



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:59 AM UTC

PDB ID : 3C0K / pdb_00003c0k
Title : Crystal Structure of a ribosomal RNA methyltransferase
Authors : Subramanian, S.; Jayaraman, S.; Bujnicki, J.
Deposited on : 2008-01-21
Resolution : 2.00 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

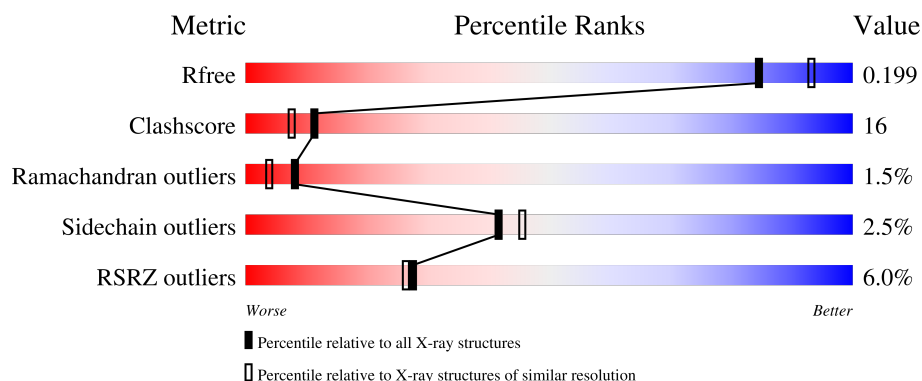
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	396	8% 65% 30% .
1	B	396	4% 73% 24% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6587 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 UPF0064 protein yccW.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	Se	0	0	0
			3064	1933	547	570	6	8			
1	B	395	Total	C	N	O	S	Se	0	0	0
			3065	1934	547	570	6	8			

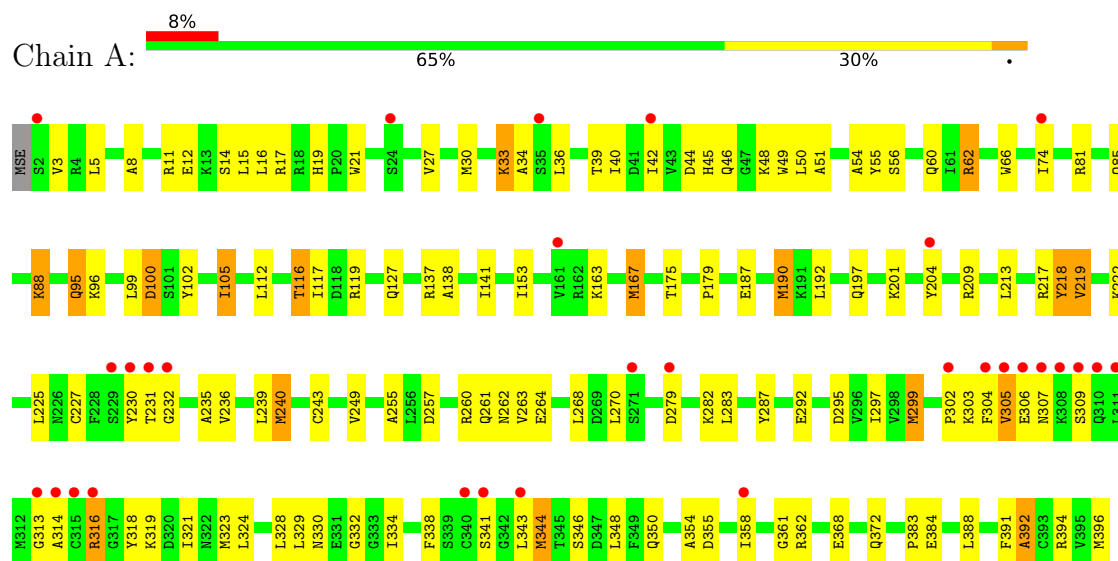
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	164	Total	O	0	0
			164	164		
2	B	294	Total	O	0	0
			294	294		

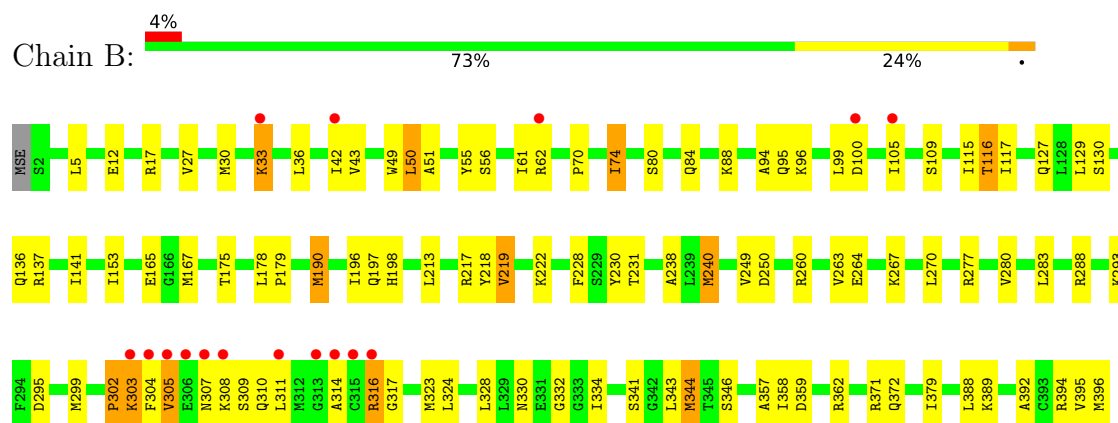
3 Residue-property plots

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: UPF0064 protein yccW



• Molecule 1: UPF0064 protein yccW



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.31Å 80.88Å 66.16Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	42.25 – 2.00 42.25 – 2.04	Depositor EDS
% Data completeness (in resolution range)	92.9 (42.25-2.00) 99.6 (42.25-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.242 0.203 , 0.199	Depositor DCC
R_{free} test set	2157 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6587	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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	0.52	8/3111 (0.3%)	0.91	8/4179 (0.2%)
1	B	0.54	8/3112 (0.3%)	0.94	9/4181 (0.2%)
All	All	0.53	16/6223 (0.3%)	0.92	17/8360 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	MSE	SE-CE	-8.42	1.70	1.95
1	B	167	MSE	SE-CE	-7.29	1.73	1.95
1	A	299	MSE	SE-CE	-6.53	1.75	1.95
1	B	190	MSE	SE-CE	-6.52	1.75	1.95
1	A	240	MSE	SE-CE	-6.48	1.76	1.95
1	A	323	MSE	SE-CE	-6.43	1.76	1.95
1	B	323	MSE	SE-CE	-6.24	1.76	1.95
1	B	344	MSE	SE-CE	-5.83	1.77	1.95
1	B	299	MSE	SE-CE	-5.72	1.78	1.95
1	A	344	MSE	SE-CE	-5.44	1.79	1.95
1	A	396	MSE	SE-CE	-5.40	1.79	1.95
1	A	190	MSE	SE-CE	-5.37	1.79	1.95
1	A	167	MSE	SE-CE	-5.36	1.79	1.95
1	A	344	MSE	CG-SE	-5.30	1.79	1.95
1	B	396	MSE	SE-CE	-5.25	1.79	1.95
1	B	344	MSE	CG-SE	-5.23	1.79	1.95

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	VAL	N-CA-C	11.62	124.34	112.83
1	B	317	GLY	N-CA-C	-11.62	100.25	114.66
1	B	219	VAL	N-CA-C	10.80	123.53	112.83
1	A	201	LYS	CB-CA-C	-6.59	108.26	117.23
1	A	100	ASP	N-CA-C	-6.30	104.06	112.94
1	B	100	ASP	N-CA-C	-6.04	105.73	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ILE	N-CA-C	-6.01	99.78	106.21
1	A	60	GLN	N-CA-C	-5.99	104.87	111.82
1	A	338	PHE	N-CA-C	5.50	117.77	109.41
1	A	218	TYR	N-CA-C	5.39	119.85	113.28
1	A	392	ALA	N-CA-C	-5.37	99.77	108.52
1	B	56	SER	CA-C-N	5.35	125.16	119.28
1	B	56	SER	C-N-CA	5.35	125.16	119.28
1	B	196	ILE	N-CA-C	5.31	115.52	110.42
1	B	392	ALA	N-CA-C	-5.22	100.00	108.52
1	B	129	LEU	N-CA-C	5.09	119.76	113.50
1	A	17	ARG	N-CA-C	-5.07	106.88	113.16

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	3064	0	3031	122	0
1	B	3065	0	3035	88	0
2	A	164	0	0	5	0
2	B	294	0	0	7	0
All	All	6587	0	6066	198	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 16.

All (198) 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:116:THR:HG23	1:A:127:GLN:HB2	1.27	1.14
1:B:116:THR:HG23	1:B:127:GLN:HB2	1.27	1.14
1:B:33:LYS:H	1:B:33:LYS:HE2	1.12	1.12
1:B:42:ILE:HD11	1:B:51:ALA:HB3	1.30	1.06
1:A:341:SER:HB2	1:A:343:LEU:HD13	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:THR:CG2	1:B:127:GLN:HB2	2.01	0.89
1:A:39:THR:OG1	1:A:74:ILE:HD11	1.75	0.87
1:B:105:ILE:HD11	1:B:115:ILE:HG22	1.61	0.82
1:A:5:LEU:HD21	1:A:27:VAL:HG22	1.62	0.80
1:A:316:ARG:NE	1:A:316:ARG:HA	1.97	0.80
1:A:105:ILE:HG23	1:A:117:ILE:HB	1.65	0.79
1:B:5:LEU:HD21	1:B:27:VAL:HG22	1.66	0.77
1:A:33:LYS:HD3	1:A:33:LYS:H	1.48	0.77
1:B:33:LYS:H	1:B:33:LYS:CE	1.94	0.77
1:A:3:VAL:HG13	1:A:40:ILE:HG22	1.68	0.75
1:B:105:ILE:HG12	1:B:117:ILE:HB	1.69	0.74
1:B:303:LYS:O	1:B:305:VAL:N	2.20	0.73
1:A:316:ARG:HA	1:A:316:ARG:HE	1.54	0.72
1:B:42:ILE:CD1	1:B:51:ALA:HB3	2.13	0.71
1:B:105:ILE:HD11	1:B:117:ILE:HG13	1.72	0.71
1:A:192:LEU:HD13	1:A:204:TYR:OH	1.89	0.70
1:A:227:CYS:SG	1:A:299:MSE:HE2	2.31	0.70
1:B:33:LYS:HE2	1:B:33:LYS:N	1.98	0.69
1:A:346:SER:O	1:A:350:GLN:HG3	1.92	0.69
1:A:8:ALA:HB3	1:A:11:ARG:HG3	1.77	0.67
1:A:3:VAL:HG11	1:A:34:ALA:HB2	1.75	0.67
1:A:116:THR:CG2	1:A:127:GLN:HB2	2.16	0.67
1:B:316:ARG:N	1:B:316:ARG:HD2	2.09	0.66
1:A:15:LEU:HG	1:A:42:ILE:HD12	1.78	0.66
1:B:307:ASN:C	1:B:309:SER:H	2.03	0.66
1:A:42:ILE:CD1	1:A:51:ALA:HB3	2.26	0.66
1:A:74:ILE:O	1:A:74:ILE:HG13	1.96	0.65
1:A:230:TYR:C	1:A:255:ALA:HB1	2.21	0.65
1:A:341:SER:C	1:A:343:LEU:H	2.04	0.65
1:A:42:ILE:HD11	1:A:51:ALA:HB3	1.78	0.64
1:A:88:LYS:HD3	1:B:394:ARG:NH2	2.13	0.64
1:A:119:ARG:HH11	1:A:119:ARG:HG3	1.61	0.63
1:A:355:ASP:O	1:A:358:ILE:HG13	1.98	0.63
1:A:236:VAL:HG23	2:A:546:HOH:O	1.97	0.63
1:A:88:LYS:HD3	1:B:394:ARG:HH21	1.63	0.63
1:A:217:ARG:HG3	1:B:96:LYS:HE2	1.79	0.63
1:B:105:ILE:HD11	1:B:115:ILE:CG2	2.27	0.63
1:A:96:LYS:HE2	1:B:217:ARG:HG3	1.81	0.63
1:A:163:LYS:HD2	1:A:167:MSE:O	1.98	0.62
1:A:42:ILE:HG13	1:A:42:ILE:O	2.00	0.62
1:A:350:GLN:HG2	1:A:391:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:CD1	1:B:115:ILE:HG22	2.28	0.62
1:B:288:ARG:HB2	1:B:328:LEU:HD11	1.82	0.62
1:A:33:LYS:HD3	1:A:33:LYS:N	2.14	0.62
1:B:74:ILE:O	1:B:74:ILE:HG13	1.98	0.62
1:A:287:TYR:CD1	1:A:292:GLU:HG3	2.35	0.61
1:B:74:ILE:HD11	1:B:136:GLN:CD	2.26	0.61
1:A:179:PRO:HG2	1:A:197:GLN:HG3	1.82	0.60
1:B:213:LEU:C	1:B:213:LEU:HD13	2.27	0.59
1:B:137:ARG:O	1:B:141:ILE:HG12	2.02	0.59
1:A:257:ASP:O	1:A:261:GLN:HG3	2.03	0.59
1:B:249:VAL:HG21	1:B:283:LEU:HD23	1.85	0.58
1:B:62:ARG:HH11	1:B:62:ARG:HG2	1.68	0.58
1:A:236:VAL:HG21	1:A:262:ASN:HB3	1.87	0.57
1:A:3:VAL:CG1	1:A:40:ILE:HG22	2.34	0.57
1:A:5:LEU:HG	1:A:30:MSE:SE	2.55	0.57
1:A:249:VAL:HG21	1:A:283:LEU:HD23	1.88	0.56
1:B:12:GLU:HB2	1:B:50:LEU:HD21	1.88	0.55
1:A:287:TYR:HB3	1:A:292:GLU:HB2	1.87	0.55
1:A:44:ASP:OD2	1:A:48:LYS:HB2	2.07	0.55
1:A:350:GLN:HG2	1:A:391:PHE:CE2	2.42	0.54
1:B:190:MSE:HB2	1:B:240:MSE:HE3	1.89	0.54
1:B:55:TYR:OH	1:B:62:ARG:NH2	2.40	0.54
1:B:153:ILE:HB	1:B:175:THR:HG22	1.88	0.54
1:B:260:ARG:O	1:B:264:GLU:HG3	2.07	0.54
1:A:329:LEU:O	1:A:362:ARG:NH1	2.34	0.53
1:A:260:ARG:O	1:A:264:GLU:HG3	2.08	0.53
1:A:316:ARG:NE	1:A:316:ARG:CA	2.71	0.53
1:A:219:VAL:O	1:A:243:CYS:HA	2.08	0.53
1:B:179:PRO:HG2	1:B:197:GLN:HG3	1.89	0.53
1:A:230:TYR:CE1	1:A:231:THR:HG23	2.44	0.52
1:B:178:LEU:HD12	1:B:179:PRO:HD2	1.89	0.52
1:B:388:LEU:C	1:B:388:LEU:HD23	2.34	0.52
1:A:116:THR:HG23	1:A:127:GLN:CB	2.18	0.52
1:B:324:LEU:O	1:B:328:LEU:HD13	2.09	0.52
1:A:88:LYS:CD	1:B:394:ARG:HH21	2.23	0.52
1:A:217:ARG:HH11	1:A:217:ARG:HG2	1.75	0.52
1:B:198:HIS:HD2	2:B:548:HOH:O	1.92	0.52
1:B:346:SER:HB2	1:B:389:LYS:HD2	1.92	0.52
1:A:344:MSE:CB	1:A:348:LEU:HD23	2.40	0.51
1:A:332:GLY:HA3	1:B:88:LYS:HE3	1.93	0.51
1:B:213:LEU:HD13	1:B:213:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LYS:C	1:B:305:VAL:H	2.17	0.51
1:A:230:TYR:CG	1:A:231:THR:N	2.67	0.50
1:B:62:ARG:HG2	1:B:62:ARG:NH1	2.27	0.50
1:B:130:SER:HA	1:B:165:GLU:HG3	1.93	0.50
1:B:218:TYR:CD1	1:B:334:ILE:HD13	2.45	0.50
1:B:362:ARG:HE	1:B:395:VAL:HG11	1.77	0.50
1:B:190:MSE:HG3	1:B:240:MSE:CE	2.42	0.50
1:B:109:SER:HA	1:B:379:ILE:HB	1.94	0.49
1:A:19:HIS:CE1	1:A:21:TRP:HB2	2.47	0.49
1:A:235:ALA:HB3	2:A:546:HOH:O	2.13	0.49
1:A:394:ARG:HH21	1:B:88:LYS:NZ	2.11	0.49
1:A:304:PHE:C	1:A:306:GLU:H	2.20	0.49
1:A:330:ASN:HA	2:A:448:HOH:O	2.13	0.49
1:B:42:ILE:HG12	1:B:51:ALA:O	2.13	0.48
1:A:249:VAL:CG2	1:A:283:LEU:HD23	2.43	0.48
1:A:217:ARG:HG2	1:A:217:ARG:NH1	2.29	0.48
1:A:257:ASP:C	1:A:261:GLN:HE21	2.21	0.48
1:A:88:LYS:HE3	1:B:332:GLY:HA3	1.96	0.48
1:B:116:THR:HG21	2:B:597:HOH:O	2.14	0.48
1:B:309:SER:O	1:B:343:LEU:HD21	2.13	0.48
1:A:153:ILE:HB	1:A:175:THR:HG22	1.95	0.48
1:A:119:ARG:HG3	1:A:119:ARG:NH1	2.28	0.48
1:B:105:ILE:CD1	1:B:115:ILE:CG2	2.90	0.48
1:A:100:ASP:OD2	1:A:100:ASP:C	2.57	0.48
1:A:318:TYR:O	1:A:321:ILE:HG22	2.13	0.48
1:B:49:TRP:CZ3	1:B:70:PRO:HG3	2.48	0.47
1:A:30:MSE:HE2	1:A:55:TYR:CE1	2.49	0.47
1:A:222:LYS:HB3	1:A:295:ASP:HB2	1.96	0.47
1:B:74:ILE:HD11	1:B:136:GLN:HG3	1.96	0.47
1:A:12:GLU:HB2	1:A:50:LEU:HD21	1.96	0.47
1:A:316:ARG:HG3	1:A:319:LYS:HD3	1.95	0.47
1:A:12:GLU:O	1:A:16:LEU:HG	2.15	0.47
1:A:341:SER:C	1:A:343:LEU:N	2.71	0.47
1:B:105:ILE:HG12	1:B:117:ILE:CB	2.43	0.47
1:A:102:TYR:CZ	1:A:119:ARG:HD3	2.51	0.46
1:B:222:LYS:HB3	1:B:295:ASP:HB2	1.97	0.46
1:A:96:LYS:CE	1:B:217:ARG:HG3	2.44	0.46
1:A:383:PRO:HG2	1:A:384:GLU:OE1	2.15	0.46
1:A:102:TYR:OH	1:A:119:ARG:HD3	2.15	0.46
1:A:39:THR:OG1	1:A:74:ILE:CD1	2.57	0.46
1:A:105:ILE:CD1	1:A:112:LEU:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:C	1:A:305:VAL:H	2.24	0.46
1:B:302:PRO:O	1:B:303:LYS:C	2.59	0.46
1:A:81:ARG:O	1:A:85:GLN:HG3	2.16	0.46
1:A:299:MSE:CE	1:A:321:ILE:HG13	2.45	0.46
2:A:768:HOH:O	1:B:358:ILE:HD12	2.16	0.45
1:A:99:LEU:HD23	1:A:187:GLU:HA	1.98	0.45
1:B:362:ARG:CZ	2:B:695:HOH:O	2.63	0.45
1:B:341:SER:OG	1:B:344:MSE:HG2	2.16	0.45
1:A:42:ILE:HG12	1:A:51:ALA:O	2.16	0.45
1:B:330:ASN:HA	2:B:709:HOH:O	2.15	0.45
1:B:250:ASP:O	1:B:277:ARG:HA	2.16	0.45
1:A:324:LEU:O	1:A:328:LEU:HD13	2.17	0.45
1:A:368:GLU:HB3	1:A:392:ALA:HB3	1.98	0.45
1:B:305:VAL:C	1:B:307:ASN:H	2.24	0.45
1:A:218:TYR:CD1	1:A:334:ILE:HD13	2.52	0.45
1:B:362:ARG:NE	2:B:695:HOH:O	2.50	0.45
1:A:33:LYS:N	1:A:33:LYS:CD	2.79	0.45
1:A:56:SER:O	1:A:62:ARG:HD2	2.17	0.45
1:A:105:ILE:HD13	1:A:112:LEU:HB2	1.98	0.45
1:A:137:ARG:O	1:A:141:ILE:HG12	2.17	0.45
1:A:187:GLU:HG3	1:A:187:GLU:O	2.17	0.44
1:B:307:ASN:O	1:B:309:SER:N	2.50	0.44
1:A:12:GLU:HB2	1:A:50:LEU:CD2	2.47	0.44
1:B:80:SER:O	1:B:84:GLN:HG3	2.18	0.44
1:B:293:LYS:NZ	2:B:612:HOH:O	2.50	0.44
1:A:358:ILE:C	1:A:358:ILE:HD12	2.42	0.44
1:A:48:LYS:N	1:A:48:LYS:HD2	2.33	0.43
1:A:54:ALA:HB2	1:A:66:TRP:NE1	2.33	0.43
1:A:88:LYS:CE	1:B:394:ARG:HH21	2.31	0.43
1:A:388:LEU:C	1:A:388:LEU:HD23	2.44	0.43
1:A:14:SER:OG	1:A:15:LEU:HD22	2.17	0.43
1:A:263:VAL:HG12	1:A:270:LEU:HD22	1.99	0.43
1:A:45:HIS:CE1	1:A:46:GLN:HG3	2.53	0.43
1:A:372:GLN:HA	1:A:388:LEU:HD13	2.00	0.43
1:A:99:LEU:HD21	1:A:209:ARG:HD3	2.01	0.42
1:A:279:ASP:HB3	1:A:282:LYS:HB3	2.00	0.42
1:A:358:ILE:CD1	1:B:17:ARG:HH22	2.31	0.42
1:A:5:LEU:C	1:A:5:LEU:HD23	2.44	0.42
1:A:5:LEU:HB2	1:A:40:ILE:HD12	2.02	0.42
1:B:74:ILE:HD11	1:B:136:GLN:CG	2.50	0.42
1:A:96:LYS:HE2	1:B:217:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:HG3	1:A:319:LYS:CD	2.49	0.42
1:A:354:ALA:O	1:A:358:ILE:HG23	2.19	0.42
1:B:228:PHE:CE1	1:B:280:VAL:HG11	2.54	0.42
1:B:219:VAL:HG21	1:B:238:ALA:HA	2.02	0.42
1:B:263:VAL:HG12	1:B:270:LEU:HD22	2.01	0.42
1:A:48:LYS:O	1:A:50:LEU:HD13	2.19	0.42
1:B:94:ALA:HA	1:B:99:LEU:HB2	2.02	0.42
1:A:49:TRP:CH2	1:A:51:ALA:HA	2.55	0.42
1:B:43:VAL:HG12	1:B:49:TRP:HA	2.02	0.42
1:A:138:ALA:HB3	2:A:474:HOH:O	2.19	0.41
1:A:12:GLU:H	1:A:12:GLU:CD	2.27	0.41
1:A:361:GLY:C	1:A:362:ARG:HG3	2.44	0.41
1:B:357:ALA:HB1	1:B:362:ARG:O	2.20	0.41
1:A:15:LEU:HG	1:A:42:ILE:CD1	2.48	0.41
1:B:230:TYR:CG	1:B:231:THR:N	2.88	0.41
1:B:302:PRO:N	2:B:664:HOH:O	2.52	0.41
1:B:307:ASN:C	1:B:309:SER:N	2.69	0.41
1:A:190:MSE:HB2	1:A:240:MSE:HE3	2.03	0.41
1:A:95:GLN:HG3	1:A:96:LYS:N	2.36	0.41
1:B:308:LYS:O	1:B:310:GLN:N	2.50	0.41
1:A:36:LEU:C	1:A:36:LEU:HD23	2.45	0.41
1:B:5:LEU:HG	1:B:30:MSE:SE	2.71	0.41
1:B:36:LEU:C	1:B:36:LEU:HD23	2.46	0.41
1:A:225:LEU:HB3	1:A:297:ILE:HG12	2.03	0.41
1:A:230:TYR:C	1:A:232:GLY:H	2.29	0.40
1:B:371:ARG:HG2	1:B:372:GLN:N	2.36	0.40
1:A:239:LEU:HB2	1:A:268:LEU:HD13	2.03	0.40
1:A:74:ILE:O	1:A:74:ILE:CG1	2.68	0.40
1:B:5:LEU:C	1:B:5:LEU:HD23	2.46	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	393/396 (99%)	373 (95%)	14 (4%)	6 (2%)	8	4
1	B	393/396 (99%)	372 (95%)	15 (4%)	6 (2%)	8	4
All	All	786/792 (99%)	745 (95%)	29 (4%)	12 (2%)	8	4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PRO
1	A	307	ASN
1	A	309	SER
1	B	304	PHE
1	B	305	VAL
1	A	313	GLY
1	B	311	LEU
1	A	314	ALA
1	B	302	PRO
1	B	303	LYS
1	B	314	ALA
1	A	305	VAL

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	317/320 (99%)	309 (98%)	8 (2%)	42	45
1	B	317/320 (99%)	309 (98%)	8 (2%)	42	45
All	All	634/640 (99%)	618 (98%)	16 (2%)	42	45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	62	ARG
1	A	88	LYS
1	A	95	GLN

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Mol	Chain	Res	Type
1	A	105	ILE
1	A	116	THR
1	A	213	LEU
1	A	316	ARG
1	B	33	LYS
1	B	50	LEU
1	B	74	ILE
1	B	95	GLN
1	B	116	THR
1	B	267	LYS
1	B	316	ARG
1	B	359	ASP

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	84	GLN
1	A	87	GLN
1	A	95	GLN
1	A	188	HIS
1	A	198	HIS
1	A	200	HIS
1	A	221	ASN
1	A	226	ASN
1	A	261	GLN
1	A	322	ASN
1	A	369	GLN
1	B	46	GLN
1	B	60	GLN
1	B	87	GLN
1	B	198	HIS
1	B	253	GLN
1	B	261	GLN

5.3.3 RNA ⓘ

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	386/396 (97%)	0.46	30 (7%) 19 18	11, 26, 46, 65	0
1	B	386/396 (97%)	0.10	16 (4%) 41 40	11, 20, 34, 51	0
All	All	772/792 (97%)	0.28	46 (5%) 27 26	11, 22, 43, 65	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	6.7
1	A	311	LEU	5.6
1	B	313	GLY	5.5
1	A	313	GLY	5.4
1	B	315	CYS	5.4
1	B	314	ALA	4.7
1	B	304	PHE	4.6
1	A	42	ILE	4.5
1	A	314	ALA	4.4
1	A	309	SER	4.3
1	B	311	LEU	4.3
1	B	305	VAL	4.2
1	B	316	ARG	3.9
1	A	230	TYR	3.9
1	A	231	THR	3.8
1	A	308	LYS	3.8
1	A	315	CYS	3.6
1	A	341	SER	3.6
1	A	307	ASN	3.5
1	A	232	GLY	3.4
1	B	308	LYS	3.2
1	A	340	CYS	3.2
1	B	306	GLU	3.1
1	A	229	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	42	ILE	2.9
1	A	310	GLN	2.8
1	B	105	ILE	2.8
1	A	35	SER	2.7
1	A	304	PHE	2.7
1	A	161	VAL	2.7
1	B	307	ASN	2.6
1	A	2	SER	2.6
1	B	100	ASP	2.6
1	A	306	GLU	2.5
1	A	74	ILE	2.5
1	A	24	SER	2.4
1	A	305	VAL	2.4
1	A	302	PRO	2.3
1	A	358	ILE	2.3
1	A	271	SER	2.3
1	A	316	ARG	2.1
1	A	204	TYR	2.1
1	B	62	ARG	2.1
1	B	303	LYS	2.1
1	A	279	ASP	2.1
1	B	33	LYS	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.