



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:45 PM UTC

PDB ID : 4AU4 / pdb_00004au4
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

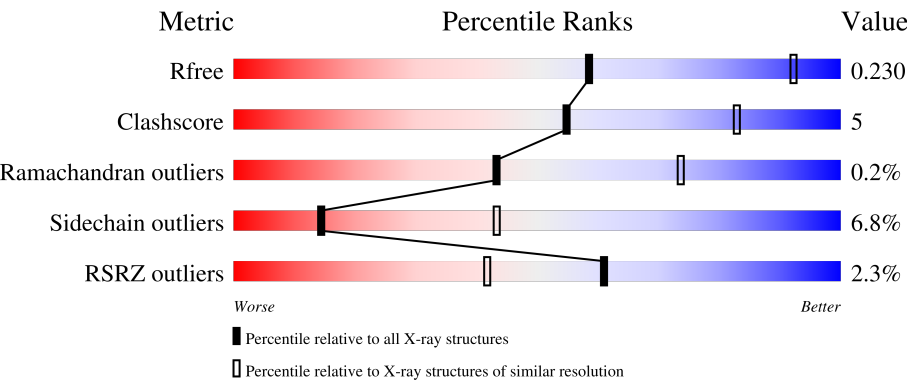
1 Overall quality at a glance i

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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 of 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 $\leq 5\%$. 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	% 75%17%• 7%
1	B	392	% 76%16%• 6%
1	C	392	3% 77%15%• 6%
1	D	392	3% 75%17%• 7%
1	E	392	2% 78%13%• 6%

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Mol	Chain	Length	Quality of chain
1	F	392	
1	G	392	

2 Entry composition

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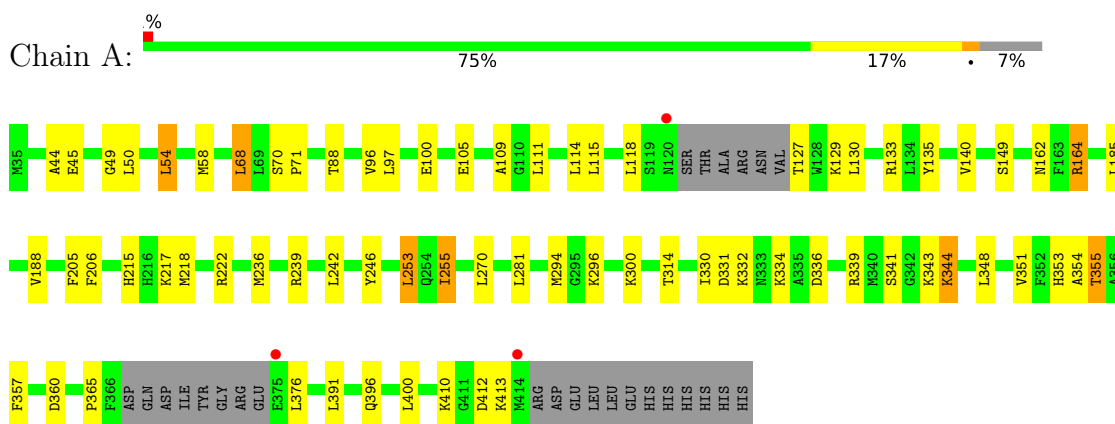
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Chain	Residue	Modelled	Actual	Comment	Reference
G	420	GLU	-	expression tag	UNP C7C419
G	421	HIS	-	expression tag	UNP C7C419
G	422	HIS	-	expression tag	UNP C7C419
G	423	HIS	-	expression tag	UNP C7C419
G	424	HIS	-	expression tag	UNP C7C419
G	425	HIS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

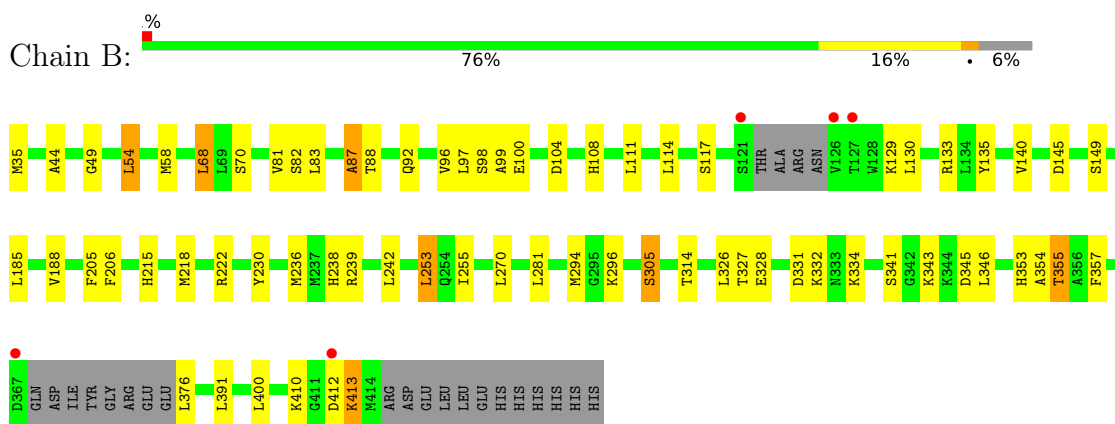
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

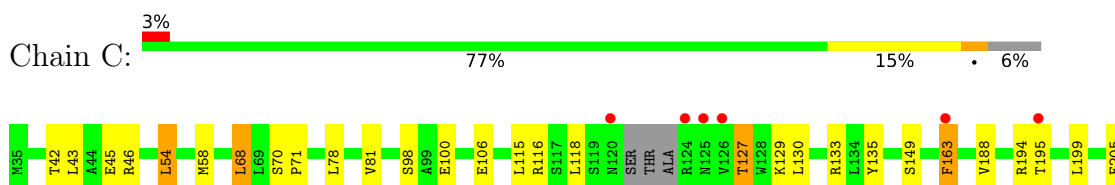
- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

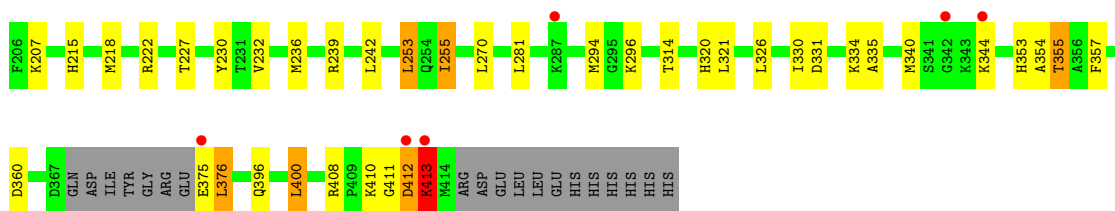


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

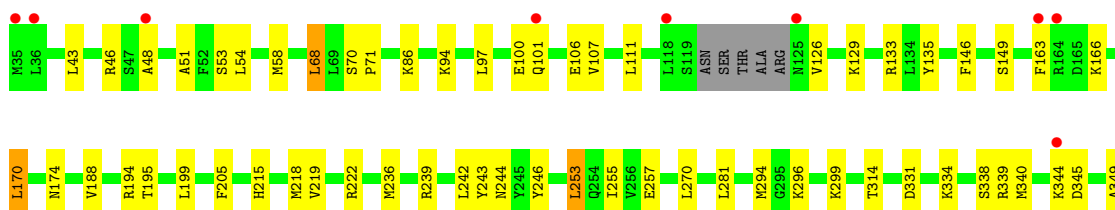
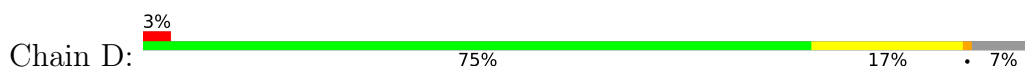


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

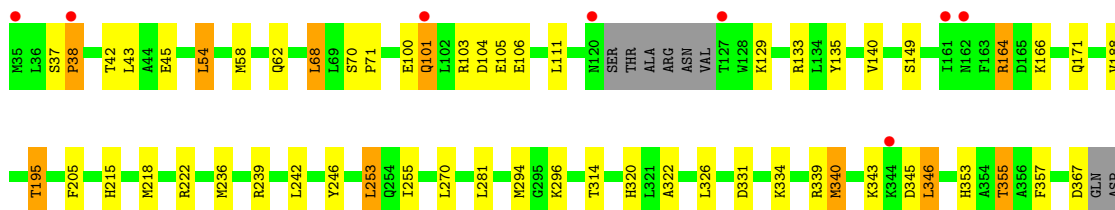
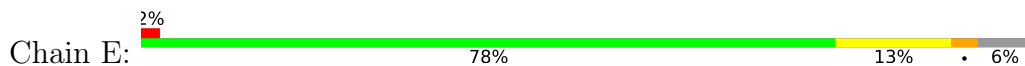




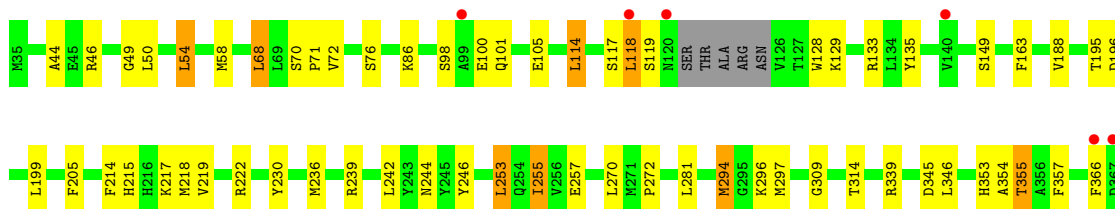
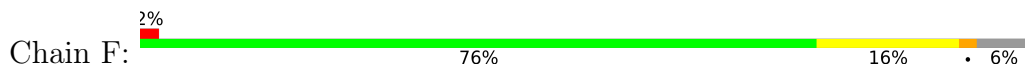
- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)



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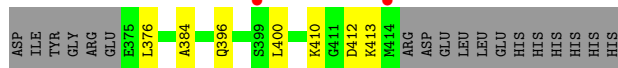
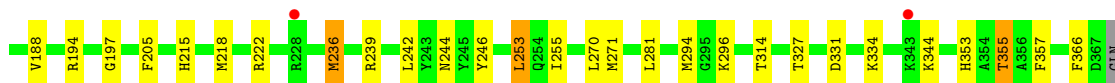
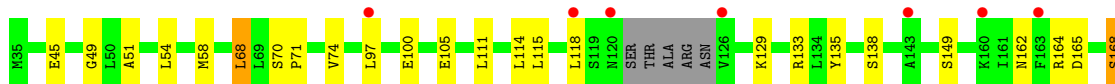
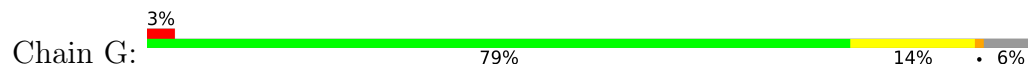


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)





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



4 Data and refinement statistics

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) 97.5 (48.17-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.180 , 0.220 0.193 , 0.230	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)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.86	0/2934	1.31	14/3954 (0.4%)
1	B	0.84	0/2949	1.31	7/3975 (0.2%)
1	C	0.87	1/2959 (0.0%)	1.36	19/3989 (0.5%)
1	D	0.81	0/2933	1.31	10/3953 (0.3%)
1	E	0.83	0/2942	1.34	10/3965 (0.3%)
1	F	0.83	1/2949 (0.0%)	1.32	9/3975 (0.2%)
1	G	0.81	1/2946 (0.0%)	1.31	6/3971 (0.2%)
All	All	0.84	3/20612 (0.0%)	1.32	75/27782 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	294	MET	SD-CE	5.44	1.93	1.79
1	C	413	LYS	CA-C	5.34	1.59	1.52
1	G	366	PHE	CA-C	5.17	1.59	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	GLU	CA-C-N	9.21	134.35	120.17
1	C	375	GLU	C-N-CA	9.21	134.35	120.17
1	A	412	ASP	CA-CB-CG	7.90	120.50	112.60
1	C	412	ASP	CA-CB-CG	7.80	120.40	112.60
1	C	194	ARG	N-CA-C	6.79	120.50	110.46
1	E	345	ASP	CA-CB-CG	6.51	119.11	112.60
1	C	335	ALA	N-CA-C	6.17	119.15	109.96
1	D	106	GLU	CA-C-N	6.09	128.32	120.70
1	D	106	GLU	C-N-CA	6.09	128.32	120.70
1	E	166	LYS	CA-C-N	6.00	130.73	121.19
1	E	166	LYS	C-N-CA	6.00	130.73	121.19
1	C	163	PHE	CA-CB-CG	5.94	119.74	113.80
1	D	345	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	330	ILE	N-CA-C	5.88	117.82	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	49	GLY	CA-C-N	5.78	128.50	120.29
1	G	49	GLY	C-N-CA	5.78	128.50	120.29
1	B	49	GLY	CA-C-N	5.76	128.01	120.28
1	B	49	GLY	C-N-CA	5.76	128.01	120.28
1	A	341	SER	N-CA-C	5.74	123.02	110.80
1	D	365	PRO	CA-C-N	5.72	132.00	121.70
1	D	365	PRO	C-N-CA	5.72	132.00	121.70
1	A	255	ILE	CB-CA-C	5.72	118.68	110.33
1	E	339	ARG	CA-C-N	5.65	128.12	120.44
1	E	339	ARG	C-N-CA	5.65	128.12	120.44
1	F	255	ILE	CB-CA-C	5.60	118.51	110.33
1	B	327	THR	CA-C-N	5.60	127.71	120.44
1	B	327	THR	C-N-CA	5.60	127.71	120.44
1	F	119	SER	CA-C-N	5.55	131.69	121.70
1	F	119	SER	C-N-CA	5.55	131.69	121.70
1	C	376	LEU	N-CA-C	-5.53	104.38	113.50
1	C	127	THR	CB-CA-C	5.50	120.63	111.51
1	D	43	LEU	CA-C-N	5.48	127.89	120.38
1	D	43	LEU	C-N-CA	5.48	127.89	120.38
1	A	164	ARG	N-CA-C	-5.48	105.86	112.54
1	E	38	PRO	CA-C-N	5.47	127.88	120.44
1	E	38	PRO	C-N-CA	5.47	127.88	120.44
1	E	195	THR	CB-CA-C	5.47	118.73	109.55
1	A	49	GLY	CA-C-N	5.44	128.01	120.29
1	A	49	GLY	C-N-CA	5.44	128.01	120.29
1	C	344	LYS	N-CA-C	-5.43	105.33	112.72
1	D	412	ASP	CA-CB-CG	5.39	117.99	112.60
1	E	166	LYS	N-CA-C	-5.35	105.34	111.07
1	C	255	ILE	CB-CA-C	5.34	118.13	110.33
1	C	411	GLY	N-CA-C	5.31	118.51	110.75
1	C	45	GLU	CA-C-N	5.31	127.83	120.29
1	C	45	GLU	C-N-CA	5.31	127.83	120.29
1	B	130	LEU	CA-C-N	5.28	125.68	121.61
1	B	130	LEU	C-N-CA	5.28	125.68	121.61
1	E	164	ARG	N-CA-C	-5.28	105.42	111.07
1	C	331	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	130	LEU	CA-C-N	5.24	125.64	121.61
1	A	130	LEU	C-N-CA	5.24	125.64	121.61
1	F	309	GLY	N-CA-C	5.23	117.19	110.96
1	B	328	GLU	N-CA-C	5.22	116.66	111.07
1	A	109	ALA	CA-C-N	5.21	125.72	119.94
1	A	109	ALA	C-N-CA	5.21	125.72	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	196	ASP	CA-CB-CG	5.19	117.79	112.60
1	G	327	THR	CA-C-N	5.17	127.47	120.65
1	G	327	THR	C-N-CA	5.17	127.47	120.65
1	C	320	HIS	CA-C-N	5.14	127.68	120.28
1	C	320	HIS	C-N-CA	5.14	127.68	120.28
1	F	345	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	365	PRO	CA-C-N	5.12	130.91	121.70
1	A	365	PRO	C-N-CA	5.12	130.91	121.70
1	C	360	ASP	CA-CB-CG	5.12	117.72	112.60
1	F	49	GLY	CA-C-N	5.11	127.55	120.29
1	F	49	GLY	C-N-CA	5.11	127.55	120.29
1	A	360	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	130	LEU	CA-C-N	5.07	125.10	121.65
1	C	130	LEU	C-N-CA	5.07	125.10	121.65
1	F	214	PHE	N-CA-C	-5.05	102.29	110.32
1	G	197	GLY	CA-C-N	5.05	127.88	120.71
1	G	197	GLY	C-N-CA	5.05	127.88	120.71
1	D	53	SER	CA-C-N	5.04	127.30	120.44
1	D	53	SER	C-N-CA	5.04	127.30	120.44

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	32	0
1	B	2891	0	2921	30	0
1	C	2901	0	2925	26	0
1	D	2875	0	2911	35	0
1	E	2884	0	2912	26	0
1	F	2891	0	2921	29	0
1	G	2889	0	2918	23	0
All	All	20207	0	20416	193	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 (193) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:344:LYS:HG3	1:F:366:PHE:CD1	2.46	0.51
1:B:133:ARG:HD3	1:B:135:TYR:CZ	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
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:D:338:SER:C	1:D:340:MET:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:68:LEU:HD13	1:F:355:THR:HB	1.97	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:43:LEU:HD23	1:E:111:LEU:HG	1.97	0.47
1:E:255:ILE:HD12	1:E:270:LEU:HG	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:HD13	1:C:355:THR:HB	2.00	0.44
1:E:68:LEU:HD13	1:E:355:THR:HB	2.00	0.44
1:E:140:VAL:HG21	1:E:346:LEU:HD13	1.99	0.44
1:A:71:PRO:HG2	1:A:400:LEU:HB3	1.99	0.44
1:E:340:MET:HE2	1:E:346:LEU:HD23	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:46:ARG:NH1	1:C:98:SER:O	2.52	0.43
1:C:54:LEU:O	1:C:58:MET:HG3	2.17	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:A:88:THR:HG23	1:F:297:MET:O	2.19	0.43
1:D:222:ARG:HB2	1:D:236:MET:HG3	1.99	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:44:ALA:HB2	1:A:114:LEU:HD21	2.01	0.42
1:A:127:THR:O	1:A:206:PHE:HA	2.18	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:A:336:ASP:OD1	1:A:336:ASP:C	2.62	0.42
1:B:97:LEU:HD21	1:B:111:LEU:HD11	2.02	0.41
1:E:54:LEU:HD23	1:E:54:LEU:HA	1.90	0.41
1:E:58:MET:HE3	1:E:320:HIS:CD2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD13	1:B:355:THR:HB	2.03	0.41
1:B:206:PHE:HD2	1:B:357:PHE:CE2	2.38	0.41
1:A:54:LEU:HD23	1:A:54:LEU:HA	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:83:LEU:HB2	1:B:108:HIS:CE1	2.55	0.41
1:B:341:SER:HB3	1:B:346:LEU:HD22	2.03	0.41
1:G:165:ASP:CG	1:G:168:SER:HB3	2.46	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:70:SER:H	1:D:353:HIS:HE1	1.67	0.40
1:D:146:PHE:HB2	1:D:339:ARG:O	2.22	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
1:C:106:GLU:CD	1:G:244:ASN:HD21	2.30	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%)	21	53
1	C	364/392 (93%)	348 (96%)	14 (4%)	2 (0%)	24	58
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%)	43	73

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%)	292 (94%)	19 (6%)	17	47
1	B	313/337 (93%)	293 (94%)	20 (6%)	16	45
1	C	313/337 (93%)	293 (94%)	20 (6%)	16	45
1	D	311/337 (92%)	291 (94%)	20 (6%)	16	45
1	E	312/337 (93%)	286 (92%)	26 (8%)	10	35
1	F	313/337 (93%)	290 (93%)	23 (7%)	13	40
1	G	313/337 (93%)	292 (93%)	21 (7%)	15	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2186/2359 (93%)	2037 (93%)	149 (7%)	14	43

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	54	LEU
1	A	68	LEU
1	A	100	GLU
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	300	LYS
1	A	332	LYS
1	A	339	ARG
1	A	344	LYS
1	A	355	THR
1	A	376	LEU
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	100	GLU
1	B	104	ASP
1	B	117	SER
1	B	145	ASP
1	B	149	SER
1	B	239	ARG
1	B	242	LEU
1	B	253	LEU
1	B	294	MET
1	B	296	LYS
1	B	305	SER
1	B	355	THR
1	B	376	LEU
1	B	410	LYS

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Mol	Chain	Res	Type
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	116	ARG
1	C	149	SER
1	C	227	THR
1	C	239	ARG
1	C	242	LEU
1	C	253	LEU
1	C	294	MET
1	C	296	LYS
1	C	330	ILE
1	C	334	LYS
1	C	340	MET
1	C	355	THR
1	C	376	LEU
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	101	GLN
1	D	126	VAL
1	D	149	SER
1	D	170	LEU
1	D	219	VAL
1	D	239	ARG
1	D	242	LEU
1	D	253	LEU
1	D	294	MET
1	D	296	LYS
1	D	344	LYS
1	D	355	THR
1	D	376	LEU
1	D	396	GLN
1	D	410	LYS
1	D	412	ASP
1	D	414	MET

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Mol	Chain	Res	Type
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	105	GLU
1	E	149	SER
1	E	164	ARG
1	E	171	GLN
1	E	195	THR
1	E	239	ARG
1	E	242	LEU
1	E	253	LEU
1	E	294	MET
1	E	296	LYS
1	E	340	MET
1	E	343	LYS
1	E	346	LEU
1	E	355	THR
1	E	367	ASP
1	E	376	LEU
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	101	GLN
1	F	105	GLU
1	F	114	LEU
1	F	117	SER
1	F	118	LEU
1	F	149	SER
1	F	219	VAL
1	F	239	ARG
1	F	242	LEU
1	F	253	LEU
1	F	294	MET

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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	396	GLN
1	F	410	LYS
1	F	412	ASP
1	G	45	GLU
1	G	68	LEU
1	G	100	GLU
1	G	105	GLU
1	G	138	SER
1	G	149	SER
1	G	168	SER
1	G	194	ARG
1	G	236	MET
1	G	239	ARG
1	G	242	LEU
1	G	253	LEU
1	G	294	MET
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	162	ASN
1	A	171	GLN
1	A	274	HIS
1	A	353	HIS
1	A	396	GLN
1	B	153	HIS
1	B	216	HIS
1	B	274	HIS
1	B	320	HIS

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Mol	Chain	Res	Type
1	B	353	HIS
1	C	153	HIS
1	C	162	ASN
1	C	216	HIS
1	C	274	HIS
1	C	353	HIS
1	D	209	HIS
1	D	216	HIS
1	D	353	HIS
1	D	364	ASN
1	E	216	HIS
1	E	353	HIS
1	F	152	GLN
1	F	162	ASN
1	F	216	HIS
1	F	353	HIS
1	G	162	ASN
1	G	216	HIS
1	G	298	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th 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%)	-0.23	3 (0%) 82 67	20, 36, 71, 107	0
1	B	368/392 (93%)	-0.13	5 (1%) 73 55	25, 42, 77, 103	0
1	C	370/392 (94%)	-0.00	12 (3%) 50 33	21, 45, 86, 109	0
1	D	366/392 (93%)	0.16	11 (3%) 52 34	21, 54, 103, 131	0
1	E	367/392 (93%)	-0.05	9 (2%) 58 39	24, 48, 84, 102	0
1	F	368/392 (93%)	0.15	8 (2%) 62 43	20, 50, 100, 129	0
1	G	368/392 (93%)	0.21	11 (2%) 52 34	22, 56, 113, 132	0
All	All	2573/2744 (93%)	0.02	59 (2%) 61 42	20, 46, 97, 132	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	366	PHE	6.7
1	B	121	SER	6.5
1	C	124	ARG	5.1
1	G	414	MET	5.0
1	C	126	VAL	4.9
1	A	375	GLU	4.3
1	C	125	ASN	4.1
1	D	125	ASN	3.9
1	D	163	PHE	3.5
1	E	375	GLU	3.4
1	F	367	ASP	3.4
1	B	126	VAL	3.2
1	F	375	GLU	3.1
1	C	120	ASN	3.0
1	B	367	ASP	3.0
1	E	120	ASN	2.9
1	G	120	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	38	PRO	2.9
1	F	120	ASN	2.9
1	A	120	ASN	2.9
1	F	140	VAL	2.8
1	D	366	PHE	2.8
1	C	287	LYS	2.8
1	F	99	ALA	2.7
1	D	48	ALA	2.7
1	E	127	THR	2.7
1	E	101	GLN	2.7
1	G	118	LEU	2.6
1	E	35	MET	2.5
1	B	412	ASP	2.5
1	D	36	LEU	2.4
1	F	118	LEU	2.4
1	G	126	VAL	2.4
1	E	161	ILE	2.4
1	D	164	ARG	2.4
1	D	35	MET	2.4
1	E	162	ASN	2.4
1	G	163	PHE	2.4
1	D	118	LEU	2.3
1	G	97	LEU	2.3
1	C	344	LYS	2.2
1	E	344	LYS	2.2
1	C	342	GLY	2.2
1	G	143	ALA	2.2
1	C	412	ASP	2.2
1	F	414	MET	2.2
1	C	413	LYS	2.2
1	B	127	THR	2.1
1	D	344	LYS	2.1
1	G	343	LYS	2.1
1	C	163	PHE	2.1
1	D	376	LEU	2.1
1	G	399	SER	2.1
1	G	160	LYS	2.1
1	C	195	THR	2.1
1	D	101	GLN	2.1
1	G	228	ARG	2.0
1	C	375	GLU	2.0
1	A	414	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.