Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2024 – 02:38 AM EDT

PDB ID	:	2GHP
Title	:	Crystal structure of the N-terminal 3 RNA binding domains of the yeast splicing factor Prp24
Authors	:	Bae, E.; Wesenberg, G.E.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2006-03-27
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

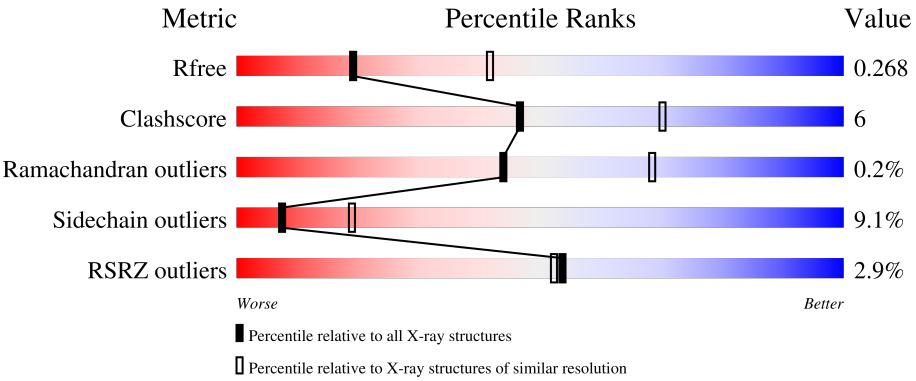
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 <=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	292	62% 15% • 21%
1	B	292	69% 12% • 18%
1	C	292	4% 61% 16% • 21%
1	D	292	63% 15% • 21%
1	E	292	66% 11% • 21%

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Mol	Chain	Length	Quality of chain
1	F	292	2% 66% 14% 18%
1	G	292	4% 61% 16% 21%
1	H	292	% 61% 17% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15219 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 U4/U6 snRNA-associated splicing factor PRP24.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	0	0
			1864	1183	328	344	5	4			
1	B	239	Total	C	N	O	S	Se	0	0	0
			1921	1218	339	355	5	4			
1	C	232	Total	C	N	O	S	Se	0	0	0
			1864	1183	328	344	5	4			
1	D	232	Total	C	N	O	S	Se	0	0	0
			1864	1183	328	344	5	4			
1	E	232	Total	C	N	O	S	Se	0	0	0
			1864	1183	328	344	5	4			
1	F	239	Total	C	N	O	S	Se	0	0	0
			1921	1218	339	355	5	4			
1	G	232	Total	C	N	O	S	Se	0	0	0
			1864	1183	328	344	5	4			
1	H	232	Total	C	N	O	S	Se	0	0	0
			1864	1183	328	344	5	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP P49960
A	1	MSE	MET	modified residue	UNP P49960
A	121	MSE	MET	modified residue	UNP P49960
A	213	MSE	MET	modified residue	UNP P49960
A	258	MSE	MET	modified residue	UNP P49960
A	272	MSE	MET	modified residue	UNP P49960
B	0	SER	-	cloning artifact	UNP P49960
B	1	MSE	MET	modified residue	UNP P49960
B	121	MSE	MET	modified residue	UNP P49960
B	213	MSE	MET	modified residue	UNP P49960
B	258	MSE	MET	modified residue	UNP P49960
B	272	MSE	MET	modified residue	UNP P49960
C	0	SER	-	cloning artifact	UNP P49960

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	MET	modified residue	UNP P49960
C	121	MSE	MET	modified residue	UNP P49960
C	213	MSE	MET	modified residue	UNP P49960
C	258	MSE	MET	modified residue	UNP P49960
C	272	MSE	MET	modified residue	UNP P49960
D	0	SER	-	cloning artifact	UNP P49960
D	1	MSE	MET	modified residue	UNP P49960
D	121	MSE	MET	modified residue	UNP P49960
D	213	MSE	MET	modified residue	UNP P49960
D	258	MSE	MET	modified residue	UNP P49960
D	272	MSE	MET	modified residue	UNP P49960
E	0	SER	-	cloning artifact	UNP P49960
E	1	MSE	MET	modified residue	UNP P49960
E	121	MSE	MET	modified residue	UNP P49960
E	213	MSE	MET	modified residue	UNP P49960
E	258	MSE	MET	modified residue	UNP P49960
E	272	MSE	MET	modified residue	UNP P49960
F	0	SER	-	cloning artifact	UNP P49960
F	1	MSE	MET	modified residue	UNP P49960
F	121	MSE	MET	modified residue	UNP P49960
F	213	MSE	MET	modified residue	UNP P49960
F	258	MSE	MET	modified residue	UNP P49960
F	272	MSE	MET	modified residue	UNP P49960
G	0	SER	-	cloning artifact	UNP P49960
G	1	MSE	MET	modified residue	UNP P49960
G	121	MSE	MET	modified residue	UNP P49960
G	213	MSE	MET	modified residue	UNP P49960
G	258	MSE	MET	modified residue	UNP P49960
G	272	MSE	MET	modified residue	UNP P49960
H	0	SER	-	cloning artifact	UNP P49960
H	1	MSE	MET	modified residue	UNP P49960
H	121	MSE	MET	modified residue	UNP P49960
H	213	MSE	MET	modified residue	UNP P49960
H	258	MSE	MET	modified residue	UNP P49960
H	272	MSE	MET	modified residue	UNP P49960

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	28	Total O 28 28	0	0

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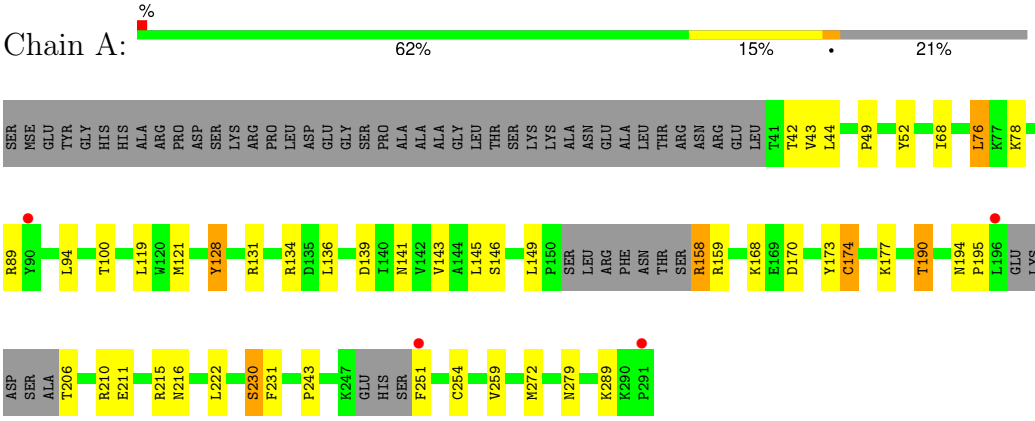
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	24	Total O 24 24	0	0
2	D	16	Total O 16 16	0	0
2	E	27	Total O 27 27	0	0
2	F	26	Total O 26 26	0	0
2	G	21	Total O 21 21	0	0
2	H	19	Total O 19 19	0	0

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.

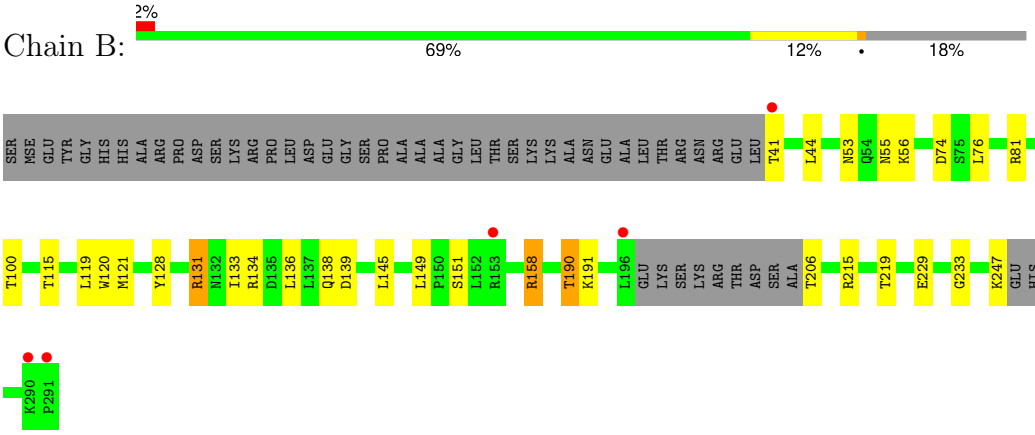
• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24

Chain A:



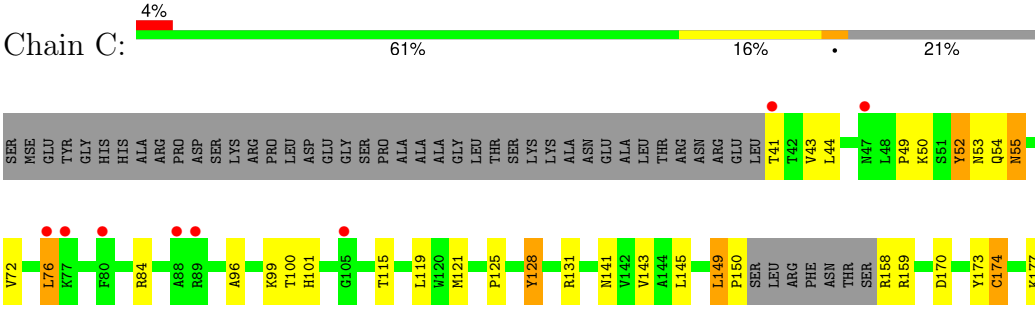
• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24

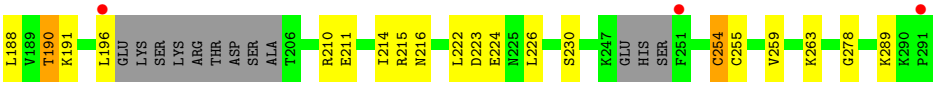
Chain B:



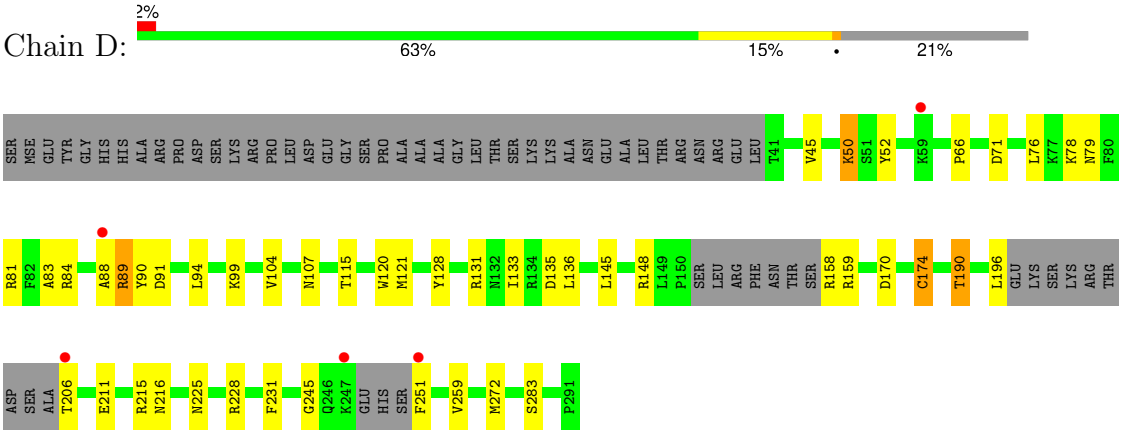
• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24

Chain C:

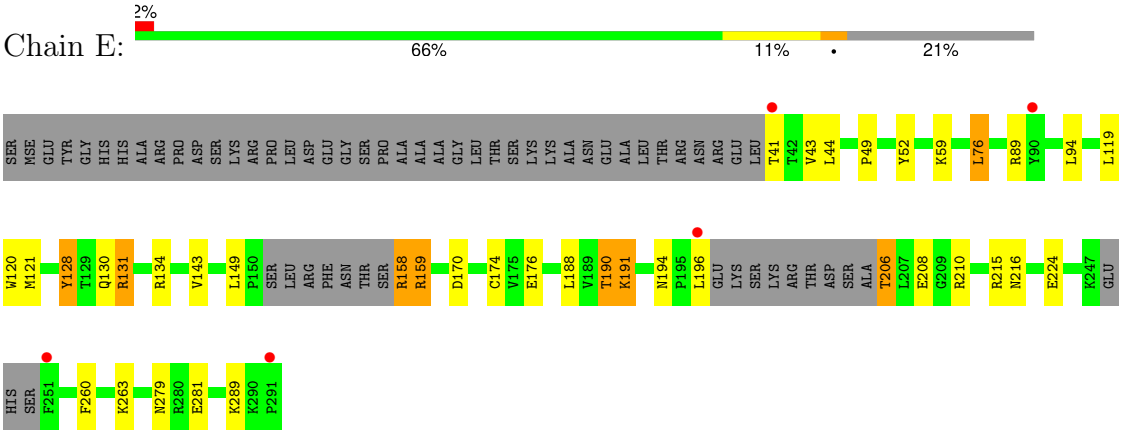




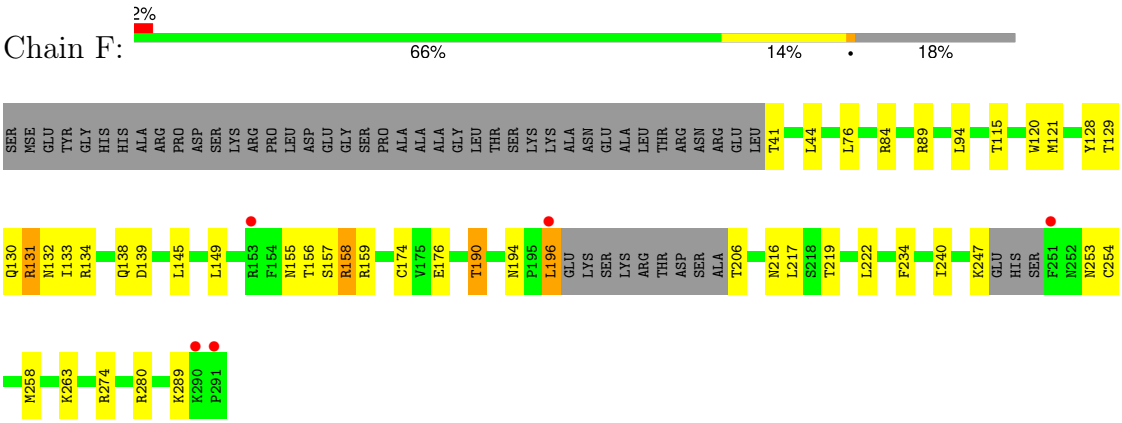
• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



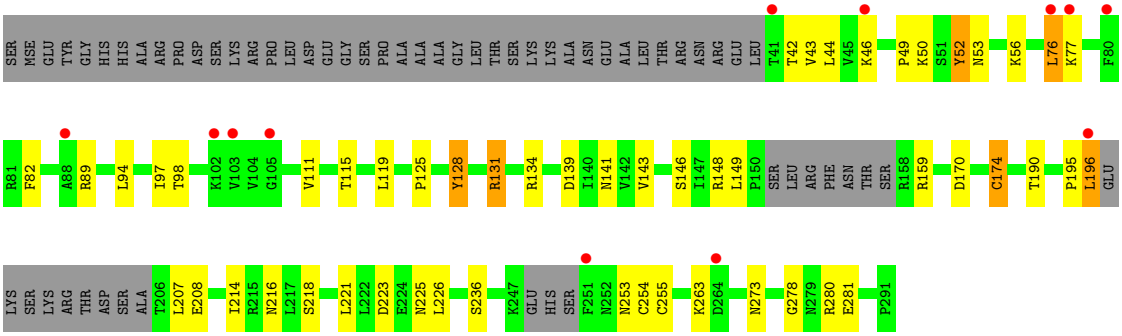
• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24

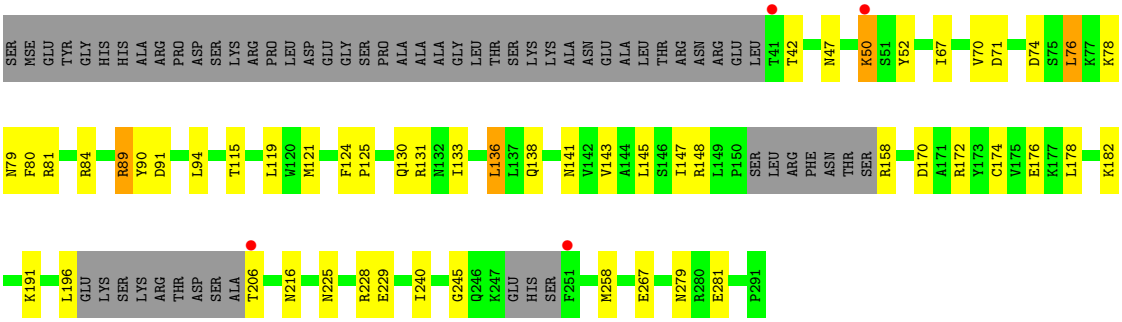


• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



• Molecule 1: U4/U6 snRNA-associated splicing factor PRP24

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.61Å 125.85Å 196.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.70 49.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.50-2.70) 94.2 (49.50-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.264 0.221 , 0.268	Depositor DCC
R_{free} test set	3738 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15219	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0758e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.59	1/1889 (0.1%)	0.72	0/2536
1	B	0.62	0/1948	0.71	0/2617
1	C	0.59	2/1889 (0.1%)	0.68	0/2536
1	D	0.57	1/1889 (0.1%)	0.67	0/2536
1	E	0.57	0/1889	0.70	0/2536
1	F	0.56	1/1948 (0.1%)	0.69	0/2617
1	G	0.59	2/1889 (0.1%)	0.68	0/2536
1	H	0.53	0/1889	0.66	0/2536
All	All	0.58	7/15230 (0.0%)	0.69	0/20450

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	CYS	CB-SG	-7.12	1.70	1.82
1	G	174	CYS	CB-SG	-7.04	1.70	1.82
1	A	174	CYS	CB-SG	-6.88	1.70	1.82
1	C	254	CYS	CB-SG	-6.44	1.71	1.82
1	G	254	CYS	CB-SG	-5.31	1.73	1.81
1	F	174	CYS	CB-SG	-5.20	1.73	1.81
1	D	99	LYS	CE-NZ	5.19	1.62	1.49

There are no bond angle outliers.

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	1864	0	1899	27	0
1	B	1921	0	1956	19	0
1	C	1864	0	1899	25	0
1	D	1864	0	1899	21	0
1	E	1864	0	1899	24	0
1	F	1921	0	1956	22	0
1	G	1864	0	1899	23	0
1	H	1864	0	1899	29	0
2	A	32	0	0	1	0
2	B	28	0	0	0	0
2	C	24	0	0	0	0
2	D	16	0	0	0	0
2	E	27	0	0	1	0
2	F	26	0	0	1	0
2	G	21	0	0	0	0
2	H	19	0	0	1	0
All	All	15219	0	15306	170	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 6.

All (170) 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:121:MSE:HE2	1:B:133:ILE:HD12	1.53	0.89
1:B:215:ARG:HH12	1:C:216:ASN:HB2	1.47	0.80
1:B:121:MSE:HE2	1:B:133:ILE:CD1	2.13	0.78
1:E:131:ARG:HH22	1:E:134:ARG:HD2	1.49	0.76
1:A:216:ASN:HB2	1:D:215:ARG:HH12	1.49	0.75
1:D:211:GLU:HG3	1:D:259:VAL:HG22	1.69	0.73
1:F:274:ARG:HD3	2:F:303:HOH:O	1.88	0.73
1:F:84:ARG:HB2	1:F:145:LEU:HG	1.71	0.71
1:A:121:MSE:HE1	1:A:136:LEU:HD12	1.71	0.71
1:B:84:ARG:HB2	1:B:145:LEU:HG	1.73	0.70
1:A:128:TYR:O	1:A:159:ARG:NH2	2.25	0.69
1:H:84:ARG:HB2	1:H:145:LEU:HG	1.73	0.69
1:E:215:ARG:NH1	1:H:216:ASN:HB2	2.08	0.67
1:E:131:ARG:NH2	1:E:134:ARG:HD2	2.09	0.67
1:B:215:ARG:NH1	1:C:216:ASN:HB2	2.10	0.66
1:H:76:LEU:HD22	1:H:143:VAL:HG23	1.78	0.66
1:G:53:ASN:HB3	1:G:56:LYS:HG3	1.78	0.66
1:H:89:ARG:HG3	1:H:90:TYR:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:ASN:ND2	1:H:281:GLU:O	2.28	0.64
1:C:49:PRO:HG2	1:C:52:TYR:CD1	2.33	0.63
1:D:50:LYS:HA	1:D:81:ARG:HG3	1.81	0.63
1:E:128:TYR:O	1:E:159:ARG:NH2	2.32	0.63
1:F:131:ARG:NH2	1:F:134:ARG:HD2	2.15	0.62
1:G:223:ASP:HB3	1:G:226:LEU:HB3	1.80	0.62
1:A:216:ASN:HB2	1:D:215:ARG:NH1	2.15	0.62
1:B:121:MSE:HB2	1:B:190:THR:HG23	1.81	0.61
1:E:215:ARG:HH12	1:H:216:ASN:HB2	1.65	0.61
1:F:121:MSE:HE2	1:F:133:ILE:CD1	2.31	0.61
1:F:216:ASN:O	1:F:216:ASN:ND2	2.34	0.60
1:H:89:ARG:HG3	1:H:90:TYR:N	2.16	0.60
1:D:121:MSE:HE2	1:D:133:ILE:CD1	2.32	0.60
1:C:76:LEU:HD13	1:C:143:VAL:HG23	1.84	0.59
1:A:215:ARG:NH2	1:D:216:ASN:HB2	2.18	0.59
1:B:219:THR:HG23	1:B:247:LYS:HD2	1.84	0.58
1:A:84:ARG:HB2	1:A:145:LEU:HD21	1.86	0.57
1:G:170:ASP:O	1:G:174:CYS:HB2	2.04	0.57
1:C:180:GLY:HA2	1:C:187:THR:HG22	1.85	0.57
1:D:225:ASN:OD1	1:D:228:ARG:NH2	2.37	0.57
1:H:47:ASN:HA	1:H:80:PHE:CD2	2.38	0.57
1:A:279:ASN:HB2	1:B:139:ASP:OD1	2.06	0.56
1:F:120:TRP:O	1:F:190:THR:HG22	2.06	0.56
1:H:121:MSE:HE2	1:H:133:ILE:CD1	2.36	0.55
1:A:76:LEU:HD13	1:A:143:VAL:HG23	1.87	0.55
1:C:53:ASN:OD1	1:C:55:ASN:HB2	2.07	0.55
1:A:231:PHE:CE2	1:A:272:MSE:HG3	2.42	0.55
1:H:225:ASN:O	1:H:229:GLU:HG3	2.06	0.55
1:C:211:GLU:HG3	1:C:259:VAL:HG22	1.89	0.54
1:G:46:LYS:HG3	1:G:82:PHE:CE1	2.42	0.54
1:C:222:LEU:HD13	1:C:254:CYS:HB3	1.89	0.54
1:H:50:LYS:HG2	1:H:79:ASN:O	2.08	0.54
1:F:121:MSE:HE2	1:F:133:ILE:HD12	1.90	0.53
1:B:120:TRP:O	1:B:190:THR:HG22	2.07	0.53
1:D:121:MSE:HE1	1:D:136:LEU:HD12	1.90	0.53
1:G:53:ASN:HB3	1:G:56:LYS:CG	2.39	0.52
1:D:84:ARG:HB2	1:D:145:LEU:HG	1.91	0.52
1:A:206:THR:HG22	1:A:210:ARG:HH21	1.75	0.52
1:H:130:GLN:HB2	2:H:307:HOH:O	2.10	0.52
1:D:89:ARG:HG3	1:D:90:TYR:H	1.75	0.51
1:E:131:ARG:HH11	1:E:131:ARG:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:ASP:OD1	1:H:81:ARG:NE	2.42	0.51
1:C:173:TYR:OH	1:C:177:LYS:HE3	2.11	0.51
1:C:84:ARG:HB2	1:C:145:LEU:HG	1.93	0.50
1:A:211:GLU:HG3	1:A:259:VAL:HG22	1.92	0.50
1:F:196:LEU:H	1:F:196:LEU:HD23	1.77	0.50
1:H:67:ILE:HG21	1:H:70:VAL:HG23	1.94	0.50
1:C:190:THR:O	1:C:191:LYS:HG2	2.12	0.49
1:G:49:PRO:HG2	1:G:52:TYR:CD1	2.48	0.49
1:A:49:PRO:HG2	1:A:52:TYR:CD1	2.47	0.49
1:H:121:MSE:HE2	1:H:133:ILE:HD13	1.95	0.49
1:A:170:ASP:O	1:A:174:CYS:HB2	2.13	0.48
1:D:121:MSE:HE2	1:D:133:ILE:HD13	1.94	0.48
1:E:210:ARG:HD2	1:E:260:PHE:O	2.13	0.48
1:B:158:ARG:HG3	1:B:233:GLY:HA3	1.96	0.48
1:G:216:ASN:ND2	1:G:281:GLU:O	2.46	0.48
1:H:133:ILE:HB	1:H:147:ILE:HD13	1.94	0.48
1:A:121:MSE:HB2	1:A:190:THR:HG23	1.95	0.48
1:A:173:TYR:OH	1:A:177:LYS:HE2	2.13	0.48
1:C:214:ILE:O	1:C:255:CYS:HA	2.13	0.47
1:E:49:PRO:HG2	1:E:52:TYR:CD1	2.49	0.47
1:E:120:TRP:CZ2	1:E:191:LYS:HG3	2.48	0.47
1:F:253:ASN:OD1	1:G:253:ASN:ND2	2.47	0.47
1:A:84:ARG:HB2	1:A:145:LEU:CD2	2.44	0.47
1:E:76:LEU:HD13	1:E:143:VAL:HG23	1.96	0.47
1:H:240:ILE:HG12	1:H:258:MSE:HE2	1.97	0.47
1:E:159:ARG:HB2	1:E:159:ARG:HH11	1.80	0.47
1:H:228:ARG:HG2	1:H:228:ARG:HH11	1.80	0.47
1:E:131:ARG:HH22	1:E:134:ARG:CD	2.26	0.46
1:H:124:PHE:HB2	1:H:125:PRO:CD	2.46	0.46
1:F:121:MSE:HE2	1:F:133:ILE:HD13	1.97	0.46
1:G:214:ILE:O	1:G:255:CYS:HA	2.15	0.46
1:C:223:ASP:HB3	1:C:226:LEU:HB3	1.96	0.46
1:E:121:MSE:HE3	1:E:188:LEU:HD11	1.98	0.46
1:A:42:THR:OG1	1:A:86:GLU:HG3	2.16	0.46
1:A:243:PRO:HB3	1:D:251:PHE:CZ	2.51	0.46
1:E:158:ARG:O	1:E:158:ARG:HG2	2.16	0.46
1:B:247:LYS:H	1:B:247:LYS:HG2	1.48	0.46
1:F:217:LEU:O	1:F:254:CYS:HB2	2.16	0.45
1:B:136:LEU:O	1:B:139:ASP:HB2	2.17	0.45
1:F:196:LEU:HD23	1:F:196:LEU:N	2.31	0.45
1:H:136:LEU:HD13	1:H:178:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:O	1:C:174:CYS:HB2	2.17	0.45
1:G:216:ASN:CG	1:G:280:ARG:HH21	2.19	0.45
1:H:121:MSE:HE1	1:H:136:LEU:HD12	1.99	0.45
1:F:176:GLU:OE1	1:H:267:GLU:OE2	2.35	0.45
1:E:279:ASN:HB2	1:F:139:ASP:OD1	2.17	0.45
1:F:155:ASN:O	1:F:156:THR:C	2.55	0.45
1:F:194:ASN:ND2	1:F:263:LYS:HD2	2.32	0.45
1:G:76:LEU:HD13	1:G:143:VAL:HG23	1.99	0.45
1:A:194:ASN:HA	1:A:195:PRO:HD2	1.78	0.44
1:F:158:ARG:HD3	1:F:234:PHE:CZ	2.52	0.44
1:B:131:ARG:NH2	1:B:134:ARG:HD2	2.33	0.44
1:D:228:ARG:HH11	1:D:228:ARG:HG3	1.82	0.44
1:B:53:ASN:OD1	1:B:56:LYS:HG3	2.18	0.44
1:G:94:LEU:HD23	1:G:97:ILE:HD12	2.00	0.44
1:A:141:ASN:O	1:C:289:LYS:HE2	2.17	0.44
1:H:172:ARG:O	1:H:176:GLU:HG2	2.18	0.44
1:B:131:ARG:HH22	1:B:134:ARG:HD2	1.83	0.43
1:B:74:ASP:OD1	1:B:81:ARG:NH2	2.51	0.43
1:D:66:PRO:HB2	1:D:88:ALA:HB2	2.00	0.43
1:H:170:ASP:O	1:H:174:CYS:HB2	2.18	0.43
1:E:170:ASP:OD1	1:G:208:GLU:OE2	2.35	0.43
1:B:253:ASN:OD1	1:C:215:ARG:HD3	2.18	0.43
1:C:121:MSE:HG2	1:C:188:LEU:HD11	2.00	0.43
1:E:191:LYS:HD3	2:E:295:HOH:O	2.17	0.43
1:G:131:ARG:HH22	1:G:134:ARG:HD2	1.82	0.43
1:F:129:THR:N	1:F:132:ASN:OD1	2.38	0.43
1:F:240:ILE:HG12	1:F:258:MSE:HE2	2.01	0.43
1:F:289:LYS:HG3	1:H:141:ASN:HB2	2.00	0.42
1:C:210:ARG:CG	1:C:263:LYS:HG2	2.49	0.42
1:E:289:LYS:HG3	1:G:141:ASN:HB2	2.01	0.42
1:B:251:PHE:O	1:B:252:ASN:HB2	2.20	0.42
1:G:218:SER:OG	1:G:221:LEU:HG	2.19	0.42
1:D:121:MSE:HE2	1:D:133:ILE:HD12	2.01	0.42
1:E:194:ASN:ND2	1:E:263:LYS:HD2	2.35	0.42
1:G:195:PRO:O	1:G:263:LYS:NZ	2.52	0.42
1:A:131:ARG:NH1	1:A:134:ARG:HD2	2.35	0.42
1:E:149:LEU:HD21	1:E:159:ARG:NE	2.35	0.42
1:G:196:LEU:HD23	1:G:196:LEU:H	1.84	0.42
1:H:121:MSE:HE2	1:H:133:ILE:HD12	2.01	0.42
1:B:121:MSE:CE	1:B:133:ILE:CD1	2.90	0.42
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:NH1	1:A:230:SER:O	2.53	0.42
1:E:131:ARG:HA	1:E:131:ARG:NH1	2.34	0.42
1:F:222:LEU:HD12	1:F:222:LEU:HA	1.90	0.42
1:A:222:LEU:HD22	1:A:254:CYS:HB3	2.02	0.42
1:E:190:THR:C	1:E:191:LYS:HG2	2.40	0.42
1:C:96:ALA:O	1:C:99:LYS:HB2	2.19	0.41
1:D:45:VAL:HB	1:D:83:ALA:HB3	2.02	0.41
1:C:54:GLN:HA	1:C:72:VAL:HG21	2.02	0.41
1:A:136:LEU:O	1:A:139:ASP:HB2	2.20	0.41
1:A:168:LYS:HG3	2:A:293:HOH:O	2.20	0.41
1:C:49:PRO:O	1:C:52:TYR:HB2	2.21	0.41
1:G:139:ASP:OD1	1:H:279:ASN:HB2	2.20	0.41
1:A:289:LYS:HG3	1:C:141:ASN:HB2	2.03	0.41
1:G:273:ASN:O	1:H:182:LYS:HE3	2.20	0.41
1:E:206:THR:HG23	1:E:208:GLU:H	1.85	0.41
1:F:216:ASN:ND2	1:F:280:ARG:HE	2.18	0.41
1:H:258:MSE:HE3	1:H:258:MSE:HB2	1.94	0.41
1:A:222:LEU:HD12	1:A:222:LEU:HA	1.90	0.41
1:D:120:TRP:O	1:D:190:THR:CG2	2.69	0.41
1:D:170:ASP:O	1:D:174:CYS:HB2	2.21	0.41
1:D:231:PHE:CE2	1:D:272:MSE:HG3	2.56	0.41
1:E:216:ASN:ND2	1:E:281:GLU:O	2.46	0.41
1:G:43:VAL:HG13	1:G:111:VAL:HG13	2.03	0.41
1:C:149:LEU:HA	1:C:150:PRO:HD2	1.71	0.41
1:C:125:PRO:O	1:C:128:TYR:HB2	2.20	0.40
1:G:125:PRO:O	1:G:128:TYR:HB2	2.20	0.40
1:G:42:THR:HG22	1:G:43:VAL:N	2.37	0.40
1:C:158:ARG:NH1	1:C:230:SER:O	2.54	0.40
1:D:120:TRP:O	1:D:190:THR:HG22	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	224/292 (77%)	218 (97%)	6 (3%)	0	100	100
1	B	233/292 (80%)	227 (97%)	6 (3%)	0	100	100
1	C	224/292 (77%)	216 (96%)	7 (3%)	1 (0%)	30	55
1	D	224/292 (77%)	211 (94%)	12 (5%)	1 (0%)	30	55
1	E	224/292 (77%)	220 (98%)	4 (2%)	0	100	100
1	F	233/292 (80%)	226 (97%)	7 (3%)	0	100	100
1	G	224/292 (77%)	213 (95%)	10 (4%)	1 (0%)	30	55
1	H	224/292 (77%)	211 (94%)	12 (5%)	1 (0%)	30	55
All	All	1810/2336 (78%)	1742 (96%)	64 (4%)	4 (0%)	44	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	GLY
1	D	245	GLY
1	G	278	GLY
1	H	245	GLY

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	208/253 (82%)	192 (92%)	16 (8%)	10	26
1	B	215/253 (85%)	197 (92%)	18 (8%)	9	22
1	C	208/253 (82%)	190 (91%)	18 (9%)	8	20
1	D	208/253 (82%)	185 (89%)	23 (11%)	5	12
1	E	208/253 (82%)	188 (90%)	20 (10%)	7	17
1	F	215/253 (85%)	196 (91%)	19 (9%)	8	20
1	G	208/253 (82%)	188 (90%)	20 (10%)	7	17
1	H	208/253 (82%)	189 (91%)	19 (9%)	7	19
All	All	1678/2024 (83%)	1525 (91%)	153 (9%)	7	19

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	44	LEU
1	A	68	ILE
1	A	76	LEU
1	A	78	LYS
1	A	89	ARG
1	A	94	LEU
1	A	100	THR
1	A	119	LEU
1	A	128	TYR
1	A	146	SER
1	A	149	LEU
1	A	158	ARG
1	A	190	THR
1	A	230	SER
1	A	251	PHE
1	B	41	THR
1	B	44	LEU
1	B	55	ASN
1	B	76	LEU
1	B	89	ARG
1	B	100	THR
1	B	115	THR
1	B	119	LEU
1	B	128	TYR
1	B	131	ARG
1	B	138	GLN
1	B	149	LEU
1	B	151	SER
1	B	158	ARG
1	B	190	THR
1	B	191	LYS
1	B	206	THR
1	B	229	GLU
1	C	41	THR
1	C	43	VAL
1	C	44	LEU
1	C	50	LYS
1	C	52	TYR
1	C	55	ASN
1	C	76	LEU
1	C	100	THR

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Mol	Chain	Res	Type
1	C	101	HIS
1	C	115	THR
1	C	119	LEU
1	C	128	TYR
1	C	131	ARG
1	C	149	LEU
1	C	159	ARG
1	C	190	THR
1	C	196	LEU
1	C	224	GLU
1	D	50	LYS
1	D	52	TYR
1	D	71	ASP
1	D	76	LEU
1	D	78	LYS
1	D	79	ASN
1	D	89	ARG
1	D	91	ASP
1	D	94	LEU
1	D	104	VAL
1	D	107	ASN
1	D	115	THR
1	D	128	TYR
1	D	131	ARG
1	D	135	ASP
1	D	148	ARG
1	D	158	ARG
1	D	159	ARG
1	D	174	CYS
1	D	190	THR
1	D	196	LEU
1	D	206	THR
1	D	283	SER
1	E	41	THR
1	E	43	VAL
1	E	44	LEU
1	E	59	LYS
1	E	76	LEU
1	E	89	ARG
1	E	94	LEU
1	E	119	LEU
1	E	128	TYR

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Mol	Chain	Res	Type
1	E	130	GLN
1	E	131	ARG
1	E	158	ARG
1	E	159	ARG
1	E	174	CYS
1	E	176	GLU
1	E	190	THR
1	E	191	LYS
1	E	196	LEU
1	E	206	THR
1	E	224	GLU
1	F	41	THR
1	F	44	LEU
1	F	76	LEU
1	F	89	ARG
1	F	94	LEU
1	F	115	THR
1	F	128	TYR
1	F	130	GLN
1	F	131	ARG
1	F	138	GLN
1	F	149	LEU
1	F	157	SER
1	F	158	ARG
1	F	159	ARG
1	F	190	THR
1	F	196	LEU
1	F	206	THR
1	F	219	THR
1	F	247	LYS
1	G	44	LEU
1	G	50	LYS
1	G	52	TYR
1	G	76	LEU
1	G	77	LYS
1	G	89	ARG
1	G	98	THR
1	G	115	THR
1	G	119	LEU
1	G	128	TYR
1	G	131	ARG
1	G	146	SER

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Mol	Chain	Res	Type
1	G	148	ARG
1	G	149	LEU
1	G	159	ARG
1	G	190	THR
1	G	196	LEU
1	G	207	LEU
1	G	225	ASN
1	G	236	SER
1	H	42	THR
1	H	50	LYS
1	H	52	TYR
1	H	71	ASP
1	H	76	LEU
1	H	78	LYS
1	H	89	ARG
1	H	91	ASP
1	H	94	LEU
1	H	115	THR
1	H	119	LEU
1	H	131	ARG
1	H	136	LEU
1	H	138	GLN
1	H	148	ARG
1	H	158	ARG
1	H	191	LYS
1	H	196	LEU
1	H	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides 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	228/292 (78%)	0.09	4 (1%)	67	67	41, 57, 73, 81	0
1	B	235/292 (80%)	0.11	6 (2%)	57	56	40, 57, 72, 78	0
1	C	228/292 (78%)	0.56	13 (5%)	30	28	39, 55, 70, 75	0
1	D	228/292 (78%)	0.36	5 (2%)	62	61	39, 54, 73, 78	0
1	E	228/292 (78%)	0.21	5 (2%)	62	61	41, 56, 71, 80	0
1	F	235/292 (80%)	0.24	5 (2%)	63	63	40, 57, 72, 80	0
1	G	228/292 (78%)	0.63	12 (5%)	33	31	39, 55, 70, 74	0
1	H	228/292 (78%)	0.30	4 (1%)	67	67	38, 54, 73, 78	0
All	All	1838/2336 (78%)	0.31	54 (2%)	54	52	38, 56, 71, 81	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	41	THR	6.4
1	C	41	THR	6.1
1	F	291	PRO	5.4
1	G	251	PHE	4.8
1	H	41	THR	4.4
1	C	196	LEU	4.1
1	C	251	PHE	3.9
1	F	196	LEU	3.5
1	G	76	LEU	3.4
1	D	251	PHE	3.4
1	G	105	GLY	3.2
1	A	291	PRO	3.1
1	C	88	ALA	3.1
1	B	196	LEU	3.1
1	A	251	PHE	3.0
1	E	251	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	76	LEU	2.9
1	C	291	PRO	2.8
1	D	59	LYS	2.8
1	E	41	THR	2.8
1	E	291	PRO	2.8
1	G	196	LEU	2.7
1	E	196	LEU	2.7
1	B	251	PHE	2.6
1	G	88	ALA	2.6
1	D	247	LYS	2.6
1	B	291	PRO	2.5
1	C	80	PHE	2.5
1	C	89	ARG	2.4
1	C	77	LYS	2.4
1	C	105	GLY	2.4
1	G	77	LYS	2.4
1	A	90	TYR	2.3
1	B	41	THR	2.3
1	G	80	PHE	2.3
1	E	90	TYR	2.3
1	G	102	LYS	2.3
1	C	66	PRO	2.3
1	H	251	PHE	2.2
1	D	88	ALA	2.2
1	G	264	ASP	2.2
1	F	251	PHE	2.2
1	H	50	LYS	2.2
1	D	206	THR	2.2
1	G	103	VAL	2.2
1	F	290	LYS	2.2
1	B	153	ARG	2.2
1	G	46	LYS	2.1
1	F	153	ARG	2.1
1	C	47	ASN	2.1
1	A	196	LEU	2.1
1	C	68	ILE	2.1
1	B	290	LYS	2.0
1	H	206	THR	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 monosaccharides 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.