Preliminary Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2020 – 01:08 PM PDT

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

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

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:

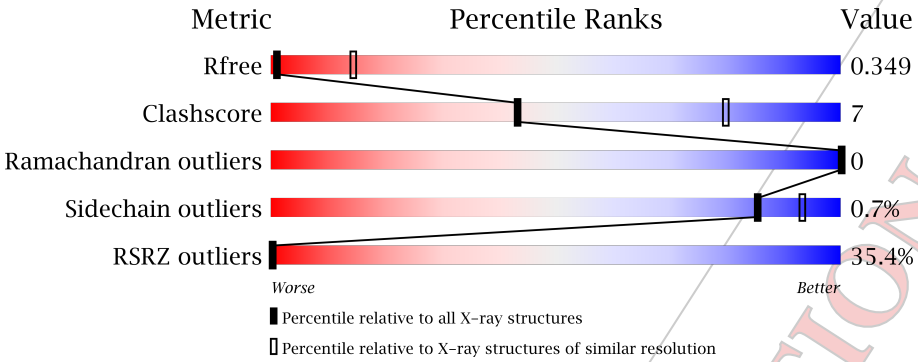
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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	329	43% 79% 21%
1	B	329	31% 81% 19%
1	C	329	34% 83% 17%
1	D	329	38% 84% 16%
1	E	329	33% 81% 19%

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Mol	Chain	Length	Quality of chain
1	F	329	31% 82% 18%
1	G	329	30% 81% 19%
1	H	329	43% 76% 24%

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	I	1	-	-	-	X
3	SO4	I	5	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21809 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.

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			

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0

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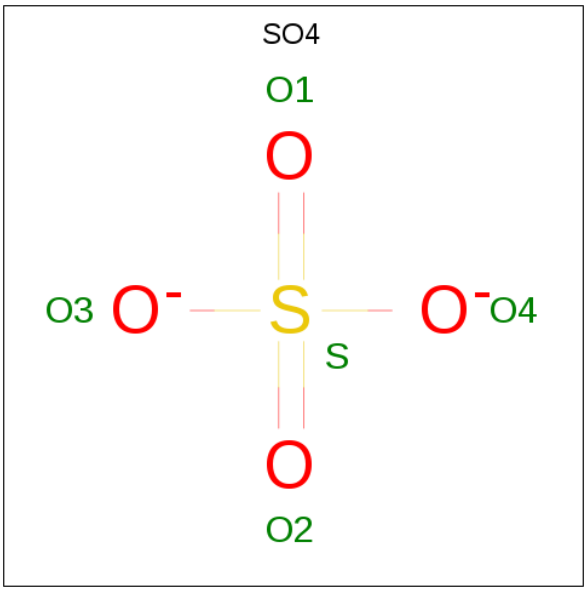
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	1	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0

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

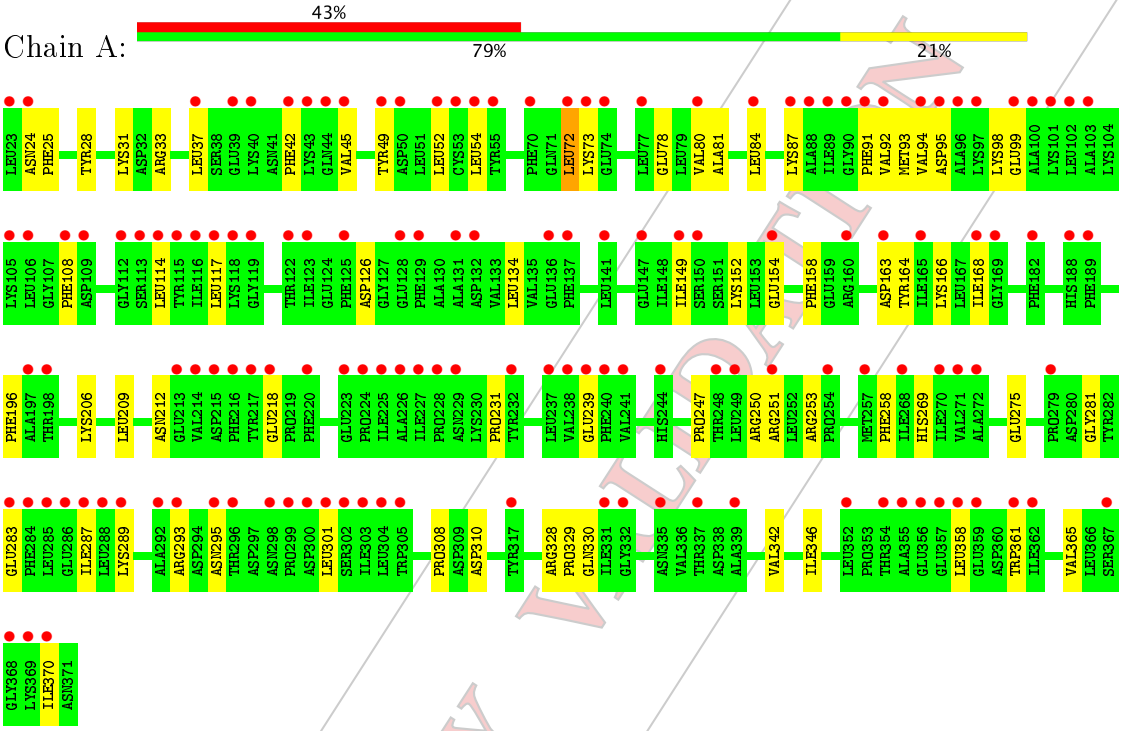


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0

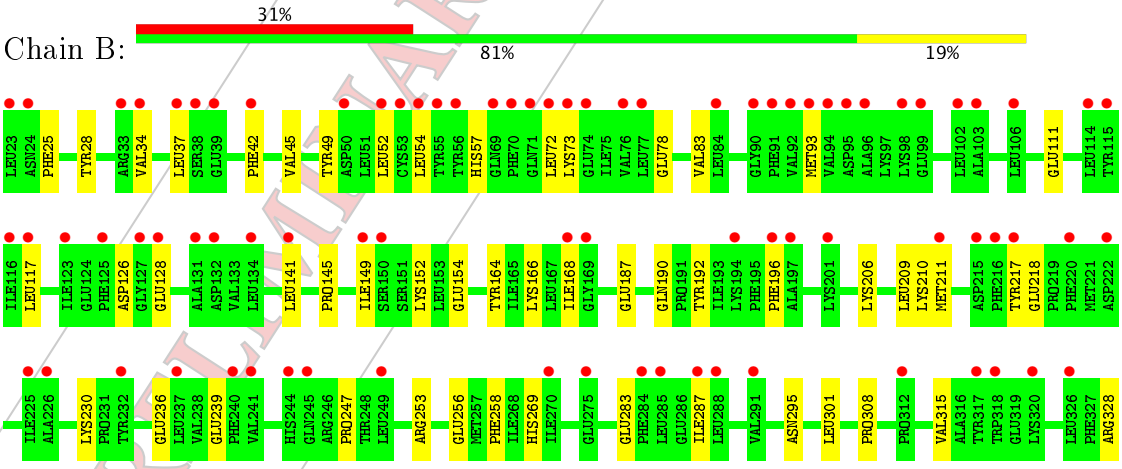
3 Residue-property plots (i)

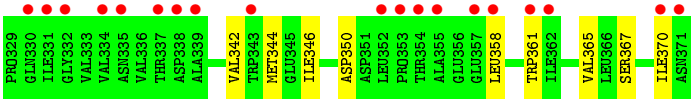
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand electron density. Residues are 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:



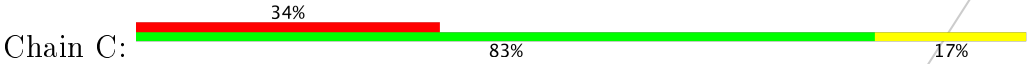
- Molecule 1:

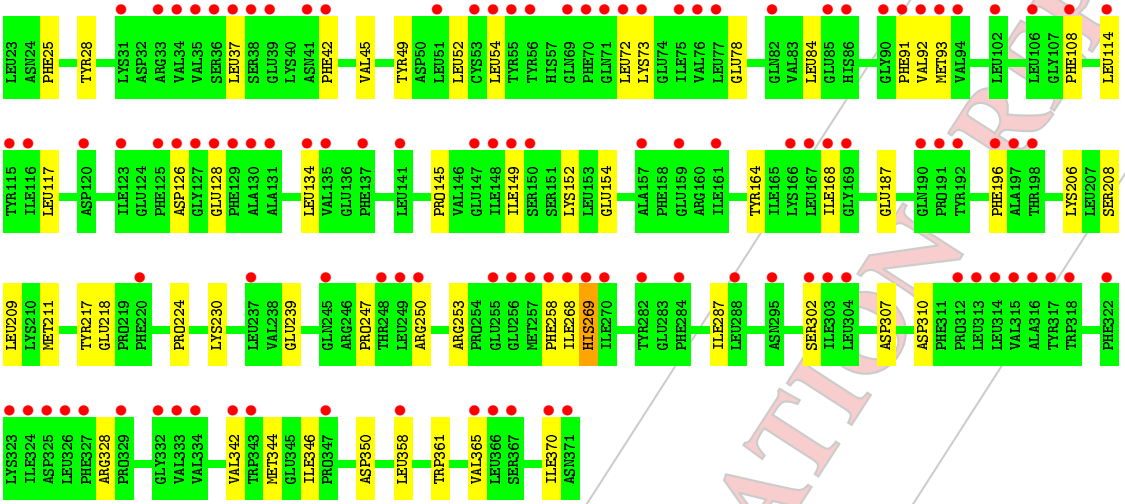




- Molecule 1:

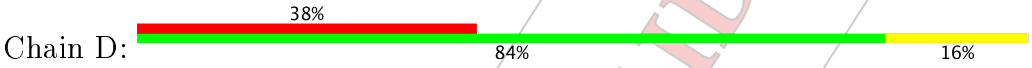
Chain C:

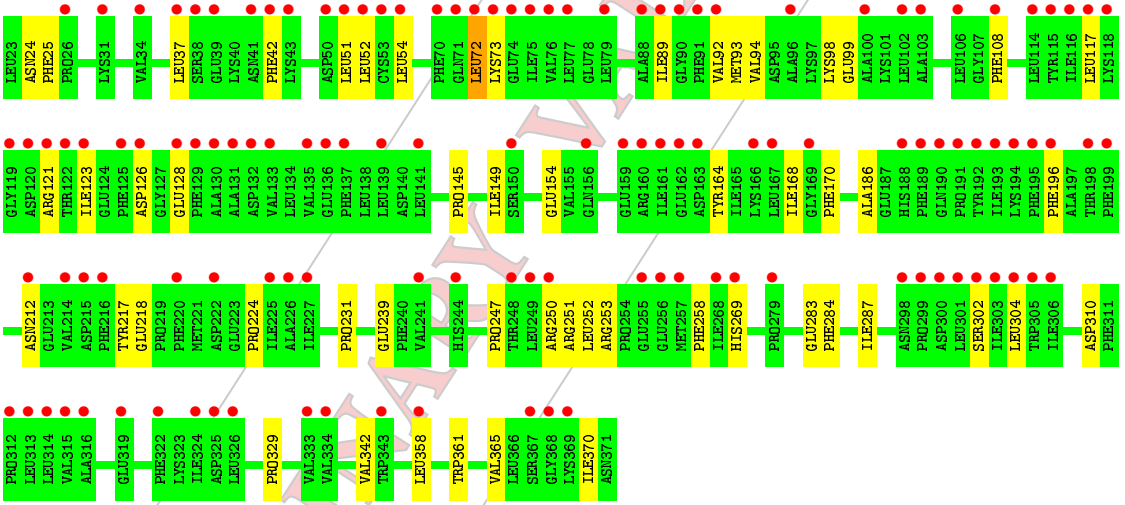




- Molecule 1:

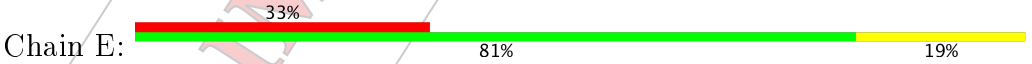
Chain D:

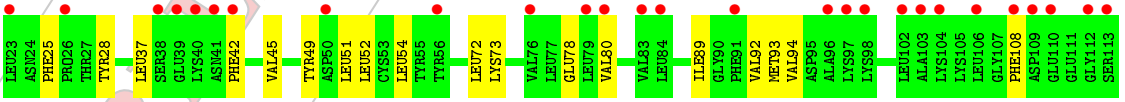


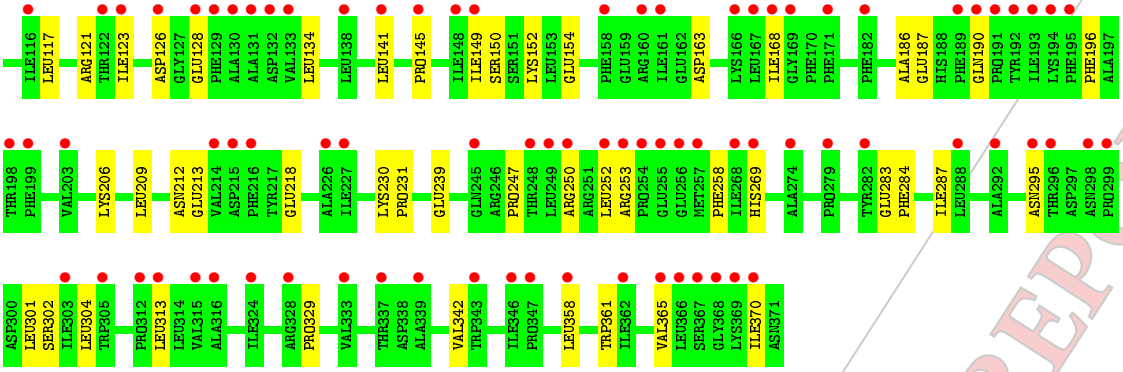


- Molecule 1:

Chain E:

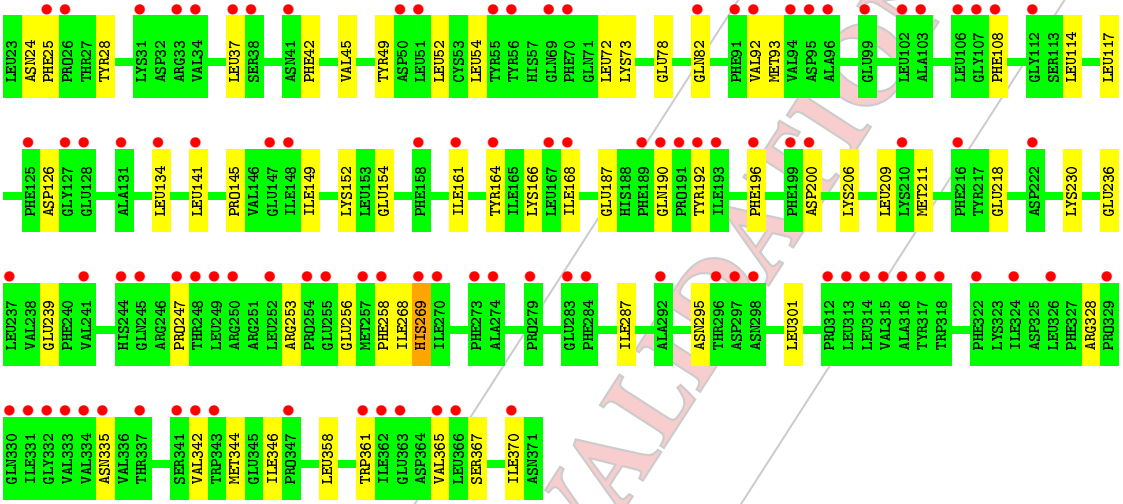






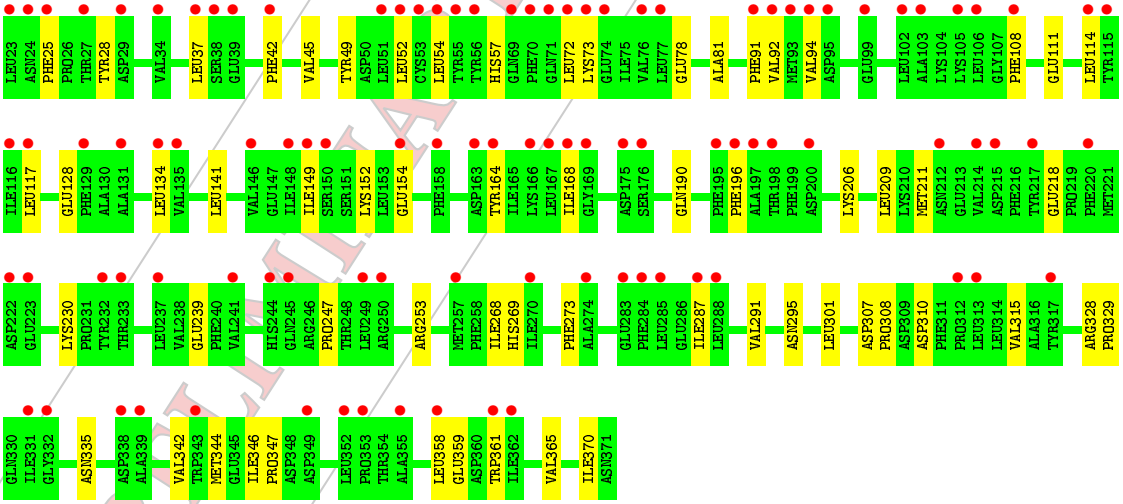
- Molecule 1:

Chain F:



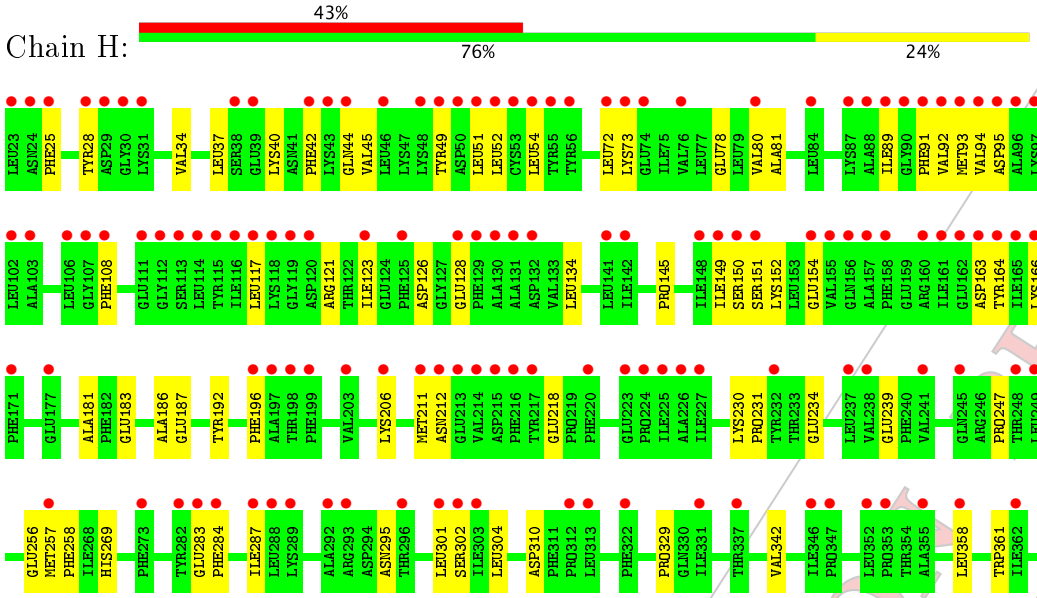
- Molecule 1:

Chain G:



- Molecule 1:

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}	0.292 , 0.341 0.299 , 0.349	Depositor DCC
R_{free} test set	1446 reflections (4.84%)	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 , 81.8	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	21809	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	0.32	0/2779	0.51	1/3758 (0.0%)
1	B	0.32	0/2779	0.51	0/3758
1	C	0.32	0/2779	0.52	0/3758
1	D	0.32	0/2779	0.51	1/3758 (0.0%)
1	E	0.32	0/2779	0.51	0/3758
1	F	0.32	0/2779	0.52	0/3758
1	G	0.32	0/2779	0.50	0/3758
1	H	0.32	0/2779	0.51	0/3758
All	All	0.32	0/22232	0.51	2/30064 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	LEU	CA-CB-CG	5.57	128.10	115.30
1	D	72	LEU	CA-CB-CG	5.25	127.38	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	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2715	0	2653	41	0
1	C	2715	0	2653	40	0
1	D	2715	0	2653	36	0
1	E	2715	0	2653	41	0
1	F	2715	0	2653	39	0
1	G	2715	0	2653	38	0
1	H	2715	0	2653	49	0
2	Y	64	0	0	0	0
3	I	25	0	0	0	0
All	All	21809	0	21224	312	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 7.

All (312) 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	2.22	0.73
1:F:211:MET:O	1:F:230:LYS:NZ	2.22	0.72
1:C:164:TYR:HD2	1:C:253:ARG:HH22	1.36	0.72
1:H:342:VAL:HG11	1:H:370:ILE:HG23	1.71	0.71
1:B:211:MET:O	1:B:230:LYS:NZ	2.25	0.69
1:F:164:TYR:HD2	1:F:253:ARG:HH22	1.39	0.68
1:A:164:TYR:HD2	1:A:253:ARG:HH22	1.41	0.68
1:G:211:MET:O	1:G:230:LYS:NZ	2.22	0.68
1:E:342:VAL:HG11	1:E:370:ILE:HG23	1.76	0.68
1:A:152:LYS:HB3	1:A:206:LYS:HE3	1.75	0.67
1:G:342:VAL:HG11	1:G:370:ILE:HG23	1.78	0.66
1:B:164:TYR:HD2	1:B:253:ARG:HH22	1.43	0.66
1:D:342:VAL:HG11	1:D:370:ILE:HG23	1.78	0.64
1:D:250:ARG:NH1	1:D:302:SER:OG	2.30	0.64
1:B:52:LEU:HB2	1:B:117:LEU:HB2	1.79	0.63
1:A:342:VAL:HG11	1:A:370:ILE:HG23	1.80	0.63
1:E:250:ARG:NH1	1:E:302:SER:OG	2.34	0.61
1:C:52:LEU:HB2	1:C:117:LEU:HB2	1.82	0.60
1:F:342:VAL:HG11	1:F:370:ILE:HG23	1.82	0.60
1:H:212:ASN:HB3	1:H:231:PRO:HB3	1.81	0.60
1:A:251:ARG:NH2	1:A:310:ASP:OD2	2.29	0.59
1:B:342:VAL:HG11	1:B:370:ILE:HG23	1.84	0.59
1:F:287:ILE:HG22	1:F:358:LEU:HD12	1.83	0.59
1:A:72:LEU:HD12	1:A:73:LYS:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HG	1:A:92:VAL:HG23	1.85	0.58
1:G:164:TYR:HD2	1:G:253:ARG:HH22	1.50	0.58
1:B:287:ILE:HG22	1:B:358:LEU:HD12	1.86	0.57
1:D:247:PRO:HD2	1:D:250:ARG:HD3	1.86	0.57
1:G:152:LYS:HB3	1:G:206:LYS:HE3	1.86	0.57
1:C:149:ILE:HG23	1:C:154:GLU:HB3	1.86	0.57
1:E:247:PRO:HD2	1:E:250:ARG:HD3	1.86	0.57
1:E:72:LEU:HD12	1:E:73:LYS:HG3	1.86	0.57
1:H:72:LEU:HD12	1:H:73:LYS:HG3	1.87	0.57
1:B:149:ILE:HG23	1:B:154:GLU:HB3	1.85	0.57
1:A:218:GLU:OE1	1:A:247:PRO:HB3	2.05	0.57
1:C:287:ILE:HG22	1:C:358:LEU:HD12	1.86	0.57
1:A:80:VAL:HG21	1:A:134:LEU:HD23	1.86	0.56
1:C:218:GLU:OE1	1:C:247:PRO:HB3	2.06	0.56
1:F:149:ILE:HG23	1:F:154:GLU:HB3	1.87	0.56
1:D:72:LEU:HD12	1:D:73:LYS:HG3	1.87	0.56
1:C:152:LYS:HB3	1:C:206:LYS:HE3	1.87	0.56
1:C:342:VAL:HG11	1:C:370:ILE:HG23	1.86	0.56
1:F:168:ILE:HG23	1:F:209:LEU:HD11	1.87	0.56
1:F:52:LEU:HB2	1:F:117:LEU:HB2	1.86	0.56
1:B:37:LEU:HD11	1:B:42:PHE:HA	1.88	0.56
1:F:152:LYS:HB3	1:F:206:LYS:HE3	1.87	0.56
1:C:168:ILE:HG23	1:C:209:LEU:HD11	1.88	0.56
1:E:126:ASP:HB3	1:E:258:PHE:HB3	1.87	0.56
1:B:152:LYS:HB3	1:B:206:LYS:HE3	1.88	0.56
1:H:250:ARG:NH1	1:H:302:SER:OG	2.39	0.56
1:D:54:LEU:HG	1:D:92:VAL:HG23	1.88	0.55
1:F:218:GLU:OE1	1:F:247:PRO:HB3	2.07	0.55
1:H:251:ARG:NH2	1:H:310:ASP:OD2	2.34	0.55
1:G:168:ILE:HG23	1:G:209:LEU:HD11	1.87	0.55
1:H:149:ILE:HG23	1:H:154:GLU:HB3	1.88	0.55
1:E:218:GLU:OE1	1:E:247:PRO:HB3	2.05	0.55
1:A:126:ASP:HB3	1:A:258:PHE:HB3	1.89	0.54
1:B:72:LEU:HD12	1:B:73:LYS:HG3	1.89	0.54
1:E:168:ILE:HG23	1:E:209:LEU:HD11	1.89	0.54
1:G:287:ILE:HG22	1:G:358:LEU:HD12	1.88	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:H:80:VAL:HG21	1:H:134:LEU:HD23	1.89	0.54
1:B:210:LYS:HB3	1:B:230:LYS:HZ1	1.73	0.54
1:G:28:TYR:CE1	1:G:78:GLU:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:SER:O	1:F:236:GLU:HA	2.07	0.53
1:H:121:ARG:NH1	1:H:123:ILE:HD11	2.23	0.53
1:F:114:LEU:HD23	1:F:134:LEU:HD11	1.91	0.53
1:E:54:LEU:HG	1:E:92:VAL:HG23	1.91	0.53
1:H:126:ASP:HB3	1:H:258:PHE:HB3	1.91	0.53
1:A:149:ILE:HG23	1:A:154:GLU:HB3	1.91	0.53
1:C:72:LEU:HD12	1:C:73:LYS:HG3	1.91	0.53
1:B:236:GLU:HA	1:F:367:SER:O	2.09	0.53
1:G:37:LEU:HD11	1:G:42:PHE:HA	1.91	0.53
1:B:141:LEU:HD23	1:B:190:GLN:HG2	1.91	0.52
1:A:283:GLU:O	1:A:287:ILE:HG12	2.09	0.52
1:H:37:LEU:HD11	1:H:42:PHE:HA	1.92	0.52
1:A:84:LEU:HD22	1:A:87:LYS:HG3	1.90	0.52
1:B:28:TYR:CE1	1:B:78:GLU:HB3	2.44	0.52
1:H:54:LEU:HG	1:H:92:VAL:HG23	1.92	0.52
1:C:344:MET:HG3	1:C:361:TRP:CD1	2.45	0.52
1:D:218:GLU:OE1	1:D:247:PRO:HB3	2.10	0.52
1:H:247:PRO:HD2	1:H:250:ARG:HD3	1.92	0.52
1:H:34:VAL:HG11	1:H:93:MET:HE3	1.91	0.52
1:H:287:ILE:HG22	1:H:358:LEU:HD12	1.92	0.52
1:A:287:ILE:HG22	1:A:358:LEU:HD12	1.91	0.52
1:H:218:GLU:OE1	1:H:247:PRO:HB3	2.10	0.51
1:E:287:ILE:HG22	1:E:358:LEU:HD12	1.92	0.51
1:B:344:MET:HG3	1:B:361:TRP:CD1	2.46	0.51
1:E:212:ASN:HB3	1:E:231:PRO:HB3	1.93	0.51
1:G:72:LEU:HD12	1:G:73:LYS:HG3	1.93	0.51
1:E:37:LEU:HD11	1:E:42:PHE:HA	1.93	0.51
1:D:126:ASP:HB3	1:D:258:PHE:HB3	1.93	0.50
1:H:164:TYR:HD2	1:H:253:ARG:HH22	1.58	0.50
1:C:45:VAL:HG13	1:C:49:TYR:CE2	2.47	0.50
1:E:252:LEU:HD13	1:E:304:LEU:HD21	1.91	0.50
1:A:37:LEU:HD11	1:A:42:PHE:HA	1.94	0.50
1:F:344:MET:HG3	1:F:361:TRP:CD1	2.47	0.50
1:F:72:LEU:HD12	1:F:73:LYS:HG3	1.94	0.50
1:G:57:HIS:ND1	1:G:111:GLU:OE2	2.45	0.50
1:C:128:GLU:HB2	1:H:25:PHE:CZ	2.47	0.49
1:C:328:ARG:NH1	1:C:346:ILE:O	2.38	0.49
1:D:25:PHE:CZ	1:G:128:GLU:HB2	2.48	0.49
1:G:218:GLU:OE1	1:G:247:PRO:HB3	2.12	0.49
1:E:80:VAL:HG21	1:E:134:LEU:HD23	1.94	0.49
1:G:328:ARG:NH1	1:G:346:ILE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:HA	1:B:315:VAL:HG21	1.95	0.49
1:D:247:PRO:HG2	1:D:250:ARG:HB3	1.94	0.49
1:B:328:ARG:NH1	1:B:346:ILE:O	2.41	0.49
1:G:308:PRO:HA	1:G:315:VAL:HG21	1.94	0.49
1:H:28:TYR:CE1	1:H:78:GLU:HB3	2.48	0.49
1:F:268:ILE:HD12	1:F:335:ASN:HA	1.95	0.48
1:E:149:ILE:HG23	1:E:154:GLU:HB3	1.95	0.48
1:F:37:LEU:HD11	1:F:42:PHE:HA	1.95	0.48
1:E:45:VAL:HG13	1:E:49:TYR:CE2	2.47	0.48
1:A:328:ARG:NH1	1:A:346:ILE:O	2.46	0.48
1:D:252:LEU:HD13	1:D:304:LEU:HD21	1.94	0.48
1:A:54:LEU:HD13	1:A:117:LEU:HG	1.96	0.48
1:B:295:ASN:HB2	1:B:301:LEU:HD23	1.94	0.48
1:C:145:PRO:HG2	1:C:187:GLU:HG2	1.96	0.47
1:C:37:LEU:HD11	1:C:42:PHE:HA	1.95	0.47
1:E:54:LEU:HD13	1:E:117:LEU:HG	1.96	0.47
1:H:247:PRO:HG2	1:H:250:ARG:HB3	1.96	0.47
1:B:350:ASP:CG	1:E:150:SER:HB2	2.34	0.47
1:E:145:PRO:HB2	1:E:186:ALA:HB1	1.95	0.47
1:A:247:PRO:HD2	1:A:250:ARG:HD3	1.95	0.47
1:E:93:MET:HE2	1:E:93:MET:HB3	1.73	0.47
1:G:54:LEU:HD13	1:G:117:LEU:HG	1.95	0.47
1:C:250:ARG:NH1	1:C:302:SER:OG	2.48	0.47
1:F:54:LEU:HD22	1:F:108:PHE:HZ	1.79	0.47
1:A:94:VAL:HG13	1:A:99:GLU:HB2	1.96	0.46
1:F:28:TYR:HA	1:F:82:GLN:OE1	2.15	0.46
1:A:168:ILE:HA	1:A:196:PHE:O	2.16	0.46
1:C:45:VAL:HG13	1:C:49:TYR:HE2	1.78	0.46
1:H:168:ILE:HA	1:H:196:PHE:O	2.15	0.46
1:A:212:ASN:HB3	1:A:231:PRO:HB3	1.97	0.46
1:B:93:MET:HE2	1:B:93:MET:HB3	1.84	0.46
1:D:145:PRO:HB2	1:D:186:ALA:HB1	1.96	0.46
1:D:37:LEU:HD11	1:D:42:PHE:HA	1.98	0.46
1:G:295:ASN:HB2	1:G:301:LEU:HD23	1.97	0.46
1:A:54:LEU:HD22	1:A:108:PHE:HZ	1.81	0.46
1:D:361:TRP:O	1:D:365:VAL:HG23	2.16	0.46
1:E:361:TRP:O	1:E:365:VAL:HG23	2.16	0.46
1:F:161:ILE:O	1:F:166:LYS:NZ	2.33	0.46
1:G:114:LEU:HD23	1:G:134:LEU:HD11	1.97	0.46
1:H:40:LYS:NZ	1:H:44:GLN:OE1	2.48	0.46
1:A:164:TYR:CE1	1:A:166:LYS:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:ARG:NH1	1:F:346:ILE:O	2.39	0.46
1:G:141:LEU:HD23	1:G:190:GLN:HG2	1.98	0.46
1:C:168:ILE:HA	1:C:196:PHE:O	2.16	0.46
1:F:54:LEU:HG	1:F:92:VAL:HG23	1.98	0.46
1:C:28:TYR:CE1	1:C:78:GLU:HB3	2.51	0.46
1:G:72:LEU:HD12	1:G:73:LYS:N	2.31	0.46
1:C:25:PHE:HE2	1:H:257:MET:HE1	1.81	0.46
1:C:307:ASP:HB3	1:C:310:ASP:OD2	2.16	0.46
1:F:45:VAL:HG13	1:F:49:TYR:CE2	2.51	0.46
1:H:181:ALA:HB1	1:H:234:GLU:N	2.31	0.46
1:H:192:TYR:CE1	1:H:256:GLU:HA	2.51	0.46
1:D:212:ASN:HB3	1:D:231:PRO:HB3	1.98	0.45
1:D:93:MET:HB3	1:D:93:MET:HE2	1.74	0.45
1:F:200:ASP:OD1	1:G:347:PRO:HB3	2.15	0.45
1:A:275:GLU:HG2	1:A:308:PRO:HD2	1.97	0.45
1:C:54:LEU:HG	1:C:92:VAL:HG23	1.97	0.45
1:D:54:LEU:HD22	1:D:108:PHE:HZ	1.81	0.45
1:G:344:MET:HG3	1:G:361:TRP:CD1	2.50	0.45
1:H:211:MET:O	1:H:230:LYS:NZ	2.44	0.45
1:G:307:ASP:HB3	1:G:310:ASP:OD2	2.15	0.45
1:A:93:MET:HE2	1:A:93:MET:HB3	1.79	0.45
1:C:114:LEU:HD23	1:C:134:LEU:HD11	1.97	0.45
1:C:268:ILE:HG22	1:C:269:HIS:ND1	2.32	0.45
1:D:287:ILE:HG22	1:D:358:LEU:HD12	1.97	0.45
1:G:45:VAL:HG13	1:G:49:TYR:CE2	2.51	0.45
1:H:163:ASP:HB3	1:H:253:ARG:HH21	1.80	0.45
1:H:52:LEU:HD23	1:H:52:LEU:HA	1.82	0.45
1:A:361:TRP:O	1:A:365:VAL:HG23	2.17	0.45
1:B:45:VAL:HG13	1:B:49:TYR:CE2	2.52	0.45
1:H:54:LEU:HD23	1:H:94:VAL:HG21	1.99	0.45
1:D:52:LEU:HB2	1:D:117:LEU:HB2	1.97	0.45
1:E:45:VAL:HG13	1:E:49:TYR:HE2	1.81	0.45
1:F:54:LEU:HD22	1:F:108:PHE:CZ	2.52	0.45
1:G:361:TRP:O	1:G:365:VAL:HG23	2.15	0.45
1:B:218:GLU:OE1	1:B:247:PRO:HB3	2.17	0.45
1:B:72:LEU:HD12	1:B:73:LYS:N	2.32	0.45
1:C:25:PHE:CZ	1:H:128:GLU:HB2	2.52	0.45
1:D:164:TYR:HD2	1:D:253:ARG:HH22	1.63	0.45
1:F:141:LEU:HD23	1:F:190:GLN:HG2	1.98	0.45
1:C:54:LEU:HD13	1:C:117:LEU:HG	1.99	0.44
1:B:25:PHE:CZ	1:E:128:GLU:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:VAL:HG13	1:G:359:GLU:HG3	1.99	0.44
1:G:54:LEU:HG	1:G:92:VAL:HG23	1.99	0.44
1:E:52:LEU:HB2	1:E:117:LEU:HB2	1.98	0.44
1:H:52:LEU:HB2	1:H:117:LEU:HB2	1.99	0.44
1:A:247:PRO:HG2	1:A:250:ARG:HB3	2.00	0.44
1:F:93:MET:HB3	1:F:93:MET:HE2	1.93	0.44
1:H:164:TYR:CE1	1:H:166:LYS:HG2	2.53	0.44
1:A:328:ARG:O	1:A:330:GLN:HG2	2.18	0.44
1:C:350:ASP:CG	1:H:150:SER:HB2	2.38	0.44
1:B:83:VAL:HG21	1:E:313:LEU:HD11	1.99	0.44
1:E:72:LEU:HD12	1:E:73:LYS:N	2.33	0.44
1:F:268:ILE:HG22	1:F:269:HIS:ND1	2.32	0.44
1:B:126:ASP:HB3	1:B:258:PHE:HD2	1.83	0.44
1:F:126:ASP:HB3	1:F:258:PHE:CD2	2.52	0.44
1:H:94:VAL:HG13	1:H:99:GLU:HB2	2.00	0.44
1:C:361:TRP:O	1:C:365:VAL:HG23	2.18	0.44
1:E:247:PRO:HG2	1:E:250:ARG:HB3	1.99	0.44
1:F:145:PRO:HG2	1:F:187:GLU:HG2	2.00	0.44
1:F:361:TRP:O	1:F:365:VAL:HG23	2.18	0.44
1:H:152:LYS:HB3	1:H:206:LYS:HE3	1.99	0.44
1:B:168:ILE:HA	1:B:196:PHE:O	2.18	0.44
1:D:94:VAL:HG13	1:D:99:GLU:HB2	1.99	0.44
1:E:54:LEU:HD22	1:E:108:PHE:HZ	1.82	0.44
1:G:54:LEU:HD22	1:G:108:PHE:HZ	1.82	0.44
1:G:268:ILE:HD12	1:G:335:ASN:HA	1.99	0.44
1:A:295:ASN:HB2	1:A:301:LEU:HD23	2.00	0.44
1:B:34:VAL:HG12	1:B:93:MET:HG2	1.99	0.44
1:D:168:ILE:HA	1:D:196:PHE:O	2.17	0.44
1:B:308:PRO:HB3	1:B:315:VAL:HG11	2.00	0.43
1:D:54:LEU:HD13	1:D:117:LEU:HG	2.00	0.43
1:D:121:ARG:NH1	1:D:123:ILE:HD11	2.33	0.43
1:F:72:LEU:HD12	1:F:73:LYS:N	2.33	0.43
1:C:208:SER:OG	1:D:98:LYS:HE3	2.17	0.43
1:E:141:LEU:HD23	1:E:190:GLN:HG2	2.00	0.43
1:H:95:ASP:HB3	1:H:98:LYS:HB3	1.99	0.43
1:G:45:VAL:HG12	1:G:52:LEU:HD21	2.01	0.43
1:H:283:GLU:O	1:H:287:ILE:HG12	2.18	0.43
1:A:28:TYR:CE1	1:A:78:GLU:HB3	2.53	0.43
1:A:81:ALA:HA	1:A:91:PHE:CE1	2.53	0.43
1:C:72:LEU:HD12	1:C:73:LYS:N	2.33	0.43
1:F:54:LEU:HD13	1:F:117:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:LEU:HD22	1:G:108:PHE:CZ	2.54	0.43
1:A:289:LYS:HB3	1:A:293:ARG:HH12	1.84	0.43
1:E:51:LEU:HB2	1:E:89:ILE:HG12	2.01	0.43
1:E:295:ASN:HB2	1:E:301:LEU:HD23	1.99	0.43
1:E:283:GLU:O	1:E:287:ILE:HG12	2.19	0.43
1:H:81:ALA:HA	1:H:91:PHE:CE1	2.54	0.43
1:B:57:HIS:ND1	1:B:111:GLU:OE2	2.52	0.43
1:B:361:TRP:O	1:B:365:VAL:HG23	2.18	0.43
1:F:126:ASP:HB3	1:F:258:PHE:HD2	1.84	0.43
1:H:72:LEU:HD12	1:H:73:LYS:N	2.34	0.43
1:E:163:ASP:HB3	1:E:253:ARG:HH21	1.84	0.43
1:G:273:PHE:O	1:G:329:PRO:HA	2.18	0.43
1:D:251:ARG:NH2	1:D:310:ASP:OD2	2.38	0.42
1:H:54:LEU:HD22	1:H:108:PHE:HZ	1.84	0.42
1:H:252:LEU:HD13	1:H:304:LEU:HD21	2.01	0.42
1:D:283:GLU:OE1	1:G:154:GLU:HG3	2.19	0.42
1:E:54:LEU:HD23	1:E:94:VAL:HG21	2.01	0.42
1:F:295:ASN:HB2	1:F:301:LEU:HD23	2.02	0.42
1:G:54:LEU:HD23	1:G:94:VAL:HG21	2.01	0.42
1:A:163:ASP:HB3	1:A:253:ARG:HH21	1.85	0.42
1:A:45:VAL:HG13	1:A:49:TYR:CE2	2.55	0.42
1:B:168:ILE:HG23	1:B:209:LEU:HD11	2.01	0.42
1:D:54:LEU:HD23	1:D:94:VAL:HG21	2.02	0.42
1:B:128:GLU:HB2	1:E:25:PHE:CZ	2.54	0.42
1:E:28:TYR:CE1	1:E:78:GLU:HB3	2.54	0.42
1:C:126:ASP:HB3	1:C:258:PHE:HD2	1.85	0.42
1:B:126:ASP:HB3	1:B:258:PHE:CD2	2.54	0.42
1:C:126:ASP:HB3	1:C:258:PHE:CD2	2.54	0.42
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.88	0.42
1:E:284:PHE:CG	1:E:329:PRO:HB3	2.55	0.42
1:D:128:GLU:HB2	1:G:25:PHE:CZ	2.55	0.42
1:H:45:VAL:HG13	1:H:49:TYR:CE2	2.55	0.42
1:A:168:ILE:HG23	1:A:209:LEU:HD11	2.01	0.42
1:A:54:LEU:HG	1:A:92:VAL:CG2	2.50	0.42
1:C:93:MET:HE2	1:C:93:MET:HB3	1.94	0.42
1:F:24:ASN:HB3	1:F:25:PHE:H	1.69	0.42
1:A:95:ASP:HB3	1:A:98:LYS:HB3	2.02	0.42
1:C:350:ASP:O	1:H:151:SER:HB2	2.20	0.42
1:D:284:PHE:CG	1:D:329:PRO:HB3	2.55	0.42
1:F:192:TYR:CE1	1:F:256:GLU:HA	2.55	0.42
1:C:84:LEU:HD12	1:C:91:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:361:TRP:O	1:H:365:VAL:HG23	2.20	0.41
1:D:170:PHE:O	1:D:212:ASN:N	2.44	0.41
1:D:72:LEU:HD12	1:D:73:LYS:N	2.36	0.41
1:G:168:ILE:HA	1:G:196:PHE:O	2.20	0.41
1:A:31:LYS:HB3	1:A:33:ARG:NH1	2.35	0.41
1:C:217:TYR:CZ	1:C:224:PRO:HB3	2.56	0.41
1:B:210:LYS:HB3	1:B:230:LYS:NZ	2.34	0.41
1:B:283:GLU:O	1:B:287:ILE:HG12	2.20	0.41
1:D:51:LEU:HB2	1:D:89:ILE:HG12	2.03	0.41
1:H:51:LEU:HB2	1:H:89:ILE:HG12	2.02	0.41
1:G:81:ALA:HA	1:G:91:PHE:CE1	2.56	0.41
1:A:126:ASP:HB3	1:A:258:PHE:CD2	2.55	0.41
1:D:149:ILE:HG23	1:D:154:GLU:HB3	2.03	0.41
1:D:24:ASN:HB3	1:D:25:PHE:H	1.71	0.41
1:D:54:LEU:HD22	1:D:108:PHE:CZ	2.55	0.41
1:F:45:VAL:HG13	1:F:49:TYR:HE2	1.84	0.41
1:A:158:PHE:HE1	1:A:196:PHE:CD1	2.39	0.41
1:B:45:VAL:HG12	1:B:52:LEU:HD21	2.03	0.41
1:E:152:LYS:HB3	1:E:206:LYS:HE3	2.02	0.41
1:H:54:LEU:HD13	1:H:117:LEU:HG	2.03	0.41
1:B:54:LEU:HD13	1:B:117:LEU:HG	2.02	0.41
1:E:121:ARG:NH1	1:E:187:GLU:O	2.54	0.41
1:A:24:ASN:HB3	1:A:25:PHE:H	1.69	0.40
1:B:145:PRO:HG2	1:B:187:GLU:HG2	2.04	0.40
1:E:168:ILE:HA	1:E:196:PHE:O	2.21	0.40
1:E:213:GLU:HB2	1:E:230:LYS:HD3	2.04	0.40
1:F:28:TYR:CE1	1:F:78:GLU:HB3	2.56	0.40
1:A:114:LEU:HD23	1:A:134:LEU:HD11	2.04	0.40
1:A:281:GLY:HA2	1:A:329:PRO:HG3	2.01	0.40
1:A:45:VAL:HG12	1:A:52:LEU:HD21	2.03	0.40
1:B:166:LYS:HB2	1:B:217:TYR:HB2	2.02	0.40
1:C:247:PRO:HG2	1:C:250:ARG:HB3	2.02	0.40
1:H:295:ASN:HB2	1:H:301:LEU:HD23	2.03	0.40
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.87	0.40
1:B:192:TYR:CE1	1:B:256:GLU:HA	2.56	0.40
1:D:217:TYR:CZ	1:D:224:PRO:HB3	2.56	0.40
1:E:121:ARG:NH1	1:E:123:ILE:HD11	2.36	0.40
1:F:168:ILE:HA	1:F:196:PHE:O	2.22	0.40
1:H:145:PRO:HB2	1:H:186:ALA:HB1	2.04	0.40
1:H:284:PHE:CG	1:H:329:PRO:HB3	2.57	0.40
1:C:54:LEU:HD22	1:C:108:PHE:HZ	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:GLU:O	1:H:187:GLU:HG3	2.22	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	323/329 (98%)	309 (96%)	14 (4%)	0	100	100
1	B	323/329 (98%)	310 (96%)	13 (4%)	0	100	100
1	C	323/329 (98%)	310 (96%)	13 (4%)	0	100	100
1	D	323/329 (98%)	310 (96%)	13 (4%)	0	100	100
1	E	323/329 (98%)	309 (96%)	14 (4%)	0	100	100
1	F	323/329 (98%)	310 (96%)	13 (4%)	0	100	100
1	G	323/329 (98%)	310 (96%)	13 (4%)	0	100	100
1	H	323/329 (98%)	310 (96%)	13 (4%)	0	100	100
All	All	2584/2632 (98%)	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	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	B	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	C	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	D	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	E	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	F	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	G	297/298 (100%)	295 (99%)	2 (1%)	85 93
1	H	297/298 (100%)	295 (99%)	2 (1%)	85 93
All	All	2376/2384 (100%)	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 (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 69 ligands modelled in this entry, 64 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	I	1	2	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	I	2	2	4,4,4	0.19	0	6,6,6	0.06	0
3	SO4	I	3	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	I	4	-	4,4,4	0.19	0	6,6,6	0.08	0
3	SO4	I	5	-	4,4,4	0.18	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	I	1	2	-	0/0/0/0	0/0/0/0
3	SO4	I	2	2	-	0/0/0/0	0/0/0/0
3	SO4	I	3	-	-	0/0/0/0	0/0/0/0
3	SO4	I	4	-	-	0/0/0/0	0/0/0/0
3	SO4	I	5	-	-	0/0/0/0	0/0/0/0

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	2
1	D	2
1	E	2
1	H	2
1	B	2
1	C	2
1	A	2
1	F	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	258:PHE	C	268:ILE	N	16.16
1	D	258:PHE	C	268:ILE	N	16.05
1	E	258:PHE	C	268:ILE	N	16.05
1	B	258:PHE	C	268:ILE	N	16.03
1	G	258:PHE	C	268:ILE	N	16.01
1	F	258:PHE	C	268:ILE	N	15.90
1	C	258:PHE	C	268:ILE	N	15.86
1	H	258:PHE	C	268:ILE	N	15.85
1	B	57:HIS	C	69:GLN	N	9.62
1	E	57:HIS	C	69:GLN	N	9.61
1	C	57:HIS	C	69:GLN	N	9.57
1	G	57:HIS	C	69:GLN	N	9.55
1	A	57:HIS	C	69:GLN	N	9.48
1	F	57:HIS	C	69:GLN	N	9.48
1	H	57:HIS	C	69:GLN	N	9.46
1	D	57:HIS	C	69:GLN	N	9.45

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	329/329 (100%)	2.12	142 (43%)	0	0	66, 99, 134, 141	0
1	B	329/329 (100%)	1.45	101 (30%)	0	0	51, 89, 137, 152	0
1	C	329/329 (100%)	1.55	113 (34%)	0	0	50, 88, 132, 154	0
1	D	329/329 (100%)	1.82	124 (37%)	0	0	58, 98, 133, 145	0
1	E	329/329 (100%)	1.64	109 (33%)	0	0	56, 97, 136, 148	0
1	F	329/329 (100%)	1.42	103 (31%)	0	0	47, 91, 133, 160	0
1	G	329/329 (100%)	1.41	100 (30%)	0	0	49, 91, 131, 156	0
1	H	329/329 (100%)	2.01	141 (42%)	0	0	60, 96, 133, 142	0
All	All	2632/2632 (100%)	1.68	933 (35%)	0	0	47, 94, 134, 160	0

All (933) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ALA	13.0
1	H	115	TYR	11.3
1	H	150	SER	10.6
1	D	257	MET	10.4
1	A	96	ALA	9.7
1	E	248	THR	9.6
1	E	257	MET	9.5
1	H	113	SER	9.3
1	C	92	VAL	8.9
1	C	127	GLY	8.8
1	C	93	MET	8.7
1	D	53	CYS	8.6
1	H	114	LEU	8.6
1	C	128	GLU	8.5
1	D	190	GLN	8.4
1	A	169	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	8.1
1	A	215	ASP	8.1
1	G	54	LEU	8.0
1	D	128	GLU	7.9
1	H	53	CYS	7.9
1	G	73	LYS	7.9
1	A	95	ASP	7.9
1	C	257	MET	7.9
1	D	248	THR	7.9
1	A	23	LEU	7.9
1	A	116	ILE	7.8
1	E	128	GLU	7.7
1	H	112	GLY	7.7
1	H	212	ASN	7.7
1	H	102	LEU	7.6
1	A	115	TYR	7.6
1	G	92	VAL	7.6
1	B	71	GLN	7.5
1	H	54	LEU	7.4
1	H	88	ALA	7.3
1	A	102	LEU	7.3
1	E	249	LEU	7.3
1	B	55	TYR	7.2
1	A	97	LYS	7.1
1	D	302	SER	7.1
1	G	116	ILE	7.1
1	H	129	PHE	7.0
1	A	227	ILE	7.0
1	A	55	TYR	7.0
1	A	150	SER	7.0
1	H	96	ALA	6.8
1	D	191	PRO	6.8
1	E	190	GLN	6.7
1	H	169	GLY	6.6
1	A	198	THR	6.6
1	D	90	GLY	6.6
1	H	149	ILE	6.5
1	E	367	SER	6.5
1	F	191	PRO	6.5
1	D	102	LEU	6.4
1	A	113	SER	6.4
1	G	94	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLU	6.4
1	E	192	TYR	6.4
1	D	91	PHE	6.3
1	C	71	GLN	6.3
1	G	55	TYR	6.3
1	G	53	CYS	6.2
1	A	54	LEU	6.2
1	H	302	SER	6.2
1	H	92	VAL	6.2
1	F	315	VAL	6.2
1	F	108	PHE	6.1
1	D	192	TYR	6.1
1	A	149	ILE	6.1
1	D	256	GLU	6.1
1	C	94	VAL	6.1
1	F	318	TRP	6.1
1	G	93	MET	6.0
1	C	37	LEU	6.0
1	F	128	GLU	6.0
1	B	94	VAL	5.9
1	H	215	ASP	5.9
1	D	71	GLN	5.9
1	A	117	LEU	5.9
1	H	44	GLN	5.9
1	A	216	PHE	5.9
1	H	226	ALA	5.8
1	C	269	HIS	5.8
1	H	296	THR	5.8
1	H	248	THR	5.8
1	E	193	ILE	5.7
1	C	91	PHE	5.7
1	F	94	VAL	5.7
1	D	74	GLU	5.6
1	H	168	ILE	5.6
1	A	301	LEU	5.6
1	A	225	ILE	5.6
1	E	191	PRO	5.6
1	B	92	VAL	5.6
1	C	258	PHE	5.5
1	A	214	VAL	5.5
1	H	55	TYR	5.5
1	C	54	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	108	PHE	5.5
1	G	56	TYR	5.5
1	H	283	GLU	5.5
1	A	355	ALA	5.5
1	G	70	PHE	5.5
1	D	301	LEU	5.4
1	G	114	LEU	5.4
1	F	192	TYR	5.4
1	E	102	LEU	5.4
1	B	91	PHE	5.4
1	B	149	ILE	5.4
1	C	75	ILE	5.4
1	H	198	THR	5.4
1	C	334	VAL	5.3
1	D	324	ILE	5.3
1	C	192	TYR	5.3
1	D	129	PHE	5.3
1	H	116	ILE	5.3
1	G	212	ASN	5.2
1	D	39	GLU	5.2
1	H	237	LEU	5.2
1	C	191	PRO	5.2
1	D	42	PHE	5.2
1	D	268	ILE	5.2
1	G	76	VAL	5.2
1	G	102	LEU	5.2
1	A	129	PHE	5.1
1	H	301	LEU	5.1
1	D	249	LEU	5.1
1	B	96	ALA	5.1
1	B	23	LEU	5.1
1	H	119	GLY	5.1
1	B	114	LEU	5.1
1	A	125	PHE	5.1
1	A	359	GLU	5.0
1	B	95	ASP	5.0
1	D	125	PHE	5.0
1	G	52	LEU	5.0
1	C	333	VAL	5.0
1	F	257	MET	5.0
1	D	70	PHE	5.0
1	B	102	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	53	CYS	5.0
1	F	50	ASP	5.0
1	E	131	ALA	4.9
1	E	366	LEU	4.9
1	A	91	PHE	4.9
1	A	132	ASP	4.9
1	F	314	LEU	4.9
1	B	196	PHE	4.9
1	F	95	ASP	4.9
1	A	286	GLU	4.9
1	E	130	ALA	4.9
1	D	54	LEU	4.9
1	B	54	LEU	4.9
1	C	318	TRP	4.9
1	H	56	TYR	4.9
1	H	117	LEU	4.8
1	A	303	ILE	4.8
1	B	106	LEU	4.8
1	D	88	ALA	4.8
1	E	41	ASN	4.8
1	E	40	LYS	4.8
1	B	38	SER	4.8
1	A	248	THR	4.8
1	C	129	PHE	4.8
1	F	190	GLN	4.8
1	D	250	ARG	4.7
1	A	53	CYS	4.7
1	D	226	ALA	4.7
1	D	73	LYS	4.7
1	E	292	ALA	4.7
1	D	106	LEU	4.7
1	F	313	LEU	4.7
1	H	99	GLU	4.7
1	A	358	LEU	4.7
1	E	109	ASP	4.7
1	A	100	ALA	4.7
1	A	123	ILE	4.7
1	A	39	GLU	4.6
1	B	72	LEU	4.6
1	A	112	GLY	4.6
1	G	115	TYR	4.6
1	H	303	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	130	ALA	4.6
1	B	116	ILE	4.6
1	E	149	ILE	4.6
1	A	295	ASN	4.6
1	B	354	THR	4.6
1	H	245	GLN	4.6
1	H	216	PHE	4.6
1	E	226	ALA	4.5
1	A	339	ALA	4.5
1	D	215	ASP	4.5
1	C	324	ILE	4.5
1	F	107	GLY	4.5
1	H	52	LEU	4.5
1	H	23	LEU	4.5
1	D	141	LEU	4.4
1	H	238	VAL	4.4
1	D	298	ASN	4.4
1	A	136	GLU	4.4
1	D	227	ILE	4.4
1	G	77	LEU	4.4
1	H	163	ASP	4.4
1	C	55	TYR	4.4
1	F	92	VAL	4.4
1	B	318	TRP	4.4
1	E	296	THR	4.4
1	A	357	GLU	4.4
1	C	38	SER	4.3
1	E	103	ALA	4.3
1	D	89	ILE	4.3
1	F	26	PRO	4.3
1	F	245	GLN	4.3
1	A	84	LEU	4.3
1	A	302	SER	4.3
1	G	117	LEU	4.3
1	B	99	GLU	4.3
1	B	361	TRP	4.3
1	B	197	ALA	4.2
1	G	74	GLU	4.2
1	F	333	VAL	4.2
1	A	99	GLU	4.2
1	E	141	LEU	4.2
1	B	370	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	LEU	4.2
1	F	37	LEU	4.2
1	C	125	PHE	4.2
1	H	337	THR	4.2
1	A	332	GLY	4.2
1	E	194	LYS	4.2
1	E	23	LEU	4.2
1	E	250	ARG	4.1
1	E	50	ASP	4.1
1	H	160	ARG	4.1
1	A	217	TYR	4.1
1	A	298	ASN	4.1
1	A	257	MET	4.1
1	D	52	LEU	4.1
1	D	96	ALA	4.0
1	D	114	LEU	4.0
1	E	123	ILE	4.0
1	B	70	PHE	4.0
1	F	112	GLY	4.0
1	D	316	ALA	4.0
1	H	43	LYS	4.0
1	H	111	GLU	4.0
1	G	241	VAL	4.0
1	E	295	ASN	4.0
1	B	84	LEU	4.0
1	A	88	ALA	4.0
1	F	91	PHE	4.0
1	B	332	GLY	4.0
1	H	217	TYR	4.0
1	D	194	LYS	4.0
1	G	95	ASP	4.0
1	A	284	PHE	3.9
1	A	94	VAL	3.9
1	H	249	LEU	3.9
1	E	145	PRO	3.9
1	E	370	ILE	3.9
1	D	50	ASP	3.9
1	B	93	MET	3.9
1	G	176	SER	3.9
1	A	87	LYS	3.9
1	E	161	ILE	3.9
1	C	33	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	36	SER	3.9
1	C	102	LEU	3.9
1	E	198	THR	3.9
1	A	141	LEU	3.8
1	E	365	VAL	3.8
1	C	313	LEU	3.8
1	C	72	LEU	3.8
1	C	82	GLN	3.8
1	H	89	ILE	3.8
1	D	137	PHE	3.8
1	D	244	HIS	3.8
1	E	97	LYS	3.8
1	D	150	SER	3.8
1	D	131	ALA	3.8
1	F	193	ILE	3.8
1	H	151	SER	3.8
1	A	197	ALA	3.8
1	E	227	ILE	3.8
1	D	161	ILE	3.8
1	D	136	GLU	3.8
1	G	217	TYR	3.7
1	G	257	MET	3.7
1	A	352	LEU	3.7
1	A	168	ILE	3.7
1	C	325	ASP	3.7
1	C	76	VAL	3.7
1	C	315	VAL	3.7
1	C	149	ILE	3.7
1	E	182	PHE	3.7
1	A	354	THR	3.7
1	D	299	PRO	3.7
1	G	169	GLY	3.7
1	E	368	GLY	3.7
1	F	366	LEU	3.7
1	F	337	THR	3.7
1	A	44	GLN	3.7
1	B	317	TYR	3.7
1	A	52	LEU	3.7
1	B	241	VAL	3.7
1	H	91	PHE	3.7
1	G	168	ILE	3.7
1	D	121	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	96	ALA	3.7
1	C	190	GLN	3.6
1	D	76	VAL	3.6
1	F	322	PHE	3.6
1	G	72	LEU	3.6
1	E	113	SER	3.6
1	G	167	LEU	3.6
1	A	154	GLU	3.6
1	C	147	GLU	3.6
1	G	222	ASP	3.6
1	H	355	ALA	3.6
1	H	220	PHE	3.6
1	F	103	ALA	3.6
1	B	74	GLU	3.6
1	F	248	THR	3.6
1	C	126	ASP	3.6
1	H	123	ILE	3.6
1	D	303	ILE	3.6
1	H	80	VAL	3.6
1	H	232	TYR	3.6
1	A	268	ILE	3.6
1	C	131	ALA	3.6
1	D	369	LYS	3.6
1	A	241	VAL	3.6
1	H	167	LEU	3.6
1	C	120	ASP	3.6
1	B	117	LEU	3.6
1	H	171	PHE	3.6
1	B	215	ASP	3.6
1	G	343	TRP	3.6
1	A	289	LYS	3.5
1	D	269	HIS	3.5
1	E	160	ARG	3.5
1	G	149	ILE	3.5
1	C	317	TYR	3.5
1	A	24	ASN	3.5
1	E	333	VAL	3.5
1	B	244	HIS	3.5
1	D	313	LEU	3.5
1	D	169	GLY	3.5
1	G	332	GLY	3.5
1	B	284	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	3.5
1	F	249	LEU	3.5
1	B	312	PRO	3.5
1	E	254	PRO	3.5
1	H	213	GLU	3.5
1	F	342	VAL	3.5
1	G	237	LEU	3.5
1	C	197	ALA	3.5
1	H	76	VAL	3.5
1	E	83	VAL	3.5
1	D	72	LEU	3.5
1	H	165	ILE	3.5
1	H	49	TYR	3.5
1	E	203	VAL	3.5
1	B	125	PHE	3.5
1	E	252	LEU	3.5
1	G	245	GLN	3.5
1	H	257	MET	3.5
1	D	123	ILE	3.4
1	B	150	SER	3.4
1	C	312	PRO	3.4
1	B	115	TYR	3.4
1	H	93	MET	3.4
1	C	347	PRO	3.4
1	E	195	PHE	3.4
1	E	167	LEU	3.4
1	A	240	PHE	3.4
1	E	215	ASP	3.4
1	H	162	GLU	3.4
1	B	222	ASP	3.4
1	E	324	ILE	3.4
1	E	313	LEU	3.4
1	B	331	ILE	3.4
1	H	39	GLU	3.4
1	A	160	ARG	3.4
1	C	196	PHE	3.4
1	H	73	LYS	3.4
1	E	268	ILE	3.4
1	E	298	ASN	3.4
1	H	288	LEU	3.4
1	C	130	ALA	3.4
1	E	305	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	245	GLN	3.4
1	A	90	GLY	3.4
1	D	120	ASP	3.4
1	F	269	HIS	3.4
1	G	313	LEU	3.3
1	A	362	ILE	3.3
1	G	129	PHE	3.3
1	H	106	LEU	3.3
1	A	119	GLY	3.3
1	B	56	TYR	3.3
1	A	42	PHE	3.3
1	F	131	ALA	3.3
1	C	134	LEU	3.3
1	A	254	PRO	3.3
1	E	362	ILE	3.3
1	B	128	GLU	3.3
1	H	132	ASP	3.3
1	C	250	ARG	3.3
1	A	89	ILE	3.3
1	D	193	ILE	3.3
1	E	339	ALA	3.3
1	B	353	PRO	3.3
1	H	94	VAL	3.3
1	H	154	GLU	3.3
1	F	33	ARG	3.3
1	D	198	THR	3.3
1	A	271	VAL	3.3
1	C	343	TRP	3.2
1	B	77	LEU	3.2
1	D	92	VAL	3.2
1	H	225	ILE	3.2
1	E	189	PHE	3.2
1	C	268	ILE	3.2
1	H	196	PHE	3.2
1	D	216	PHE	3.2
1	C	323	LYS	3.2
1	H	97	LYS	3.2
1	C	115	TYR	3.2
1	B	69	GLN	3.2
1	D	214	VAL	3.2
1	B	34	VAL	3.2
1	G	355	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	213	GLU	3.2
1	D	116	ILE	3.2
1	D	368	GLY	3.2
1	D	222	ASP	3.2
1	G	215	ASP	3.2
1	H	90	GLY	3.2
1	D	126	ASP	3.2
1	F	141	LEU	3.2
1	B	168	ILE	3.2
1	C	70	PHE	3.1
1	D	220	PHE	3.1
1	A	106	LEU	3.1
1	C	249	LEU	3.1
1	C	316	ALA	3.1
1	A	368	GLY	3.1
1	B	216	PHE	3.1
1	A	229	ASN	3.1
1	G	274	ALA	3.1
1	E	312	PRO	3.1
1	E	369	LYS	3.1
1	H	103	ALA	3.1
1	E	26	PRO	3.1
1	G	175	ASP	3.1
1	A	369	LYS	3.1
1	D	77	LEU	3.1
1	F	331	ILE	3.1
1	G	164	TYR	3.1
1	A	285	LEU	3.1
1	D	162	GLU	3.1
1	G	196	PHE	3.1
1	H	95	ASP	3.0
1	H	48	LYS	3.0
1	F	99	GLU	3.0
1	G	287	ILE	3.0
1	D	333	VAL	3.0
1	H	224	PRO	3.0
1	E	38	SER	3.0
1	F	250	ARG	3.0
1	F	341	SER	3.0
1	A	101	LYS	3.0
1	H	30	GLY	3.0
1	A	288	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	314	LEU	3.0
1	E	91	PHE	3.0
1	C	73	LYS	3.0
1	F	102	LEU	3.0
1	A	279	PRO	3.0
1	F	34	VAL	3.0
1	C	326	LEU	3.0
1	A	118	LYS	3.0
1	F	312	PRO	3.0
1	A	361	TRP	3.0
1	H	131	ALA	3.0
1	H	158	PHE	3.0
1	C	270	ILE	3.0
1	D	279	PRO	3.0
1	E	199	PHE	3.0
1	G	232	TYR	3.0
1	A	287	ILE	3.0
1	B	53	CYS	3.0
1	H	197	ALA	3.0
1	H	352	LEU	3.0
1	E	39	GLU	3.0
1	B	330	GLN	3.0
1	D	367	SER	3.0
1	H	273	PHE	3.0
1	G	331	ILE	3.0
1	C	304	LEU	3.0
1	D	122	THR	3.0
1	G	37	LEU	3.0
1	C	322	PHE	3.0
1	D	41	ASN	3.0
1	H	50	ASP	3.0
1	F	199	PHE	3.0
1	D	334	VAL	3.0
1	G	223	GLU	3.0
1	H	282	TYR	3.0
1	E	299	PRO	3.0
1	F	147	GLU	3.0
1	A	92	VAL	2.9
1	D	103	ALA	2.9
1	A	270	ILE	2.9
1	E	110	GLU	2.9
1	B	357	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	125	PHE	2.9
1	D	135	VAL	2.9
1	E	158	PHE	2.9
1	G	108	PHE	2.9
1	F	332	GLY	2.9
1	C	86	HIS	2.9
1	D	79	LEU	2.9
1	G	99	GLU	2.9
1	F	317	TYR	2.9
1	E	256	GLU	2.9
1	H	31	LYS	2.9
1	B	37	LEU	2.9
1	B	141	LEU	2.9
1	A	296	THR	2.9
1	E	122	THR	2.9
1	H	42	PHE	2.9
1	G	69	GLN	2.9
1	F	270	ILE	2.9
1	C	329	PRO	2.9
1	A	220	PHE	2.9
1	G	361	TRP	2.9
1	A	223	GLU	2.9
1	B	343	TRP	2.9
1	B	123	ILE	2.9
1	H	313	LEU	2.9
1	C	135	VAL	2.9
1	D	38	SER	2.9
1	D	315	VAL	2.9
1	A	367	SER	2.9
1	B	288	LEU	2.8
1	F	38	SER	2.8
1	B	73	LYS	2.8
1	E	214	VAL	2.8
1	G	29	ASP	2.8
1	H	177	GLU	2.8
1	C	161	ILE	2.8
1	H	284	PHE	2.8
1	F	127	GLY	2.8
1	H	241	VAL	2.8
1	F	96	ALA	2.8
1	F	335	ASN	2.8
1	A	337	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	28	TYR	2.8
1	H	214	VAL	2.8
1	H	370	ILE	2.8
1	C	90	GLY	2.8
1	B	249	LEU	2.8
1	C	39	GLU	2.8
1	B	355	ALA	2.8
1	G	270	ILE	2.8
1	C	35	VAL	2.8
1	G	284	PHE	2.8
1	C	370	ILE	2.8
1	C	108	PHE	2.8
1	C	69	GLN	2.8
1	E	84	LEU	2.8
1	H	203	VAL	2.8
1	E	166	LYS	2.8
1	C	137	PHE	2.8
1	E	288	LEU	2.8
1	F	189	PHE	2.8
1	F	334	VAL	2.8
1	H	227	ILE	2.8
1	B	169	GLY	2.8
1	B	226	ALA	2.8
1	C	42	PHE	2.8
1	E	106	LEU	2.8
1	E	274	ALA	2.8
1	F	279	PRO	2.7
1	H	322	PHE	2.7
1	A	251	ARG	2.7
1	E	337	THR	2.7
1	F	254	PRO	2.7
1	B	103	ALA	2.7
1	F	365	VAL	2.7
1	C	167	LEU	2.7
1	B	50	ASP	2.7
1	G	135	VAL	2.7
1	A	105	LYS	2.7
1	G	349	ASP	2.7
1	G	353	PRO	2.7
1	H	148	ILE	2.7
1	E	255	GLU	2.7
1	H	74	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	284	PHE	2.7
1	F	106	LEU	2.7
1	G	288	LEU	2.7
1	D	212	ASN	2.7
1	D	326	LEU	2.7
1	E	79	LEU	2.7
1	F	56	TYR	2.7
1	G	91	PHE	2.7
1	A	163	ASP	2.7
1	B	287	ILE	2.7
1	C	114	LEU	2.7
1	E	216	PHE	2.7
1	C	85	GLU	2.7
1	H	141	LEU	2.7
1	C	148	ILE	2.7
1	D	255	GLU	2.7
1	E	42	PHE	2.7
1	F	330	GLN	2.7
1	C	303	ILE	2.7
1	E	346	ILE	2.7
1	H	87	LYS	2.7
1	A	73	LYS	2.7
1	F	326	LEU	2.7
1	H	128	GLU	2.7
1	B	98	LYS	2.7
1	E	245	GLN	2.7
1	E	116	ILE	2.7
1	E	269	HIS	2.7
1	F	168	ILE	2.7
1	B	39	GLU	2.6
1	B	352	LEU	2.6
1	C	237	LEU	2.6
1	H	108	PHE	2.6
1	C	256	GLU	2.6
1	H	223	GLU	2.6
1	G	150	SER	2.6
1	A	77	LEU	2.6
1	B	291	VAL	2.6
1	B	371	ASN	2.6
1	B	335	ASN	2.6
1	F	158	PHE	2.6
1	B	194	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	289	LYS	2.6
1	H	362	ILE	2.6
1	D	312	PRO	2.6
1	F	316	ALA	2.6
1	H	166	LYS	2.6
1	E	169	GLY	2.6
1	D	241	VAL	2.6
1	G	103	ALA	2.6
1	D	189	PHE	2.6
1	E	171	PHE	2.6
1	D	300	ASP	2.6
1	H	51	LEU	2.6
1	F	222	ASP	2.6
1	G	200	ASP	2.6
1	A	74	GLU	2.6
1	B	33	ARG	2.6
1	B	131	ALA	2.6
1	D	119	GLY	2.6
1	G	38	SER	2.6
1	F	244	HIS	2.6
1	A	108	PHE	2.6
1	A	122	THR	2.6
1	E	303	ILE	2.6
1	F	252	LEU	2.6
1	A	293	ARG	2.6
1	D	325	ASP	2.6
1	D	34	VAL	2.6
1	H	156	GLN	2.6
1	E	253	ARG	2.6
1	C	141	LEU	2.5
1	G	358	LEU	2.5
1	B	211	MET	2.5
1	C	157	ALA	2.5
1	B	225	ILE	2.5
1	D	43	LYS	2.5
1	G	148	ILE	2.5
1	D	100	ALA	2.5
1	A	331	ILE	2.5
1	B	134	LEU	2.5
1	G	134	LEU	2.5
1	A	370	ILE	2.5
1	F	55	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	217	TYR	2.5
1	F	324	ILE	2.5
1	E	129	PHE	2.5
1	E	279	PRO	2.5
1	F	343	TRP	2.5
1	H	312	PRO	2.5
1	C	245	GLN	2.5
1	D	132	ASP	2.5
1	D	163	ASP	2.5
1	G	220	PHE	2.5
1	H	211	MET	2.5
1	H	157	ALA	2.5
1	A	80	VAL	2.5
1	G	39	GLU	2.5
1	G	283	GLU	2.5
1	C	31	LYS	2.5
1	B	127	GLY	2.5
1	B	270	ILE	2.5
1	D	26	PRO	2.5
1	H	164	TYR	2.5
1	A	137	PHE	2.5
1	B	337	THR	2.4
1	E	343	TRP	2.4
1	B	237	LEU	2.4
1	C	56	TYR	2.4
1	F	200	ASP	2.4
1	G	154	GLU	2.4
1	F	69	GLN	2.4
1	H	358	LEU	2.4
1	D	108	PHE	2.4
1	F	25	PHE	2.4
1	D	156	GLN	2.4
1	H	155	VAL	2.4
1	F	284	PHE	2.4
1	A	305	TRP	2.4
1	B	232	TYR	2.4
1	F	241	VAL	2.4
1	E	148	ILE	2.4
1	F	329	PRO	2.4
1	C	34	VAL	2.4
1	E	282	TYR	2.4
1	B	132	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	220	PHE	2.4
1	C	169	GLY	2.4
1	A	43	LYS	2.4
1	D	196	PHE	2.4
1	F	370	ILE	2.4
1	F	298	ASN	2.4
1	A	147	GLU	2.4
1	H	118	LYS	2.4
1	C	342	VAL	2.4
1	F	347	PRO	2.4
1	A	165	ILE	2.4
1	E	112	GLY	2.4
1	D	358	LEU	2.4
1	G	197	ALA	2.4
1	D	159	GLU	2.4
1	F	255	GLU	2.4
1	D	118	LYS	2.4
1	C	198	THR	2.4
1	G	166	LYS	2.4
1	E	98	LYS	2.4
1	B	90	GLY	2.4
1	C	332	GLY	2.4
1	D	160	ARG	2.4
1	A	49	TYR	2.4
1	A	182	PHE	2.4
1	C	371	ASN	2.3
1	A	272	ALA	2.3
1	A	304	LEU	2.3
1	D	322	PHE	2.3
1	F	363	GLU	2.3
1	A	299	PRO	2.3
1	G	51	LEU	2.3
1	A	50	ASP	2.3
1	H	293	ARG	2.3
1	F	362	ILE	2.3
1	H	331	ILE	2.3
1	A	45	VAL	2.3
1	D	343	TRP	2.3
1	G	27	THR	2.3
1	G	163	ASP	2.3
1	F	216	PHE	2.3
1	G	195	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLU	2.3
1	F	161	ILE	2.3
1	H	161	ILE	2.3
1	E	76	VAL	2.3
1	E	358	LEU	2.3
1	C	123	ILE	2.3
1	D	139	LEU	2.3
1	H	46	LEU	2.3
1	B	24	ASN	2.3
1	H	365	VAL	2.3
1	A	37	LEU	2.3
1	A	128	GLU	2.3
1	D	51	LEU	2.3
1	C	220	PHE	2.3
1	F	274	ALA	2.3
1	C	116	ILE	2.3
1	F	148	ILE	2.3
1	C	51	LEU	2.3
1	A	335	ASN	2.3
1	C	166	LYS	2.3
1	F	237	LEU	2.3
1	H	130	ALA	2.3
1	F	167	LEU	2.3
1	G	312	PRO	2.3
1	H	347	PRO	2.3
1	B	240	PHE	2.3
1	D	75	ILE	2.3
1	D	188	HIS	2.3
1	E	168	ILE	2.3
1	B	285	LEU	2.3
1	C	302	SER	2.3
1	H	287	ILE	2.3
1	D	166	LYS	2.3
1	F	296	THR	2.3
1	A	244	HIS	2.3
1	E	80	VAL	2.3
1	G	244	HIS	2.3
1	D	167	LEU	2.3
1	B	76	VAL	2.2
1	A	317	TYR	2.2
1	E	126	ASP	2.2
1	H	353	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	237	LEU	2.2
1	D	304	LEU	2.2
1	F	361	TRP	2.2
1	G	23	LEU	2.2
1	G	249	LEU	2.2
1	D	115	TYR	2.2
1	H	292	ALA	2.2
1	F	164	TYR	2.2
1	D	37	LEU	2.2
1	B	201	LYS	2.2
1	C	295	ASN	2.2
1	D	314	LEU	2.2
1	F	82	GLN	2.2
1	G	131	ALA	2.2
1	G	233	THR	2.2
1	H	84	LEU	2.2
1	F	70	PHE	2.2
1	H	24	ASN	2.2
1	B	338	ASP	2.2
1	E	132	ASP	2.2
1	F	247	PRO	2.2
1	G	198	THR	2.2
1	A	40	LYS	2.2
1	E	316	ALA	2.2
1	G	25	PHE	2.2
1	A	232	TYR	2.2
1	G	24	ASN	2.2
1	C	365	VAL	2.2
1	F	134	LEU	2.2
1	G	338	ASP	2.2
1	D	225	ILE	2.2
1	C	288	LEU	2.2
1	G	158	PHE	2.2
1	B	326	LEU	2.2
1	G	34	VAL	2.2
1	F	210	LYS	2.2
1	E	56	TYR	2.2
1	C	77	LEU	2.2
1	D	117	LEU	2.2
1	D	133	VAL	2.2
1	D	305	TRP	2.2
1	G	71	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	285	LEU	2.2
1	D	195	PHE	2.2
1	F	51	LEU	2.2
1	F	292	ALA	2.1
1	B	358	LEU	2.1
1	D	306	ILE	2.1
1	H	142	ILE	2.1
1	C	41	ASN	2.1
1	F	41	ASN	2.1
1	G	146	VAL	2.1
1	C	150	SER	2.1
1	F	31	LYS	2.1
1	H	25	PHE	2.1
1	A	228	PRO	2.1
1	B	339	ALA	2.1
1	E	347	PRO	2.1
1	H	72	LEU	2.1
1	B	362	ILE	2.1
1	D	31	LYS	2.1
1	A	103	ALA	2.1
1	A	238	VAL	2.1
1	A	218	GLU	2.1
1	C	248	THR	2.1
1	C	367	SER	2.1
1	E	133	VAL	2.1
1	G	339	ALA	2.1
1	A	109	ASP	2.1
1	F	196	PHE	2.1
1	C	168	ILE	2.1
1	B	320	LYS	2.1
1	H	101	LYS	2.1
1	A	131	ALA	2.1
1	A	292	ALA	2.1
1	D	199	PHE	2.1
1	F	273	PHE	2.1
1	B	334	VAL	2.1
1	E	328	ARG	2.1
1	G	214	VAL	2.1
1	F	258	PHE	2.1
1	G	42	PHE	2.1
1	E	104	LYS	2.1
1	G	352	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	ASP	2.1
1	H	120	ASP	2.1
1	H	346	ILE	2.1
1	E	138	LEU	2.1
1	B	42	PHE	2.1
1	F	297	ASP	2.1
1	H	29	ASP	2.1
1	C	159	GLU	2.1
1	C	255	GLU	2.1
1	D	319	GLU	2.1
1	H	107	GLY	2.1
1	A	224	PRO	2.0
1	G	250	ARG	2.0
1	B	275	GLU	2.0
1	F	283	GLU	2.0
1	G	105	LYS	2.0
1	H	38	SER	2.0
1	C	106	LEU	2.0
1	H	199	PHE	2.0
1	A	189	PHE	2.0
1	C	327	PHE	2.0
1	F	125	PHE	2.0
1	A	356	GLU	2.0
1	G	106	LEU	2.0
1	H	170	PHE	2.0
1	H	206	LYS	2.0
1	C	282	TYR	2.0
1	A	70	PHE	2.0
1	C	358	LEU	2.0
1	G	317	TYR	2.0
1	G	362	ILE	2.0
1	A	72	LEU	2.0
1	C	366	LEU	2.0
1	E	315	VAL	2.0
1	A	188	HIS	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	Y	15	1/?	0.47	0.14	134,134,134,134	1
2	YB	Y	42	1/?	0.51	0.15	118,118,118,118	1
2	YB	Y	47	1/?	0.57	0.10	204,204,204,204	0
2	YB	Y	51	1/?	0.69	0.15	91,91,91,91	1
2	YB	Y	34	1/?	0.71	0.17	129,129,129,129	1
2	YB	Y	83	1/?	0.71	0.15	92,92,92,92	1
2	YB	Y	10	1/?	0.73	0.09	166,166,166,166	1
2	YB	Y	27	1/?	0.76	0.19	112,112,112,112	1
2	YB	Y	35	1/?	0.77	0.12	183,183,183,183	1
2	YB	Y	77	1/?	0.78	0.10	100,100,100,100	1
2	YB	Y	23	1/?	0.78	0.05	184,184,184,184	0
2	YB	Y	38	1/?	0.79	0.15	161,161,161,161	0
2	YB	Y	80	1/?	0.81	0.17	187,187,187,187	1
2	YB	Y	6	1/?	0.81	0.14	129,129,129,129	0
2	YB	Y	11	1/?	0.82	0.13	127,127,127,127	1
2	YB	Y	86	1/?	0.84	0.10	213,213,213,213	1
2	YB	Y	55	1/?	0.85	0.12	126,126,126,126	1
2	YB	Y	75	1/?	0.86	0.18	125,125,125,125	1
2	YB	Y	9	1/?	0.86	0.09	144,144,144,144	1
2	YB	Y	54	1/?	0.87	0.18	86,86,86,86	1
2	YB	Y	4	1/?	0.89	0.11	149,149,149,149	1
2	YB	Y	26	1/?	0.89	0.07	151,151,151,151	1
2	YB	Y	1	1/?	0.91	0.13	115,115,115,115	0
2	YB	Y	28	1/?	0.91	0.27	126,126,126,126	1
2	YB	Y	48	1/?	0.92	0.22	94,94,94,94	1
2	YB	Y	32	1/?	0.92	0.17	170,170,170,170	1
2	YB	Y	36	1/?	0.92	0.09	83,83,83,83	1
2	YB	Y	3	1/?	0.92	0.13	122,122,122,122	0
2	YB	Y	31	1/?	0.92	0.18	134,134,134,134	1
2	YB	Y	22	1/?	0.92	0.07	127,127,127,127	1
2	YB	Y	70	1/?	0.93	0.21	109,109,109,109	1
2	YB	Y	21	1/?	0.93	0.09	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YB	Y	2	1/?	0.93	0.12	111,111,111,111	0
2	YB	Y	19	1/?	0.94	0.10	164,164,164,164	0
2	YB	Y	81	1/?	0.94	0.14	132,132,132,132	1
2	YB	Y	8	1/?	0.95	0.19	161,161,161,161	1
2	YB	Y	45	1/?	0.99	0.07	168,168,168,168	0
2	YB	Y	79	1/?	-	-	131,131,131,131	1
2	YB	Y	85	1/?	0.52	0.20	191,191,191,191	1
2	YB	Y	24	1/?	0.57	0.09	127,127,127,127	1
2	YB	Y	87	1/?	0.67	0.11	222,222,222,222	1
3	SO4	I	1	5/?	0.68	0.60	121,127,147,149	0
2	YB	Y	14	1/?	0.75	0.12	139,139,139,139	1
3	SO4	I	3	5/?	0.75	0.25	103,110,117,120	0
2	YB	Y	33	1/?	0.77	0.09	172,172,172,172	0
2	YB	Y	37	1/?	0.77	0.27	117,117,117,117	1
2	YB	Y	76	1/?	0.77	0.15	113,113,113,113	1
2	YB	Y	57	1/?	0.78	0.17	124,124,124,124	1
3	SO4	I	5	5/?	0.79	0.50	114,118,124,126	0
2	YB	Y	40	1/?	0.79	0.07	153,153,153,153	1
2	YB	Y	41	1/?	0.80	0.17	99,99,99,99	1
2	YB	Y	13	1/?	0.81	0.08	148,148,148,148	1
2	YB	Y	82	1/?	0.81	0.32	173,173,173,173	1
2	YB	Y	12	1/?	0.82	0.11	140,140,140,140	1
2	YB	Y	20	1/?	0.82	0.16	130,130,130,130	1
2	YB	Y	16	1/?	0.82	0.15	125,125,125,125	1
2	YB	Y	7	1/?	0.84	0.19	150,150,150,150	1
2	YB	Y	78	1/?	0.84	0.26	116,116,116,116	1
2	YB	Y	84	1/?	0.84	0.17	327,327,327,327	1
3	SO4	I	2	5/?	0.85	0.19	101,104,109,112	0
2	YB	Y	49	1/?	0.85	0.14	112,112,112,112	1
2	YB	Y	30	1/?	0.85	0.11	161,161,161,161	0
3	SO4	I	4	5/?	0.86	0.19	97,105,113,114	0
2	YB	Y	53	1/?	0.87	0.17	103,103,103,103	1
2	YB	Y	73	1/?	0.87	0.19	110,110,110,110	1
2	YB	Y	18	1/?	0.87	0.17	114,114,114,114	1
2	YB	Y	5	1/?	0.92	0.18	155,155,155,155	1
2	YB	Y	29	1/?	0.93	0.07	95,95,95,95	1
2	YB	Y	17	1/?	0.96	0.20	106,106,106,106	1

6.5 Other polymers

There are no such residues in this entry.