Full wwPDB X-ray Structure Validation Report (i)

May 6, 2020 – 04:10 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 (1)) were used in the production of this report:

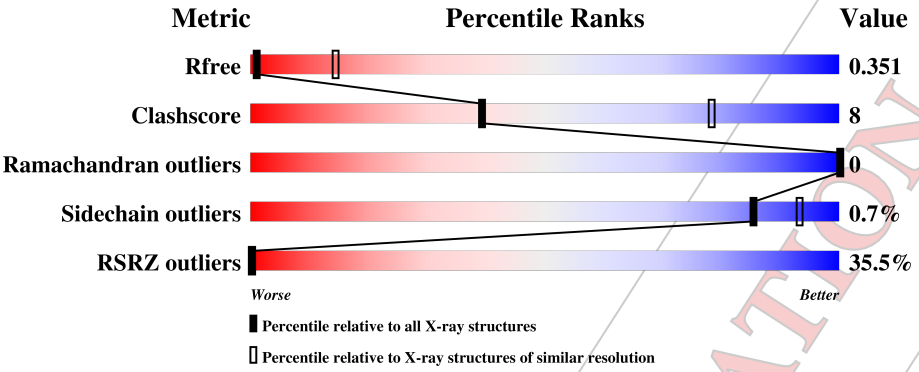
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 respectively. 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	36% 65% 19% 15%
1	B	387	26% 68% 17% 15%
1	C	387	28% 67% 17% • 15%
1	D	387	32% 71% 14% 15%
1	E	387	30% 66% 19% 15%

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Mol	Chain	Length	Quality of chain
1	F	387	27% 70% 15% 15%
1	G	387	26% 68% 17% 15%
1	H	387	36% 64% 21% 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
3	SO4	A	410	-	-	-	X
3	SO4	F	408	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21808 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
			2715	1771	416	522	6			
1	B	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	C	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	D	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	E	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	F	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	G	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	H	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	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	8	Total Yb 8 8	0	0
2	D	8	Total Yb 8 8	0	0
2	E	9	Total Yb 9 9	0	0
2	H	6	Total Yb 6 6	0	0
2	B	7	Total Yb 7 7	0	0

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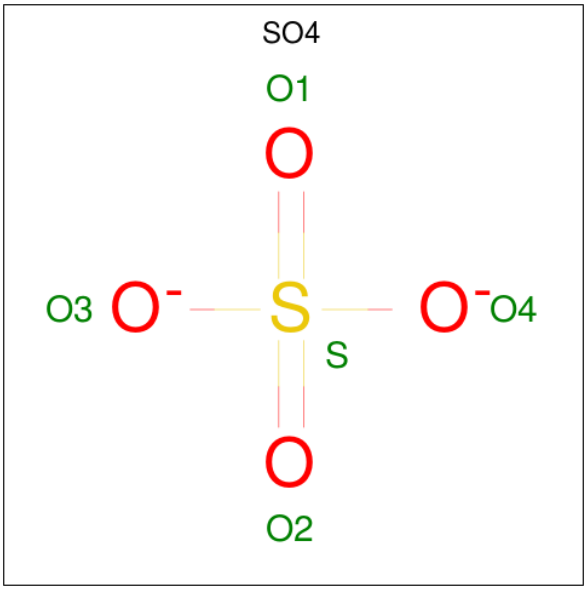
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	9	Total Yb 9 9	0	0
2	A	9	Total Yb 9 9	0	0
2	F	7	Total Yb 7 7	0	0

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



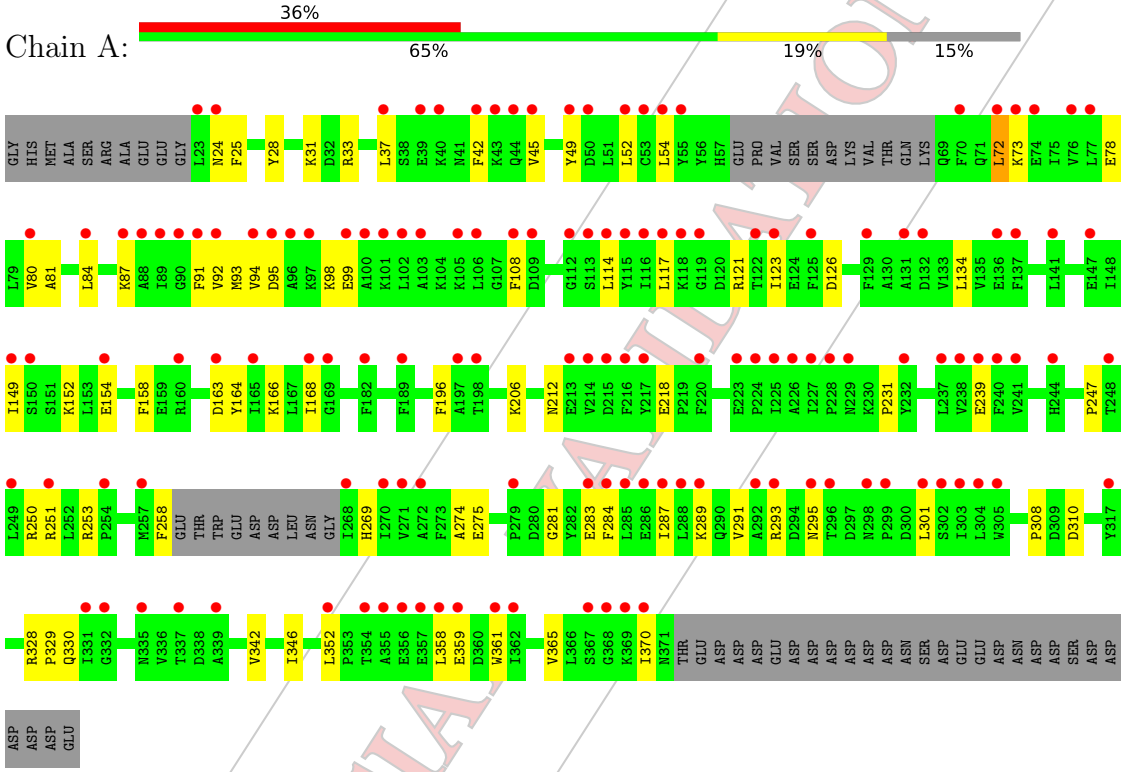
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

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 geometry and 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.

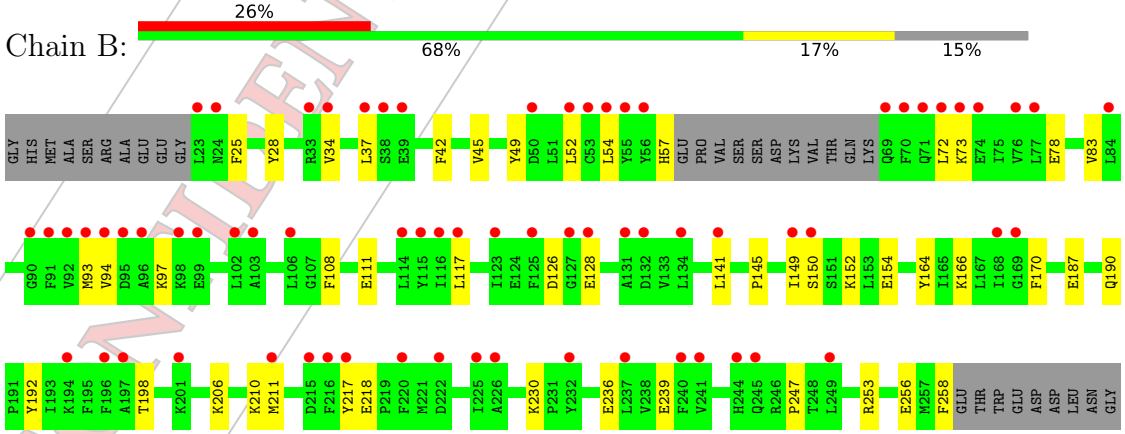
• Molecule 1: Calsequestrin-2

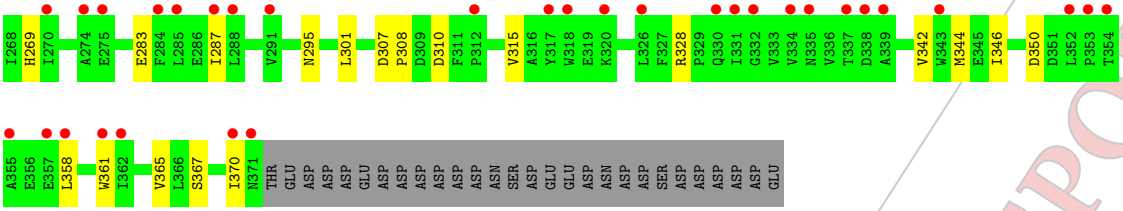
Chain A:



• Molecule 1: Calsequestrin-2

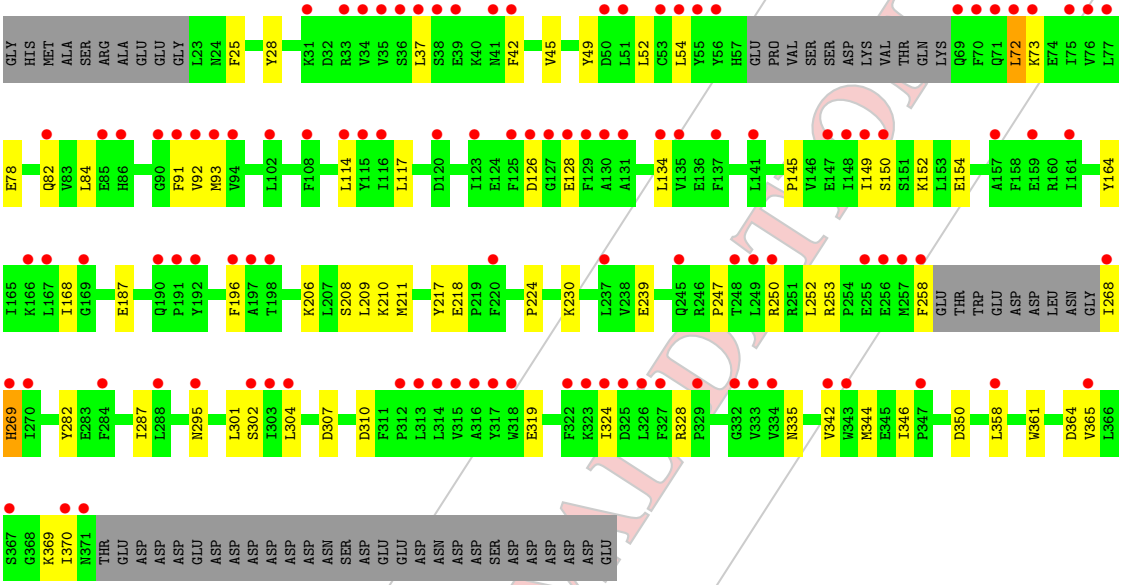
Chain B:





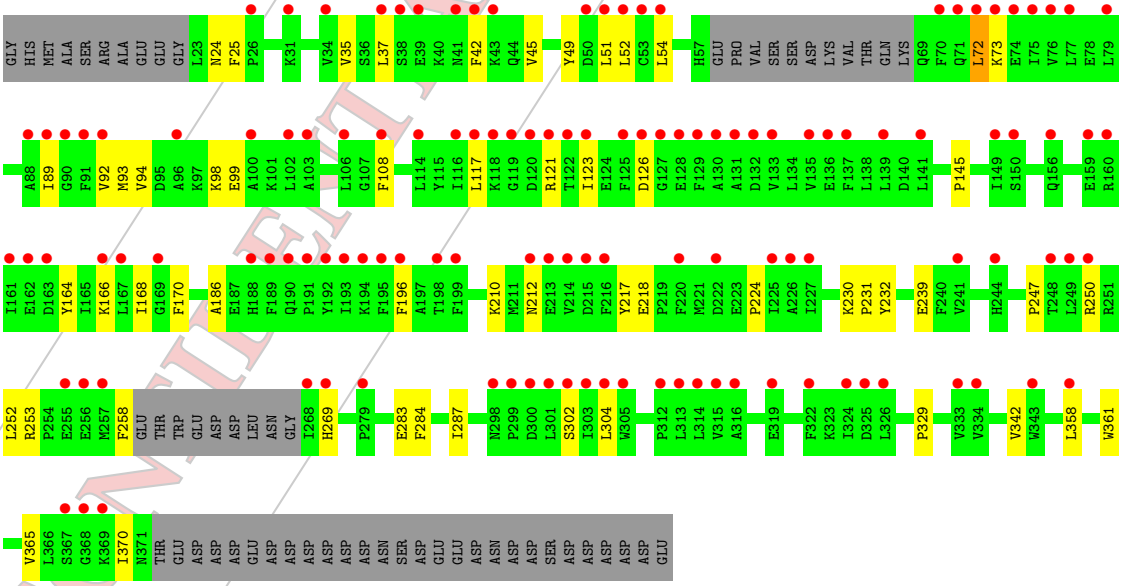
• Molecule 1: Calsequestrin-2

Chain C:



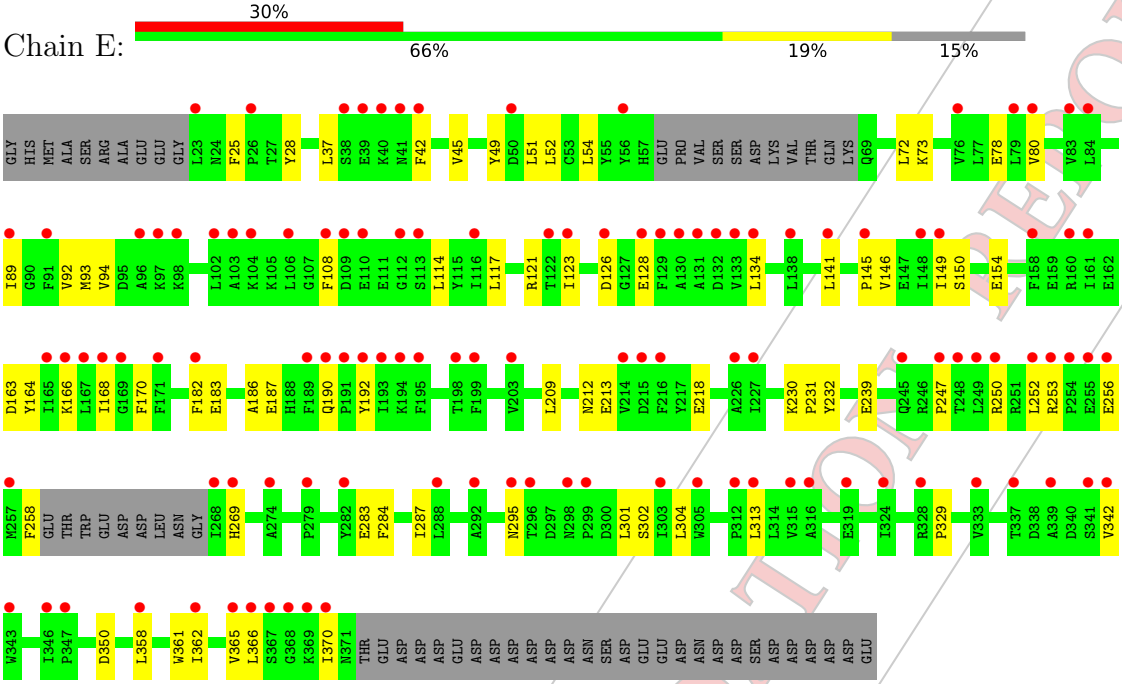
• Molecule 1: Calsequestrin-2

Chain D:



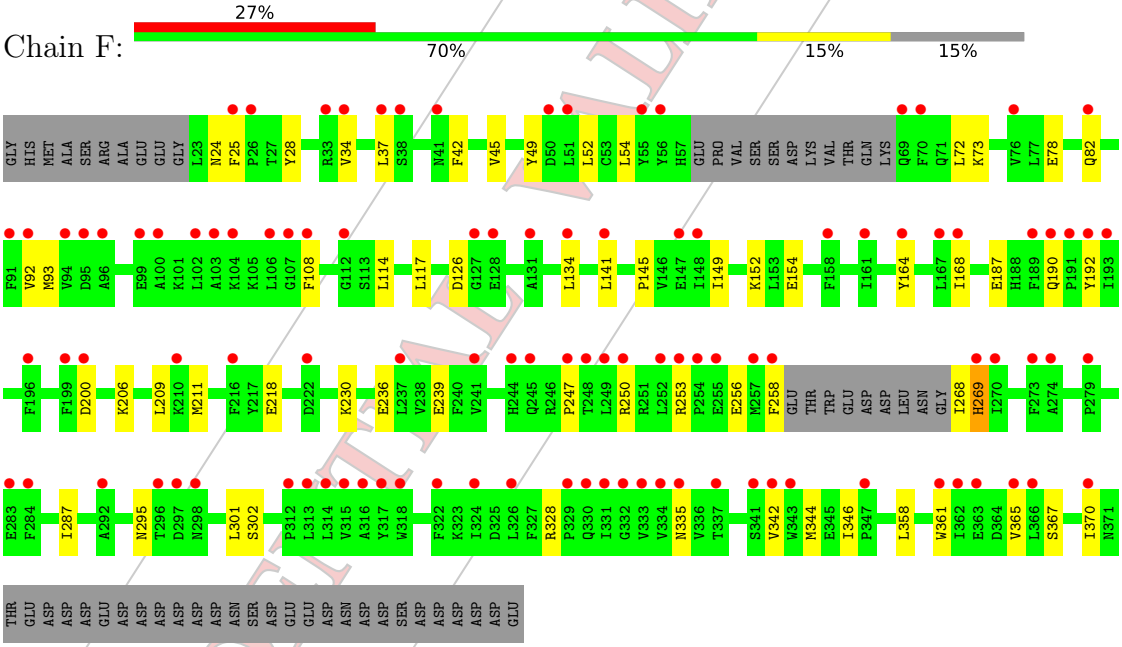
• Molecule 1: Calsequestrin-2

Chain E:



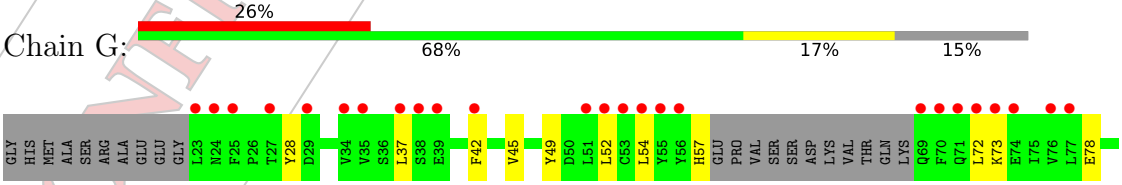
• Molecule 1: Calsequestrin-2

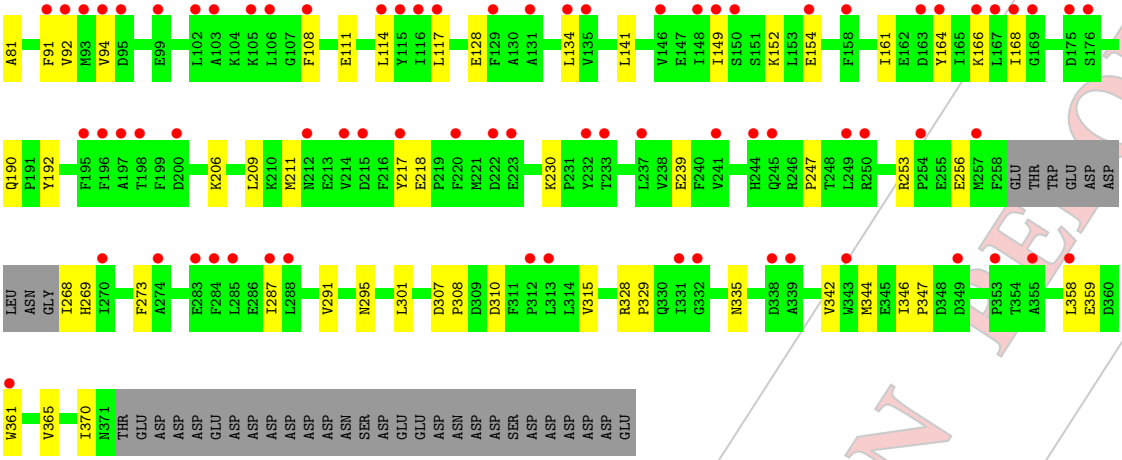
Chain F:



• Molecule 1: Calsequestrin-2

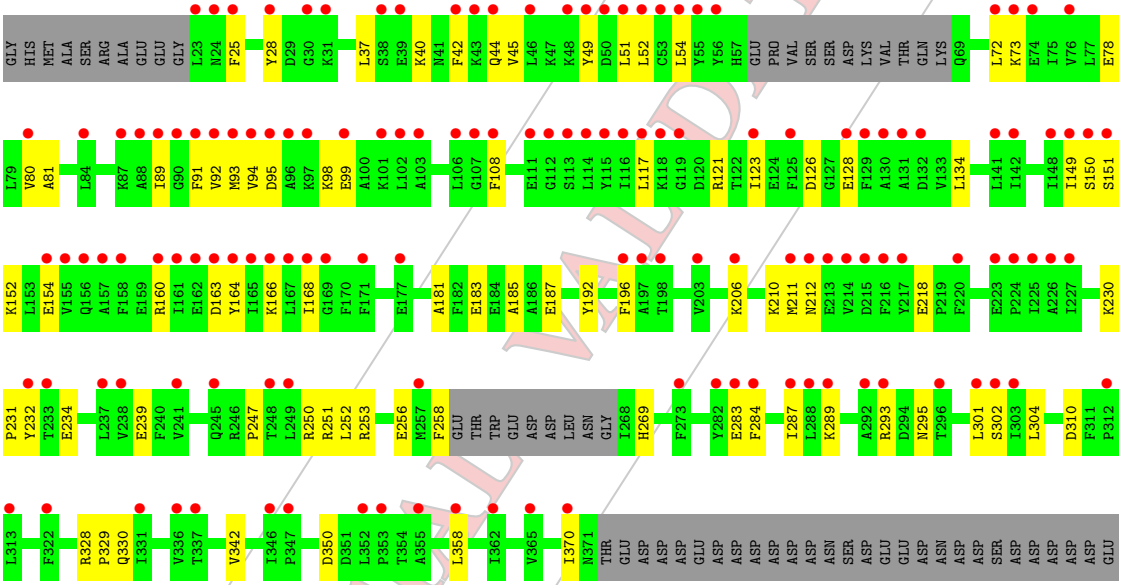
Chain G:





- 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)	214.34 – 3.84 214.34 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.4 (214.34-3.84) 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}	0.290 , 0.340 0.296 , 0.351	Depositor DCC
R_{free} test set	1440 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 , 81.2	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	0.86	EDS
Total number of atoms	21808	wwPDB-VP
Average B, all atoms (Å^2)	98.0	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

5.1 Standard geometry

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	0.38	0/2779	0.56	1/3758 (0.0%)
1	B	0.40	0/2779	0.57	0/3758
1	C	0.40	0/2779	0.58	1/3758 (0.0%)
1	D	0.39	0/2779	0.57	1/3758 (0.0%)
1	E	0.40	0/2779	0.56	0/3758
1	F	0.40	0/2779	0.58	0/3758
1	G	0.40	0/2779	0.56	0/3758
1	H	0.39	0/2779	0.57	0/3758
All	All	0.40	0/22232	0.57	3/30064 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	LEU	CA-CB-CG	5.98	129.05	115.30
1	D	72	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	72	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2715	0	2653	49	0
1	B	2715	0	2653	45	0
1	C	2715	0	2653	49	0
1	D	2715	0	2653	37	0
1	E	2715	0	2653	48	0
1	F	2715	0	2653	42	0
1	G	2715	0	2653	41	0
1	H	2715	0	2653	53	0
2	A	9	0	0	0	0
2	B	7	0	0	0	0
2	C	9	0	0	0	0
2	D	8	0	0	0	0
2	E	9	0	0	0	0
2	F	7	0	0	0	0
2	G	8	0	0	0	0
2	H	6	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
All	All	21808	0	21224	346	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 8.

All (346) 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:C:211:MET:O	1:C:230:LYS:NZ	2.19	0.76
1:F:211:MET:O	1:F:230:LYS:NZ	2.19	0.73
1:H:342:VAL:HG11	1:H:370:ILE:HG23	1.70	0.71
1:C:164:TYR:HD2	1:C:253:ARG:HH22	1.38	0.71
1:A:152:LYS:HB3	1:A:206:LYS:HE3	1.73	0.69
1:B:211:MET:O	1:B:230:LYS:NZ	2.25	0.69
1:G:211:MET:O	1:G:230:LYS:NZ	2.22	0.68
1:D:250:ARG:NH1	1:D:302:SER:OG	2.26	0.68
1:G:342:VAL:HG11	1:G:370:ILE:HG23	1.76	0.67
1:E:342:VAL:HG11	1:E:370:ILE:HG23	1.77	0.66
1:F:164:TYR:HD2	1:F:253:ARG:HH22	1.42	0.66
1:D:342:VAL:HG11	1:D:370:ILE:HG23	1.77	0.66
1:E:250:ARG:NH1	1:E:302:SER:OG	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TYR:HD2	1:A:253:ARG:HH22	1.45	0.65
1:A:342:VAL:HG11	1:A:370:ILE:HG23	1.79	0.64
1:B:164:TYR:HD2	1:B:253:ARG:HH22	1.45	0.64
1:G:161:ILE:O	1:G:166:LYS:NZ	2.23	0.64
1:B:52:LEU:HB2	1:B:117:LEU:HB2	1.79	0.63
1:F:287:ILE:HG22	1:F:358:LEU:HD12	1.79	0.63
1:B:287:ILE:HG22	1:B:358:LEU:HD12	1.81	0.62
1:F:342:VAL:HG11	1:F:370:ILE:HG23	1.81	0.62
1:H:212:ASN:HB3	1:H:231:PRO:HB3	1.80	0.62
1:C:52:LEU:HB2	1:C:117:LEU:HB2	1.81	0.62
1:C:287:ILE:HG22	1:C:358:LEU:HD12	1.82	0.61
1:A:251:ARG:NH2	1:A:310:ASP:OD2	2.28	0.60
1:A:218:GLU:OE1	1:A:247:PRO:HB3	2.02	0.60
1:B:37:LEU:HD11	1:B:42:PHE:HA	1.84	0.60
1:B:342:VAL:HG11	1:B:370:ILE:HG23	1.84	0.59
1:A:54:LEU:HG	1:A:92:VAL:HG23	1.84	0.59
1:F:168:ILE:HG23	1:F:209:LEU:HD11	1.84	0.59
1:H:250:ARG:NH1	1:H:302:SER:OG	2.36	0.59
1:A:72:LEU:HD12	1:A:73:LYS:HG3	1.85	0.59
1:C:218:GLU:OE1	1:C:247:PRO:HB3	2.03	0.59
1:E:72:LEU:HD12	1:E:73:LYS:HG3	1.85	0.58
1:E:126:ASP:HB3	1:E:258:PHE:HB3	1.85	0.58
1:H:121:ARG:NH1	1:H:123:ILE:HD11	2.18	0.58
1:A:80:VAL:HG21	1:A:134:LEU:HD23	1.86	0.58
1:E:247:PRO:HD2	1:E:250:ARG:HD3	1.86	0.58
1:B:149:ILE:HG23	1:B:154:GLU:HB3	1.85	0.58
1:D:247:PRO:HD2	1:D:250:ARG:HD3	1.85	0.58
1:G:152:LYS:HB3	1:G:206:LYS:HE3	1.86	0.58
1:C:149:ILE:HG23	1:C:154:GLU:HB3	1.86	0.57
1:E:218:GLU:OE1	1:E:247:PRO:HB3	2.03	0.57
1:F:218:GLU:OE1	1:F:247:PRO:HB3	2.05	0.57
1:B:72:LEU:HD12	1:B:73:LYS:HG3	1.86	0.57
1:H:72:LEU:HD12	1:H:73:LYS:HG3	1.86	0.57
1:G:168:ILE:HG23	1:G:209:LEU:HD11	1.85	0.57
1:C:342:VAL:HG11	1:C:370:ILE:HG23	1.85	0.57
1:G:287:ILE:HG22	1:G:358:LEU:HD12	1.85	0.57
1:B:152:LYS:HB3	1:B:206:LYS:HE3	1.87	0.56
1:A:84:LEU:HD22	1:A:87:LYS:HG3	1.85	0.56
1:F:52:LEU:HB2	1:F:117:LEU:HB2	1.86	0.56
1:B:367:SER:O	1:F:236:GLU:HA	2.04	0.56
1:D:72:LEU:HD12	1:D:73:LYS:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:TYR:CE1	1:G:78:GLU:HB3	2.40	0.56
1:H:149:ILE:HG23	1:H:154:GLU:HB3	1.88	0.56
1:A:283:GLU:O	1:A:287:ILE:HG12	2.06	0.56
1:A:126:ASP:HB3	1:A:258:PHE:HB3	1.88	0.55
1:D:54:LEU:HG	1:D:92:VAL:HG23	1.88	0.55
1:G:164:TYR:HD2	1:G:253:ARG:HH22	1.53	0.55
1:C:168:ILE:HG23	1:C:209:LEU:HD11	1.88	0.55
1:D:218:GLU:OE1	1:D:247:PRO:HB3	2.06	0.55
1:B:28:TYR:CE1	1:B:78:GLU:HB3	2.41	0.55
1:F:149:ILE:HG23	1:F:154:GLU:HB3	1.89	0.55
1:C:152:LYS:HB3	1:C:206:LYS:HE3	1.88	0.55
1:F:152:LYS:HB3	1:F:206:LYS:HE3	1.88	0.55
1:H:126:ASP:HB3	1:H:258:PHE:HB3	1.89	0.55
1:C:72:LEU:HD12	1:C:73:LYS:HG3	1.88	0.54
1:H:218:GLU:OE1	1:H:247:PRO:HB3	2.07	0.54
1:G:37:LEU:HD11	1:G:42:PHE:HA	1.89	0.54
1:G:149:ILE:HG23	1:G:154:GLU:HB3	1.88	0.54
1:G:52:LEU:HB2	1:G:117:LEU:HB2	1.88	0.54
1:B:141:LEU:HD23	1:B:190:GLN:HG2	1.90	0.54
1:C:45:VAL:HG13	1:C:49:TYR:CE2	2.43	0.53
1:H:80:VAL:HG21	1:H:134:LEU:HD23	1.89	0.53
1:A:149:ILE:HG23	1:A:154:GLU:HB3	1.91	0.53
1:E:287:ILE:HG22	1:E:358:LEU:HD12	1.91	0.53
1:H:54:LEU:HG	1:H:92:VAL:HG23	1.91	0.53
1:A:287:ILE:HG22	1:A:358:LEU:HD12	1.90	0.53
1:E:168:ILE:HG23	1:E:209:LEU:HD11	1.91	0.53
1:G:308:PRO:HA	1:G:315:VAL:HG21	1.90	0.53
1:G:328:ARG:NH1	1:G:346:ILE:O	2.41	0.53
1:H:37:LEU:HD11	1:H:42:PHE:HA	1.91	0.53
1:E:54:LEU:HG	1:E:92:VAL:HG23	1.91	0.52
1:C:344:MET:HG3	1:C:361:TRP:CD1	2.44	0.52
1:E:37:LEU:HD11	1:E:42:PHE:HA	1.91	0.52
1:F:37:LEU:HD11	1:F:42:PHE:HA	1.91	0.52
1:B:236:GLU:HA	1:F:367:SER:O	2.10	0.52
1:H:247:PRO:HD2	1:H:250:ARG:HD3	1.91	0.52
1:F:268:ILE:HD12	1:F:335:ASN:HA	1.91	0.52
1:D:126:ASP:HB3	1:D:258:PHE:HB3	1.92	0.52
1:H:287:ILE:HG22	1:H:358:LEU:HD12	1.92	0.52
1:G:218:GLU:OE1	1:G:247:PRO:HB3	2.09	0.52
1:E:212:ASN:HB3	1:E:231:PRO:HB3	1.92	0.52
1:G:72:LEU:HD12	1:G:73:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:MET:HG3	1:B:361:TRP:CD1	2.45	0.52
1:F:72:LEU:HD12	1:F:73:LYS:HG3	1.92	0.51
1:F:114:LEU:HD23	1:F:134:LEU:HD11	1.92	0.51
1:C:37:LEU:HD11	1:C:42:PHE:HA	1.92	0.51
1:G:57:HIS:ND1	1:G:111:GLU:OE2	2.43	0.51
1:H:251:ARG:NH2	1:H:310:ASP:OD2	2.38	0.51
1:E:252:LEU:HD13	1:E:304:LEU:HD21	1.91	0.51
1:F:344:MET:HG3	1:F:361:TRP:CD1	2.46	0.51
1:C:328:ARG:NH1	1:C:346:ILE:O	2.37	0.50
1:E:45:VAL:HG13	1:E:49:TYR:CE2	2.45	0.50
1:A:37:LEU:HD11	1:A:42:PHE:HA	1.94	0.50
1:C:45:VAL:HG13	1:C:49:TYR:HE2	1.74	0.50
1:C:28:TYR:CE1	1:C:78:GLU:HB3	2.46	0.50
1:D:252:LEU:HD13	1:D:304:LEU:HD21	1.92	0.50
1:F:328:ARG:NH1	1:F:346:ILE:O	2.35	0.50
1:B:308:PRO:HA	1:B:315:VAL:HG21	1.94	0.50
1:E:149:ILE:HG23	1:E:154:GLU:HB3	1.94	0.50
1:D:25:PHE:CZ	1:G:128:GLU:HB2	2.48	0.49
1:C:128:GLU:HB2	1:H:25:PHE:CZ	2.47	0.49
1:G:307:ASP:HB3	1:G:310:ASP:OD2	2.12	0.49
1:H:28:TYR:CE1	1:H:78:GLU:HB3	2.47	0.49
1:A:164:TYR:CE1	1:A:166:LYS:HG2	2.48	0.49
1:B:350:ASP:CG	1:E:150:SER:HB2	2.33	0.49
1:D:247:PRO:HG2	1:D:250:ARG:HB3	1.94	0.48
1:A:247:PRO:HD2	1:A:250:ARG:HD3	1.94	0.48
1:B:295:ASN:HB2	1:B:301:LEU:HD23	1.93	0.48
1:F:45:VAL:HG13	1:F:49:TYR:CE2	2.49	0.48
1:G:114:LEU:HD23	1:G:134:LEU:HD11	1.95	0.48
1:G:54:LEU:HD13	1:G:117:LEU:HG	1.94	0.48
1:F:28:TYR:HA	1:F:82:GLN:OE1	2.13	0.48
1:H:163:ASP:HB3	1:H:253:ARG:HH21	1.78	0.48
1:C:210:LYS:HB3	1:C:230:LYS:HZ1	1.79	0.48
1:C:307:ASP:HB3	1:C:310:ASP:OD2	2.12	0.48
1:E:80:VAL:HG21	1:E:134:LEU:HD23	1.95	0.48
1:F:200:ASP:OD1	1:G:347:PRO:HB3	2.13	0.48
1:D:37:LEU:HD11	1:D:42:PHE:HA	1.96	0.48
1:G:45:VAL:HG13	1:G:49:TYR:CE2	2.49	0.48
1:C:250:ARG:NH1	1:C:302:SER:OG	2.47	0.48
1:H:192:TYR:CE1	1:H:256:GLU:HA	2.49	0.48
1:A:289:LYS:HB3	1:A:293:ARG:HH12	1.79	0.47
1:E:45:VAL:HG13	1:E:49:TYR:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:ASN:HB2	1:G:301:LEU:HD23	1.96	0.47
1:B:45:VAL:HG13	1:B:49:TYR:CE2	2.50	0.47
1:E:145:PRO:HB2	1:E:186:ALA:HB1	1.95	0.47
1:B:210:LYS:HB3	1:B:230:LYS:NZ	2.30	0.47
1:A:212:ASN:HB3	1:A:231:PRO:HB3	1.96	0.47
1:A:275:GLU:HG2	1:A:308:PRO:HD2	1.95	0.47
1:H:54:LEU:HD23	1:H:94:VAL:HG21	1.97	0.47
1:A:328:ARG:O	1:A:330:GLN:HG2	2.15	0.47
1:D:210:LYS:HB3	1:D:230:LYS:HZ3	1.80	0.47
1:D:287:ILE:HG22	1:D:358:LEU:HD12	1.95	0.47
1:E:54:LEU:HD13	1:E:117:LEU:HG	1.96	0.47
1:A:328:ARG:NH1	1:A:346:ILE:O	2.47	0.47
1:D:93:MET:HB3	1:D:93:MET:HE2	1.73	0.47
1:C:145:PRO:HG2	1:C:187:GLU:HG2	1.96	0.47
1:A:54:LEU:HD13	1:A:117:LEU:HG	1.97	0.47
1:D:145:PRO:HB2	1:D:186:ALA:HB1	1.96	0.47
1:B:57:HIS:ND1	1:B:111:GLU:OE2	2.48	0.47
1:D:54:LEU:HD22	1:D:108:PHE:HZ	1.80	0.47
1:F:141:LEU:HD23	1:F:190:GLN:HG2	1.97	0.47
1:H:164:TYR:CE1	1:H:166:LYS:HG2	2.50	0.47
1:H:247:PRO:HG2	1:H:250:ARG:HB3	1.97	0.47
1:A:54:LEU:HD22	1:A:108:PHE:HZ	1.80	0.46
1:F:54:LEU:HD22	1:F:108:PHE:HZ	1.79	0.46
1:G:268:ILE:HD12	1:G:335:ASN:HA	1.96	0.46
1:G:344:MET:HG3	1:G:361:TRP:CD1	2.49	0.46
1:E:54:LEU:HD23	1:E:94:VAL:HG21	1.97	0.46
1:G:54:LEU:HD22	1:G:108:PHE:HZ	1.80	0.46
1:C:114:LEU:HD23	1:C:134:LEU:HD11	1.97	0.46
1:C:54:LEU:HG	1:C:92:VAL:HG23	1.97	0.46
1:G:291:VAL:HG13	1:G:359:GLU:HG3	1.98	0.46
1:A:168:ILE:HA	1:A:196:PHE:O	2.16	0.46
1:G:72:LEU:HD12	1:G:73:LYS:N	2.31	0.46
1:H:152:LYS:HB3	1:H:206:LYS:HE3	1.97	0.46
1:D:212:ASN:HB3	1:D:231:PRO:HB3	1.98	0.46
1:G:54:LEU:HD22	1:G:108:PHE:CZ	2.51	0.46
1:G:141:LEU:HD23	1:G:190:GLN:HG2	1.98	0.46
1:H:40:LYS:NZ	1:H:44:GLN:OE1	2.49	0.46
1:C:54:LEU:HD13	1:C:117:LEU:HG	1.98	0.45
1:G:361:TRP:O	1:G:365:VAL:HG23	2.15	0.45
1:B:34:VAL:HG12	1:B:93:MET:HG2	1.97	0.45
1:B:93:MET:HE2	1:B:93:MET:HB3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ASP:HB3	1:E:253:ARG:HH21	1.81	0.45
1:E:230:LYS:HB3	1:E:232:TYR:OH	2.16	0.45
1:F:54:LEU:HG	1:F:92:VAL:HG23	1.98	0.45
1:A:93:MET:HE2	1:A:93:MET:HB3	1.76	0.45
1:E:283:GLU:O	1:E:287:ILE:HG12	2.16	0.45
1:F:54:LEU:HD22	1:F:108:PHE:CZ	2.51	0.45
1:D:121:ARG:NH1	1:D:123:ILE:HD11	2.32	0.45
1:A:81:ALA:HA	1:A:91:PHE:CE1	2.51	0.45
1:A:94:VAL:HG13	1:A:99:GLU:HB2	1.98	0.45
1:B:218:GLU:OE1	1:B:247:PRO:HB3	2.17	0.45
1:D:361:TRP:O	1:D:365:VAL:HG23	2.17	0.45
1:H:81:ALA:HA	1:H:91:PHE:CE1	2.52	0.45
1:A:295:ASN:HB2	1:A:301:LEU:HD23	1.99	0.45
1:A:284:PHE:HB2	1:A:352:LEU:HD13	1.99	0.45
1:D:54:LEU:HD23	1:D:94:VAL:HG21	1.99	0.45
1:H:181:ALA:HB1	1:H:234:GLU:N	2.32	0.45
1:B:192:TYR:CE1	1:B:256:GLU:HA	2.51	0.45
1:E:361:TRP:O	1:E:365:VAL:HG23	2.17	0.45
1:E:51:LEU:HB2	1:E:89:ILE:HG12	1.99	0.45
1:F:54:LEU:HD13	1:F:117:LEU:HG	1.98	0.45
1:G:273:PHE:O	1:G:329:PRO:HA	2.17	0.45
1:D:230:LYS:HB3	1:D:232:TYR:OH	2.16	0.45
1:E:295:ASN:HB2	1:E:301:LEU:HD23	1.97	0.45
1:F:145:PRO:HG2	1:F:187:GLU:HG2	1.99	0.45
1:H:283:GLU:O	1:H:287:ILE:HG12	2.17	0.45
1:H:93:MET:HE2	1:H:93:MET:HB3	1.72	0.45
1:B:166:LYS:HB2	1:B:217:TYR:HB2	1.98	0.45
1:F:28:TYR:CE1	1:F:78:GLU:HB3	2.52	0.45
1:G:81:ALA:HA	1:G:91:PHE:CE1	2.52	0.45
1:H:95:ASP:HB3	1:H:98:LYS:HB3	1.98	0.45
1:D:52:LEU:HB2	1:D:117:LEU:HB2	1.98	0.44
1:E:52:LEU:HB2	1:E:117:LEU:HB2	1.98	0.44
1:F:45:VAL:HG13	1:F:49:TYR:HE2	1.81	0.44
1:B:126:ASP:HB3	1:B:258:PHE:HD2	1.83	0.44
1:B:361:TRP:O	1:B:365:VAL:HG23	2.17	0.44
1:C:168:ILE:HA	1:C:196:PHE:O	2.18	0.44
1:C:84:LEU:HD12	1:C:91:PHE:HZ	1.82	0.44
1:E:54:LEU:HD22	1:E:108:PHE:HZ	1.82	0.44
1:E:284:PHE:CG	1:E:329:PRO:HB3	2.53	0.44
1:F:295:ASN:HB2	1:F:301:LEU:HD23	2.00	0.44
1:D:283:GLU:OE1	1:G:154:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASP:CG	1:H:150:SER:HB2	2.38	0.44
1:F:126:ASP:HB3	1:F:258:PHE:CD2	2.52	0.44
1:C:350:ASP:O	1:H:151:SER:HB2	2.18	0.44
1:H:230:LYS:HB3	1:H:232:TYR:OH	2.17	0.44
1:B:308:PRO:HB3	1:B:315:VAL:HG11	2.00	0.44
1:H:52:LEU:HB2	1:H:117:LEU:HB2	1.99	0.44
1:C:268:ILE:HG22	1:C:269:HIS:ND1	2.33	0.44
1:E:121:ARG:NH1	1:E:123:ILE:HD11	2.33	0.44
1:G:166:LYS:HB2	1:G:217:TYR:HB2	1.98	0.44
1:G:54:LEU:HG	1:G:92:VAL:HG23	2.00	0.44
1:G:54:LEU:HD23	1:G:94:VAL:HG21	2.00	0.44
1:B:25:PHE:CZ	1:E:128:GLU:HB2	2.53	0.44
1:F:126:ASP:HB3	1:F:258:PHE:HD2	1.83	0.44
1:F:192:TYR:CE1	1:F:256:GLU:HA	2.53	0.44
1:H:183:GLU:O	1:H:187:GLU:HG3	2.18	0.44
1:A:247:PRO:HG2	1:A:250:ARG:HB3	2.00	0.43
1:A:163:ASP:HB3	1:A:253:ARG:HH21	1.83	0.43
1:H:168:ILE:HA	1:H:196:PHE:O	2.18	0.43
1:A:28:TYR:CE1	1:A:78:GLU:HB3	2.53	0.43
1:A:54:LEU:HG	1:A:92:VAL:CG2	2.49	0.43
1:B:72:LEU:HD12	1:B:73:LYS:N	2.33	0.43
1:C:361:TRP:O	1:C:365:VAL:HG23	2.19	0.43
1:D:51:LEU:HB2	1:D:89:ILE:HG12	2.01	0.43
1:E:28:TYR:CE1	1:E:78:GLU:HB3	2.53	0.43
1:H:52:LEU:HD23	1:H:52:LEU:HA	1.79	0.43
1:D:24:ASN:HB3	1:D:25:PHE:H	1.69	0.43
1:E:93:MET:HE2	1:E:93:MET:HB3	1.73	0.43
1:H:54:LEU:HD22	1:H:108:PHE:HZ	1.83	0.43
1:A:361:TRP:O	1:A:365:VAL:HG23	2.19	0.43
1:E:141:LEU:HD23	1:E:190:GLN:HG2	2.00	0.43
1:A:95:ASP:HB3	1:A:98:LYS:HB3	2.00	0.43
1:H:211:MET:O	1:H:230:LYS:NZ	2.47	0.43
1:D:170:PHE:O	1:D:212:ASN:N	2.43	0.43
1:F:268:ILE:HG22	1:F:269:HIS:ND1	2.33	0.43
1:F:361:TRP:O	1:F:365:VAL:HG23	2.19	0.43
1:A:45:VAL:HG13	1:A:49:TYR:CE2	2.54	0.43
1:D:54:LEU:HD13	1:D:117:LEU:HG	2.00	0.43
1:E:183:GLU:O	1:E:187:GLU:HG3	2.19	0.43
1:C:25:PHE:CZ	1:H:128:GLU:HB2	2.54	0.43
1:B:150:SER:HB2	1:E:350:ASP:CG	2.38	0.42
1:B:145:PRO:HG2	1:B:187:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:TYR:CZ	1:C:224:PRO:HB3	2.54	0.42
1:B:328:ARG:NH1	1:B:346:ILE:O	2.38	0.42
1:B:54:LEU:HD22	1:B:108:PHE:CZ	2.54	0.42
1:D:168:ILE:HA	1:D:196:PHE:O	2.18	0.42
1:F:72:LEU:HD12	1:F:73:LYS:N	2.33	0.42
1:B:45:VAL:HG13	1:B:49:TYR:HE2	1.84	0.42
1:C:252:LEU:HB2	1:C:304:LEU:HD11	2.01	0.42
1:E:284:PHE:CD2	1:E:329:PRO:HB3	2.54	0.42
1:E:72:LEU:HD12	1:E:73:LYS:N	2.34	0.42
1:H:45:VAL:HG13	1:H:49:TYR:CE2	2.54	0.42
1:D:54:LEU:HD22	1:D:108:PHE:CZ	2.54	0.42
1:B:128:GLU:HB2	1:E:25:PHE:CZ	2.53	0.42
1:A:114:LEU:HD23	1:A:134:LEU:HD11	2.02	0.42
1:B:170:PHE:HA	1:B:198:THR:O	2.19	0.42
1:B:283:GLU:O	1:B:287:ILE:HG12	2.19	0.42
1:E:247:PRO:HG2	1:E:250:ARG:HB3	2.01	0.42
1:D:164:TYR:CE1	1:D:166:LYS:HG2	2.55	0.42
1:E:213:GLU:HB2	1:E:230:LYS:HD3	2.02	0.42
1:H:284:PHE:CG	1:H:329:PRO:HB3	2.55	0.42
1:H:94:VAL:HG13	1:H:99:GLU:HB2	2.02	0.42
1:C:319:GLU:HG2	1:C:324:ILE:O	2.18	0.42
1:E:164:TYR:CE1	1:E:166:LYS:HG2	2.55	0.42
1:G:45:VAL:HG13	1:G:49:TYR:HE2	1.85	0.42
1:H:164:TYR:HD2	1:H:253:ARG:HH22	1.66	0.42
1:C:150:SER:HB2	1:H:350:ASP:CG	2.40	0.42
1:C:126:ASP:HB3	1:C:258:PHE:HD2	1.85	0.42
1:D:94:VAL:HG13	1:D:99:GLU:HB2	2.01	0.42
1:H:252:LEU:HD13	1:H:304:LEU:HD21	2.01	0.42
1:A:24:ASN:HB3	1:A:25:PHE:H	1.68	0.42
1:D:284:PHE:CG	1:D:329:PRO:HB3	2.55	0.42
1:F:24:ASN:HB3	1:F:25:PHE:H	1.69	0.42
1:B:126:ASP:HB3	1:B:258:PHE:CD2	2.54	0.42
1:C:268:ILE:HD12	1:C:335:ASN:HA	2.02	0.42
1:D:35:VAL:O	1:D:92:VAL:HA	2.20	0.42
1:B:83:VAL:HG21	1:E:313:LEU:HD11	2.01	0.42
1:H:51:LEU:HB2	1:H:89:ILE:HG12	2.01	0.42
1:C:126:ASP:HB3	1:C:258:PHE:CD2	2.55	0.41
1:C:364:ASP:O	1:C:369:LYS:HB2	2.19	0.41
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.79	0.41
1:E:114:LEU:HD23	1:E:134:LEU:HD11	2.01	0.41
1:F:93:MET:HB3	1:F:93:MET:HE2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:VAL:HG12	1:G:52:LEU:HD21	2.02	0.41
1:A:281:GLY:HA2	1:A:329:PRO:HG3	2.01	0.41
1:B:210:LYS:HB3	1:B:230:LYS:HZ1	1.86	0.41
1:A:289:LYS:HB3	1:A:293:ARG:NH1	2.36	0.41
1:C:72:LEU:HD12	1:C:73:LYS:N	2.35	0.41
1:E:362:ILE:O	1:E:366:LEU:HG	2.21	0.41
1:F:54:LEU:O	1:F:114:LEU:HD12	2.20	0.41
1:A:158:PHE:HE1	1:A:196:PHE:CD1	2.39	0.41
1:A:284:PHE:CD2	1:A:329:PRO:HB3	2.55	0.41
1:F:250:ARG:NH1	1:F:302:SER:OG	2.53	0.41
1:D:164:TYR:HD2	1:D:253:ARG:HH22	1.68	0.41
1:A:121:ARG:NH1	1:A:123:ILE:HD11	2.36	0.41
1:C:295:ASN:HB2	1:C:301:LEU:HD23	2.02	0.41
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.86	0.41
1:F:200:ASP:CG	1:G:347:PRO:HB3	2.41	0.41
1:C:282:TYR:OH	1:H:160:ARG:HD3	2.21	0.41
1:A:274:ALA:HB1	1:A:281:GLY:O	2.20	0.41
1:A:291:VAL:HG13	1:A:359:GLU:HG3	2.03	0.41
1:B:54:LEU:HD23	1:B:94:VAL:HG21	2.02	0.41
1:H:295:ASN:HB2	1:H:301:LEU:HD23	2.02	0.41
1:H:328:ARG:O	1:H:330:GLN:HG2	2.20	0.41
1:A:126:ASP:HB3	1:A:258:PHE:CD2	2.56	0.41
1:C:37:LEU:HD21	1:C:42:PHE:HD1	1.86	0.41
1:D:217:TYR:CZ	1:D:224:PRO:HB3	2.56	0.41
1:E:146:VAL:HG13	1:E:182:PHE:HE2	1.86	0.41
1:G:192:TYR:CE1	1:G:256:GLU:HA	2.55	0.41
1:H:72:LEU:HD12	1:H:73:LYS:N	2.36	0.41
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.86	0.40
1:B:54:LEU:HD13	1:B:117:LEU:HG	2.02	0.40
1:D:45:VAL:HG13	1:D:49:TYR:CE2	2.55	0.40
1:B:307:ASP:HB3	1:B:310:ASP:OD2	2.20	0.40
1:B:57:HIS:CE1	1:B:97:LYS:HE2	2.56	0.40
1:F:247:PRO:HD2	1:F:250:ARG:HD3	2.02	0.40
1:A:31:LYS:HB3	1:A:33:ARG:NH1	2.36	0.40
1:C:28:TYR:HA	1:C:82:GLN:OE1	2.21	0.40
1:E:170:PHE:O	1:E:212:ASN:N	2.46	0.40
1:H:210:LYS:HB3	1:H:230:LYS:HZ3	1.87	0.40
1:H:185:ALA:N	1:H:234:GLU:HG3	2.36	0.40
1:C:208:SER:OG	1:D:98:LYS:HE3	2.21	0.40
1:C:247:PRO:HG2	1:C:250:ARG:HB3	2.03	0.40
1:C:93:MET:HE2	1:C:93:MET:HB3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:VAL:HG12	1:F:93:MET:HG2	2.04	0.40
1:H:289:LYS:HB3	1:H:293:ARG:HH12	1.86	0.40
1:A:54:LEU:HD23	1:A:94:VAL:HG21	2.02	0.40
1:E:192:TYR:CE1	1:E:256:GLU:HA	2.57	0.40
1:H:54:LEU:HD13	1:H:117:LEU:HG	2.04	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%)	309 (96%)	14 (4%)	0	100	100
1	B	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	C	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	D	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	E	323/387 (84%)	309 (96%)	14 (4%)	0	100	100
1	F	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	G	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	H	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
All	All	2584/3096 (84%)	2478 (96%)	106 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	B	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	C	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	D	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	E	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	F	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	G	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	H	297/351 (85%)	295 (99%)	2 (1%)	85	93
All	All	2376/2808 (85%)	2360 (99%)	16 (1%)	85	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	269	HIS
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	HIS
1	F	188	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 68 ligands modelled in this entry, 63 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	B	408	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	H	407	-	4,4,4	0.16	0	6,6,6	0.19	0
3	SO4	D	409	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	F	408	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	410	2	4,4,4	0.15	0	6,6,6	0.15	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%)	2.15	139 (42%)	0 0	69, 99, 134, 141	0
1	B	329/387 (85%)	1.46	101 (30%)	0 0	54, 89, 137, 152	0
1	C	329/387 (85%)	1.53	110 (33%)	0 0	51, 87, 132, 154	0
1	D	329/387 (85%)	1.79	125 (37%)	0 0	57, 99, 133, 146	0
1	E	329/387 (85%)	1.64	116 (35%)	0 0	56, 97, 137, 148	0
1	F	329/387 (85%)	1.43	105 (31%)	0 0	48, 91, 133, 160	0
1	G	329/387 (85%)	1.40	99 (30%)	0 0	50, 92, 132, 156	0
1	H	329/387 (85%)	2.01	139 (42%)	0 0	61, 96, 133, 143	0
All	All	2632/3096 (85%)	1.68	934 (35%)	0 0	48, 94, 135, 160	0

All (934) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ALA	13.0
1	H	115	TYR	11.6
1	H	150	SER	10.5
1	D	257	MET	10.4
1	A	96	ALA	10.4
1	E	248	THR	9.6
1	H	113	SER	9.3
1	E	257	MET	9.3
1	C	127	GLY	8.9
1	H	114	LEU	8.9
1	C	92	VAL	8.7
1	A	114	LEU	8.7
1	D	190	GLN	8.6
1	C	128	GLU	8.6
1	A	169	GLY	8.6
1	C	93	MET	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	215	ASP	8.4
1	G	54	LEU	8.2
1	A	95	ASP	8.0
1	G	73	LYS	8.0
1	A	116	ILE	7.9
1	H	53	CYS	7.9
1	A	23	LEU	7.9
1	C	257	MET	7.8
1	E	128	GLU	7.8
1	A	115	TYR	7.8
1	H	102	LEU	7.7
1	H	112	GLY	7.7
1	H	54	LEU	7.6
1	G	92	VAL	7.6
1	B	71	GLN	7.6
1	D	128	GLU	7.6
1	H	212	ASN	7.5
1	D	248	THR	7.4
1	A	102	LEU	7.4
1	A	113	SER	7.3
1	H	88	ALA	7.3
1	D	53	CYS	7.2
1	A	97	LYS	7.2
1	G	116	ILE	7.2
1	A	55	TYR	7.2
1	E	249	LEU	7.1
1	B	55	TYR	7.1
1	H	129	PHE	7.0
1	A	227	ILE	7.0
1	A	150	SER	7.0
1	H	169	GLY	6.9
1	H	96	ALA	6.9
1	D	302	SER	6.9
1	D	191	PRO	6.7
1	E	190	GLN	6.6
1	A	283	GLU	6.6
1	A	198	THR	6.6
1	F	191	PRO	6.5
1	G	55	TYR	6.5
1	H	149	ILE	6.5
1	G	94	VAL	6.4
1	H	92	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	LEU	6.4
1	F	108	PHE	6.4
1	F	315	VAL	6.4
1	C	71	GLN	6.3
1	G	53	CYS	6.3
1	H	302	SER	6.2
1	D	71	GLN	6.2
1	A	149	ILE	6.2
1	E	192	TYR	6.2
1	G	93	MET	6.2
1	H	44	GLN	6.2
1	D	192	TYR	6.1
1	D	90	GLY	6.1
1	H	226	ALA	6.0
1	D	256	GLU	6.0
1	F	128	GLU	6.0
1	B	94	VAL	6.0
1	F	318	TRP	6.0
1	C	269	HIS	6.0
1	H	215	ASP	6.0
1	D	102	LEU	5.9
1	G	70	PHE	5.9
1	A	216	PHE	5.9
1	A	117	LEU	5.9
1	H	248	THR	5.8
1	D	91	PHE	5.8
1	E	108	PHE	5.8
1	H	168	ILE	5.8
1	A	355	ALA	5.8
1	A	225	ILE	5.7
1	G	56	TYR	5.7
1	E	226	ALA	5.7
1	H	283	GLU	5.7
1	C	37	LEU	5.7
1	F	94	VAL	5.7
1	D	324	ILE	5.7
1	H	55	TYR	5.7
1	D	74	GLU	5.7
1	E	193	ILE	5.7
1	B	92	VAL	5.6
1	E	367	SER	5.6
1	A	214	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	5.6
1	C	94	VAL	5.5
1	G	114	LEU	5.5
1	H	296	THR	5.5
1	C	334	VAL	5.5
1	C	258	PHE	5.5
1	F	192	TYR	5.5
1	E	191	PRO	5.4
1	C	54	LEU	5.4
1	B	96	ALA	5.4
1	B	149	ILE	5.4
1	D	268	ILE	5.4
1	B	23	LEU	5.4
1	C	192	TYR	5.4
1	H	198	THR	5.4
1	B	95	ASP	5.4
1	B	91	PHE	5.4
1	A	359	GLU	5.3
1	C	75	ILE	5.3
1	C	191	PRO	5.3
1	D	301	LEU	5.3
1	H	116	ILE	5.3
1	D	129	PHE	5.2
1	E	130	ALA	5.2
1	A	129	PHE	5.2
1	E	102	LEU	5.2
1	H	119	GLY	5.2
1	D	70	PHE	5.1
1	G	76	VAL	5.1
1	G	212	ASN	5.1
1	C	91	PHE	5.1
1	F	314	LEU	5.1
1	A	286	GLU	5.1
1	B	102	LEU	5.1
1	G	102	LEU	5.1
1	H	237	LEU	5.1
1	E	141	LEU	5.1
1	C	333	VAL	5.1
1	E	131	ALA	5.1
1	D	42	PHE	5.1
1	F	257	MET	5.1
1	D	125	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	129	PHE	5.0
1	C	318	TRP	5.0
1	D	39	GLU	5.0
1	F	95	ASP	5.0
1	B	114	LEU	4.9
1	A	132	ASP	4.9
1	E	109	ASP	4.9
1	E	41	ASN	4.9
1	B	54	LEU	4.9
1	D	249	LEU	4.9
1	A	125	PHE	4.9
1	B	38	SER	4.9
1	H	117	LEU	4.9
1	H	301	LEU	4.9
1	B	196	PHE	4.9
1	G	52	LEU	4.9
1	A	100	ALA	4.9
1	H	56	TYR	4.9
1	A	358	LEU	4.9
1	A	303	ILE	4.9
1	F	190	GLN	4.9
1	B	116	ILE	4.9
1	F	50	ASP	4.8
1	A	112	GLY	4.8
1	E	40	LYS	4.8
1	F	107	GLY	4.8
1	E	366	LEU	4.8
1	D	226	ALA	4.8
1	A	248	THR	4.8
1	D	73	LYS	4.8
1	D	130	ALA	4.8
1	A	123	ILE	4.8
1	A	357	GLU	4.8
1	A	91	PHE	4.7
1	B	106	LEU	4.7
1	E	292	ALA	4.7
1	A	295	ASN	4.7
1	B	72	LEU	4.7
1	A	39	GLU	4.7
1	D	88	ALA	4.7
1	G	115	TYR	4.7
1	A	339	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	313	LEU	4.7
1	B	354	THR	4.7
1	H	99	GLU	4.7
1	D	250	ARG	4.7
1	H	216	PHE	4.6
1	H	303	ILE	4.6
1	D	54	LEU	4.6
1	B	361	TRP	4.6
1	B	99	GLU	4.6
1	C	53	CYS	4.6
1	E	149	ILE	4.5
1	A	53	CYS	4.5
1	A	136	GLU	4.5
1	G	77	LEU	4.5
1	H	52	LEU	4.5
1	C	324	ILE	4.5
1	H	23	LEU	4.5
1	D	215	ASP	4.5
1	A	302	SER	4.5
1	G	74	GLU	4.5
1	H	245	GLN	4.5
1	E	296	THR	4.4
1	D	141	LEU	4.4
1	D	194	LYS	4.4
1	C	38	SER	4.4
1	H	238	VAL	4.4
1	H	151	SER	4.4
1	G	117	LEU	4.4
1	H	163	ASP	4.4
1	B	318	TRP	4.4
1	D	106	LEU	4.4
1	D	227	ILE	4.3
1	C	125	PHE	4.3
1	E	103	ALA	4.3
1	A	84	LEU	4.3
1	F	26	PRO	4.3
1	B	197	ALA	4.3
1	D	89	ILE	4.2
1	H	43	LYS	4.2
1	F	333	VAL	4.2
1	B	370	ILE	4.2
1	F	92	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	194	LYS	4.2
1	H	337	THR	4.2
1	D	298	ASN	4.2
1	E	295	ASN	4.2
1	H	217	TYR	4.2
1	A	298	ASN	4.2
1	E	50	ASP	4.1
1	C	55	TYR	4.1
1	D	50	ASP	4.1
1	F	245	GLN	4.1
1	A	94	VAL	4.1
1	E	370	ILE	4.1
1	F	37	LEU	4.1
1	E	250	ARG	4.1
1	D	96	ALA	4.1
1	D	72	LEU	4.1
1	H	160	ARG	4.1
1	D	316	ALA	4.0
1	E	23	LEU	4.0
1	H	249	LEU	4.0
1	D	114	LEU	4.0
1	B	70	PHE	4.0
1	A	217	TYR	4.0
1	G	176	SER	4.0
1	A	249	LEU	4.0
1	B	93	MET	4.0
1	C	82	GLN	4.0
1	E	123	ILE	4.0
1	G	217	TYR	4.0
1	E	161	ILE	4.0
1	A	354	THR	3.9
1	A	284	PHE	3.9
1	A	168	ILE	3.9
1	B	332	GLY	3.9
1	F	337	THR	3.9
1	C	126	ASP	3.9
1	G	95	ASP	3.9
1	A	87	LYS	3.9
1	H	111	GLU	3.9
1	H	355	ALA	3.9
1	A	88	ALA	3.9
1	E	145	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	161	ILE	3.9
1	A	141	LEU	3.9
1	A	257	MET	3.9
1	F	91	PHE	3.9
1	G	241	VAL	3.9
1	B	84	LEU	3.9
1	C	313	LEU	3.9
1	E	160	ARG	3.8
1	E	368	GLY	3.8
1	B	284	PHE	3.8
1	G	169	GLY	3.8
1	A	154	GLU	3.8
1	B	117	LEU	3.8
1	D	52	LEU	3.8
1	A	352	LEU	3.8
1	C	72	LEU	3.8
1	D	269	HIS	3.8
1	A	197	ALA	3.8
1	F	193	ILE	3.8
1	H	89	ILE	3.8
1	A	332	GLY	3.8
1	E	227	ILE	3.8
1	A	368	GLY	3.8
1	E	198	THR	3.8
1	G	257	MET	3.8
1	A	44	GLN	3.8
1	C	190	GLN	3.8
1	F	112	GLY	3.8
1	C	325	ASP	3.8
1	D	137	PHE	3.8
1	F	322	PHE	3.7
1	A	289	LYS	3.7
1	G	72	LEU	3.7
1	F	103	ALA	3.7
1	D	131	ALA	3.7
1	E	365	VAL	3.7
1	F	366	LEU	3.7
1	D	244	HIS	3.7
1	C	76	VAL	3.7
1	D	369	LYS	3.7
1	B	241	VAL	3.7
1	C	315	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	121	ARG	3.7
1	D	150	SER	3.7
1	G	168	ILE	3.7
1	C	102	LEU	3.7
1	B	52	LEU	3.7
1	A	24	ASN	3.7
1	F	342	VAL	3.7
1	G	167	LEU	3.6
1	H	91	PHE	3.6
1	H	165	ILE	3.6
1	H	232	TYR	3.6
1	E	333	VAL	3.6
1	G	222	ASP	3.6
1	B	74	GLU	3.6
1	A	241	VAL	3.6
1	H	73	LYS	3.6
1	C	147	GLU	3.6
1	C	33	ARG	3.6
1	A	99	GLU	3.6
1	C	149	ILE	3.6
1	D	368	GLY	3.6
1	H	39	GLU	3.6
1	H	213	GLU	3.6
1	H	76	VAL	3.6
1	C	317	TYR	3.6
1	E	324	ILE	3.6
1	D	123	ILE	3.6
1	D	76	VAL	3.6
1	E	182	PHE	3.6
1	G	245	GLN	3.6
1	C	120	ASP	3.6
1	A	52	LEU	3.6
1	C	36	SER	3.6
1	H	167	LEU	3.6
1	B	245	GLN	3.6
1	E	113	SER	3.5
1	D	313	LEU	3.5
1	H	220	PHE	3.5
1	B	244	HIS	3.5
1	C	197	ALA	3.5
1	A	240	PHE	3.5
1	A	119	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	312	PRO	3.5
1	D	303	ILE	3.5
1	H	80	VAL	3.5
1	H	93	MET	3.5
1	H	132	ASP	3.5
1	H	171	PHE	3.5
1	H	49	TYR	3.5
1	E	97	LYS	3.5
1	E	313	LEU	3.5
1	B	353	PRO	3.5
1	E	254	PRO	3.5
1	H	257	MET	3.5
1	H	97	LYS	3.5
1	H	288	LEU	3.5
1	E	96	ALA	3.5
1	C	130	ALA	3.4
1	F	248	THR	3.4
1	D	120	ASP	3.4
1	B	115	TYR	3.4
1	G	237	LEU	3.4
1	D	299	PRO	3.4
1	H	94	VAL	3.4
1	B	317	TYR	3.4
1	C	196	PHE	3.4
1	B	331	ILE	3.4
1	D	136	GLU	3.4
1	B	312	PRO	3.4
1	E	305	TRP	3.4
1	D	169	GLY	3.4
1	H	154	GLU	3.4
1	E	203	VAL	3.4
1	C	134	LEU	3.4
1	G	343	TRP	3.4
1	E	252	LEU	3.4
1	E	369	LYS	3.4
1	B	215	ASP	3.4
1	C	347	PRO	3.4
1	E	83	VAL	3.4
1	E	195	PHE	3.4
1	E	298	ASN	3.4
1	A	285	LEU	3.4
1	A	362	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	149	ILE	3.4
1	H	123	ILE	3.4
1	A	160	ARG	3.4
1	D	198	THR	3.3
1	B	150	SER	3.3
1	F	131	ALA	3.3
1	A	268	ILE	3.3
1	G	355	ALA	3.3
1	H	90	GLY	3.3
1	C	343	TRP	3.3
1	G	332	GLY	3.3
1	F	269	HIS	3.3
1	E	268	ILE	3.3
1	D	122	THR	3.3
1	E	167	LEU	3.3
1	H	106	LEU	3.3
1	H	225	ILE	3.3
1	B	125	PHE	3.3
1	C	323	LYS	3.3
1	B	222	ASP	3.3
1	B	168	ILE	3.3
1	C	268	ILE	3.3
1	H	48	LYS	3.3
1	G	313	LEU	3.3
1	A	213	GLU	3.3
1	C	250	ARG	3.3
1	D	222	ASP	3.3
1	A	101	LYS	3.3
1	E	312	PRO	3.2
1	F	335	ASN	3.2
1	A	42	PHE	3.2
1	D	193	ILE	3.2
1	E	362	ILE	3.2
1	F	341	SER	3.2
1	B	56	TYR	3.2
1	A	287	ILE	3.2
1	E	215	ASP	3.2
1	H	162	GLU	3.2
1	D	367	SER	3.2
1	F	249	LEU	3.2
1	B	216	PHE	3.2
1	E	339	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	288	LEU	3.2
1	C	115	TYR	3.2
1	F	250	ARG	3.2
1	A	89	ILE	3.2
1	A	361	TRP	3.2
1	G	129	PHE	3.2
1	D	214	VAL	3.2
1	E	122	THR	3.2
1	B	128	GLU	3.2
1	C	314	LEU	3.2
1	G	287	ILE	3.2
1	H	196	PHE	3.2
1	B	69	GLN	3.2
1	G	215	ASP	3.2
1	A	106	LEU	3.2
1	F	33	ARG	3.1
1	A	279	PRO	3.1
1	H	95	ASP	3.1
1	D	41	ASN	3.1
1	H	282	TYR	3.1
1	E	189	PHE	3.1
1	C	249	LEU	3.1
1	C	326	LEU	3.1
1	F	141	LEU	3.1
1	B	77	LEU	3.1
1	G	274	ALA	3.1
1	D	220	PHE	3.1
1	B	34	VAL	3.1
1	E	110	GLU	3.1
1	G	196	PHE	3.1
1	D	126	ASP	3.1
1	D	162	GLU	3.1
1	A	118	LYS	3.1
1	H	30	GLY	3.1
1	F	99	GLU	3.1
1	A	254	PRO	3.1
1	C	70	PHE	3.1
1	D	216	PHE	3.1
1	A	271	VAL	3.1
1	D	334	VAL	3.1
1	G	69	GLN	3.1
1	C	316	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	229	ASN	3.0
1	D	333	VAL	3.0
1	D	279	PRO	3.0
1	B	330	GLN	3.0
1	C	108	PHE	3.0
1	E	91	PHE	3.0
1	E	158	PHE	3.0
1	H	224	PRO	3.0
1	B	53	CYS	3.0
1	A	369	LYS	3.0
1	D	116	ILE	3.0
1	H	103	ALA	3.0
1	A	296	THR	3.0
1	B	357	GLU	3.0
1	F	34	VAL	3.0
1	H	42	PHE	3.0
1	A	223	GLU	3.0
1	C	322	PHE	3.0
1	F	147	GLU	3.0
1	F	102	LEU	3.0
1	F	331	ILE	3.0
1	D	77	LEU	3.0
1	A	92	VAL	3.0
1	C	161	ILE	3.0
1	G	108	PHE	3.0
1	H	197	ALA	3.0
1	H	273	PHE	3.0
1	F	317	TYR	3.0
1	C	90	GLY	2.9
1	F	199	PHE	2.9
1	B	287	ILE	2.9
1	C	256	GLU	2.9
1	E	26	PRO	2.9
1	E	299	PRO	2.9
1	G	99	GLU	2.9
1	C	86	HIS	2.9
1	B	141	LEU	2.9
1	H	177	GLU	2.9
1	H	125	PHE	2.9
1	H	284	PHE	2.9
1	B	123	ILE	2.9
1	E	256	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	92	VAL	2.9
1	C	131	ALA	2.9
1	G	175	ASP	2.9
1	B	355	ALA	2.9
1	F	96	ALA	2.9
1	H	289	LYS	2.9
1	E	106	LEU	2.9
1	G	232	TYR	2.9
1	A	270	ILE	2.9
1	B	37	LEU	2.9
1	D	135	VAL	2.9
1	D	315	VAL	2.9
1	H	214	VAL	2.9
1	H	31	LYS	2.9
1	G	223	GLU	2.9
1	H	158	PHE	2.9
1	E	269	HIS	2.9
1	F	312	PRO	2.9
1	A	105	LYS	2.9
1	A	90	GLY	2.9
1	B	288	LEU	2.9
1	F	279	PRO	2.9
1	G	361	TRP	2.9
1	H	352	LEU	2.9
1	H	313	LEU	2.9
1	E	38	SER	2.8
1	G	331	ILE	2.8
1	F	127	GLY	2.8
1	A	337	THR	2.8
1	B	352	LEU	2.8
1	C	270	ILE	2.8
1	C	304	LEU	2.8
1	C	69	GLN	2.8
1	C	329	PRO	2.8
1	E	199	PHE	2.8
1	G	284	PHE	2.8
1	H	370	ILE	2.8
1	E	214	VAL	2.8
1	A	73	LYS	2.8
1	D	79	LEU	2.8
1	B	73	LYS	2.8
1	C	39	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	139	LEU	2.8
1	H	74	GLU	2.8
1	H	241	VAL	2.8
1	B	169	GLY	2.8
1	F	56	TYR	2.8
1	F	334	VAL	2.8
1	A	122	THR	2.8
1	F	189	PHE	2.8
1	G	353	PRO	2.8
1	E	255	GLU	2.8
1	E	274	ALA	2.8
1	F	332	GLY	2.8
1	C	137	PHE	2.8
1	D	103	ALA	2.8
1	F	252	LEU	2.8
1	F	316	ALA	2.8
1	H	227	ILE	2.7
1	A	220	PHE	2.7
1	B	249	LEU	2.7
1	B	343	TRP	2.7
1	F	106	LEU	2.7
1	C	35	VAL	2.7
1	E	42	PHE	2.7
1	C	85	GLU	2.7
1	B	103	ALA	2.7
1	F	326	LEU	2.7
1	H	108	PHE	2.7
1	C	114	LEU	2.7
1	G	91	PHE	2.7
1	H	28	TYR	2.7
1	E	245	GLN	2.7
1	F	158	PHE	2.7
1	F	270	ILE	2.7
1	H	148	ILE	2.7
1	A	367	SER	2.7
1	E	288	LEU	2.7
1	H	87	LYS	2.7
1	G	288	LEU	2.7
1	G	270	ILE	2.7
1	E	79	LEU	2.7
1	C	135	VAL	2.7
1	G	135	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	24	ASN	2.7
1	D	159	GLU	2.7
1	B	217	TYR	2.7
1	F	365	VAL	2.7
1	H	131	ALA	2.7
1	B	98	LYS	2.7
1	B	335	ASN	2.7
1	H	223	GLU	2.7
1	H	203	VAL	2.7
1	H	128	GLU	2.7
1	D	189	PHE	2.7
1	D	326	LEU	2.7
1	F	244	HIS	2.7
1	A	251	ARG	2.7
1	D	132	ASP	2.7
1	F	38	SER	2.7
1	E	337	THR	2.7
1	B	194	LYS	2.7
1	B	371	ASN	2.7
1	D	212	ASN	2.7
1	H	166	LYS	2.7
1	G	37	LEU	2.6
1	H	322	PHE	2.7
1	A	370	ILE	2.6
1	F	330	GLN	2.6
1	C	284	PHE	2.6
1	C	148	ILE	2.6
1	C	370	ILE	2.6
1	C	73	LYS	2.6
1	F	254	PRO	2.6
1	G	29	ASP	2.6
1	E	39	GLU	2.6
1	H	362	ILE	2.6
1	A	77	LEU	2.6
1	A	163	ASP	2.6
1	D	255	GLU	2.6
1	G	283	GLU	2.6
1	F	324	ILE	2.6
1	C	167	LEU	2.6
1	D	312	PRO	2.6
1	F	298	ASN	2.6
1	A	45	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	131	ALA	2.6
1	A	74	GLU	2.6
1	A	108	PHE	2.6
1	E	216	PHE	2.6
1	E	346	ILE	2.6
1	C	237	LEU	2.6
1	A	293	ARG	2.6
1	B	39	GLU	2.6
1	E	253	ARG	2.6
1	A	331	ILE	2.6
1	E	116	ILE	2.6
1	F	168	ILE	2.6
1	D	241	VAL	2.6
1	B	50	ASP	2.6
1	A	43	LYS	2.6
1	H	141	LEU	2.6
1	C	42	PHE	2.6
1	D	325	ASP	2.6
1	F	200	ASP	2.6
1	C	157	ALA	2.6
1	E	282	TYR	2.5
1	G	38	SER	2.5
1	B	132	ASP	2.5
1	D	156	GLN	2.5
1	E	279	PRO	2.5
1	G	103	ALA	2.5
1	C	141	LEU	2.5
1	E	129	PHE	2.5
1	G	349	ASP	2.5
1	D	108	PHE	2.5
1	E	84	LEU	2.5
1	G	358	LEU	2.5
1	D	26	PRO	2.5
1	F	343	TRP	2.5
1	B	225	ILE	2.5
1	A	137	PHE	2.5
1	E	166	LYS	2.5
1	H	156	GLN	2.5
1	C	342	VAL	2.5
1	G	148	ILE	2.5
1	B	33	ARG	2.5
1	B	337	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	245	GLN	2.5
1	E	171	PHE	2.5
1	D	163	ASP	2.5
1	G	164	TYR	2.5
1	G	134	LEU	2.5
1	B	270	ILE	2.5
1	H	155	VAL	2.5
1	G	200	ASP	2.4
1	A	237	LEU	2.4
1	H	358	LEU	2.4
1	A	239	GLU	2.4
1	G	39	GLU	2.4
1	G	166	LYS	2.4
1	F	255	GLU	2.4
1	H	164	TYR	2.4
1	E	303	ILE	2.4
1	G	197	ALA	2.4
1	E	343	TRP	2.4
1	G	220	PHE	2.4
1	G	105	LYS	2.4
1	A	165	ILE	2.4
1	A	299	PRO	2.4
1	F	161	ILE	2.4
1	F	222	ASP	2.4
1	H	287	ILE	2.4
1	B	226	ALA	2.4
1	A	305	TRP	2.4
1	A	80	VAL	2.4
1	A	147	GLU	2.4
1	F	241	VAL	2.4
1	F	284	PHE	2.4
1	H	312	PRO	2.4
1	H	211	MET	2.4
1	B	237	LEU	2.4
1	H	51	LEU	2.4
1	C	31	LYS	2.4
1	C	371	ASN	2.4
1	D	119	GLY	2.4
1	E	316	ALA	2.4
1	H	157	ALA	2.4
1	G	249	LEU	2.4
1	G	233	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	154	GLU	2.4
1	D	188	HIS	2.4
1	G	71	GLN	2.4
1	A	182	PHE	2.4
1	C	303	ILE	2.4
1	D	118	LYS	2.4
1	C	51	LEU	2.4
1	F	69	GLN	2.4
1	C	123	ILE	2.4
1	E	76	VAL	2.4
1	F	283	GLU	2.4
1	F	329	PRO	2.4
1	F	363	GLU	2.4
1	G	195	PHE	2.4
1	C	332	GLY	2.4
1	D	160	ARG	2.4
1	C	169	GLY	2.4
1	D	51	LEU	2.4
1	H	46	LEU	2.4
1	C	327	PHE	2.4
1	D	300	ASP	2.4
1	E	132	ASP	2.4
1	F	55	TYR	2.4
1	F	370	ILE	2.3
1	F	347	PRO	2.3
1	B	211	MET	2.3
1	C	116	ILE	2.3
1	G	163	ASP	2.3
1	G	312	PRO	2.3
1	C	198	THR	2.3
1	D	358	LEU	2.3
1	A	244	HIS	2.3
1	B	127	GLY	2.3
1	B	285	LEU	2.3
1	D	43	LYS	2.3
1	H	24	ASN	2.3
1	F	274	ALA	2.3
1	G	338	ASP	2.3
1	H	331	ILE	2.3
1	B	291	VAL	2.3
1	C	302	SER	2.3
1	E	169	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	322	PHE	2.3
1	F	296	THR	2.3
1	A	304	LEU	2.3
1	C	34	VAL	2.3
1	D	37	LEU	2.3
1	H	365	VAL	2.3
1	B	240	PHE	2.3
1	F	362	ILE	2.3
1	B	76	VAL	2.3
1	D	314	LEU	2.3
1	F	210	LYS	2.3
1	H	293	ARG	2.3
1	E	358	LEU	2.3
1	G	34	VAL	2.3
1	H	347	PRO	2.3
1	D	196	PHE	2.3
1	D	75	ILE	2.3
1	H	118	LYS	2.3
1	A	103	ALA	2.3
1	A	272	ALA	2.3
1	B	90	GLY	2.3
1	C	56	TYR	2.3
1	A	356	GLU	2.2
1	C	220	PHE	2.3
1	A	335	ASN	2.2
1	D	343	TRP	2.2
1	B	232	TYR	2.2
1	G	25	PHE	2.2
1	B	275	GLU	2.2
1	D	34	VAL	2.2
1	E	315	VAL	2.2
1	F	148	ILE	2.2
1	F	237	LEU	2.2
1	H	84	LEU	2.2
1	F	216	PHE	2.2
1	C	166	LYS	2.2
1	G	339	ALA	2.2
1	H	130	ALA	2.2
1	F	164	TYR	2.2
1	G	24	ASN	2.2
1	A	224	PRO	2.2
1	B	339	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	23	LEU	2.2
1	E	104	LYS	2.2
1	A	238	VAL	2.2
1	D	167	LEU	2.2
1	E	112	GLY	2.2
1	B	201	LYS	2.2
1	D	199	PHE	2.2
1	G	244	HIS	2.2
1	G	254	PRO	2.2
1	H	50	ASP	2.2
1	H	72	LEU	2.2
1	A	49	TYR	2.2
1	B	220	PHE	2.2
1	E	328	ARG	2.2
1	F	82	GLN	2.2
1	C	295	ASN	2.2
1	D	133	VAL	2.2
1	E	80	VAL	2.2
1	H	353	PRO	2.2
1	B	338	ASP	2.2
1	D	166	LYS	2.2
1	C	50	ASP	2.2
1	G	158	PHE	2.2
1	B	358	LEU	2.2
1	F	167	LEU	2.2
1	G	250	ARG	2.2
1	F	258	PHE	2.2
1	C	367	SER	2.2
1	D	100	ALA	2.2
1	G	131	ALA	2.2
1	E	133	VAL	2.2
1	F	134	LEU	2.2
1	B	362	ILE	2.2
1	F	25	PHE	2.2
1	H	25	PHE	2.2
1	G	214	VAL	2.2
1	E	148	ILE	2.2
1	E	165	ILE	2.2
1	F	361	TRP	2.2
1	H	101	LYS	2.2
1	C	255	GLU	2.2
1	F	100	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	304	LEU	2.1
1	H	38	SER	2.1
1	D	305	TRP	2.1
1	F	273	PHE	2.1
1	H	292	ALA	2.1
1	D	213	GLU	2.1
1	C	365	VAL	2.1
1	G	51	LEU	2.1
1	G	285	LEU	2.1
1	G	27	THR	2.1
1	G	150	SER	2.1
1	H	107	GLY	2.1
1	A	72	LEU	2.1
1	E	347	PRO	2.1
1	E	56	TYR	2.1
1	E	168	ILE	2.1
1	F	70	PHE	2.1
1	H	161	ILE	2.1
1	A	131	ALA	2.1
1	G	146	VAL	2.1
1	A	70	PHE	2.1
1	E	319	GLU	2.1
1	E	126	ASP	2.1
1	F	76	VAL	2.1
1	D	195	PHE	2.1
1	F	247	PRO	2.1
1	A	40	LYS	2.1
1	A	232	TYR	2.1
1	F	196	PHE	2.1
1	A	50	ASP	2.1
1	E	98	LYS	2.1
1	A	37	LEU	2.1
1	E	134	LEU	2.1
1	B	320	LYS	2.1
1	D	31	LYS	2.1
1	D	38	SER	2.1
1	A	109	ASP	2.1
1	D	225	ILE	2.1
1	E	341	SER	2.1
1	C	77	LEU	2.1
1	E	342	VAL	2.1
1	A	317	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	89	ILE	2.1
1	B	334	VAL	2.1
1	C	159	GLU	2.1
1	E	138	LEU	2.1
1	A	292	ALA	2.1
1	C	288	LEU	2.1
1	H	233	THR	2.1
1	F	253	ARG	2.1
1	B	134	LEU	2.0
1	F	41	ASN	2.0
1	A	228	PRO	2.0
1	C	248	THR	2.0
1	F	297	ASP	2.0
1	D	149	ILE	2.0
1	A	76	VAL	2.0
1	B	326	LEU	2.0
1	F	51	LEU	2.0
1	G	106	LEU	2.0
1	B	274	ALA	2.0
1	C	41	ASN	2.0
1	E	247	PRO	2.0
1	H	142	ILE	2.0
1	C	150	SER	2.0
1	D	127	GLY	2.0
1	G	198	THR	2.0
1	C	358	LEU	2.0
1	G	35	VAL	2.0
1	H	206	LYS	2.0
1	D	319	GLU	2.0
1	F	292	ALA	2.0
1	H	346	ILE	2.0
1	F	104	LYS	2.0
1	H	336	VAL	2.0
1	A	189	PHE	2.0
1	D	117	LEU	2.0
1	G	42	PHE	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	E	403	1/1	0.48	0.14	133,133,133,133	1
2	YB	E	407	1/1	0.53	0.16	115,115,115,115	1
2	YB	B	404	1/1	0.58	0.10	202,202,202,202	0
2	YB	B	402	1/1	0.59	0.10	124,124,124,124	1
3	SO4	A	410	5/5	0.68	0.61	119,129,144,148	0
2	YB	A	408	1/1	0.69	0.14	94,94,94,94	1
2	YB	F	404	1/1	0.71	0.17	129,129,129,129	1
2	YB	C	407	1/1	0.73	0.14	88,88,88,88	1
2	YB	H	402	1/1	0.73	0.08	165,165,165,165	1
2	YB	H	404	1/1	0.74	0.17	159,159,159,159	0
3	SO4	H	407	5/5	0.75	0.23	105,113,123,123	0
2	YB	G	407	1/1	0.75	0.17	100,100,100,100	1
2	YB	F	402	1/1	0.76	0.11	135,135,135,135	1
2	YB	A	407	1/1	0.76	0.15	105,105,105,105	1
2	YB	C	405	1/1	0.76	0.16	129,129,129,129	1
2	YB	G	403	1/1	0.77	0.19	111,111,111,111	1
2	YB	H	406	1/1	0.77	0.12	307,307,307,307	0
2	YB	A	404	1/1	0.78	0.07	149,149,149,149	1
2	YB	F	405	1/1	0.78	0.27	116,116,116,116	1
2	YB	E	408	1/1	0.78	0.17	120,120,120,120	1
3	SO4	F	408	5/5	0.78	0.53	112,121,124,127	0
2	YB	G	406	1/1	0.78	0.12	182,182,182,182	1
2	YB	D	408	1/1	0.79	0.17	347,347,347,347	1
2	YB	B	407	1/1	0.79	0.10	97,97,97,97	1
2	YB	F	403	1/1	0.80	0.05	184,184,184,184	0
2	YB	H	405	1/1	0.81	0.18	184,184,184,184	1
2	YB	E	405	1/1	0.81	0.09	170,170,170,170	0
2	YB	C	402	1/1	0.81	0.07	149,149,149,149	1
2	YB	H	403	1/1	0.81	0.13	130,130,130,130	1
2	YB	A	403	1/1	0.82	0.16	123,123,123,123	1
2	YB	G	408	1/1	0.82	0.31	169,169,169,169	1
2	YB	C	403	1/1	0.83	0.16	120,120,120,120	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YB	A	402	1/1	0.84	0.11	134,134,134,134	1
2	YB	F	407	1/1	0.84	0.18	325,325,325,325	1
2	YB	B	401	1/1	0.85	0.14	127,127,127,127	0
2	YB	D	407	1/1	0.85	0.17	130,130,130,130	1
2	YB	A	406	1/1	0.85	0.14	115,115,115,115	1
2	YB	D	401	1/1	0.85	0.19	149,149,149,149	1
2	YB	E	409	1/1	0.85	0.26	116,116,116,116	1
2	YB	B	406	1/1	0.85	0.19	109,109,109,109	1
3	SO4	B	408	5/5	0.85	0.20	99,100,111,111	0
2	YB	E	402	1/1	0.86	0.08	148,148,148,148	1
2	YB	D	403	1/1	0.87	0.11	161,161,161,161	0
2	YB	B	405	1/1	0.87	0.12	123,123,123,123	1
3	SO4	D	409	5/5	0.87	0.17	100,107,113,117	0
2	YB	A	409	1/1	0.87	0.14	315,315,315,315	0
2	YB	G	401	1/1	0.87	0.13	165,165,165,165	0
2	YB	C	408	1/1	0.88	0.16	100,100,100,100	1
2	YB	D	404	1/1	0.88	0.11	166,166,166,166	1
2	YB	D	405	1/1	0.88	0.16	85,85,85,85	1
2	YB	E	401	1/1	0.90	0.11	153,153,153,153	1
2	YB	B	403	1/1	0.90	0.07	150,150,150,150	1
2	YB	A	405	1/1	0.91	0.22	92,92,92,92	1
2	YB	F	406	1/1	0.91	0.09	160,160,160,160	0
2	YB	C	401	1/1	0.91	0.13	142,142,142,142	0
2	YB	G	404	1/1	0.91	0.27	122,122,122,122	1
2	YB	E	406	1/1	0.92	0.09	94,94,94,94	1
2	YB	F	401	1/1	0.92	0.13	134,134,134,134	0
2	YB	G	405	1/1	0.93	0.17	129,129,129,129	1
2	YB	H	401	1/1	0.93	0.17	158,158,158,158	1
2	YB	G	402	1/1	0.93	0.09	162,162,162,162	0
2	YB	D	406	1/1	0.93	0.21	137,137,137,137	1
2	YB	C	406	1/1	0.93	0.07	130,130,130,130	1
2	YB	A	401	1/1	0.94	0.19	157,157,157,157	1
2	YB	E	404	1/1	0.94	0.06	92,92,92,92	1
2	YB	C	404	1/1	0.95	0.11	161,161,161,161	1
2	YB	D	402	1/1	0.96	0.19	115,115,115,115	1
2	YB	C	409	1/1	0.96	0.14	130,130,130,130	1

6.5 Other polymers

There are no such residues in this entry.