



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:53 PM UTC

PDB ID : 1SZ1 / pdb_00001sz1
Title : Mechanism of CCA-adding enzymes specificity revealed by crystal structures of ternary complexes
Authors : Xiong, Y.; Steitz, T.A.
Deposited on : 2004-04-02
Resolution : 6.21 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

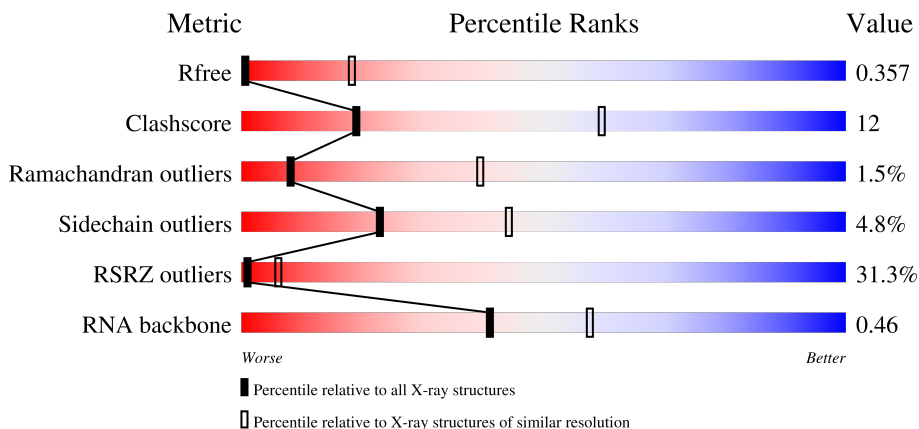
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.21 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	1148 (8.40-4.00)
Clashscore	190562	1009 (8.40-4.02)
Ramachandran outliers	187476	1037 (8.40-4.00)
Sidechain outliers	187428	1003 (8.40-4.00)
RSRZ outliers	180081	1141 (8.40-4.00)
RNA backbone	3983	1054 (8.70-3.10)

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	E	76	11% 39% 39% 16% 5%
1	F	76	13% 43% 34% 17% 5%
2	A	437	35% 80% 17% .
2	B	437	32% 80% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	H2U	E	16	-	-	-	X
1	H2U	E	17	-	-	-	X
1	H2U	F	16	-	-	-	X
1	H2U	F	17	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10556 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 RNA chain called T-RNA (76-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	76	Total	C	N	O	P	0	0	0
			1648	746	294	533	75			
1	F	76	Total	C	N	O	P	0	0	0
			1648	746	294	533	75			

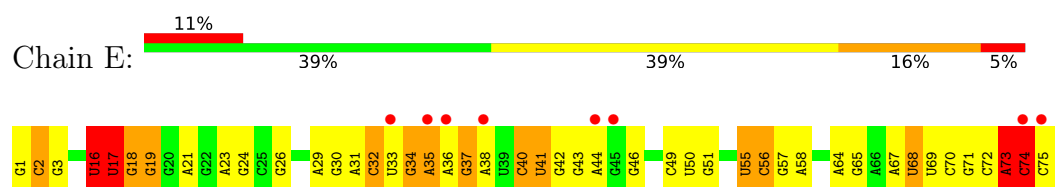
- Molecule 2 is a protein called tRNA nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
2	B	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

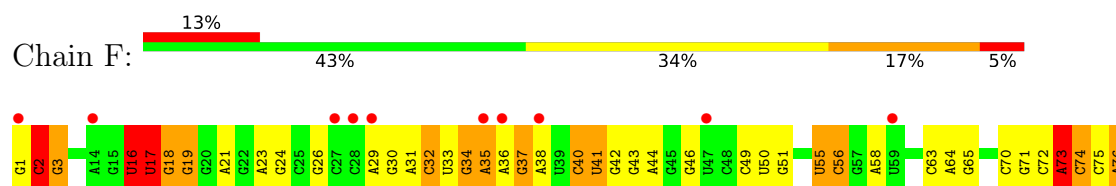
3 Residue-property plots [i](#)

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.

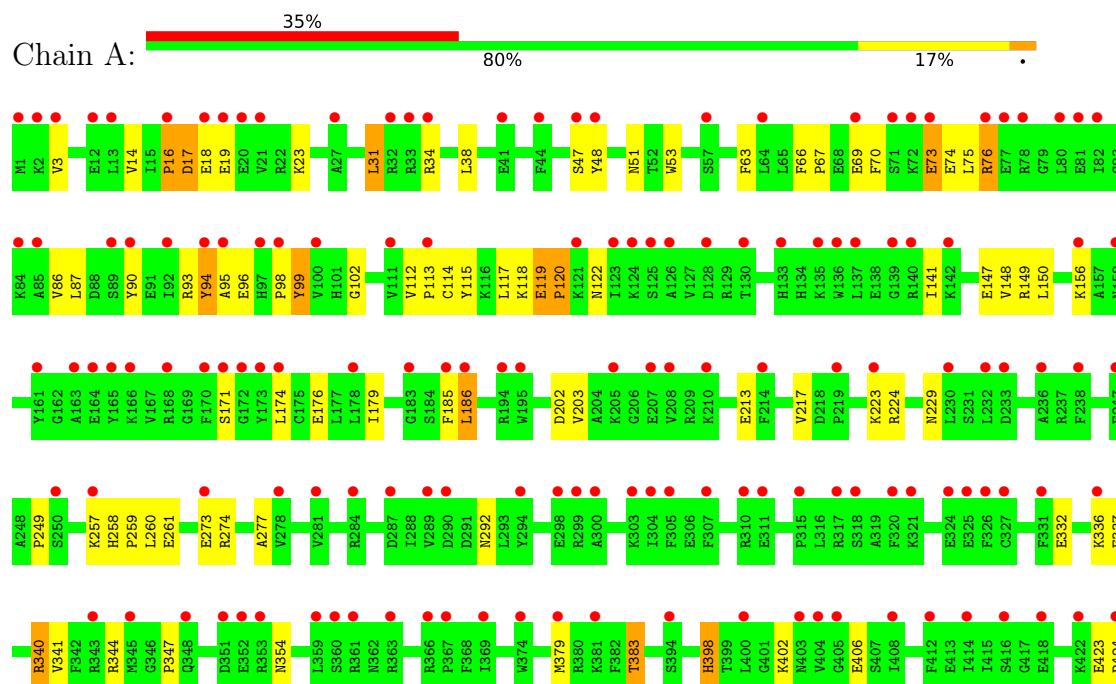
• Molecule 1: T-RNA (76-MER)

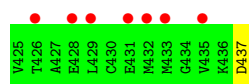


• Molecule 1: T-RNA (76-MER)

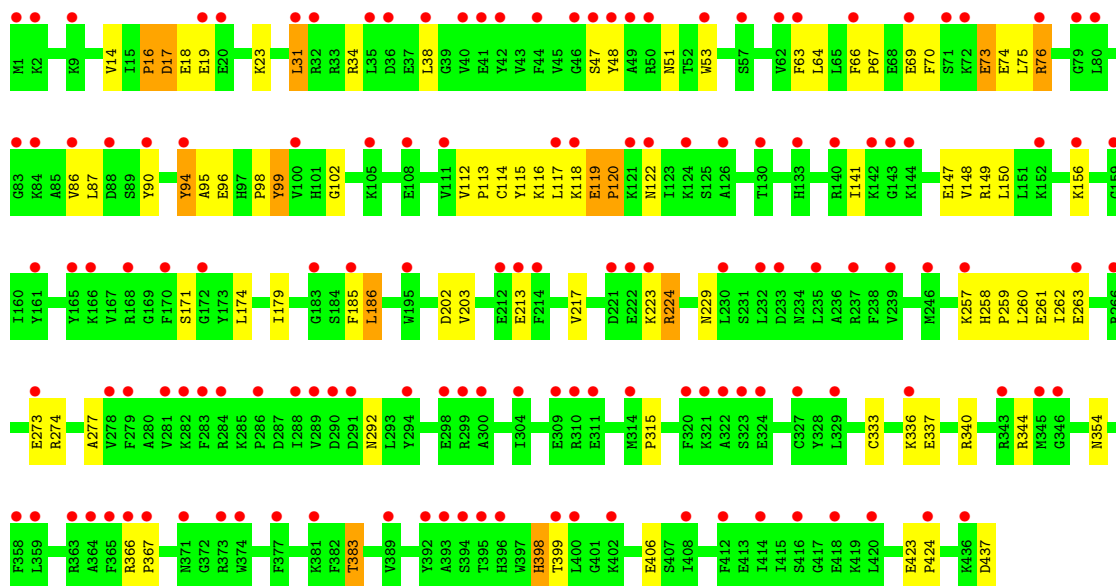
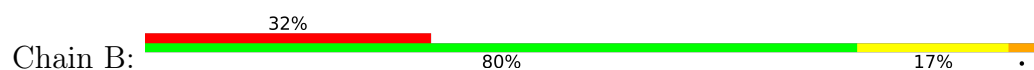


• Molecule 2: tRNA nucleotidyltransferase





• Molecule 2: tRNA nucleotidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.40Å 218.40Å 170.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.72 – 6.21 44.72 – 6.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.72-6.21) 98.0 (44.72-6.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 6.14Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.360 , 0.380 0.345 , 0.357	Depositor DCC
R_{free} test set	574 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	124.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	10556	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: H2U, 2MG, 7MG, M2G, 1MA, 5MU, OMC, OMG, 5MC, YG, PSU

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	E	0.72	3/1483 (0.2%)	1.06	8/2311 (0.3%)
1	F	0.73	2/1483 (0.1%)	1.14	12/2311 (0.5%)
2	A	0.42	0/3713	0.82	1/4987 (0.0%)
2	B	0.42	0/3713	0.81	1/4987 (0.0%)
All	All	0.53	5/10392 (0.0%)	0.91	22/14596 (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	E	0	1
1	F	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	56	C	O3'-P	-10.56	1.45	1.61
1	E	58	1MA	O3'-P	-9.47	1.47	1.61
1	F	58	1MA	O3'-P	6.52	1.71	1.61
1	E	56	C	O3'-P	5.42	1.69	1.61
1	E	55	PSU	O3'-P	-5.17	1.53	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	58	1MA	P-O3'-C3'	16.99	145.69	120.20
1	F	58	1MA	O3'-P-O5'	13.09	123.64	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	58	1MA	OP2-P-O3'	-8.40	82.78	108.00
1	E	56	C	P-O3'-C3'	-8.15	107.97	120.20
1	F	2	C	O3'-P-O5'	-7.29	93.06	104.00
1	E	68	U	P-O3'-C3'	-6.97	109.74	120.20
1	E	58	1MA	O3'-P-O5'	6.93	114.40	104.00
1	F	2	C	C3'-C2'-C1'	-6.53	94.77	101.30
1	F	18	G	C5'-C4'-O4'	-6.50	99.35	109.10
1	E	18	G	C5'-C4'-O4'	-6.46	99.42	109.10
1	F	2	C	O4'-C4'-C3'	-6.29	97.71	104.00
1	F	56	C	P-O3'-C3'	-6.02	111.16	120.20
1	F	2	C	C5'-C4'-C3'	-5.85	107.23	116.00
1	E	73	A	C4'-C3'-C2'	-5.75	96.85	102.60
1	F	73	A	C4'-C3'-C2'	-5.75	96.85	102.60
1	E	58	1MA	P-O3'-C3'	5.73	128.79	120.20
1	E	68	U	C4'-C3'-C2'	5.64	108.24	102.60
2	B	90	TYR	N-CA-C	5.53	118.09	109.52
1	E	74	C	N1-C1'-C2'	5.45	120.17	112.00
2	A	90	TYR	N-CA-C	5.39	117.87	109.52
1	F	2	C	C2'-C3'-O3'	5.25	121.57	113.70
1	F	55	PSU	P-O3'-C3'	-5.06	112.60	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	19	G	Sidechain
1	F	19	G	Sidechain

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	E	1648	0	862	64	0
1	F	1648	0	862	69	0
2	A	3630	0	3633	69	0
2	B	3630	0	3633	68	0
All	All	10556	0	8990	229	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 12.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:G:H2'	1:F:2:C:H5'	1.50	0.94
1:F:55:PSU:H5'	2:B:344:ARG:HH21	1.37	0.90
1:F:41:U:H6	1:F:41:U:H5'	1.37	0.90
1:E:1:G:H2'	1:E:2:C:H5'	1.53	0.89
1:E:41:U:H5'	1:E:41:U:H6	1.38	0.88
1:E:1:G:C2'	1:E:2:C:H5'	2.06	0.85
1:E:55:PSU:H5'	2:A:344:ARG:HH21	1.40	0.84
1:F:1:G:C2'	1:F:2:C:H5'	2.06	0.84
1:E:74:C:N4	2:A:95:ALA:HB1	1.93	0.83
2:B:76:ARG:NH2	2:B:113:PRO:HG2	1.94	0.83
2:A:76:ARG:NH2	2:A:113:PRO:HG2	1.94	0.82
1:E:74:C:H42	2:A:95:ALA:HB1	1.43	0.80
1:F:2:C:H5''	2:B:292:ASN:CG	2.06	0.80
1:E:35:A:H5'	1:E:35:A:H8	1.50	0.77
1:F:35:A:H5'	1:F:35:A:H8	1.50	0.77
1:F:55:PSU:H5'	2:B:344:ARG:NH2	2.00	0.76
1:E:34:OMG:C2'	1:E:35:A:H5''	2.17	0.74
1:E:56:C:O2	2:A:354:ASN:HB3	1.87	0.74
1:F:34:OMG:C2'	1:F:35:A:H5''	2.18	0.74
1:F:74:C:H42	2:B:95:ALA:HB1	1.52	0.74
1:F:73:A:H2'	1:F:74:C:C6	2.22	0.74
1:F:74:C:N4	2:B:95:ALA:HB1	2.03	0.73
1:F:72:C:P	2:B:224:ARG:HH12	2.12	0.73
2:B:185:PHE:O	2:B:186:LEU:HB2	1.88	0.73
1:F:2:C:H5''	2:B:292:ASN:OD1	1.87	0.73
2:A:94:TYR:HA	2:A:98:PRO:HA	1.70	0.73
1:E:73:A:H2'	1:E:74:C:C6	2.25	0.72
2:B:94:TYR:HA	2:B:98:PRO:HA	1.72	0.71
1:E:33:U:O2'	1:E:35:A:N7	2.22	0.71
1:E:34:OMG:H2'	1:E:35:A:H5''	1.72	0.71
2:B:76:ARG:HH22	2:B:113:PRO:HG2	1.53	0.71
1:F:33:U:O2'	1:F:35:A:N7	2.22	0.70
1:F:34:OMG:H2'	1:F:35:A:H5''	1.73	0.70
1:E:34:OMG:H8	1:E:34:OMG:OP1	1.74	0.70
2:A:185:PHE:O	2:A:186:LEU:HB2	1.91	0.70
1:F:34:OMG:H8	1:F:34:OMG:OP1	1.73	0.70
1:F:70:C:H2'	1:F:71:G:O4'	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:76:ARG:HA	2:A:76:ARG:CZ	2.24	0.67
1:F:1:G:O2'	2:B:292:ASN:ND2	2.28	0.66
2:A:260:LEU:HD11	2:A:437:ASP:HB3	1.77	0.66
2:B:17:ASP:C	2:B:19:GLU:H	2.03	0.66
1:F:37:YG:H31	1:F:37:YG:H1'	1.77	0.66
1:E:37:YG:H1'	1:E:37:YG:H31	1.77	0.65
2:B:260:LEU:HD11	2:B:437:ASP:HB3	1.77	0.65
2:A:17:ASP:C	2:A:19:GLU:H	2.05	0.65
2:B:185:PHE:O	2:B:186:LEU:CB	2.46	0.64
1:F:26:M2G:HM22	1:F:44:A:C2	2.33	0.64
2:B:202:ASP:HA	2:B:217:VAL:HB	1.79	0.63
1:E:26:M2G:HM22	1:E:44:A:C2	2.33	0.63
1:E:70:C:H2'	1:E:71:G:O4'	1.98	0.63
1:F:64:A:OP1	2:B:398:HIS:C	2.41	0.63
2:B:148:VAL:HA	2:B:179:ILE:HG13	1.82	0.62
1:F:2:C:O3'	1:F:2:C:O5'	2.17	0.62
2:A:202:ASP:HA	2:A:217:VAL:HB	1.80	0.62
2:B:76:ARG:CZ	2:B:76:ARG:HA	2.30	0.62
2:A:148:VAL:HA	2:A:179:ILE:HG13	1.81	0.61
1:E:72:C:P	2:A:224:ARG:HH12	2.24	0.61
1:F:40:5MC:H2'	1:F:41:U:H5'	1.83	0.61
2:B:99:TYR:CD1	2:B:112:VAL:HG22	2.36	0.61
1:E:34:OMG:H2'	1:E:35:A:C5'	2.30	0.61
2:A:185:PHE:O	2:A:186:LEU:CB	2.48	0.60
2:B:73:GLU:O	2:B:76:ARG:HB2	2.01	0.60
1:E:73:A:H5'	2:A:229:ASN:HD21	1.65	0.60
2:B:337:GLU:HG3	2:B:383:THR:HG23	1.84	0.60
1:E:2:C:H2'	1:E:3:G:O4'	2.02	0.60
1:F:34:OMG:H2'	1:F:35:A:C5'	2.31	0.60
1:E:40:5MC:H2'	1:E:41:U:H5'	1.83	0.60
2:A:76:ARG:HH22	2:A:113:PRO:HG2	1.65	0.59
1:F:41:U:H2'	1:F:42:G:O4'	2.03	0.59
2:A:337:GLU:HG3	2:A:383:THR:HG23	1.84	0.58
1:E:41:U:H5'	1:E:41:U:C6	2.30	0.58
1:E:64:A:H2'	1:E:65:G:O4'	2.04	0.58
1:E:41:U:H2'	1:E:42:G:O4'	2.03	0.57
2:A:47:SER:HB3	2:A:53:TRP:HB3	1.86	0.57
2:A:99:TYR:CD1	2:A:112:VAL:HG22	2.38	0.57
1:F:64:A:OP1	2:B:399:THR:HA	2.05	0.57
2:B:47:SER:HB3	2:B:53:TRP:HB3	1.87	0.57
1:F:64:A:H2'	1:F:65:G:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:A:H5'	2:B:229:ASN:HD21	1.69	0.57
1:F:35:A:H2'	1:F:36:A:O4'	2.06	0.56
1:E:56:C:H1'	2:A:354:ASN:HB3	1.86	0.56
1:E:56:C:C2	2:A:347:PRO:HB3	2.41	0.55
1:E:35:A:H2'	1:E:36:A:O4'	2.06	0.55
2:A:34:ARG:HD2	2:A:86:VAL:HA	1.87	0.55
1:F:75:C:H2'	2:B:99:TYR:CE2	2.42	0.55
1:F:64:A:OP1	2:B:399:THR:N	2.39	0.55
1:E:1:G:O2'	2:A:292:ASN:ND2	2.40	0.55
1:E:35:A:H2'	1:E:36:A:C8	2.42	0.54
1:E:55:PSU:H5'	2:A:344:ARG:NH2	2.16	0.54
2:A:76:ARG:HG3	2:A:76:ARG:HH11	1.72	0.54
1:E:41:U:H6	1:E:41:U:C5'	2.16	0.54
2:B:34:ARG:HD2	2:B:86:VAL:HA	1.90	0.54
1:F:35:A:H2'	1:F:36:A:C8	2.43	0.54
2:B:34:ARG:HB2	2:B:86:VAL:HG13	1.89	0.54
1:F:73:A:H5'	2:B:229:ASN:ND2	2.22	0.54
1:E:37:YG:H31	1:E:37:YG:C1'	2.38	0.53
1:F:37:YG:H31	1:F:37:YG:C1'	2.38	0.53
2:B:147:GLU:HA	2:B:150:LEU:HD12	1.88	0.53
1:E:29:A:O2'	1:E:30:G:H5'	2.09	0.53
1:E:73:A:H5'	2:A:229:ASN:ND2	2.24	0.53
2:B:115:TYR:C	2:B:117:LEU:H	2.17	0.53
1:E:64:A:OP1	2:A:398:HIS:C	2.52	0.52
1:F:29:A:O2'	1:F:30:G:H5'	2.09	0.52
2:A:147:GLU:HA	2:A:150:LEU:HD12	1.92	0.52
2:A:34:ARG:HB2	2:A:86:VAL:HG13	1.90	0.52
2:A:70:PHE:CD2	2:A:74:GLU:HG2	2.45	0.51
1:F:2:C:H2'	1:F:3:G:O4'	2.11	0.51
1:F:72:C:H2'	1:F:73:A:O4'	2.10	0.51
2:A:31:LEU:HD12	2:A:86:VAL:HG11	1.92	0.51
2:B:48:TYR:HA	2:B:53:TRP:CE3	2.46	0.51
1:E:37:YG:H32	1:E:38:A:O4'	2.11	0.50
1:F:16:H2U:C1'	1:F:17:H2U:P	2.99	0.50
1:F:41:U:H6	1:F:41:U:C5'	2.16	0.50
1:F:37:YG:H32	1:F:38:A:O4'	2.11	0.50
1:E:72:C:H2'	1:E:73:A:O4'	2.11	0.50
2:A:115:TYR:C	2:A:117:LEU:H	2.19	0.50
1:E:64:A:OP1	2:A:398:HIS:HB2	2.12	0.50
2:B:277:ALA:HB2	2:B:336:LYS:HG2	1.92	0.50
1:F:35:A:H5'	1:F:35:A:C8	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:A:H5'	1:E:35:A:C8	2.38	0.50
1:F:33:U:O2	1:F:36:A:OP2	2.31	0.49
1:F:1:G:C3'	1:F:2:C:H5'	2.42	0.49
1:F:41:U:H5'	1:F:41:U:C6	2.29	0.49
2:A:48:TYR:HA	2:A:53:TRP:CE3	2.48	0.49
1:E:75:C:H2'	2:A:99:TYR:CE2	2.47	0.49
1:F:40:5MC:H2'	1:F:41:U:C5'	2.42	0.49
1:F:2:C:C2'	1:F:3:G:O5'	2.61	0.49
2:B:70:PHE:CD2	2:B:74:GLU:HG2	2.47	0.49
1:E:33:U:O2	1:E:36:A:OP2	2.31	0.48
1:E:75:C:O2'	2:A:93:ARG:HB3	2.13	0.48
2:A:70:PHE:HD2	2:A:74:GLU:HG2	1.77	0.48
1:F:64:A:OP1	2:B:399:THR:CA	2.61	0.48
1:E:40:5MC:H2'	1:E:41:U:C5'	2.43	0.48
1:E:56:C:N4	1:E:57:G:C6	2.82	0.48
1:F:2:C:H3'	1:F:2:C:C6	2.49	0.48
1:E:1:G:C3'	1:E:2:C:H5'	2.43	0.48
1:E:30:G:O2'	1:E:31:A:H5'	2.14	0.48
2:B:16:PRO:O	2:B:18:GLU:N	2.47	0.48
2:B:87:LEU:HD13	2:B:102:GLY:HA3	1.95	0.47
2:A:274:ARG:NE	2:A:332:GLU:OE2	2.45	0.47
2:B:70:PHE:HD2	2:B:74:GLU:HG2	1.80	0.47
2:B:75:LEU:HD11	2:B:115:TYR:CZ	2.50	0.47
2:A:66:PHE:HB3	2:A:75:LEU:HD22	1.97	0.47
1:F:3:G:C2	1:F:71:G:C2	3.03	0.47
2:A:87:LEU:HD13	2:A:102:GLY:HA3	1.96	0.47
2:B:14:VAL:CG1	2:B:149:ARG:HB3	2.45	0.47
1:F:30:G:O2'	1:F:31:A:H5'	2.14	0.47
1:E:16:H2U:H1'	1:E:17:H2U:OP2	2.15	0.46
2:A:277:ALA:HB2	2:A:336:LYS:HG2	1.97	0.46
1:F:2:C:H5''	2:B:292:ASN:ND2	2.29	0.46
2:A:120:PRO:C	2:A:122:ASN:H	2.23	0.46
1:E:67:A:O2'	1:E:68:U:H5'	2.15	0.46
2:A:76:ARG:HH21	2:A:113:PRO:HG2	1.78	0.46
1:E:23:A:O2'	1:E:24:G:H5'	2.15	0.46
2:A:14:VAL:CG1	2:A:149:ARG:HB3	2.46	0.45
2:A:341:VAL:HG21	2:B:274:ARG:HG2	1.98	0.45
2:B:31:LEU:HD12	2:B:86:VAL:HG11	1.99	0.45
1:F:23:A:O2'	1:F:24:G:H5'	2.16	0.45
2:A:51:ASN:HA	2:A:53:TRP:CZ3	2.51	0.45
1:F:34:OMG:C2'	1:F:35:A:C5'	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:PHE:HB3	2:B:75:LEU:HD22	1.99	0.44
2:B:120:PRO:C	2:B:122:ASN:H	2.25	0.44
1:E:56:C:O2	2:A:354:ASN:CB	2.62	0.44
2:B:258:HIS:HB2	2:B:259:PRO:HD2	2.00	0.44
1:F:23:A:H2'	1:F:24:G:C8	2.52	0.44
2:A:73:GLU:HA	2:A:76:ARG:HB2	1.99	0.44
2:A:75:LEU:HD11	2:A:115:TYR:CZ	2.53	0.44
2:A:141:ILE:HD11	2:A:148:VAL:HG21	2.00	0.44
2:B:64:LEU:N	2:B:112:VAL:O	2.32	0.44
1:F:43:G:H2'	1:F:44:A:C8	2.53	0.44
2:A:16:PRO:O	2:A:18:GLU:N	2.50	0.44
2:B:99:TYR:HD1	2:B:112:VAL:HG22	1.82	0.44
2:A:67:PRO:C	2:A:69:GLU:H	2.26	0.43
2:A:70:PHE:HD2	2:A:74:GLU:CG	2.31	0.43
2:B:118:LYS:O	2:B:119:GLU:HB2	2.17	0.43
2:B:171:SER:O	2:B:174:LEU:HB3	2.18	0.43
2:B:51:ASN:HA	2:B:53:TRP:CZ3	2.53	0.43
1:E:23:A:H2'	1:E:24:G:C8	2.53	0.43
1:E:50:U:O2'	1:E:51:G:H5'	2.19	0.43
1:F:72:C:OP1	2:B:224:ARG:NH1	2.51	0.43
1:F:50:U:O2'	1:F:51:G:H5'	2.19	0.43
1:E:43:G:H2'	1:E:44:A:C8	2.53	0.43
2:A:340:ARG:HG2	2:A:379:MET:HE3	2.00	0.43
1:E:32:OMC:H6	1:E:32:OMC:O5'	2.02	0.42
1:E:37:YG:C21	1:E:37:YG:H101	2.50	0.42
1:F:37:YG:C21	1:F:37:YG:H101	2.49	0.42
1:F:63:C:H5''	2:B:399:THR:HB	2.01	0.42
2:A:148:VAL:HG11	2:A:176:GLU:HG2	2.01	0.42
2:A:171:SER:O	2:A:174:LEU:HB3	2.20	0.42
2:A:258:HIS:HB2	2:A:259:PRO:HD2	2.01	0.42
1:F:55:PSU:C5'	2:B:344:ARG:HH21	2.20	0.42
1:E:1:G:C6	1:E:2:C:C4	3.07	0.42
1:F:32:OMC:O5'	1:F:32:OMC:H6	2.03	0.42
2:A:63:PHE:CD2	2:A:114:CYS:SG	3.13	0.42
2:A:99:TYR:HD1	2:A:112:VAL:HG22	1.84	0.42
2:B:141:ILE:HD11	2:B:148:VAL:HG21	2.01	0.42
1:E:75:C:H2'	2:A:99:TYR:HE2	1.84	0.41
2:A:63:PHE:HD2	2:A:114:CYS:SG	2.43	0.41
2:A:118:LYS:O	2:A:119:GLU:HB2	2.20	0.41
2:A:67:PRO:HB2	2:A:70:PHE:CD1	2.55	0.41
2:B:63:PHE:CD2	2:B:114:CYS:SG	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:G:H2'	1:E:72:C:O5'	2.20	0.41
2:B:70:PHE:HD2	2:B:74:GLU:CG	2.32	0.41
1:E:34:OMG:C2'	1:E:35:A:C5'	2.91	0.41
2:B:63:PHE:HD2	2:B:114:CYS:SG	2.43	0.41
2:B:67:PRO:C	2:B:69:GLU:H	2.28	0.41
2:B:315:PRO:HA	2:B:333:CYS:HA	2.02	0.41
1:F:56:C:H1'	2:B:354:ASN:HB3	2.02	0.41
1:F:75:C:H5''	1:F:76:A:P	2.61	0.41
1:E:50:U:C2'	1:E:51:G:H5'	2.51	0.41
1:E:69:U:H2'	1:E:70:C:C6	2.55	0.41
1:F:50:U:C2'	1:F:51:G:H5'	2.51	0.41
1:F:75:C:H2'	2:B:99:TYR:HE2	1.83	0.41
2:A:423:GLU:HB3	2:A:424:PRO:HD2	2.02	0.41
1:F:64:A:H5''	2:B:398:HIS:HB2	2.01	0.41
2:A:3:VAL:HG22	2:A:249:PRO:HG2	2.03	0.41
2:A:67:PRO:HB2	2:A:70:PHE:HD1	1.86	0.41
2:A:94:TYR:HA	2:A:98:PRO:CA	2.46	0.40
2:B:366:ARG:HA	2:B:367:PRO:HD3	1.91	0.40
2:B:423:GLU:HB3	2:B:424:PRO:HD2	2.03	0.40
1:F:36:A:H2'	1:F:37:YG:O4'	2.21	0.40
2:B:262:ILE:HG22	2:B:263:GLU:N	2.36	0.40
1:E:2:C:OP1	2:A:402:LYS:CB	2.69	0.40
1:F:37:YG:C3	1:F:37:YG:C2'	2.99	0.40
2:A:119:GLU:HA	2:A:120:PRO:HD3	1.82	0.40
2:B:16:PRO:HB2	2:B:17:ASP:H	1.74	0.40
1:E:36:A:H2'	1:E:37:YG:O4'	2.21	0.40
1:E:37:YG:C1'	1:E:37:YG:C3	3.00	0.40
1:F:74:C:H3'	1:F:75:C:O4'	2.22	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	
2	A	435/437 (100%)	397 (91%)	32 (7%)	6 (1%)	9	40
2	B	435/437 (100%)	397 (91%)	31 (7%)	7 (2%)	7	37
All	All	870/874 (100%)	794 (91%)	63 (7%)	13 (2%)	8	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	17	ASP
2	A	186	LEU
2	B	17	ASP
2	B	186	LEU
2	A	16	PRO
2	A	261	GLU
2	B	16	PRO
2	B	261	GLU
2	A	119	GLU
2	B	119	GLU
2	B	116	LYS
2	A	120	PRO
2	B	120	PRO

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	
2	A	387/387 (100%)	369 (95%)	18 (5%)	23	44
2	B	387/387 (100%)	368 (95%)	19 (5%)	22	43
All	All	774/774 (100%)	737 (95%)	37 (5%)	23	44

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	23	LYS
2	A	31	LEU
2	A	38	LEU

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Mol	Chain	Res	Type
2	A	73	GLU
2	A	76	ARG
2	A	94	TYR
2	A	96	GLU
2	A	99	TYR
2	A	156	LYS
2	A	203	VAL
2	A	213	GLU
2	A	223	LYS
2	A	257	LYS
2	A	273	GLU
2	A	340	ARG
2	A	383	THR
2	A	398	HIS
2	A	406	GLU
2	B	23	LYS
2	B	31	LEU
2	B	38	LEU
2	B	73	GLU
2	B	76	ARG
2	B	94	TYR
2	B	96	GLU
2	B	99	TYR
2	B	156	LYS
2	B	203	VAL
2	B	213	GLU
2	B	223	LYS
2	B	224	ARG
2	B	257	LYS
2	B	273	GLU
2	B	340	ARG
2	B	383	THR
2	B	398	HIS
2	B	406	GLU

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

Mol	Chain	Res	Type
2	A	191	ASN
2	A	229	ASN
2	A	258	HIS
2	A	292	ASN

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Mol	Chain	Res	Type
2	B	191	ASN
2	B	229	ASN
2	B	258	HIS
2	B	292	ASN
2	B	398	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	73/76 (96%)	10 (13%)	2 (2%)
1	F	73/76 (96%)	11 (15%)	3 (4%)
All	All	146/152 (96%)	21 (14%)	5 (3%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	2	C
1	E	17	H2U
1	E	18	G
1	E	19	G
1	E	21	A
1	E	35	A
1	E	41	U
1	E	73	A
1	E	74	C
1	E	76	A
1	F	2	C
1	F	3	G
1	F	17	H2U
1	F	18	G
1	F	19	G
1	F	21	A
1	F	35	A
1	F	41	U
1	F	73	A
1	F	74	C
1	F	76	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	16	H2U
1	E	18	G
1	F	2	C
1	F	16	H2U
1	F	18	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

28 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	F	55	1	18,21,22	0.67	0	21,30,33	0.84	0
1	OMG	F	34	1	23,26,27	0.52	0	32,38,41	0.51	1 (3%)
1	OMC	E	32	1	19,22,23	0.42	0	25,31,34	0.59	1 (4%)
1	OMC	F	32	1	19,22,23	0.40	0	25,31,34	0.59	1 (4%)
1	2MG	E	10	1	23,26,27	0.48	0	33,38,41	0.42	0
1	OMG	E	34	1	23,26,27	0.53	0	32,38,41	0.51	1 (3%)
1	PSU	E	55	1	18,21,22	0.67	0	21,30,33	0.83	0
1	5MC	E	40	1	19,22,23	0.60	0	26,32,35	0.66	1 (3%)
1	5MU	F	54	1	19,22,23	0.45	0	27,32,35	0.64	0
1	YG	F	37	1	38,42,43	0.90	2 (5%)	45,62,65	2.18	10 (22%)
1	7MG	F	46	1	23,26,27	1.00	2 (8%)	27,39,42	1.24	2 (7%)
1	H2U	E	17	1	18,21,22	1.14	2 (11%)	19,30,33	0.87	0
1	1MA	F	58	1	21,25,26	1.94	2 (9%)	30,37,40	1.62	7 (23%)
1	PSU	F	39	1	18,21,22	0.61	0	21,30,33	0.65	0
1	2MG	F	10	1	23,26,27	0.49	0	33,38,41	0.42	0
1	M2G	F	26	1	24,27,28	0.46	0	33,40,43	0.42	0
1	PSU	E	39	1	18,21,22	0.59	0	21,30,33	0.65	0
1	5MC	F	40	1	19,22,23	0.61	1 (5%)	26,32,35	0.66	1 (3%)
1	H2U	F	17	1	18,21,22	1.42	2 (11%)	19,30,33	0.77	0
1	7MG	E	46	1	23,26,27	1.02	3 (13%)	27,39,42	1.25	2 (7%)
1	M2G	E	26	1	24,27,28	0.45	0	33,40,43	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	F	49	1	19,22,23	0.70	0	26,32,35	0.71	1 (3%)
1	H2U	F	16	1	18,21,22	1.14	2 (11%)	19,30,33	0.91	0
1	5MU	E	54	1	19,22,23	0.47	0	27,32,35	0.63	0
1	YG	E	37	1	38,42,43	0.90	2 (5%)	45,62,65	2.20	10 (22%)
1	H2U	E	16	1	18,21,22	1.15	2 (11%)	19,30,33	0.91	0
1	5MC	E	49	1	19,22,23	0.70	0	26,32,35	0.71	1 (3%)
1	1MA	E	58	1	21,25,26	1.93	2 (9%)	30,37,40	1.63	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	F	55	1	-	1/7/25/26	0/2/2/2
1	OMG	F	34	1	-	1/9/27/28	0/3/3/3
1	OMC	E	32	1	-	0/9/27/28	0/2/2/2
1	OMC	F	32	1	-	0/9/27/28	0/2/2/2
1	2MG	E	10	1	-	0/9/27/28	0/3/3/3
1	OMG	E	34	1	-	1/9/27/28	0/3/3/3
1	PSU	E	55	1	-	1/7/25/26	0/2/2/2
1	5MC	E	40	1	-	1/7/25/26	0/2/2/2
1	5MU	F	54	1	-	0/7/25/26	0/2/2/2
1	YG	F	37	1	-	7/24/42/43	0/4/4/4
1	7MG	F	46	1	-	2/7/37/38	0/3/3/3
1	H2U	E	17	1	-	0/7/38/39	0/2/2/2
1	1MA	F	58	1	-	0/7/25/26	0/3/3/3
1	PSU	F	39	1	-	0/7/25/26	0/2/2/2
1	2MG	F	10	1	-	0/9/27/28	0/3/3/3
1	M2G	F	26	1	-	0/11/29/30	0/3/3/3
1	PSU	E	39	1	-	0/7/25/26	0/2/2/2
1	5MC	F	40	1	-	1/7/25/26	0/2/2/2
1	H2U	F	17	1	-	2/7/38/39	0/2/2/2
1	7MG	E	46	1	-	2/7/37/38	0/3/3/3
1	M2G	E	26	1	-	0/11/29/30	0/3/3/3
1	5MC	F	49	1	-	0/7/25/26	0/2/2/2
1	H2U	F	16	1	-	4/7/38/39	0/2/2/2
1	5MU	E	54	1	-	0/7/25/26	0/2/2/2
1	YG	E	37	1	-	7/24/42/43	0/4/4/4
1	H2U	E	16	1	-	4/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	E	49	1	-	0/7/25/26	0/2/2/2
1	1MA	E	58	1	-	0/7/25/26	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	1MA	C6-N6	7.80	1.46	1.28
1	E	58	1MA	C6-N6	7.72	1.46	1.28
1	F	17	H2U	C1'-N1	5.10	1.56	1.46
1	F	58	1MA	C2-N3	3.64	1.37	1.30
1	E	58	1MA	C2-N3	3.64	1.37	1.30
1	E	17	H2U	C6-C5	-3.48	1.43	1.52
1	E	16	H2U	C6-C5	-3.27	1.44	1.52
1	F	16	H2U	C6-C5	-3.21	1.44	1.52
1	F	37	YG	C2-N2	3.01	1.38	1.33
1	E	37	YG	C2-N2	3.00	1.38	1.33
1	F	46	7MG	C5-N7	2.72	1.39	1.35
1	E	16	H2U	C2-N1	2.71	1.39	1.35
1	F	17	H2U	C2-N1	2.69	1.39	1.35
1	F	16	H2U	C2-N1	2.68	1.39	1.35
1	E	46	7MG	C5-N7	2.67	1.39	1.35
1	E	17	H2U	C2-N1	2.60	1.39	1.35
1	E	46	7MG	C4-N9	2.37	1.40	1.37
1	F	46	7MG	C4-N9	2.35	1.40	1.37
1	F	40	5MC	C5-C4	-2.06	1.42	1.44
1	E	46	7MG	C8-N9	-2.06	1.44	1.45
1	F	37	YG	C3-N3	2.03	1.50	1.47
1	E	37	YG	C3-N3	2.02	1.50	1.47

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	YG	C11-C12-N1	7.82	110.82	105.31
1	F	37	YG	C11-C12-N1	7.77	110.79	105.31
1	E	37	YG	C24-O23-C21	6.40	123.04	115.63
1	F	37	YG	C24-O23-C21	6.28	122.91	115.63
1	E	46	7MG	C4-C5-N7	4.68	110.90	105.38
1	E	37	YG	O23-C21-N20	4.64	118.58	110.77
1	F	46	7MG	C4-C5-N7	4.58	110.79	105.38
1	F	37	YG	O23-C21-N20	4.56	118.43	110.77
1	E	37	YG	C5-C4-N3	4.00	127.24	123.99
1	F	58	1MA	N1-C2-N3	4.00	130.75	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	58	1MA	N1-C2-N3	3.98	130.73	126.00
1	F	37	YG	C5-C4-N3	3.91	127.17	123.99
1	F	58	1MA	CM1-N1-C6	-3.82	114.23	120.15
1	E	58	1MA	CM1-N1-C6	-3.80	114.26	120.15
1	F	58	1MA	CM1-N1-C2	3.78	128.24	120.50
1	E	58	1MA	CM1-N1-C2	3.76	128.19	120.50
1	E	37	YG	O23-C21-O22	-3.55	119.44	124.62
1	F	37	YG	C10-C11-N2	3.55	126.44	119.32
1	E	37	YG	C10-C11-N2	3.50	126.35	119.32
1	F	37	YG	O23-C21-O22	-3.48	119.56	124.62
1	E	37	YG	C2-N1-C12	-3.39	103.84	109.94
1	F	37	YG	C2-N1-C12	-3.34	103.93	109.94
1	F	37	YG	N3-C2-N2	-3.16	122.26	126.62
1	E	37	YG	N3-C2-N2	-3.16	122.26	126.62
1	E	46	7MG	N9-C8-N7	3.13	107.81	103.37
1	F	46	7MG	N9-C8-N7	3.11	107.78	103.37
1	E	58	1MA	C6-C5-N7	-2.82	127.18	132.16
1	F	58	1MA	C6-C5-N7	-2.78	127.24	132.16
1	F	37	YG	C19-O18-C16	2.78	122.21	115.92
1	E	37	YG	C19-O18-C16	2.70	122.04	115.92
1	F	37	YG	O18-C16-C15	2.48	117.81	111.49
1	E	37	YG	O18-C16-C15	2.47	117.78	111.49
1	E	58	1MA	N1-C6-N6	2.47	125.91	119.71
1	F	58	1MA	N1-C6-N6	2.47	125.91	119.71
1	E	49	5MC	C5-C6-N1	-2.43	120.67	123.31
1	F	49	5MC	C5-C6-N1	-2.42	120.68	123.31
1	E	40	5MC	C5-C6-N1	-2.27	120.85	123.31
1	F	40	5MC	C5-C6-N1	-2.25	120.87	123.31
1	E	34	OMG	CM2-O2'-C2'	2.09	119.85	114.47
1	E	58	1MA	C6-C5-C4	2.07	122.70	118.32
1	F	58	1MA	C5-C4-N3	-2.06	124.24	127.27
1	E	58	1MA	C5-C4-N3	-2.06	124.25	127.27
1	F	32	OMC	CM2-O2'-C2'	2.05	119.74	114.47
1	F	58	1MA	C6-C5-C4	2.05	122.67	118.32
1	F	34	OMG	CM2-O2'-C2'	2.03	119.69	114.47
1	E	32	OMC	CM2-O2'-C2'	2.03	119.68	114.47

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	16	H2U	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	E	16	H2U	O4'-C1'-N1-C6
1	E	46	7MG	C2'-C1'-N9-C8
1	F	16	H2U	O4'-C1'-N1-C2
1	F	16	H2U	O4'-C1'-N1-C6
1	F	37	YG	C15-C16-O18-C19
1	F	46	7MG	C2'-C1'-N9-C8
1	E	37	YG	O17-C16-O18-C19
1	F	37	YG	O17-C16-O18-C19
1	E	37	YG	C15-C16-O18-C19
1	E	16	H2U	C2'-C1'-N1-C6
1	E	37	YG	C12-C13-C14-C15
1	F	37	YG	C12-C13-C14-C15
1	F	16	H2U	C2'-C1'-N1-C6
1	E	16	H2U	C2'-C1'-N1-C2
1	E	37	YG	C13-C14-C15-C16
1	F	37	YG	C13-C14-C15-C16
1	F	16	H2U	C2'-C1'-N1-C2
1	F	17	H2U	O4'-C4'-C5'-O5'
1	F	17	H2U	C3'-C4'-C5'-O5'
1	E	34	OMG	C4'-C5'-O5'-P
1	F	34	OMG	C4'-C5'-O5'-P
1	F	40	5MC	O4'-C4'-C5'-O5'
1	E	46	7MG	C2'-C1'-N9-C4
1	F	46	7MG	C2'-C1'-N9-C4
1	E	40	5MC	O4'-C4'-C5'-O5'
1	E	55	PSU	O4'-C1'-C5-C6
1	F	55	PSU	O4'-C1'-C5-C6
1	E	37	YG	C13-C14-C15-N20
1	F	37	YG	C13-C14-C15-N20
1	E	37	YG	C14-C15-C16-O18
1	F	37	YG	C14-C15-C16-O18
1	F	37	YG	C14-C15-C16-O17
1	E	37	YG	C14-C15-C16-O17

There are no ring outliers.

16 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	55	PSU	3	0
1	F	34	OMG	5	0
1	E	32	OMC	1	0
1	F	32	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	34	OMG	5	0
1	E	55	PSU	2	0
1	E	40	5MC	2	0
1	F	37	YG	6	0
1	E	17	H2U	1	0
1	F	26	M2G	1	0
1	F	40	5MC	2	0
1	F	17	H2U	1	0
1	E	26	M2G	1	0
1	F	16	H2U	1	0
1	E	37	YG	6	0
1	E	16	H2U	1	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	57:G	O3'	58:1MA	P	1.25

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	E	62/76 (81%)	1.01	8 (12%) 7 15	101, 102, 102, 102	0
1	F	62/76 (81%)	1.17	10 (16%) 4 12	101, 102, 102, 102	0
2	A	437/437 (100%)	1.62	153 (35%) 1 5	102, 102, 102, 107	0
2	B	437/437 (100%)	1.60	141 (32%) 1 6	102, 102, 102, 107	0
All	All	998/1026 (97%)	1.55	312 (31%) 1 6	101, 102, 102, 107	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	165	TYR	8.6
2	B	76	ARG	6.4
2	B	223	LYS	5.6
2	A	170	PHE	5.6
2	B	365	PHE	5.6
2	A	431	GLU	5.5
2	A	400	LEU	5.3
2	B	364	ALA	5.2
2	B	377	PHE	5.2
2	B	327	CYS	5.1
2	A	92	ILE	5.1
2	B	1	MET	5.0
2	B	366	ARG	4.9
2	A	366	ARG	4.9
2	B	345	MET	4.7
2	A	136	TRP	4.7
2	B	381	LYS	4.7
2	A	433	MET	4.5
2	A	130	THR	4.4
2	A	124	LYS	4.4
2	A	166	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	A	416	SER	4.3
2	B	233	ASP	4.3
2	B	168	ARG	4.3
2	A	81	GLU	4.2
2	A	294	TYR	4.2
2	B	283	PHE	4.2
2	B	282	LYS	4.2
2	A	331	PHE	4.2
2	B	321	LYS	4.2
2	B	105	LYS	4.1
2	B	170	PHE	4.1
2	A	310	ARG	4.1
2	B	122	ASN	4.1
2	B	324	GLU	4.1
2	A	78	ARG	4.1
2	B	183	GLY	4.0
2	B	126	ALA	4.0
2	A	299	ARG	4.0
2	A	2	LYS	4.0
2	B	161	TYR	3.9
2	B	393	ALA	3.9
2	A	100	VAL	3.9
2	B	400	LEU	3.9
2	A	19	GLU	3.9
2	A	336	LYS	3.9
2	A	207	GLU	3.9
1	E	35	A	3.8
2	A	135	LYS	3.8
2	A	85	ALA	3.7
2	B	195	TRP	3.7
2	B	310	ARG	3.7
2	A	44	PHE	3.7
2	A	47	SER	3.7
2	A	82	ILE	3.7
2	B	121	LYS	3.7
2	A	133	HIS	3.6
1	F	47	U	3.6
2	B	130	THR	3.6
2	B	38	LEU	3.6
2	A	97	HIS	3.6
2	A	381	LYS	3.6
2	A	214	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	44	PHE	3.5
2	B	48	TYR	3.5
2	B	49	ALA	3.5
2	A	321	LYS	3.5
2	B	336	LYS	3.5
2	B	374	TRP	3.5
2	A	210	LYS	3.5
2	A	121	LYS	3.4
2	B	281	VAL	3.4
2	B	363	ARG	3.4
2	A	290	ASP	3.4
2	A	171	SER	3.4
2	A	374	TRP	3.4
2	B	2	LYS	3.4
2	A	404	VAL	3.4
2	B	235	LEU	3.3
2	B	142	LYS	3.3
2	B	239	VAL	3.3
2	B	298	GLU	3.3
2	A	422	LYS	3.3
2	B	47	SER	3.3
2	A	230	LEU	3.3
2	B	358	PHE	3.3
2	B	100	VAL	3.2
2	B	80	LEU	3.2
2	B	309	GLU	3.2
2	A	205	LYS	3.2
1	E	36	A	3.2
2	B	63	PHE	3.2
2	A	317	ARG	3.2
2	A	111	VAL	3.1
2	B	90	TYR	3.1
2	A	195	TRP	3.1
2	A	289	VAL	3.1
2	A	345	MET	3.1
2	A	223	LYS	3.1
2	B	46	GLY	3.1
2	A	408	ILE	3.1
2	B	402	LYS	3.1
2	B	31	LEU	3.1
2	B	35	LEU	3.1
2	B	40	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	45	G	3.1
2	A	351	ASP	3.1
2	A	12	GLU	3.1
2	B	79	GLY	3.0
2	A	125	SER	3.0
2	A	163	ALA	3.0
2	B	117	LEU	3.0
2	A	71	SER	3.0
2	A	140	ARG	3.0
2	A	428	GLU	3.0
2	A	318	SER	3.0
2	B	71	SER	3.0
2	B	290	ASP	3.0
2	B	83	GLY	3.0
2	B	19	GLU	3.0
2	B	41	GLU	3.0
2	A	98	PRO	2.9
2	A	363	ARG	2.9
2	A	20	GLU	2.9
2	A	247	GLU	2.9
2	A	304	ILE	2.9
2	A	326	PHE	2.9
2	B	323	SER	2.9
2	A	164	GLU	2.9
2	A	142	LYS	2.9
2	A	77	GLU	2.9
2	B	311	GLU	2.9
1	F	35	A	2.8
2	B	322	ALA	2.8
2	A	156	LYS	2.8
2	A	360	SER	2.8
2	B	371	ASN	2.8
2	A	178	LEU	2.8
2	A	57	SER	2.8
2	A	325	GLU	2.8
2	B	346	GLY	2.8
1	E	44	A	2.8
2	A	257	LYS	2.8
2	B	143	GLY	2.8
2	A	161	TYR	2.8
2	A	76	ARG	2.8
2	B	111	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	156	LYS	2.8
2	B	389	VAL	2.7
2	A	348	GLN	2.7
2	A	305	PHE	2.7
2	B	320	PHE	2.7
2	B	246	MET	2.7
2	A	72	LYS	2.7
2	A	233	ASP	2.7
2	B	32	ARG	2.7
2	B	278	VAL	2.7
2	A	361	ARG	2.7
2	A	432	MET	2.7
2	A	48	TYR	2.7
2	A	418	GLU	2.7
2	A	435	VAL	2.7
2	A	158	ASN	2.7
2	A	34	ARG	2.7
2	B	273	GLU	2.7
2	A	185	PHE	2.7
2	B	88	ASP	2.6
2	B	86	VAL	2.6
1	E	74	C	2.6
2	B	291	ASP	2.6
2	B	212	GLU	2.6
2	B	152	LYS	2.6
2	B	237	ARG	2.6
1	F	1	G	2.6
2	A	324	GLU	2.6
2	A	412	PHE	2.6
2	B	373	ARG	2.6
1	F	38	A	2.6
2	A	126	ALA	2.5
2	A	123	ILE	2.5
2	A	21	VAL	2.5
2	A	172	GLY	2.5
2	A	16	PRO	2.5
2	A	13	LEU	2.5
2	A	64	LEU	2.5
2	A	89	SER	2.5
2	B	118	LYS	2.5
2	B	144	LYS	2.5
2	A	307	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	420	LEU	2.5
2	A	281	VAL	2.5
2	A	343	ARG	2.5
2	A	379	MET	2.5
2	B	343	ARG	2.5
2	B	36	ASP	2.5
2	B	257	LYS	2.5
2	A	424	PRO	2.5
2	A	95	ALA	2.5
2	B	394	SER	2.5
2	A	273	GLU	2.5
2	B	166	LYS	2.5
2	B	42	TYR	2.5
2	A	32	ARG	2.5
2	A	1	MET	2.4
2	A	84	LYS	2.4
2	B	9	LYS	2.4
1	E	75	C	2.4
2	B	94	TYR	2.4
2	A	183	GLY	2.4
2	A	80	LEU	2.4
2	A	320	PHE	2.4
2	B	414	ILE	2.4
2	B	399	THR	2.4
2	A	113	PRO	2.4
2	B	172	GLY	2.4
2	B	412	PHE	2.4
2	B	62	VAL	2.4
2	A	298	GLU	2.4
2	B	108	GLU	2.4
2	B	279	PHE	2.4
2	A	128	ASP	2.4
2	A	33	ARG	2.4
2	B	294	TYR	2.4
2	B	396	HIS	2.4
2	A	232	LEU	2.4
2	B	424	PRO	2.4
2	A	250	SER	2.4
2	B	53	TRP	2.4
2	A	174	LEU	2.3
2	B	232	LEU	2.3
2	A	367	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	367	PRO	2.3
2	B	159	GLY	2.3
2	B	222	GLU	2.3
1	F	27	C	2.3
1	F	28	C	2.3
2	A	3	VAL	2.3
2	B	266	ARG	2.3
2	B	436	LYS	2.3
2	A	287	ASP	2.3
2	A	403	ASN	2.3
2	B	416	SER	2.3
2	B	263	GLU	2.3
1	E	33	U	2.3
2	A	137	LEU	2.3
2	A	359	LEU	2.3
2	B	284	ARG	2.3
2	A	41	GLU	2.2
2	A	139	GLY	2.2
2	A	236	ALA	2.2
2	A	194	ARG	2.2
2	B	69	GLU	2.2
2	A	173	TYR	2.2
2	A	315	PRO	2.2
2	A	284	ARG	2.2
2	A	353	ARG	2.2
2	B	286	PRO	2.2
2	A	394	SER	2.2
2	B	304	ILE	2.2
2	A	90	TYR	2.2
2	B	329	LEU	2.2
2	A	238	PHE	2.2
2	A	18	GLU	2.2
1	E	38	A	2.2
1	F	29	A	2.2
2	B	213	GLU	2.2
2	B	50	ARG	2.2
2	A	405	GLY	2.2
1	F	59	U	2.2
2	B	84	LYS	2.2
2	B	57	SER	2.2
2	B	124	LYS	2.1
2	A	311	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	327	CYS	2.1
2	A	219	PRO	2.1
2	A	429	LEU	2.1
2	B	72	LYS	2.1
2	A	165	TYR	2.1
2	B	230	LEU	2.1
2	B	392	TYR	2.1
2	A	73	GLU	2.1
2	A	426	THR	2.1
2	A	186	LEU	2.1
2	B	214	PHE	2.1
2	B	418	GLU	2.1
2	B	140	ARG	2.1
2	B	314	MET	2.1
2	A	27	ALA	2.1
2	B	395	THR	2.1
2	B	408	ILE	2.1
2	B	20	GLU	2.1
2	B	221	ASP	2.1
2	A	303	LYS	2.1
2	B	359	LEU	2.1
1	F	36	A	2.1
2	B	185	PHE	2.1
2	B	300	ALA	2.1
2	B	299	ARG	2.0
2	B	289	VAL	2.0
2	A	168	ARG	2.0
2	A	369	ILE	2.0
2	A	414	ILE	2.0
2	B	288	ILE	2.0
1	F	14	A	2.0
2	A	352	GLU	2.0
2	A	94	TYR	2.0
2	B	66	PHE	2.0
2	A	300	ALA	2.0
2	B	133	HIS	2.0
2	A	208	VAL	2.0
2	A	278	VAL	2.0
2	A	69	GLU	2.0

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

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
1	OMG	F	34	24/25	0.27	0.37	102,102,102,102	0
1	OMC	F	32	21/22	0.44	0.29	101,102,102,102	0
1	M2G	E	26	25/26	0.46	0.30	101,101,101,101	0
1	OMC	E	32	21/22	0.53	0.26	101,102,102,102	0
1	YG	F	37	39/40	0.53	0.35	101,102,102,102	0
1	5MC	F	40	21/22	0.53	0.27	102,102,102,102	0
1	PSU	E	39	20/21	0.56	0.19	101,101,101,101	0
1	2MG	F	10	24/25	0.57	0.22	101,102,102,102	0
1	H2U	F	17	20/21	0.59	0.52	101,101,101,101	10
1	PSU	F	39	20/21	0.61	0.23	101,101,101,101	0
1	H2U	E	17	20/21	0.61	0.56	101,101,101,101	4
1	YG	E	37	39/40	0.62	0.38	101,102,102,102	0
1	7MG	F	46	24/25	0.62	0.22	101,101,102,102	0
1	2MG	E	10	24/25	0.63	0.20	101,102,102,102	0
1	7MG	E	46	24/25	0.66	0.19	101,102,102,102	0
1	H2U	E	16	20/21	0.67	0.57	101,101,101,101	13
1	OMG	E	34	24/25	0.74	0.30	101,102,102,102	0
1	5MC	E	40	21/22	0.75	0.17	101,101,102,102	0
1	H2U	F	16	20/21	0.77	0.53	101,101,101,101	13
1	M2G	F	26	25/26	0.77	0.21	101,102,102,102	0
1	5MC	F	49	21/22	0.81	0.21	101,101,102,102	0
1	5MC	E	49	21/22	0.85	0.21	101,101,102,102	0
1	1MA	F	58	23/24	0.87	0.21	101,101,101,101	0
1	1MA	E	58	23/24	0.89	0.15	101,101,101,101	0
1	PSU	F	55	20/21	0.92	0.17	101,101,101,101	0
1	5MU	E	54	21/22	0.93	0.17	101,101,101,101	0
1	PSU	E	55	20/21	0.95	0.15	101,101,101,101	0
1	5MU	F	54	21/22	0.95	0.12	101,101,101,101	0

6.3 Carbohydrates ⓘ

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.