L:281:PHE:HD2	2.36	0.49
1:J:245:LYS:CD	1:K:232:GLU:CD	2.81	0.49
1:L:245:LYS:CD	1:M:232:GLU:CD	2.81	0.49
1:H:85:ALA:C	1:H:405:ALA:CB	2.50	0.49
1:F:49:ILE:CG1	1:G:513:LEU:HD22	2.42	0.49
1:N:496:PRO:O	1:N:499:VAL:HG22	2.13	0.49
1:K:349:ILE:HA	1:K:352:GLN:HG2	1.93	0.49
1:M:349:ILE:HA	1:M:352:GLN:HG2	1.93	0.49
1:A:39:VAL:CA	1:B:517:THR:HG23	2.43	0.48
1:A:513:LEU:HD22	1:G:49:ILE:CG1	2.42	0.48
1:C:349:ILE:HA	1:C:352:GLN:HG2	1.93	0.48
1:M:248:LEU:HD22	1:M:323:VAL:HG11	1.94	0.48
1:N:248:LEU:HD22	1:N:323:VAL:HG11	1.94	0.48
1:J:248:LEU:HD22	1:J:323:VAL:HG11	1.94	0.48
1:A:62:LEU:N	1:A:62:LEU:HD12	2.27	0.48
1:A:47:PRO:CB	1:B:73:MET:HG2	2.41	0.48
1:K:245:LYS:CD	1:L:232:GLU:CD	2.81	0.48
1:M:245:LYS:CD	1:N:232:GLU:CD	2.81	0.48
1:M:496:PRO:O	1:M:499:VAL:HG22	2.13	0.48
1:N:86:GLY:HA3	1:N:405:ALA:HB2	1.93	0.48
1:J:321:LYS:HB3	1:J:334:ASP:HB3	1.95	0.48
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.96	0.48
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.96	0.48
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.95	0.48
1:N:207:LYS:HE2	1:N:214:GLU:HB2	1.95	0.48
1:C:47:PRO:HD2	1:D:73:MET:HG2	0.51	0.48
1:L:86:GLY:HA3	1:L:405:ALA:HB2	1.93	0.48
1:N:86:GLY:CA	1:N:405:ALA:CB	2.88	0.48



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap $( ext{Å})$
1:E:217:SER:HA	1:E:320:ALA:O	2.13	0.48
1:I:321:LYS:HB3	1:I:334:ASP:HB3	1.95	0.48
1:K:321:LYS:HB3	1:K:334:ASP:HB3	1.95	0.48
1:K:475:ASN:ND2	1:K:489:ILE:HD12	2.28	0.48
1:D:217:SER:HA	1:D:320:ALA:O	2.13	0.48
1:G:475:ASN:ND2	1:G:489:ILE:HD12	2.28	0.48
1:B:62:LEU:HD12	1:B:62:LEU:N	2.27	0.48
1:M:270:ILE:HG21	1:N:229:ASN:O	2.00	0.48
1:L:39:VAL:CB	1:M:69:MET:HE1	2.43	0.48
1:A:49:ILE:CG1	1:B:513:LEU:HD22	2.42	0.48
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.95	0.48
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.96	0.48
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.95	0.48
1:L:421:ARG:CZ	1:L:474:GLY:HA2	2.44	0.48
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.95	0.48
1:L:496:PRO:O	1:L:499:VAL:HG22	2.13	0.48
1:G:496:PRO:O	1:G:499:VAL:HG22	2.13	0.48
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.96	0.48
1:J:349:ILE:HA	1:J:352:GLN:HG2	1.93	0.48
1:M:217:SER:HA	1:M:320:ALA:O	2.14	0.48
1:J:475:ASN:ND2	1:J:489:ILE:HD12	2.28	0.48
1:K:421:ARG:CZ	1:K:474:GLY:HA2	2.44	0.48
1:H:475:ASN:ND2	1:H:489:ILE:HD12	2.28	0.48
1:E:475:ASN:ND2	1:E:489:ILE:HD12	2.28	0.48
1:M:475:ASN:ND2	1:M:489:ILE:HD12	2.28	0.48
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.95	0.48
1:G:421:ARG:CZ	1:G:474:GLY:HA2	2.44	0.48
1:A:421:ARG:CZ	1:A:474:GLY:HA2	2.44	0.48
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.95	0.48
1:F:150:ILE:CD1	1:F:411:VAL:CB	2.87	0.48
1:E:49:ILE:CG1	1:F:513:LEU:HD22	2.42	0.48
1:A:496:PRO:O	1:A:499:VAL:HG22	2.13	0.48
1:N:475:ASN:ND2	1:N:489:ILE:HD12	2.28	0.48
1:N:217:SER:HA	1:N:320:ALA:O	2.13	0.48
1:D:475:ASN:ND2	1:D:489:ILE:HD12	2.28	0.48
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.95	0.48
1:M:421:ARG:CZ	1:M:474:GLY:HA2	2.44	0.48
1:H:421:ARG:CZ	1:H:474:GLY:HA2	2.44	0.48
1:F:47:PRO:HD2	1:G:73:MET:CA	2.44	0.48
1:D:386:GLU:CD	1:E:281:PHE:CZ	2.87	0.48
1:A:386:GLU:CD	1:B:281:PHE:CZ	2.87	0.48



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:H:270:ILE:HD13	1:I:231:ARG:HG3	1.96	0.48
1:H:496:PRO:O	1:H:499:VAL:HG22	2.13	0.48
1:M:86:GLY:HA3	1:M:405:ALA:HB2	1.93	0.48
1:A:26:ALA:CB	1:B:8:PHE:CE2	2.77	0.48
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.95	0.48
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.96	0.48
1:J:421:ARG:CZ	1:J:474:GLY:HA2	2.44	0.48
1:D:421:ARG:CZ	1:D:474:GLY:HA2	2.44	0.48
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.95	0.48
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.95	0.48
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.95	0.48
1:E:207:LYS:HE2	1:E:214:GLU:HB2	1.95	0.48
1:L:475:ASN:ND2	1:L:489:ILE:HD12	2.28	0.48
1:I:421:ARG:CZ	1:I:474:GLY:HA2	2.44	0.48
1:E:421:ARG:CZ	1:E:474:GLY:HA2	2.44	0.48
1:H:86:GLY:HA3	1:H:405:ALA:HB2	1.93	0.48
1:D:49:ILE:HG21	1:E:513:LEU:HD22	1.94	0.48
1:D:496:PRO:O	1:D:499:VAL:HG22	2.13	0.48
1:E:496:PRO:O	1:E:499:VAL:HG22	2.13	0.48
1:C:496:PRO:O	1:C:499:VAL:HG22	2.13	0.48
1:L:349:ILE:HA	1:L:352:GLN:HG2	1.93	0.48
1:C:475:ASN:ND2	1:C:489:ILE:HD12	2.28	0.48
1:K:179:ASP:HB3	1:L:282:GLY:HA2	1.96	0.48
1:H:207:LYS:HE2	1:H:214:GLU:HB2	1.95	0.48
1:H:179:ASP:HB3	1:I:282:GLY:HA2	1.96	0.48
1:D:207:LYS:HE2	1:D:214:GLU:HB2	1.95	0.48
1:C:217:SER:HA	1:C:320:ALA:O	2.13	0.48
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.95	0.48
1:H:282:GLY:HA2	1:N:179:ASP:HB3	1.96	0.48
1:M:207:LYS:HE2	1:M:214:GLU:HB2	1.95	0.48
1:A:207:LYS:HE2	1:A:214:GLU:HB2	1.95	0.48
1:B:39:VAL:CB	1:C:517:THR:HG21	1.94	0.48
1:A:281:PHE:CZ	1:G:386:GLU:CD	2.87	0.48
1:B:496:PRO:O	1:B:499:VAL:HG22	2.13	0.48
1:B:233:MET:O	1:B:237:LEU:HG	2.14	0.48
1:E:233:MET:O	1:E:237:LEU:HG	2.14	0.48
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.96	0.48
1:A:475:ASN:HD21	1:A:489:ILE:HD12	1.79	0.48
1:B:475:ASN:ND2	1:B:489:ILE:HD12	2.28	0.48
1:E:47:PRO:HD2	1:F:73:MET:CA	2.44	0.48
1:F:37:ASN:H	1:G:516:THR:HG22	1.70	0.48



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
1:L:522:THR:HG22	1:L:523:ASP:N	2.29	0.48
1:L:321:LYS:HB3	1:L:334:ASP:HB3	1.95	0.48
1:D:233:MET:O	1:D:237:LEU:HG	2.14	0.48
1:C:421:ARG:CZ	1:C:474:GLY:HA2	2.44	0.48
1:G:207:LYS:HE2	1:G:214:GLU:HB2	1.95	0.48
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.95	0.48
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.95	0.48
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.95	0.48
1:A:73:MET:HG2	1:G:47:PRO:CB	2.41	0.47
1:F:386:GLU:CD	1:G:281:PHE:CZ	2.87	0.47
1:J:245:LYS:HB2	1:J:246:PRO:HD3	1.96	0.47
1:M:522:THR:HG22	1:M:523:ASP:N	2.29	0.47
1:K:522:THR:HG22	1:K:523:ASP:N	2.29	0.47
1:A:245:LYS:HB2	1:A:246:PRO:HD3	1.96	0.47
1:B:229:ASN:O	1:B:231:ARG:N	2.45	0.47
1:G:245:LYS:HB2	1:G:246:PRO:HD3	1.96	0.47
1:C:233:MET:O	1:C:237:LEU:HG	2.14	0.47
1:A:321:LYS:HB3	1:A:334:ASP:HB3	1.95	0.47
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.95	0.47
1:L:217:SER:HA	1:L:320:ALA:O	2.14	0.47
1:B:47:PRO:HD2	1:C:73:MET:CA	2.44	0.47
1:A:73:MET:CA	1:G:47:PRO:HD2	2.44	0.47
1:C:386:GLU:CD	1:D:281:PHE:CZ	2.87	0.47
1:E:386:GLU:CD	1:F:281:PHE:CZ	2.87	0.47
1:B:386:GLU:CD	1:C:281:PHE:CZ	2.87	0.47
1:I:245:LYS:HB2	1:I:246:PRO:HD3	1.96	0.47
1:H:231:ARG:HG3	1:N:270:ILE:HD13	1.96	0.47
1:M:41:ASP:CG	1:N:522:THR:HG23	2.35	0.47
1:E:270:ILE:HG22	1:F:229:ASN:C	2.31	0.47
1:F:245:LYS:HB2	1:F:246:PRO:HD3	1.96	0.47
1:K:146:GLN:NE2	1:K:494:LEU:CD1	2.70	0.47
1:H:233:MET:O	1:H:237:LEU:HG	2.14	0.47
1:B:475:ASN:HD21	1:B:489:ILE:HD12	1.79	0.47
1:F:217:SER:HA	1:F:320:ALA:O	2.13	0.47
1:J:207:LYS:HE2	1:J:214:GLU:HB2	1.95	0.47
1:J:179:ASP:HB3	1:K:282:GLY:HA2	1.95	0.47
1:A:47:PRO:HD2	1:B:73:MET:CA	2.44	0.47
1:H:232:GLU:CD	1:N:245:LYS:CD	2.82	0.47
1:H:522:THR:HG23	1:N:41:ASP:CG	2.35	0.47
1:F:49:ILE:HG21	1:G:513:LEU:CA	2.45	0.47
1:D:49:ILE:HG21	1:E:513:LEU:CA	2.45	0.47



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:I:41:ASP:CG	1:J:522:THR:HG23	2.35	0.47
1:H:321:LYS:HB3	1:H:334:ASP:HB3	1.95	0.47
1:L:475:ASN:HD21	1:L:489:ILE:HD12	1.79	0.47
1:I:207:LYS:HE2	1:I:214:GLU:HB2	1.95	0.47
1:L:179:ASP:HB3	1:M:282:GLY:HA2	1.95	0.47
1:F:207:LYS:HE2	1:F:214:GLU:HB2	1.95	0.47
1:F:38:VAL:CG1	1:G:519:CYS:HB3	2.37	0.47
1:L:41:ASP:CG	1:M:522:THR:HG23	2.35	0.47
1:K:496:PRO:O	1:K:499:VAL:HG22	2.13	0.47
1:B:36:ARG:CZ	1:C:113:PRO:HD2	2.45	0.47
1:F:496:PRO:O	1:F:499:VAL:HG22	2.13	0.47
1:N:233:MET:O	1:N:237:LEU:HG	2.14	0.47
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.96	0.47
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.95	0.47
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.95	0.47
1:N:421:ARG:CZ	1:N:474:GLY:HA2	2.44	0.47
1:B:321:LYS:HB3	1:B:334:ASP:HB3	1.95	0.47
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.95	0.47
1:A:217:SER:HA	1:A:320:ALA:O	2.13	0.47
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.95	0.47
1:B:421:ARG:CZ	1:B:474:GLY:HA2	2.44	0.47
1:B:37:ASN:O	1:C:518:GLU:HB2	2.15	0.47
1:H:245:LYS:CD	1:I:232:GLU:CD	2.81	0.47
1:M:270:ILE:HD13	1:N:231:ARG:HG3	1.96	0.47
1:E:49:ILE:HG13	1:F:513:LEU:CD2	2.45	0.47
1:A:113:PRO:HD2	1:G:36:ARG:CZ	2.45	0.47
1:C:36:ARG:CZ	1:D:113:PRO:HD2	2.45	0.47
1:A:36:ARG:CZ	1:B:113:PRO:HD2	2.45	0.47
1:M:321:LYS:HB3	1:M:334:ASP:HB3	1.95	0.47
1:I:233:MET:O	1:I:237:LEU:HG	2.14	0.47
1:E:475:ASN:HD21	1:E:489:ILE:HD12	1.79	0.47
1:C:207:LYS:HE2	1:C:214:GLU:HB2	1.95	0.47
1:K:217:SER:HA	1:K:320:ALA:O	2.13	0.47
1:C:39:VAL:HG11	1:D:73:MET:SD	2.55	0.47
1:B:39:VAL:HG11	1:C:73:MET:SD	2.55	0.47
1:F:37:ASN:O	1:G:518:GLU:HB2	2.15	0.47
1:K:41:ASP:CG	1:L:522:THR:HG23	2.35	0.47
1:J:41:ASP:CG	1:K:522:THR:HG23	2.35	0.47
1:N:321:LYS:HB3	1:N:334:ASP:HB3	1.95	0.47
1:A:233:MET:O	1:A:237:LEU:HG	2.14	0.47
1:I:475:ASN:HD21	1:I:489:ILE:HD12	1.79	0.47



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	$overlap(\AA)$
1:D:475:ASN:HD21	1:D:489:ILE:HD12	1.79	0.47
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.95	0.47
1:K:207:LYS:HE2	1:K:214:GLU:HB2	1.95	0.47
1:J:217:SER:HA	1:J:320:ALA:O	2.13	0.47
1:D:47:PRO:HD2	1:E:73:MET:CA	2.44	0.47
1:A:39:VAL:HG11	1:B:73:MET:SD	2.55	0.47
1:A:73:MET:SD	1:G:39:VAL:HG11	2.55	0.47
1:G:522:THR:HG22	1:G:523:ASP:N	2.30	0.47
1:A:517:THR:HG23	1:G:39:VAL:CA	2.43	0.47
1:A:518:GLU:HB2	1:G:37:ASN:O	2.15	0.47
1:A:73:MET:CG	1:G:47:PRO:CB	2.88	0.47
1:A:73:MET:HE2	1:G:47:PRO:HG2	1.97	0.47
1:H:217:SER:HA	1:H:320:ALA:O	2.14	0.47
1:K:245:LYS:HB2	1:K:246:PRO:HD3	1.96	0.47
1:H:41:ASP:CG	1:I:522:THR:HG23	2.35	0.47
1:A:49:ILE:HG21	1:B:513:LEU:CA	2.45	0.47
1:B:245:LYS:HB2	1:B:246:PRO:HD3	1.96	0.47
1:F:522:THR:HG22	1:F:523:ASP:N	2.30	0.47
1:J:522:THR:HG22	1:J:523:ASP:N	2.29	0.47
1:M:26:ALA:HA	1:N:8:PHE:HE2	1.80	0.47
1:L:233:MET:O	1:L:237:LEU:HG	2.14	0.47
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.95	0.47
1:G:272:LYS:HB3	1:G:273:VAL:H	1.51	0.47
1:F:475:ASN:HD21	1:F:489:ILE:HD12	1.79	0.47
1:J:475:ASN:HD21	1:J:489:ILE:HD12	1.79	0.47
1:M:475:ASN:HD21	1:M:489:ILE:HD12	1.79	0.47
1:B:217:SER:HA	1:B:320:ALA:O	2.13	0.47
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.95	0.47
1:F:421:ARG:CZ	1:F:474:GLY:HA2	2.44	0.47
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.95	0.47
1:I:179:ASP:HB3	1:J:282:GLY:HA2	1.96	0.47
1:G:217:SER:HA	1:G:320:ALA:O	2.13	0.47
1:G:174:VAL:CG2	1:G:370:ALA:O	2.63	0.47
1:M:179:ASP:HB3	1:N:282:GLY:HA2	1.96	0.47
1:L:207:LYS:HE2	1:L:214:GLU:HB2	1.95	0.47
1:E:522:THR:HG22	1:E:523:ASP:N	2.30	0.47
1:F:39:VAL:HG11	1:G:73:MET:SD	2.55	0.47
1:I:245:LYS:CD	1:J:232:GLU:CD	2.81	0.47
1:N:522:THR:HG22	1:N:523:ASP:N	2.30	0.47
1:I:522:THR:HG22	1:I:523:ASP:N	2.29	0.47
1:I:496:PRO:O	1:I:499:VAL:HG22	2.13	0.47



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	ous page	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:L:36:ARG:HB3	1:M:518:GLU:CB	2.28	0.47
1:M:233:MET:O	1:M:237:LEU:HG	2.14	0.47
1:G:233:MET:O	1:G:237:LEU:HG	2.14	0.47
1:F:233:MET:O	1:F:237:LEU:HG	2.14	0.47
1:B:207:LYS:HE2	1:B:214:GLU:HB2	1.95	0.47
1:C:47:PRO:HD2	1:D:73:MET:CA	2.44	0.47
1:A:37:ASN:O	1:B:518:GLU:HB2	2.15	0.47
1:H:245:LYS:HB2	1:H:246:PRO:HD3	1.96	0.47
1:F:49:ILE:HG13	1:G:513:LEU:CD2	2.44	0.47
1:J:496:PRO:O	1:J:499:VAL:HG22	2.13	0.47
1:B:49:ILE:HG21	1:C:513:LEU:CA	2.45	0.47
1:C:245:LYS:HB2	1:C:246:PRO:HD3	1.96	0.47
1:D:245:LYS:HB2	1:D:246:PRO:HD3	1.96	0.47
1:D:36:ARG:CZ	1:E:113:PRO:HD2	2.45	0.47
1:N:458:CYS:SG	1:N:480:ALA:HB1	2.55	0.47
1:J:233:MET:O	1:J:237:LEU:HG	2.14	0.47
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.95	0.47
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.97	0.47
1:H:475:ASN:HD21	1:H:489:ILE:HD12	1.79	0.47
1:F:321:LYS:HB3	1:F:334:ASP:HB3	1.95	0.47
1:D:174:VAL:CG2	1:D:370:ALA:O	2.63	0.47
1:E:174:VAL:CG2	1:E:370:ALA:O	2.63	0.47
1:C:37:ASN:O	1:D:518:GLU:HB2	2.15	0.47
1:A:522:THR:HG22	1:A:523:ASP:N	2.30	0.47
1:F:36:ARG:CZ	1:G:113:PRO:HD2	2.45	0.47
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.55	0.47
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.96	0.47
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.97	0.47
1:K:381:VAL:HG11	1:K:393:LYS:HA	1.97	0.47
1:C:174:VAL:CG2	1:C:370:ALA:O	2.63	0.47
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.95	0.47
1:D:37:ASN:H	1:E:516:THR:HG22	1.70	0.46
1:E:37:ASN:H	1:F:516:THR:HG22	1.70	0.46
1:E:39:VAL:HG11	1:F:73:MET:SD	2.55	0.46
1:M:245:LYS:HB2	1:M:246:PRO:HD3	1.96	0.46
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.55	0.46
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.97	0.46
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.98	0.46
1:F:174:VAL:CG2	1:F:370:ALA:O	2.63	0.46
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.95	0.46
1:D:522:THR:HG22	1:D:523:ASP:N	2.30	0.46



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$ \text{overlap } (\mathring{\mathrm{A}})$
1:D:39:VAL:HG11	1:E:73:MET:SD	2.55	0.46
1:C:522:THR:HG22	1:C:523:ASP:N	2.30	0.46
1:H:522:THR:HG22	1:H:523:ASP:N	2.30	0.46
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.56	0.46
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.55	0.46
1:L:26:ALA:HA	1:M:8:PHE:HE2	1.80	0.46
1:J:381:VAL:HG11	1:J:393:LYS:HA	1.98	0.46
1:G:475:ASN:HD21	1:G:489:ILE:HD12	1.79	0.46
1:A:174:VAL:CG2	1:A:370:ALA:O	2.63	0.46
1:B:458:CYS:SG	1:B:480:ALA:HB1	2.55	0.46
1:A:461:GLU:OE2	1:L:463:SER:HB3	2.16	0.46
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.95	0.46
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.56	0.46
1:E:37:ASN:O	1:F:518:GLU:HB2	2.15	0.46
1:J:39:VAL:CB	1:K:69:MET:HE1	2.45	0.46
1:E:245:LYS:HB2	1:E:246:PRO:HD3	1.96	0.46
1:C:461:GLU:OE2	1:J:463:SER:HB3	2.16	0.46
1:B:461:GLU:OE2	1:K:463:SER:HB3	2.16	0.46
1:A:516:THR:HG22	1:G:37:ASN:H	1.70	0.46
1:F:47:PRO:CB	1:G:73:MET:HG2	2.42	0.46
1:L:245:LYS:HB2	1:L:246:PRO:HD3	1.96	0.46
1:L:270:ILE:CG2	1:M:229:ASN:CA	2.82	0.46
1:H:39:VAL:CB	1:I:69:MET:HE1	2.46	0.46
1:C:49:ILE:HG21	1:D:513:LEU:CA	2.45	0.46
1:M:36:ARG:HB3	1:N:518:GLU:CB	2.28	0.46
1:H:146:GLN:NE2	1:H:494:LEU:CD1	2.70	0.46
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.55	0.46
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.97	0.46
1:D:384:ALA:O	1:D:388:GLU:HB2	2.16	0.46
1:A:384:ALA:O	1:A:388:GLU:HB2	2.16	0.46
1:K:475:ASN:HD21	1:K:489:ILE:HD12	1.79	0.46
1:G:461:GLU:OE2	1:M:463:SER:HB3	2.16	0.46
1:B:47:PRO:CB	1:C:73:MET:CG	2.88	0.46
1:A:513:LEU:CD2	1:G:49:ILE:HG13	2.45	0.46
1:A:513:LEU:CA	1:G:49:ILE:HG21	2.45	0.46
1:K:86:GLY:CA	1:K:405:ALA:CB	2.88	0.46
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.56	0.46
1:K:233:MET:O	1:K:237:LEU:HG	2.14	0.46
1:L:381:VAL:HG11	1:L:393:LYS:HA	1.97	0.46
1:F:384:ALA:O	1:F:388:GLU:HB2	2.16	0.46
1:B:145:ALA:O	1:B:149:THR:HG23	2.16	0.46



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$\text{overlap } (\mathring{\mathbf{A}})$
1:I:217:SER:HA	1:I:320:ALA:O	2.14	0.46
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.97	0.46
1:C:390:LYS:HD2	1:C:390:LYS:N	2.31	0.46
1:E:390:LYS:N	1:E:390:LYS:HD2	2.31	0.46
1:C:47:PRO:HG2	1:D:73:MET:CE	2.45	0.46
1:D:47:PRO:HG2	1:E:73:MET:CE	2.45	0.46
1:A:73:MET:CE	1:G:47:PRO:HG2	2.45	0.46
1:I:270:ILE:HG21	1:J:229:ASN:O	2.00	0.46
1:N:245:LYS:HB2	1:N:246:PRO:HD3	1.96	0.46
1:A:49:ILE:HG13	1:B:513:LEU:CD2	2.45	0.46
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.96	0.46
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.97	0.46
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.97	0.46
1:N:381:VAL:HG11	1:N:393:LYS:HA	1.97	0.46
1:N:475:ASN:HD21	1:N:489:ILE:HD12	1.79	0.46
1:J:106:ALA:O	1:J:111:MET:HB2	2.16	0.46
1:E:458:CYS:SG	1:E:480:ALA:HB1	2.56	0.46
1:B:106:ALA:O	1:B:111:MET:HB2	2.16	0.46
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.56	0.46
1:G:106:ALA:O	1:G:111:MET:HB2	2.16	0.46
1:D:458:CYS:SG	1:D:480:ALA:HB1	2.55	0.46
1:B:522:THR:HG22	1:B:523:ASP:N	2.30	0.46
1:E:49:ILE:HG21	1:F:513:LEU:CA	2.45	0.46
1:B:49:ILE:HG13	1:C:513:LEU:CD2	2.45	0.46
1:H:518:GLU:CB	1:N:36:ARG:HB3	2.28	0.46
1:H:272:LYS:HB3	1:H:273:VAL:H	1.51	0.46
1:B:384:ALA:O	1:B:388:GLU:HB2	2.16	0.46
1:E:384:ALA:O	1:E:388:GLU:HB2	2.16	0.46
1:C:475:ASN:HD21	1:C:489:ILE:HD12	1.79	0.46
1:C:145:ALA:O	1:C:149:THR:HG23	2.16	0.46
1:E:36:ARG:CZ	1:F:113:PRO:HD2	2.45	0.46
1:J:182:GLY:N	1:K:283:ASP:HB2	2.25	0.46
1:B:236:VAL:O	1:B:240:VAL:HG23	2.16	0.46
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.97	0.46
1:M:381:VAL:HG11	1:M:393:LYS:HA	1.98	0.46
1:F:461:GLU:OE2	1:N:463:SER:HB3	2.16	0.46
1:D:461:GLU:OE2	1:I:463:SER:HB3	2.16	0.46
1:B:390:LYS:HD2	1:B:390:LYS:N	2.31	0.46
1:A:47:PRO:HG2	1:B:73:MET:CE	2.45	0.46
1:A:47:PRO:HG2	1:B:73:MET:HE2	1.98	0.46
1:F:47:PRO:HG2	1:G:73:MET:CE	2.45	0.46



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:D:386:GLU:CG	1:E:281:PHE:HE2	2.07	0.46
1:K:270:ILE:HD13	1:L:231:ARG:HG3	1.96	0.46
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.97	0.46
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.97	0.46
1:H:381:VAL:HG11	1:H:393:LYS:HA	1.97	0.46
1:C:103:GLY:O	1:C:107:VAL:HG23	2.16	0.46
1:A:145:ALA:O	1:A:149:THR:HG23	2.16	0.46
1:B:174:VAL:CG2	1:B:370:ALA:O	2.63	0.46
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.56	0.46
1:F:150:ILE:CG1	1:F:494:LEU:HD12	2.39	0.46
1:L:270:ILE:HD13	1:M:231:ARG:HG3	1.96	0.46
1:B:35:GLY:O	1:C:114:MET:HE1	2.10	0.46
1:I:236:VAL:O	1:I:240:VAL:HG23	2.16	0.46
1:B:103:GLY:O	1:B:107:VAL:HG23	2.16	0.46
1:N:106:ALA:O	1:N:111:MET:HB2	2.16	0.46
1:E:106:ALA:O	1:E:111:MET:HB2	2.16	0.46
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.97	0.46
1:D:390:LYS:HD2	1:D:390:LYS:N	2.31	0.46
1:D:37:ASN:O	1:E:518:GLU:HB2	2.15	0.45
1:E:47:PRO:HG2	1:F:73:MET:HE2	1.98	0.45
1:E:150:ILE:CD1	1:E:411:VAL:CB	2.87	0.45
1:H:69:MET:HE1	1:N:39:VAL:CB	2.47	0.45
1:L:146:GLN:NE2	1:L:494:LEU:CD1	2.70	0.45
1:K:26:ALA:HA	1:L:8:PHE:HE2	1.80	0.45
1:N:219:PHE:HB3	1:N:317:LEU:HD23	1.98	0.45
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.97	0.45
1:I:381:VAL:HG11	1:I:393:LYS:HA	1.97	0.45
1:E:461:GLU:OE2	1:H:463:SER:HB3	2.16	0.45
1:L:106:ALA:O	1:L:111:MET:HB2	2.16	0.45
1:M:111:MET:HG3	1:M:435:ASP:OD1	2.17	0.45
1:D:106:ALA:O	1:D:111:MET:HB2	2.16	0.45
1:E:47:PRO:HG2	1:F:73:MET:CE	2.45	0.45
1:F:37:ASN:H	1:G:516:THR:CG2	2.28	0.45
1:F:39:VAL:CA	1:G:517:THR:HG23	2.43	0.45
1:I:182:GLY:N	1:J:283:ASP:HB2	2.25	0.45
1:B:230:ILE:O	1:B:233:MET:HB2	2.17	0.45
1:C:230:ILE:O	1:C:233:MET:HB2	2.17	0.45
1:H:236:VAL:O	1:H:240:VAL:HG23	2.16	0.45
1:L:111:MET:HG3	1:L:435:ASP:OD1	2.17	0.45
1:M:106:ALA:O	1:M:111:MET:HB2	2.16	0.45
1:I:111:MET:HG3	1:I:435:ASP:OD1	2.17	0.45



Continued from previous page...

Continued from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap (\AA)$
1:F:145:ALA:O	1:F:149:THR:HG23	2.16	0.45
1:E:122:LYS:HE2	1:E:430:ARG:O	2.17	0.45
1:B:47:PRO:HG2	1:C:73:MET:CE	2.45	0.45
1:C:49:ILE:HG13	1:D:513:LEU:CD2	2.45	0.45
1:C:272:LYS:HB3	1:C:273:VAL:H	1.51	0.45
1:E:111:MET:HG3	1:E:435:ASP:OD1	2.17	0.45
1:M:122:LYS:HE2	1:M:430:ARG:O	2.17	0.45
1:E:145:ALA:O	1:E:149:THR:HG23	2.16	0.45
1:H:111:MET:HG3	1:H:435:ASP:OD1	2.16	0.45
1:E:37:ASN:H	1:F:516:THR:CG2	2.28	0.45
1:H:229:ASN:O	1:N:270:ILE:HG21	2.00	0.45
1:J:236:VAL:O	1:J:240:VAL:HG23	2.16	0.45
1:C:236:VAL:O	1:C:240:VAL:HG23	2.16	0.45
1:G:384:ALA:O	1:G:388:GLU:HB2	2.16	0.45
1:L:122:LYS:HE2	1:L:430:ARG:O	2.17	0.45
1:C:458:CYS:SG	1:C:480:ALA:HB1	2.56	0.45
1:H:325:ILE:HG23	1:H:330:THR:OG1	2.17	0.45
1:J:122:LYS:HE2	1:J:430:ARG:O	2.17	0.45
1:K:122:LYS:HE2	1:K:430:ARG:O	2.17	0.45
1:D:230:ILE:O	1:D:233:MET:HB2	2.17	0.45
1:I:90:THR:O	1:I:94:VAL:HG13	2.17	0.45
1:L:90:THR:O	1:L:94:VAL:HG13	2.17	0.45
1:C:384:ALA:O	1:C:388:GLU:HB2	2.16	0.45
1:N:111:MET:HG3	1:N:435:ASP:OD1	2.17	0.45
1:F:122:LYS:HE2	1:F:430:ARG:O	2.17	0.45
1:F:325:ILE:HG23	1:F:330:THR:OG1	2.17	0.45
1:E:47:PRO:CB	1:F:73:MET:HG2	2.41	0.45
1:J:270:ILE:HD13	1:K:231:ARG:HG3	1.96	0.45
1:K:39:VAL:CB	1:L:69:MET:HE1	2.46	0.45
1:J:146:GLN:NE2	1:J:494:LEU:CD1	2.70	0.45
1:N:230:ILE:O	1:N:233:MET:HB2	2.17	0.45
1:J:111:MET:HG3	1:J:435:ASP:OD1	2.17	0.45
1:D:111:MET:HG3	1:D:435:ASP:OD1	2.17	0.45
1:H:106:ALA:O	1:H:111:MET:HB2	2.16	0.45
1:E:90:THR:O	1:E:94:VAL:HG13	2.17	0.45
1:C:325:ILE:HG23	1:C:330:THR:OG1	2.17	0.45
1:K:106:ALA:O	1:K:111:MET:HB2	2.16	0.45
1:F:111:MET:HG3	1:F:435:ASP:OD1	2.17	0.45
1:M:103:GLY:O	1:M:107:VAL:HG23	2.16	0.45
1:E:325:ILE:HG23	1:E:330:THR:OG1	2.17	0.45
1:M:389:MET:SD	1:N:281:PHE:CD2	3.10	0.45



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:K:230:ILE:O	1:K:233:MET:HB2	2.16	0.45
1:E:230:ILE:O	1:E:233:MET:HB2	2.17	0.45
1:A:236:VAL:O	1:A:240:VAL:HG23	2.16	0.45
1:E:236:VAL:O	1:E:240:VAL:HG23	2.16	0.45
1:M:90:THR:O	1:M:94:VAL:HG13	2.17	0.45
1:D:90:THR:O	1:D:94:VAL:HG13	2.17	0.45
1:F:106:ALA:O	1:F:111:MET:HB2	2.16	0.45
1:K:267:MET:O	1:K:268:ARG:HB2	2.17	0.45
1:N:122:LYS:HE2	1:N:430:ARG:O	2.17	0.45
1:D:103:GLY:O	1:D:107:VAL:HG23	2.16	0.45
1:D:325:ILE:HG23	1:D:330:THR:OG1	2.17	0.45
1:I:267:MET:O	1:I:268:ARG:HB2	2.17	0.45
1:J:267:MET:O	1:J:268:ARG:HB2	2.17	0.45
1:H:389:MET:SD	1:I:281:PHE:CD2	3.10	0.45
1:E:386:GLU:CG	1:F:281:PHE:HE2	2.07	0.45
1:A:230:ILE:O	1:A:233:MET:HB2	2.17	0.45
1:L:236:VAL:O	1:L:240:VAL:HG23	2.16	0.45
1:K:236:VAL:O	1:K:240:VAL:HG23	2.16	0.45
1:L:272:LYS:HB3	1:L:273:VAL:H	1.51	0.45
1:K:90:THR:O	1:K:94:VAL:HG13	2.17	0.45
1:L:325:ILE:HG23	1:L:330:THR:OG1	2.17	0.45
1:H:103:GLY:O	1:H:107:VAL:HG23	2.16	0.45
1:G:325:ILE:HG23	1:G:330:THR:OG1	2.17	0.45
1:A:106:ALA:O	1:A:111:MET:HB2	2.16	0.45
1:J:90:THR:O	1:J:94:VAL:HG13	2.17	0.45
1:D:122:LYS:HE2	1:D:430:ARG:O	2.17	0.45
1:J:389:MET:SD	1:K:281:PHE:CD2	3.10	0.45
1:I:389:MET:SD	1:J:281:PHE:CD2	3.10	0.45
1:L:230:ILE:O	1:L:233:MET:HB2	2.17	0.45
1:M:230:ILE:O	1:M:233:MET:HB2	2.17	0.45
1:H:230:ILE:O	1:H:233:MET:HB2	2.17	0.45
1:F:230:ILE:O	1:F:233:MET:HB2	2.17	0.45
1:G:236:VAL:O	1:G:240:VAL:HG23	2.16	0.45
1:K:111:MET:HG3	1:K:435:ASP:OD1	2.17	0.45
1:C:106:ALA:O	1:C:111:MET:HB2	2.16	0.45
1:L:267:MET:O	1:L:268:ARG:HB2	2.17	0.45
1:J:403:THR:O	1:J:407:VAL:HG23	2.17	0.45
1:C:267:MET:O	1:C:268:ARG:HB2	2.17	0.45
1:D:47:PRO:HG2	1:E:73:MET:HE2	1.99	0.45
1:I:270:ILE:HD13	1:J:231:ARG:HG3	1.96	0.45
1:L:270:ILE:HG21	1:M:229:ASN:O	2.00	0.45



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$overlap(\AA)$
1:G:230:ILE:O	1:G:233:MET:HB2	2.17	0.45
1:H:90:THR:O	1:H:94:VAL:HG13	2.17	0.45
1:G:145:ALA:O	1:G:149:THR:HG23	2.16	0.45
1:A:325:ILE:HG23	1:A:330:THR:OG1	2.17	0.45
1:B:325:ILE:HG23	1:B:330:THR:OG1	2.17	0.45
1:N:325:ILE:HG23	1:N:330:THR:OG1	2.17	0.45
1:K:103:GLY:O	1:K:107:VAL:HG23	2.16	0.45
1:A:122:LYS:HE2	1:A:430:ARG:O	2.17	0.45
1:G:390:LYS:HD2	1:G:390:LYS:N	2.31	0.45
1:A:390:LYS:HD2	1:A:390:LYS:N	2.31	0.45
1:H:281:PHE:CD2	1:N:389:MET:SD	3.10	0.44
1:H:270:ILE:HG21	1:I:229:ASN:O	2.00	0.44
1:D:35:GLY:O	1:E:114:MET:HE1	2.10	0.44
1:M:146:GLN:NE2	1:M:494:LEU:CD1	2.70	0.44
1:N:236:VAL:O	1:N:240:VAL:HG23	2.16	0.44
1:J:272:LYS:HB3	1:J:273:VAL:H	1.51	0.44
1:J:103:GLY:O	1:J:107:VAL:HG23	2.16	0.44
1:A:103:GLY:O	1:A:107:VAL:HG23	2.16	0.44
1:G:202:PRO:O	1:G:203:TYR:HB2	2.17	0.44
1:N:103:GLY:O	1:N:107:VAL:HG23	2.17	0.44
1:B:73:MET:O	1:B:76:GLU:HB2	2.18	0.44
1:L:389:MET:SD	1:M:281:PHE:CD2	3.10	0.44
1:K:389:MET:SD	1:L:281:PHE:CD2	3.10	0.44
1:K:270:ILE:CG2	1:L:229:ASN:CA	2.82	0.44
1:L:73:MET:O	1:L:76:GLU:HB2	2.18	0.44
1:D:270:ILE:HG22	1:E:229:ASN:C	2.31	0.44
1:A:434:GLU:O	1:A:438:VAL:HG23	2.18	0.44
1:J:230:ILE:O	1:J:233:MET:HB2	2.17	0.44
1:D:236:VAL:O	1:D:240:VAL:HG23	2.16	0.44
1:L:103:GLY:O	1:L:107:VAL:HG23	2.16	0.44
1:K:403:THR:O	1:K:407:VAL:HG23	2.17	0.44
1:A:202:PRO:O	1:A:203:TYR:HB2	2.17	0.44
1:F:390:LYS:HD2	1:F:390:LYS:N	2.31	0.44
1:E:47:PRO:CB	1:F:73:MET:CG	2.87	0.44
1:C:150:ILE:CG1	1:C:494:LEU:HD12	2.39	0.44
1:D:49:ILE:HG13	1:E:513:LEU:CD2	2.45	0.44
1:H:434:GLU:O	1:H:438:VAL:HG23	2.18	0.44
1:G:111:MET:HG3	1:G:435:ASP:OD1	2.17	0.44
1:A:111:MET:HG3	1:A:435:ASP:OD1	2.17	0.44
1:I:103:GLY:O	1:I:107:VAL:HG23	2.16	0.44
1:F:267:MET:O	1:F:268:ARG:HB2	2.17	0.44



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:H:267:MET:O	1:H:268:ARG:HB2	2.17	0.44
1:D:145:ALA:O	1:D:149:THR:HG23	2.16	0.44
1:E:73:MET:O	1:E:76:GLU:HB2	2.18	0.44
1:H:26:ALA:HA	1:I:8:PHE:HE2	1.80	0.44
1:M:236:VAL:O	1:M:240:VAL:HG23	2.16	0.44
1:M:325:ILE:HG23	1:M:330:THR:OG1	2.17	0.44
1:D:267:MET:O	1:D:268:ARG:HB2	2.17	0.44
1:I:122:LYS:HE2	1:I:430:ARG:O	2.17	0.44
1:M:267:MET:O	1:M:268:ARG:HB2	2.17	0.44
1:I:325:ILE:HG23	1:I:330:THR:OG1	2.17	0.44
1:B:122:LYS:HE2	1:B:430:ARG:O	2.17	0.44
1:F:103:GLY:O	1:F:107:VAL:HG23	2.16	0.44
1:A:73:MET:O	1:A:76:GLU:HB2	2.18	0.44
1:N:73:MET:O	1:N:76:GLU:HB2	2.18	0.44
1:H:73:MET:O	1:H:76:GLU:HB2	2.18	0.44
1:K:182:GLY:N	1:L:283:ASP:HB2	2.25	0.44
1:N:434:GLU:O	1:N:438:VAL:HG23	2.18	0.44
1:I:230:ILE:O	1:I:233:MET:HB2	2.17	0.44
1:I:434:GLU:O	1:I:438:VAL:HG23	2.18	0.44
1:F:236:VAL:O	1:F:240:VAL:HG23	2.16	0.44
1:B:272:LYS:HB3	1:B:273:VAL:H	1.51	0.44
1:F:461:GLU:HA	1:F:462:PRO:HD2	1.90	0.44
1:I:106:ALA:O	1:I:111:MET:HB2	2.16	0.44
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.99	0.44
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.99	0.44
1:J:202:PRO:O	1:J:203:TYR:HB2	2.18	0.44
1:K:202:PRO:O	1:K:203:TYR:HB2	2.17	0.44
1:C:122:LYS:HE2	1:C:430:ARG:O	2.17	0.44
1:F:202:PRO:O	1:F:203:TYR:HB2	2.17	0.44
1:D:73:MET:O	1:D:76:GLU:HB2	2.18	0.44
1:E:150:ILE:CD1	1:E:494:LEU:CD1	2.94	0.44
1:K:73:MET:O	1:K:76:GLU:HB2	2.18	0.44
1:C:111:MET:HG3	1:C:435:ASP:OD1	2.17	0.44
1:E:267:MET:O	1:E:268:ARG:HB2	2.17	0.44
1:H:205:ILE:HA	1:H:213:VAL:HG22	1.99	0.44
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.99	0.44
1:B:267:MET:O	1:B:268:ARG:HB2	2.17	0.44
1:M:403:THR:O	1:M:407:VAL:HG23	2.17	0.44
1:C:434:GLU:O	1:C:438:VAL:HG23	2.18	0.44
1:M:434:GLU:O	1:M:438:VAL:HG23	2.18	0.44
1:F:90:THR:O	1:F:94:VAL:HG13	2.17	0.44



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:F:430:ARG:HA	1:F:430:ARG:HD3	1.84	0.44
1:N:403:THR:O	1:N:407:VAL:HG23	2.17	0.44
1:G:122:LYS:HE2	1:G:430:ARG:O	2.17	0.44
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.99	0.44
1:E:103:GLY:O	1:E:107:VAL:HG23	2.16	0.44
1:G:103:GLY:O	1:G:107:VAL:HG23	2.16	0.44
1:K:325:ILE:HG23	1:K:330:THR:OG1	2.17	0.44
1:C:73:MET:O	1:C:76:GLU:HB2	2.18	0.44
1:G:179:ASP:HB3	1:G:389:MET:HE1	2.00	0.44
1:B:90:THR:O	1:B:94:VAL:HG13	2.17	0.44
1:B:111:MET:HG3	1:B:435:ASP:OD1	2.17	0.44
1:D:202:PRO:O	1:D:203:TYR:HB2	2.17	0.44
1:G:267:MET:O	1:G:268:ARG:HB2	2.17	0.44
1:J:205:ILE:HA	1:J:213:VAL:HG22	1.99	0.44
1:N:267:MET:O	1:N:268:ARG:HB2	2.17	0.44
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.99	0.44
1:G:73:MET:O	1:G:76:GLU:HB2	2.18	0.44
1:I:26:ALA:HA	1:J:8:PHE:HE2	1.80	0.44
1:E:272:LYS:HB3	1:E:273:VAL:H	1.51	0.44
1:A:90:THR:O	1:A:94:VAL:HG13	2.17	0.44
1:B:202:PRO:O	1:B:203:TYR:HB2	2.18	0.44
1:K:16:MET:O	1:K:20:VAL:HG13	2.18	0.44
1:J:16:MET:O	1:J:20:VAL:HG13	2.18	0.44
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.99	0.44
1:I:46:ALA:HA	1:I:47:PRO:HD3	1.89	0.44
1:A:16:MET:O	1:A:20:VAL:HG13	2.18	0.44
1:H:122:LYS:HE2	1:H:430:ARG:O	2.17	0.44
1:J:325:ILE:HG23	1:J:330:THR:OG1	2.17	0.44
1:M:202:PRO:O	1:M:203:TYR:HB2	2.18	0.44
1:C:37:ASN:H	1:D:516:THR:CG2	2.28	0.43
1:F:47:PRO:HG2	1:G:73:MET:HE2	1.98	0.43
1:D:150:ILE:CD1	1:D:494:LEU:CD1	2.94	0.43
1:G:90:THR:O	1:G:94:VAL:HG13	2.17	0.43
1:C:90:THR:O	1:C:94:VAL:HG13	2.17	0.43
1:G:149:THR:HG23	1:G:159:GLY:HA3	2.00	0.43
1:B:430:ARG:HA	1:B:430:ARG:HD3	1.84	0.43
1:D:464:VAL:HG22	1:I:464:VAL:HA	2.00	0.43
1:I:202:PRO:O	1:I:203:TYR:HB2	2.17	0.43
1:N:90:THR:O	1:N:94:VAL:HG13	2.17	0.43
1:I:403:THR:O	1:I:407:VAL:HG23	2.17	0.43
1:N:202:PRO:O	1:N:203:TYR:HB2	2.18	0.43



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$overlap(\AA)$
1:B:37:ASN:H	1:C:516:THR:CG2	2.28	0.43
1:L:408:GLU:N	1:L:498:LYS:HE2	2.33	0.43
1:M:182:GLY:N	1:N:283:ASP:HB2	2.25	0.43
1:B:434:GLU:O	1:B:438:VAL:HG23	2.18	0.43
1:K:434:GLU:O	1:K:438:VAL:HG23	2.18	0.43
1:L:434:GLU:O	1:L:438:VAL:HG23	2.18	0.43
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.99	0.43
1:L:120:ILE:O	1:L:124:VAL:HG23	2.19	0.43
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.99	0.43
1:I:146:GLN:NE2	1:I:494:LEU:CD1	2.70	0.43
1:J:434:GLU:O	1:J:438:VAL:HG23	2.18	0.43
1:L:149:THR:HG22	1:L:156:GLU:HA	2.01	0.43
1:G:461:GLU:HA	1:G:462:PRO:HD2	1.90	0.43
1:H:120:ILE:O	1:H:124:VAL:HG23	2.18	0.43
1:L:16:MET:O	1:L:20:VAL:HG13	2.18	0.43
1:G:16:MET:O	1:G:20:VAL:HG13	2.18	0.43
1:H:202:PRO:O	1:H:203:TYR:HB2	2.18	0.43
1:M:61:GLU:O	1:N:3:ALA:HA	2.19	0.43
1:A:150:ILE:CG1	1:A:494:LEU:CD1	2.97	0.43
1:I:386:GLU:HB2	1:J:284:ARG:CD	2.40	0.43
1:J:73:MET:O	1:J:76:GLU:HB2	2.18	0.43
1:H:182:GLY:N	1:I:283:ASP:HB2	2.25	0.43
1:M:26:ALA:HA	1:N:8:PHE:CZ	2.54	0.43
1:K:149:THR:HG22	1:K:156:GLU:HA	2.00	0.43
1:B:461:GLU:HA	1:B:462:PRO:HD2	1.90	0.43
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.99	0.43
1:J:120:ILE:O	1:J:124:VAL:HG23	2.19	0.43
1:D:120:ILE:O	1:D:124:VAL:HG23	2.19	0.43
1:E:464:VAL:HG22	1:H:464:VAL:HA	2.00	0.43
1:D:16:MET:O	1:D:20:VAL:HG13	2.18	0.43
1:J:386:GLU:HB2	1:K:284:ARG:CD	2.40	0.43
1:D:305:ILE:HG23	1:D:308:GLU:HG3	2.00	0.43
1:C:149:THR:HG23	1:C:159:GLY:HA3	2.00	0.43
1:N:120:ILE:O	1:N:124:VAL:HG23	2.19	0.43
1:E:350:ARG:O	1:E:353:ILE:HG12	2.19	0.43
1:N:501:ARG:HG3	1:N:502:SER:N	2.34	0.43
1:E:202:PRO:O	1:E:203:TYR:HB2	2.18	0.43
1:B:16:MET:O	1:B:20:VAL:HG13	2.18	0.43
1:K:61:GLU:O	1:L:3:ALA:HA	2.19	0.43
1:H:61:GLU:O	1:I:3:ALA:HA	2.19	0.43
1:K:205:ILE:HA	1:K:213:VAL:HG22	1.99	0.43



Continued from previous page...

Continuea from previ	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	overlap $(Å)$
1:C:47:PRO:CB	1:D:73:MET:CG	2.88	0.43
1:A:229:ASN:C	1:G:270:ILE:HG22	2.31	0.43
1:L:183:LEU:HA	1:L:183:LEU:HD23	1.90	0.43
1:E:305:ILE:HG23	1:E:308:GLU:HG3	2.00	0.43
1:G:434:GLU:O	1:G:438:VAL:HG23	2.18	0.43
1:F:434:GLU:O	1:F:438:VAL:HG23	2.18	0.43
1:M:149:THR:HG22	1:M:156:GLU:HA	2.01	0.43
1:F:149:THR:HG23	1:F:159:GLY:HA3	2.00	0.43
1:C:464:VAL:HG22	1:J:464:VAL:HA	2.00	0.43
1:B:120:ILE:O	1:B:124:VAL:HG23	2.19	0.43
1:F:16:MET:O	1:F:20:VAL:HG13	2.18	0.43
1:C:120:ILE:O	1:C:124:VAL:HG23	2.19	0.43
1:H:350:ARG:O	1:H:353:ILE:HG12	2.19	0.43
1:L:202:PRO:O	1:L:203:TYR:HB2	2.18	0.43
1:I:16:MET:O	1:I:20:VAL:HG13	2.18	0.43
1:F:120:ILE:O	1:F:124:VAL:HG23	2.19	0.43
1:L:403:THR:O	1:L:407:VAL:HG23	2.17	0.43
1:A:150:ILE:CD1	1:A:494:LEU:CD1	2.94	0.43
1:H:386:GLU:HA	1:I:281:PHE:N	2.34	0.43
1:J:245:LYS:CE	1:K:232:GLU:CG	2.91	0.43
1:I:73:MET:O	1:I:76:GLU:HB2	2.18	0.43
1:C:245:LYS:CE	1:D:232:GLU:HG3	2.45	0.43
1:A:229:ASN:C	1:G:270:ILE:HG23	2.30	0.43
1:M:183:LEU:HA	1:M:183:LEU:HD23	1.90	0.43
1:L:26:ALA:HA	1:M:8:PHE:CZ	2.54	0.43
1:L:27:VAL:HG12	1:L:90:THR:HG23	2.01	0.43
1:D:27:VAL:HG12	1:D:90:THR:HG23	2.01	0.43
1:A:461:GLU:HA	1:A:462:PRO:HD2	1.90	0.43
1:A:149:THR:HG23	1:A:159:GLY:HA3	2.00	0.43
1:E:91:THR:O	1:E:94:VAL:HG22	2.19	0.43
1:C:158:VAL:HG21	1:C:395:ARG:HD2	2.01	0.43
1:D:158:VAL:HG21	1:D:395:ARG:HD2	2.01	0.43
1:M:16:MET:O	1:M:20:VAL:HG13	2.18	0.43
1:A:267:MET:O	1:A:268:ARG:HB2	2.17	0.43
1:N:350:ARG:O	1:N:353:ILE:HG12	2.19	0.43
1:N:16:MET:O	1:N:20:VAL:HG13	2.18	0.43
1:I:350:ARG:O	1:I:353:ILE:HG12	2.19	0.43
1:A:150:ILE:CG1	1:A:494:LEU:HD12	2.39	0.43
1:F:73:MET:O	1:F:76:GLU:HB2	2.18	0.43
1:G:150:ILE:CG1	1:G:494:LEU:CD1	2.97	0.43
1:F:150:ILE:CG1	1:F:494:LEU:CD1	2.97	0.43



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Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:H:281:PHE:N	1:N:386:GLU:HA	2.34	0.43
1:M:73:MET:O	1:M:76:GLU:HB2	2.18	0.43
1:M:408:GLU:N	1:M:498:LYS:HE2	2.33	0.43
1:A:245:LYS:CE	1:B:232:GLU:HG3	2.45	0.43
1:F:91:THR:O	1:F:94:VAL:HG22	2.19	0.43
1:H:403:THR:O	1:H:407:VAL:HG23	2.18	0.43
1:I:61:GLU:O	1:J:3:ALA:HA	2.19	0.43
1:F:436:GLN:O	1:F:440:ILE:HG13	2.19	0.43
1:F:350:ARG:O	1:F:353:ILE:HG12	2.19	0.43
1:G:120:ILE:O	1:G:124:VAL:HG23	2.19	0.43
1:G:436:GLN:O	1:G:440:ILE:HG13	2.19	0.43
1:D:350:ARG:O	1:D:353:ILE:HG12	2.19	0.43
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.99	0.43
1:G:150:ILE:CD1	1:G:494:LEU:CD1	2.94	0.43
1:A:37:ASN:H	1:B:516:THR:CG2	2.28	0.43
1:A:516:THR:CG2	1:G:37:ASN:H	2.28	0.43
1:K:386:GLU:HA	1:L:281:PHE:N	2.34	0.43
1:M:39:VAL:HG11	1:N:69:MET:CE	2.34	0.43
1:I:305:ILE:HG23	1:I:308:GLU:HG3	2.00	0.43
1:E:434:GLU:O	1:E:438:VAL:HG23	2.18	0.43
1:D:149:THR:HG23	1:D:159:GLY:HA3	2.00	0.43
1:I:120:ILE:O	1:I:124:VAL:HG23	2.19	0.43
1:E:158:VAL:HG21	1:E:395:ARG:HD2	2.01	0.43
1:B:418:ALA:O	1:B:422:VAL:HG23	2.19	0.43
1:A:120:ILE:O	1:A:124:VAL:HG23	2.19	0.43
1:D:501:ARG:HG3	1:D:502:SER:N	2.34	0.43
1:C:16:MET:O	1:C:20:VAL:HG13	2.18	0.43
1:C:150:ILE:CG1	1:C:494:LEU:CD1	2.97	0.43
1:D:150:ILE:CD1	1:D:411:VAL:CB	2.87	0.43
1:M:245:LYS:CE	1:N:232:GLU:CG	2.91	0.43
1:N:305:ILE:HG23	1:N:308:GLU:HG3	2.00	0.43
1:J:305:ILE:HG23	1:J:308:GLU:HG3	2.01	0.43
1:D:434:GLU:O	1:D:438:VAL:HG23	2.18	0.43
1:H:91:THR:O	1:H:94:VAL:HG22	2.19	0.43
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.01	0.43
1:B:91:THR:O	1:B:94:VAL:HG22	2.19	0.43
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.01	0.43
1:N:91:THR:O	1:N:94:VAL:HG22	2.19	0.43
1:M:501:ARG:HG3	1:M:502:SER:N	2.34	0.43
1:H:501:ARG:HG3	1:H:502:SER:N	2.34	0.43
1:B:158:VAL:HG21	1:B:395:ARG:HD2	2.01	0.43



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; ({\rm \AA})$	overlap (Å)
1:N:443:ALA:O	1:N:447:MET:HG3	2.19	0.43
1:L:61:GLU:O	1:M:3:ALA:HA	2.19	0.43
1:J:443:ALA:O	1:J:447:MET:HG3	2.19	0.43
1:E:150:ILE:CG1	1:E:494:LEU:CD1	2.97	0.42
1:M:387:VAL:HA	1:N:281:PHE:CD1	2.50	0.42
1:H:408:GLU:N	1:H:498:LYS:HE2	2.33	0.42
1:B:49:ILE:CG2	1:C:513:LEU:CD2	2.92	0.42
1:M:168:LYS:CD	1:M:189:VAL:HG23	2.46	0.42
1:G:305:ILE:HG23	1:G:308:GLU:HG3	2.00	0.42
1:J:149:THR:HG22	1:J:156:GLU:HA	2.00	0.42
1:M:91:THR:O	1:M:94:VAL:HG22	2.19	0.42
1:K:91:THR:O	1:K:94:VAL:HG22	2.19	0.42
1:D:91:THR:O	1:D:94:VAL:HG22	2.19	0.42
1:A:91:THR:O	1:A:94:VAL:HG22	2.19	0.42
1:E:436:GLN:O	1:E:440:ILE:HG13	2.19	0.42
1:A:501:ARG:HG3	1:A:502:SER:N	2.34	0.42
1:C:202:PRO:O	1:C:203:TYR:HB2	2.18	0.42
1:H:16:MET:O	1:H:20:VAL:HG13	2.18	0.42
1:H:443:ALA:O	1:H:447:MET:HG3	2.19	0.42
1:K:120:ILE:O	1:K:124:VAL:HG23	2.19	0.42
1:I:443:ALA:O	1:I:447:MET:HG3	2.19	0.42
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.99	0.42
1:H:3:ALA:HA	1:N:61:GLU:O	2.19	0.42
1:J:386:GLU:HA	1:K:281:PHE:N	2.34	0.42
1:I:386:GLU:HA	1:J:281:PHE:N	2.34	0.42
1:I:408:GLU:N	1:I:498:LYS:HE2	2.33	0.42
1:B:49:ILE:HG12	1:C:513:LEU:HD13	1.99	0.42
1:C:49:ILE:CG2	1:D:513:LEU:CD2	2.92	0.42
1:N:408:GLU:N	1:N:498:LYS:HE2	2.33	0.42
1:L:190:VAL:O	1:L:191:GLU:O	2.38	0.42
1:H:26:ALA:HA	1:I:8:PHE:CZ	2.54	0.42
1:H:8:PHE:CZ	1:N:26:ALA:HA	2.54	0.42
1:J:26:ALA:HA	1:K:8:PHE:HE2	1.80	0.42
1:K:350:ARG:O	1:K:353:ILE:HG12	2.19	0.42
1:L:350:ARG:O	1:L:353:ILE:HG12	2.19	0.42
1:A:436:GLN:O	1:A:440:ILE:HG13	2.19	0.42
1:A:350:ARG:O	1:A:353:ILE:HG12	2.19	0.42
1:B:436:GLN:O	1:B:440:ILE:HG13	2.19	0.42
1:F:464:VAL:HG22	1:N:464:VAL:HA	2.00	0.42
1:E:179:ASP:HB3	1:E:389:MET:HE1	2.02	0.42
1:K:190:VAL:O	1:K:191:GLU:O	2.38	0.42



Continued from previous page...

Atom-1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$ \text{overlap } (\text{\AA})$
1:L:305:ILE:HG23	1:L:308:GLU:HG3	2.00	0.42
1:H:8:PHE:HE2	1:N:26:ALA:HA	1.80	0.42
1:I:91:THR:O	1:I:94:VAL:HG22	2.19	0.42
1:K:27:VAL:HG12	1:K:90:THR:HG23	2.01	0.42
1:B:27:VAL:HG12	1:B:90:THR:HG23	2.01	0.42
1:B:149:THR:HG23	1:B:159:GLY:HA3	2.00	0.42
1:M:120:ILE:O	1:M:124:VAL:HG23	2.19	0.42
1:E:16:MET:O	1:E:20:VAL:HG13	2.18	0.42
1:L:436:GLN:O	1:L:440:ILE:HG13	2.19	0.42
1:G:418:ALA:O	1:G:422:VAL:HG23	2.19	0.42
1:B:464:VAL:HG22	1:K:464:VAL:HA	2.01	0.42
1:H:418:ALA:O	1:H:422:VAL:HG23	2.19	0.42
1:J:61:GLU:O	1:K:3:ALA:HA	2.19	0.42
1:C:501:ARG:HG3	1:C:502:SER:N	2.34	0.42
1:D:436:GLN:O	1:D:440:ILE:HG13	2.19	0.42
1:D:37:ASN:H	1:E:516:THR:CG2	2.28	0.42
1:A:46:ALA:HA	1:A:47:PRO:HD3	1.89	0.42
1:I:85:ALA:C	1:I:405:ALA:CB	2.50	0.42
1:J:408:GLU:N	1:J:498:LYS:HE2	2.33	0.42
1:E:27:VAL:HG12	1:E:90:THR:HG23	2.01	0.42
1:N:27:VAL:HG12	1:N:90:THR:HG23	2.01	0.42
1:B:350:ARG:O	1:B:353:ILE:HG12	2.19	0.42
1:C:47:PRO:HG2	1:D:73:MET:HE2	2.00	0.42
1:H:386:GLU:HB2	1:I:284:ARG:CD	2.40	0.42
1:M:386:GLU:HA	1:N:281:PHE:N	2.34	0.42
1:A:49:ILE:HG12	1:B:513:LEU:HD13	1.99	0.42
1:F:35:GLY:O	1:G:114:MET:HE1	2.12	0.42
1:M:190:VAL:O	1:M:191:GLU:O	2.38	0.42
1:K:443:ALA:O	1:K:447:MET:HG3	2.19	0.42
1:F:524:LEU:HA	1:F:525:PRO:HD3	1.94	0.42
1:M:436:GLN:O	1:M:440:ILE:HG13	2.19	0.42
1:G:464:VAL:HG22	1:M:464:VAL:HA	2.00	0.42
1:A:464:VAL:HG22	1:L:464:VAL:HA	2.00	0.42
1:N:197:ARG:HD2	1:N:277:LYS:HG3	2.02	0.42
1:H:197:ARG:HD2	1:H:277:LYS:HG3	2.02	0.42
1:C:179:ASP:HB3	1:C:389:MET:HE1	2.02	0.42
1:C:305:ILE:HG23	1:C:308:GLU:HG3	2.00	0.42
1:J:26:ALA:HA	1:K:8:PHE:CZ	2.54	0.42
1:G:91:THR:O	1:G:94:VAL:HG22	2.19	0.42
1:N:436:GLN:O	1:N:440:ILE:HG13	2.19	0.42
1:C:350:ARG:O	1:C:353:ILE:HG12	2.19	0.42



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:J:350:ARG:O	1:J:353:ILE:HG12	2.19	0.42
1:K:85:ALA:C	1:K:405:ALA:CB	2.50	0.42
1:A:180:GLY:N	1:A:389:MET:HE1	2.35	0.42
1:A:305:ILE:HG23	1:A:308:GLU:HG3	2.00	0.42
1:F:305:ILE:HG23	1:F:308:GLU:HG3	2.00	0.42
1:H:305:ILE:HG23	1:H:308:GLU:HG3	2.00	0.42
1:K:26:ALA:HA	1:L:8:PHE:CZ	2.54	0.42
1:H:149:THR:HG22	1:H:156:GLU:HA	2.01	0.42
1:I:149:THR:HG22	1:I:156:GLU:HA	2.00	0.42
1:C:91:THR:O	1:C:94:VAL:HG22	2.19	0.42
1:J:91:THR:O	1:J:94:VAL:HG22	2.19	0.42
1:F:158:VAL:HG21	1:F:395:ARG:HD2	2.01	0.42
1:A:418:ALA:O	1:A:422:VAL:HG23	2.19	0.42
1:M:350:ARG:O	1:M:353:ILE:HG12	2.19	0.42
1:I:418:ALA:O	1:I:422:VAL:HG23	2.19	0.42
1:H:436:GLN:O	1:H:440:ILE:HG13	2.19	0.42
1:J:524:LEU:HA	1:J:525:PRO:HD3	1.94	0.42
1:A:158:VAL:HG21	1:A:395:ARG:HD2	2.01	0.42
1:B:47:PRO:HG2	1:C:73:MET:HE2	2.00	0.42
1:L:387:VAL:HA	1:M:281:PHE:CD1	2.50	0.42
1:D:179:ASP:HB3	1:D:389:MET:HE1	2.02	0.42
1:J:190:VAL:O	1:J:191:GLU:O	2.38	0.42
1:N:190:VAL:O	1:N:191:GLU:O	2.38	0.42
1:N:168:LYS:CD	1:N:189:VAL:HG23	2.46	0.42
1:B:305:ILE:HG23	1:B:308:GLU:HG3	2.00	0.42
1:K:305:ILE:HG23	1:K:308:GLU:HG3	2.00	0.42
1:N:149:THR:HG22	1:N:156:GLU:HA	2.01	0.42
1:H:430:ARG:HA	1:H:430:ARG:HD3	1.85	0.42
1:I:197:ARG:HD2	1:I:277:LYS:HG3	2.02	0.42
1:M:443:ALA:O	1:M:447:MET:HG3	2.19	0.42
1:G:350:ARG:O	1:G:353:ILE:HG12	2.19	0.42
1:E:120:ILE:O	1:E:124:VAL:HG23	2.19	0.42
1:D:418:ALA:O	1:D:422:VAL:HG23	2.19	0.42
1:C:443:ALA:O	1:C:447:MET:HG3	2.20	0.42
1:E:501:ARG:HG3	1:E:502:SER:N	2.34	0.42
1:L:386:GLU:HA	1:M:281:PHE:N	2.34	0.42
1:M:39:VAL:HB	1:N:69:MET:HE1	2.02	0.42
1:K:408:GLU:N	1:K:498:LYS:HE2	2.33	0.42
1:L:182:GLY:N	1:M:283:ASP:HB2	2.25	0.42
1:H:27:VAL:HG12	1:H:90:THR:HG23	2.01	0.42
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.01	0.42



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:E:149:THR:HG23	1:E:159:GLY:HA3	2.00	0.42
1:I:77:VAL:HG12	1:I:92:ALA:HB1	2.02	0.42
1:N:418:ALA:O	1:N:422:VAL:HG23	2.19	0.42
1:B:443:ALA:O	1:B:447:MET:HG3	2.19	0.42
1:I:436:GLN:O	1:I:440:ILE:HG13	2.19	0.42
1:E:418:ALA:O	1:E:422:VAL:HG23	2.19	0.42
1:G:77:VAL:HG12	1:G:92:ALA:HB1	2.02	0.42
1:C:46:ALA:HA	1:C:47:PRO:HD3	1.89	0.42
1:J:405:ALA:O	1:J:498:LYS:HE3	2.16	0.42
1:B:270:ILE:HD11	1:C:231:ARG:HG3	2.01	0.42
1:I:174:VAL:HG11	1:I:331:THR:HG1	1.74	0.42
1:M:305:ILE:HG23	1:M:308:GLU:HG3	2.00	0.42
1:I:26:ALA:HA	1:J:8:PHE:CZ	2.54	0.42
1:G:27:VAL:HG12	1:G:90:THR:HG23	2.01	0.42
1:M:430:ARG:HD3	1:M:430:ARG:HA	1.85	0.42
1:K:430:ARG:HD3	1:K:430:ARG:HA	1.85	0.42
1:J:197:ARG:HD2	1:J:277:LYS:HG3	2.02	0.42
1:G:501:ARG:HG3	1:G:502:SER:N	2.34	0.42
1:C:436:GLN:O	1:C:440:ILE:HG13	2.19	0.42
1:F:77:VAL:HG12	1:F:92:ALA:HB1	2.01	0.42
1:E:150:ILE:CG1	1:E:494:LEU:HD12	2.39	0.41
1:C:49:ILE:HG12	1:D:513:LEU:HD13	1.99	0.41
1:D:443:ALA:O	1:D:447:MET:HG3	2.19	0.41
1:A:128:VAL:O	1:A:132:LYS:HG2	2.20	0.41
1:L:501:ARG:HG3	1:L:502:SER:N	2.34	0.41
1:K:197:ARG:HD2	1:K:277:LYS:HG3	2.02	0.41
1:F:443:ALA:O	1:F:447:MET:HG3	2.19	0.41
1:H:77:VAL:HG12	1:H:92:ALA:HB1	2.02	0.41
1:A:524:LEU:HA	1:A:525:PRO:HD3	1.94	0.41
1:A:443:ALA:O	1:A:447:MET:HG3	2.20	0.41
1:M:197:ARG:HD2	1:M:277:LYS:HG3	2.02	0.41
1:G:150:ILE:CD1	1:G:411:VAL:HG21	2.50	0.41
1:L:168:LYS:CD	1:L:189:VAL:HG23	2.46	0.41
1:L:91:THR:O	1:L:94:VAL:HG22	2.19	0.41
1:I:430:ARG:HD3	1:I:430:ARG:HA	1.84	0.41
1:M:128:VAL:O	1:M:132:LYS:HG2	2.20	0.41
1:J:40:LEU:HD23	1:K:521:VAL:HB	2.02	0.41
1:K:40:LEU:HD23	1:L:521:VAL:HB	2.02	0.41
1:M:418:ALA:O	1:M:422:VAL:HG23	2.19	0.41
1:I:40:LEU:HD23	1:J:521:VAL:HB	2.02	0.41
1:F:501:ARG:HG3	1:F:502:SER:N	2.34	0.41



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:G:443:ALA:O	1:G:447:MET:HG3	2.19	0.41
1:K:436:GLN:O	1:K:440:ILE:HG13	2.19	0.41
1:H:521:VAL:HB	1:N:40:LEU:HD23	2.02	0.41
1:K:128:VAL:O	1:K:132:LYS:HG2	2.20	0.41
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.56	0.41
1:H:40:LEU:HD23	1:I:521:VAL:HB	2.02	0.41
1:D:524:LEU:HA	1:D:525:PRO:HD3	1.94	0.41
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.56	0.41
1:J:436:GLN:O	1:J:440:ILE:HG13	2.19	0.41
1:B:150:ILE:CD1	1:B:411:VAL:HG21	2.51	0.41
1:B:245:LYS:CE	1:C:232:GLU:HG3	2.46	0.41
1:D:245:LYS:CE	1:E:232:GLU:HG3	2.46	0.41
1:I:219:PHE:O	1:I:247:LEU:HD12	2.20	0.41
1:I:27:VAL:HG12	1:I:90:THR:HG23	2.01	0.41
1:L:197:ARG:HD2	1:L:277:LYS:HG3	2.02	0.41
1:F:418:ALA:O	1:F:422:VAL:HG23	2.19	0.41
1:I:501:ARG:HG3	1:I:502:SER:N	2.34	0.41
1:G:197:ARG:HD2	1:G:277:LYS:HG3	2.02	0.41
1:J:418:ALA:O	1:J:422:VAL:HG23	2.19	0.41
1:A:197:ARG:HD2	1:A:277:LYS:HG3	2.02	0.41
1:H:281:PHE:CD1	1:N:387:VAL:HA	2.50	0.41
1:I:65:LYS:O	1:I:69:MET:HG3	2.21	0.41
1:B:26:ALA:CB	1:C:8:PHE:CE2	2.77	0.41
1:I:190:VAL:O	1:I:191:GLU:O	2.38	0.41
1:M:272:LYS:HB3	1:M:273:VAL:H	1.51	0.41
1:J:27:VAL:HG12	1:J:90:THR:HG23	2.01	0.41
1:C:472:GLY:HA3	1:C:476:TYR:CD2	2.56	0.41
1:K:472:GLY:HA3	1:K:476:TYR:CD2	2.56	0.41
1:F:472:GLY:HA3	1:F:476:TYR:CD2	2.56	0.41
1:J:77:VAL:HG12	1:J:92:ALA:HB1	2.02	0.41
1:G:472:GLY:HA3	1:G:476:TYR:CD2	2.55	0.41
1:G:158:VAL:HG21	1:G:395:ARG:HD2	2.01	0.41
1:L:418:ALA:O	1:L:422:VAL:HG23	2.19	0.41
1:E:65:LYS:O	1:E:69:MET:HG3	2.21	0.41
1:B:150:ILE:CD1	1:B:494:LEU:CD1	2.94	0.41
1:N:65:LYS:O	1:N:69:MET:HG3	2.21	0.41
1:L:65:LYS:O	1:L:69:MET:HG3	2.21	0.41
1:M:405:ALA:O	1:M:498:LYS:HE3	2.16	0.41
1:H:190:VAL:O	1:H:191:GLU:O	2.38	0.41
1:H:283:ASP:HB2	1:N:182:GLY:N	2.25	0.41
1:H:219:PHE:O	1:H:247:LEU:HD12	2.21	0.41



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A 1 4	ous page	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	$overlap(\AA)$
1:G:430:ARG:HD3	1:G:430:ARG:HA	1.84	0.41
1:G:128:VAL:O	1:G:132:LYS:HG2	2.20	0.41
1:N:128:VAL:O	1:N:132:LYS:HG2	2.20	0.41
1:C:77:VAL:HG12	1:C:92:ALA:HB1	2.02	0.41
1:K:46:ALA:HA	1:K:47:PRO:HD3	1.89	0.41
1:L:40:LEU:HD23	1:M:521:VAL:HB	2.02	0.41
1:M:40:LEU:HD23	1:N:521:VAL:HB	2.02	0.41
1:F:197:ARG:HD2	1:F:277:LYS:HG3	2.02	0.41
1:B:222:LEU:HD23	1:B:250:ILE:HB	2.03	0.41
1:J:128:VAL:O	1:J:132:LYS:HG2	2.20	0.41
1:C:418:ALA:O	1:C:422:VAL:HG23	2.19	0.41
1:M:461:GLU:HA	1:M:462:PRO:HD2	1.90	0.41
1:D:77:VAL:HG12	1:D:92:ALA:HB1	2.02	0.41
1:N:461:GLU:HA	1:N:462:PRO:HD2	1.90	0.41
1:K:501:ARG:HG3	1:K:502:SER:N	2.34	0.41
1:B:150:ILE:CG1	1:B:494:LEU:CD1	2.97	0.41
1:C:219:PHE:O	1:C:247:LEU:HD12	2.20	0.41
1:F:27:VAL:HG12	1:F:90:THR:HG23	2.01	0.41
1:B:128:VAL:O	1:B:132:LYS:HG2	2.20	0.41
1:D:128:VAL:O	1:D:132:LYS:HG2	2.20	0.41
1:L:472:GLY:HA3	1:L:476:TYR:CD2	2.56	0.41
1:K:222:LEU:HD23	1:K:250:ILE:HB	2.03	0.41
1:K:418:ALA:O	1:K:422:VAL:HG23	2.19	0.41
1:C:65:LYS:O	1:C:69:MET:HG3	2.21	0.41
1:A:513:LEU:HD13	1:G:49:ILE:HG12	1.99	0.41
1:A:232:GLU:HG3	1:G:245:LYS:CE	2.46	0.41
1:N:85:ALA:C	1:N:405:ALA:CB	2.50	0.41
1:L:321:LYS:CB	1:L:334:ASP:HB3	2.51	0.41
1:K:321:LYS:CB	1:K:334:ASP:HB3	2.51	0.41
1:B:219:PHE:O	1:B:247:LEU:HD12	2.21	0.41
1:G:219:PHE:O	1:G:247:LEU:HD12	2.20	0.41
1:J:219:PHE:O	1:J:247:LEU:HD12	2.21	0.41
1:C:461:GLU:HA	1:C:462:PRO:HD2	1.90	0.41
1:E:443:ALA:O	1:E:447:MET:HG3	2.19	0.41
1:A:77:VAL:HG12	1:A:92:ALA:HB1	2.02	0.41
1:E:472:GLY:HA3	1:E:476:TYR:CD2	2.56	0.41
1:E:46:ALA:HA	1:E:47:PRO:HD3	1.89	0.41
1:D:150:ILE:CD1	1:D:411:VAL:HG21	2.51	0.41
1:J:321:LYS:CB	1:J:334:ASP:HB3	2.51	0.41
1:D:219:PHE:O	1:D:247:LEU:HD12	2.20	0.41
1:G:23:LEU:O	1:G:27:VAL:HG23	2.21	0.41



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap(\AA)$
1:C:321:LYS:CB	1:C:334:ASP:HB3	2.51	0.41
1:A:430:ARG:HD3	1:A:430:ARG:HA	1.84	0.41
1:N:222:LEU:HD23	1:N:250:ILE:HB	2.03	0.41
1:H:128:VAL:O	1:H:132:LYS:HG2	2.20	0.41
1:D:472:GLY:HA3	1:D:476:TYR:CD2	2.55	0.41
1:M:524:LEU:HA	1:M:525:PRO:HD3	1.94	0.41
1:B:501:ARG:HG3	1:B:502:SER:N	2.34	0.41
1:J:501:ARG:HG3	1:J:502:SER:N	2.34	0.41
1:L:77:VAL:HG12	1:L:92:ALA:HB1	2.02	0.41
1:C:150:ILE:CD1	1:C:494:LEU:CD1	2.94	0.41
1:A:65:LYS:O	1:A:69:MET:HG3	2.21	0.41
1:D:150:ILE:CG1	1:D:494:LEU:CD1	2.97	0.41
1:I:387:VAL:HA	1:J:281:PHE:CD1	2.50	0.41
1:I:245:LYS:CE	1:J:232:GLU:CG	2.91	0.41
1:K:65:LYS:O	1:K:69:MET:HG3	2.21	0.41
1:F:179:ASP:HB3	1:F:389:MET:HE1	2.03	0.41
1:B:180:GLY:N	1:B:389:MET:HE1	2.36	0.41
1:E:26:ALA:CB	1:F:8:PHE:CE2	2.77	0.41
1:I:321:LYS:CB	1:I:334:ASP:HB3	2.51	0.41
1:K:168:LYS:CD	1:K:189:VAL:HG23	2.46	0.41
1:A:219:PHE:O	1:A:247:LEU:HD12	2.20	0.41
1:L:273:VAL:HG12	1:L:274:ALA:N	2.36	0.41
1:A:23:LEU:O	1:A:27:VAL:HG23	2.21	0.41
1:G:321:LYS:CB	1:G:334:ASP:HB3	2.51	0.41
1:D:321:LYS:CB	1:D:334:ASP:HB3	2.51	0.41
1:E:321:LYS:CB	1:E:334:ASP:HB3	2.51	0.41
1:F:321:LYS:CB	1:F:334:ASP:HB3	2.51	0.41
1:A:222:LEU:HD23	1:A:250:ILE:HB	2.03	0.41
1:B:77:VAL:HG12	1:B:92:ALA:HB1	2.01	0.41
1:J:472:GLY:HA3	1:J:476:TYR:CD2	2.56	0.41
1:E:197:ARG:HD2	1:E:277:LYS:HG3	2.02	0.41
1:I:472:GLY:HA3	1:I:476:TYR:CD2	2.56	0.41
1:F:400:LEU:O	1:F:404:ARG:HG3	2.21	0.41
1:N:77:VAL:HG12	1:N:92:ALA:HB1	2.02	0.41
1:L:222:LEU:HD23	1:L:250:ILE:HB	2.03	0.41
1:L:443:ALA:O	1:L:447:MET:HG3	2.19	0.41
1:N:524:LEU:HA	1:N:525:PRO:HD3	1.94	0.41
1:J:222:LEU:HD23	1:J:250:ILE:HB	2.03	0.41
1:E:222:LEU:HD23	1:E:250:ILE:HB	2.03	0.41
1:A:150:ILE:CD1	1:A:411:VAL:HG21	2.51	0.41
1:G:65:LYS:O	1:G:69:MET:HG3	2.21	0.41



Continued from previous page...

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap (\AA)$
1:L:245:LYS:HE2	1:M:232:GLU:CD	2.42	0.41
1:E:219:PHE:O	1:E:247:LEU:HD12	2.20	0.41
1:M:273:VAL:HG12	1:M:274:ALA:N	2.36	0.41
1:M:23:LEU:O	1:M:27:VAL:HG23	2.21	0.41
1:D:23:LEU:O	1:D:27:VAL:HG23	2.21	0.41
1:B:321:LYS:CB	1:B:334:ASP:HB3	2.51	0.41
1:D:149:THR:CG2	1:D:159:GLY:HA3	2.52	0.41
1:G:132:LYS:HA	1:G:132:LYS:HD3	1.92	0.41
1:M:77:VAL:HG12	1:M:92:ALA:HB1	2.02	0.41
1:B:400:LEU:O	1:B:404:ARG:HG3	2.21	0.41
1:I:128:VAL:O	1:I:132:LYS:HG2	2.20	0.41
1:E:77:VAL:HG12	1:E:92:ALA:HB1	2.02	0.41
1:E:128:VAL:O	1:E:132:LYS:HG2	2.20	0.41
1:B:197:ARG:HD2	1:B:277:LYS:HG3	2.02	0.41
1:F:128:VAL:O	1:F:132:LYS:HG2	2.20	0.41
1:C:150:ILE:CD1	1:C:411:VAL:CB	2.87	0.40
1:E:150:ILE:CD1	1:E:411:VAL:HG21	2.51	0.40
1:H:65:LYS:O	1:H:69:MET:HG3	2.21	0.40
1:M:321:LYS:CB	1:M:334:ASP:HB3	2.51	0.40
1:F:219:PHE:O	1:F:247:LEU:HD12	2.20	0.40
1:B:273:VAL:HG12	1:B:274:ALA:N	2.36	0.40
1:K:23:LEU:O	1:K:27:VAL:HG23	2.21	0.40
1:E:430:ARG:HA	1:E:430:ARG:HD3	1.84	0.40
1:K:273:VAL:HG12	1:K:274:ALA:N	2.36	0.40
1:C:128:VAL:O	1:C:132:LYS:HG2	2.20	0.40
1:D:82:ASN:O	1:D:86:GLY:HA2	2.22	0.40
1:M:472:GLY:HA3	1:M:476:TYR:CD2	2.56	0.40
1:E:400:LEU:O	1:E:404:ARG:HG3	2.21	0.40
1:K:77:VAL:HG12	1:K:92:ALA:HB1	2.01	0.40
1:N:46:ALA:HA	1:N:47:PRO:HD3	1.89	0.40
1:L:128:VAL:O	1:L:132:LYS:HG2	2.20	0.40
1:G:400:LEU:O	1:G:404:ARG:HG3	2.21	0.40
1:A:82:ASN:O	1:A:86:GLY:HA2	2.22	0.40
1:B:65:LYS:O	1:B:69:MET:HG3	2.21	0.40
1:F:150:ILE:CD1	1:F:494:LEU:CD1	2.94	0.40
1:E:49:ILE:HG12	1:F:513:LEU:HD13	1.99	0.40
1:M:82:ASN:O	1:M:86:GLY:HA2	2.22	0.40
1:N:219:PHE:O	1:N:247:LEU:HD12	2.20	0.40
1:C:273:VAL:HG12	1:C:274:ALA:N	2.36	0.40
1:I:23:LEU:O	1:I:27:VAL:HG23	2.21	0.40
1:G:222:LEU:HD23	1:G:250:ILE:HB	2.03	0.40



Continued from previous page...

Continuea from previ		Interatomic	Clash	
Atom-1	Atom-2	${f distance} \; ({f \AA})$	$overlap( ext{\AA})$	
1:L:461:GLU:HA	1:L:462:PRO:HD2	1.90	0.40	
1:D:222:LEU:HD23	1:D:250:ILE:HB	2.03	0.40	
1:E:82:ASN:O	1:E:86:GLY:HA2	2.21	0.40	
1:M:86:GLY:CA	1:M:405:ALA:HB1	2.52	0.40	
1:N:82:ASN:O	1:N:86:GLY:HA2	2.22	0.40	
1:E:217:SER:N	1:E:218:PRO:HD3	2.37	0.40	
1:F:180:GLY:N	1:F:389:MET:HE1	2.37	0.40	
1:J:183:LEU:HA	1:J:183:LEU:HD23	1.90	0.40	
1:C:160:LYS:HB3	1:C:160:LYS:HZ2	1.85	0.40	
1:L:219:PHE:O	1:L:247:LEU:HD12	2.20	0.40	
1:H:23:LEU:O	1:H:27:VAL:HG23	2.21	0.40	
1:F:23:LEU:O	1:F:27:VAL:HG23	2.21	0.40	
1:L:23:LEU:O	1:L:27:VAL:HG23	2.21	0.40	
1:C:149:THR:CG2	1:C:159:GLY:HA3	2.52	0.40	
1:M:132:LYS:HD3	1:M:132:LYS:HA	1.92	0.40	
1:B:82:ASN:O	1:B:86:GLY:HA2	2.22	0.40	
1:I:222:LEU:HD23	1:I:250:ILE:HB	2.03	0.40	
1:N:472:GLY:HA3	1:N:476:TYR:CD2	2.56	0.40	
1:D:304:GLU:H	1:D:304:GLU:HG2	1.72	0.40	
1:D:65:LYS:O	1:D:69:MET:HG3	2.21	0.40	
1:H:284:ARG:CD	1:N:386:GLU:HB2	2.40	0.40	
1:C:386:GLU:CG	1:D:281:PHE:HE2	2.07	0.40	
1:M:65:LYS:O	1:M:69:MET:HG3	2.21	0.40	
1:F:49:ILE:HG12	1:G:513:LEU:HD13	1.99	0.40	
1:N:86:GLY:CA	1:N:405:ALA:HB1	2.52	0.40	
1:E:245:LYS:CE	1:F:232:GLU:HG3	2.45	0.40	
1:H:321:LYS:CB	1:H:334:ASP:HB3	2.51	0.40	
1:C:23:LEU:O	1:C:27:VAL:HG23	2.21	0.40	
1:A:321:LYS:CB	1:A:334:ASP:HB3	2.51	0.40	
1:A:400:LEU:O	1:A:404:ARG:HG3	2.21	0.40	
1:D:197:ARG:HD2	1:D:277:LYS:HG3	2.02	0.40	
1:C:82:ASN:O	1:C:86:GLY:HA2	2.22	0.40	
1:C:197:ARG:HD2	1:C:277:LYS:HG3	2.02	0.40	
1:D:400:LEU:O	1:D:404:ARG:HG3	2.21	0.40	
1:A:273:VAL:HG12	1:A:274:ALA:N	2.36	0.40	
1:I:524:LEU:HA	1:I:525:PRO:HD3	1.94	0.40	
1:G:82:ASN:O	1:G:86:GLY:HA2	2.21	0.40	
1:H:472:GLY:HA3	1:H:476:TYR:CD2	2.56	0.40	
1:J:516:THR:O	1:J:516:THR:HG22	2.22	0.40	
1:C:150:ILE:CD1	1:C:411:VAL:HG21	2.51	0.40	
1:H:217:SER:N	1:H:218:PRO:HD3	2.37	0.40	



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Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance} & ( ext{Å}) \end{array}$	Clash overlap (Å)
1:L:82:ASN:O	1:L:86:GLY:HA2	2.22	0.40
1:F:270:ILE:HG23	1:G:229:ASN:C	2.30	0.40
1:F:245:LYS:CE	1:G:232:GLU:HG3	2.45	0.40
1:J:273:VAL:HG12	1:J:274:ALA:N	2.36	0.40
1:G:14:VAL:O	1:G:18:ARG:HG3	2.22	0.40
1:B:23:LEU:O	1:B:27:VAL:HG23	2.21	0.40
1:A:149:THR:CG2	1:A:159:GLY:HA3	2.52	0.40
1:L:430:ARG:HD3	1:L:430:ARG:HA	1.85	0.40
1:F:385:THR:C	1:F:387:VAL:H	2.25	0.40
1:H:461:GLU:HA	1:H:462:PRO:HD2	1.90	0.40

There are no symmetry-related clashes.

#### 6.3 Torsion angles (i)

#### 6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	A	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	В	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	С	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	D	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	E	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	F	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	G	507/547~(93%)	473 (93%)	26 (5%)	8 (2%)	12	56
1	Н	507/547~(93%)	469 (92%)	29 (6%)	9 (2%)	11	53
1	I	507/547~(93%)	469 (92%)	29 (6%)	9 (2%)	11	53
1	J	507/547~(93%)	469 (92%)	29 (6%)	9 (2%)	11	53
1	K	507/547~(93%)	469 (92%)	29 (6%)	9 (2%)	11	53
1	L	507/547~(93%)	469 (92%)	29 (6%)	9 (2%)	11	53



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	М	507/547 (93%)	469 (92%)	29 (6%)	9 (2%)	11	53
1	N	507/547 (93%)	469 (92%)	29 (6%)	9 (2%)	11	53
All	All	$7098/7658 \; (93\%)$	6594 (93%)	385 (5%)	119 (2%)	16	55

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	270	ILE
1	A	340	ALA
1	В	185	ASP
1	В	270	ILE ALA ASP ILE ALA
1	B C C	340	ALA
1	С	185	ASP
1	С	270	ILE
1	С	340	ALA
1	D	185	ASP ILE
1	D	270	ILE
1	D	340	ALA ASP
1	Е	185	ASP
1	Е	270	ILE ALA
1	Е	340	ALA
1	F	185	ASP
1	F	270	ILE
1	F	340	ALA ASP
1	G	185	ASP
1	G	270	ILE
1	G	340	ALA
1	Н	270	ILE
1	Н	340	ALA
1	Н	386	GLU
1	I	270	ILE
1	I	340	ALA
1	I	386	GLU
1	J	270	ILE
1	J	340	ALA
1	J	386	GLU
1	K	270	ILE
1	K	340	ALA
1	K	386	GLU
1	L	270	ILE



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Mol	Chain	Res	Type		
1	L	340	ALA		
1	L	386	GLU		
1	M	270	ILE		
1	M	340	ALA		
1	M	386	GLU		
1	N	270	ILE		
1	N	340	ALA		
1	N	386	GLU		
1	A	334	ASP		
1	B C	334	ASP		
1	С	334	ASP		
1	D	334	ASP		
1	Е	334	ASP		
1	F	334	ASP		
1	G	334	ASP		
1	Н	334	ASP		
1	Н	385	THR		
1	I	334	ASP		
1	I	385	THR		
1	J	334	ASP		
1	J	385	THR		
1	K	334	ASP		
1	K	385	THR		
1	L	334	ASP		
1	L	385	THR		
1	M	334	ASP		
1	M	385	THR		
1	N	334	ASP		
1	N	385	THR		
1	A	243	ALA		
1	A	337	GLY		
1	В	243	ALA GLY ALA GLY		
1	B C	337	GLY		
1	С	243	ALA		
1	С	337	GLY		
1	D	243	ALA GLY		
1	D	337	GLY		
1	Е	243	ALA		
1	Е	337	GLY		
1	F	243	ALA		
1	F	337	GLY		
1	G	243	ALA		



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Conti	Continued from previous page					
Mol	Chain	Res	Type			
1	G	337	GLY			
1	Н	243	ALA			
1	Н	337	GLY			
1	I	243	ALA			
1	I	337	GLY			
1	J	243	ALA			
1	J	337	GLY			
1	K	243	ALA			
1	K	337	GLY			
1	L	243	ALA			
1	L	337	GLY			
1	M	243	ALA			
1	M	337	GLY			
1	N	243	ALA			
1	N	337	GLY			
1	A	202	PRO			
1	В	202	PRO			
1	С	202	PRO			
1	D	202	PRO			
1	Е	202	PRO			
1	F	202	PRO			
1	G	202	PRO			
1	Н	202	PRO			
1	I	202	PRO			
1	J	202	PRO			
1	K	202	PRO			
1	L	202	PRO			
1	M	202	PRO			
1	N	202	PRO			
1	A	230	ILE			
1	В	230	ILE			
1	С	230	ILE			
1	F	230	ILE			
1	G	230	ILE			
1	D	230	ILE			
1	E	230	ILE			
1	Н	230	ILE			
1	I	230	ILE			
1	J	230	ILE			
1	K	230	ILE			
1	L	230	ILE			
1	M	230	ILE			



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Mol	Chain	Res	Type
1	N	230	ILE

#### 6.3.2 Protein sidechains (i)

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In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	401/414 (97%)	384 (96%)	17 (4%)	36 70
1	В	401/414~(97%)	384 (96%)	17 (4%)	36 70
1	С	401/414 (97%)	384 (96%)	17 (4%)	36 70
1	D	401/414 (97%)	384 (96%)	17 (4%)	36 70
1	E	401/414 (97%)	384 (96%)	17 (4%)	36 70
1	F	401/414 (97%)	384 (96%)	17 (4%)	36 70
1	G	401/414 (97%)	384 (96%)	17 (4%)	36 70
1	Н	401/414 (97%)	385 (96%)	16 (4%)	38 71
1	I	401/414 (97%)	385 (96%)	16 (4%)	38 71
1	J	401/414 (97%)	385 (96%)	16 (4%)	38 71
1	K	401/414 (97%)	385 (96%)	16 (4%)	38 71
1	L	401/414 (97%)	385 (96%)	16 (4%)	38 71
1	М	401/414 (97%)	385 (96%)	16 (4%)	38 71
1	N	401/414 (97%)	385 (96%)	16 (4%)	38 71
All	All	5614/5796 (97%)	5383 (96%)	231 (4%)	42 71

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	MET
1	A	138	CYS
1	A	178	GLU
1	A	189	VAL
1	A	231	ARG
1	A	264	VAL



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Conti	Continued from previous page					
Mol	Chain	Res	Type			
1	A	265	ASN			
1	A	270	ILE			
1	A	271	VAL			
1	A	283	ASP			
1	A	290	GLN			
1	A	307	MET			
1	A	313	THR			
1	A	329	THR			
1	A	360	TYR			
1	A	389	MET			
1	A	483	GLU			
1	В	111	MET			
1	В	138	CYS			
1	В	178	GLU			
1	В	189	VAL			
1	В	231	ARG			
1	В	264	VAL			
1	В	265	ASN			
1	В	270	ILE			
1	В	271	VAL			
1	В	283	ASP			
1	В	290	GLN			
1	В	307	MET			
1	В	313	THR			
1	В	329	THR			
1	В	360	TYR			
1	В	389	MET			
1	В	483	GLU			
1	С	111	MET			
1	C C C C C C C C	138	CYS			
1	С	178	GLU			
1	С	189	VAL			
1	С	231	ARG VAL			
1	С	264	VAL			
1	С	265	ASN			
1	С	270	ILE VAL ASP			
1	С	271	VAL			
1	С	283	ASP			
1	С	290	GLN			
1	C	307	MET THR			
1	C	313	THR			
1	C	329	THR			



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Mol	Chain	Res	Type		
1	С	360	TYR		
1	С	389	MET		
1	C C D	483	GLU		
1		111	MET		
1	D	138	CYS		
1	D	178	GLU		
1	D	189	VAL		
1	D	231	ARG		
1	D	264	VAL		
1	D	265	ASN		
1	D	270	ILE		
1	D	271	VAL		
1	D	283	ASP		
1	D	290	GLN		
1	D	307	MET		
1	D	313	THR		
1	D	329	THR		
1	D	360	TYR		
1	D	389	MET		
1	D	483	GLU		
1	Е	111	MET		
1	Е	138	CYS		
1	Е	178	GLU		
1	Е	189	VAL		
1	Е	231	ARG		
1	Е	264	VAL		
1	Е	265	ASN		
1	Е	270	ILE		
1	Е	271	VAL		
1	Е	283	ASP		
1	Е	290	GLN		
1	Е	307	MET		
1	Е	313	THR		
1	Е	329	THR		
1	Е	360	THR TYR		
1	Е	389	MET		
1	Е	483	GLU		
1	F	111	MET		
1	F	138	CYS		
1	F	178	GLU		
1	F	189	VAL		
1	F	231	ARG		



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Mol	Chain	Res	Type	
1	F	264	VAL	
1	F	265	ASN	
1	F	270	ILE	
1	F	271	VAL	
1	F	283	ASP	
1	F	290	GLN	
1	F	307	MET	
1	F	313	THR	
1	F	329	THR	
1	F	360	TYR	
1	F	389	MET	
1	F	483	GLU	
1	G	111	MET	
1	G	138	CYS	
1	G	178	GLU	
1	G	189	VAL	
1	G	231	ARG	
1	G	264	VAL	
1	G	265	ASN	
1	G	270	ILE	
1	G	271	VAL	
1	G	283	ASP	
1	G	290	GLN	
1	G	307	MET	
1	G	313	THR	
1	G	329	THR	
1	G	360	TYR	
1	G	389	MET	
1	G	483	GLU	
1	Н	111	MET	
1	Н	156	GLU	
1	Н	186	GLU	
1	Н	231	ARG	
1	Н	264	VAL	
1	Н	265	ASN	
1	Н	270	ILE	
1	Н	271	VAL	
1	Н	283	ASP	
1	Н	290	GLN	
1	Н	307	MET	
1	Н	313	THR	
1	Н	329	THR	



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Mol	Chain	Res	Type	
1	Н	360	TYR	
1	Н	398	ASP	
1	Н	483	GLU	
1	I	111	MET	
1	I	156	GLU	
1	I	186	GLU	
1	I	231	ARG	
1	I	264	VAL	
1	I	265	ASN	
1	I	270	ILE	
1	I	271	VAL	
1	I	283	ASP	
1	I	290	GLN	
1	I	307	MET	
1	I	313	THR	
1	I	329	THR	
1	I	360	TYR	
1	I	398	ASP	
1	I	483	GLU	
1	J	111	MET	
1	J	156	GLU	
1	J	186	GLU	
1	J	231	ARG	
1	J	264	VAL	
1	J	265	ASN	
1	J	270	ILE	
1	J	271	VAL	
1	J	283	ASP	
1	J	290	GLN	
1	J	307	MET	
1	J	313	THR	
1	J	329	THR	
1	J	360	TYR	
1	J	398	ASP	
1	J	483	GLU	
1	K	111	MET	
1	K	156	GLU	
1	K	186	GLU	
1	K	231	ARG	
1	K	264	VAL	
1	K	265	ASN	
1	K	270	ILE	



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Mol	Chain	Res	Type		
1	K	271	VAL		
1	K	283	ASP		
1	K	290	GLN		
1	K	307	MET		
1	K	313	THR		
1	K	329	THR		
1	K	360	TYR		
1	K	398	ASP		
1	K	483	GLU		
1	L	111	MET		
1	L	156	GLU		
1	L	186	GLU		
1	L	231	ARG		
1	L	264	VAL		
1	L	265	ASN		
1	L	270	ILE		
1	L	271	VAL		
1	L	283	ASP		
1	L	290	GLN		
1	L	307	MET		
1	L	313	THR		
1	L	329	THR		
1	L	360	TYR		
1	L	398	ASP		
1	L	483	GLU		
1	M	111	MET		
1	M	156	GLU		
1	M	186	GLU		
1	M	231	ARG		
1	M	264	VAL		
1	M	265	ASN		
1	M	270	ILE		
1	M	271	VAL		
1	M	283	ASP		
1	М	290	GLN		
1	М	307	MET		
1	M	313	THR		
1	M	329	THR		
1	M	360	TYR		
1	M	398	ASP		
1	M	483	GLU		
1	N	111	MET		

 $oxed{ \begin{bmatrix} N & | \ 111 \ \end{bmatrix} & \text{MET} \\ Continued on next page... }$ 



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Mol	Chain	Res	Type
1	N	156	GLU
1	N	186	GLU
1	N	231	ARG
1	N	264	VAL
1	N	265	ASN
1	N	270	ILE
1	N	271	VAL
1	N	283	ASP
1	N	290	GLN
1	N	307	MET
1	N	313	THR
1	N	329	THR
1	N	360	TYR
1	N	398	ASP
1	N	483	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	290	GLN
1	A	366	GLN
1	A	401	HIS
1	A	437	ASN
1	A	453	GLN
1	В	265	ASN
1	В	290	GLN
1	В	366	GLN
1	В	437	ASN
1	В	475	ASN
1	С	265	ASN
1	С	290	GLN
1	C C C	366	GLN
1	С	437	ASN
1	С	453	GLN
1	D	265	ASN
1	D	290	GLN
1	D	366	GLN
1	D	437	ASN
1	D	453	GLN
1	E	265	ASN
1	Е	290	GLN

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Mol	Chain	Res	Type	
1	Ε	366	GLN	
1	Ε	437	ASN	
1	E	453	GLN	
1	E	475	ASN	
1	F	265	ASN	
1	F	290	GLN	
1	F	366	GLN	
1	F	437	ASN	
1	F	453	GLN	
1	F	475	ASN	
1	G	265	ASN	
1	G	290	GLN	
1	G	366	GLN	
1	G	437	ASN	
1	G	453	GLN	
1	G	475	ASN	
1	Н	146	GLN	
1	Н	265	ASN	
1	Н	290	GLN	
1	Н	366	GLN	
1	Н	437	ASN	
1	Н	453	GLN	
1	Н	467	ASN	
1	Н	475	ASN	
1	I	146	GLN	
1	I	265	ASN	
1	I	290	GLN	
1	I	366	GLN	
1	I	437	ASN	
1	I	453	GLN	
1	I	467	ASN	
1	I	475	ASN	
1	J	146	GLN $ $	
1	J	265	ASN	
1	J	290	GLN	
1	J	366	GLN	
1	J	437	ASN	
1	J	453	GLN	
1	J	467	ASN	
1	J	475	ASN	
1	K	146	GLN	
1	K	265	ASN	



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Mol	Chain	Res	$egin{array}{c}  ext{Type} \end{array}$
1	K	290	GLN
1	K	366	GLN
1	K	437	ASN
1	K	453	GLN
1	K	467	ASN
1	K	475	ASN
1	L	146	GLN
1	L	265	ASN
1	L	290	GLN
1	L	366	GLN
1	L	437	ASN
1	L	453	GLN
1	L	467	ASN
1	M	146	GLN
1	M	265	ASN
1	M	290	GLN
1	M	366	GLN
1	M	437	ASN
1	M	453	GLN
1	M	467	ASN
1	М	475	ASN
1	N	146	GLN
1	N	265	ASN
1	N	290	GLN
1	N	366	GLN
1	N	437	ASN
1	N	453	GLN
1	N	467	ASN
1	N	475	ASN

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains (i)

Mogul was not executed - this section is therefore empty.

### 6.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.



# 6.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

## 6.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

### 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

