



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:05 PM UTC

PDB ID : 6K6S / pdb_00006k6s
Title : Structure of RNase J1 from Staphylococcus epidermidis
Authors : Raj, R.; Gopal, B.
Deposited on : 2019-06-04
Resolution : 2.99 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

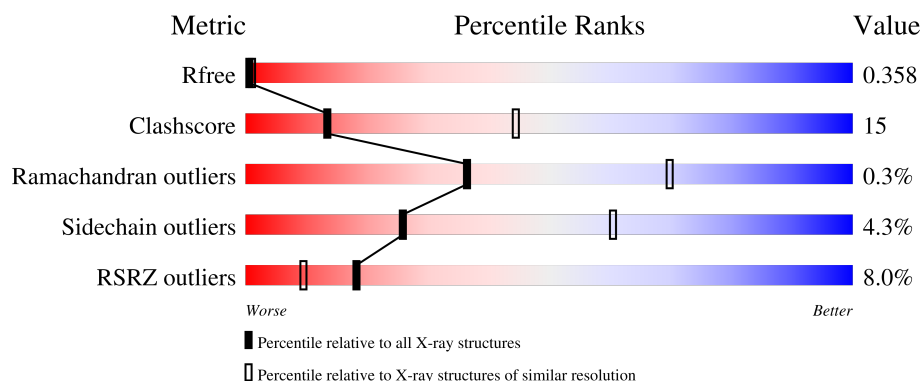
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	574	5% 57% 18% • 23%
1	B	574	7% 63% 13% • 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5837 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 Ribonuclease J 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			2972	1879	522	562	9			
1	B	441	Total	C	N	O	S	0	0	0
			2861	1796	509	549	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q8CT16
A	-12	GLY	-	expression tag	UNP Q8CT16
A	-11	SER	-	expression tag	UNP Q8CT16
A	-10	SER	-	expression tag	UNP Q8CT16
A	-9	HIS	-	expression tag	UNP Q8CT16
A	-8	HIS	-	expression tag	UNP Q8CT16
A	-7	HIS	-	expression tag	UNP Q8CT16
A	-6	HIS	-	expression tag	UNP Q8CT16
A	-5	HIS	-	expression tag	UNP Q8CT16
A	-4	HIS	-	expression tag	UNP Q8CT16
A	-3	SER	-	expression tag	UNP Q8CT16
A	-2	GLN	-	expression tag	UNP Q8CT16
A	-1	ASP	-	expression tag	UNP Q8CT16
A	0	PRO	-	expression tag	UNP Q8CT16
B	-13	MET	-	initiating methionine	UNP Q8CT16
B	-12	GLY	-	expression tag	UNP Q8CT16
B	-11	SER	-	expression tag	UNP Q8CT16
B	-10	SER	-	expression tag	UNP Q8CT16
B	-9	HIS	-	expression tag	UNP Q8CT16
B	-8	HIS	-	expression tag	UNP Q8CT16
B	-7	HIS	-	expression tag	UNP Q8CT16
B	-6	HIS	-	expression tag	UNP Q8CT16
B	-5	HIS	-	expression tag	UNP Q8CT16
B	-4	HIS	-	expression tag	UNP Q8CT16
B	-3	SER	-	expression tag	UNP Q8CT16

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP Q8CT16
B	-1	ASP	-	expression tag	UNP Q8CT16
B	0	PRO	-	expression tag	UNP Q8CT16

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.07Å 86.07Å 486.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.58 – 2.99 50.58 – 2.99	Depositor EDS
% Data completeness (in resolution range)	84.0 (50.58-2.99) 84.0 (50.58-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.297 , 0.337 0.321 , 0.358	Depositor DCC
R_{free} test set	971 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 127.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5837	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.46	0/3036	0.97	10/4174 (0.2%)
1	B	0.42	0/2922	0.93	7/4026 (0.2%)
All	All	0.44	0/5958	0.95	17/8200 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	LEU	N-CA-C	-8.66	101.84	111.28
1	A	60	LEU	N-CA-C	-8.06	100.13	110.53
1	B	203	ASP	N-CA-C	6.80	118.07	108.00
1	B	257	ARG	N-CA-C	6.39	118.24	111.28
1	A	361	SER	N-CA-C	-6.18	98.83	108.90
1	A	68	VAL	N-CA-C	6.11	117.66	111.00
1	A	67	ILE	N-CA-C	5.55	117.62	109.63
1	A	62	GLN	N-CA-C	-5.52	105.26	111.28
1	B	358	SER	N-CA-C	5.30	116.74	111.07
1	A	202	PRO	CA-N-CD	-5.29	104.59	112.00
1	A	65	ASP	N-CA-C	5.27	118.81	112.38
1	B	255	PHE	O-C-N	-5.20	116.47	123.23
1	B	28	GLU	N-CA-C	5.18	117.69	109.50
1	A	425	THR	N-CA-C	-5.16	101.52	109.52
1	B	36	ILE	N-CA-C	5.12	115.34	110.53
1	A	281	GLU	CA-C-N	5.05	125.33	119.47
1	A	281	GLU	C-N-CA	5.05	125.33	119.47

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	2972	0	2478	91	0
1	B	2861	0	2249	65	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	5837	0	4727	155	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 15.

All (155) 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:A:307:ALA:O	1:A:311:ILE:HG13	1.52	1.08
1:A:71:PHE:CE2	1:A:135:ILE:HD11	1.95	1.00
1:A:135:ILE:HG22	1:A:152:VAL:HG12	1.51	0.93
1:A:202:PRO:HB3	1:A:371:GLN:OE1	1.71	0.91
1:B:204:PHE:CE1	1:B:372:GLY:C	2.51	0.88
1:B:145:PRO:HG2	1:B:235:ILE:HD11	1.57	0.86
1:A:300:SER:HB2	1:A:331:SER:HB3	1.57	0.85
1:A:311:ILE:HG23	1:A:319:ILE:O	1.77	0.85
1:A:135:ILE:CG2	1:A:152:VAL:HG12	2.08	0.82
1:B:41:LYS:C	1:B:42:PHE:HD1	1.91	0.77
1:B:299:GLY:HA3	1:B:308:LEU:CB	2.17	0.75
1:B:308:LEU:O	1:B:311:ILE:HG22	1.87	0.74
1:A:425:THR:OG1	1:A:428:SER:CB	2.39	0.71
1:B:140:THR:HG22	1:B:141:THR:N	2.06	0.71
1:A:33:ILE:HG22	1:A:67:ILE:HA	1.71	0.71
1:B:140:THR:HG21	1:B:165:PHE:HB2	1.74	0.69
1:A:140:THR:HG22	1:A:141:THR:N	2.07	0.69
1:A:33:ILE:HG22	1:A:67:ILE:CA	2.23	0.68
1:A:272:ILE:HD13	1:A:272:ILE:C	2.18	0.68
1:A:275:PRO:CB	1:A:276:PRO:HA	2.24	0.68
1:A:266:GLY:C	1:A:272:ILE:HG22	2.18	0.67
1:A:139:LEU:HG	1:A:140:THR:N	2.09	0.67
1:B:304:PRO:HG2	1:B:305:MET:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLY:C	1:A:272:ILE:CG2	2.69	0.66
1:B:257:ARG:HH12	1:B:306:ALA:HA	1.61	0.66
1:B:372:GLY:HA2	1:B:375:GLN:HE21	1.61	0.65
1:B:257:ARG:NH1	1:B:306:ALA:HA	2.12	0.65
1:A:140:THR:HG21	1:A:165:PHE:HB2	1.77	0.65
1:A:276:PRO:HG2	1:A:277:GLU:H	1.61	0.65
1:B:204:PHE:CE1	1:B:373:ASP:N	2.64	0.64
1:A:257:ARG:NH2	1:A:305:MET:O	2.22	0.64
1:B:378:LEU:HD21	1:B:403:GLY:HA2	1.80	0.62
1:A:425:THR:OG1	1:A:428:SER:N	2.33	0.62
1:A:276:PRO:HG2	1:A:277:GLU:N	2.15	0.61
1:A:256:GLY:O	1:A:260:GLU:N	2.32	0.61
1:A:43:PRO:HB2	1:A:46:ASN:CB	2.31	0.60
1:B:304:PRO:HG2	1:B:305:MET:N	2.16	0.60
1:A:345:ILE:HA	1:A:348:LEU:HD12	1.83	0.60
1:A:12:TYR:OH	1:A:33:ILE:HD11	2.01	0.60
1:A:272:ILE:HG23	1:A:272:ILE:O	2.01	0.59
1:A:309:SER:O	1:A:313:ASN:HB2	2.03	0.58
1:B:304:PRO:CG	1:B:305:MET:H	2.16	0.58
1:B:145:PRO:HG2	1:B:235:ILE:CD1	2.32	0.57
1:B:7:ASN:O	1:B:7:ASN:ND2	2.38	0.57
1:B:257:ARG:NH1	1:B:305:MET:O	2.39	0.56
1:A:71:PHE:CE2	1:A:135:ILE:CD1	2.79	0.56
1:B:143:SER:O	1:B:234:ASN:ND2	2.39	0.56
1:A:139:LEU:HG	1:A:140:THR:H	1.70	0.55
1:A:266:GLY:O	1:A:272:ILE:HG22	2.07	0.54
1:A:140:THR:CG2	1:A:141:THR:N	2.71	0.54
1:A:28:GLU:CB	1:A:33:ILE:HG13	2.38	0.54
1:A:144:ILE:HD12	1:A:145:PRO:HD2	1.90	0.53
1:A:435:ILE:HG13	1:A:436:PRO:HD2	1.90	0.53
1:B:306:ALA:O	1:B:307:ALA:HB3	2.08	0.53
1:A:159:ILE:HG23	1:A:191:CYS:HB3	1.91	0.52
1:B:140:THR:CG2	1:B:141:THR:N	2.73	0.52
1:B:328:VAL:HG22	1:B:356:ILE:HD12	1.90	0.52
1:A:71:PHE:CZ	1:A:135:ILE:HD11	2.43	0.52
1:A:203:ASP:O	1:A:372:GLY:N	2.42	0.52
1:A:143:SER:O	1:A:234:ASN:ND2	2.43	0.52
1:A:256:GLY:O	1:A:260:GLU:HB2	2.10	0.52
1:B:42:PHE:CD1	1:B:42:PHE:N	2.77	0.52
1:B:42:PHE:HD1	1:B:42:PHE:N	2.08	0.51
1:B:259:MET:HA	1:B:262:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:PRO:CG	1:B:305:MET:N	2.70	0.51
1:A:341:ILE:O	1:A:345:ILE:HG13	2.11	0.51
1:A:140:THR:CG2	1:A:165:PHE:HB2	2.40	0.51
1:A:41:LYS:HD2	1:A:43:PRO:HG3	1.93	0.50
1:A:189:VAL:HG21	1:A:381:ILE:HG23	1.93	0.50
1:B:308:LEU:O	1:B:311:ILE:CG2	2.58	0.50
1:A:275:PRO:HB3	1:A:276:PRO:HA	1.92	0.50
1:A:18:GLY:HA2	1:A:392:GLU:HA	1.94	0.50
1:A:276:PRO:CG	1:A:277:GLU:H	2.25	0.50
1:B:159:ILE:HG23	1:B:191:CYS:HB3	1.94	0.49
1:A:291:HIS:CE1	1:A:292:GLU:HG2	2.47	0.49
1:B:381:ILE:O	1:B:383:PRO:HD3	2.12	0.49
1:A:381:ILE:O	1:A:383:PRO:HD3	2.12	0.49
1:B:41:LYS:C	1:B:42:PHE:CD1	2.82	0.49
1:B:238:VAL:HG13	1:B:296:LEU:HD21	1.95	0.49
1:B:18:GLY:HA2	1:B:392:GLU:HA	1.94	0.49
1:B:298:THR:O	1:B:308:LEU:CB	2.60	0.49
1:A:289:PRO:HB2	1:A:292:GLU:HG3	1.94	0.49
1:B:401:GLU:O	1:B:404:VAL:HG12	2.13	0.48
1:A:276:PRO:CG	1:A:277:GLU:N	2.76	0.48
1:B:140:THR:HG22	1:B:141:THR:H	1.75	0.48
1:A:312:ALA:HA	1:A:321:ILE:HD11	1.96	0.48
1:A:342:ASN:O	1:A:346:ASN:ND2	2.46	0.48
1:B:399:HIS:HA	1:B:402:THR:HG22	1.94	0.48
1:B:73:THR:OG1	1:B:74:HIS:N	2.47	0.48
1:B:257:ARG:HH12	1:B:306:ALA:CA	2.26	0.48
1:A:151:ILE:HG22	1:A:160:VAL:HG22	1.95	0.48
1:A:327:VAL:HG21	1:A:348:LEU:HD22	1.96	0.48
1:B:341:ILE:O	1:B:344:THR:OG1	2.23	0.48
1:A:180:LYS:HA	1:A:183:GLN:HG2	1.96	0.47
1:A:96:GLY:O	1:A:121:GLU:HA	2.14	0.47
1:A:256:GLY:O	1:A:260:GLU:CB	2.62	0.47
1:B:200:LEU:HD11	1:B:394:ARG:HG2	1.96	0.47
1:B:345:ILE:HA	1:B:348:LEU:HD12	1.96	0.47
1:A:135:ILE:HG22	1:A:152:VAL:CG1	2.35	0.47
1:A:203:ASP:O	1:A:372:GLY:HA3	2.15	0.47
1:A:388:PRO:HG2	1:A:396:LEU:HG	1.97	0.47
1:A:330:SER:O	1:A:364:HIS:CG	2.68	0.46
1:A:399:HIS:HA	1:A:402:THR:HG22	1.97	0.46
1:A:73:THR:OG1	1:A:74:HIS:N	2.49	0.46
1:A:275:PRO:CB	1:A:276:PRO:CA	2.91	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HG12	1:A:294:LEU:HD23	1.98	0.46
1:B:140:THR:CG2	1:B:165:PHE:HB2	2.44	0.46
1:B:24:THR:HG23	1:B:37:ASP:O	2.16	0.46
1:A:140:THR:HG22	1:A:141:THR:H	1.78	0.46
1:A:272:ILE:HD13	1:A:272:ILE:O	2.17	0.45
1:A:30:LYS:CB	1:A:132:HIS:NE2	2.79	0.45
1:A:291:HIS:ND1	1:A:292:GLU:HG2	2.32	0.45
1:A:346:ASN:HD21	1:B:394:ARG:NH1	2.14	0.44
1:B:189:VAL:HG21	1:B:381:ILE:HG23	1.98	0.44
1:A:14:LEU:HD12	1:A:55:PRO:HB2	1.99	0.44
1:A:52:TYR:CE2	1:A:444:GLY:HA3	2.52	0.44
1:A:178:ILE:HG23	1:A:380:LEU:HD21	2.00	0.44
1:A:263:ILE:O	1:A:267:MET:N	2.47	0.44
1:A:81:GLY:HA2	1:A:107:LYS:NZ	2.33	0.44
1:B:6:SER:O	1:B:8:GLU:HG2	2.17	0.44
1:B:414:PHE:HE2	1:B:429:ALA:HB1	1.83	0.44
1:B:59:TYR:HB2	1:B:436:PRO:HG2	2.00	0.44
1:A:272:ILE:C	1:A:272:ILE:CD1	2.85	0.43
1:B:129:LYS:HA	1:B:134:GLU:HA	2.00	0.43
1:B:25:TYR:CE2	1:B:389:ILE:HD12	2.53	0.43
1:B:100:ALA:O	1:B:104:ILE:HG13	2.18	0.43
1:B:40:ILE:HG22	1:B:54:ILE:HD13	2.01	0.43
1:B:345:ILE:HD13	1:B:355:VAL:HG11	2.00	0.43
1:A:135:ILE:O	1:A:135:ILE:HG13	2.16	0.42
1:A:202:PRO:HA	1:A:203:ASP:HA	1.63	0.42
1:B:144:ILE:HD12	1:B:145:PRO:HD2	2.00	0.42
1:B:143:SER:C	1:B:234:ASN:HD22	2.26	0.42
1:B:204:PHE:HE1	1:B:372:GLY:C	2.19	0.42
1:A:15:GLY:HA2	1:A:418:ILE:HD13	2.01	0.42
1:A:257:ARG:H	1:A:257:ARG:HD2	1.84	0.42
1:B:178:ILE:HG23	1:B:380:LEU:HD21	2.01	0.42
1:A:203:ASP:O	1:A:372:GLY:CA	2.68	0.42
1:A:301:GLN:NE2	1:A:331:SER:HB2	2.35	0.42
1:B:303:GLU:H	1:B:303:GLU:HG3	1.69	0.42
1:B:145:PRO:HG3	1:B:236:TYR:CE1	2.54	0.42
1:A:139:LEU:HA	1:A:139:LEU:HD12	1.88	0.41
1:A:25:TYR:CE2	1:A:389:ILE:HD12	2.55	0.41
1:A:40:ILE:HG22	1:A:54:ILE:HD13	2.01	0.41
1:B:204:PHE:CZ	1:B:372:GLY:HA3	2.55	0.41
1:B:204:PHE:CZ	1:B:372:GLY:C	2.97	0.41
1:A:140:THR:CG2	1:A:141:THR:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:HG23	1:A:37:ASP:O	2.20	0.41
1:B:204:PHE:CE1	1:B:372:GLY:CA	3.03	0.41
1:B:304:PRO:CD	1:B:305:MET:H	2.34	0.40
1:B:378:LEU:CD2	1:B:403:GLY:HA2	2.50	0.40
1:A:10:GLY:O	1:A:27:VAL:HA	2.21	0.40
1:B:238:VAL:O	1:B:242:VAL:HG23	2.22	0.40
1:A:53:VAL:HG23	1:A:439:ASN:HB3	2.04	0.40
1:A:60:LEU:O	1:A:61:GLU:CB	2.70	0.40
1:A:235:ILE:HA	1:A:238:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/574 (77%)	406 (92%)	33 (8%)	2 (0%)	24	60
1	B	439/574 (76%)	408 (93%)	30 (7%)	1 (0%)	43	76
All	All	880/1148 (77%)	814 (92%)	63 (7%)	3 (0%)	36	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	PRO
1	A	202	PRO
1	A	333	PRO

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	236/497 (48%)	224 (95%)	12 (5%)	21	55
1	B	206/497 (41%)	199 (97%)	7 (3%)	32	66
All	All	442/994 (44%)	423 (96%)	19 (4%)	26	60

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	132	HIS
1	A	202	PRO
1	A	203	ASP
1	A	237	ARG
1	A	272	ILE
1	A	292	GLU
1	A	322	ILE
1	A	380	LEU
1	A	396	LEU
1	A	413	VAL
1	A	435	ILE
1	B	8	GLU
1	B	53	VAL
1	B	237	ARG
1	B	257	ARG
1	B	345	ILE
1	B	380	LEU
1	B	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	183	GLN
1	A	313	ASN
1	A	346	ASN
1	A	374	GLN
1	B	111	HIS
1	B	337	ASN
1	B	362	ASN

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Mol	Chain	Res	Type
1	B	374	GLN
1	B	375	GLN
1	B	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	443/574 (77%)	0.62	29 (6%)	25 13	26, 100, 128, 184	0
1	B	441/574 (76%)	0.73	42 (9%)	14 7	30, 103, 140, 201	0
All	All	884/1148 (77%)	0.67	71 (8%)	18 9	26, 102, 136, 201	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	TYR	7.8
1	B	14	LEU	6.8
1	A	14	LEU	5.9
1	B	46	ASN	5.2
1	B	29	TYR	4.6
1	B	72	ILE	3.8
1	B	161	HIS	3.8
1	B	39	GLY	3.5
1	A	276	PRO	3.5
1	A	12	TYR	3.5
1	A	193	LEU	3.5
1	B	306	ALA	3.4
1	A	27	VAL	3.3
1	A	330	SER	3.3
1	B	104	ILE	3.3
1	B	92	VAL	3.2
1	B	307	ALA	3.1
1	B	52	TYR	3.1
1	A	366	SER	3.1
1	A	329	PHE	3.0
1	A	334	ILE	3.0
1	B	348	LEU	2.9
1	B	329	PHE	2.9
1	A	160	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	45	ASP	2.9
1	A	443	ASP	2.8
1	B	357	HIS	2.8
1	A	59	TYR	2.7
1	B	402	THR	2.6
1	B	336	GLY	2.6
1	B	230	THR	2.6
1	B	358	SER	2.6
1	B	100	ALA	2.6
1	A	83	VAL	2.6
1	B	51	ASP	2.5
1	B	120	HIS	2.5
1	B	31	ASP	2.4
1	B	75	GLY	2.4
1	A	258	SER	2.4
1	B	181	MET	2.4
1	A	161	HIS	2.4
1	B	47	LEU	2.4
1	B	168	ASP	2.3
1	A	303	GLU	2.3
1	A	53	VAL	2.3
1	B	49	GLY	2.3
1	A	192	LEU	2.3
1	A	80	ILE	2.3
1	A	315	THR	2.3
1	B	99	LEU	2.3
1	A	61	GLU	2.2
1	B	50	ILE	2.2
1	A	377	MET	2.2
1	B	101	LEU	2.2
1	B	95	TYR	2.2
1	A	302	GLY	2.2
1	B	137	PHE	2.2
1	B	122	ILE	2.1
1	B	159	ILE	2.1
1	A	58	THR	2.1
1	A	154	THR	2.1
1	A	86	LEU	2.1
1	A	133	PHE	2.1
1	B	117	THR	2.1
1	B	333	PRO	2.1
1	A	91	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASP	2.1
1	B	377	MET	2.0
1	B	337	ASN	2.0
1	B	428	SER	2.0
1	A	51	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	B	601	1/1	0.96	0.08	82,82,82,82	0
2	MN	B	602	1/1	0.96	0.12	77,77,77,77	0
2	MN	A	601	1/1	0.98	0.09	65,65,65,65	0
2	MN	A	602	1/1	0.98	0.05	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.