



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 08:01 AM UTC

PDB ID : 8BYW / pdb_00008byw
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	:	4-5-2 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

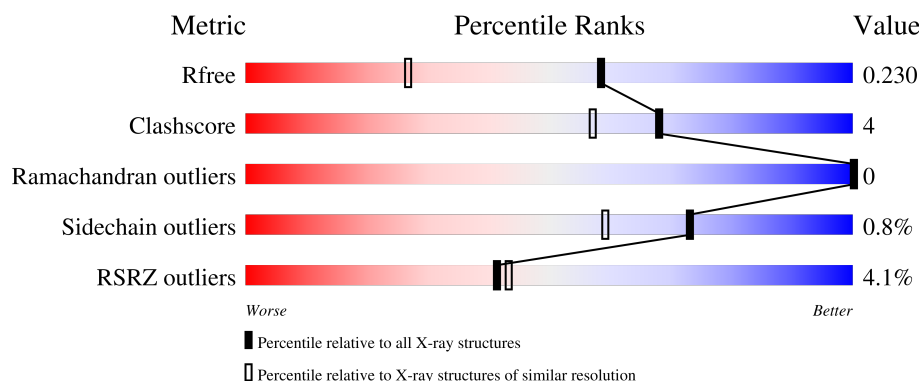
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

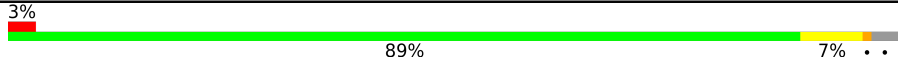
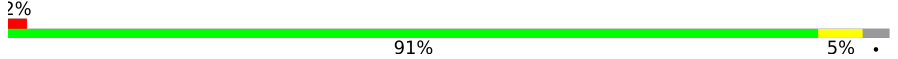
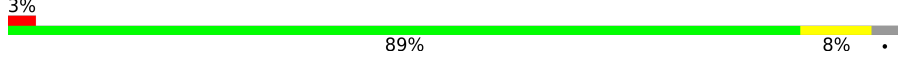
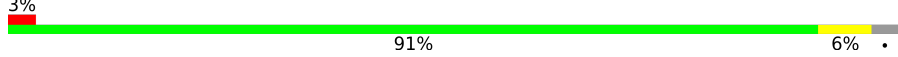
The reported resolution of this entry is 1.59 Å.

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.



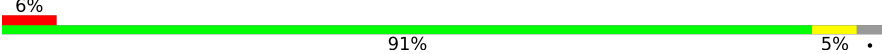
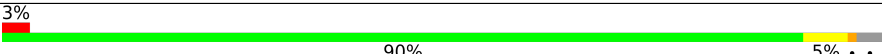
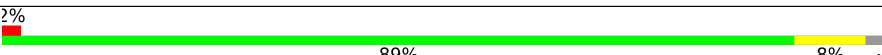
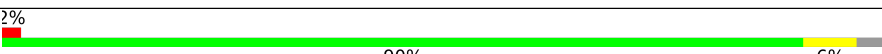
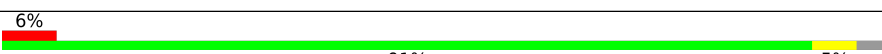
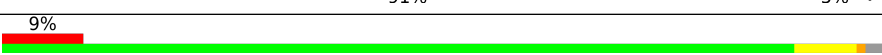
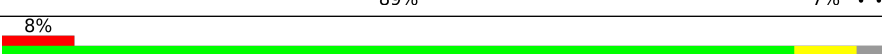
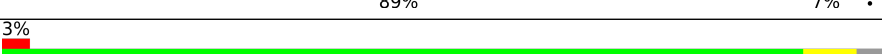
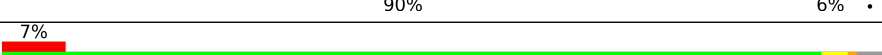
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

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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

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			

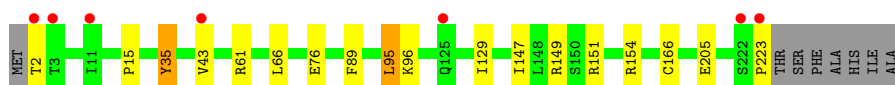
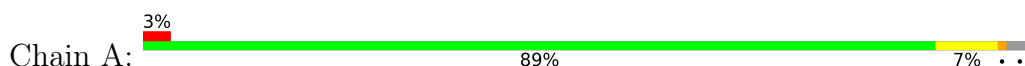
- Molecule 2 is water.

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

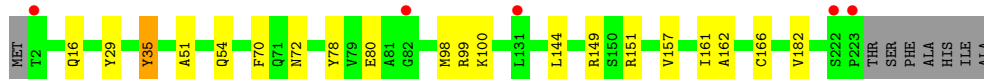
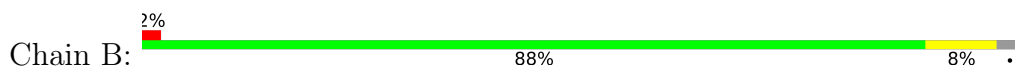
3 Residue-property plots [i](#)

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



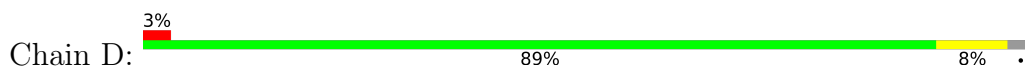
- Molecule 1: Ureidoacrylate amidohydrolase RutB



- Molecule 1: Ureidoacrylate amidohydrolase RutB



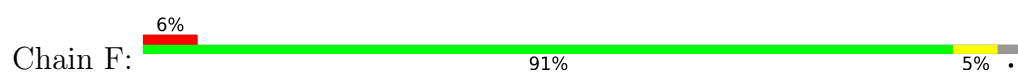
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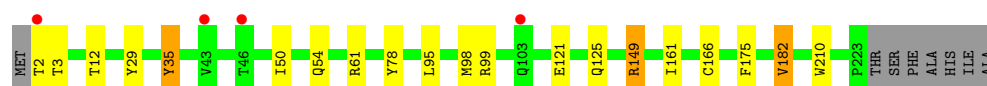
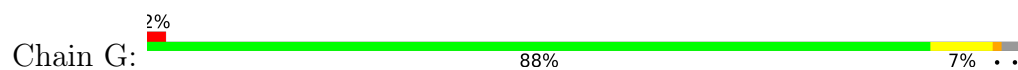
- Molecule 1: Ureidoacrylate amidohydrolase RutB



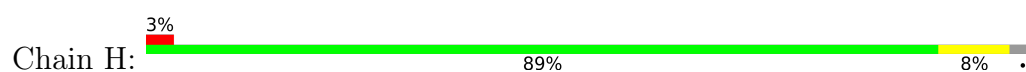
- Molecule 1: Ureidoacrylate amidohydrolase RutB



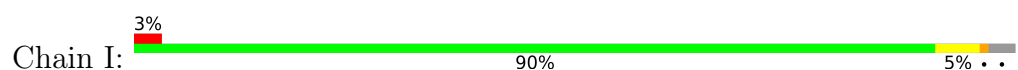
• Molecule 1: Ureidoacrylate amidohydrolase RutB



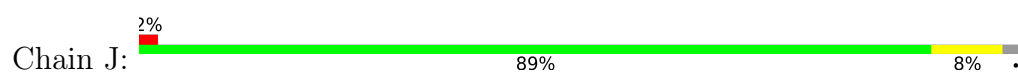
• Molecule 1: Ureidoacrylate amidohydrolase RutB



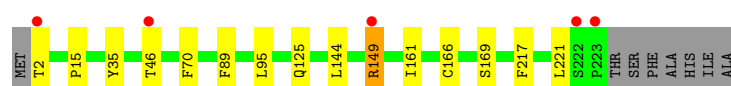
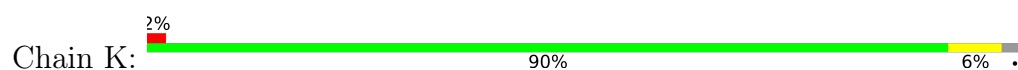
• Molecule 1: Ureidoacrylate amidohydrolase RutB



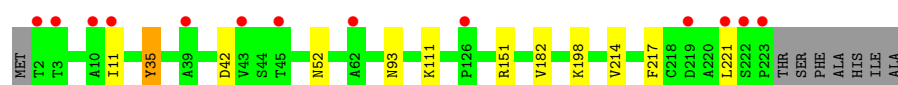
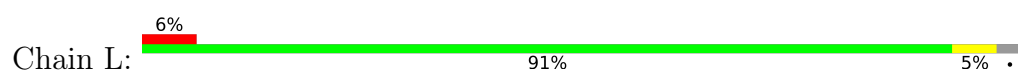
• Molecule 1: Ureidoacrylate amidohydrolase RutB



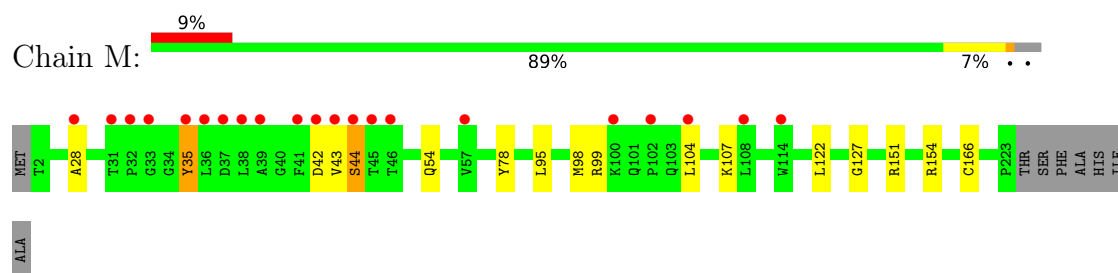
• Molecule 1: Ureidoacrylate amidohydrolase RutB



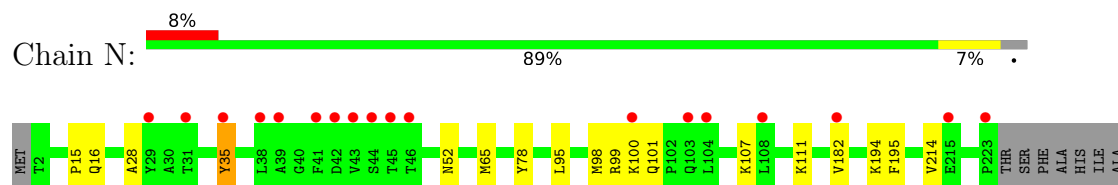
• Molecule 1: Ureidoacrylate amidohydrolase RutB



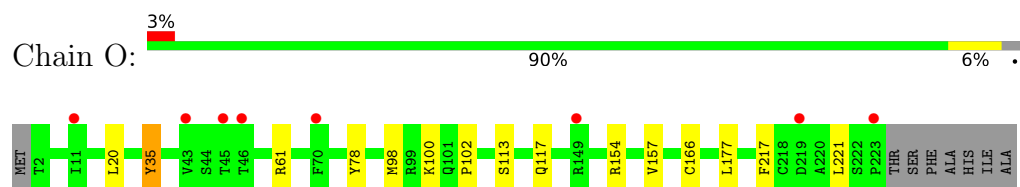
- Molecule 1: Ureidoacrylate amidohydrolase RutB



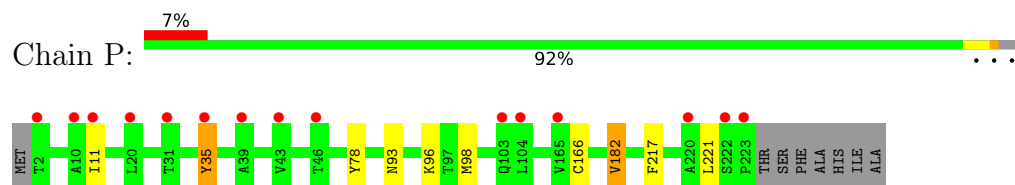
- Molecule 1: Ureidoacrylate amidohydrolase RutB



- Molecule 1: Ureidoacrylate amidohydrolase RutB



- Molecule 1: Ureidoacrylate amidohydrolase RutB



4 Data and refinement statistics

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 48.71 – 1.59	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.71-1.59) 93.0 (48.71-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.18rc2	Depositor
R, R_{free}	0.206 , 0.233 0.205 , 0.230	Depositor DCC
R_{free} test set	22459 reflections (4.80%)	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)	0.39 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

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

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	0.33	0/1760	0.55	0/2401
1	B	0.31	0/1760	0.52	0/2401
1	C	0.31	0/1760	0.52	0/2401
1	D	0.34	0/1760	0.55	0/2401
1	E	0.32	0/1760	0.53	0/2401
1	F	0.29	0/1760	0.52	1/2401 (0.0%)
1	G	0.31	0/1760	0.55	1/2401 (0.0%)
1	H	0.30	0/1760	0.51	0/2401
1	I	0.30	0/1760	0.51	0/2401
1	J	0.29	0/1760	0.52	0/2401
1	K	0.33	0/1760	0.53	1/2401 (0.0%)
1	L	0.28	0/1760	0.50	0/2401
1	M	0.27	0/1753	0.49	0/2392
1	N	0.29	0/1756	0.50	0/2396
1	O	0.32	0/1760	0.53	0/2401
1	P	0.25	0/1760	0.48	0/2401
All	All	0.30	0/28149	0.52	3/38402 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	K	149	ARG	CB-CG-CD	-6.75	95.78	111.30
1	F	3	THR	CB-CA-C	5.97	119.60	109.75

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	1715	0	1675	17	0
1	B	1715	0	1675	15	0
1	C	1715	0	1675	10	0
1	D	1715	0	1675	19	0
1	E	1715	0	1675	12	0
1	F	1715	0	1675	10	0
1	G	1715	0	1675	19	0
1	H	1715	0	1675	16	0
1	I	1715	0	1675	13	0
1	J	1715	0	1675	14	0
1	K	1715	0	1675	11	1
1	L	1715	0	1675	10	0
1	M	1708	0	1669	12	0
1	N	1711	0	1671	10	0
1	O	1715	0	1675	11	1
1	P	1715	0	1675	7	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	4	6
2	M	158	0	0	4	0
2	N	153	0	0	3	4
2	O	179	0	0	5	1
2	P	142	0	0	1	1
All	All	30533	0	26790	196	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 4.

All (196) 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:N:107:LYS:NZ	2:N:302:HOH:O	2.18	0.77
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:100:LYS:NZ	2:D:301:HOH:O	2.07	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:D:87:PRO:C	2:D:305:HOH:O	2.52	0.52
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:L:111:LYS:NZ	2:L:307:HOH:O	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:103:GLN:H	1:C:103:GLN:CD	2.19	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:N:78:TYR:CZ	1:N:98:MET:HE1	2.47	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: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:G:78:TYR:CZ	1:G:98:MET:HE1	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:100:LYS:NZ	2:O:309:HOH:O	2.45	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:H:78:TYR:CZ	1:H:98:MET:HE1	2.50	0.45
1:B:78:TYR:CZ	1:B:98:MET:HE1	2.51	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:M:78:TYR:CZ	1:M:98:MET:HE1	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:O:78:TYR:CZ	1:O:98:MET:HE1	2.53	0.44
1:I:35:TYR:CD1	1:I:35:TYR:C	2.96	0.43
1:D:35:TYR:CD1	1:D:35:TYR:C	2.96	0.43
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:P:78:TYR:CZ	1:P:98:MET:HE1	2.54	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:F:78:TYR:CZ	1:F:98:MET:HE1	2.55	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:A:35:TYR:CD1	1:A:35:TYR:C	2.98	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:P:35:TYR:CD1	1:P:35:TYR:C	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:111:LYS:NZ	2:N:308:HOH:O	2.44	0.42
1:O:35:TYR:CD1	1:O:35:TYR:C	2.97	0.42
1:B:35:TYR:CD1	1:B:35:TYR:C	2.98	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:K:35:TYR:CD1	1:K:35:TYR:C	2.98	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:J:35:TYR:CD1	1:J:35:TYR:C	2.98	0.41
1:C:35:TYR:CD1	1:C:35:TYR:C	2.98	0.41
1:J:78:TYR:CZ	1:J:98:MET:HE1	2.55	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
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:E:35:TYR:CD1	1:E:35:TYR:C	2.97	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:L:35:TYR:CD1	1:L:35:TYR:C	2.99	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
1:G:35:TYR:CD1	1:G:35:TYR:C	2.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	179 (99%)	2 (1%)	65	46
1	B	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	C	181/188 (96%)	179 (99%)	2 (1%)	65	46
1	D	181/188 (96%)	181 (100%)	0	100	100
1	E	181/188 (96%)	181 (100%)	0	100	100
1	F	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	G	181/188 (96%)	179 (99%)	2 (1%)	65	46
1	H	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	I	181/188 (96%)	178 (98%)	3 (2%)	53	30
1	J	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	K	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	L	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	M	179/188 (95%)	177 (99%)	2 (1%)	65	46
1	N	180/188 (96%)	177 (98%)	3 (2%)	53	30
1	O	181/188 (96%)	180 (99%)	1 (1%)	78	66
1	P	181/188 (96%)	179 (99%)	2 (1%)	65	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2893/3008 (96%)	2870 (99%)	23 (1%)	73 59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	A	95	LEU
1	B	35	TYR
1	C	35	TYR
1	C	182	VAL
1	F	35	TYR
1	G	35	TYR
1	G	182	VAL
1	H	35	TYR
1	I	35	TYR
1	I	45	THR
1	I	149	ARG
1	J	95	LEU
1	K	169	SER
1	L	35	TYR
1	M	35	TYR
1	M	44	SER
1	N	16	GLN
1	N	35	TYR
1	N	182	VAL
1	O	35	TYR
1	P	35	TYR
1	P	182	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	54	GLN
1	B	72	ASN
1	D	17	GLN
1	D	125	GLN
1	G	54	GLN
1	H	71	GLN
1	H	189	HIS
1	I	16	GLN

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Mol	Chain	Res	Type
1	J	54	GLN
1	K	125	GLN
1	M	16	GLN
1	M	72	ASN
1	M	93	ASN
1	M	141	ASN
1	N	72	ASN
1	N	101	GLN
1	O	17	GLN
1	O	72	ASN
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 oligosaccharides 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, 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	222/230 (96%)	0.25	7 (3%) 50 53	12, 18, 27, 41	0
1	B	222/230 (96%)	0.44	5 (2%) 61 64	13, 20, 29, 49	0
1	C	222/230 (96%)	0.46	4 (1%) 67 71	12, 21, 33, 45	0
1	D	222/230 (96%)	0.32	6 (2%) 56 59	12, 19, 29, 42	0
1	E	222/230 (96%)	0.27	6 (2%) 56 59	13, 19, 27, 42	0
1	F	222/230 (96%)	0.63	14 (6%) 26 26	13, 23, 38, 53	0
1	G	222/230 (96%)	0.49	4 (1%) 67 71	12, 21, 33, 41	0
1	H	222/230 (96%)	0.46	6 (2%) 56 59	13, 20, 31, 56	0
1	I	222/230 (96%)	0.62	8 (3%) 46 48	13, 23, 37, 54	0
1	J	222/230 (96%)	0.61	4 (1%) 67 71	14, 22, 32, 48	0
1	K	222/230 (96%)	0.36	5 (2%) 61 64	15, 20, 30, 41	0
1	L	222/230 (96%)	0.67	13 (5%) 28 29	15, 25, 41, 57	0
1	M	222/230 (96%)	0.87	21 (9%) 14 14	15, 25, 44, 55	0
1	N	222/230 (96%)	0.72	18 (8%) 18 18	14, 24, 40, 49	0
1	O	222/230 (96%)	0.71	8 (3%) 46 48	16, 23, 34, 52	0
1	P	222/230 (96%)	0.83	15 (6%) 23 24	16, 27, 43, 57	0
All	All	3552/3680 (96%)	0.54	144 (4%) 41 43	12, 21, 36, 57	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	PRO	6.4
1	O	223	PRO	5.7
1	H	223	PRO	5.6
1	F	223	PRO	4.8
1	M	43	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	2	THR	4.5
1	I	223	PRO	4.5
1	P	223	PRO	4.2
1	A	2	THR	4.1
1	J	223	PRO	4.1
1	E	2	THR	4.0
1	N	43	VAL	3.9
1	I	2	THR	3.9
1	L	11	ILE	3.7
1	G	2	THR	3.7
1	H	2	THR	3.7
1	M	39	ALA	3.7
1	K	2	THR	3.6
1	L	223	PRO	3.6
1	K	46	THR	3.6
1	L	2	THR	3.6
1	E	223	PRO	3.5
1	O	219	ASP	3.4
1	A	223	PRO	3.4
1	M	35	TYR	3.4
1	P	43	VAL	3.3
1	N	46	THR	3.3
1	P	222	SER	3.3
1	P	11	ILE	3.2
1	D	223	PRO	3.2
1	L	43	VAL	3.2
1	M	41	PHE	3.2
1	I	11	ILE	3.2
1	E	222	SER	3.2
1	M	38	LEU	3.1
1	I	222	SER	3.0
1	D	11	ILE	3.0
1	F	222	SER	3.0
1	O	43	VAL	3.0
1	M	104	LEU	2.9
1	L	221	LEU	2.9
1	C	103	GLN	2.9
1	K	222	SER	2.9
1	P	10	ALA	2.8
1	J	46	THR	2.8
1	P	2	THR	2.8
1	N	104	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	2.7
1	K	223	PRO	2.7
1	L	222	SER	2.7
1	D	70	PHE	2.7
1	D	222	SER	2.7
1	M	44	SER	2.7
1	C	43	VAL	2.7
1	O	149	ARG	2.6
1	N	215	GLU	2.6
1	M	36	LEU	2.6
1	N	45	THR	2.6
1	K	149	ARG	2.6
1	F	215	GLU	2.6
1	I	221	LEU	2.6
1	E	43	VAL	2.6
1	M	102	PRO	2.6
1	B	222	SER	2.6
1	F	39	ALA	2.5
1	M	114	TRP	2.5
1	M	33	GLY	2.5
1	F	43	VAL	2.5
1	F	63	ALA	2.5
1	N	35	TYR	2.5
1	N	223	PRO	2.5
1	I	43	VAL	2.5
1	O	46	THR	2.5
1	B	131	LEU	2.5
1	F	221	LEU	2.5
1	P	104	LEU	2.5
1	B	2	THR	2.5
1	D	43	VAL	2.5
1	I	45	THR	2.4
1	P	165	VAL	2.4
1	J	222	SER	2.4
1	P	39	ALA	2.4
1	P	103	GLN	2.4
1	C	34	GLY	2.4
1	L	126	PRO	2.4
1	F	44	SER	2.4
1	G	43	VAL	2.4
1	M	42	ASP	2.4
1	H	11	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	38	LEU	2.4
1	N	41	PHE	2.4
1	O	70	PHE	2.4
1	N	39	ALA	2.3
1	M	32	PRO	2.3
1	F	46	THR	2.3
1	M	45	THR	2.3
1	F	11	ILE	2.3
1	O	11	ILE	2.3
1	N	108	LEU	2.3
1	P	20	LEU	2.3
1	D	2	THR	2.3
1	G	103	GLN	2.3
1	L	62	ALA	2.3
1	H	70	PHE	2.3
1	A	125	GLN	2.3
1	N	100	LYS	2.3
1	A	11	ILE	2.3
1	P	35	TYR	2.3
1	P	46	THR	2.2
1	L	219	ASP	2.2
1	G	46	THR	2.2
1	M	31	THR	2.2
1	C	35	TYR	2.2
1	E	16	GLN	2.2
1	L	10	ALA	2.1
1	M	28	ALA	2.1
1	A	222	SER	2.1
1	N	182	VAL	2.1
1	H	222	SER	2.1
1	F	60	ALA	2.1
1	N	31	THR	2.1
1	N	42	ASP	2.1
1	J	194	LYS	2.1
1	M	37	ASP	2.1
1	A	3	THR	2.1
1	F	220	ALA	2.1
1	M	46	THR	2.1
1	O	45	THR	2.1
1	M	108	LEU	2.1
1	M	100	LYS	2.1
1	L	3	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	45	THR	2.0
1	L	39	ALA	2.0
1	F	36	LEU	2.0
1	N	29	TYR	2.0
1	N	44	SER	2.0
1	B	82	GLY	2.0
1	I	3	THR	2.0
1	P	31	THR	2.0
1	N	103	GLN	2.0
1	P	220	ALA	2.0
1	E	70	PHE	2.0
1	H	13	PHE	2.0
1	M	57	VAL	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.