Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2019 – 02:16 PM EDT

PDB ID	:	6OWW
Title	:	Crystal structure of a Human Cardiac Calsequestrin Filament Complexed with Ytterbium
Deposited on	:	2019-05-12
Resolution	:	3.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

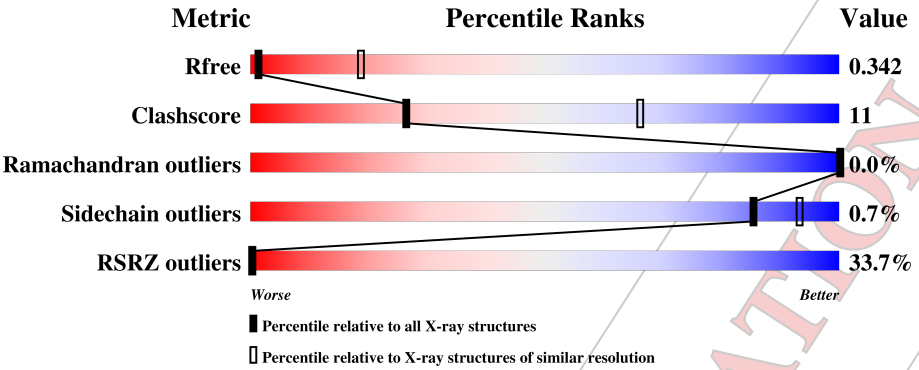
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.3.2
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.3.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1018 (4.08-3.60)
Clashscore	122126	1087 (4.08-3.60)
Ramachandran outliers	120053	1050 (4.08-3.60)
Sidechain outliers	120020	1044 (4.08-3.60)
RSRZ outliers	108989	1002 (4.10-3.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	25% 64% 20% • 15%
1	B	387	33% 61% 24% 15%
1	C	387	23% 67% 18% 15%
1	D	387	30% 62% 23% 15%
1	E	387	35% 60% 25% 15%

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Mol	Chain	Length	Quality of chain
1	F	387	23% 61% 24% 15%
1	G	387	36% 63% 22% 15%
1	H	387	24% 65% 20% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	YB	G	407	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21752 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Calsequestrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2708	1768	416	518	6			
1	B	329	Total	C	N	O	S	0	0	0
			2708	1768	416	518	6			
1	C	329	Total	C	N	O	S	0	0	0
			2708	1768	416	518	6			
1	D	329	Total	C	N	O	S	0	0	0
			2712	1770	416	520	6			
1	E	329	Total	C	N	O	S	0	0	0
			2708	1768	416	518	6			
1	F	329	Total	C	N	O	S	0	0	0
			2708	1768	416	518	6			
1	G	329	Total	C	N	O	S	0	0	0
			2705	1767	416	516	6			
1	H	329	Total	C	N	O	S	0	0	0
			2708	1768	416	518	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O14958
A	14	HIS	-	expression tag	UNP O14958
A	15	MET	-	expression tag	UNP O14958
A	16	ALA	-	expression tag	UNP O14958
A	17	SER	-	expression tag	UNP O14958
B	13	GLY	-	expression tag	UNP O14958
B	14	HIS	-	expression tag	UNP O14958
B	15	MET	-	expression tag	UNP O14958
B	16	ALA	-	expression tag	UNP O14958
B	17	SER	-	expression tag	UNP O14958
C	13	GLY	-	expression tag	UNP O14958
C	14	HIS	-	expression tag	UNP O14958
C	15	MET	-	expression tag	UNP O14958

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	ALA	-	expression tag	UNP O14958
C	17	SER	-	expression tag	UNP O14958
D	13	GLY	-	expression tag	UNP O14958
D	14	HIS	-	expression tag	UNP O14958
D	15	MET	-	expression tag	UNP O14958
D	16	ALA	-	expression tag	UNP O14958
D	17	SER	-	expression tag	UNP O14958
E	13	GLY	-	expression tag	UNP O14958
E	14	HIS	-	expression tag	UNP O14958
E	15	MET	-	expression tag	UNP O14958
E	16	ALA	-	expression tag	UNP O14958
E	17	SER	-	expression tag	UNP O14958
F	13	GLY	-	expression tag	UNP O14958
F	14	HIS	-	expression tag	UNP O14958
F	15	MET	-	expression tag	UNP O14958
F	16	ALA	-	expression tag	UNP O14958
F	17	SER	-	expression tag	UNP O14958
G	13	GLY	-	expression tag	UNP O14958
G	14	HIS	-	expression tag	UNP O14958
G	15	MET	-	expression tag	UNP O14958
G	16	ALA	-	expression tag	UNP O14958
G	17	SER	-	expression tag	UNP O14958
H	13	GLY	-	expression tag	UNP O14958
H	14	HIS	-	expression tag	UNP O14958
H	15	MET	-	expression tag	UNP O14958
H	16	ALA	-	expression tag	UNP O14958
H	17	SER	-	expression tag	UNP O14958

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	9	Total Yb 9 9	0	0
2	D	11	Total Yb 11 11	0	0
2	E	10	Total Yb 10 10	0	0
2	H	5	Total Yb 5 5	0	0
2	B	7	Total Yb 7 7	0	0

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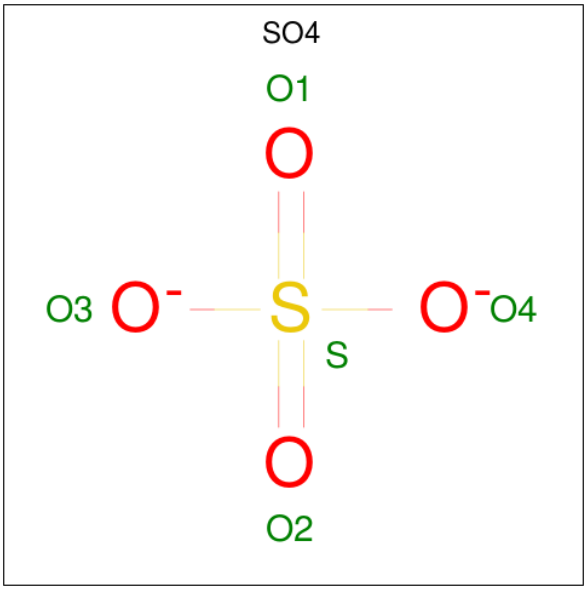
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	6	Total Yb 6 6	0	0
2	A	7	Total Yb 7 7	0	0
2	F	7	Total Yb 7 7	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



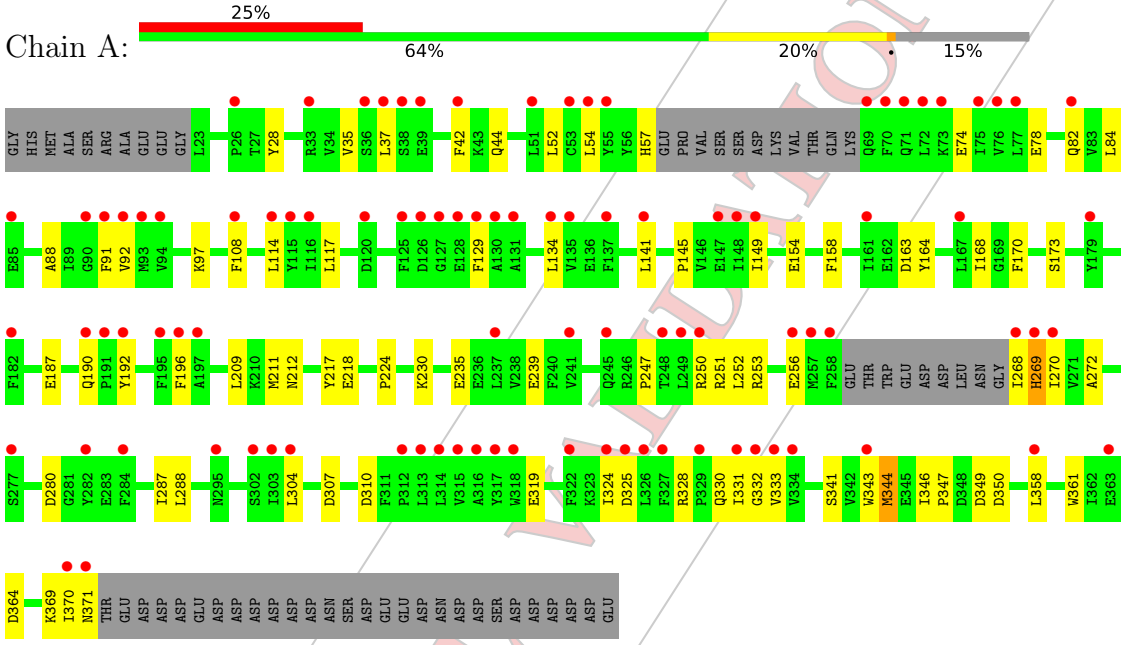
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

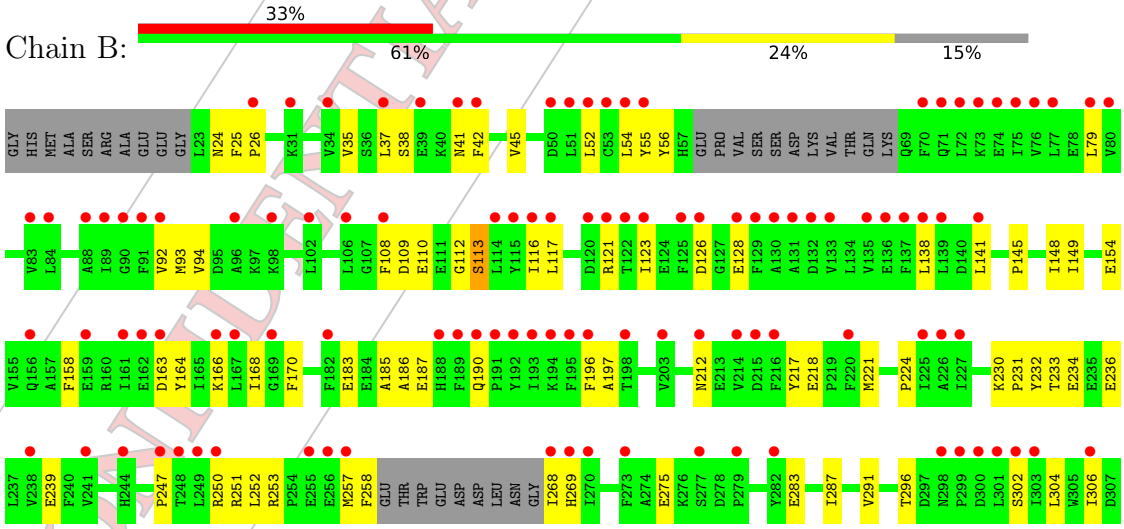
• Molecule 1: Calsequestrin-2

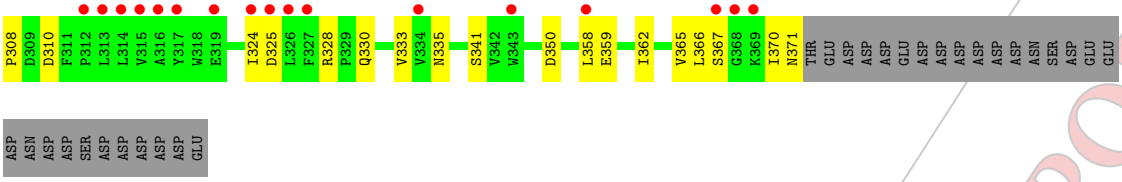
Chain A:



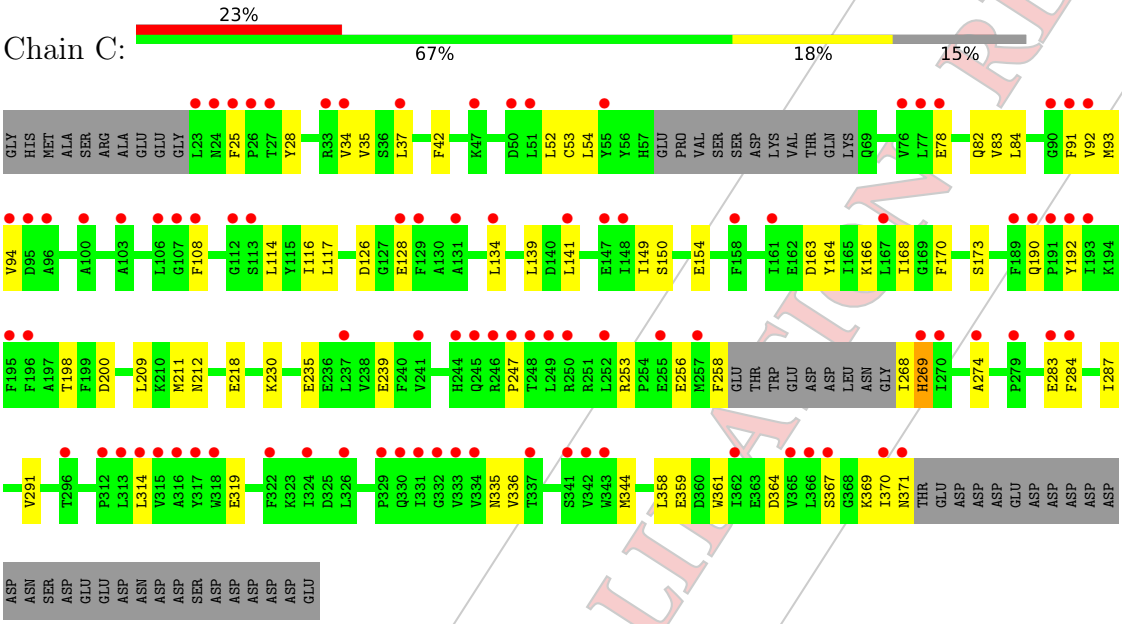
• Molecule 1: Calsequestrin-2

Chain B:

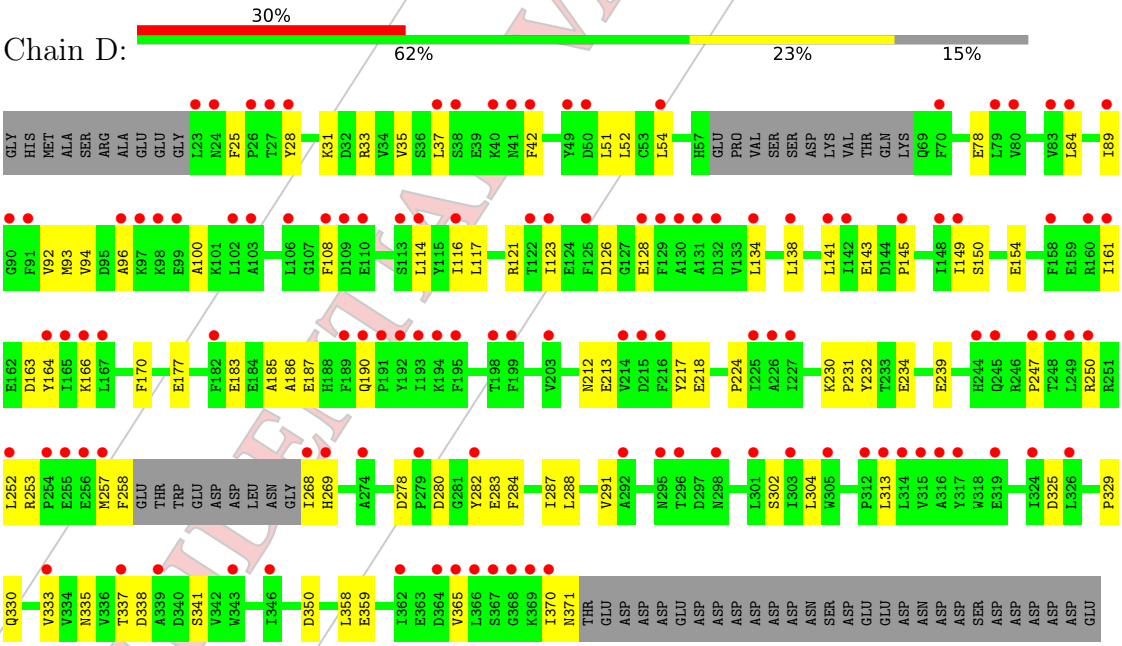




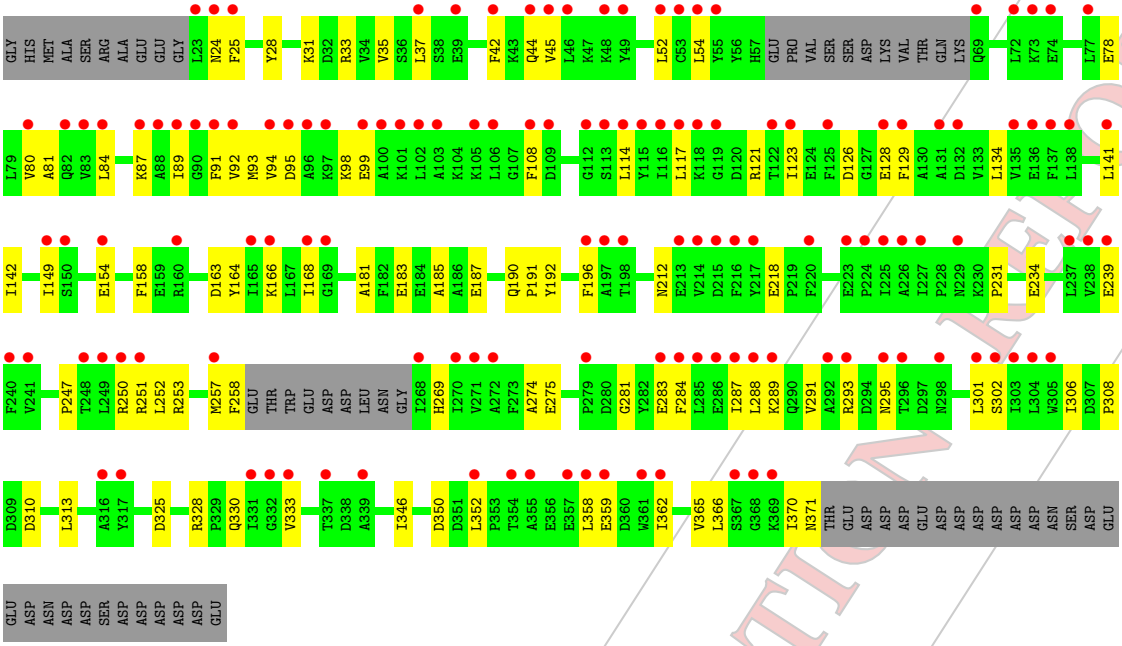
• Molecule 1: Calsequestrin-2



• Molecule 1: Calsequestrin-2

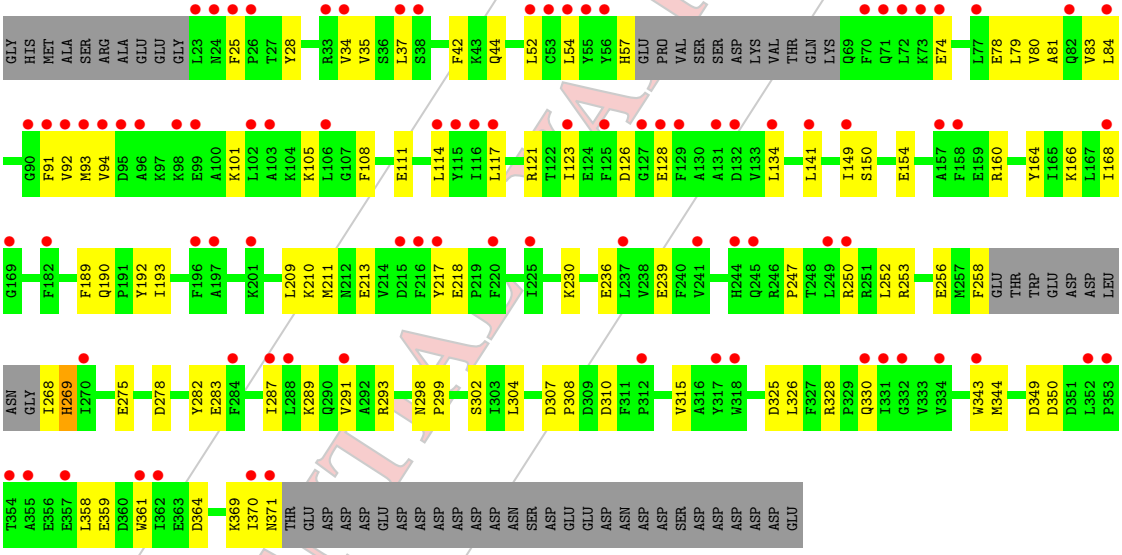


• Molecule 1: Calsequestrin-2



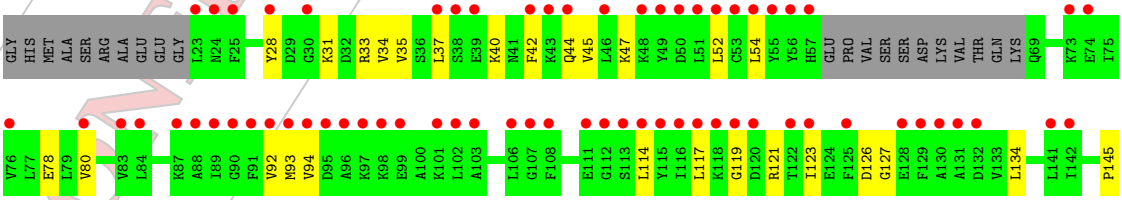
• Molecule 1: Calsequestrin-2

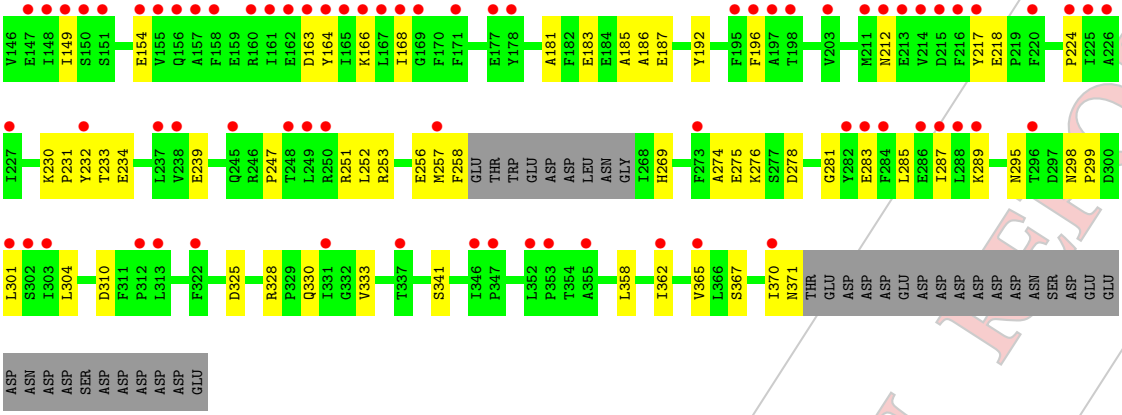
Chain F:



• Molecule 1: Calsequestrin-2

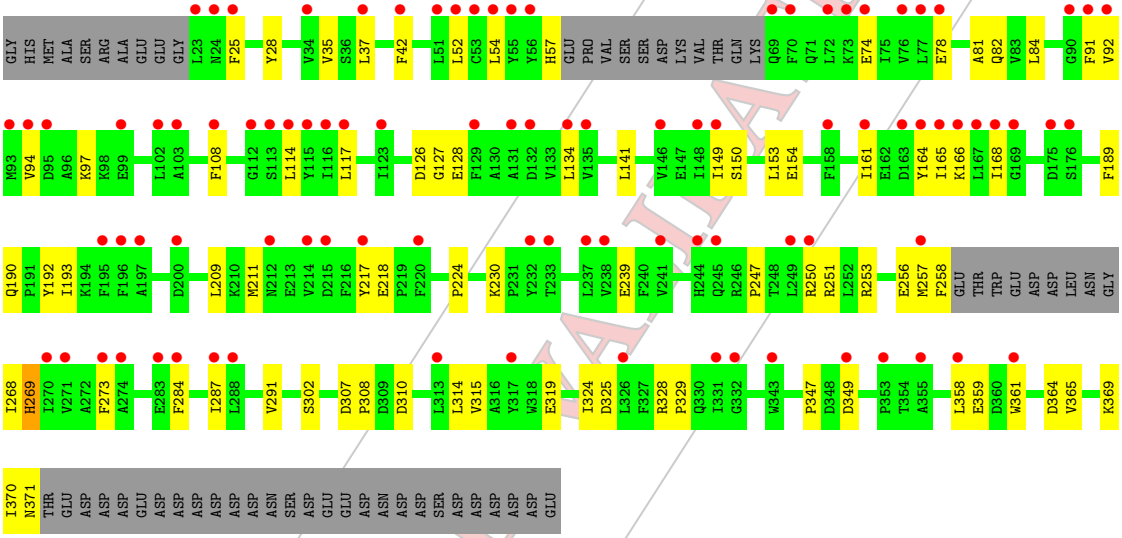
Chain G:





- Molecule 1: Calsequestrin-2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.83Å 86.02Å 214.34Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	107.20 – 3.84 214.34 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.4 (107.20-3.84) 98.0 (214.34-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.89Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.284 , 0.330 0.291 , 0.342	Depositor DCC
R_{free} test set	1439 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 87.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.266 for k,h,-l 0.266 for -k,-h,-l 0.266 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	21752	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: YB, SO4

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/2772	0.66	1/3749 (0.0%)
1	B	0.43	0/2772	0.65	1/3749 (0.0%)
1	C	0.43	0/2772	0.63	0/3749
1	D	0.43	0/2776	0.63	1/3754 (0.0%)
1	E	0.41	0/2772	0.62	1/3749 (0.0%)
1	F	0.43	0/2772	0.61	0/3749
1	G	0.43	0/2769	0.61	0/3745
1	H	0.44	0/2772	0.63	0/3749
All	All	0.43	0/22177	0.63	4/29993 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	SER	N-CA-C	6.78	129.32	111.00
1	A	288	LEU	CB-CG-CD2	-6.06	100.70	111.00
1	E	288	LEU	CA-CB-CG	5.70	128.40	115.30
1	D	288	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	PRO	Peptide

5.2 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	2708	0	2647	65	0
1	B	2708	0	2647	69	0
1	C	2708	0	2647	56	0
1	D	2712	0	2651	68	0
1	E	2708	0	2647	67	0
1	F	2708	0	2647	64	0
1	G	2705	0	2645	60	0
1	H	2708	0	2647	58	0
2	A	7	0	0	0	0
2	B	7	0	0	0	0
2	C	6	0	0	0	0
2	D	11	0	0	0	0
2	E	10	0	0	0	0
2	F	7	0	0	0	0
2	G	9	0	0	0	0
2	H	5	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
All	All	21752	0	21178	475	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 11.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HG21	1:A:343:TRP:CH2	2.13	0.84
1:B:250:ARG:NH1	1:B:302:SER:OG	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLY:HA2	1:A:343:TRP:HB2	1.67	0.77
1:E:35:VAL:HG23	1:E:92:VAL:HG12	1.67	0.75
1:B:126:ASP:HB3	1:B:258:PHE:HB3	1.71	0.72
1:D:35:VAL:HG23	1:D:92:VAL:HG12	1.70	0.72
1:D:250:ARG:NH1	1:D:302:SER:OG	2.23	0.72
1:A:324:ILE:HG21	1:A:343:TRP:HH2	1.52	0.71
1:F:35:VAL:HG23	1:F:92:VAL:HG12	1.72	0.71
1:E:126:ASP:HB3	1:E:258:PHE:HB3	1.73	0.71
1:A:211:MET:O	1:A:230:LYS:NZ	2.22	0.71
1:F:364:ASP:HB3	1:F:369:LYS:HB2	1.72	0.71
1:B:56:TYR:HB3	1:B:113:SER:HA	1.72	0.70
1:A:84:LEU:HD12	1:A:91:PHE:HZ	1.57	0.70
1:B:35:VAL:HG23	1:B:92:VAL:HG12	1.72	0.70
1:F:52:LEU:HB2	1:F:117:LEU:HB2	1.73	0.70
1:A:324:ILE:HD13	1:A:343:TRP:CH2	2.27	0.70
1:H:211:MET:O	1:H:230:LYS:NZ	2.23	0.69
1:F:211:MET:O	1:F:230:LYS:NZ	2.26	0.69
1:D:121:ARG:CZ	1:D:123:ILE:HD11	2.23	0.69
1:A:149:ILE:HG23	1:A:154:GLU:HB3	1.74	0.68
1:G:212:ASN:HB3	1:G:231:PRO:HB3	1.75	0.68
1:B:252:LEU:HD13	1:B:304:LEU:HD21	1.75	0.68
1:A:52:LEU:HB2	1:A:117:LEU:HB2	1.77	0.67
1:C:164:TYR:HD2	1:C:253:ARG:HH22	1.43	0.67
1:D:126:ASP:HB3	1:D:258:PHE:HB3	1.77	0.66
1:G:126:ASP:HB3	1:G:258:PHE:HB3	1.76	0.66
1:B:109:ASP:OD1	1:B:110:GLU:N	2.28	0.65
1:C:149:ILE:HG23	1:C:154:GLU:HB3	1.77	0.65
1:D:252:LEU:HD13	1:D:304:LEU:HD21	1.77	0.65
1:H:149:ILE:HG23	1:H:154:GLU:HB3	1.78	0.65
1:A:164:TYR:HD2	1:A:253:ARG:HH22	1.42	0.65
1:C:218:GLU:OE1	1:C:247:PRO:HB3	1.96	0.65
1:A:324:ILE:HG21	1:A:343:TRP:CZ2	2.32	0.64
1:F:149:ILE:HG23	1:F:154:GLU:HB3	1.80	0.64
1:F:287:ILE:HG22	1:F:358:LEU:HD12	1.80	0.64
1:E:251:ARG:NH2	1:E:310:ASP:OD2	2.29	0.63
1:G:121:ARG:HH12	1:G:123:ILE:HD11	1.64	0.63
1:F:164:TYR:HD2	1:F:253:ARG:HH22	1.44	0.63
1:G:35:VAL:HG23	1:G:92:VAL:HG12	1.81	0.62
1:H:28:TYR:CE1	1:H:78:GLU:HB3	2.34	0.62
1:A:333:VAL:H	1:A:343:TRP:HB3	1.63	0.62
1:E:218:GLU:OE1	1:E:247:PRO:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:VAL:HG23	1:H:92:VAL:HG12	1.81	0.62
1:C:211:MET:O	1:C:230:LYS:NZ	2.23	0.62
1:D:212:ASN:HB3	1:D:231:PRO:HB3	1.82	0.61
1:A:364:ASP:O	1:A:369:LYS:N	2.33	0.61
1:D:218:GLU:OE1	1:D:247:PRO:HB3	2.01	0.61
1:E:54:LEU:HG	1:E:92:VAL:HG23	1.82	0.61
1:B:218:GLU:OE1	1:B:247:PRO:HB3	2.00	0.61
1:B:251:ARG:NH2	1:B:310:ASP:OD2	2.29	0.60
1:E:287:ILE:HG22	1:E:358:LEU:HD12	1.84	0.60
1:C:287:ILE:HG22	1:C:358:LEU:HD12	1.84	0.59
1:F:114:LEU:HD23	1:F:134:LEU:HD11	1.84	0.59
1:E:80:VAL:HG21	1:E:134:LEU:HD23	1.85	0.59
1:G:121:ARG:NH1	1:G:123:ILE:HD11	2.17	0.59
1:A:344:MET:HB2	1:A:361:TRP:CE2	2.37	0.59
1:E:250:ARG:NH1	1:E:302:SER:OG	2.36	0.59
1:E:84:LEU:HD22	1:E:87:LYS:HG3	1.85	0.59
1:A:341:SER:HB2	1:A:343:TRP:HD1	1.67	0.59
1:G:149:ILE:HG23	1:G:154:GLU:HB3	1.85	0.59
1:H:52:LEU:HB2	1:H:117:LEU:HB2	1.85	0.58
1:G:28:TYR:CE1	1:G:78:GLU:HB3	2.38	0.58
1:B:367:SER:HB2	1:G:233:THR:HG21	1.86	0.58
1:D:283:GLU:OE1	1:F:154:GLU:HG3	2.03	0.58
1:A:324:ILE:HD13	1:A:343:TRP:HH2	1.67	0.58
1:C:364:ASP:HB3	1:C:369:LYS:HB2	1.86	0.58
1:G:127:GLY:HA2	1:G:257:MET:SD	2.43	0.58
1:E:283:GLU:O	1:E:287:ILE:HG12	2.05	0.57
1:F:141:LEU:HD23	1:F:190:GLN:HG2	1.86	0.57
1:A:287:ILE:HG22	1:A:358:LEU:HD12	1.87	0.57
1:B:38:SER:HB2	1:B:41:ASN:HD22	1.69	0.57
1:F:101:LYS:HB3	1:F:105:LYS:HE3	1.86	0.57
1:E:212:ASN:HB3	1:E:231:PRO:HB3	1.87	0.57
1:C:367:SER:HB2	1:F:236:GLU:HG2	1.86	0.57
1:B:121:ARG:HH12	1:B:123:ILE:HD11	1.69	0.57
1:D:114:LEU:HD23	1:D:134:LEU:HD11	1.87	0.57
1:H:308:PRO:HA	1:H:315:VAL:HG21	1.87	0.57
1:D:333:VAL:HG21	1:D:365:VAL:HG11	1.86	0.56
1:B:145:PRO:HB2	1:B:186:ALA:HB1	1.88	0.56
1:D:54:LEU:HG	1:D:92:VAL:HG23	1.87	0.56
1:B:54:LEU:HD23	1:B:94:VAL:HG21	1.88	0.56
1:E:247:PRO:HG2	1:E:250:ARG:HB3	1.88	0.56
1:F:28:TYR:CE1	1:F:78:GLU:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HG23	1:A:209:LEU:HD11	1.87	0.56
1:A:218:GLU:OE1	1:A:247:PRO:HB3	2.06	0.56
1:A:114:LEU:HD23	1:A:134:LEU:HD11	1.87	0.56
1:B:121:ARG:NH1	1:B:123:ILE:HD11	2.21	0.56
1:B:325:ASP:HB3	1:B:328:ARG:HE	1.71	0.55
1:C:52:LEU:HB2	1:C:117:LEU:HB2	1.88	0.55
1:D:287:ILE:HG22	1:D:358:LEU:HD12	1.87	0.55
1:H:291:VAL:HG13	1:H:359:GLU:HG3	1.89	0.55
1:A:268:ILE:HG22	1:A:269:HIS:ND1	2.21	0.55
1:A:341:SER:HB2	1:A:343:TRP:CD1	2.41	0.55
1:C:35:VAL:HG23	1:C:92:VAL:HG12	1.87	0.55
1:A:57:HIS:HE1	1:A:97:LYS:HE2	1.71	0.54
1:C:268:ILE:HD13	1:C:336:VAL:HG12	1.89	0.54
1:F:289:LYS:HE2	1:F:293:ARG:HH12	1.72	0.54
1:D:145:PRO:HB2	1:D:186:ALA:HB1	1.90	0.54
1:C:114:LEU:HD23	1:C:134:LEU:HD11	1.89	0.54
1:B:128:GLU:HB2	1:H:25:PHE:CZ	2.43	0.54
1:F:364:ASP:O	1:F:369:LYS:N	2.40	0.54
1:G:183:GLU:O	1:G:187:GLU:HG3	2.08	0.54
1:G:192:TYR:CD1	1:G:256:GLU:HA	2.43	0.54
1:A:332:GLY:HA2	1:A:343:TRP:CB	2.35	0.54
1:A:35:VAL:HG23	1:A:92:VAL:HG12	1.89	0.54
1:G:283:GLU:O	1:G:287:ILE:HG12	2.08	0.54
1:C:54:LEU:HD22	1:C:108:PHE:CZ	2.43	0.54
1:D:54:LEU:HD23	1:D:94:VAL:HG21	1.90	0.53
1:A:272:ALA:HA	1:A:331:ILE:HA	1.89	0.53
1:G:163:ASP:HB3	1:G:253:ARG:HH21	1.74	0.53
1:H:287:ILE:HG22	1:H:358:LEU:HD12	1.90	0.53
1:C:28:TYR:HA	1:C:82:GLN:OE1	2.09	0.53
1:C:168:ILE:HG23	1:C:209:LEU:HD11	1.89	0.53
1:G:34:VAL:HG11	1:G:93:MET:HE3	1.90	0.53
1:A:319:GLU:HG2	1:A:324:ILE:O	2.09	0.53
1:D:31:LYS:HB2	1:D:33:ARG:CZ	2.39	0.53
1:D:52:LEU:HB2	1:D:117:LEU:HB2	1.90	0.53
1:C:314:LEU:HB2	1:E:25:PHE:CE1	2.43	0.53
1:G:325:ASP:HB3	1:G:328:ARG:HE	1.74	0.52
1:G:54:LEU:HG	1:G:92:VAL:HG23	1.92	0.52
1:G:54:LEU:HD23	1:G:94:VAL:HG21	1.91	0.52
1:E:275:GLU:HG2	1:E:308:PRO:HD2	1.92	0.52
1:A:332:GLY:CA	1:A:343:TRP:HB2	2.39	0.52
1:D:25:PHE:CZ	1:F:128:GLU:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:GLU:OE1	1:F:247:PRO:HB3	2.09	0.52
1:H:114:LEU:HD23	1:H:134:LEU:HD11	1.90	0.52
1:E:274:ALA:HB1	1:E:281:GLY:O	2.09	0.52
1:D:213:GLU:HB2	1:D:230:LYS:HD3	1.91	0.52
1:D:149:ILE:HG23	1:D:154:GLU:HB3	1.91	0.52
1:E:164:TYR:HD2	1:E:253:ARG:HH22	1.56	0.52
1:E:289:LYS:HB3	1:E:293:ARG:HH12	1.74	0.52
1:A:280:ASP:OD2	1:A:349:ASP:HB3	2.10	0.52
1:B:233:THR:HG21	1:G:367:SER:HB2	1.91	0.52
1:G:164:TYR:CE1	1:G:166:LYS:HG2	2.45	0.52
1:B:110:GLU:C	1:B:112:GLY:H	2.12	0.52
1:D:313:LEU:HD11	1:F:83:VAL:HG21	1.91	0.52
1:E:164:TYR:CE1	1:E:166:LYS:HG2	2.45	0.52
1:C:268:ILE:HD12	1:C:335:ASN:HA	1.93	0.51
1:E:289:LYS:HB3	1:E:293:ARG:NH1	2.26	0.51
1:A:28:TYR:CE1	1:A:78:GLU:HB3	2.46	0.51
1:D:54:LEU:HD13	1:D:117:LEU:HG	1.91	0.51
1:E:149:ILE:HG23	1:E:154:GLU:HB3	1.91	0.51
1:H:127:GLY:HA2	1:H:257:MET:SD	2.51	0.51
1:A:54:LEU:HD22	1:A:108:PHE:CZ	2.46	0.51
1:C:126:ASP:HB3	1:C:258:PHE:CD2	2.46	0.51
1:C:84:LEU:HD12	1:C:91:PHE:HZ	1.76	0.51
1:G:287:ILE:HG22	1:G:358:LEU:HD12	1.93	0.51
1:E:163:ASP:HB3	1:E:253:ARG:HH21	1.76	0.51
1:E:284:PHE:HB2	1:E:352:LEU:HD13	1.93	0.50
1:H:218:GLU:OE1	1:H:247:PRO:HB3	2.10	0.50
1:E:94:VAL:HG13	1:E:99:GLU:HB2	1.93	0.50
1:A:370:ILE:HG22	1:A:371:ASN:N	2.26	0.50
1:B:170:PHE:O	1:B:212:ASN:N	2.40	0.50
1:C:54:LEU:HD22	1:C:108:PHE:HZ	1.76	0.50
1:E:121:ARG:HH12	1:E:123:ILE:HD11	1.76	0.50
1:A:192:TYR:CD1	1:A:256:GLU:HA	2.47	0.50
1:H:161:ILE:O	1:H:166:LYS:NZ	2.26	0.50
1:E:181:ALA:HB1	1:E:234:GLU:N	2.27	0.50
1:F:80:VAL:HG21	1:F:134:LEU:HD23	1.94	0.50
1:A:54:LEU:HD22	1:A:108:PHE:HZ	1.77	0.50
1:C:192:TYR:CE1	1:C:256:GLU:HA	2.47	0.50
1:B:247:PRO:HD2	1:B:250:ARG:HD3	1.93	0.50
1:D:141:LEU:HD23	1:D:190:GLN:HG2	1.94	0.50
1:G:333:VAL:HG21	1:G:365:VAL:HG11	1.94	0.50
1:D:164:TYR:CE1	1:D:166:LYS:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:HD23	1:E:134:LEU:HD11	1.93	0.50
1:G:192:TYR:CE1	1:G:256:GLU:HA	2.46	0.50
1:F:308:PRO:HA	1:F:315:VAL:HG21	1.93	0.49
1:B:212:ASN:HB3	1:B:231:PRO:HB3	1.94	0.49
1:E:185:ALA:N	1:E:234:GLU:HG3	2.27	0.49
1:C:370:ILE:HG22	1:C:371:ASN:N	2.26	0.49
1:G:218:GLU:OE1	1:G:247:PRO:HB3	2.12	0.49
1:A:168:ILE:HA	1:A:196:PHE:O	2.12	0.49
1:C:192:TYR:CD1	1:C:256:GLU:HA	2.47	0.49
1:F:275:GLU:HG2	1:F:278:ASP:HB3	1.94	0.49
1:H:84:LEU:HD12	1:H:91:PHE:HZ	1.78	0.49
1:B:185:ALA:N	1:B:234:GLU:HG3	2.26	0.49
1:G:185:ALA:N	1:G:234:GLU:HG3	2.27	0.49
1:A:74:GLU:O	1:A:78:GLU:HG2	2.13	0.49
1:C:141:LEU:HD23	1:C:190:GLN:HG2	1.95	0.49
1:D:163:ASP:HB3	1:D:253:ARG:HH21	1.78	0.49
1:D:37:LEU:HD11	1:D:42:PHE:HA	1.95	0.48
1:D:333:VAL:O	1:D:341:SER:HA	2.14	0.48
1:F:370:ILE:HG22	1:F:371:ASN:N	2.29	0.48
1:C:128:GLU:HB2	1:E:25:PHE:CZ	2.47	0.48
1:E:328:ARG:NH1	1:E:346:ILE:O	2.46	0.48
1:F:268:ILE:HG22	1:F:269:HIS:ND1	2.28	0.48
1:E:121:ARG:NH1	1:E:123:ILE:HD11	2.28	0.48
1:D:150:SER:HB2	1:F:350:ASP:CG	2.33	0.48
1:G:276:LYS:HB3	1:G:276:LYS:HE3	1.63	0.48
1:B:230:LYS:HB3	1:B:232:TYR:OH	2.14	0.48
1:F:291:VAL:HG13	1:F:359:GLU:HG3	1.95	0.48
1:C:283:GLU:O	1:C:287:ILE:HG12	2.13	0.48
1:F:252:LEU:HD13	1:F:304:LEU:HD21	1.95	0.48
1:G:40:LYS:NZ	1:G:44:GLN:OE1	2.41	0.48
1:H:126:ASP:HB3	1:H:258:PHE:HB3	1.96	0.48
1:D:170:PHE:O	1:D:212:ASN:N	2.41	0.48
1:E:158:PHE:HE1	1:E:196:PHE:CD1	2.32	0.48
1:E:45:VAL:HG23	1:E:52:LEU:HD11	1.94	0.48
1:E:54:LEU:HG	1:E:92:VAL:CG2	2.44	0.48
1:E:183:GLU:O	1:E:187:GLU:HG3	2.14	0.47
1:F:344:MET:HG3	1:F:361:TRP:CD1	2.48	0.47
1:F:54:LEU:HD22	1:F:108:PHE:CE2	2.49	0.47
1:D:126:ASP:CB	1:D:258:PHE:HB3	2.44	0.47
1:E:247:PRO:HD2	1:E:250:ARG:HD3	1.95	0.47
1:C:268:ILE:HG22	1:C:269:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:TYR:CE1	1:E:78:GLU:HB3	2.49	0.47
1:G:80:VAL:HG21	1:G:134:LEU:HD23	1.95	0.47
1:H:54:LEU:HD22	1:H:108:PHE:CZ	2.48	0.47
1:H:164:TYR:HB3	1:H:253:ARG:NH2	2.30	0.47
1:D:93:MET:HB3	1:D:93:MET:HE2	1.68	0.47
1:G:217:TYR:CZ	1:G:224:PRO:HB3	2.49	0.47
1:A:344:MET:HB2	1:A:361:TRP:NE1	2.30	0.47
1:B:145:PRO:HB2	1:B:186:ALA:CB	2.44	0.47
1:B:287:ILE:HG22	1:B:358:LEU:HD12	1.97	0.47
1:G:251:ARG:NH2	1:G:310:ASP:OD2	2.45	0.47
1:C:364:ASP:O	1:C:369:LYS:N	2.47	0.47
1:E:370:ILE:HG22	1:E:371:ASN:N	2.28	0.47
1:F:57:HIS:ND1	1:F:111:GLU:OE2	2.46	0.47
1:F:370:ILE:HG22	1:F:371:ASN:H	1.79	0.47
1:F:37:LEU:HD11	1:F:42:PHE:HA	1.97	0.47
1:G:333:VAL:HG21	1:G:365:VAL:CG1	2.45	0.47
1:D:161:ILE:HD11	1:F:282:TYR:HB2	1.97	0.47
1:D:183:GLU:O	1:D:187:GLU:HG3	2.14	0.47
1:B:283:GLU:OE1	1:H:154:GLU:HG3	2.15	0.47
1:H:284:PHE:CE1	1:H:358:LEU:HD11	2.50	0.47
1:G:252:LEU:HD13	1:G:304:LEU:HD21	1.97	0.47
1:G:370:ILE:HG22	1:G:371:ASN:N	2.30	0.47
1:H:251:ARG:NH2	1:H:310:ASP:OD2	2.34	0.47
1:H:370:ILE:HG22	1:H:371:ASN:N	2.30	0.47
1:B:168:ILE:HA	1:B:196:PHE:O	2.14	0.47
1:H:268:ILE:HG22	1:H:269:HIS:ND1	2.29	0.47
1:C:154:GLU:HG3	1:E:283:GLU:OE1	2.15	0.47
1:F:54:LEU:HD23	1:F:94:VAL:HG21	1.97	0.47
1:G:34:VAL:CG1	1:G:93:MET:HE3	2.45	0.47
1:C:344:MET:HG3	1:C:361:TRP:CD1	2.50	0.46
1:D:370:ILE:HG22	1:D:371:ASN:N	2.30	0.46
1:D:128:GLU:HB2	1:F:25:PHE:CZ	2.50	0.46
1:G:114:LEU:HD23	1:G:134:LEU:HD11	1.97	0.46
1:A:332:GLY:CA	1:A:343:TRP:CB	2.92	0.46
1:H:192:TYR:CD1	1:H:256:GLU:HA	2.50	0.46
1:H:273:PHE:O	1:H:329:PRO:HA	2.15	0.46
1:H:319:GLU:HG2	1:H:324:ILE:O	2.15	0.46
1:E:37:LEU:HD11	1:E:42:PHE:HA	1.97	0.46
1:C:28:TYR:CE1	1:C:78:GLU:HB3	2.50	0.46
1:D:54:LEU:HD22	1:D:108:PHE:HZ	1.80	0.46
1:C:83:VAL:HG21	1:E:313:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:VAL:HG21	1:D:365:VAL:CG1	2.45	0.46
1:G:230:LYS:HB3	1:G:232:TYR:OH	2.15	0.46
1:H:358:LEU:HA	1:H:358:LEU:HD23	1.82	0.46
1:A:217:TYR:CZ	1:A:224:PRO:HB3	2.51	0.46
1:A:364:ASP:HB3	1:A:369:LYS:HB2	1.97	0.46
1:B:141:LEU:HD23	1:B:190:GLN:HG2	1.98	0.46
1:D:350:ASP:CG	1:F:150:SER:HB2	2.36	0.46
1:B:25:PHE:CE1	1:H:314:LEU:HB2	2.51	0.46
1:E:325:ASP:O	1:E:330:GLN:NE2	2.37	0.46
1:C:173:SER:HB3	1:H:325:ASP:HB2	1.98	0.46
1:E:370:ILE:HG22	1:E:371:ASN:H	1.81	0.46
1:G:47:LYS:NZ	1:G:119:GLY:HA2	2.31	0.46
1:H:37:LEU:HD11	1:H:42:PHE:HA	1.98	0.46
1:H:141:LEU:HD23	1:H:190:GLN:HG2	1.97	0.46
1:C:53:CYS:SG	1:C:116:ILE:HD12	2.57	0.45
1:D:313:LEU:HD21	1:F:79:LEU:HD21	1.97	0.45
1:E:333:VAL:HG21	1:E:365:VAL:HG11	1.98	0.45
1:B:217:TYR:CZ	1:B:224:PRO:HB3	2.51	0.45
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.77	0.45
1:A:37:LEU:HD11	1:A:42:PHE:HA	1.96	0.45
1:B:268:ILE:HD12	1:B:335:ASN:HA	1.98	0.45
1:B:183:GLU:O	1:B:187:GLU:HG3	2.16	0.45
1:H:28:TYR:HA	1:H:82:GLN:OE1	2.16	0.45
1:B:164:TYR:CE1	1:B:166:LYS:HG2	2.52	0.45
1:C:25:PHE:CZ	1:E:128:GLU:HB2	2.52	0.45
1:D:247:PRO:HD2	1:D:250:ARG:HD3	1.97	0.45
1:H:364:ASP:O	1:H:369:LYS:N	2.50	0.45
1:B:25:PHE:HD1	1:B:26:PRO:HD2	1.81	0.45
1:F:325:ASP:O	1:F:330:GLN:NE2	2.43	0.45
1:H:81:ALA:HA	1:H:91:PHE:CE2	2.51	0.45
1:B:252:LEU:HD22	1:B:306:ILE:HG12	1.99	0.45
1:C:150:SER:HB2	1:E:350:ASP:CG	2.37	0.45
1:F:192:TYR:CD1	1:F:256:GLU:HA	2.52	0.45
1:H:164:TYR:HB3	1:H:253:ARG:HH22	1.81	0.45
1:B:93:MET:HE2	1:B:93:MET:HB3	1.67	0.45
1:D:284:PHE:CG	1:D:329:PRO:HB3	2.52	0.45
1:E:295:ASN:HB2	1:E:301:LEU:HD23	1.98	0.45
1:E:54:LEU:HD23	1:E:94:VAL:HG21	1.99	0.45
1:F:168:ILE:HG23	1:F:209:LEU:HD11	1.99	0.45
1:C:126:ASP:HB3	1:C:258:PHE:HD2	1.80	0.45
1:C:34:VAL:HG12	1:C:93:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ARG:NH2	1:F:123:ILE:HD11	2.32	0.45
1:H:164:TYR:HD2	1:H:253:ARG:HH22	1.64	0.45
1:C:319:GLU:OE1	1:E:87:LYS:NZ	2.37	0.44
1:D:121:ARG:NH1	1:D:123:ILE:HD11	2.32	0.44
1:D:31:LYS:HB2	1:D:33:ARG:NH1	2.32	0.44
1:B:367:SER:HB2	1:G:233:THR:CG2	2.47	0.44
1:G:275:GLU:HG3	1:G:278:ASP:HB3	1.99	0.44
1:C:37:LEU:HD21	1:C:42:PHE:HD1	1.81	0.44
1:D:185:ALA:N	1:D:234:GLU:HG3	2.32	0.44
1:E:81:ALA:HA	1:E:91:PHE:CE1	2.52	0.44
1:H:217:TYR:CZ	1:H:224:PRO:HB3	2.53	0.44
1:H:307:ASP:HB3	1:H:310:ASP:OD2	2.16	0.44
1:F:44:GLN:HB2	1:F:44:GLN:HE21	1.68	0.44
1:A:28:TYR:HA	1:A:82:GLN:OE1	2.17	0.44
1:A:88:ALA:HB2	1:D:177:GLU:HA	1.99	0.44
1:D:325:ASP:O	1:D:330:GLN:NE2	2.31	0.44
1:D:51:LEU:HB2	1:D:89:ILE:HG12	1.99	0.44
1:G:168:ILE:HA	1:G:196:PHE:O	2.17	0.44
1:B:24:ASN:HB3	1:B:25:PHE:H	1.71	0.44
1:D:370:ILE:HG22	1:D:371:ASN:H	1.82	0.44
1:F:364:ASP:HB3	1:F:369:LYS:HD3	1.99	0.44
1:H:328:ARG:HD2	1:H:349:ASP:OD2	2.16	0.44
1:A:141:LEU:HD23	1:A:190:GLN:HG2	2.00	0.44
1:B:370:ILE:HG22	1:B:371:ASN:N	2.32	0.44
1:C:163:ASP:HB3	1:C:253:ARG:HH21	1.83	0.44
1:F:84:LEU:HD12	1:F:91:PHE:HZ	1.82	0.44
1:G:370:ILE:HG22	1:G:371:ASN:H	1.83	0.44
1:A:114:LEU:HB2	1:A:129:PHE:HE2	1.83	0.44
1:D:28:TYR:CE1	1:D:78:GLU:HB3	2.53	0.44
1:G:126:ASP:CB	1:G:258:PHE:HB3	2.44	0.44
1:D:116:ILE:HD12	1:D:138:LEU:HD21	2.00	0.44
1:F:192:TYR:CE1	1:F:256:GLU:HA	2.53	0.44
1:G:212:ASN:CB	1:G:231:PRO:HB3	2.47	0.44
1:B:55:TYR:CD1	1:B:113:SER:HB2	2.53	0.43
1:D:230:LYS:HB3	1:D:232:TYR:OH	2.18	0.43
1:D:247:PRO:HG2	1:D:250:ARG:HB3	1.99	0.43
1:D:257:MET:HE1	1:F:25:PHE:HE2	1.83	0.43
1:F:326:LEU:HD21	1:F:343:TRP:CH2	2.53	0.43
1:G:145:PRO:HB2	1:G:186:ALA:HB1	2.00	0.43
1:H:166:LYS:HB2	1:H:217:TYR:HB2	2.00	0.43
1:A:252:LEU:HB2	1:A:304:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ASP:N	1:A:350:ASP:OD1	2.50	0.43
1:H:54:LEU:HD23	1:H:94:VAL:HG21	1.99	0.43
1:A:57:HIS:CE1	1:A:97:LYS:HE2	2.52	0.43
1:E:252:LEU:HD22	1:E:306:ILE:HG12	1.99	0.43
1:H:57:HIS:CE1	1:H:97:LYS:HE2	2.53	0.43
1:A:328:ARG:HD2	1:A:349:ASP:OD2	2.18	0.43
1:B:275:GLU:HG2	1:B:308:PRO:HD2	2.00	0.43
1:E:54:LEU:HD13	1:E:117:LEU:HG	2.00	0.43
1:A:145:PRO:HG2	1:A:187:GLU:HG2	2.01	0.43
1:B:324:ILE:HG12	1:B:330:GLN:NE2	2.34	0.43
1:D:217:TYR:CZ	1:D:224:PRO:HB3	2.53	0.43
1:E:168:ILE:HA	1:E:196:PHE:O	2.18	0.43
1:F:250:ARG:NH1	1:F:302:SER:OG	2.50	0.43
1:G:275:GLU:HG3	1:G:278:ASP:CB	2.48	0.43
1:H:165:ILE:HA	1:H:217:TYR:O	2.19	0.43
1:H:192:TYR:CE1	1:H:256:GLU:HA	2.53	0.43
1:A:251:ARG:NH1	3:A:408:SO4:O4	2.52	0.43
1:A:44:GLN:HB2	1:A:44:GLN:HE21	1.59	0.43
1:F:328:ARG:HD2	1:F:349:ASP:OD2	2.18	0.43
1:B:149:ILE:HG23	1:B:154:GLU:HB3	1.99	0.43
1:C:235:GLU:H	1:C:235:GLU:CD	2.22	0.43
1:B:350:ASP:OD2	1:H:150:SER:HB2	2.17	0.43
1:B:247:PRO:HG2	1:B:250:ARG:HB3	2.00	0.43
1:C:54:LEU:HD23	1:C:94:VAL:HG21	2.00	0.43
1:E:141:LEU:HD23	1:E:190:GLN:HG2	2.01	0.43
1:E:44:GLN:HE21	1:E:44:GLN:HB2	1.60	0.43
1:F:34:VAL:HG12	1:F:93:MET:HG2	2.01	0.43
1:C:200:ASP:OD1	1:H:347:PRO:HB3	2.18	0.43
1:G:295:ASN:HB2	1:G:301:LEU:HD23	2.00	0.43
1:G:358:LEU:O	1:G:362:ILE:HG12	2.18	0.43
1:H:250:ARG:NH1	1:H:302:SER:OG	2.52	0.43
1:B:54:LEU:HG	1:B:92:VAL:HG23	2.00	0.43
1:A:247:PRO:HG2	1:A:250:ARG:HB3	2.00	0.42
1:C:37:LEU:HD11	1:C:42:PHE:HA	2.01	0.42
1:H:74:GLU:O	1:H:78:GLU:HG2	2.19	0.42
1:C:170:PHE:O	1:C:212:ASN:N	2.37	0.42
1:D:283:GLU:O	1:D:287:ILE:HG12	2.19	0.42
1:E:328:ARG:O	1:E:330:GLN:HG2	2.19	0.42
1:A:307:ASP:HB3	1:A:310:ASP:OD2	2.19	0.42
1:A:330:GLN:HA	1:A:346:ILE:HD12	2.01	0.42
1:C:170:PHE:CD2	1:C:211:MET:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:ILE:O	1:E:366:LEU:HG	2.19	0.42
1:F:307:ASP:HB3	1:F:310:ASP:OD2	2.20	0.42
1:G:126:ASP:HB3	1:G:258:PHE:CD2	2.54	0.42
1:A:235:GLU:H	1:A:235:GLU:CD	2.23	0.42
1:A:270:ILE:HG12	1:A:333:VAL:HG22	2.01	0.42
1:B:54:LEU:HD22	1:B:108:PHE:HZ	1.85	0.42
1:E:24:ASN:HB3	1:E:25:PHE:H	1.70	0.42
1:E:89:ILE:HD11	1:E:142:ILE:HD12	2.01	0.42
1:G:52:LEU:HB2	1:G:117:LEU:HB2	2.00	0.42
1:A:364:ASP:HB3	1:A:369:LYS:HD3	2.01	0.42
1:B:148:ILE:CD1	1:B:197:ALA:HB3	2.49	0.42
1:B:291:VAL:HG13	1:B:359:GLU:HG3	2.01	0.42
1:D:143:GLU:O	1:D:190:GLN:NE2	2.53	0.42
1:D:84:LEU:HD13	1:D:89:ILE:HD12	2.02	0.42
1:G:333:VAL:O	1:G:341:SER:HA	2.20	0.42
1:B:25:PHE:CZ	1:H:128:GLU:HB2	2.55	0.42
1:H:168:ILE:HG23	1:H:209:LEU:HD11	2.01	0.42
1:B:221:MET:CE	1:B:296:THR:HG22	2.49	0.42
1:B:163:ASP:HB3	1:B:253:ARG:HH21	1.85	0.42
1:B:333:VAL:HG21	1:B:365:VAL:HG11	2.02	0.42
1:C:370:ILE:HG22	1:C:371:ASN:H	1.85	0.42
1:F:74:GLU:O	1:F:78:GLU:HG2	2.20	0.42
1:B:333:VAL:HG21	1:B:365:VAL:CG1	2.50	0.42
1:C:54:LEU:HD13	1:C:117:LEU:HG	2.02	0.42
1:C:291:VAL:HG13	1:C:359:GLU:HG3	2.01	0.42
1:G:164:TYR:HD2	1:G:253:ARG:HH22	1.68	0.42
1:A:54:LEU:HD13	1:A:117:LEU:HG	2.02	0.42
1:D:278:ASP:OD1	1:D:280:ASP:HB2	2.20	0.42
1:B:116:ILE:HD12	1:B:138:LEU:HD21	2.01	0.42
1:B:126:ASP:HB2	1:B:257:MET:O	2.20	0.42
1:D:96:ALA:O	1:D:100:ALA:HB2	2.20	0.42
1:E:93:MET:HE2	1:E:93:MET:HB3	1.68	0.42
1:G:181:ALA:HB1	1:G:234:GLU:N	2.35	0.42
1:A:163:ASP:HB3	1:A:253:ARG:HH21	1.85	0.41
1:B:158:PHE:HE1	1:B:196:PHE:CD1	2.38	0.41
1:D:54:LEU:HD23	1:D:94:VAL:CG2	2.49	0.41
1:E:333:VAL:HG21	1:E:365:VAL:CG1	2.50	0.41
1:G:54:LEU:HG	1:G:92:VAL:CG2	2.50	0.41
1:A:114:LEU:HB2	1:A:129:PHE:CE2	2.56	0.41
1:E:54:LEU:HD22	1:E:108:PHE:HZ	1.85	0.41
1:F:126:ASP:HB3	1:F:258:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LEU:HD11	1:G:42:PHE:HA	2.02	0.41
1:G:52:LEU:HA	1:G:52:LEU:HD23	1.72	0.41
1:D:145:PRO:HB2	1:D:186:ALA:CB	2.49	0.41
1:F:213:GLU:HB2	1:F:230:LYS:HD3	2.02	0.41
1:D:150:SER:HB2	1:F:350:ASP:OD1	2.21	0.41
1:F:81:ALA:HA	1:F:91:PHE:CE2	2.56	0.41
1:B:370:ILE:HG22	1:B:371:ASN:H	1.86	0.41
1:B:38:SER:HB2	1:B:41:ASN:ND2	2.33	0.41
1:D:282:TYR:OH	1:F:160:ARG:HD3	2.19	0.41
1:E:31:LYS:HB3	1:E:33:ARG:NH1	2.35	0.41
1:H:189:PHE:CD1	1:H:193:ILE:HD12	2.56	0.41
1:A:319:GLU:OE2	1:A:325:ASP:HA	2.20	0.41
1:B:54:LEU:HD22	1:B:108:PHE:CZ	2.56	0.41
1:C:170:PHE:HA	1:C:198:THR:O	2.20	0.41
1:F:189:PHE:CD1	1:F:193:ILE:HD12	2.56	0.41
1:A:170:PHE:O	1:A:212:ASN:N	2.40	0.41
1:C:164:TYR:CE1	1:C:166:LYS:HG2	2.56	0.41
1:E:257:MET:HE3	1:E:257:MET:HB2	1.83	0.41
1:H:308:PRO:HB3	1:H:315:VAL:HG11	2.03	0.41
1:F:164:TYR:CE1	1:F:166:LYS:HG2	2.56	0.41
1:F:210:LYS:HB3	1:F:230:LYS:HZ1	1.86	0.41
1:F:166:LYS:HB2	1:F:217:TYR:HB2	2.02	0.41
1:G:42:PHE:O	1:G:45:VAL:HG22	2.21	0.41
1:B:283:GLU:O	1:B:287:ILE:HG12	2.20	0.41
1:D:163:ASP:HB3	1:D:253:ARG:NH2	2.35	0.41
1:E:95:ASP:HB3	1:E:98:LYS:HB3	2.02	0.41
1:F:283:GLU:O	1:F:287:ILE:HG12	2.20	0.41
1:G:285:LEU:HG	1:G:289:LYS:HE3	2.03	0.41
1:D:268:ILE:HD12	1:D:335:ASN:HA	2.03	0.41
1:B:333:VAL:O	1:B:341:SER:HA	2.21	0.41
1:D:291:VAL:HG13	1:D:359:GLU:HG3	2.03	0.41
1:D:54:LEU:HD22	1:D:108:PHE:CZ	2.55	0.41
1:G:274:ALA:HB1	1:G:281:GLY:O	2.21	0.41
1:H:247:PRO:HG2	1:H:250:ARG:HB3	2.02	0.41
1:B:52:LEU:HB2	1:B:117:LEU:HB2	2.03	0.40
1:B:42:PHE:O	1:B:45:VAL:HG22	2.22	0.40
1:B:54:LEU:HD13	1:B:117:LEU:HG	2.03	0.40
1:G:328:ARG:O	1:G:330:GLN:HG2	2.22	0.40
1:H:114:LEU:CD2	1:H:134:LEU:HD11	2.51	0.40
1:A:173:SER:HB3	1:F:325:ASP:HB2	2.03	0.40
1:B:37:LEU:HD11	1:B:42:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:LYS:HB3	1:G:33:ARG:CZ	2.51	0.40
1:H:361:TRP:O	1:H:365:VAL:HG23	2.22	0.40
1:B:232:TYR:HA	1:B:236:GLU:OE2	2.21	0.40
1:C:93:MET:HE2	1:C:93:MET:HB3	1.99	0.40
1:D:257:MET:HE1	1:F:25:PHE:CE2	2.56	0.40
1:H:52:LEU:HD23	1:H:52:LEU:HA	1.79	0.40
1:A:158:PHE:HE1	1:A:196:PHE:CD1	2.40	0.40
1:B:362:ILE:O	1:B:366:LEU:HG	2.22	0.40
1:C:274:ALA:HB2	1:C:284:PHE:HD2	1.87	0.40
1:D:337:THR:OG1	1:D:338:ASP:N	2.55	0.40
1:E:114:LEU:HB2	1:E:129:PHE:HE2	1.85	0.40
1:H:54:LEU:HD13	1:H:117:LEU:HG	2.02	0.40
1:H:153:LEU:HA	1:H:153:LEU:HD13	1.81	0.40
1:H:57:HIS:HE1	1:H:97:LYS:HE2	1.86	0.40
1:B:25:PHE:CD1	1:B:26:PRO:HD2	2.57	0.40
1:C:139:LEU:HA	1:C:139:LEU:HD23	1.91	0.40
1:C:370:ILE:HG21	1:C:370:ILE:HD13	1.86	0.40
1:C:54:LEU:O	1:C:114:LEU:HD12	2.21	0.40
1:E:191:PRO:HD2	1:E:192:TYR:CE1	2.57	0.40
1:E:291:VAL:HG13	1:E:359:GLU:HG3	2.03	0.40
1:F:298:ASN:HA	1:F:299:PRO:HD3	1.89	0.40
1:G:298:ASN:HA	1:G:299:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	Percentiles
1	A	323/387 (84%)	301 (93%)	21 (6%)	1 (0%)	43 79
1	B	323/387 (84%)	306 (95%)	17 (5%)	0	100 100
1	C	323/387 (84%)	307 (95%)	16 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	323/387 (84%)	307 (95%)	16 (5%)	0	100	100
1	E	323/387 (84%)	307 (95%)	16 (5%)	0	100	100
1	F	323/387 (84%)	307 (95%)	16 (5%)	0	100	100
1	G	323/387 (84%)	307 (95%)	16 (5%)	0	100	100
1	H	323/387 (84%)	308 (95%)	15 (5%)	0	100	100
All	All	2584/3096 (84%)	2450 (95%)	133 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	295/351 (84%)	293 (99%)	2 (1%)	85	93
1	B	295/351 (84%)	292 (99%)	3 (1%)	78	89
1	C	295/351 (84%)	293 (99%)	2 (1%)	85	93
1	D	296/351 (84%)	294 (99%)	2 (1%)	85	93
1	E	295/351 (84%)	293 (99%)	2 (1%)	85	93
1	F	295/351 (84%)	293 (99%)	2 (1%)	85	93
1	G	294/351 (84%)	292 (99%)	2 (1%)	85	93
1	H	295/351 (84%)	293 (99%)	2 (1%)	85	93
All	All	2360/2808 (84%)	2343 (99%)	17 (1%)	85	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	269	HIS

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	239	GLU
1	B	269	HIS
1	C	239	GLU
1	C	269	HIS
1	D	239	GLU
1	D	269	HIS
1	E	239	GLU
1	E	269	HIS
1	F	239	GLU
1	F	269	HIS
1	G	239	GLU
1	G	269	HIS
1	H	239	GLU
1	H	269	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 62 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	408	-	4,4,4	0.11	0	6,6,6	0.17	0
3	SO4	B	408	-	4,4,4	0.19	0	6,6,6	0.16	0
3	SO4	D	412	2	4,4,4	0.19	0	6,6,6	0.14	0
3	SO4	E	411	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	G	410	2	4,4,4	0.12	0	6,6,6	0.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	329/387 (85%)	1.39	96 (29%) 0 0	47, 88, 131, 153	0
1	B	329/387 (85%)	1.76	126 (38%) 0 0	58, 97, 135, 146	0
1	C	329/387 (85%)	1.32	90 (27%) 0 0	50, 90, 132, 152	0
1	D	329/387 (85%)	1.58	118 (35%) 0 0	57, 95, 133, 152	0
1	E	329/387 (85%)	1.98	136 (41%) 0 0	63, 96, 137, 145	0
1	F	329/387 (85%)	1.29	88 (26%) 0 0	57, 88, 138, 158	0
1	G	329/387 (85%)	1.88	140 (42%) 0 0	61, 95, 134, 151	0
1	H	329/387 (85%)	1.33	94 (28%) 0 0	51, 89, 137, 150	0
All	All	2632/3096 (85%)	1.57	888 (33%) 0 0	47, 93, 135, 158	0

All (888) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	226	ALA	12.2
1	B	53	CYS	10.4
1	G	115	TYR	10.3
1	D	248	THR	9.7
1	E	96	ALA	9.6
1	E	102	LEU	9.2
1	E	114	LEU	8.9
1	G	150	SER	8.7
1	G	114	LEU	8.7
1	F	55	TYR	8.5
1	D	128	GLU	8.5
1	B	257	MET	8.5
1	E	215	ASP	8.5
1	E	116	ILE	8.3
1	A	92	VAL	8.2
1	E	169	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	E	97	LYS	8.2
1	G	113	SER	8.1
1	E	95	ASP	8.0
1	G	302	SER	7.8
1	B	128	GLU	7.7
1	E	115	TYR	7.7
1	E	225	ILE	7.6
1	H	73	LYS	7.6
1	B	302	SER	7.4
1	G	53	CYS	7.4
1	B	248	THR	7.3
1	G	102	LEU	7.2
1	A	93	MET	7.1
1	H	92	VAL	7.1
1	D	257	MET	7.0
1	H	114	LEU	7.0
1	H	116	ILE	6.9
1	D	249	LEU	6.9
1	E	113	SER	6.8
1	F	114	LEU	6.8
1	C	318	TRP	6.7
1	F	71	GLN	6.7
1	G	212	ASN	6.7
1	A	258	PHE	6.6
1	H	54	LEU	6.6
1	G	112	GLY	6.6
1	E	55	TYR	6.6
1	G	88	ALA	6.5
1	D	102	LEU	6.5
1	B	190	GLN	6.5
1	G	149	ILE	6.4
1	E	23	LEU	6.4
1	D	190	GLN	6.4
1	H	93	MET	6.4
1	H	53	CYS	6.4
1	C	26	PRO	6.3
1	A	128	GLU	6.3
1	G	119	GLY	6.3
1	E	54	LEU	6.3
1	B	74	GLU	6.2
1	G	169	GLY	6.2
1	B	130	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	E	332	GLY	6.2
1	B	90	GLY	6.2
1	G	54	LEU	6.1
1	G	92	VAL	6.1
1	F	23	LEU	6.1
1	C	108	PHE	6.1
1	E	117	LEU	6.1
1	B	125	PHE	6.0
1	G	248	THR	5.9
1	B	91	PHE	5.9
1	B	191	PRO	5.9
1	B	102	LEU	5.9
1	G	116	ILE	5.9
1	B	268	ILE	5.8
1	A	127	GLY	5.8
1	A	91	PHE	5.8
1	C	128	GLU	5.8
1	G	129	PHE	5.8
1	A	54	LEU	5.7
1	C	191	PRO	5.7
1	H	55	TYR	5.7
1	D	130	ALA	5.7
1	B	54	LEU	5.7
1	E	198	THR	5.7
1	C	315	VAL	5.6
1	B	249	LEU	5.6
1	G	55	TYR	5.6
1	A	269	HIS	5.6
1	E	125	PHE	5.6
1	C	314	LEU	5.6
1	E	149	ILE	5.6
1	H	94	VAL	5.6
1	G	198	THR	5.6
1	H	52	LEU	5.6
1	E	150	SER	5.6
1	E	358	LEU	5.5
1	B	324	ILE	5.5
1	G	168	ILE	5.5
1	E	216	PHE	5.5
1	F	361	TRP	5.5
1	A	318	TRP	5.5
1	E	132	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	248	THR	5.4
1	A	129	PHE	5.4
1	D	226	ALA	5.4
1	F	94	VAL	5.4
1	D	193	ILE	5.4
1	F	92	VAL	5.4
1	G	117	LEU	5.4
1	G	303	ILE	5.3
1	D	192	TYR	5.3
1	G	44	GLN	5.3
1	B	301	LEU	5.2
1	G	283	GLU	5.2
1	E	283	GLU	5.2
1	A	38	SER	5.2
1	A	192	TYR	5.2
1	B	88	ALA	5.2
1	A	333	VAL	5.1
1	G	249	LEU	5.1
1	E	303	ILE	5.1
1	E	301	LEU	5.1
1	F	38	SER	5.1
1	H	74	GLU	5.1
1	F	116	ILE	5.1
1	D	145	PRO	5.1
1	H	115	TYR	5.1
1	A	53	CYS	5.1
1	E	286	GLU	5.1
1	G	226	ALA	5.1
1	D	191	PRO	5.1
1	C	91	PHE	5.0
1	B	192	TYR	5.0
1	G	52	LEU	5.0
1	B	129	PHE	5.0
1	E	302	SER	5.0
1	E	227	ILE	5.0
1	A	71	GLN	5.0
1	B	71	GLN	5.0
1	C	337	THR	4.9
1	B	250	ARG	4.9
1	H	76	VAL	4.9
1	C	313	LEU	4.9
1	B	269	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	367	SER	4.9
1	A	37	LEU	4.8
1	B	73	LYS	4.8
1	G	23	LEU	4.8
1	D	109	ASP	4.8
1	A	257	MET	4.8
1	B	42	PHE	4.8
1	G	301	LEU	4.8
1	F	91	PHE	4.8
1	E	359	GLU	4.8
1	E	91	PHE	4.7
1	E	53	CYS	4.7
1	G	215	ASP	4.7
1	H	77	LEU	4.7
1	D	108	PHE	4.7
1	D	365	VAL	4.7
1	F	54	LEU	4.7
1	B	194	LYS	4.7
1	C	193	ILE	4.7
1	E	129	PHE	4.7
1	C	92	VAL	4.7
1	G	99	GLU	4.7
1	B	89	ILE	4.7
1	A	75	ILE	4.7
1	D	123	ILE	4.6
1	B	256	GLU	4.6
1	B	121	ARG	4.6
1	E	214	VAL	4.6
1	C	192	TYR	4.6
1	D	366	LEU	4.6
1	G	56	TYR	4.6
1	G	163	ASP	4.6
1	C	190	GLN	4.5
1	G	245	GLN	4.5
1	B	215	ASP	4.5
1	H	70	PHE	4.5
1	G	296	THR	4.5
1	D	131	ALA	4.5
1	D	23	LEU	4.5
1	F	72	LEU	4.5
1	D	26	PRO	4.5
1	B	141	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	123	ILE	4.5
1	H	56	TYR	4.5
1	D	250	ARG	4.5
1	E	355	ALA	4.4
1	E	84	LEU	4.4
1	G	165	ILE	4.4
1	B	316	ALA	4.4
1	F	96	ALA	4.4
1	D	194	LYS	4.4
1	C	245	GLN	4.4
1	B	52	LEU	4.4
1	C	333	VAL	4.4
1	C	94	VAL	4.4
1	A	76	VAL	4.4
1	E	52	LEU	4.3
1	E	39	GLU	4.3
1	F	95	ASP	4.3
1	H	212	ASN	4.3
1	F	354	THR	4.3
1	E	357	GLU	4.3
1	E	141	LEU	4.3
1	A	191	PRO	4.3
1	F	215	ASP	4.3
1	A	55	TYR	4.3
1	B	123	ILE	4.3
1	F	149	ILE	4.3
1	H	117	LEU	4.3
1	F	196	PHE	4.2
1	B	137	PHE	4.2
1	E	249	LEU	4.2
1	B	131	ALA	4.2
1	E	295	ASN	4.2
1	B	226	ALA	4.2
1	C	103	ALA	4.2
1	C	107	GLY	4.2
1	A	317	TYR	4.2
1	B	114	LEU	4.2
1	D	103	ALA	4.2
1	D	141	LEU	4.1
1	F	332	GLY	4.1
1	D	149	ILE	4.1
1	A	334	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	238	VAL	4.1
1	A	147	GLU	4.1
1	C	257	MET	4.1
1	H	95	ASP	4.1
1	G	216	PHE	4.1
1	E	168	ILE	4.1
1	D	369	LYS	4.1
1	B	368	GLY	4.1
1	G	237	LEU	4.1
1	H	169	GLY	4.1
1	C	112	GLY	4.1
1	G	89	ILE	4.0
1	A	313	LEU	4.0
1	B	92	VAL	4.0
1	F	84	LEU	4.0
1	C	322	PHE	4.0
1	B	136	GLU	4.0
1	B	76	VAL	4.0
1	C	248	THR	4.0
1	H	168	ILE	3.9
1	A	94	VAL	3.9
1	D	110	GLU	3.9
1	F	244	HIS	3.9
1	F	318	TRP	3.9
1	B	26	PRO	3.9
1	C	37	LEU	3.9
1	H	72	LEU	3.9
1	G	220	PHE	3.9
1	D	91	PHE	3.9
1	A	72	LEU	3.9
1	G	49	TYR	3.9
1	G	132	ASP	3.8
1	C	33	ARG	3.8
1	D	337	THR	3.8
1	F	56	TYR	3.8
1	H	129	PHE	3.8
1	A	130	ALA	3.8
1	C	95	ASP	3.8
1	F	99	GLU	3.8
1	C	269	HIS	3.8
1	G	151	SER	3.8
1	A	125	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	48	LYS	3.8
1	B	369	LYS	3.8
1	B	303	ILE	3.7
1	D	313	LEU	3.7
1	A	134	LEU	3.7
1	B	227	ILE	3.7
1	B	244	HIS	3.7
1	B	50	ASP	3.7
1	G	197	ALA	3.7
1	A	371	ASN	3.7
1	A	324	ILE	3.7
1	F	131	ALA	3.7
1	A	316	ALA	3.7
1	F	74	GLU	3.7
1	A	332	GLY	3.7
1	B	298	ASN	3.7
1	E	289	LYS	3.7
1	A	82	GLN	3.7
1	D	50	ASP	3.7
1	F	117	LEU	3.7
1	E	108	PHE	3.6
1	G	90	GLY	3.6
1	A	114	LEU	3.6
1	D	195	PHE	3.6
1	H	270	ILE	3.6
1	D	316	ALA	3.6
1	E	88	ALA	3.6
1	E	331	ILE	3.6
1	D	227	ILE	3.6
1	E	106	LEU	3.6
1	G	196	PHE	3.6
1	E	197	ALA	3.6
1	E	109	ASP	3.6
1	E	119	GLY	3.6
1	G	73	LYS	3.6
1	D	298	ASN	3.6
1	H	355	ALA	3.6
1	D	122	THR	3.6
1	B	70	PHE	3.6
1	B	313	LEU	3.6
1	D	41	ASN	3.6
1	E	42	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	161	ILE	3.6
1	F	353	PRO	3.6
1	D	324	ILE	3.6
1	C	25	PHE	3.6
1	F	331	ILE	3.6
1	B	135	VAL	3.6
1	H	332	GLY	3.6
1	A	149	ILE	3.5
1	G	24	ASN	3.5
1	B	326	LEU	3.5
1	G	123	ILE	3.5
1	G	131	ALA	3.5
1	F	132	ASP	3.5
1	E	241	VAL	3.5
1	G	217	TYR	3.5
1	A	326	LEU	3.5
1	E	87	LYS	3.5
1	D	83	VAL	3.5
1	A	270	ILE	3.5
1	D	252	LEU	3.5
1	F	168	ILE	3.5
1	A	315	VAL	3.5
1	G	167	LEU	3.5
1	E	339	ALA	3.5
1	B	39	GLU	3.5
1	B	77	LEU	3.5
1	G	43	LYS	3.5
1	E	105	LYS	3.5
1	H	91	PHE	3.5
1	G	166	LYS	3.5
1	F	102	LEU	3.5
1	E	136	GLU	3.5
1	E	298	ASN	3.4
1	A	115	TYR	3.4
1	F	225	ILE	3.4
1	A	26	PRO	3.4
1	D	113	SER	3.4
1	B	34	VAL	3.4
1	G	355	ALA	3.4
1	H	149	ILE	3.4
1	H	102	LEU	3.4
1	E	270	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	134	LEU	3.4
1	A	250	ARG	3.4
1	H	196	PHE	3.4
1	B	188	HIS	3.4
1	D	368	GLY	3.4
1	D	182	PHE	3.4
1	F	106	LEU	3.4
1	E	279	PRO	3.4
1	E	362	ILE	3.4
1	F	53	CYS	3.4
1	G	125	PHE	3.4
1	A	131	ALA	3.4
1	E	80	VAL	3.4
1	G	164	TYR	3.4
1	C	270	ILE	3.4
1	B	120	ASP	3.4
1	D	97	LYS	3.4
1	G	118	LYS	3.4
1	H	287	ILE	3.4
1	F	216	PHE	3.4
1	D	129	PHE	3.4
1	F	284	PHE	3.4
1	D	38	SER	3.3
1	G	96	ALA	3.3
1	C	341	SER	3.3
1	D	274	ALA	3.3
1	E	89	ILE	3.3
1	C	332	GLY	3.3
1	H	176	SER	3.3
1	H	237	LEU	3.3
1	H	313	LEU	3.3
1	G	160	ARG	3.3
1	F	169	GLY	3.3
1	C	131	ALA	3.3
1	C	250	ARG	3.3
1	D	339	ALA	3.3
1	C	331	ILE	3.3
1	H	131	ALA	3.3
1	C	147	GLU	3.3
1	H	343	TRP	3.3
1	H	135	VAL	3.3
1	B	126	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	249	LEU	3.3
1	A	329	PRO	3.3
1	D	98	LYS	3.3
1	A	73	LYS	3.3
1	D	254	PRO	3.3
1	E	100	ALA	3.3
1	B	216	PHE	3.3
1	A	126	ASP	3.3
1	B	299	PRO	3.3
1	E	352	LEU	3.3
1	E	154	GLU	3.3
1	G	111	GLU	3.3
1	E	284	PHE	3.2
1	F	123	ILE	3.2
1	F	52	LEU	3.2
1	C	246	ARG	3.2
1	G	97	LYS	3.2
1	C	279	PRO	3.2
1	E	112	GLY	3.2
1	H	24	ASN	3.2
1	F	73	LYS	3.2
1	E	293	ARG	3.2
1	G	37	LEU	3.2
1	B	80	VAL	3.2
1	G	224	PRO	3.2
1	D	364	ASP	3.2
1	E	367	SER	3.2
1	H	217	TYR	3.2
1	G	80	VAL	3.2
1	D	296	THR	3.2
1	G	331	ILE	3.2
1	D	292	ALA	3.2
1	H	233	THR	3.2
1	G	287	ILE	3.2
1	E	369	LYS	3.2
1	C	50	ASP	3.2
1	G	106	LEU	3.2
1	H	51	LEU	3.2
1	B	315	VAL	3.2
1	E	268	ILE	3.2
1	A	325	ASP	3.2
1	B	116	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	326	LEU	3.2
1	E	217	TYR	3.2
1	A	190	GLN	3.2
1	G	288	LEU	3.2
1	B	133	VAL	3.2
1	B	334	VAL	3.2
1	H	37	LEU	3.1
1	G	91	PHE	3.1
1	G	250	ARG	3.1
1	E	165	ILE	3.1
1	E	361	TRP	3.1
1	H	69	GLN	3.1
1	G	289	LYS	3.1
1	C	141	LEU	3.1
1	H	158	PHE	3.1
1	E	250	ARG	3.1
1	A	312	PRO	3.1
1	F	125	PHE	3.1
1	G	103	ALA	3.1
1	D	203	VAL	3.1
1	G	313	LEU	3.1
1	C	317	TYR	3.1
1	G	38	SER	3.1
1	G	156	GLN	3.1
1	G	158	PHE	3.1
1	C	342	VAL	3.1
1	D	317	TYR	3.1
1	H	108	PHE	3.1
1	D	165	ILE	3.1
1	G	148	ILE	3.1
1	H	195	PHE	3.1
1	D	245	GLN	3.0
1	E	271	VAL	3.0
1	H	163	ASP	3.0
1	E	90	GLY	3.0
1	D	189	PHE	3.0
1	F	115	TYR	3.0
1	A	39	GLU	3.0
1	D	167	LEU	3.0
1	E	101	LYS	3.0
1	F	141	LEU	3.0
1	G	352	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	248	THR	3.0
1	E	292	ALA	3.0
1	B	122	THR	3.0
1	F	270	ILE	3.0
1	G	155	VAL	3.0
1	B	312	PRO	3.0
1	A	196	PHE	3.0
1	B	159	GLU	3.0
1	B	79	LEU	3.0
1	A	148	ILE	3.0
1	A	249	LEU	3.0
1	B	162	GLU	3.0
1	H	331	ILE	3.0
1	B	106	LEU	3.0
1	C	366	LEU	3.0
1	A	161	ILE	2.9
1	E	99	GLU	2.9
1	G	51	LEU	2.9
1	H	167	LEU	2.9
1	D	158	PHE	2.9
1	G	76	VAL	2.9
1	G	130	ALA	2.9
1	D	160	ARG	2.9
1	F	355	ALA	2.9
1	A	331	ILE	2.9
1	H	112	GLY	2.9
1	D	215	ASP	2.9
1	G	50	ASP	2.9
1	D	80	VAL	2.9
1	A	197	ALA	2.9
1	F	287	ILE	2.9
1	D	84	LEU	2.9
1	A	284	PHE	2.9
1	E	354	THR	2.9
1	H	241	VAL	2.9
1	D	303	ILE	2.9
1	G	30	GLY	2.9
1	B	72	LEU	2.9
1	A	90	GLY	2.9
1	H	288	LEU	2.9
1	E	288	LEU	2.9
1	F	77	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	250	ARG	2.9
1	G	141	LEU	2.9
1	G	42	PHE	2.9
1	G	154	GLU	2.9
1	B	317	TYR	2.9
1	E	24	ASN	2.9
1	E	317	TYR	2.9
1	C	252	LEU	2.9
1	F	217	TYR	2.9
1	G	171	PHE	2.9
1	H	146	VAL	2.9
1	A	314	LEU	2.9
1	G	161	ILE	2.9
1	D	333	VAL	2.8
1	B	319	GLU	2.8
1	E	287	ILE	2.8
1	F	134	LEU	2.8
1	H	215	ASP	2.8
1	D	214	VAL	2.8
1	E	73	LYS	2.8
1	F	24	ASN	2.8
1	D	198	THR	2.8
1	D	89	ILE	2.8
1	G	362	ILE	2.8
1	C	334	VAL	2.8
1	C	255	GLU	2.8
1	B	169	GLY	2.8
1	C	365	VAL	2.8
1	F	197	ALA	2.8
1	A	343	TRP	2.8
1	F	370	ILE	2.8
1	H	361	TRP	2.8
1	B	247	PRO	2.8
1	C	316	ALA	2.8
1	F	371	ASN	2.8
1	C	77	LEU	2.8
1	B	132	ASP	2.8
1	B	220	PHE	2.8
1	H	25	PHE	2.8
1	D	312	PRO	2.8
1	E	368	GLY	2.8
1	A	304	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLU	2.8
1	B	241	VAL	2.8
1	D	247	PRO	2.8
1	E	316	ALA	2.8
1	H	166	LYS	2.8
1	B	195	PHE	2.8
1	G	273	PHE	2.8
1	E	285	LEU	2.8
1	F	70	PHE	2.8
1	D	346	ILE	2.8
1	B	166	LYS	2.8
1	E	166	LYS	2.8
1	F	93	MET	2.8
1	H	257	MET	2.8
1	C	78	GLU	2.7
1	G	257	MET	2.7
1	E	103	ALA	2.7
1	H	90	GLY	2.7
1	G	346	ILE	2.7
1	D	295	ASN	2.7
1	E	49	TYR	2.7
1	H	164	TYR	2.7
1	A	77	LEU	2.7
1	C	296	THR	2.7
1	F	357	GLU	2.7
1	F	317	TYR	2.7
1	G	232	TYR	2.7
1	C	100	ALA	2.7
1	E	92	VAL	2.7
1	H	103	ALA	2.7
1	B	196	PHE	2.7
1	F	288	LEU	2.7
1	A	137	PHE	2.7
1	G	178	TYR	2.7
1	F	245	GLN	2.7
1	A	370	ILE	2.7
1	E	272	ALA	2.7
1	G	39	GLU	2.7
1	B	214	VAL	2.7
1	D	116	ILE	2.7
1	E	37	LEU	2.7
1	G	353	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	128	GLU	2.7
1	E	238	VAL	2.7
1	G	282	TYR	2.7
1	D	96	ALA	2.7
1	D	326	LEU	2.6
1	H	250	ARG	2.6
1	H	148	ILE	2.6
1	G	98	LYS	2.6
1	A	42	PHE	2.6
1	F	129	PHE	2.6
1	G	46	LEU	2.6
1	G	157	ALA	2.6
1	H	99	GLU	2.6
1	G	108	PHE	2.6
1	A	277	SER	2.6
1	G	94	VAL	2.6
1	G	177	GLU	2.6
1	E	213	GLU	2.6
1	B	193	ILE	2.6
1	B	83	VAL	2.6
1	H	284	PHE	2.6
1	B	117	LEU	2.6
1	F	352	LEU	2.6
1	E	118	LYS	2.6
1	E	251	ARG	2.6
1	G	225	ILE	2.6
1	A	303	ILE	2.6
1	G	93	MET	2.6
1	H	232	TYR	2.6
1	H	358	LEU	2.6
1	B	300	ASP	2.6
1	B	41	ASN	2.6
1	B	277	SER	2.6
1	G	25	PHE	2.6
1	F	330	GLN	2.6
1	H	161	ILE	2.6
1	C	189	PHE	2.6
1	D	166	LYS	2.6
1	E	94	VAL	2.6
1	A	141	LEU	2.5
1	B	161	ILE	2.5
1	G	74	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	49	TYR	2.5
1	G	57	HIS	2.5
1	H	197	ALA	2.5
1	D	343	TRP	2.5
1	E	296	THR	2.5
1	D	42	PHE	2.5
1	A	237	LEU	2.5
1	B	51	LEU	2.5
1	D	305	TRP	2.5
1	A	33	ARG	2.5
1	A	245	GLN	2.5
1	E	333	VAL	2.5
1	G	370	ILE	2.5
1	G	162	GLU	2.5
1	G	284	PHE	2.5
1	A	36	SER	2.5
1	B	367	SER	2.5
1	D	319	GLU	2.5
1	C	312	PRO	2.5
1	D	279	PRO	2.5
1	A	327	PHE	2.5
1	E	74	GLU	2.5
1	B	314	LEU	2.5
1	B	75	ILE	2.5
1	B	325	ASP	2.5
1	B	198	THR	2.5
1	H	271	VAL	2.5
1	G	128	GLU	2.5
1	F	33	ARG	2.5
1	E	45	VAL	2.5
1	E	135	VAL	2.5
1	F	343	TRP	2.5
1	C	34	VAL	2.5
1	A	182	PHE	2.5
1	F	26	PRO	2.4
1	H	113	SER	2.4
1	C	371	ASN	2.4
1	E	44	GLN	2.4
1	H	200	ASP	2.4
1	A	358	LEU	2.4
1	A	268	ILE	2.4
1	C	158	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	163	ASP	2.4
1	C	241	VAL	2.4
1	G	214	VAL	2.4
1	B	189	PHE	2.4
1	F	201	LYS	2.4
1	C	76	VAL	2.4
1	H	326	LEU	2.4
1	A	116	ILE	2.4
1	E	122	THR	2.4
1	G	213	GLU	2.4
1	A	167	LEU	2.4
1	C	237	LEU	2.4
1	G	83	VAL	2.4
1	H	245	GLN	2.4
1	D	256	GLU	2.4
1	A	120	ASP	2.4
1	E	131	ALA	2.4
1	B	139	LEU	2.4
1	E	138	LEU	2.4
1	D	282	TYR	2.4
1	C	24	ASN	2.4
1	E	239	GLU	2.4
1	C	90	GLY	2.4
1	H	274	ALA	2.4
1	B	156	GLN	2.4
1	H	220	PHE	2.4
1	G	95	ASP	2.4
1	B	98	LYS	2.4
1	E	160	ARG	2.4
1	A	51	LEU	2.4
1	D	79	LEU	2.4
1	E	83	VAL	2.4
1	B	115	TYR	2.4
1	G	84	LEU	2.3
1	H	214	VAL	2.3
1	B	84	LEU	2.3
1	H	34	VAL	2.3
1	C	284	PHE	2.3
1	D	27	THR	2.3
1	B	225	ILE	2.3
1	C	161	ILE	2.3
1	D	362	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	54	LEU	2.3
1	F	34	VAL	2.3
1	E	48	LYS	2.3
1	D	269	HIS	2.3
1	H	42	PHE	2.3
1	G	227	ILE	2.3
1	H	123	ILE	2.3
1	B	358	LEU	2.3
1	D	37	LEU	2.3
1	F	241	VAL	2.3
1	F	25	PHE	2.3
1	H	244	HIS	2.3
1	A	302	SER	2.3
1	D	70	PHE	2.3
1	D	216	PHE	2.3
1	E	240	PHE	2.3
1	F	249	LEU	2.3
1	H	23	LEU	2.3
1	F	90	GLY	2.3
1	C	247	PRO	2.3
1	G	337	THR	2.3
1	D	40	LYS	2.3
1	B	96	ALA	2.3
1	C	343	TRP	2.3
1	E	257	MET	2.3
1	F	103	ALA	2.3
1	C	329	PRO	2.3
1	G	101	LYS	2.3
1	E	196	PHE	2.3
1	C	367	SER	2.3
1	F	334	VAL	2.3
1	D	90	GLY	2.3
1	A	282	TYR	2.3
1	D	125	PHE	2.3
1	C	96	ALA	2.3
1	G	211	MET	2.3
1	A	363	GLU	2.3
1	C	330	GLN	2.3
1	A	70	PHE	2.3
1	E	337	THR	2.3
1	F	312	PRO	2.3
1	G	195	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	25	PHE	2.3
1	D	138	LEU	2.2
1	D	132	ASP	2.2
1	E	220	PHE	2.2
1	G	28	TYR	2.2
1	B	255	GLU	2.2
1	E	304	LEU	2.2
1	B	212	ASN	2.2
1	B	167	LEU	2.2
1	C	196	PHE	2.2
1	D	199	PHE	2.2
1	B	273	PHE	2.2
1	F	98	LYS	2.2
1	A	241	VAL	2.2
1	C	195	PHE	2.2
1	F	220	PHE	2.2
1	G	312	PRO	2.2
1	H	317	TYR	2.2
1	G	286	GLU	2.2
1	H	249	LEU	2.2
1	F	182	PHE	2.2
1	D	301	LEU	2.2
1	A	108	PHE	2.2
1	H	349	ASP	2.2
1	E	77	LEU	2.2
1	G	147	GLU	2.2
1	B	182	PHE	2.2
1	E	224	PRO	2.2
1	E	305	TRP	2.2
1	C	244	HIS	2.2
1	C	324	ILE	2.2
1	E	223	GLU	2.2
1	F	362	ILE	2.2
1	A	135	VAL	2.2
1	C	283	GLU	2.2
1	F	37	LEU	2.2
1	F	291	VAL	2.2
1	G	87	LYS	2.2
1	H	175	ASP	2.2
1	C	55	TYR	2.2
1	A	85	GLU	2.2
1	C	51	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	315	VAL	2.2
1	E	69	GLN	2.2
1	E	82	GLN	2.2
1	B	306	ILE	2.2
1	G	122	THR	2.2
1	G	120	ASP	2.2
1	C	106	LEU	2.2
1	G	365	VAL	2.2
1	D	142	ILE	2.2
1	G	347	PRO	2.1
1	B	203	VAL	2.1
1	C	47	LYS	2.1
1	D	314	LEU	2.1
1	G	107	GLY	2.1
1	D	255	GLU	2.1
1	F	158	PHE	2.1
1	D	134	LEU	2.1
1	F	237	LEU	2.1
1	C	274	ALA	2.1
1	C	134	LEU	2.1
1	D	106	LEU	2.1
1	H	78	GLU	2.1
1	C	148	ILE	2.1
1	C	23	LEU	2.1
1	E	229	ASN	2.1
1	G	203	VAL	2.1
1	B	343	TRP	2.1
1	D	28	TYR	2.1
1	E	128	GLU	2.1
1	E	237	LEU	2.1
1	A	295	ASN	2.1
1	H	353	PRO	2.1
1	F	157	ALA	2.1
1	H	273	PHE	2.1
1	C	362	ILE	2.1
1	H	238	VAL	2.1
1	H	283	GLU	2.1
1	B	138	LEU	2.1
1	D	114	LEU	2.1
1	B	327	PHE	2.1
1	C	27	THR	2.1
1	A	322	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	322	PHE	2.1
1	E	72	LEU	2.1
1	D	244	HIS	2.1
1	A	179	TYR	2.1
1	B	270	ILE	2.1
1	C	167	LEU	2.1
1	B	279	PRO	2.0
1	H	132	ASP	2.0
1	C	129	PHE	2.0
1	E	137	PHE	2.0
1	D	268	ILE	2.0
1	B	282	TYR	2.0
1	B	108	PHE	2.0
1	B	55	TYR	2.0
1	C	113	SER	2.0
1	H	165	ILE	2.0
1	F	82	GLN	2.0
1	D	164	TYR	2.0
1	A	195	PHE	2.0
1	B	37	LEU	2.0
1	E	46	LEU	2.0
1	D	24	ASN	2.0
1	D	148	ILE	2.0
1	B	238	VAL	2.0
1	C	370	ILE	2.0
1	D	370	ILE	2.0
1	B	31	LYS	2.0
1	F	127	GLY	2.0
1	A	69	GLN	2.0
1	D	225	ILE	2.0
1	G	142	ILE	2.0
1	D	99	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YB	D	403	1/1	0.30	0.17	136,136,136,136	1
2	YB	E	409	1/1	0.39	0.21	188,188,188,188	1
2	YB	E	408	1/1	0.53	0.19	171,171,171,171	1
2	YB	F	407	1/1	0.57	0.18	173,173,173,173	1
3	SO4	A	408	5/5	0.62	0.36	96,99,100,101	5
2	YB	D	409	1/1	0.64	0.30	144,144,144,144	1
2	YB	E	405	1/1	0.65	0.10	152,152,152,152	1
2	YB	A	403	1/1	0.67	0.22	121,121,121,121	1
2	YB	E	410	1/1	0.68	0.09	226,226,226,226	1
2	YB	D	410	1/1	0.69	0.18	170,170,170,170	1
2	YB	H	405	1/1	0.70	0.16	113,113,113,113	1
2	YB	C	403	1/1	0.70	0.20	136,136,136,136	1
3	SO4	E	411	5/5	0.72	0.35	104,108,114,114	0
2	YB	A	406	1/1	0.72	0.12	107,107,107,107	1
2	YB	G	409	1/1	0.72	0.20	221,221,221,221	0
2	YB	D	411	1/1	0.75	0.27	119,119,119,119	1
2	YB	F	404	1/1	0.75	0.08	186,186,186,186	0
2	YB	E	406	1/1	0.75	0.19	144,144,144,144	1
2	YB	B	406	1/1	0.75	0.23	214,214,214,214	0
2	YB	G	407	1/1	0.79	0.42	195,195,195,195	1
2	YB	G	403	1/1	0.79	0.08	153,153,153,153	1
2	YB	G	408	1/1	0.80	0.15	135,135,135,135	1
2	YB	E	403	1/1	0.80	0.10	165,165,165,165	0
2	YB	C	402	1/1	0.81	0.06	174,174,174,174	0
3	SO4	G	410	5/5	0.81	0.20	101,101,112,113	5
2	YB	C	404	1/1	0.82	0.34	117,117,117,117	1
2	YB	G	401	1/1	0.82	0.12	145,145,145,145	1
2	YB	G	402	1/1	0.83	0.14	113,113,113,113	1
2	YB	H	404	1/1	0.84	0.08	173,173,173,173	0
2	YB	A	402	1/1	0.85	0.08	156,156,156,156	1
2	YB	F	402	1/1	0.86	0.10	139,139,139,139	1
2	YB	E	404	1/1	0.86	0.20	110,110,110,110	1
2	YB	E	407	1/1	0.87	0.08	122,122,122,122	1
2	YB	D	402	1/1	0.87	0.08	119,119,119,119	1
2	YB	B	407	1/1	0.87	0.17	250,250,250,250	0
2	YB	E	402	1/1	0.87	0.13	131,131,131,131	1
2	YB	E	401	1/1	0.87	0.16	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YB	D	404	1/1	0.87	0.21	99,99,99,99	1
2	YB	D	405	1/1	0.87	0.06	159,159,159,159	1
2	YB	A	401	1/1	0.87	0.14	126,126,126,126	0
2	YB	G	406	1/1	0.88	0.20	115,115,115,115	1
2	YB	H	402	1/1	0.88	0.17	109,109,109,109	1
2	YB	B	403	1/1	0.89	0.07	182,182,182,182	1
2	YB	F	406	1/1	0.89	0.10	82,82,82,82	1
2	YB	F	401	1/1	0.89	0.11	135,135,135,135	0
3	SO4	D	412	5/5	0.89	0.22	101,106,108,111	0
3	SO4	B	408	5/5	0.89	0.24	99,110,114,116	0
2	YB	B	402	1/1	0.90	0.12	171,171,171,171	0
2	YB	B	405	1/1	0.91	0.26	125,125,125,125	1
2	YB	D	406	1/1	0.91	0.11	104,104,104,104	1
2	YB	C	406	1/1	0.91	0.23	122,122,122,122	1
2	YB	F	405	1/1	0.91	0.16	123,123,123,123	1
2	YB	G	404	1/1	0.92	0.08	166,166,166,166	1
2	YB	G	405	1/1	0.92	0.28	147,147,147,147	1
2	YB	A	405	1/1	0.92	0.14	160,160,160,160	0
2	YB	A	404	1/1	0.93	0.06	150,150,150,150	1
2	YB	D	407	1/1	0.93	0.13	107,107,107,107	1
2	YB	B	404	1/1	0.94	0.08	173,173,173,173	0
2	YB	B	401	1/1	0.95	0.23	149,149,149,149	1
2	YB	A	407	1/1	0.95	0.16	108,108,108,108	1
2	YB	D	408	1/1	0.95	0.08	190,190,190,190	0
2	YB	F	403	1/1	0.95	0.27	129,129,129,129	1
2	YB	H	403	1/1	0.96	0.21	130,130,130,130	1
2	YB	H	401	1/1	0.96	0.13	99,99,99,99	0
2	YB	D	401	1/1	0.97	0.15	137,137,137,137	1
2	YB	C	401	1/1	0.97	0.14	127,127,127,127	0
2	YB	C	405	1/1	0.98	0.06	179,179,179,179	0

6.5 Other polymers

There are no such residues in this entry.