



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 AM UTC

PDB ID : 3BU2 / pdb_00003bu2
Title : Crystal structure of a tRNA-binding protein from *Staphylococcus saprophyticus* subsp. *saprophyticus*. Northeast Structural Genomics Consortium target SyR77
Authors : Seetharaman, J.; Su, M.; Forouhar, F.; Wang, D.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xia, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2007-12-31
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

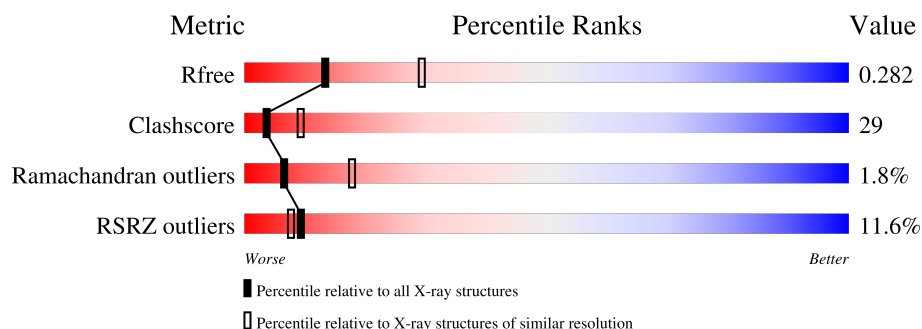
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	199	10% 59% 37% ..
1	B	199	11% 54% 42% ..
1	C	199	12% 54% 42% ..
1	D	199	12% 59% 35% ..

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6099 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 Putative tRNA-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1477	940	236	293	2	6			
1	B	195	Total	C	N	O	S	Se	0	0	0
			1477	940	236	293	2	6			
1	C	195	Total	C	N	O	S	Se	0	0	0
			1477	940	236	293	2	6			
1	D	195	Total	C	N	O	S	Se	0	0	0
			1477	940	236	293	2	6			

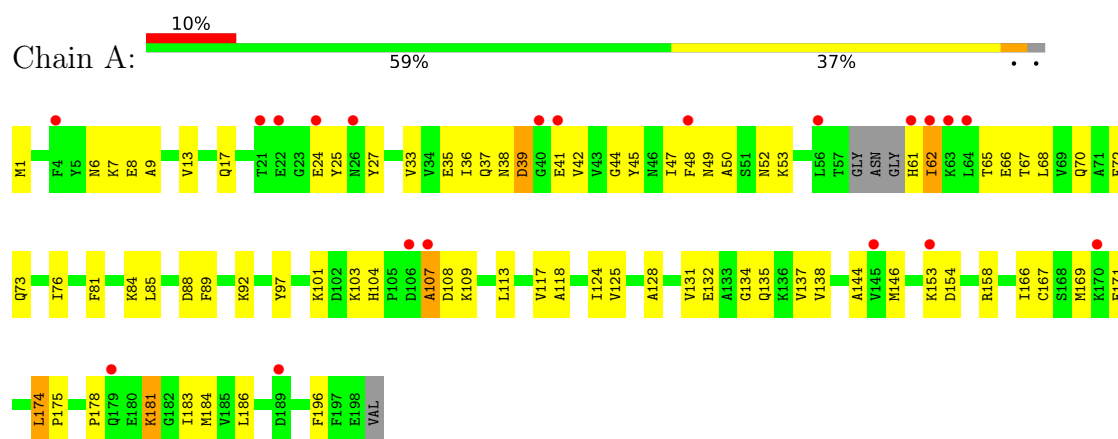
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	57	Total	O	0	0
			57	57		
2	C	41	Total	O	0	0
			41	41		
2	D	56	Total	O	0	0
			56	56		

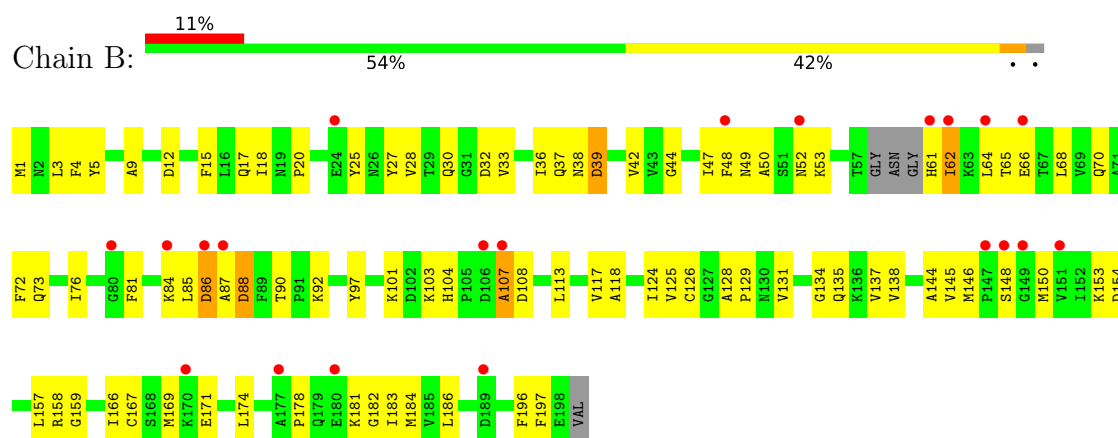
3 Residue-property plots [i](#)

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.

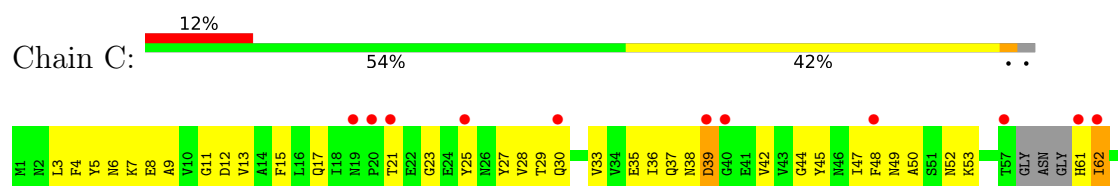
• Molecule 1: Putative tRNA-binding protein

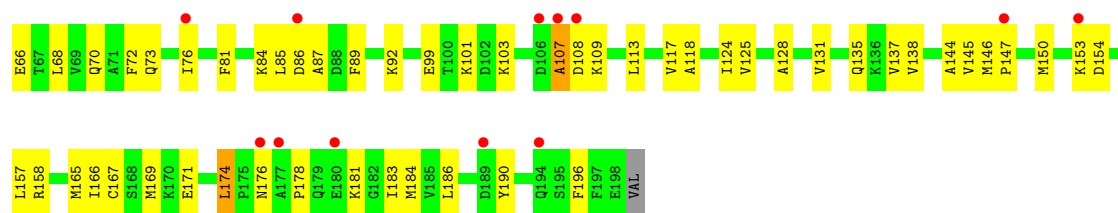


• Molecule 1: Putative tRNA-binding protein

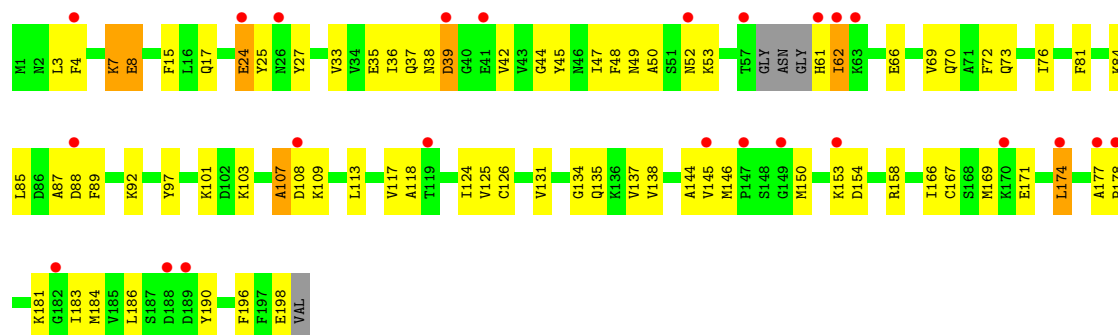


• Molecule 1: Putative tRNA-binding protein





● Molecule 1: Putative tRNA-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.90Å 79.80Å 139.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.10 – 2.70 40.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.4 (40.10-2.70) 90.9 (40.10-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.54 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.273 0.259 , 0.282	Depositor DCC
R_{free} test set	2100 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6099	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/1495	0.94	5/2016 (0.2%)
1	B	0.45	0/1495	0.92	3/2016 (0.1%)
1	C	0.48	0/1495	0.95	4/2016 (0.2%)
1	D	0.47	0/1495	0.97	6/2016 (0.3%)
All	All	0.46	0/5980	0.95	18/8064 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	CYS	N-CA-C	6.54	119.38	110.55
1	A	167	CYS	N-CA-C	6.52	119.36	110.55
1	C	167	CYS	N-CA-C	6.42	119.21	110.55
1	B	167	CYS	N-CA-C	6.39	119.17	110.55
1	A	107	ALA	N-CA-C	-5.84	107.96	114.62
1	B	107	ALA	N-CA-C	-5.83	107.97	114.62
1	D	24	GLU	N-CA-C	5.71	119.09	110.64
1	C	107	ALA	N-CA-C	-5.60	108.23	114.62
1	D	107	ALA	N-CA-C	-5.60	108.24	114.62
1	D	8	GLU	N-CA-C	5.42	117.89	111.33
1	C	174	LEU	CA-C-N	5.30	126.47	119.84
1	C	174	LEU	C-N-CA	5.30	126.47	119.84
1	D	174	LEU	CA-C-N	5.22	126.37	119.84
1	D	174	LEU	C-N-CA	5.22	126.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	LYS	N-CA-C	5.11	119.20	112.92
1	B	181	LYS	N-CA-C	5.10	119.19	112.92
1	A	174	LEU	CA-C-N	5.06	126.17	119.84
1	A	174	LEU	C-N-CA	5.06	126.17	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	ASP	Peptide

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	1477	0	1471	90	0
1	B	1477	0	1471	97	0
1	C	1477	0	1471	89	0
1	D	1477	0	1471	87	0
2	A	37	0	0	14	0
2	B	57	0	0	19	0
2	C	41	0	0	9	0
2	D	56	0	0	11	0
All	All	6099	0	5884	344	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:VAL:HG12	2:B:227:HOH:O	1.67	0.92
1:B:68:LEU:HD12	2:B:226:HOH:O	1.71	0.90
1:C:28:VAL:HG12	2:C:228:HOH:O	1.73	0.87
1:A:184:MSE:HE3	1:A:186:LEU:HD21	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MSE:HE3	1:C:186:LEU:HD21	1.59	0.83
1:C:169:MSE:HE3	1:C:174:LEU:HD22	1.59	0.83
1:B:169:MSE:HE3	1:B:174:LEU:HD22	1.60	0.83
1:B:184:MSE:HE3	1:B:186:LEU:HD21	1.60	0.83
1:C:47:ILE:HD11	1:C:50:ALA:HA	1.62	0.82
1:D:184:MSE:HE3	1:D:186:LEU:HD21	1.60	0.82
1:A:169:MSE:HE3	1:A:174:LEU:HD22	1.61	0.82
1:D:8:GLU:H	1:D:8:GLU:CD	1.88	0.82
1:D:169:MSE:HE3	1:D:174:LEU:HD22	1.60	0.82
1:B:47:ILE:HD11	1:B:50:ALA:HA	1.62	0.81
1:B:47:ILE:HD13	1:B:53:LYS:HD2	1.63	0.80
1:B:196:PHE:HZ	1:C:169:MSE:HE2	1.48	0.79
1:D:47:ILE:HD11	1:D:50:ALA:HA	1.63	0.79
1:A:47:ILE:HD11	1:A:50:ALA:HA	1.64	0.78
1:D:47:ILE:HD13	1:D:53:LYS:HD2	1.64	0.78
1:A:47:ILE:HD13	1:A:53:LYS:HD2	1.65	0.77
1:A:196:PHE:HZ	1:D:169:MSE:HE2	1.51	0.76
1:B:129:PRO:HD2	2:B:202:HOH:O	1.86	0.75
1:C:47:ILE:HD13	1:C:53:LYS:HD2	1.67	0.74
1:A:24:GLU:H	1:A:24:GLU:CD	1.94	0.74
1:A:1:MSE:HB2	1:A:17:GLN:O	1.89	0.73
1:B:182:GLY:HA2	2:B:202:HOH:O	1.89	0.73
1:A:137:VAL:HG23	2:A:201:HOH:O	1.90	0.71
1:A:50:ALA:HB3	2:A:237:HOH:O	1.91	0.70
1:C:48:PHE:CE2	1:D:158:ARG:HG3	2.25	0.70
1:D:72:PHE:O	1:D:76:ILE:HG23	1.92	0.70
1:D:47:ILE:CD1	1:D:53:LYS:HD2	2.23	0.69
1:B:30:GLN:HG3	2:B:227:HOH:O	1.92	0.69
1:D:38:ASN:O	1:D:39:ASP:HB2	1.92	0.69
1:A:169:MSE:HE2	1:D:196:PHE:HZ	1.58	0.68
1:A:9:ALA:O	1:A:128:ALA:HB2	1.93	0.68
1:C:73:GLN:HE22	1:C:84:LYS:HA	1.58	0.68
1:D:73:GLN:HE22	1:D:84:LYS:HA	1.58	0.68
1:B:38:ASN:O	1:B:39:ASP:HB2	1.95	0.67
1:C:38:ASN:O	1:C:39:ASP:HB2	1.94	0.67
1:B:15:PHE:HE1	1:B:157:LEU:HD11	1.58	0.67
1:B:47:ILE:CD1	1:B:53:LYS:HD2	2.23	0.67
1:B:73:GLN:HE22	1:B:85:LEU:H	1.39	0.67
1:A:38:ASN:O	1:A:39:ASP:HB2	1.95	0.67
1:A:47:ILE:CD1	1:A:53:LYS:HD2	2.24	0.67
1:A:158:ARG:HG3	1:B:48:PHE:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:PHE:O	1:B:76:ILE:HG23	1.94	0.66
1:A:137:VAL:HG21	1:A:166:ILE:CG2	2.26	0.66
1:A:72:PHE:O	1:A:76:ILE:HG23	1.94	0.66
1:C:30:GLN:HG3	2:C:228:HOH:O	1.94	0.65
1:B:73:GLN:HE22	1:B:84:LYS:HA	1.61	0.65
1:A:73:GLN:HE22	1:A:84:LYS:HA	1.60	0.65
1:C:137:VAL:HG21	1:C:166:ILE:CG2	2.25	0.65
1:D:73:GLN:HE22	1:D:85:LEU:H	1.43	0.65
1:C:72:PHE:O	1:C:76:ILE:HG23	1.97	0.65
1:A:137:VAL:CG2	2:A:201:HOH:O	2.45	0.64
1:C:73:GLN:HE22	1:C:85:LEU:H	1.44	0.64
1:B:73:GLN:NE2	1:B:85:LEU:H	1.96	0.64
1:B:137:VAL:HG21	1:B:166:ILE:CG2	2.28	0.64
1:B:159:GLY:HA3	2:B:242:HOH:O	1.97	0.63
1:C:47:ILE:CD1	1:C:53:LYS:HD2	2.27	0.63
1:C:15:PHE:HE1	1:C:157:LEU:HD11	1.64	0.63
1:A:52:ASN:HB2	2:A:202:HOH:O	1.98	0.63
1:A:73:GLN:HE22	1:A:85:LEU:H	1.44	0.63
1:B:137:VAL:CG2	2:B:203:HOH:O	2.46	0.63
1:B:137:VAL:HG23	2:B:203:HOH:O	1.99	0.62
1:B:62:ILE:HB	2:B:247:HOH:O	1.98	0.62
1:C:99:GLU:HB3	2:C:247:HOH:O	2.00	0.62
1:D:88:ASP:CG	1:D:89:PHE:H	2.08	0.62
1:C:158:ARG:HG3	1:D:48:PHE:CE2	2.34	0.61
1:A:137:VAL:HG21	1:A:166:ILE:HG23	1.81	0.61
1:D:137:VAL:HG21	1:D:166:ILE:CG2	2.29	0.61
1:C:8:GLU:HG3	1:C:181:LYS:HB3	1.81	0.61
1:D:92:LYS:HB3	1:D:144:ALA:HB2	1.83	0.61
1:C:137:VAL:HG21	1:C:166:ILE:HG23	1.82	0.60
1:A:48:PHE:CE2	1:B:158:ARG:HG3	2.35	0.60
1:C:92:LYS:HB3	1:C:144:ALA:HB2	1.83	0.60
1:D:137:VAL:CG2	2:D:205:HOH:O	2.50	0.60
1:A:109:LYS:NZ	2:A:205:HOH:O	2.33	0.60
1:B:92:LYS:HB3	1:B:144:ALA:HB2	1.83	0.60
1:B:3:LEU:HD22	1:B:4:PHE:N	2.17	0.60
1:D:88:ASP:OD2	1:D:89:PHE:N	2.29	0.59
1:D:137:VAL:HG23	2:D:205:HOH:O	2.01	0.59
1:D:4:PHE:HB2	2:D:219:HOH:O	2.02	0.59
1:C:137:VAL:HG23	2:C:258:HOH:O	2.02	0.59
1:C:62:ILE:HD13	1:C:62:ILE:N	2.18	0.59
1:A:113:LEU:HG	2:A:234:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:VAL:HG21	1:D:166:ILE:HG23	1.83	0.58
1:C:17:GLN:NE2	1:C:150:MSE:HG3	2.18	0.58
1:C:73:GLN:HE22	1:C:85:LEU:N	2.02	0.58
1:B:73:GLN:HE22	1:B:85:LEU:N	2.01	0.58
1:D:73:GLN:HE22	1:D:85:LEU:N	2.01	0.58
1:D:117:VAL:O	1:D:117:VAL:HG13	2.03	0.58
1:B:62:ILE:N	1:B:62:ILE:HD13	2.19	0.58
1:B:137:VAL:HG21	1:B:166:ILE:HG23	1.85	0.58
1:D:69:VAL:HG11	1:D:87:ALA:HB2	1.86	0.57
1:A:92:LYS:HB3	1:A:144:ALA:HB2	1.85	0.57
1:D:73:GLN:NE2	1:D:85:LEU:H	2.02	0.57
1:A:117:VAL:HG13	1:A:117:VAL:O	2.03	0.57
1:D:8:GLU:CD	1:D:8:GLU:N	2.61	0.57
1:A:73:GLN:HE22	1:A:85:LEU:N	2.03	0.57
1:B:117:VAL:HG13	1:B:117:VAL:O	2.02	0.57
1:D:8:GLU:HG3	1:D:181:LYS:HB3	1.87	0.56
1:A:62:ILE:HD13	1:A:62:ILE:N	2.20	0.56
1:B:150:MSE:HB3	2:B:240:HOH:O	2.06	0.56
1:C:7:LYS:HA	1:C:11:GLY:O	2.04	0.56
1:C:73:GLN:NE2	1:C:85:LEU:H	2.02	0.56
1:A:137:VAL:HG22	1:A:138:VAL:N	2.19	0.56
1:A:158:ARG:NE	2:A:209:HOH:O	2.38	0.56
1:B:65:THR:N	2:B:226:HOH:O	2.38	0.56
1:A:73:GLN:NE2	1:A:85:LEU:H	2.04	0.56
1:D:169:MSE:HG2	2:D:243:HOH:O	2.06	0.55
1:C:137:VAL:HG22	1:C:138:VAL:N	2.21	0.55
2:A:237:HOH:O	1:B:12:ASP:C	2.50	0.55
1:B:15:PHE:CE1	1:B:157:LEU:HD11	2.41	0.55
1:B:137:VAL:HG22	1:B:138:VAL:N	2.20	0.55
1:C:169:MSE:HE3	1:C:174:LEU:CD2	2.35	0.55
1:B:84:LYS:HD2	2:B:209:HOH:O	2.06	0.55
1:A:1:MSE:HE2	1:A:1:MSE:N	2.22	0.55
1:D:137:VAL:HG22	1:D:138:VAL:N	2.21	0.55
1:C:109:LYS:HB2	2:C:254:HOH:O	2.07	0.54
1:C:117:VAL:O	1:C:117:VAL:HG13	2.07	0.54
1:B:62:ILE:HG12	1:B:62:ILE:O	2.07	0.54
1:A:6:ASN:CG	1:A:9:ALA:HB3	2.32	0.54
1:C:15:PHE:CE1	1:C:157:LEU:HD11	2.43	0.54
1:D:62:ILE:HG12	1:D:62:ILE:O	2.07	0.54
1:D:109:LYS:HB2	2:D:226:HOH:O	2.07	0.53
1:C:62:ILE:HG12	1:C:62:ILE:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:HG13	1:B:47:ILE:O	2.07	0.53
1:D:62:ILE:N	1:D:62:ILE:HD13	2.23	0.53
1:C:27:TYR:CE1	1:C:36:ILE:HD12	2.44	0.53
1:A:47:ILE:HG13	1:A:47:ILE:O	2.09	0.53
1:B:33:VAL:HG22	1:B:81:PHE:CE2	2.44	0.53
1:B:27:TYR:CE1	1:B:36:ILE:HD12	2.44	0.52
1:A:103:LYS:NZ	1:A:103:LYS:HB3	2.25	0.52
1:C:147:PRO:HB2	2:C:234:HOH:O	2.09	0.52
1:A:27:TYR:CE1	1:A:36:ILE:HD12	2.44	0.52
1:D:88:ASP:O	1:D:89:PHE:HB2	2.10	0.52
1:C:6:ASN:CG	1:C:9:ALA:HB3	2.35	0.52
1:A:1:MSE:HE2	1:A:1:MSE:H1	1.75	0.52
1:A:8:GLU:CD	1:A:8:GLU:H	2.16	0.52
1:C:33:VAL:HG22	1:C:81:PHE:CE2	2.45	0.52
1:D:169:MSE:HE3	1:D:174:LEU:CD2	2.38	0.51
1:C:153:LYS:HE3	1:C:154:ASP:H	1.75	0.51
1:B:103:LYS:NZ	1:B:103:LYS:HB3	2.25	0.51
1:A:62:ILE:HG12	1:A:62:ILE:O	2.09	0.51
1:C:47:ILE:HG13	1:C:47:ILE:O	2.10	0.51
1:B:104:HIS:HB3	2:B:212:HOH:O	2.10	0.51
1:D:145:VAL:HB	2:D:218:HOH:O	2.10	0.51
1:B:86:ASP:CG	1:B:87:ALA:N	2.69	0.51
1:D:103:LYS:HB3	1:D:103:LYS:NZ	2.26	0.51
1:A:138:VAL:HG11	1:A:184:MSE:HE2	1.93	0.51
1:D:47:ILE:O	1:D:47:ILE:HG13	2.11	0.51
1:D:33:VAL:HG22	1:D:81:PHE:CE2	2.45	0.50
1:D:17:GLN:CD	1:D:150:MSE:HE3	2.36	0.50
1:D:27:TYR:CE1	1:D:36:ILE:HD12	2.46	0.50
1:C:25:TYR:CE2	1:C:38:ASN:HB2	2.47	0.50
1:B:138:VAL:HG11	1:B:184:MSE:HE2	1.94	0.50
1:A:169:MSE:HB2	1:A:178:PRO:HG2	1.93	0.50
1:D:153:LYS:HE3	1:D:154:ASP:H	1.76	0.50
1:A:153:LYS:HE3	1:A:154:ASP:H	1.77	0.50
1:B:108:ASP:N	2:B:212:HOH:O	2.43	0.50
1:B:169:MSE:HB2	1:B:178:PRO:HG2	1.93	0.50
1:B:169:MSE:HE2	1:C:196:PHE:HZ	1.76	0.50
1:B:37:GLN:HB3	1:B:42:VAL:HA	1.94	0.50
1:B:25:TYR:CE2	1:B:38:ASN:HB2	2.47	0.50
1:B:124:ILE:HD12	1:B:125:VAL:N	2.27	0.50
1:C:3:LEU:HD12	1:C:4:PHE:H	1.77	0.50
1:C:12:ASP:OD2	1:D:49:ASN:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG22	1:A:81:PHE:CE2	2.46	0.49
1:C:47:ILE:C	1:C:47:ILE:HD12	2.37	0.49
1:D:146:MSE:CE	1:D:171:GLU:HG3	2.41	0.49
1:A:25:TYR:CE2	1:A:38:ASN:HB2	2.48	0.49
1:B:153:LYS:HE3	1:B:154:ASP:H	1.76	0.49
1:C:37:GLN:HB3	1:C:42:VAL:HA	1.94	0.49
1:D:124:ILE:HD12	1:D:125:VAL:N	2.27	0.49
1:D:183:ILE:HD12	1:D:183:ILE:C	2.37	0.49
1:B:86:ASP:OD2	1:B:87:ALA:N	2.41	0.49
1:D:4:PHE:HB3	1:D:15:PHE:HB2	1.93	0.49
1:D:62:ILE:HD12	2:D:244:HOH:O	2.13	0.49
1:C:9:ALA:O	1:C:128:ALA:HB2	2.11	0.49
1:A:181:LYS:HZ1	1:D:198:GLU:CD	2.20	0.49
1:A:183:ILE:C	1:A:183:ILE:HD12	2.37	0.49
1:C:138:VAL:HG11	1:C:184:MSE:HE2	1.93	0.49
1:D:169:MSE:HB2	1:D:178:PRO:HG2	1.94	0.49
1:A:169:MSE:HE3	1:A:174:LEU:CD2	2.37	0.49
1:D:25:TYR:CE2	1:D:38:ASN:HB2	2.48	0.48
1:C:66:GLU:O	1:C:70:GLN:HG3	2.14	0.48
1:C:103:LYS:NZ	1:C:103:LYS:HB3	2.29	0.48
1:D:138:VAL:HG11	1:D:184:MSE:HE2	1.95	0.48
1:D:88:ASP:CG	1:D:89:PHE:N	2.70	0.48
2:B:236:HOH:O	1:C:169:MSE:HG3	2.12	0.48
1:A:37:GLN:HB3	1:A:42:VAL:HA	1.95	0.48
1:C:169:MSE:HB2	1:C:178:PRO:HG2	1.96	0.48
1:B:1:MSE:HA	1:B:17:GLN:O	2.13	0.48
1:C:146:MSE:CE	1:C:171:GLU:HG3	2.43	0.48
1:C:47:ILE:HD11	1:C:50:ALA:CA	2.40	0.47
1:D:37:GLN:HB3	1:D:42:VAL:HA	1.96	0.47
1:A:24:GLU:CD	1:A:24:GLU:N	2.68	0.47
1:C:124:ILE:HD12	1:C:125:VAL:N	2.30	0.47
1:B:36:ILE:HG23	1:B:44:GLY:C	2.40	0.47
1:B:66:GLU:O	1:B:70:GLN:HG3	2.15	0.47
1:C:107:ALA:O	1:C:108:ASP:HB3	2.15	0.47
1:B:1:MSE:HE2	1:B:18:ILE:HG12	1.96	0.47
1:B:124:ILE:HD12	1:B:125:VAL:C	2.38	0.47
1:B:61:HIS:O	1:B:62:ILE:C	2.57	0.47
1:B:145:VAL:HG22	2:B:201:HOH:O	2.14	0.47
1:B:148:SER:HB2	2:B:219:HOH:O	2.15	0.47
1:C:138:VAL:CG1	1:C:184:MSE:HE2	2.45	0.47
1:D:101:LYS:HG3	1:D:113:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:C	1:A:47:ILE:HD12	2.39	0.47
2:A:237:HOH:O	1:B:5:TYR:HE1	1.97	0.47
1:B:107:ALA:O	1:B:108:ASP:HB3	2.15	0.47
1:B:3:LEU:HD22	1:B:3:LEU:C	2.40	0.47
1:A:1:MSE:HG2	1:B:64:LEU:HD11	1.97	0.46
1:A:107:ALA:O	1:A:108:ASP:HB3	2.16	0.46
1:A:117:VAL:O	1:A:118:ALA:HB3	2.15	0.46
1:B:169:MSE:HE3	1:B:174:LEU:CD2	2.37	0.46
1:B:183:ILE:HD12	1:B:183:ILE:C	2.41	0.46
1:B:9:ALA:O	1:B:128:ALA:HB2	2.15	0.46
1:A:8:GLU:HG3	1:A:181:LYS:HB3	1.98	0.46
1:B:47:ILE:HD12	1:B:47:ILE:C	2.40	0.46
1:B:101:LYS:HG3	1:B:113:LEU:CD2	2.45	0.46
1:C:183:ILE:C	1:C:183:ILE:HD12	2.39	0.46
1:B:146:MSE:CE	1:B:171:GLU:HG3	2.45	0.46
1:C:5:TYR:OH	1:C:12:ASP:OD1	2.26	0.46
1:A:61:HIS:O	1:A:62:ILE:C	2.58	0.46
1:A:138:VAL:CG1	1:A:184:MSE:HE2	2.45	0.46
1:C:101:LYS:HG3	1:C:113:LEU:CD2	2.46	0.46
1:A:36:ILE:HG23	1:A:44:GLY:C	2.41	0.46
1:A:124:ILE:HD12	1:A:125:VAL:N	2.31	0.46
1:A:174:LEU:HD23	1:A:178:PRO:HG3	1.98	0.46
1:D:107:ALA:O	1:D:108:ASP:HB3	2.16	0.46
1:D:124:ILE:HD12	1:D:125:VAL:C	2.41	0.46
1:A:8:GLU:HG3	1:A:181:LYS:CB	2.46	0.45
1:C:61:HIS:O	1:C:62:ILE:C	2.58	0.45
1:B:33:VAL:HG22	1:B:81:PHE:HE2	1.80	0.45
1:B:65:THR:HG23	2:B:226:HOH:O	2.15	0.45
1:D:174:LEU:HD23	1:D:178:PRO:HG3	1.98	0.45
1:B:138:VAL:CG1	1:B:184:MSE:HE2	2.46	0.45
1:C:29:THR:C	2:C:228:HOH:O	2.59	0.45
1:B:124:ILE:HD12	1:B:125:VAL:O	2.16	0.45
1:C:174:LEU:HD23	1:C:178:PRO:HG3	1.99	0.45
1:D:61:HIS:O	1:D:62:ILE:C	2.59	0.44
1:D:36:ILE:HG23	1:D:44:GLY:C	2.42	0.44
1:A:146:MSE:CE	1:A:171:GLU:HG3	2.47	0.44
1:C:117:VAL:O	1:C:118:ALA:HB3	2.17	0.44
1:C:146:MSE:HE2	1:C:165:MSE:SE	2.68	0.44
1:D:47:ILE:HD12	1:D:47:ILE:C	2.42	0.44
1:A:101:LYS:HG3	1:A:113:LEU:CD2	2.47	0.44
1:C:36:ILE:HG23	1:C:44:GLY:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD23	1:B:178:PRO:HG3	1.99	0.44
1:B:197:PHE:CE1	1:C:176:ASN:HB2	2.53	0.44
1:C:72:PHE:HE2	1:D:3:LEU:HD22	1.83	0.44
1:C:124:ILE:HD12	1:C:125:VAL:C	2.42	0.44
1:D:138:VAL:CG1	1:D:184:MSE:HE2	2.48	0.44
1:A:66:GLU:O	1:A:70:GLN:HG3	2.17	0.44
1:B:47:ILE:HD11	1:B:50:ALA:CA	2.42	0.44
1:B:103:LYS:HB3	1:B:103:LYS:HZ2	1.83	0.44
1:B:88:ASP:OD2	1:B:90:THR:OG1	2.33	0.44
1:A:174:LEU:HA	1:A:175:PRO:HD3	1.86	0.43
1:D:118:ALA:HA	2:D:231:HOH:O	2.18	0.43
1:C:66:GLU:HA	1:C:89:PHE:HE1	1.83	0.43
1:D:35:GLU:HG3	1:D:45:TYR:CE1	2.53	0.43
1:D:66:GLU:O	1:D:70:GLN:HG3	2.19	0.43
1:D:33:VAL:HG22	1:D:81:PHE:HE2	1.83	0.43
1:A:50:ALA:N	2:A:237:HOH:O	2.48	0.43
1:B:39:ASP:HB3	2:B:248:HOH:O	2.18	0.43
1:B:117:VAL:O	1:B:118:ALA:HB3	2.18	0.43
1:D:97:TYR:OH	1:D:134:GLY:HA2	2.18	0.43
1:A:6:ASN:C	1:A:6:ASN:HD22	2.27	0.43
1:A:41:GLU:HB3	1:B:20:PRO:HB3	2.01	0.43
1:B:86:ASP:CG	1:B:87:ALA:H	2.27	0.43
1:C:8:GLU:HG3	1:C:181:LYS:CB	2.46	0.43
1:C:8:GLU:CD	1:C:8:GLU:H	2.25	0.43
1:A:33:VAL:HG22	1:A:81:PHE:HE2	1.82	0.43
1:A:103:LYS:HB3	1:A:103:LYS:HZ2	1.82	0.43
1:B:38:ASN:O	1:B:39:ASP:CB	2.66	0.43
1:C:33:VAL:HG22	1:C:81:PHE:HE2	1.82	0.43
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.90	0.42
1:A:73:GLN:HE22	1:A:84:LYS:CA	2.30	0.42
1:B:131:VAL:HA	1:B:135:GLN:HE22	1.84	0.42
1:D:84:LYS:HG2	2:D:200:HOH:O	2.17	0.42
1:A:66:GLU:HA	1:A:89:PHE:CE1	2.54	0.42
1:A:124:ILE:HD12	1:A:125:VAL:C	2.44	0.42
1:D:49:ASN:O	1:D:52:ASN:OD1	2.37	0.42
1:D:61:HIS:N	2:D:228:HOH:O	2.52	0.42
1:C:138:VAL:HG11	1:C:184:MSE:CE	2.48	0.42
1:D:73:GLN:NE2	1:D:85:LEU:N	2.64	0.42
1:B:124:ILE:HD11	1:B:126:CYS:HB2	2.01	0.42
1:C:73:GLN:NE2	1:C:85:LEU:N	2.64	0.42
1:D:38:ASN:O	1:D:39:ASP:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:HD23	1:C:68:LEU:HA	1.91	0.42
1:C:124:ILE:HD12	1:C:125:VAL:O	2.20	0.42
1:B:49:ASN:O	1:B:52:ASN:OD1	2.37	0.42
1:C:137:VAL:CG2	2:C:258:HOH:O	2.65	0.42
1:C:73:GLN:HE22	1:C:84:LYS:CA	2.29	0.42
1:A:132:GLU:H	1:A:135:GLN:NE2	2.18	0.42
1:C:146:MSE:HE3	1:C:171:GLU:HG3	2.01	0.42
1:A:73:GLN:NE2	1:A:85:LEU:N	2.67	0.42
1:A:13:VAL:HG22	1:B:48:PHE:CD2	2.54	0.41
1:B:104:HIS:HB3	1:B:107:ALA:HB3	2.02	0.41
1:A:7:LYS:N	2:A:235:HOH:O	2.52	0.41
1:A:67:THR:CG2	2:A:232:HOH:O	2.68	0.41
1:C:13:VAL:HG22	1:D:48:PHE:CD2	2.55	0.41
1:A:137:VAL:CG2	1:A:138:VAL:N	2.83	0.41
1:B:73:GLN:NE2	1:B:85:LEU:N	2.64	0.41
1:C:35:GLU:HG3	1:C:45:TYR:CE1	2.56	0.41
1:A:97:TYR:OH	1:A:134:GLY:HA2	2.20	0.41
1:A:131:VAL:HA	1:A:135:GLN:HE22	1.85	0.41
1:C:186:LEU:HB3	1:C:190:TYR:CD1	2.56	0.41
1:B:196:PHE:CZ	1:C:169:MSE:HE2	2.40	0.41
1:D:117:VAL:O	1:D:118:ALA:HB3	2.21	0.41
1:D:177:ALA:HA	1:D:178:PRO:HD3	1.89	0.41
1:D:124:ILE:HD11	1:D:126:CYS:HB2	2.01	0.41
1:A:169:MSE:HE2	1:D:196:PHE:CZ	2.47	0.41
1:B:32:ASP:O	1:B:48:PHE:HD1	2.04	0.41
1:D:73:GLN:HE22	1:D:84:LYS:CA	2.28	0.41
1:A:35:GLU:HG3	1:A:45:TYR:CE1	2.55	0.41
1:A:38:ASN:O	1:A:39:ASP:CB	2.66	0.41
1:A:65:THR:HB	2:A:232:HOH:O	2.20	0.41
1:A:67:THR:HG22	2:A:232:HOH:O	2.20	0.41
1:B:25:TYR:CD1	1:B:36:ILE:HD11	2.55	0.41
1:B:73:GLN:HE22	1:B:84:LYS:CA	2.31	0.41
1:B:138:VAL:HG11	1:B:184:MSE:CE	2.50	0.41
1:C:6:ASN:ND2	1:C:171:GLU:OE2	2.53	0.41
1:C:49:ASN:O	1:C:52:ASN:OD1	2.38	0.41
1:C:137:VAL:CG2	1:C:138:VAL:N	2.84	0.41
1:D:25:TYR:CD1	1:D:36:ILE:HD11	2.56	0.41
1:D:158:ARG:NE	2:D:203:HOH:O	2.28	0.41
1:D:7:LYS:HB2	1:D:7:LYS:HE3	1.86	0.41
1:D:146:MSE:HE3	1:D:171:GLU:HG3	2.03	0.41
1:D:186:LEU:HB3	1:D:190:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLN:HE22	1:C:150:MSE:HG3	1.84	0.40
1:A:88:ASP:OD2	1:A:88:ASP:C	2.63	0.40
1:B:97:TYR:OH	1:B:134:GLY:HA2	2.21	0.40
1:C:131:VAL:HA	1:C:135:GLN:HE22	1.86	0.40
1:D:24:GLU:H	1:D:24:GLU:HG3	1.53	0.40
1:D:124:ILE:HD12	1:D:125:VAL:O	2.21	0.40
1:A:1:MSE:HG2	1:B:64:LEU:CD1	2.52	0.40
1:A:49:ASN:O	1:A:52:ASN:OD1	2.39	0.40
1:A:104:HIS:HB3	1:A:107:ALA:HB3	2.02	0.40
1:C:28:VAL:C	2:C:228:HOH:O	2.64	0.40
1:C:145:VAL:HG23	1:C:145:VAL:O	2.22	0.40
1:D:131:VAL:HA	1:D:135:GLN:HE22	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/199 (96%)	173 (91%)	16 (8%)	2 (1%)	12	32
1	B	191/199 (96%)	170 (89%)	18 (9%)	3 (2%)	7	20
1	C	191/199 (96%)	170 (89%)	15 (8%)	6 (3%)	3	8
1	D	191/199 (96%)	170 (89%)	18 (9%)	3 (2%)	7	20
All	All	764/796 (96%)	683 (89%)	67 (9%)	14 (2%)	6	18

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	B	62	ILE
1	B	88	ASP

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Mol	Chain	Res	Type
1	C	62	ILE
1	D	62	ILE
1	C	21	THR
1	A	39	ASP
1	B	39	ASP
1	C	39	ASP
1	D	39	ASP
1	C	86	ASP
1	C	87	ALA
1	D	7	LYS
1	C	23	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

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	189/199 (94%)	0.74	20 (10%) 11 9	6, 20, 37, 51	0
1	B	189/199 (94%)	0.65	21 (11%) 10 8	4, 18, 36, 52	0
1	C	189/199 (94%)	0.76	23 (12%) 8 7	5, 18, 35, 52	0
1	D	189/199 (94%)	0.82	24 (12%) 8 7	5, 20, 36, 51	0
All	All	756/796 (94%)	0.74	88 (11%) 9 8	4, 19, 37, 52	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	HIS	6.1
1	A	62	ILE	6.1
1	D	62	ILE	6.1
1	A	61	HIS	5.6
1	C	62	ILE	5.0
1	C	61	HIS	4.9
1	D	39	ASP	4.8
1	A	21	THR	4.1
1	B	61	HIS	3.8
1	D	26	ASN	3.6
1	C	30	GLN	3.6
1	B	86	ASP	3.5
1	C	21	THR	3.5
1	D	153	LYS	3.4
1	A	189	ASP	3.4
1	D	88	ASP	3.4
1	C	39	ASP	3.3
1	B	62	ILE	3.3
1	B	147	PRO	3.2
1	C	107	ALA	3.2
1	C	108	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	180	GLU	3.0
1	C	57	THR	3.0
1	C	153	LYS	3.0
1	D	170	LYS	3.0
1	A	26	ASN	3.0
1	D	108	ASP	3.0
1	B	64	LEU	2.9
1	C	86	ASP	2.9
1	D	189	ASP	2.9
1	A	106	ASP	2.8
1	B	149	GLY	2.8
1	D	41	GLU	2.8
1	B	148	SER	2.8
1	D	63	LYS	2.8
1	A	4	PHE	2.8
1	C	20	PRO	2.7
1	B	48	PHE	2.7
1	A	63	LYS	2.7
1	B	24	GLU	2.7
1	A	48	PHE	2.7
1	A	107	ALA	2.6
1	A	153	LYS	2.6
1	A	24	GLU	2.6
1	C	106	ASP	2.6
1	B	66	GLU	2.6
1	D	149	GLY	2.6
1	C	19	ASN	2.6
1	B	106	ASP	2.5
1	B	80	GLY	2.5
1	C	176	ASN	2.5
1	A	41	GLU	2.5
1	B	84	LYS	2.5
1	C	189	ASP	2.5
1	B	180	GLU	2.5
1	C	40	GLY	2.5
1	C	48	PHE	2.5
1	D	178	PRO	2.4
1	C	194	GLN	2.4
1	D	52	ASN	2.4
1	B	107	ALA	2.4
1	D	177	ALA	2.4
1	A	64	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	24	GLU	2.3
1	B	170	LYS	2.3
1	C	25	TYR	2.3
1	D	145	VAL	2.3
1	B	177	ALA	2.2
1	A	170	LYS	2.2
1	C	177	ALA	2.2
1	D	188	ASP	2.2
1	A	40	GLY	2.2
1	D	147	PRO	2.1
1	B	52	ASN	2.1
1	D	174	LEU	2.1
1	D	182	GLY	2.1
1	B	151	VAL	2.1
1	D	4	PHE	2.1
1	B	87	ALA	2.1
1	D	57	THR	2.1
1	B	189	ASP	2.1
1	A	22	GLU	2.0
1	D	119	THR	2.0
1	C	147	PRO	2.0
1	A	56	LEU	2.0
1	A	145	VAL	2.0
1	A	179	GLN	2.0
1	C	76	ILE	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 ⓘ

There are no such residues in this entry.