Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:11 am BST

PDB ID	:	4AU4
Title	:	Crystal Structure of Hsp47
Authors	:	Widmer, C.; Gebauer, J.M.; Brunstein, E.; Rodenbaum, S.; Zaucke, F.; Drogemuller, C.; Leeb, T.; Baumann, U.
Deposited on	:	2012-05-14
Resolution	:	2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

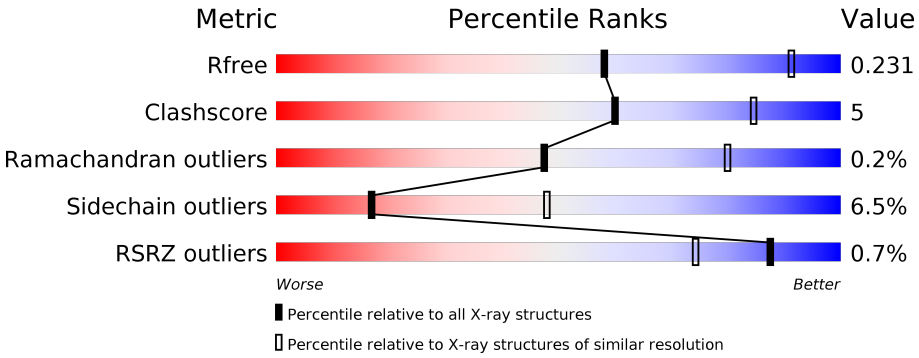
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.97 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	392	77% 16% • 7%
1	B	392	78% 15% • 6%
1	C	392	% 80% 13% • 6%
1	D	392	77% 15% • 7%
1	E	392	% 79% 13% • 6%
1	F	392	78% 14% • 6%

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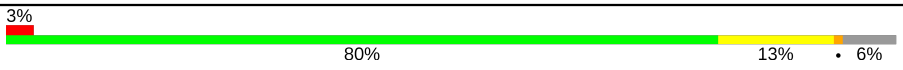
Mol	Chain	Length	Quality of chain
1	G	392	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20207 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 SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2876	1833	500	529	14			
1	B	368	Total	C	N	O	S	0	0	0
			2891	1842	502	533	14			
1	C	370	Total	C	N	O	S	0	0	0
			2901	1848	504	535	14			
1	D	366	Total	C	N	O	S	0	0	0
			2875	1834	499	528	14			
1	E	367	Total	C	N	O	S	0	0	0
			2884	1837	501	532	14			
1	F	368	Total	C	N	O	S	0	0	0
			2891	1842	502	533	14			
1	G	368	Total	C	N	O	S	0	0	0
			2889	1838	502	535	14			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP C7C419
A	419	LEU	-	expression tag	UNP C7C419
A	420	GLU	-	expression tag	UNP C7C419
A	421	HIS	-	expression tag	UNP C7C419
A	422	HIS	-	expression tag	UNP C7C419
A	423	HIS	-	expression tag	UNP C7C419
A	424	HIS	-	expression tag	UNP C7C419
A	425	HIS	-	expression tag	UNP C7C419
A	426	HIS	-	expression tag	UNP C7C419
B	35	MET	-	expression tag	UNP C7C419
B	419	LEU	-	expression tag	UNP C7C419
B	420	GLU	-	expression tag	UNP C7C419
B	421	HIS	-	expression tag	UNP C7C419
B	422	HIS	-	expression tag	UNP C7C419

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Chain	Residue	Modelled	Actual	Comment	Reference
B	423	HIS	-	expression tag	UNP C7C419
B	424	HIS	-	expression tag	UNP C7C419
B	425	HIS	-	expression tag	UNP C7C419
B	426	HIS	-	expression tag	UNP C7C419
C	35	MET	-	expression tag	UNP C7C419
C	419	LEU	-	expression tag	UNP C7C419
C	420	GLU	-	expression tag	UNP C7C419
C	421	HIS	-	expression tag	UNP C7C419
C	422	HIS	-	expression tag	UNP C7C419
C	423	HIS	-	expression tag	UNP C7C419
C	424	HIS	-	expression tag	UNP C7C419
C	425	HIS	-	expression tag	UNP C7C419
C	426	HIS	-	expression tag	UNP C7C419
D	35	MET	-	expression tag	UNP C7C419
D	419	LEU	-	expression tag	UNP C7C419
D	420	GLU	-	expression tag	UNP C7C419
D	421	HIS	-	expression tag	UNP C7C419
D	422	HIS	-	expression tag	UNP C7C419
D	423	HIS	-	expression tag	UNP C7C419
D	424	HIS	-	expression tag	UNP C7C419
D	425	HIS	-	expression tag	UNP C7C419
D	426	HIS	-	expression tag	UNP C7C419
E	35	MET	-	expression tag	UNP C7C419
E	419	LEU	-	expression tag	UNP C7C419
E	420	GLU	-	expression tag	UNP C7C419
E	421	HIS	-	expression tag	UNP C7C419
E	422	HIS	-	expression tag	UNP C7C419
E	423	HIS	-	expression tag	UNP C7C419
E	424	HIS	-	expression tag	UNP C7C419
E	425	HIS	-	expression tag	UNP C7C419
E	426	HIS	-	expression tag	UNP C7C419
F	35	MET	-	expression tag	UNP C7C419
F	419	LEU	-	expression tag	UNP C7C419
F	420	GLU	-	expression tag	UNP C7C419
F	421	HIS	-	expression tag	UNP C7C419
F	422	HIS	-	expression tag	UNP C7C419
F	423	HIS	-	expression tag	UNP C7C419
F	424	HIS	-	expression tag	UNP C7C419
F	425	HIS	-	expression tag	UNP C7C419
F	426	HIS	-	expression tag	UNP C7C419
G	35	MET	-	expression tag	UNP C7C419
G	419	LEU	-	expression tag	UNP C7C419

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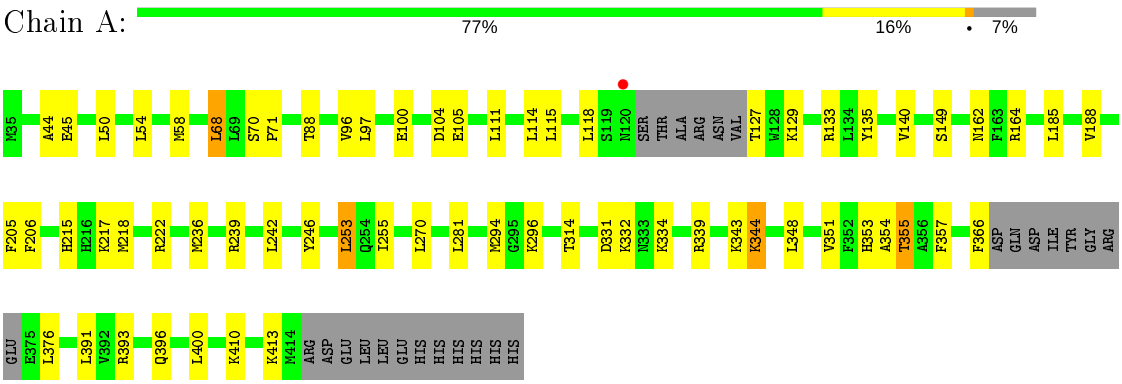
Chain	Residue	Modelled	Actual	Comment	Reference
G	420	GLU	-	expression tag	UNP C7C419
G	421	HIS	-	expression tag	UNP C7C419
G	422	HIS	-	expression tag	UNP C7C419
G	423	HIS	-	expression tag	UNP C7C419
G	424	HIS	-	expression tag	UNP C7C419
G	425	HIS	-	expression tag	UNP C7C419
G	426	HIS	-	expression tag	UNP C7C419

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.

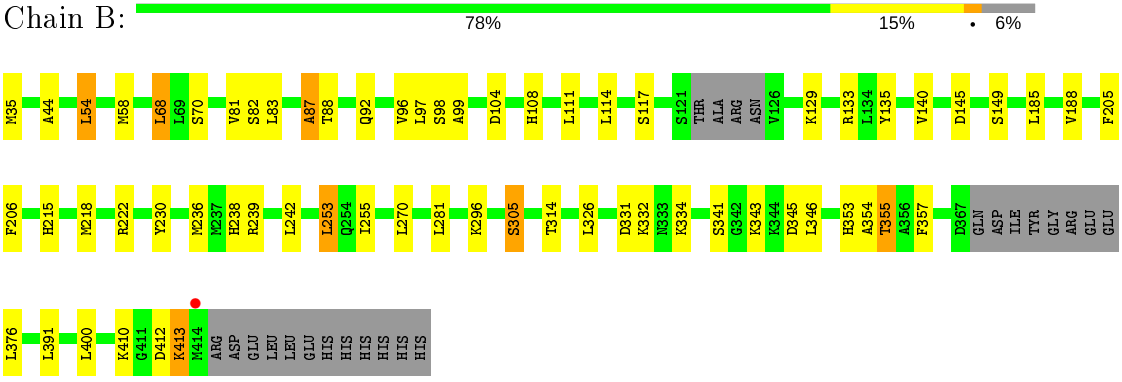
• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

Chain A:



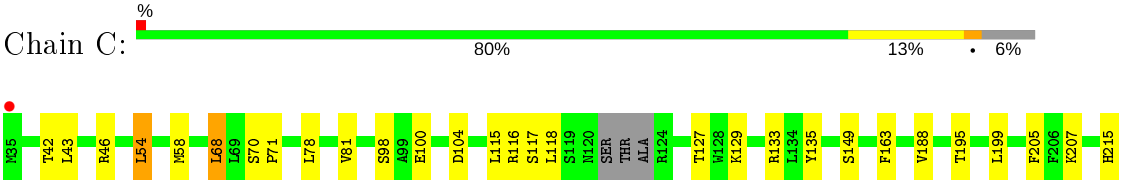
• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

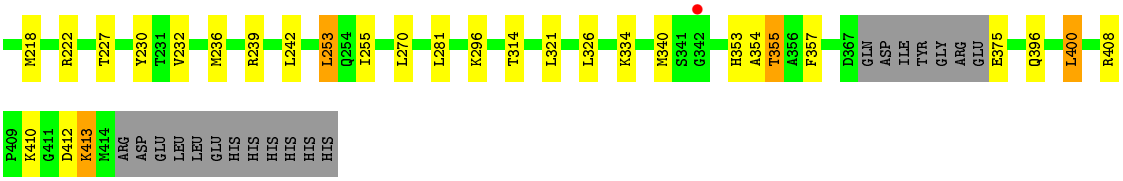
Chain B:



• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

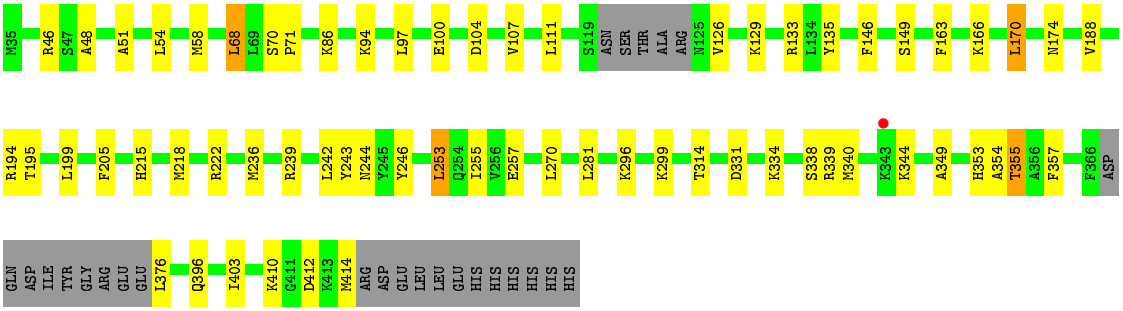
Chain C:





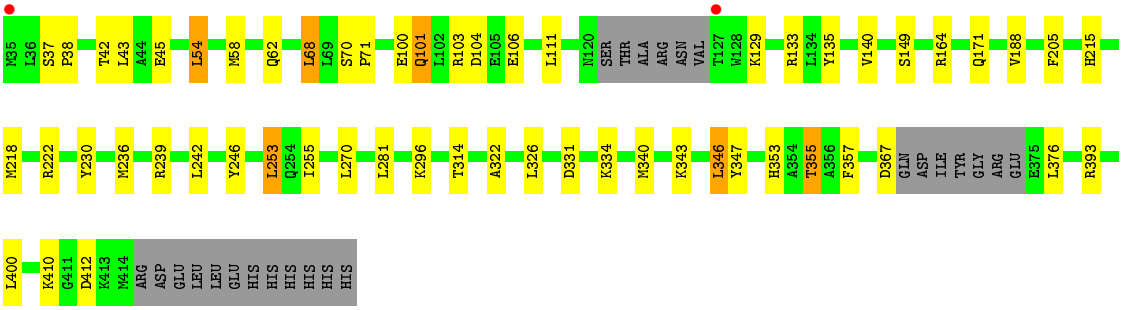
• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

Chain D:



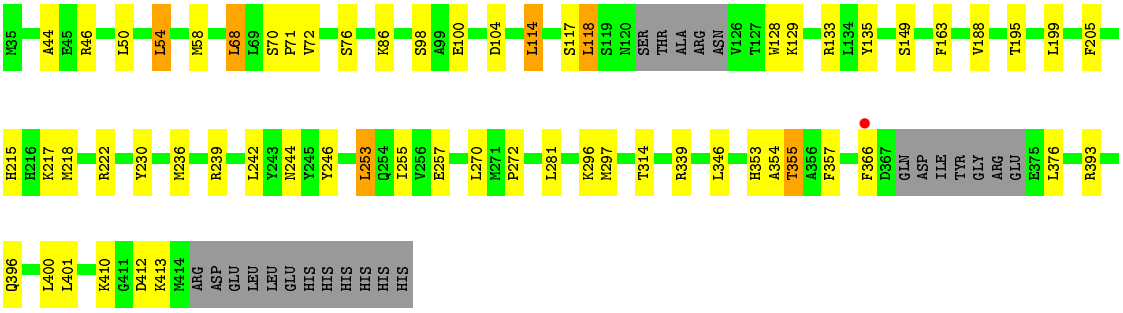
• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

Chain E:



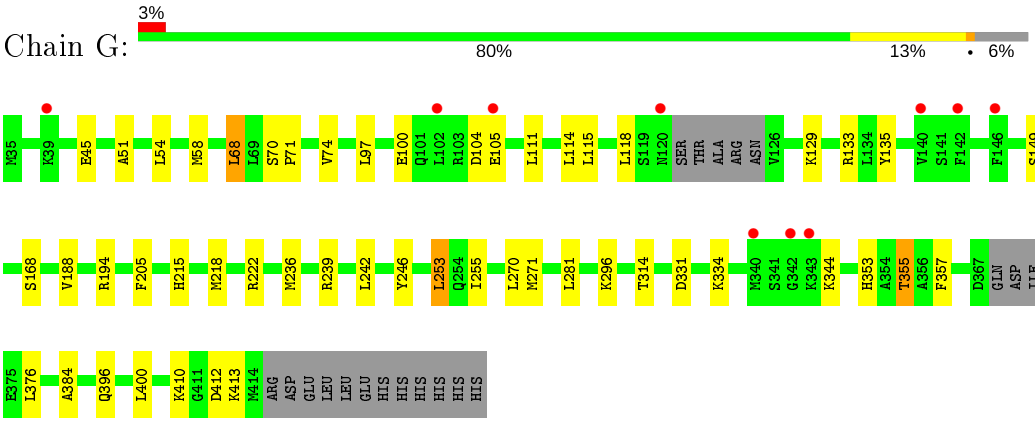
• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

Chain F:



• Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	178.78Å 115.11Å 188.28Å 90.00° 107.69° 90.00°	Depositor
Resolution (Å)	48.17 – 2.97 48.17 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.17-2.97) 97.6 (48.17-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.180 , 0.220 0.193 , 0.231	Depositor DCC
R_{free} test set	3660 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20207	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

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	0.53	0/2934	0.73	0/3954
1	B	0.52	0/2949	0.71	0/3975
1	C	0.53	0/2959	0.73	1/3989 (0.0%)
1	D	0.50	0/2933	0.70	0/3953
1	E	0.51	0/2942	0.72	0/3965
1	F	0.51	0/2949	0.71	0/3975
1	G	0.49	0/2946	0.70	0/3971
All	All	0.51	0/20612	0.72	1/27782 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	375	GLU	C-N-CA	5.06	134.35	121.70

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	2876	0	2908	31	0
1	B	2891	0	2921	30	0
1	C	2901	0	2925	25	0
1	D	2875	0	2911	35	0
1	E	2884	0	2912	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2891	0	2921	29	0
1	G	2889	0	2918	21	0
All	All	20207	0	20416	188	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 5.

All (188) 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:B:140:VAL:HG22	1:B:343:LYS:HG3	1.61	0.81
1:B:68:LEU:HD11	1:B:357:PHE:HB2	1.66	0.78
1:A:68:LEU:HD11	1:A:357:PHE:HB2	1.68	0.75
1:C:68:LEU:HD11	1:C:357:PHE:HB2	1.67	0.75
1:D:68:LEU:HD11	1:D:357:PHE:HB2	1.71	0.73
1:G:68:LEU:HD11	1:G:357:PHE:HB2	1.71	0.73
1:E:68:LEU:HD11	1:E:357:PHE:HB2	1.73	0.71
1:B:230:TYR:CE1	1:B:413:LYS:HD3	2.27	0.70
1:F:163:PHE:HE1	1:F:199:LEU:HD22	1.57	0.70
1:F:68:LEU:HD11	1:F:357:PHE:HB2	1.72	0.70
1:D:163:PHE:HB3	1:D:195:THR:HB	1.74	0.69
1:F:253:LEU:HD13	1:F:281:LEU:HD11	1.76	0.67
1:B:44:ALA:HB2	1:B:114:LEU:HD21	1.77	0.67
1:C:163:PHE:HB2	1:C:195:THR:HG23	1.77	0.67
1:F:54:LEU:O	1:F:58:MET:HG3	1.98	0.64
1:B:140:VAL:HG22	1:B:343:LYS:CG	2.29	0.62
1:B:331:ASP:HB3	1:B:334:LYS:HB2	1.82	0.62
1:D:194:ARG:HG3	1:D:349:ALA:HB1	1.79	0.62
1:D:70:SER:H	1:D:353:HIS:CE1	2.18	0.62
1:C:127:THR:HG23	1:C:207:LYS:HB3	1.83	0.59
1:G:54:LEU:O	1:G:58:MET:HG3	2.02	0.59
1:F:71:PRO:HG2	1:F:400:LEU:HB3	1.85	0.59
1:C:71:PRO:HG2	1:C:400:LEU:HB3	1.84	0.59
1:B:54:LEU:O	1:B:58:MET:HG3	2.02	0.58
1:F:230:TYR:CZ	1:F:413:LYS:HG3	2.39	0.58
1:A:188:VAL:O	1:A:314:THR:HG21	2.04	0.57
1:D:215:HIS:HB3	1:D:218:MET:HG2	1.86	0.57
1:G:71:PRO:HG2	1:G:400:LEU:HB3	1.86	0.57
1:G:133:ARG:HD3	1:G:135:TYR:CZ	2.39	0.57
1:A:331:ASP:HB3	1:A:334:LYS:HB2	1.87	0.57
1:G:215:HIS:HB3	1:G:218:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ARG:CZ	1:F:98:SER:HB3	2.35	0.56
1:E:37:SER:HB2	1:E:38:PRO:HD2	1.88	0.56
1:A:50:LEU:HD11	1:A:96:VAL:HG12	1.88	0.56
1:F:188:VAL:O	1:F:314:THR:HG21	2.06	0.56
1:G:331:ASP:HB3	1:G:334:LYS:HB2	1.88	0.55
1:D:94:LYS:HE3	1:D:107:VAL:HG21	1.88	0.55
1:E:322:ALA:HA	1:E:326:LEU:O	2.07	0.55
1:C:188:VAL:O	1:C:314:THR:HG21	2.07	0.55
1:G:97:LEU:HD21	1:G:111:LEU:HD11	1.89	0.55
1:E:188:VAL:O	1:E:314:THR:HG21	2.08	0.54
1:B:188:VAL:O	1:B:314:THR:HG21	2.08	0.54
1:D:188:VAL:O	1:D:314:THR:HG21	2.08	0.54
1:F:163:PHE:HB3	1:F:195:THR:HB	1.89	0.54
1:A:255:ILE:HD12	1:A:270:LEU:HG	1.90	0.53
1:D:299:LYS:HD2	1:E:103:ARG:HG2	1.89	0.53
1:A:140:VAL:HG22	1:A:343:LYS:HG2	1.91	0.53
1:G:115:LEU:HA	1:G:118:LEU:HD12	1.90	0.53
1:A:215:HIS:HB3	1:A:218:MET:HG2	1.91	0.53
1:D:163:PHE:HE1	1:D:199:LEU:HD22	1.73	0.53
1:D:163:PHE:CE1	1:D:199:LEU:HD22	2.44	0.53
1:A:133:ARG:HD3	1:A:135:TYR:CZ	2.44	0.53
1:B:215:HIS:HB3	1:B:218:MET:HG2	1.91	0.53
1:G:222:ARG:HB2	1:G:236:MET:HG3	1.91	0.53
1:D:243:TYR:HA	1:E:103:ARG:HH22	1.75	0.52
1:F:133:ARG:HD3	1:F:135:TYR:CZ	2.45	0.52
1:C:115:LEU:HA	1:C:118:LEU:HD12	1.92	0.51
1:E:331:ASP:HB3	1:E:334:LYS:HB2	1.92	0.51
1:D:194:ARG:HD2	1:D:349:ALA:O	2.11	0.51
1:G:188:VAL:O	1:G:314:THR:HG21	2.10	0.51
1:E:133:ARG:HD3	1:E:135:TYR:CZ	2.46	0.51
1:F:230:TYR:CE1	1:F:413:LYS:HG3	2.45	0.51
1:F:255:ILE:HD12	1:F:270:LEU:HG	1.92	0.51
1:A:185:LEU:HD21	1:A:354:ALA:HB1	1.92	0.51
1:C:70:SER:H	1:C:353:HIS:CE1	2.29	0.51
1:B:133:ARG:HD3	1:B:135:TYR:CZ	2.46	0.51
1:A:344:LYS:HG3	1:F:366:PHE:CD1	2.46	0.51
1:F:70:SER:H	1:F:353:HIS:CE1	2.30	0.50
1:D:331:ASP:HB3	1:D:334:LYS:HB2	1.92	0.50
1:E:215:HIS:HB3	1:E:218:MET:HG2	1.94	0.50
1:A:70:SER:H	1:A:353:HIS:CE1	2.30	0.50
1:C:232:VAL:HG22	1:C:413:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:HD3	1:D:135:TYR:CZ	2.47	0.50
1:C:133:ARG:HD3	1:C:135:TYR:CZ	2.47	0.50
1:D:97:LEU:HD21	1:D:111:LEU:HD11	1.93	0.49
1:A:348:LEU:HD21	1:A:351:VAL:CG2	2.42	0.49
1:G:70:SER:H	1:G:353:HIS:CE1	2.29	0.49
1:B:70:SER:H	1:B:353:HIS:CE1	2.31	0.49
1:D:170:LEU:HD23	1:D:174:ASN:HD21	1.77	0.49
1:G:253:LEU:HD13	1:G:281:LEU:HD11	1.95	0.49
1:D:253:LEU:HD13	1:D:281:LEU:HD11	1.95	0.48
1:B:332:LYS:HG2	1:B:345:ASP:HB3	1.96	0.48
1:C:253:LEU:HD13	1:C:281:LEU:HD11	1.96	0.48
1:E:129:LYS:HB2	1:E:205:PHE:HB3	1.95	0.48
1:A:162:ASN:HD21	1:A:164:ARG:HB2	1.79	0.48
1:D:255:ILE:HD12	1:D:270:LEU:HG	1.96	0.48
1:G:255:ILE:HD12	1:G:270:LEU:HG	1.95	0.48
1:A:253:LEU:HD13	1:A:281:LEU:HD11	1.96	0.48
1:D:244:ASN:ND2	1:E:106:GLU:OE2	2.33	0.47
1:D:243:TYR:HA	1:E:103:ARG:NH2	2.29	0.47
1:E:253:LEU:HD13	1:E:281:LEU:HD11	1.95	0.47
1:B:238:HIS:ND1	1:B:305:SER:HB3	2.30	0.47
1:F:129:LYS:HB2	1:F:205:PHE:HB3	1.97	0.47
1:G:51:ALA:CB	1:G:71:PRO:HG3	2.44	0.47
1:F:68:LEU:HD13	1:F:355:THR:HB	1.97	0.47
1:C:222:ARG:HB2	1:C:236:MET:HG3	1.96	0.47
1:E:101:GLN:NE2	1:E:101:GLN:H	2.12	0.47
1:C:408:ARG:HD3	1:C:413:LYS:HE3	1.96	0.47
1:C:129:LYS:HB2	1:C:205:PHE:HB3	1.97	0.47
1:C:255:ILE:HD12	1:C:270:LEU:HG	1.97	0.47
1:E:255:ILE:HD12	1:E:270:LEU:HG	1.95	0.47
1:E:43:LEU:HD23	1:E:111:LEU:HG	1.97	0.47
1:F:215:HIS:HB3	1:F:218:MET:HG2	1.95	0.46
1:A:115:LEU:HA	1:A:118:LEU:HD12	1.95	0.46
1:B:253:LEU:HD13	1:B:281:LEU:HD11	1.96	0.46
1:F:222:ARG:HB2	1:F:236:MET:HG3	1.98	0.46
1:B:255:ILE:HD12	1:B:270:LEU:HG	1.97	0.46
1:A:97:LEU:HD21	1:A:111:LEU:HD11	1.96	0.46
1:D:129:LYS:HB2	1:D:205:PHE:HB3	1.97	0.46
1:F:118:LEU:HG	1:F:401:LEU:HG	1.97	0.46
1:G:129:LYS:HB2	1:G:205:PHE:HB3	1.98	0.45
1:G:68:LEU:HD13	1:G:355:THR:HB	1.99	0.45
1:G:54:LEU:HD12	1:G:74:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:SER:C	1:D:340:MET:H	2.20	0.45
1:C:81:VAL:HG11	1:C:326:LEU:HD11	1.99	0.45
1:E:222:ARG:HB2	1:E:236:MET:HG3	1.97	0.45
1:D:54:LEU:O	1:D:58:MET:HG3	2.17	0.44
1:E:70:SER:H	1:E:353:HIS:CE1	2.35	0.44
1:G:246:TYR:HB3	1:G:255:ILE:HG23	1.98	0.44
1:A:129:LYS:HB2	1:A:205:PHE:HB3	1.99	0.44
1:C:68:LEU:HD13	1:C:355:THR:HB	2.00	0.44
1:E:140:VAL:HG21	1:E:346:LEU:HD13	1.99	0.44
1:E:68:LEU:HD13	1:E:355:THR:HB	2.00	0.44
1:A:71:PRO:HG2	1:A:400:LEU:HB3	1.99	0.44
1:G:111:LEU:HA	1:G:114:LEU:HD12	1.99	0.44
1:A:54:LEU:O	1:A:58:MET:HG3	2.17	0.44
1:D:48:ALA:O	1:D:51:ALA:HB3	2.17	0.43
1:C:54:LEU:O	1:C:58:MET:HG3	2.17	0.43
1:C:46:ARG:NH1	1:C:98:SER:O	2.52	0.43
1:D:86:LYS:HG3	1:D:339:ARG:HG3	1.99	0.43
1:F:246:TYR:HB3	1:F:255:ILE:HG23	2.00	0.43
1:A:246:TYR:HB3	1:A:255:ILE:HG23	1.99	0.43
1:F:72:VAL:HG13	1:F:114:LEU:HB3	2.00	0.43
1:F:86:LYS:HG3	1:F:339:ARG:HG3	2.00	0.43
1:D:222:ARG:HB2	1:D:236:MET:HG3	1.99	0.43
1:A:88:THR:HG23	1:F:297:MET:O	2.19	0.43
1:C:68:LEU:HD11	1:C:357:PHE:CB	2.45	0.43
1:D:244:ASN:HB2	1:D:257:GLU:HB3	2.00	0.43
1:E:54:LEU:O	1:E:58:MET:HG3	2.17	0.43
1:A:222:ARG:HB2	1:A:236:MET:HG3	2.00	0.42
1:D:246:TYR:HB3	1:D:255:ILE:HG23	2.01	0.42
1:A:185:LEU:HD21	1:A:354:ALA:CB	2.50	0.42
1:A:127:THR:O	1:A:206:PHE:HA	2.18	0.42
1:A:44:ALA:HB2	1:A:114:LEU:HD21	2.01	0.42
1:F:44:ALA:HB2	1:F:114:LEU:HD21	1.99	0.42
1:F:118:LEU:HD22	1:F:128:TRP:CE2	2.54	0.42
1:B:97:LEU:O	1:B:99:ALA:N	2.53	0.42
1:E:246:TYR:HB3	1:E:255:ILE:HG23	2.01	0.42
1:F:314:THR:HG23	1:F:354:ALA:HB2	2.02	0.42
1:B:92:GLN:O	1:B:96:VAL:HG23	2.20	0.42
1:G:271:MET:SD	1:G:384:ALA:HA	2.60	0.42
1:C:163:PHE:HE1	1:C:199:LEU:HD22	1.85	0.42
1:A:68:LEU:HD11	1:A:357:PHE:CB	2.45	0.42
1:B:97:LEU:HD21	1:B:111:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:HA	1:E:54:LEU:HD23	1.90	0.41
1:A:215:HIS:CE1	1:A:217:LYS:HB2	2.55	0.41
1:D:51:ALA:HB2	1:D:71:PRO:HG3	2.02	0.41
1:F:215:HIS:CE1	1:F:217:LYS:HB2	2.54	0.41
1:B:206:PHE:HD2	1:B:357:PHE:CE2	2.38	0.41
1:B:68:LEU:HD13	1:B:355:THR:HB	2.03	0.41
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.83	0.41
1:A:294:MET:O	1:B:87:ALA:HA	2.19	0.41
1:D:51:ALA:HB1	1:D:403:ILE:HG21	2.02	0.41
1:F:272:PRO:HD3	1:F:281:LEU:HD22	2.01	0.41
1:B:391:LEU:HD22	1:B:400:LEU:HD11	2.02	0.41
1:C:42:THR:O	1:C:46:ARG:HG2	2.21	0.41
1:B:81:VAL:HG11	1:B:326:LEU:HD11	2.03	0.41
1:B:88:THR:O	1:B:92:GLN:HG3	2.21	0.41
1:A:391:LEU:HD22	1:A:400:LEU:HD11	2.02	0.41
1:B:341:SER:HB3	1:B:346:LEU:HD22	2.03	0.41
1:B:83:LEU:HB2	1:B:108:HIS:CE1	2.55	0.41
1:B:222:ARG:HB2	1:B:236:MET:HG3	2.03	0.41
1:C:230:TYR:OH	1:C:413:LYS:HB3	2.20	0.41
1:D:166:LYS:O	1:D:170:LEU:HB2	2.21	0.41
1:B:129:LYS:HB2	1:B:205:PHE:HB3	2.02	0.41
1:E:71:PRO:HG2	1:E:400:LEU:HB3	2.02	0.41
1:F:244:ASN:HB2	1:F:257:GLU:HB3	2.03	0.41
1:A:68:LEU:HD13	1:A:355:THR:HB	2.02	0.40
1:B:400:LEU:HD12	1:B:400:LEU:HA	1.98	0.40
1:C:215:HIS:HB3	1:C:218:MET:HG2	2.02	0.40
1:C:314:THR:HG23	1:C:354:ALA:HB2	2.02	0.40
1:B:185:LEU:HD21	1:B:354:ALA:HB1	2.02	0.40
1:C:78:LEU:HD21	1:C:321:LEU:HD22	2.02	0.40
1:D:146:PHE:HB2	1:D:339:ARG:O	2.22	0.40
1:D:70:SER:H	1:D:353:HIS:HE1	1.67	0.40
1:D:68:LEU:HD13	1:D:355:THR:HB	2.03	0.40
1:G:162:ASN:HD21	1:G:164:ARG:HB2	1.87	0.40
1:D:314:THR:HG23	1:D:354:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	360/392 (92%)	351 (98%)	9 (2%)	0	100 100
1	B	362/392 (92%)	351 (97%)	9 (2%)	2 (1%)	25 61
1	C	364/392 (93%)	348 (96%)	14 (4%)	2 (0%)	29 66
1	D	360/392 (92%)	348 (97%)	12 (3%)	0	100 100
1	E	361/392 (92%)	347 (96%)	14 (4%)	0	100 100
1	F	362/392 (92%)	353 (98%)	9 (2%)	0	100 100
1	G	362/392 (92%)	350 (97%)	12 (3%)	0	100 100
All	All	2531/2744 (92%)	2448 (97%)	79 (3%)	4 (0%)	47 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	SER
1	C	412	ASP
1	B	87	ALA
1	C	413	LYS

5.3.2 Protein sidechains

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	311/337 (92%)	291 (94%)	20 (6%)	17 49
1	B	313/337 (93%)	295 (94%)	18 (6%)	20 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	313/337 (93%)	294 (94%)	19 (6%)	18 51
1	D	311/337 (92%)	293 (94%)	18 (6%)	20 53
1	E	312/337 (93%)	286 (92%)	26 (8%)	11 37
1	F	313/337 (93%)	292 (93%)	21 (7%)	16 47
1	G	313/337 (93%)	294 (94%)	19 (6%)	18 51
All	All	2186/2359 (93%)	2045 (94%)	141 (6%)	17 48

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	68	LEU
1	A	100	GLU
1	A	104	ASP
1	A	105	GLU
1	A	149	SER
1	A	239	ARG
1	A	242	LEU
1	A	253	LEU
1	A	296	LYS
1	A	332	LYS
1	A	339	ARG
1	A	344	LYS
1	A	355	THR
1	A	366	PHE
1	A	376	LEU
1	A	393	ARG
1	A	396	GLN
1	A	410	LYS
1	A	413	LYS
1	B	35	MET
1	B	54	LEU
1	B	68	LEU
1	B	82	SER
1	B	104	ASP
1	B	117	SER
1	B	145	ASP
1	B	149	SER
1	B	239	ARG
1	B	242	LEU

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Mol	Chain	Res	Type
1	B	253	LEU
1	B	296	LYS
1	B	305	SER
1	B	355	THR
1	B	376	LEU
1	B	410	LYS
1	B	412	ASP
1	B	413	LYS
1	C	43	LEU
1	C	54	LEU
1	C	68	LEU
1	C	100	GLU
1	C	104	ASP
1	C	116	ARG
1	C	117	SER
1	C	149	SER
1	C	227	THR
1	C	239	ARG
1	C	242	LEU
1	C	253	LEU
1	C	296	LYS
1	C	334	LYS
1	C	340	MET
1	C	355	THR
1	C	396	GLN
1	C	400	LEU
1	C	410	LYS
1	D	46	ARG
1	D	68	LEU
1	D	100	GLU
1	D	104	ASP
1	D	126	VAL
1	D	149	SER
1	D	170	LEU
1	D	239	ARG
1	D	242	LEU
1	D	253	LEU
1	D	296	LYS
1	D	344	LYS
1	D	355	THR
1	D	376	LEU
1	D	396	GLN

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Mol	Chain	Res	Type
1	D	410	LYS
1	D	412	ASP
1	D	414	MET
1	E	42	THR
1	E	45	GLU
1	E	54	LEU
1	E	62	GLN
1	E	68	LEU
1	E	100	GLU
1	E	101	GLN
1	E	104	ASP
1	E	149	SER
1	E	164	ARG
1	E	171	GLN
1	E	230	TYR
1	E	239	ARG
1	E	242	LEU
1	E	253	LEU
1	E	296	LYS
1	E	340	MET
1	E	343	LYS
1	E	346	LEU
1	E	347	TYR
1	E	355	THR
1	E	367	ASP
1	E	376	LEU
1	E	393	ARG
1	E	410	LYS
1	E	412	ASP
1	F	50	LEU
1	F	54	LEU
1	F	68	LEU
1	F	76	SER
1	F	100	GLU
1	F	104	ASP
1	F	114	LEU
1	F	117	SER
1	F	118	LEU
1	F	149	SER
1	F	239	ARG
1	F	242	LEU
1	F	253	LEU

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Mol	Chain	Res	Type
1	F	296	LYS
1	F	346	LEU
1	F	355	THR
1	F	376	LEU
1	F	393	ARG
1	F	396	GLN
1	F	410	LYS
1	F	412	ASP
1	G	45	GLU
1	G	68	LEU
1	G	100	GLU
1	G	104	ASP
1	G	105	GLU
1	G	149	SER
1	G	168	SER
1	G	194	ARG
1	G	239	ARG
1	G	242	LEU
1	G	253	LEU
1	G	296	LYS
1	G	344	LYS
1	G	355	THR
1	G	376	LEU
1	G	396	GLN
1	G	410	LYS
1	G	412	ASP
1	G	413	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	353	HIS
1	B	153	HIS
1	B	353	HIS
1	C	120	ASN
1	C	353	HIS
1	D	353	HIS
1	E	353	HIS
1	F	152	GLN
1	F	162	ASN
1	F	353	HIS

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Mol	Chain	Res	Type
1	G	353	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	366/392 (93%)	-0.50	1 (0%)	94	87	20, 36, 71, 107	0
1	B	368/392 (93%)	-0.40	1 (0%)	94	87	25, 42, 77, 103	0
1	C	370/392 (94%)	-0.48	2 (0%)	91	80	21, 45, 86, 109	0
1	D	366/392 (93%)	-0.30	1 (0%)	94	87	21, 54, 103, 131	0
1	E	367/392 (93%)	-0.48	2 (0%)	91	80	24, 48, 84, 102	0
1	F	368/392 (93%)	-0.35	1 (0%)	94	87	20, 50, 100, 129	0
1	G	368/392 (93%)	-0.10	11 (2%)	50	31	22, 56, 113, 132	0
All	All	2573/2744 (93%)	-0.37	19 (0%)	87	74	20, 46, 97, 132	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	366	PHE	5.5
1	G	140	VAL	3.4
1	G	120	ASN	3.3
1	E	35	MET	3.0
1	G	39	LYS	2.9
1	G	102	LEU	2.9
1	G	342	GLY	2.9
1	G	343	LYS	2.8
1	B	414	MET	2.6
1	A	120	ASN	2.6
1	G	105	GLU	2.4
1	C	35	MET	2.4
1	C	342	GLY	2.3
1	G	163	PHE	2.2
1	E	127	THR	2.2
1	G	340	MET	2.2
1	G	142	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	146	PHE	2.1
1	D	343	LYS	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.