Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 01:19 pm GMT

PDB ID	:	8BYW
Title	:	Rut B structure
Authors	:	Rajendran, C.; Sterner, R.; Busch, M.
Deposited on	:	2022-12-14
Resolution	:	1.59 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:

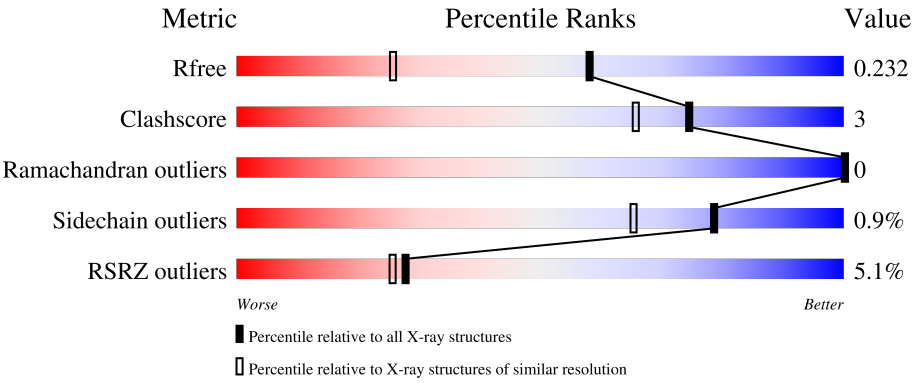
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	230	2% 89% 7%
1	B	230	% 89% 8%
1	C	230	3% 92%
1	D	230	% 89% 7%
1	E	230	2% 91% 6%

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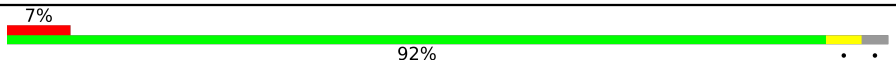
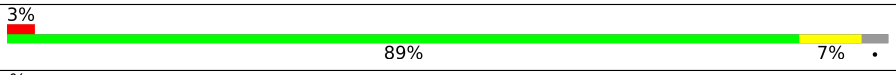
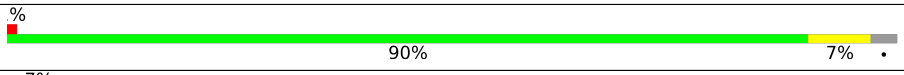
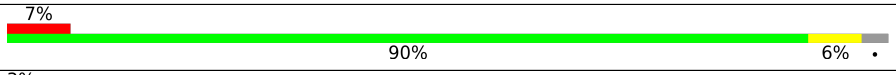
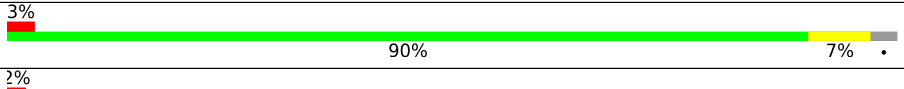
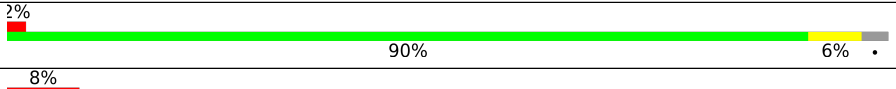
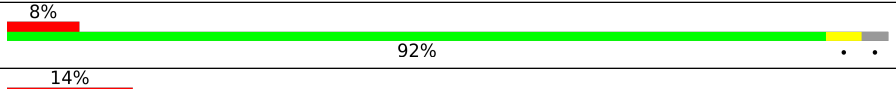
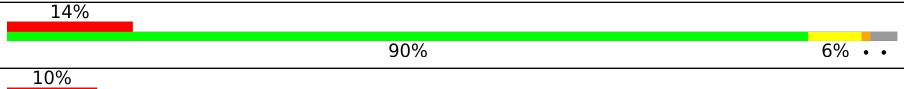
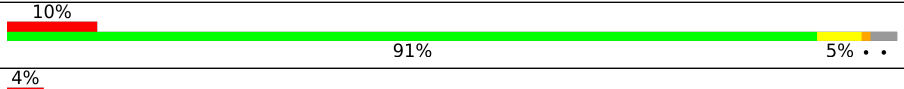
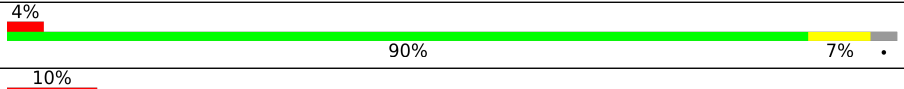
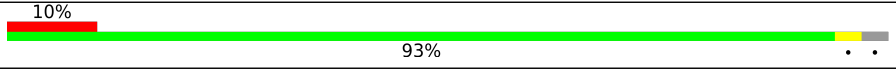
Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	
1	K	230	
1	L	230	
1	M	230	
1	N	230	
1	O	230	
1	P	230	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30533 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 Ureidoacrylate amidohydrolase RutB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	B	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	C	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	D	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	E	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	F	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	G	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	H	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	I	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	J	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	K	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	L	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	M	222	Total	C	N	O	S	0	0	0
			1708	1101	285	317	5			
1	N	222	Total	C	N	O	S	0	0	0
			1711	1102	285	319	5			
1	O	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			
1	P	222	Total	C	N	O	S	0	0	0
			1715	1104	285	321	5			

- Molecule 2 is water.

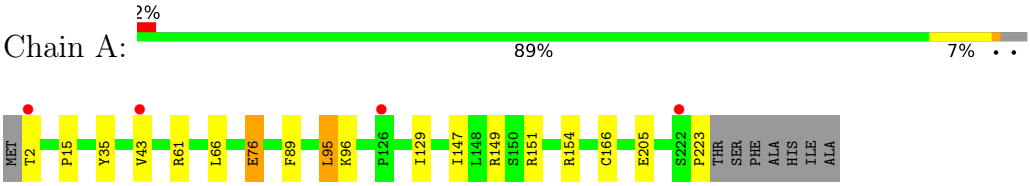
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	240	Total O 240 240	0	0
2	B	226	Total O 226 226	0	0
2	C	191	Total O 191 191	0	0
2	D	231	Total O 231 231	0	0
2	E	231	Total O 231 231	0	0
2	F	188	Total O 188 188	0	0
2	G	195	Total O 195 195	0	0
2	H	200	Total O 200 200	0	0
2	I	198	Total O 198 198	0	0
2	J	198	Total O 198 198	0	0
2	K	203	Total O 203 203	0	0
2	L	171	Total O 171 171	0	0
2	M	158	Total O 158 158	0	0
2	N	153	Total O 153 153	0	0
2	O	179	Total O 179 179	0	0
2	P	142	Total O 142 142	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.

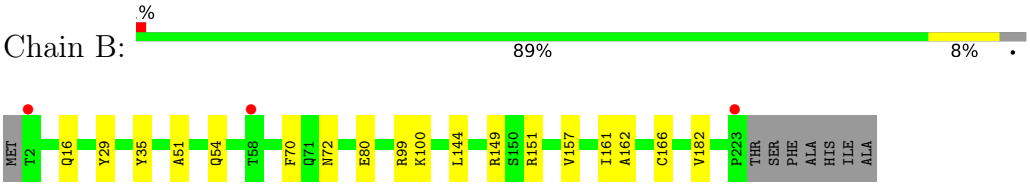
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain A:



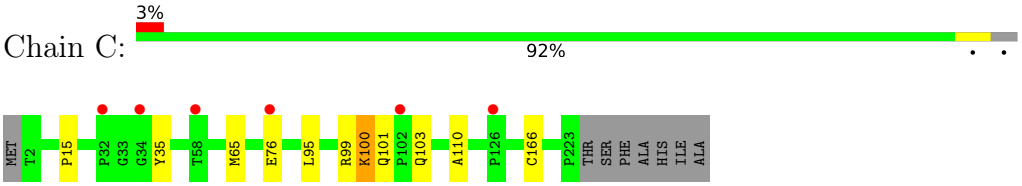
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain B:



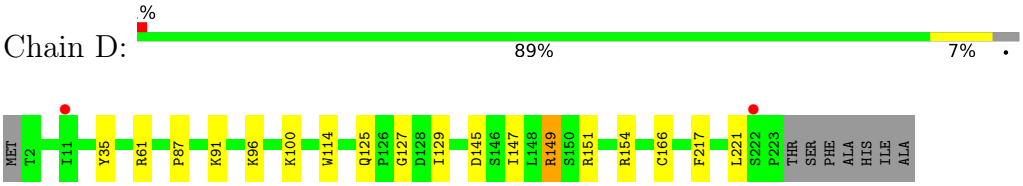
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain C:



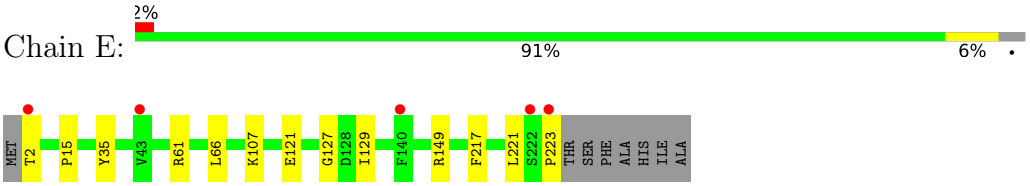
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain D:



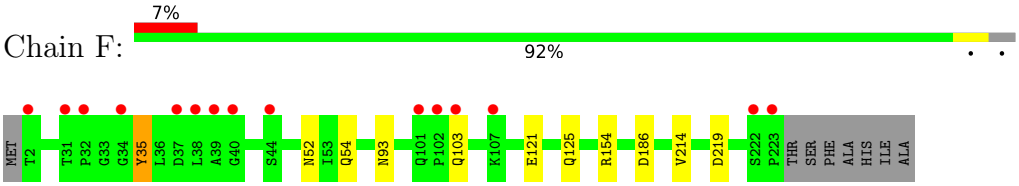
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain E:



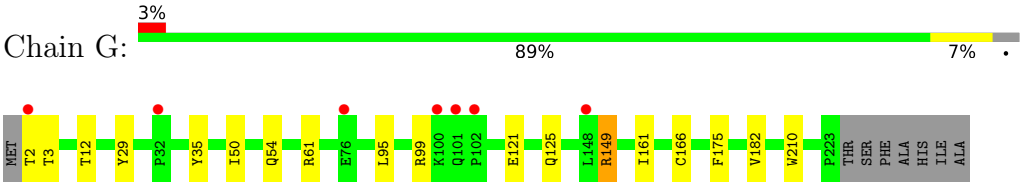
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain F:



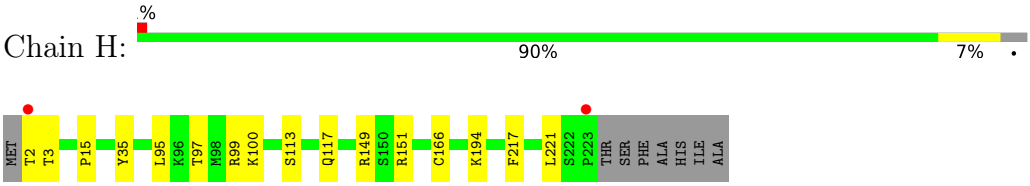
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain G:



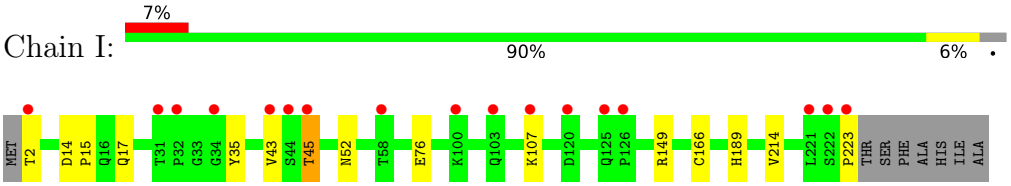
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain H:



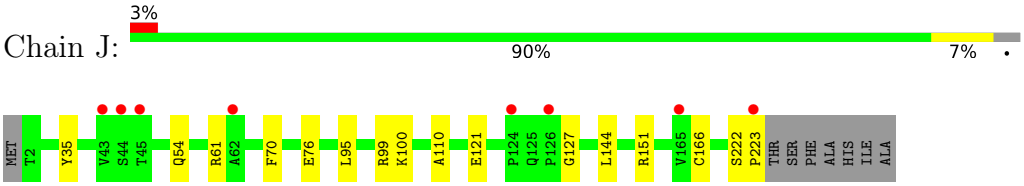
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain I:



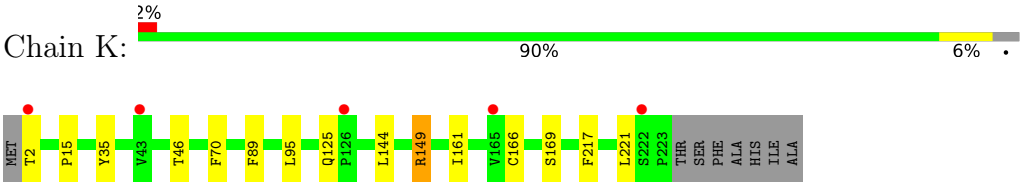
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain J:



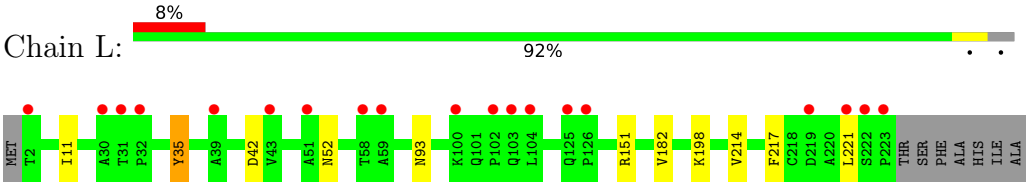
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain K:



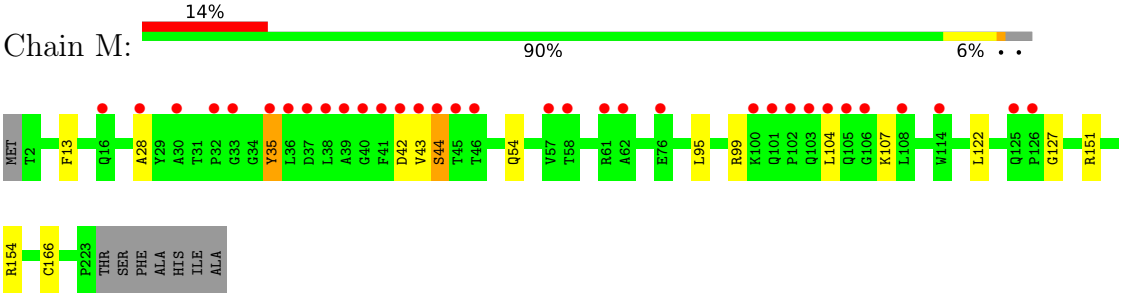
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain L:



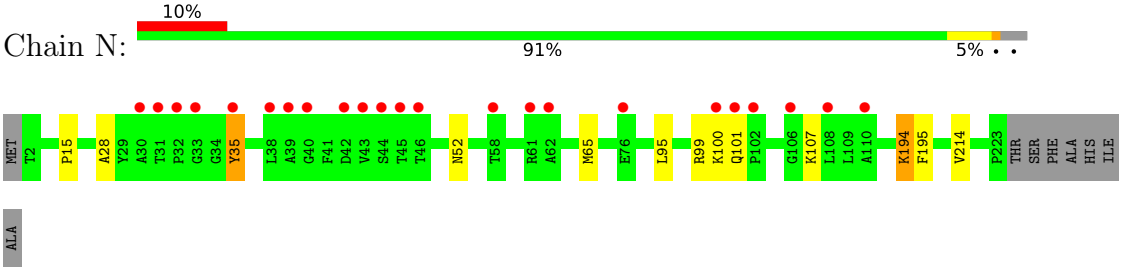
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain M:



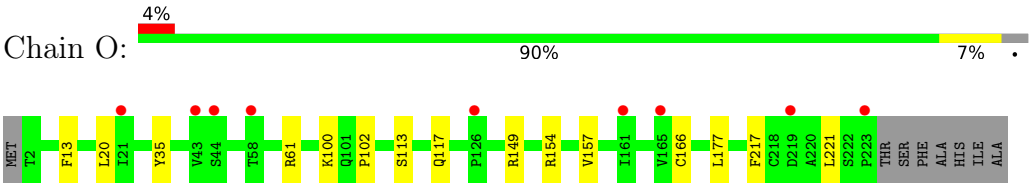
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain N:



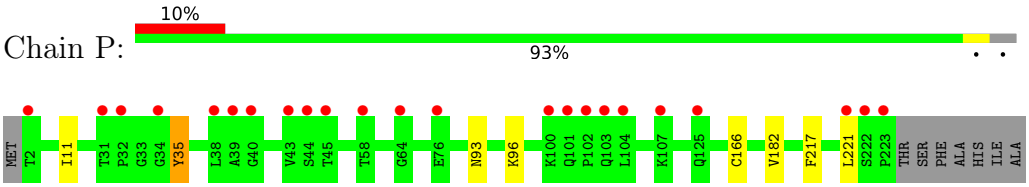
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain O:



• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.56Å 108.25Å 123.74Å 85.74° 83.33° 74.27°	Depositor
Resolution (Å)	48.71 – 1.59 47.59 – 1.59	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.71-1.59) 92.4 (47.59-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.18rc2	Depositor
R, R_{free}	0.206 , 0.233 0.206 , 0.232	Depositor DCC
R_{free} test set	21602 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	30533	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% 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	0.40	0/1760	0.59	0/2401
1	B	0.38	0/1760	0.58	0/2401
1	C	0.37	0/1760	0.56	0/2401
1	D	0.40	0/1760	0.63	2/2401 (0.1%)
1	E	0.39	0/1760	0.57	0/2401
1	F	0.37	0/1760	0.54	0/2401
1	G	0.39	0/1760	0.61	2/2401 (0.1%)
1	H	0.37	0/1760	0.56	0/2401
1	I	0.37	0/1760	0.55	0/2401
1	J	0.37	0/1760	0.57	0/2401
1	K	0.40	0/1760	0.56	1/2401 (0.0%)
1	L	0.35	0/1760	0.53	0/2401
1	M	0.35	0/1753	0.53	0/2392
1	N	0.37	0/1756	0.54	0/2396
1	O	0.39	1/1760 (0.1%)	0.61	2/2401 (0.1%)
1	P	0.34	0/1760	0.53	0/2401
All	All	0.38	1/28149 (0.0%)	0.57	7/38402 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	149	ARG	CG-CD	5.58	1.66	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	149	ARG	NE-CZ-NH2	11.12	125.86	120.30
1	O	149	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	D	149	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	D	149	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	K	149	ARG	CB-CG-CD	-6.08	95.78	111.60
1	G	149	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	O	149	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1715	0	1675	16	0
1	B	1715	0	1675	13	0
1	C	1715	0	1675	9	0
1	D	1715	0	1675	18	0
1	E	1715	0	1675	11	0
1	F	1715	0	1675	9	0
1	G	1715	0	1675	17	0
1	H	1715	0	1675	15	0
1	I	1715	0	1675	12	0
1	J	1715	0	1675	12	0
1	K	1715	0	1675	10	1
1	L	1715	0	1675	8	0
1	M	1708	0	1669	11	0
1	N	1711	0	1671	8	0
1	O	1715	0	1675	8	1
1	P	1715	0	1675	5	0
2	A	240	0	0	8	0
2	B	226	0	0	6	0
2	C	191	0	0	3	3
2	D	231	0	0	16	0
2	E	231	0	0	7	1
2	F	188	0	0	4	3
2	G	195	0	0	4	1
2	H	200	0	0	4	3
2	I	198	0	0	7	2
2	J	198	0	0	7	5
2	K	203	0	0	5	0
2	L	171	0	0	3	6
2	M	158	0	0	4	0
2	N	153	0	0	2	4
2	O	179	0	0	4	1
2	P	142	0	0	1	1
All	All	30533	0	26790	172	16

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 3.

All (172) 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:G:3:THR:HG23	1:H:3:THR:H	1.26	1.00
1:B:29:TYR:OH	2:B:301:HOH:O	1.85	0.92
1:J:222:SER:OG	2:J:301:HOH:O	1.88	0.92
1:J:76:GLU:HG2	1:J:110:ALA:HB1	1.59	0.82
1:G:2:THR:HG23	2:G:442:HOH:O	1.79	0.81
1:A:205:GLU:OE1	2:A:301:HOH:O	1.98	0.78
1:D:61:ARG:NH1	2:D:303:HOH:O	2.14	0.78
1:A:149:ARG:HH11	1:H:149:ARG:HH11	1.32	0.78
2:D:305:HOH:O	1:G:175:PHE:HE1	1.67	0.78
1:F:219:ASP:O	2:F:301:HOH:O	2.02	0.78
1:M:42:ASP:OD1	1:M:44:SER:OG	2.03	0.76
2:D:305:HOH:O	1:G:175:PHE:CE1	2.37	0.76
1:A:151:ARG:NH2	2:A:304:HOH:O	2.21	0.73
1:F:154:ARG:NH1	2:F:304:HOH:O	2.21	0.73
1:G:3:THR:HG23	1:H:3:THR:N	2.03	0.73
1:L:42:ASP:OD2	2:L:301:HOH:O	2.06	0.73
1:D:145:ASP:O	1:D:149:ARG:HG3	1.90	0.72
1:E:61:ARG:NH1	2:E:303:HOH:O	2.19	0.71
1:D:151:ARG:NH2	2:D:304:HOH:O	2.20	0.71
1:D:125:GLN:OE1	2:D:302:HOH:O	2.08	0.70
1:C:100:LYS:NZ	2:C:301:HOH:O	2.26	0.68
1:N:107:LYS:NZ	2:N:302:HOH:O	2.18	0.68
1:B:16:GLN:OE1	2:B:302:HOH:O	2.10	0.67
1:E:223:PRO:O	2:E:301:HOH:O	2.12	0.67
1:C:99:ARG:HD2	1:I:223:PRO:HA	1.77	0.67
1:E:121:GLU:OE2	2:E:302:HOH:O	2.13	0.67
1:K:125:GLN:OE1	2:K:301:HOH:O	2.14	0.66
1:E:127:GLY:N	2:E:304:HOH:O	2.22	0.66
1:F:125:GLN:OE1	2:F:302:HOH:O	2.14	0.66
1:B:72:ASN:ND2	2:B:301:HOH:O	2.29	0.65
1:K:2:THR:HG22	2:K:403:HOH:O	1.96	0.65
1:C:76:GLU:HG3	1:C:110:ALA:HB1	1.79	0.64
1:M:151:ARG:NH2	2:M:302:HOH:O	2.30	0.64
1:E:149:ARG:NH2	2:E:306:HOH:O	2.30	0.64
1:G:166:CYS:SG	2:G:419:HOH:O	2.42	0.63
1:I:76:GLU:HG2	2:I:308:HOH:O	1.97	0.63
1:G:3:THR:OG1	1:H:3:THR:HB	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.63	0.62
1:H:97:THR:HA	1:H:100:LYS:HE2	1.83	0.61
1:I:107:LYS:NZ	2:I:304:HOH:O	2.34	0.60
1:N:194:LYS:HD2	1:N:195:PHE:N	2.16	0.60
1:I:52:ASN:HB3	1:I:214:VAL:HG21	1.85	0.59
1:J:61:ARG:HG3	2:J:310:HOH:O	2.02	0.59
1:M:28:ALA:HB1	1:M:35:TYR:HB3	1.85	0.59
1:O:100:LYS:NZ	2:O:302:HOH:O	2.35	0.59
1:D:166:CYS:SG	2:D:455:HOH:O	2.53	0.58
1:B:80:GLU:OE2	2:B:303:HOH:O	2.17	0.58
1:B:151:ARG:NH2	2:B:307:HOH:O	2.37	0.58
1:D:87:PRO:HB2	2:D:305:HOH:O	2.03	0.58
1:D:61:ARG:HD2	2:D:434:HOH:O	2.04	0.57
1:A:149:ARG:HD2	1:H:149:ARG:NH1	2.19	0.57
1:D:100:LYS:NZ	2:D:301:HOH:O	2.07	0.57
1:N:100:LYS:HG3	1:N:101:GLN:HG3	1.85	0.57
1:A:61:ARG:NH1	2:A:303:HOH:O	2.21	0.56
1:D:91:LYS:HG2	2:D:305:HOH:O	2.05	0.56
1:G:3:THR:CG2	1:H:3:THR:H	2.08	0.56
1:B:149:ARG:NE	2:D:306:HOH:O	2.39	0.56
1:H:151:ARG:NH2	2:H:303:HOH:O	2.37	0.56
1:D:149:ARG:NH2	2:D:306:HOH:O	2.30	0.56
1:O:61:ARG:HG3	2:O:339:HOH:O	2.05	0.56
1:G:95:LEU:O	1:G:99:ARG:HG3	2.05	0.55
1:M:104:LEU:HA	1:M:107:LYS:HD2	1.88	0.55
1:O:154:ARG:NH1	2:O:305:HOH:O	2.40	0.55
1:G:125:GLN:NE2	2:G:301:HOH:O	2.28	0.55
1:K:149:ARG:NH1	2:K:306:HOH:O	2.40	0.55
1:F:54:GLN:HE22	1:F:121:GLU:HB3	1.71	0.55
1:J:70:PHE:HZ	1:J:144:LEU:HD22	1.71	0.55
1:K:2:THR:HG23	1:K:15:PRO:HD3	1.88	0.55
1:D:151:ARG:NE	2:D:304:HOH:O	2.38	0.55
1:E:2:THR:HG23	1:E:15:PRO:HD3	1.89	0.55
1:E:2:THR:HG22	2:E:369:HOH:O	2.06	0.53
1:J:151:ARG:NH2	2:J:309:HOH:O	2.41	0.53
1:J:127:GLY:HA3	2:J:315:HOH:O	2.07	0.53
1:A:76:GLU:HG3	2:A:476:HOH:O	2.09	0.53
1:K:46:THR:HG21	1:K:161:ILE:HD11	1.92	0.52
1:L:151:ARG:NH2	2:L:305:HOH:O	2.39	0.52
1:D:127:GLY:N	2:D:307:HOH:O	2.34	0.52
1:J:127:GLY:N	2:J:303:HOH:O	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH1	2:A:310:HOH:O	2.43	0.52
1:A:223:PRO:HA	1:B:99:ARG:HD2	1.90	0.52
1:C:166:CYS:SG	2:C:429:HOH:O	2.50	0.52
1:A:2:THR:HG23	1:A:15:PRO:HD3	1.92	0.51
1:H:149:ARG:NE	2:H:305:HOH:O	2.43	0.51
1:J:166:CYS:SG	2:J:446:HOH:O	2.42	0.51
1:P:35:TYR:OH	1:P:93:ASN:HB2	2.10	0.51
1:B:100:LYS:N	1:B:100:LYS:HD3	2.26	0.51
1:I:43:VAL:O	2:I:303:HOH:O	2.20	0.50
1:K:166:CYS:SG	2:K:446:HOH:O	2.46	0.50
1:C:100:LYS:N	1:C:100:LYS:HD3	2.26	0.50
1:A:2:THR:HG22	2:A:319:HOH:O	2.10	0.50
1:N:28:ALA:HB1	1:N:35:TYR:HB3	1.93	0.50
1:M:166:CYS:SG	2:M:403:HOH:O	2.52	0.50
1:I:17:GLN:HG3	2:I:301:HOH:O	2.12	0.50
1:D:154:ARG:NH1	2:D:311:HOH:O	2.44	0.49
1:I:14:ASP:OD1	2:I:302:HOH:O	2.19	0.49
1:J:54:GLN:OE1	1:J:121:GLU:HB3	2.12	0.49
1:K:125:GLN:HG2	2:K:343:HOH:O	2.11	0.49
1:B:70:PHE:HZ	1:B:144:LEU:HD22	1.77	0.49
1:F:54:GLN:NE2	1:F:121:GLU:HB3	2.27	0.49
1:G:3:THR:HG22	1:G:12:THR:HG22	1.95	0.49
1:F:186:ASP:OD2	2:F:303:HOH:O	2.20	0.48
1:D:96:LYS:O	1:D:100:LYS:HG2	2.13	0.48
1:A:89:PHE:HA	1:A:95:LEU:HD23	1.95	0.48
1:L:35:TYR:OH	1:L:93:ASN:HB2	2.14	0.48
1:D:87:PRO:C	2:D:305:HOH:O	2.52	0.48
1:A:43:VAL:HG23	2:A:366:HOH:O	2.13	0.47
1:A:96:LYS:HE2	2:C:443:HOH:O	2.13	0.47
1:P:11:ILE:HD11	1:P:182:VAL:HG11	1.96	0.47
1:B:166:CYS:SG	2:B:463:HOH:O	2.56	0.47
1:C:101:GLN:HB3	1:C:103:GLN:NE2	2.30	0.47
1:L:52:ASN:HB3	1:L:214:VAL:HG21	1.97	0.47
1:A:129:ILE:HD13	1:A:147:ILE:HG21	1.97	0.47
1:D:114:TRP:CG	1:O:102:PRO:HB2	2.49	0.47
1:P:217:PHE:CZ	1:P:221:LEU:HD11	2.50	0.47
1:E:107:LYS:NZ	2:E:308:HOH:O	2.33	0.47
1:I:2:THR:HG23	1:I:15:PRO:HD3	1.96	0.46
1:C:95:LEU:O	1:C:99:ARG:HG3	2.16	0.46
1:L:217:PHE:CZ	1:L:221:LEU:HD11	2.51	0.46
1:J:99:ARG:HG2	2:J:318:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:15:PRO:O	1:N:65:MET:HG2	2.16	0.46
1:O:113:SER:O	1:O:117:GLN:HG3	2.16	0.46
1:A:66:LEU:HD21	1:A:129:ILE:HD12	1.97	0.46
1:C:103:GLN:H	1:C:103:GLN:CD	2.19	0.45
1:I:166:CYS:SG	2:I:419:HOH:O	2.56	0.45
1:L:11:ILE:HD11	1:L:182:VAL:HG21	1.97	0.45
1:M:28:ALA:HA	1:M:35:TYR:H	1.81	0.45
1:M:154:ARG:NH1	2:M:308:HOH:O	2.49	0.45
1:H:95:LEU:O	1:H:99:ARG:HG3	2.17	0.45
1:G:29:TYR:HB3	1:G:161:ILE:CG2	2.47	0.44
1:K:217:PHE:CZ	1:K:221:LEU:HD11	2.53	0.44
1:G:50:ILE:HG22	1:G:54:GLN:NE2	2.31	0.44
1:G:54:GLN:NE2	1:G:121:GLU:HB3	2.31	0.44
1:A:166:CYS:SG	2:A:455:HOH:O	2.58	0.44
1:F:54:GLN:NE2	1:F:121:GLU:O	2.41	0.44
1:I:149:ARG:HG3	2:I:452:HOH:O	2.17	0.44
1:H:166:CYS:SG	2:H:435:HOH:O	2.58	0.43
1:F:52:ASN:HB3	1:F:214:VAL:HG21	2.01	0.43
1:H:217:PHE:CZ	1:H:221:LEU:HD11	2.54	0.43
1:N:194:LYS:HG3	2:N:425:HOH:O	2.18	0.43
1:P:166:CYS:SG	2:P:376:HOH:O	2.62	0.43
1:G:61:ARG:HG3	2:G:310:HOH:O	2.19	0.43
1:E:66:LEU:HD11	1:E:129:ILE:HG13	2.01	0.43
1:O:166:CYS:SG	2:O:426:HOH:O	2.58	0.42
1:H:113:SER:O	1:H:117:GLN:HG3	2.19	0.42
1:K:89:PHE:HA	1:K:95:LEU:HD12	2.01	0.42
1:M:54:GLN:HG3	1:M:122:LEU:HD23	2.02	0.42
1:M:95:LEU:O	1:M:99:ARG:HG3	2.19	0.42
1:N:52:ASN:HB3	1:N:214:VAL:HG21	2.01	0.42
1:I:45:THR:HB	1:I:189:HIS:NE2	2.34	0.42
1:L:151:ARG:NE	2:L:305:HOH:O	2.50	0.42
1:L:198:LYS:HB3	1:L:198:LYS:HE3	1.73	0.42
1:G:149:ARG:CZ	1:I:149:ARG:HD3	2.50	0.41
1:H:2:THR:HG23	1:H:15:PRO:HD3	2.02	0.41
1:J:222:SER:OG	1:J:223:PRO:HD3	2.20	0.41
1:P:93:ASN:HA	1:P:96:LYS:HB2	2.02	0.41
1:C:15:PRO:O	1:C:65:MET:HG2	2.19	0.41
1:D:217:PHE:CZ	1:D:221:LEU:HD11	2.56	0.41
1:E:217:PHE:CZ	1:E:221:LEU:HD11	2.56	0.41
1:M:127:GLY:N	2:M:301:HOH:O	2.26	0.41
1:O:217:PHE:CZ	1:O:221:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ARG:HH11	1:E:61:ARG:HD2	1.66	0.41
1:D:129:ILE:HD12	1:D:147:ILE:HG21	2.03	0.41
1:J:100:LYS:HB2	1:J:100:LYS:HE2	1.79	0.41
1:K:70:PHE:CZ	1:K:144:LEU:HD22	2.56	0.41
1:M:43:VAL:O	1:M:43:VAL:HG12	2.21	0.41
1:N:95:LEU:O	1:N:99:ARG:HG3	2.21	0.41
1:F:35:TYR:OH	1:F:93:ASN:HB2	2.21	0.41
1:G:182:VAL:HA	1:G:210:TRP:O	2.21	0.40
1:H:194:LYS:HG3	2:H:407:HOH:O	2.21	0.40
1:B:157:VAL:HA	1:B:182:VAL:HG13	2.04	0.40
1:O:20:LEU:HD12	1:O:157:VAL:O	2.22	0.40
1:B:161:ILE:HA	1:B:162:ALA:HA	1.89	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:HOH:O	2:I:482:HOH:O[1_465]	1.94	0.26
2:J:456:HOH:O	2:N:437:HOH:O[1_545]	1.94	0.26
2:L:469:HOH:O	2:N:453:HOH:O[1_446]	1.96	0.24
2:F:441:HOH:O	2:H:309:HOH:O[1_655]	1.98	0.22
2:J:464:HOH:O	2:L:434:HOH:O[1_654]	1.98	0.22
1:K:149:ARG:NH1	1:O:177:LEU:O[1_554]	1.98	0.22
2:F:338:HOH:O	2:H:444:HOH:O[1_655]	1.99	0.21
2:F:429:HOH:O	2:H:467:HOH:O[1_655]	2.07	0.13
2:L:314:HOH:O	2:N:401:HOH:O[1_446]	2.09	0.11
2:C:306:HOH:O	2:G:439:HOH:O[1_565]	2.12	0.08
2:O:304:HOH:O	2:P:412:HOH:O[1_556]	2.12	0.08
2:J:464:HOH:O	2:L:415:HOH:O[1_654]	2.16	0.04
2:J:448:HOH:O	2:N:360:HOH:O[1_545]	2.17	0.03
2:C:489:HOH:O	2:I:497:HOH:O[1_465]	2.18	0.02
2:E:392:HOH:O	2:L:421:HOH:O[1_655]	2.18	0.02
2:J:343:HOH:O	2:L:435:HOH:O[1_654]	2.19	0.01

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	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	B	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	C	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	D	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	E	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	F	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	G	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	H	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	I	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	J	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	K	220/230 (96%)	218 (99%)	2 (1%)	0	100	100
1	L	220/230 (96%)	218 (99%)	2 (1%)	0	100	100
1	M	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	N	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	O	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	P	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
All	All	3520/3680 (96%)	3465 (98%)	55 (2%)	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	181/188 (96%)	178 (98%)	3 (2%)	60	38
1	B	181/188 (96%)	180 (99%)	1 (1%)	86	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	181/188 (96%)	179 (99%)	2 (1%)	73 57
1	D	181/188 (96%)	180 (99%)	1 (1%)	86 77
1	E	181/188 (96%)	180 (99%)	1 (1%)	86 77
1	F	181/188 (96%)	179 (99%)	2 (1%)	73 57
1	G	181/188 (96%)	180 (99%)	1 (1%)	86 77
1	H	181/188 (96%)	180 (99%)	1 (1%)	86 77
1	I	181/188 (96%)	179 (99%)	2 (1%)	73 57
1	J	181/188 (96%)	179 (99%)	2 (1%)	73 57
1	K	181/188 (96%)	179 (99%)	2 (1%)	73 57
1	L	181/188 (96%)	180 (99%)	1 (1%)	86 77
1	M	179/188 (95%)	176 (98%)	3 (2%)	60 38
1	N	180/188 (96%)	178 (99%)	2 (1%)	73 57
1	O	181/188 (96%)	179 (99%)	2 (1%)	73 57
1	P	181/188 (96%)	180 (99%)	1 (1%)	86 77
All	All	2893/3008 (96%)	2866 (99%)	27 (1%)	78 65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	A	76	GLU
1	A	95	LEU
1	B	35	TYR
1	C	35	TYR
1	C	100	LYS
1	D	35	TYR
1	E	35	TYR
1	F	35	TYR
1	F	103	GLN
1	G	35	TYR
1	H	35	TYR
1	I	35	TYR
1	I	45	THR
1	J	35	TYR
1	J	95	LEU
1	K	35	TYR
1	K	169	SER

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Mol	Chain	Res	Type
1	L	35	TYR
1	M	13	PHE
1	M	35	TYR
1	M	44	SER
1	N	35	TYR
1	N	194	LYS
1	O	13	PHE
1	O	35	TYR
1	P	35	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	D	125	GLN
1	F	155	HIS
1	I	16	GLN
1	K	125	GLN
1	L	155	HIS
1	M	16	GLN
1	N	101	GLN
1	O	189	HIS

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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, 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	222/230 (96%)	0.20	4 (1%) 68 67	12, 18, 27, 41	0
1	B	222/230 (96%)	0.27	3 (1%) 75 75	13, 20, 29, 49	0
1	C	222/230 (96%)	0.31	6 (2%) 54 52	12, 21, 33, 45	0
1	D	222/230 (96%)	0.22	2 (0%) 84 84	12, 19, 29, 42	0
1	E	222/230 (96%)	0.26	5 (2%) 60 59	13, 19, 27, 42	0
1	F	222/230 (96%)	0.60	15 (6%) 17 16	13, 23, 38, 53	0
1	G	222/230 (96%)	0.44	7 (3%) 47 44	12, 21, 33, 41	0
1	H	222/230 (96%)	0.25	2 (0%) 84 84	13, 20, 31, 56	0
1	I	222/230 (96%)	0.47	17 (7%) 13 11	13, 23, 37, 54	0
1	J	222/230 (96%)	0.36	8 (3%) 42 40	14, 22, 32, 48	0
1	K	222/230 (96%)	0.18	5 (2%) 60 59	15, 20, 30, 41	0
1	L	222/230 (96%)	0.64	19 (8%) 10 9	15, 25, 41, 57	0
1	M	222/230 (96%)	0.84	33 (14%) 2 1	15, 25, 44, 55	0
1	N	222/230 (96%)	0.64	23 (10%) 6 5	14, 24, 40, 49	0
1	O	222/230 (96%)	0.40	9 (4%) 37 34	16, 23, 34, 52	0
1	P	222/230 (96%)	0.74	23 (10%) 6 5	16, 27, 43, 57	0
All	All	3552/3680 (96%)	0.42	181 (5%) 28 26	12, 21, 36, 57	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	223	PRO	8.0
1	M	39	ALA	6.6
1	B	223	PRO	6.5
1	M	44	SER	5.6
1	P	43	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	M	100	LYS	5.0
1	M	102	PRO	4.7
1	P	103	GLN	4.6
1	F	103	GLN	4.6
1	M	32	PRO	4.5
1	P	222	SER	4.5
1	M	43	VAL	4.5
1	L	223	PRO	4.5
1	I	223	PRO	4.4
1	P	223	PRO	4.3
1	P	44	SER	4.3
1	L	103	GLN	4.3
1	I	103	GLN	4.2
1	N	43	VAL	4.2
1	N	100	LYS	4.2
1	L	126	PRO	4.1
1	M	126	PRO	4.1
1	J	223	PRO	4.1
1	J	44	SER	4.1
1	F	32	PRO	4.0
1	L	39	ALA	4.0
1	N	102	PRO	3.9
1	F	39	ALA	3.9
1	F	223	PRO	3.9
1	P	102	PRO	3.9
1	P	104	LEU	3.9
1	E	222	SER	3.9
1	L	102	PRO	3.8
1	F	2	THR	3.7
1	A	2	THR	3.6
1	N	58	THR	3.6
1	M	28	ALA	3.6
1	O	223	PRO	3.6
1	N	46	THR	3.6
1	L	43	VAL	3.5
1	M	103	GLN	3.5
1	D	11	ILE	3.5
1	M	114	TRP	3.4
1	I	31	THR	3.4
1	L	58	THR	3.4
1	M	35	TYR	3.4
1	E	43	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	100	LYS	3.4
1	M	106	GLY	3.4
1	M	104	LEU	3.3
1	M	42	ASP	3.3
1	E	2	THR	3.2
1	N	45	THR	3.2
1	O	219	ASP	3.2
1	K	2	THR	3.2
1	M	38	LEU	3.2
1	M	41	PHE	3.2
1	I	125	GLN	3.2
1	O	43	VAL	3.2
1	P	221	LEU	3.1
1	M	58	THR	3.1
1	L	221	LEU	3.1
1	L	222	SER	3.1
1	L	100	LYS	3.1
1	N	44	SER	3.1
1	P	45	THR	3.0
1	P	101	GLN	3.0
1	I	32	PRO	3.0
1	F	222	SER	3.0
1	N	106	GLY	2.9
1	F	44	SER	2.9
1	M	76	GLU	2.9
1	N	101	GLN	2.9
1	L	219	ASP	2.9
1	N	35	TYR	2.8
1	N	38	LEU	2.8
1	O	44	SER	2.8
1	L	104	LEU	2.8
1	M	40	GLY	2.8
1	P	40	GLY	2.8
1	A	43	VAL	2.8
1	D	222	SER	2.8
1	M	101	GLN	2.8
1	G	100	LYS	2.7
1	P	31	THR	2.7
1	G	148	LEU	2.7
1	L	125	GLN	2.7
1	I	34	GLY	2.7
1	C	32	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	126	PRO	2.7
1	M	33	GLY	2.7
1	N	76	GLU	2.7
1	M	46	THR	2.6
1	H	2	THR	2.6
1	F	102	PRO	2.6
1	P	107	LYS	2.6
1	F	37	ASP	2.6
1	O	165	VAL	2.6
1	I	44	SER	2.6
1	P	32	PRO	2.6
1	P	34	GLY	2.5
1	I	2	THR	2.5
1	M	45	THR	2.5
1	J	62	ALA	2.5
1	F	34	GLY	2.5
1	L	31	THR	2.5
1	M	105	GLN	2.5
1	P	125	GLN	2.5
1	I	45	THR	2.5
1	A	222	SER	2.4
1	C	102	PRO	2.4
1	E	223	PRO	2.4
1	B	58	THR	2.4
1	F	107	LYS	2.4
1	G	32	PRO	2.4
1	M	108	LEU	2.4
1	J	43	VAL	2.4
1	N	108	LEU	2.4
1	P	39	ALA	2.4
1	P	2	THR	2.4
1	N	42	ASP	2.4
1	M	61	ARG	2.3
1	F	101	GLN	2.3
1	M	36	LEU	2.3
1	F	31	THR	2.3
1	K	126	PRO	2.3
1	N	32	PRO	2.3
1	K	165	VAL	2.3
1	L	2	THR	2.3
1	I	107	LYS	2.3
1	I	222	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	43	VAL	2.3
1	P	64	GLY	2.3
1	L	32	PRO	2.3
1	G	76	GLU	2.3
1	I	43	VAL	2.3
1	N	110	ALA	2.2
1	J	45	THR	2.2
1	G	102	PRO	2.2
1	M	57	VAL	2.2
1	N	30	ALA	2.2
1	N	62	ALA	2.2
1	C	34	GLY	2.2
1	C	126	PRO	2.2
1	O	21	ILE	2.2
1	P	38	LEU	2.2
1	I	100	LYS	2.2
1	I	58	THR	2.2
1	M	125	GLN	2.2
1	C	76	GLU	2.2
1	J	165	VAL	2.2
1	M	37	ASP	2.2
1	J	126	PRO	2.2
1	N	39	ALA	2.1
1	O	58	THR	2.1
1	P	58	THR	2.1
1	F	38	LEU	2.1
1	O	161	ILE	2.1
1	K	222	SER	2.1
1	N	33	GLY	2.1
1	N	40	GLY	2.1
1	L	30	ALA	2.1
1	J	124	PRO	2.1
1	E	140	PHE	2.1
1	G	2	THR	2.1
1	N	31	THR	2.1
1	N	61	ARG	2.1
1	L	59	ALA	2.1
1	M	30	ALA	2.1
1	P	76	GLU	2.1
1	I	221	LEU	2.1
1	L	51	ALA	2.1
1	B	2	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	16	GLN	2.0
1	A	126	PRO	2.0
1	M	62	ALA	2.0
1	I	120	ASP	2.0
1	F	40	GLY	2.0
1	G	101	GLN	2.0
1	C	58	THR	2.0
1	I	126	PRO	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.