



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:08 AM UTC

PDB ID : 8BLN / pdb_00008bln
Title : Structure of RutB
Authors : Rajendran, C.
Deposited on : 2022-11-09
Resolution : 1.88 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

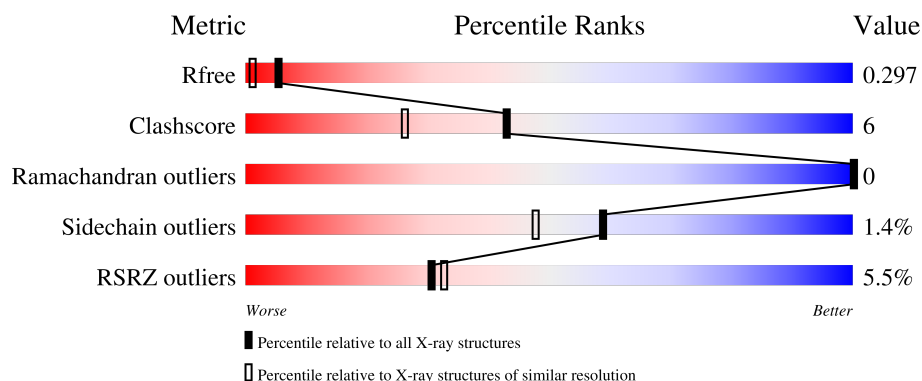
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	% 87% 10% .
1	B	230	4% 83% 13% .
1	C	230	17% 80% 15% . .
1	D	230	% 81% 14% .
1	E	230	% 83% 13% . .

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Mol	Chain	Length	Quality of chain
1	F	230	 2% 78% 18% •
1	G	230	 14% 83% 13% ••
1	H	230	 2% 85% 11% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14553 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	286	320	5			
1	B	222	Total	C	N	O	S	0	0	0
			1715	1104	286	320	5			
1	C	221	Total	C	N	O	S	0	0	0
			1705	1098	285	317	5			
1	D	221	Total	C	N	O	S	0	0	0
			1704	1097	285	317	5			
1	E	221	Total	C	N	O	S	0	0	0
			1708	1099	285	319	5			
1	F	220	Total	C	N	O	S	0	0	0
			1702	1096	284	317	5			
1	G	222	Total	C	N	O	S	0	0	0
			1690	1089	279	318	4			
1	H	222	Total	C	N	O	S	0	0	0
			1715	1104	286	320	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ASN	ASP	conflict	UNP C9QZ65
B	24	ASN	ASP	conflict	UNP C9QZ65
C	24	ASN	ASP	conflict	UNP C9QZ65
D	24	ASN	ASP	conflict	UNP C9QZ65
E	24	ASN	ASP	conflict	UNP C9QZ65
F	24	ASN	ASP	conflict	UNP C9QZ65
G	24	ASN	ASP	conflict	UNP C9QZ65
H	24	ASN	ASP	conflict	UNP C9QZ65

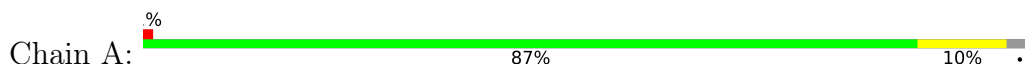
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total 106	O 106	0	0
2	B	93	Total 93	O 93	0	0
2	C	83	Total 83	O 83	0	0
2	D	149	Total 149	O 149	0	0
2	E	139	Total 139	O 139	0	0
2	F	137	Total 137	O 137	0	0
2	G	77	Total 77	O 77	0	0
2	H	115	Total 115	O 115	0	0

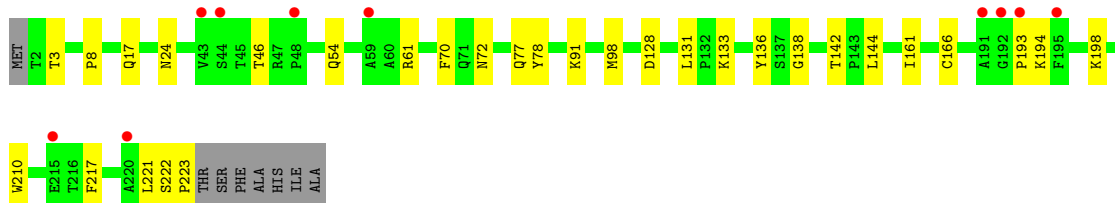
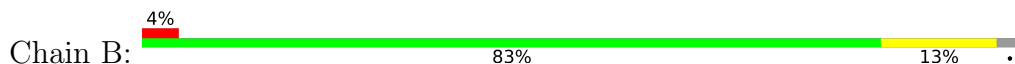
3 Residue-property plots [i](#)

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.

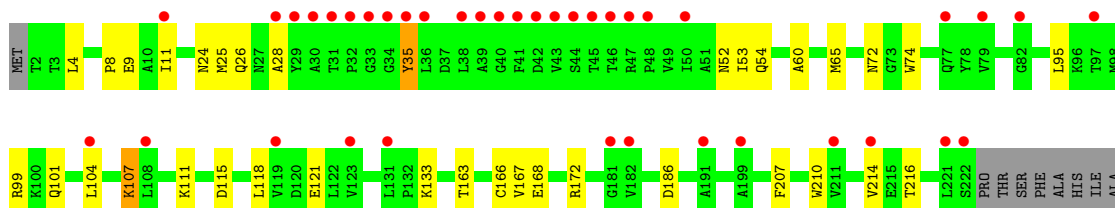
- Molecule 1: Ureidoacrylate amidohydrolase RutB



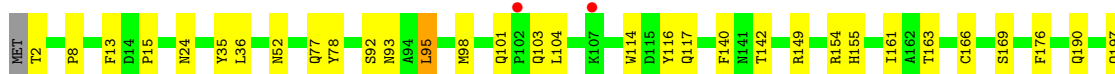
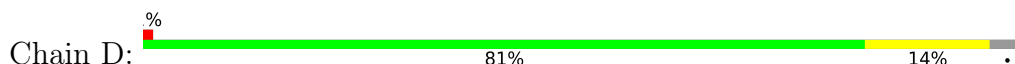
- Molecule 1: Ureidoacrylate amidohydrolase RutB

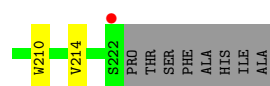


- Molecule 1: Ureidoacrylate amidohydrolase RutB

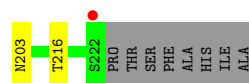
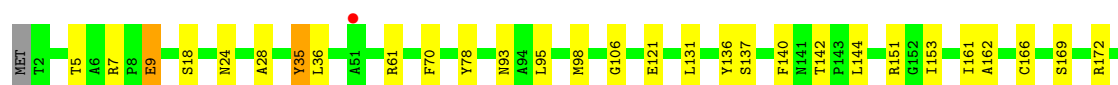
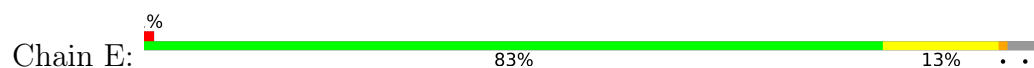


- Molecule 1: Ureidoacrylate amidohydrolase RutB

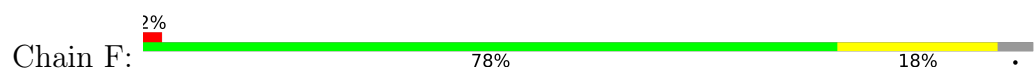




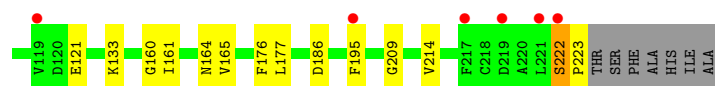
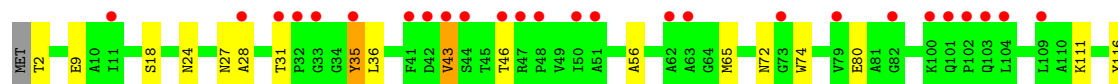
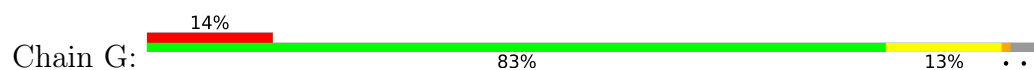
• Molecule 1: Ureidoacrylate amidohydrolase RutB



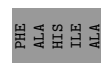
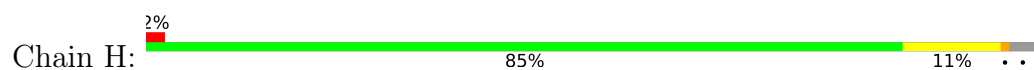
• Molecule 1: Ureidoacrylate amidohydrolase RutB



• Molecule 1: Ureidoacrylate amidohydrolase RutB



• Molecule 1: Ureidoacrylate amidohydrolase RutB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.12Å 125.11Å 123.27Å 90.00° 93.22° 90.00°	Depositor
Resolution (Å)	41.00 – 1.88 41.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.00-1.88) 97.3 (41.00-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.18rc2_3793, PHENIX 1.18rc2_3793	Depositor
R, R_{free}	0.250 , 0.296 0.251 , 0.297	Depositor DCC
R_{free} test set	6979 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14553	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 45.74 % 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 1.2663e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/1760	0.57	0/2401
1	B	0.34	0/1760	0.56	0/2401
1	C	0.29	0/1749	0.48	0/2385
1	D	0.33	0/1748	0.55	0/2384
1	E	0.33	0/1752	0.53	0/2389
1	F	0.33	0/1746	0.54	0/2381
1	G	0.31	0/1735	0.51	1/2373 (0.0%)
1	H	0.35	0/1760	0.56	0/2401
All	All	0.33	0/14010	0.54	1/19115 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	160	GLY	N-CA-C	5.02	118.10	111.52

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	1677	15	1
1	B	1715	0	1677	19	0
1	C	1705	0	1668	23	0
1	D	1704	0	1666	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1708	0	1670	25	0
1	F	1702	0	1665	27	1
1	G	1690	0	1625	23	1
1	H	1715	0	1677	17	0
2	A	106	0	0	6	0
2	B	93	0	0	7	1
2	C	83	0	0	3	0
2	D	149	0	0	7	2
2	E	139	0	0	7	1
2	F	137	0	0	4	0
2	G	77	0	0	4	1
2	H	115	0	0	6	0
All	All	14553	0	13325	167	5

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 (167) 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:F:25:MET:HE3	1:F:160:GLY:HA2	1.53	0.90
1:D:149:ARG:NH2	2:D:301:HOH:O	2.12	0.81
1:F:70:PHE:HE2	1:F:131:LEU:HD23	1.46	0.80
1:F:25:MET:HE1	1:F:161:ILE:HD12	1.64	0.79
1:E:151:ARG:NH1	2:E:301:HOH:O	2.15	0.79
1:B:194:LYS:NZ	2:B:302:HOH:O	2.15	0.78
1:C:52:ASN:HB3	1:C:214:VAL:HG21	1.66	0.77
1:A:145:ASP:OD2	2:A:301:HOH:O	2.06	0.74
1:B:17:GLN:O	2:B:301:HOH:O	2.07	0.72
1:A:149:ARG:NH1	2:A:305:HOH:O	2.24	0.70
1:D:114:TRP:HA	1:D:117:GLN:HG3	1.77	0.66
1:G:121:GLU:N	1:G:121:GLU:OE1	2.28	0.66
1:G:2:THR:N	2:G:304:HOH:O	2.29	0.65
1:H:189:HIS:N	2:H:301:HOH:O	2.17	0.65
1:E:137:SER:HB2	1:E:169:SER:HB3	1.79	0.65
1:D:103:GLN:HG2	1:D:104:LEU:HD12	1.79	0.64
1:D:154:ARG:NH1	2:D:305:HOH:O	2.26	0.64
1:A:123:VAL:N	2:A:306:HOH:O	2.25	0.64
1:F:54:GLN:O	2:F:301:HOH:O	2.14	0.64
1:F:161:ILE:HG12	1:F:189:HIS:HB3	1.80	0.63
1:E:9:GLU:OE1	2:E:302:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ASP:O	1:F:149:ARG:HG3	2.00	0.62
1:H:78:TYR:CZ	1:H:98:MET:HE1	2.35	0.61
1:G:80:GLU:OE2	2:G:302:HOH:O	2.16	0.61
1:F:52:ASN:HB3	1:F:214:VAL:HG21	1.82	0.60
1:A:222:SER:O	2:A:303:HOH:O	2.17	0.60
1:D:77:GLN:O	2:D:302:HOH:O	2.16	0.60
1:E:106:GLY:O	2:E:303:HOH:O	2.16	0.59
1:F:154:ARG:NH1	2:F:309:HOH:O	2.35	0.59
1:A:70:PHE:CE2	1:A:131:LEU:HD23	2.37	0.59
1:C:24:ASN:HD21	1:C:133:LYS:HE3	1.69	0.57
1:A:96:LYS:O	1:A:100:LYS:HG3	2.04	0.56
1:C:207:PHE:O	1:F:136:TYR:OH	2.19	0.56
1:F:24:ASN:HB2	1:F:161:ILE:O	2.05	0.56
1:E:70:PHE:HE1	1:E:131:LEU:HD23	1.71	0.56
1:G:27:ASN:OD1	1:G:31:THR:HG21	2.05	0.56
1:G:27:ASN:HA	1:G:31:THR:HG23	1.87	0.55
1:D:101:GLN:HB2	1:D:104:LEU:HD13	1.88	0.55
1:F:103:GLN:NE2	2:F:313:HOH:O	2.39	0.55
1:B:61:ARG:NH2	1:B:128:ASP:OD2	2.36	0.54
1:A:70:PHE:HZ	1:A:144:LEU:HD22	1.72	0.54
1:D:92:SER:HB3	1:D:95:LEU:HD22	1.88	0.54
1:F:140:PHE:O	1:F:142:THR:HG23	2.08	0.54
1:E:70:PHE:HZ	1:E:144:LEU:HD22	1.71	0.53
1:G:28:ALA:HB1	1:G:35:TYR:HB3	1.90	0.53
1:D:2:THR:HG23	1:D:15:PRO:HD3	1.90	0.53
1:B:193:PRO:HA	2:B:304:HOH:O	2.08	0.53
1:C:28:ALA:HB1	1:C:35:TYR:HB3	1.91	0.53
1:H:188:THR:HB	2:H:301:HOH:O	2.09	0.53
1:A:149:ARG:CZ	2:A:301:HOH:O	2.56	0.52
1:F:3:THR:OG1	1:F:12:THR:HG22	2.10	0.52
1:A:166:CYS:SG	2:A:389:HOH:O	2.34	0.52
1:B:24:ASN:HB2	1:B:161:ILE:O	2.10	0.52
1:F:198:LYS:O	1:F:198:LYS:HD3	2.10	0.52
1:F:93:ASN:OD1	2:F:303:HOH:O	2.19	0.52
1:H:70:PHE:HZ	1:H:144:LEU:HD22	1.75	0.52
1:B:222:SER:HB3	1:B:223:PRO:HD3	1.92	0.52
1:F:26:GLN:HA	1:F:118:LEU:HA	1.92	0.51
1:D:8:PRO:HD2	1:D:210:TRP:CD1	2.45	0.51
1:D:24:ASN:HB2	1:D:161:ILE:O	2.10	0.51
1:C:72:ASN:OD1	1:C:133:LYS:NZ	2.39	0.51
1:D:78:TYR:CZ	1:D:98:MET:HE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLN:HB2	1:C:104:LEU:HD12	1.93	0.50
1:B:166:CYS:SG	2:B:354:HOH:O	2.51	0.50
1:D:101:GLN:NE2	2:D:312:HOH:O	2.43	0.50
1:A:193:PRO:HG2	1:A:195:PHE:CE2	2.47	0.50
1:F:164:ASN:OD1	1:F:164:ASN:N	2.40	0.50
1:B:46:THR:N	2:B:307:HOH:O	2.43	0.49
1:G:31:THR:HG22	2:G:364:HOH:O	2.12	0.49
1:F:113:SER:O	1:F:117:GLN:HG3	2.12	0.49
1:E:70:PHE:CE1	1:E:131:LEU:HD23	2.46	0.49
1:G:186:ASP:OD1	1:G:214:VAL:HG23	2.12	0.49
1:B:46:THR:HG23	2:B:319:HOH:O	2.12	0.49
1:C:107:LYS:NZ	1:C:115:ASP:H	2.10	0.49
1:C:9:GLU:OE2	1:C:210:TRP:NE1	2.34	0.49
1:G:165:VAL:HB	2:G:321:HOH:O	2.12	0.49
1:A:78:TYR:CZ	1:A:98:MET:HE1	2.48	0.48
1:D:176:PHE:CE1	1:E:136:TYR:HB2	2.48	0.48
1:D:176:PHE:HE1	1:E:136:TYR:HB2	1.78	0.47
1:E:203:ASN:OD1	2:E:304:HOH:O	2.20	0.47
1:D:116:TYR:OH	2:D:303:HOH:O	2.18	0.47
1:H:90:HIS:O	1:H:96:LYS:HE3	2.15	0.47
1:H:117:GLN:HG2	1:H:118:LEU:O	2.15	0.47
1:D:169:SER:OG	1:E:172:ARG:NH1	2.48	0.47
1:E:166:CYS:SG	2:E:388:HOH:O	2.39	0.47
1:C:74:TRP:N	2:C:313:HOH:O	2.47	0.46
1:B:77:GLN:HG2	2:B:363:HOH:O	2.15	0.46
1:B:91:LYS:NZ	1:G:209:GLY:O	2.38	0.45
1:H:153:ILE:HD11	2:H:403:HOH:O	2.16	0.45
1:H:145:ASP:CG	1:H:149:ARG:HE	2.24	0.45
1:D:13:PHE:HB3	1:D:155:HIS:CD2	2.52	0.45
1:E:35:TYR:OH	1:E:93:ASN:HB2	2.15	0.45
1:F:163:THR:HA	1:F:167:VAL:HB	1.98	0.45
1:F:98:MET:SD	1:F:108:LEU:HB2	2.57	0.45
1:F:207:PHE:HB2	1:F:208:PHE:CD2	2.52	0.45
1:G:28:ALA:HA	1:G:35:TYR:H	1.82	0.45
1:A:89:PHE:HA	1:A:95:LEU:HD12	1.99	0.45
1:F:107:LYS:HB3	1:F:107:LYS:HE3	1.79	0.45
1:B:138:GLY:O	1:B:142:THR:OG1	2.34	0.44
1:C:168:GLU:O	1:C:172:ARG:HG3	2.17	0.44
1:E:7:ARG:HD2	2:E:319:HOH:O	2.17	0.44
1:C:168:GLU:OE2	1:C:172:ARG:NH2	2.44	0.44
1:G:24:ASN:HB2	1:G:161:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:HA	1:C:167:VAL:HB	2.00	0.44
1:G:222:SER:HB2	1:G:223:PRO:HD3	1.99	0.44
1:H:28:ALA:HB1	1:H:35:TYR:HB3	2.00	0.44
1:E:24:ASN:HB2	1:E:161:ILE:O	2.18	0.44
1:A:60:ALA:O	1:A:65:MET:HB2	2.17	0.44
1:D:190:GLN:HB3	1:D:197:GLN:HB2	1.98	0.44
1:C:25:MET:HE2	1:C:53:ILE:HD12	2.00	0.44
1:E:28:ALA:HB1	1:E:35:TYR:HB3	2.00	0.43
1:E:35:TYR:CD1	1:E:35:TYR:C	2.96	0.43
1:A:194:LYS:HE3	1:A:194:LYS:HB3	1.82	0.43
1:C:166:CYS:SG	2:C:340:HOH:O	2.49	0.43
1:E:61:ARG:HA	2:E:307:HOH:O	2.17	0.43
1:E:5:THR:HB	1:E:216:THR:HG21	2.00	0.43
1:C:26:GLN:HA	1:C:118:LEU:HA	2.00	0.43
1:C:186:ASP:OD1	1:C:214:VAL:HG23	2.18	0.43
1:G:36:LEU:HD12	1:G:36:LEU:HA	1.72	0.43
1:H:207:PHE:HB2	1:H:208:PHE:CD2	2.54	0.43
1:B:198:LYS:HE3	1:G:195:PHE:CE2	2.54	0.43
1:D:93:ASN:ND2	2:D:306:HOH:O	2.27	0.43
1:H:180:PHE:HA	2:H:397:HOH:O	2.18	0.43
1:F:25:MET:HE1	1:F:161:ILE:CD1	2.43	0.43
1:G:72:ASN:OD1	1:G:133:LYS:NZ	2.51	0.42
1:B:136:TYR:HB2	1:G:176:PHE:CE1	2.54	0.42
1:C:11:ILE:HG21	1:C:210:TRP:CE2	2.54	0.42
1:H:172:ARG:HG2	1:H:208:PHE:CD1	2.55	0.42
1:D:140:PHE:O	1:D:142:THR:HG23	2.19	0.42
1:E:18:SER:HA	1:E:153:ILE:HG23	2.01	0.42
1:F:197:GLN:HE21	1:F:201:LEU:HD11	1.83	0.42
1:C:8:PRO:HG2	1:C:9:GLU:OE1	2.18	0.42
1:D:52:ASN:HB3	1:D:214:VAL:HG21	2.01	0.42
1:E:121:GLU:OE1	1:E:121:GLU:N	2.46	0.42
1:E:140:PHE:O	1:E:142:THR:HG23	2.19	0.42
1:C:95:LEU:O	1:C:99:ARG:HG3	2.19	0.42
1:H:166:CYS:SG	2:H:391:HOH:O	2.55	0.42
1:D:103:GLN:H	1:D:103:GLN:CD	2.26	0.42
1:H:215:GLU:HG3	2:H:360:HOH:O	2.20	0.42
1:G:74:TRP:HB3	1:G:80:GLU:HB2	2.02	0.42
1:C:4:LEU:HD12	1:C:216:THR:HG22	2.02	0.41
1:H:89:PHE:HA	1:H:95:LEU:HD23	2.01	0.41
1:B:8:PRO:HD2	1:B:210:TRP:CD1	2.56	0.41
1:E:161:ILE:HA	1:E:162:ALA:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ALA:O	1:C:65:MET:HB2	2.21	0.41
1:B:72:ASN:OD1	1:B:133:LYS:NZ	2.51	0.41
1:B:78:TYR:CZ	1:B:98:MET:HE1	2.56	0.41
1:C:111:LYS:HG3	2:C:313:HOH:O	2.20	0.41
1:F:122:LEU:HD23	1:F:122:LEU:HA	1.88	0.41
1:D:166:CYS:SG	2:D:387:HOH:O	2.37	0.41
1:E:36:LEU:HD23	1:E:36:LEU:HA	1.90	0.41
1:G:18:SER:HB3	1:G:65:MET:HE3	2.03	0.41
1:C:54:GLN:NE2	1:C:121:GLU:O	2.54	0.41
1:E:78:TYR:CZ	1:E:98:MET:HE1	2.56	0.41
1:F:195:PHE:CD1	1:F:195:PHE:C	2.99	0.41
1:G:43:VAL:HG12	1:G:46:THR:OG1	2.21	0.41
1:B:70:PHE:HZ	1:B:144:LEU:HD22	1.86	0.40
1:G:56:ALA:HB2	1:G:214:VAL:HG13	2.03	0.40
1:G:111:LYS:HA	1:G:116:TYR:CD2	2.56	0.40
1:G:164:ASN:OD1	1:G:164:ASN:N	2.52	0.40
1:H:140:PHE:O	1:H:142:THR:HG23	2.20	0.40
1:F:148:LEU:HD13	1:F:156:LEU:HD21	2.03	0.40
1:A:111:LYS:HA	1:A:116:TYR:CD2	2.56	0.40
1:B:217:PHE:CZ	1:B:221:LEU:HD11	2.57	0.40
1:D:35:TYR:CD1	1:D:35:TYR:C	2.99	0.40
1:H:121:GLU:OE1	1:H:121:GLU:N	2.45	0.40
1:D:154:ARG:HH11	1:D:154:ARG:HG3	1.87	0.40

All (5) 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)
1:A:149:ARG:NH2	1:F:177:LEU:O[2_545]	1.95	0.25
1:D:149:ARG:NH2	1:G:177:LEU:O[2_655]	2.09	0.11
2:B:383:HOH:O	2:G:352:HOH:O[1_455]	2.18	0.02
2:D:429:HOH:O	2:E:435:HOH:O[1_455]	2.19	0.01
2:D:433:HOH:O	2:D:441:HOH:O[1_655]	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%)	213 (97%)	7 (3%)	0	100	100
1	B	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	C	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	D	219/230 (95%)	213 (97%)	6 (3%)	0	100	100
1	E	219/230 (95%)	215 (98%)	4 (2%)	0	100	100
1	F	218/230 (95%)	209 (96%)	9 (4%)	0	100	100
1	G	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
1	H	220/230 (96%)	212 (96%)	8 (4%)	0	100	100
All	All	1755/1840 (95%)	1699 (97%)	56 (3%)	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%)	180 (99%)	1 (1%)	78	72
1	B	181/188 (96%)	178 (98%)	3 (2%)	53	40
1	C	179/188 (95%)	177 (99%)	2 (1%)	65	56
1	D	179/188 (95%)	176 (98%)	3 (2%)	53	40
1	E	180/188 (96%)	177 (98%)	3 (2%)	53	40
1	F	179/188 (95%)	178 (99%)	1 (1%)	78	72
1	G	175/188 (93%)	171 (98%)	4 (2%)	44	29
1	H	181/188 (96%)	178 (98%)	3 (2%)	53	40
All	All	1435/1504 (95%)	1415 (99%)	20 (1%)	59	48

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	B	3	THR
1	B	54	GLN
1	B	131	LEU
1	C	35	TYR
1	C	107	LYS
1	D	36	LEU
1	D	95	LEU
1	D	163	THR
1	E	9	GLU
1	E	35	TYR
1	E	95	LEU
1	F	16	GLN
1	G	9	GLU
1	G	35	TYR
1	G	43	VAL
1	G	222	SER
1	H	54	GLN
1	H	95	LEU
1	H	117	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	16	GLN
1	B	141	ASN
1	B	189	HIS
1	C	24	ASN
1	C	52	ASN
1	C	103	GLN
1	D	125	GLN
1	E	71	GLN
1	E	125	GLN
1	F	93	ASN
1	F	103	GLN
1	G	93	ASN
1	H	17	GLN
1	H	77	GLN
1	H	125	GLN
1	H	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	3 (1%) 73 79	12, 21, 29, 38	0
1	B	222/230 (96%)	0.67	10 (4%) 38 41	16, 24, 35, 42	0
1	C	221/230 (96%)	1.20	39 (17%) 4 4	18, 32, 46, 57	0
1	D	221/230 (96%)	0.37	3 (1%) 73 79	14, 22, 33, 39	0
1	E	221/230 (96%)	0.40	2 (0%) 81 85	15, 23, 31, 38	0
1	F	220/230 (95%)	0.69	4 (1%) 67 73	18, 26, 33, 40	0
1	G	222/230 (96%)	1.08	32 (14%) 6 6	16, 32, 48, 54	0
1	H	222/230 (96%)	0.35	4 (1%) 67 73	13, 21, 31, 40	0
All	All	1771/1840 (96%)	0.63	97 (5%) 30 33	12, 24, 40, 57	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	THR	4.3
1	C	43	VAL	4.2
1	C	39	ALA	4.1
1	G	43	VAL	4.0
1	C	32	PRO	3.7
1	G	33	GLY	3.5
1	C	11	ILE	3.5
1	G	28	ALA	3.5
1	G	102	PRO	3.4
1	C	33	GLY	3.4
1	C	34	GLY	3.4
1	G	119	VAL	3.3
1	C	191	ALA	3.1
1	C	44	SER	3.1
1	D	222	SER	3.1
1	G	62	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	123	VAL	3.0
1	G	222	SER	3.0
1	C	222	SER	2.9
1	C	45	THR	2.9
1	C	28	ALA	2.9
1	C	42	ASP	2.9
1	C	31	THR	2.9
1	C	30	ALA	2.9
1	G	46	THR	2.8
1	C	119	VAL	2.8
1	B	195	PHE	2.8
1	C	97	THR	2.8
1	G	104	LEU	2.8
1	A	222	SER	2.7
1	C	82	GLY	2.7
1	C	36	LEU	2.7
1	B	191	ALA	2.7
1	G	73	GLY	2.7
1	G	103	GLN	2.7
1	F	82	GLY	2.7
1	A	70	PHE	2.7
1	C	41	PHE	2.7
1	C	48	PRO	2.7
1	C	214	VAL	2.7
1	G	31	THR	2.6
1	H	104	LEU	2.6
1	A	223	PRO	2.5
1	G	32	PRO	2.5
1	B	43	VAL	2.5
1	C	35	TYR	2.5
1	C	50	ILE	2.5
1	G	42	ASP	2.5
1	G	100	LYS	2.5
1	G	219	ASP	2.5
1	C	40	GLY	2.4
1	G	47	ARG	2.4
1	C	38	LEU	2.4
1	G	44	SER	2.4
1	E	222	SER	2.4
1	C	131	LEU	2.4
1	D	107	LYS	2.4
1	F	191	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	102	PRO	2.3
1	G	82	GLY	2.3
1	G	221	LEU	2.3
1	B	220	ALA	2.3
1	G	63	ALA	2.3
1	G	11	ILE	2.3
1	G	101	GLN	2.3
1	H	77	GLN	2.3
1	C	108	LEU	2.3
1	G	217	PHE	2.3
1	B	59	ALA	2.3
1	G	48	PRO	2.3
1	B	192	GLY	2.3
1	B	44	SER	2.3
1	G	50	ILE	2.2
1	B	48	PRO	2.2
1	C	77	GLN	2.2
1	C	104	LEU	2.2
1	G	79	VAL	2.1
1	C	221	LEU	2.1
1	F	195	PHE	2.1
1	G	41	PHE	2.1
1	B	215	GLU	2.1
1	C	199	ALA	2.1
1	E	51	ALA	2.1
1	G	195	PHE	2.1
1	C	79	VAL	2.1
1	C	182	VAL	2.1
1	C	211	VAL	2.1
1	H	43	VAL	2.1
1	G	109	LEU	2.1
1	C	47	ARG	2.1
1	C	29	TYR	2.0
1	G	35	TYR	2.0
1	B	193	PRO	2.0
1	G	51	ALA	2.0
1	F	189	HIS	2.0
1	C	181	GLY	2.0
1	H	103	GLN	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.