



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:15 AM UTC

PDB ID : 2BX2 / pdb_00002bx2
Title : Catalytic domain of E. coli RNase E
Authors : Marcaida, M.J.; Callaghan, A.J.; Scott, W.G.; Luisi, B.F.
Deposited on : 2005-07-21
Resolution : 2.85 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

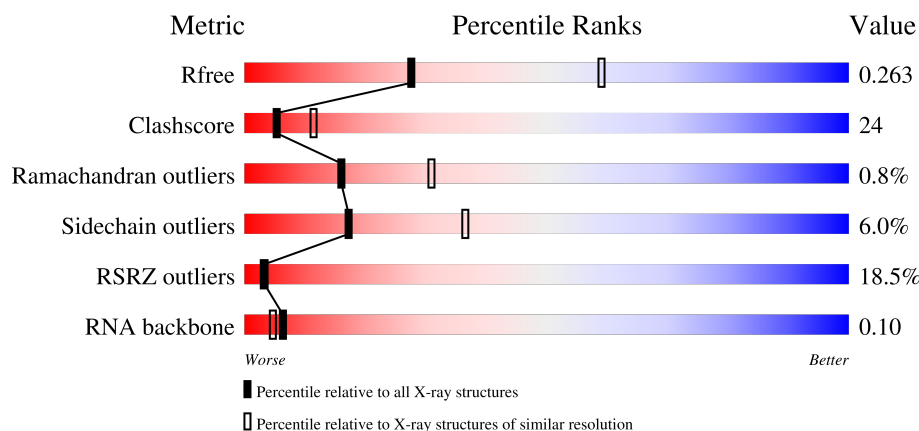
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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	L	517	16% 64% 28% • •
2	R	15	80% 13% 33% 33% 13% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4135 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 E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	500	Total	C	N	O	S	0	0	0
			3783	2361	700	710	12			

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*UP*AP*CP*AP*GP*UP*AP*UP*UP*UP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	14	Total	C	N	O	P	0	0	0
			293	131	44	104	14			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Zn	0	0
			1	1		

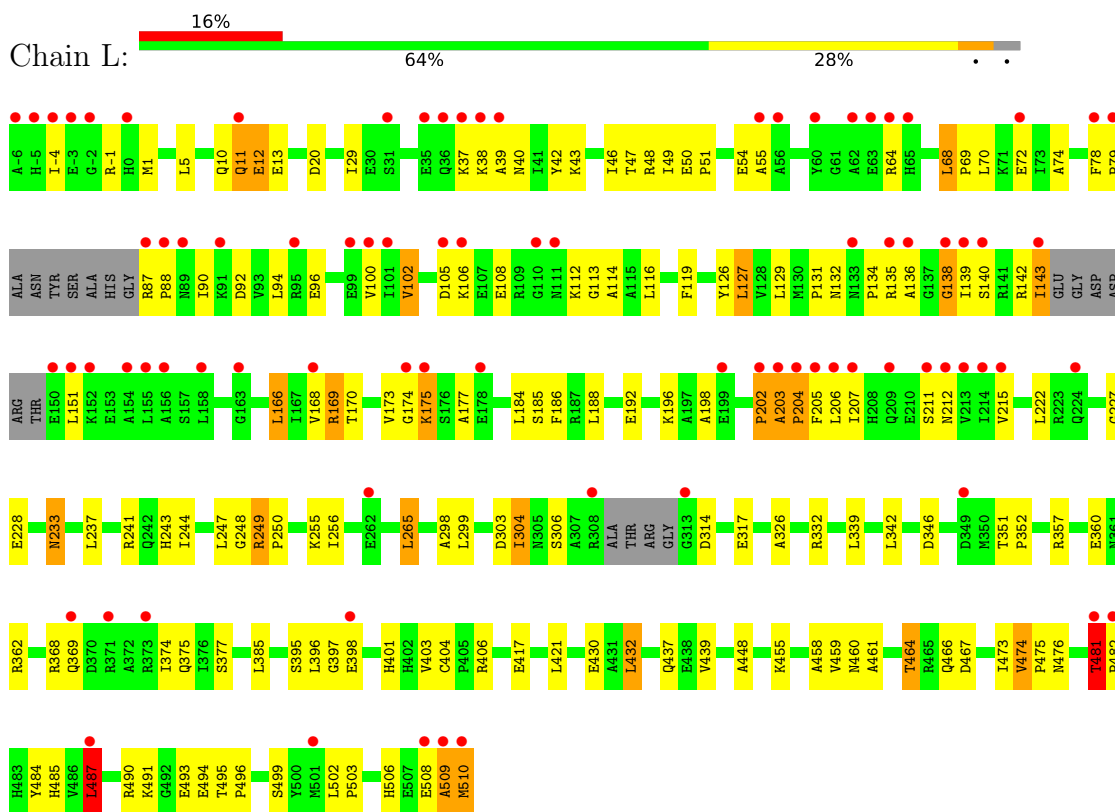
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	53	Total	O	0	0
			53	53		
5	R	3	Total	O	0	0
			3	3		

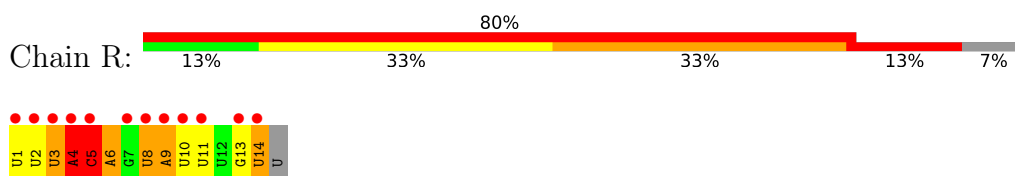
3 Residue-property plots [i](#)

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: RIBONUCLEASE E



• Molecule 2: RNA (5'-R(*UP*UP*UP*AP*CP*AP*GP*UP*AP*UP*UP* UP*GP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	195.84Å 195.84Å 143.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.85 25.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-2.85) 99.3 (25.00-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.257 0.236 , 0.263	Depositor DCC
R_{free} test set	1906 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.7	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	0.91	EDS
Total number of atoms	4135	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: MG, ZN

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	L	0.69	2/3843 (0.1%)	0.95	8/5209 (0.2%)
2	R	0.63	0/325	1.11	4/501 (0.8%)
All	All	0.68	2/4168 (0.0%)	0.97	12/5710 (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	L	1	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	487	LEU	C-N	-5.86	1.25	1.33
1	L	177	ALA	C-O	5.01	1.30	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	474	VAL	N-CA-C	7.41	115.97	107.89
1	L	233	ASN	CA-C-N	6.98	126.50	119.24
1	L	233	ASN	C-N-CA	6.98	126.50	119.24
2	R	5	C	O4'-C1'-C2'	-6.43	101.17	107.60
1	L	138	GLY	N-CA-C	6.00	117.96	110.29
2	R	4	A	O4'-C1'-C2'	-5.93	101.67	107.60
2	R	5	C	C3'-C2'-C1'	-5.90	95.40	101.30
1	L	473	ILE	CA-C-N	-5.38	117.52	123.43
1	L	473	ILE	C-N-CA	-5.38	117.52	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	102	VAL	N-CA-C	5.33	115.80	108.12
1	L	51	PRO	N-CA-C	-5.29	106.63	113.57
2	R	11	U	C3'-C2'-O2'	5.23	118.55	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	509	ALA	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	151	LEU	Peptide
1	L	202	PRO	Peptide
1	L	306	SER	Peptide
1	L	406	ARG	Peptide
1	L	481	THR	Peptide
1	L	509	ALA	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	L	3783	0	3674	158	3
2	R	293	0	147	37	3
3	L	2	0	0	0	0
4	L	1	0	0	0	0
5	L	53	0	0	3	0
5	R	3	0	0	0	0
All	All	4135	0	3821	191	3

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 24.

All (191) 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)
2:R:5:C:C6	2:R:5:C:H3'	1.77	1.19
1:L:1:MET:HE3	1:L:227:GLY:HA3	1.35	1.06
1:L:-4:ILE:HD12	1:L:-1:ARG:NH1	1.73	1.01
2:R:5:C:C6	2:R:5:C:C3'	2.44	1.01
2:R:8:U:H2'	2:R:9:A:C8	1.94	1.01
2:R:8:U:H2'	2:R:9:A:H8	1.26	0.99
1:L:138:GLY:HA3	2:R:3:U:OP1	1.63	0.97
2:R:3:U:H6	2:R:3:U:H3'	1.31	0.96
2:R:8:U:H4'	2:R:9:A:OP1	1.61	0.96
1:L:129:LEU:HG	1:L:131:PRO:HD3	1.48	0.94
1:L:43:LYS:O	1:L:203:ALA:O	1.88	0.92
1:L:244:ILE:CD1	1:L:256:ILE:HD11	2.03	0.89
2:R:5:C:H3'	2:R:5:C:H6	1.22	0.88
1:L:55:ALA:HB2	1:L:69:PRO:HA	1.53	0.88
2:R:3:U:H3'	2:R:3:U:C6	2.10	0.87
1:L:244:ILE:HD11	1:L:256:ILE:HD11	1.58	0.85
1:L:1:MET:CE	1:L:227:GLY:HA3	2.07	0.84
1:L:499:SER:O	1:L:502:LEU:HB2	1.77	0.83
1:L:303:ASP:OD2	5:L:2021:HOH:O	1.95	0.83
1:L:460:ASN:O	1:L:464:THR:HG22	1.79	0.83
1:L:346:ASP:OD2	5:L:2021:HOH:O	1.98	0.82
1:L:244:ILE:HD12	1:L:256:ILE:CD1	2.11	0.81
2:R:5:C:C3'	2:R:5:C:H6	1.85	0.80
1:L:169:ARG:HG3	2:R:1:U:OP2	1.83	0.79
1:L:69:PRO:HG2	1:L:72:GLU:CG	2.13	0.78
1:L:203:ALA:N	1:L:204:PRO:HD2	1.99	0.77
1:L:203:ALA:N	1:L:204:PRO:CD	2.46	0.77
1:L:108:GLU:HA	1:L:113:GLY:O	1.85	0.77
1:L:237:LEU:C	1:L:237:LEU:HD23	2.11	0.76
2:R:3:U:C6	2:R:3:U:C3'	2.70	0.74
1:L:55:ALA:CB	1:L:69:PRO:HA	2.16	0.74
1:L:43:LYS:O	1:L:204:PRO:HA	1.89	0.73
1:L:119:PHE:HA	1:L:132:ASN:HD22	1.51	0.73
1:L:243:HIS:O	1:L:247:LEU:HB2	1.88	0.73
1:L:244:ILE:CD1	1:L:256:ILE:CD1	2.67	0.71
1:L:487:LEU:HD12	1:L:487:LEU:N	2.07	0.70
1:L:244:ILE:HD12	1:L:256:ILE:HD12	1.74	0.68
2:R:5:C:H6	2:R:5:C:C5'	2.07	0.68
2:R:4:A:C8	2:R:4:A:C5'	2.77	0.68
1:L:166:LEU:HD23	1:L:166:LEU:O	1.94	0.68
1:L:64:ARG:NH1	1:L:112:LYS:O	2.26	0.68
1:L:102:VAL:HG11	1:L:116:LEU:HD13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:GLU:HG2	1:L:113:GLY:O	1.93	0.67
1:L:203:ALA:H	1:L:204:PRO:HD2	1.60	0.66
2:R:3:U:H6	2:R:3:U:C3'	2.03	0.66
1:L:74:ALA:HB2	1:L:132:ASN:HD21	1.61	0.66
1:L:203:ALA:H	1:L:204:PRO:CD	2.09	0.66
1:L:134:PRO:C	1:L:136:ALA:H	2.05	0.65
2:R:5:C:C6	2:R:5:C:C4'	2.79	0.65
1:L:69:PRO:HG2	1:L:72:GLU:HG2	1.78	0.65
2:R:4:A:H8	2:R:4:A:H5''	1.60	0.65
1:L:508:GLU:O	1:L:509:ALA:HB2	1.97	0.64
1:L:64:ARG:HD2	1:L:113:GLY:HA2	1.78	0.64
2:R:5:C:C6	2:R:5:C:C5'	2.80	0.64
1:L:43:LYS:C	1:L:203:ALA:O	2.39	0.64
1:L:1:MET:HE1	1:L:228:GLU:HG3	1.80	0.64
1:L:485:HIS:HB3	1:L:487:LEU:HD11	1.78	0.64
2:R:5:C:H6	2:R:5:C:H5''	1.62	0.64
1:L:314:ASP:HB3	1:L:317:GLU:HB3	1.81	0.63
1:L:506:HIS:O	1:L:510:MET:HB3	1.99	0.63
1:L:299:LEU:C	1:L:299:LEU:HD12	2.24	0.63
1:L:68:LEU:CD2	1:L:68:LEU:C	2.71	0.63
1:L:102:VAL:HG13	1:L:116:LEU:HB3	1.81	0.62
1:L:134:PRO:O	1:L:136:ALA:N	2.33	0.62
1:L:237:LEU:HD23	1:L:237:LEU:O	2.00	0.62
2:R:9:A:H2'	2:R:10:U:O2	1.99	0.62
1:L:138:GLY:CA	2:R:3:U:OP1	2.43	0.62
1:L:68:LEU:C	1:L:68:LEU:HD23	2.26	0.61
1:L:105:ASP:C	1:L:106:LYS:HG3	2.23	0.61
1:L:502:LEU:H	1:L:503:PRO:HD2	1.64	0.61
2:R:5:C:H6	2:R:5:C:C4'	2.13	0.61
1:L:38:LYS:O	1:L:39:ALA:HB3	1.99	0.61
2:R:4:A:C8	2:R:4:A:H5''	2.35	0.61
1:L:508:GLU:O	1:L:509:ALA:CB	2.48	0.61
1:L:461:ALA:HA	1:L:464:THR:HG23	1.83	0.60
1:L:126:TYR:CZ	1:L:175:LYS:HG3	2.36	0.60
2:R:8:U:C4'	2:R:9:A:OP1	2.43	0.58
1:L:233:ASN:OD1	1:L:233:ASN:C	2.46	0.57
2:R:5:C:H2'	2:R:6:A:O5'	2.03	0.57
1:L:54:GLU:O	1:L:70:LEU:CB	2.52	0.57
1:L:69:PRO:HG2	1:L:72:GLU:HG3	1.87	0.57
1:L:108:GLU:CG	1:L:113:GLY:O	2.53	0.57
1:L:143:ILE:HD11	1:L:170:THR:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:502:LEU:N	1:L:503:PRO:HD2	2.20	0.57
1:L:494:GLU:OE1	1:L:494:GLU:N	2.30	0.56
1:L:466:GLN:NE2	1:L:466:GLN:HA	2.21	0.56
1:L:484:TYR:C	1:L:484:TYR:CD1	2.83	0.56
1:L:11:GLN:H	1:L:11:GLN:CD	2.12	0.56
1:L:485:HIS:CE1	1:L:510:MET:HG3	2.41	0.55
2:R:5:C:C6	2:R:5:C:H5''	2.41	0.55
1:L:126:TYR:OH	1:L:175:LYS:HE3	2.07	0.55
1:L:395:SER:OG	1:L:398:GLU:HG3	2.07	0.55
1:L:377:SER:O	1:L:385:LEU:HD11	2.07	0.54
1:L:1:MET:HE3	1:L:227:GLY:CA	2.23	0.54
1:L:202:PRO:O	1:L:205:PHE:CE2	2.60	0.54
1:L:237:LEU:C	1:L:237:LEU:CD2	2.80	0.53
1:L:139:ILE:O	2:R:2:U:H5''	2.08	0.53
1:L:437:GLN:HB2	1:L:491:LYS:HA	1.91	0.53
1:L:47:THR:O	1:L:96:GLU:HG3	2.08	0.53
2:R:14:U:O2	2:R:14:U:H5''	2.09	0.52
1:L:502:LEU:N	1:L:503:PRO:CD	2.72	0.52
1:L:461:ALA:HA	1:L:464:THR:CG2	2.39	0.52
1:L:47:THR:HG22	1:L:48:ARG:N	2.23	0.52
1:L:490:ARG:O	1:L:493:GLU:HG2	2.10	0.52
1:L:49:ILE:HG22	1:L:50:GLU:N	2.25	0.51
1:L:49:ILE:CG2	1:L:50:GLU:N	2.73	0.51
1:L:166:LEU:HD23	1:L:166:LEU:C	2.36	0.51
1:L:212:ASN:C	1:L:212:ASN:OD1	2.53	0.51
1:L:303:ASP:C	1:L:304:ILE:HG12	2.35	0.50
1:L:466:GLN:O	1:L:467:ASP:C	2.54	0.50
2:R:4:A:C8	2:R:4:A:C3'	2.94	0.50
1:L:126:TYR:CE1	1:L:175:LYS:HG3	2.47	0.50
1:L:192:GLU:OE2	1:L:192:GLU:HA	2.10	0.49
1:L:129:LEU:HG	1:L:131:PRO:CD	2.33	0.49
1:L:487:LEU:N	1:L:487:LEU:CD1	2.75	0.49
1:L:108:GLU:HG2	1:L:113:GLY:C	2.38	0.49
1:L:481:THR:O	1:L:481:THR:OG1	2.30	0.49
1:L:351:THR:N	1:L:352:PRO:CD	2.75	0.49
1:L:502:LEU:H	1:L:503:PRO:CD	2.26	0.49
2:R:10:U:O2	2:R:10:U:O4'	2.31	0.48
1:L:-4:ILE:CD1	1:L:-1:ARG:NH1	2.63	0.48
1:L:5:LEU:HB3	1:L:265:LEU:HD13	1.96	0.48
2:R:8:U:O2'	2:R:9:A:P	2.72	0.48
1:L:417:GLU:OE2	1:L:417:GLU:N	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:GLY:O	1:L:255:LYS:HG2	2.14	0.47
1:L:12:GLU:H	1:L:12:GLU:CD	2.21	0.47
1:L:206:LEU:HD12	1:L:207:ILE:N	2.29	0.47
2:R:4:A:C8	2:R:4:A:H3'	2.49	0.47
1:L:357:ARG:HH11	1:L:357:ARG:HA	1.80	0.47
1:L:140:SER:C	1:L:142:ARG:H	2.23	0.47
1:L:357:ARG:NH1	1:L:360:GLU:OE2	2.48	0.47
1:L:476:ASN:C	1:L:476:ASN:OD1	2.57	0.46
1:L:244:ILE:HD12	1:L:256:ILE:HD11	1.76	0.46
1:L:368:ARG:HE	1:L:368:ARG:HB2	1.45	0.46
1:L:377:SER:O	1:L:385:LEU:CD1	2.63	0.46
1:L:78:PHE:O	1:L:79:PRO:C	2.57	0.46
1:L:430:GLU:HA	1:L:430:GLU:OE1	2.16	0.45
1:L:206:LEU:HD12	1:L:207:ILE:H	1.81	0.45
1:L:185:SER:O	1:L:186:PHE:C	2.59	0.45
1:L:42:TYR:CD2	1:L:206:LEU:HA	2.52	0.45
1:L:458:ALA:O	1:L:459:VAL:C	2.59	0.45
1:L:13:GLU:HG2	1:L:29:ILE:HG23	1.98	0.44
1:L:448:ALA:HB3	1:L:475:PRO:HB3	1.99	0.44
1:L:-4:ILE:HD12	1:L:-1:ARG:HH12	1.69	0.44
1:L:202:PRO:O	1:L:205:PHE:CD2	2.70	0.44
1:L:87:ARG:HA	1:L:88:PRO:HD3	1.78	0.44
1:L:222:LEU:HD23	1:L:222:LEU:HA	1.82	0.44
1:L:403:VAL:O	1:L:404:CYS:C	2.61	0.44
1:L:90:ILE:C	1:L:92:ASP:N	2.76	0.43
1:L:455:LYS:HA	1:L:455:LYS:HD2	1.67	0.43
2:R:4:A:H8	2:R:4:A:H3'	1.84	0.43
1:L:1:MET:CE	1:L:227:GLY:CA	2.88	0.43
1:L:90:ILE:C	1:L:92:ASP:H	2.26	0.43
1:L:173:VAL:CG1	1:L:174:GLY:N	2.81	0.43
1:L:448:ALA:CB	1:L:475:PRO:HB3	2.48	0.43
2:R:4:A:C5'	2:R:4:A:H8	2.21	0.43
1:L:46:ILE:CD1	1:L:94:LEU:CB	2.97	0.43
1:L:304:ILE:HD13	1:L:326:ALA:HB1	2.01	0.43
1:L:1:MET:HB3	1:L:1:MET:HE2	1.59	0.42
1:L:37:LYS:HA	1:L:40:ASN:ND2	2.34	0.42
1:L:43:LYS:O	1:L:203:ALA:C	2.59	0.42
1:L:100:VAL:HG13	1:L:102:VAL:HG23	2.01	0.42
1:L:102:VAL:CG1	1:L:116:LEU:HD22	2.48	0.42
2:R:5:C:C2'	2:R:6:A:O5'	2.67	0.42
1:L:342:LEU:HA	1:L:342:LEU:HD12	1.75	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:LYS:C	1:L:198:ALA:H	2.26	0.42
1:L:339:LEU:HA	1:L:339:LEU:HD23	1.73	0.42
2:R:8:U:C2'	2:R:9:A:H8	2.14	0.42
1:L:352:PRO:HA	5:L:2034:HOH:O	2.19	0.42
1:L:397:GLY:O	1:L:401:HIS:HB2	2.19	0.42
1:L:432:LEU:HD12	1:L:432:LEU:HA	1.85	0.42
1:L:127:LEU:HD12	1:L:127:LEU:HA	1.89	0.42
1:L:249:ARG:N	1:L:250:PRO:CD	2.82	0.42
1:L:140:SER:C	1:L:142:ARG:N	2.75	0.42
1:L:248:GLY:C	1:L:249:ARG:HG2	2.45	0.42
1:L:70:LEU:C	1:L:72:GLU:H	2.28	0.41
1:L:485:HIS:HB3	1:L:487:LEU:CD1	2.45	0.41
2:R:4:A:C8	2:R:4:A:C4'	3.03	0.41
1:L:495:THR:HB	1:L:496:PRO:CD	2.51	0.41
1:L:20:ASP:OD1	1:L:20:ASP:C	2.63	0.41
1:L:298:ALA:O	1:L:299:LEU:HB3	2.21	0.41
1:L:55:ALA:HB1	1:L:68:LEU:O	2.20	0.41
1:L:374:ILE:CG2	1:L:375:GLN:N	2.82	0.41
1:L:396:LEU:HD23	1:L:396:LEU:HA	1.75	0.41
1:L:184:LEU:O	1:L:188:LEU:HG	2.20	0.41
1:L:38:LYS:O	1:L:39:ALA:CB	2.64	0.40
1:L:127:LEU:HD12	1:L:168:VAL:HA	2.02	0.40
1:L:421:LEU:HD21	1:L:455:LYS:HE2	2.04	0.40
1:L:12:GLU:CD	1:L:12:GLU:N	2.79	0.40
1:L:211:SER:HB3	1:L:215:VAL:HB	2.04	0.40
1:L:173:VAL:HG13	1:L:174:GLY:N	2.36	0.40

All (3) 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:L:113:GLY:N	2:R:13:G:N2[11_655]	1.99	0.21
1:L:113:GLY:CA	2:R:13:G:N2[11_655]	2.08	0.12
1:L:114:ALA:N	2:R:13:G:N2[11_655]	2.18	0.02

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	L	492/517 (95%)	441 (90%)	47 (10%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	204	PRO
1	L	482	PRO
1	L	135	ARG
1	L	203	ALA

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	L	382/439 (87%)	359 (94%)	23 (6%)	17	36

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

Mol	Chain	Res	Type
1	L	10	GLN
1	L	11	GLN
1	L	12	GLU
1	L	68	LEU
1	L	127	LEU
1	L	143	ILE
1	L	166	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	169	ARG
1	L	175	LYS
1	L	241	ARG
1	L	249	ARG
1	L	265	LEU
1	L	304	ILE
1	L	332	ARG
1	L	362	ARG
1	L	369	GLN
1	L	432	LEU
1	L	439	VAL
1	L	464	THR
1	L	474	VAL
1	L	481	THR
1	L	487	LEU
1	L	510	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	10	GLN
1	L	22	GLN
1	L	36	GLN
1	L	132	ASN
1	L	190	HIS
1	L	280	GLN
1	L	355	HIS
1	L	375	GLN
1	L	466	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	13/15 (86%)	6 (46%)	2 (15%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	U
2	R	4	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	5	C
2	R	6	A
2	R	9	A
2	R	14	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	4	A
2	R	8	U

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](#)

Of 3 ligands modelled in this entry, 3 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 [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	L	500/517 (96%)	0.84	83 (16%) 4 4	25, 54, 69, 100	0
2	R	14/15 (93%)	4.81	12 (85%) 0 0	40, 60, 91, 95	0
All	All	514/532 (96%)	0.95	95 (18%) 3 3	25, 54, 71, 100	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	1	U	13.2
2	R	2	U	9.3
1	L	203	ALA	7.7
1	L	308	ARG	6.8
2	R	14	U	5.8
1	L	139	ILE	5.7
1	L	63	GLU	5.0
1	L	135	ARG	5.0
1	L	204	PRO	4.9
2	R	13	G	4.9
2	R	5	C	4.8
2	R	4	A	4.8
1	L	481	THR	4.5
2	R	9	A	4.3
2	R	3	U	4.3
1	L	150	GLU	4.0
2	R	7	G	3.9
1	L	143	ILE	3.9
1	L	206	LEU	3.8
1	L	39	ALA	3.7
1	L	214	ILE	3.7
1	L	487	LEU	3.6
1	L	91	LYS	3.6
1	L	79	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	508	GLU	3.5
1	L	-6	ALA	3.5
1	L	56	ALA	3.5
1	L	36	GLN	3.4
2	R	10	U	3.4
1	L	37	LYS	3.3
1	L	207	ILE	3.3
1	L	138	GLY	3.3
1	L	106	LYS	3.2
1	L	510	MET	3.2
1	L	100	VAL	3.2
2	R	8	U	3.2
1	L	373	ARG	3.2
1	L	11	GLN	3.2
1	L	-3	GLU	3.2
1	L	213	VAL	3.1
1	L	174	GLY	3.1
1	L	371	ARG	3.0
1	L	202	PRO	3.0
1	L	175	LYS	2.9
1	L	215	VAL	2.9
1	L	178	GLU	2.8
1	L	-5	HIS	2.8
1	L	349	ASP	2.8
1	L	313	GLY	2.8
1	L	87	ARG	2.8
1	L	110	GLY	2.8
1	L	199	GLU	2.7
1	L	78	PHE	2.7
1	L	211	SER	2.7
1	L	140	SER	2.7
1	L	224	GLN	2.6
1	L	501	MET	2.6
1	L	31	SER	2.6
1	L	151	LEU	2.6
1	L	60	TYR	2.5
1	L	111	ASN	2.5
1	L	65	HIS	2.5
1	L	0	HIS	2.5
1	L	89	ASN	2.5
1	L	38	LYS	2.4
1	L	212	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	99	GLU	2.4
1	L	136	ALA	2.4
1	L	155	LEU	2.4
1	L	158	LEU	2.4
1	L	95	ARG	2.4
1	L	101	ILE	2.4
1	L	62	ALA	2.3
1	L	72	GLU	2.3
1	L	509	ALA	2.3
1	L	168	VAL	2.3
1	L	152	LYS	2.3
1	L	482	PRO	2.3
1	L	105	ASP	2.3
1	L	-2	GLY	2.3
1	L	-4	ILE	2.2
1	L	154	ALA	2.2
1	L	398	GLU	2.2
2	R	11	U	2.2
1	L	64	ARG	2.2
1	L	156	ALA	2.2
1	L	88	PRO	2.1
1	L	369	GLN	2.1
1	L	55	ALA	2.1
1	L	35	GLU	2.1
1	L	209	GLN	2.1
1	L	205	PHE	2.1
1	L	262	GLU	2.0
1	L	133	ASN	2.0
1	L	163	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
3	MG	L	1511	1/1	0.97	0.18	62,62,62,62	0
3	MG	L	1510	1/1	0.98	0.11	45,45,45,45	1
4	ZN	L	1512	1/1	0.99	0.16	40,40,40,40	1

6.5 Other polymers [i](#)

There are no such residues in this entry.