Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 07:05 PM EDT

PDB ID	:	1SZ1
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 (i) 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 (i)) were used in the production of this report:

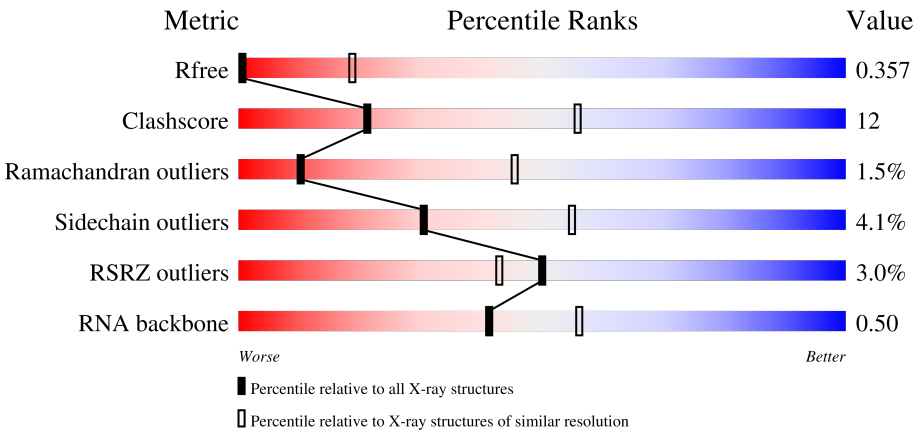
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1007 (8.50-3.88)
Clashscore	141614	1056 (8.50-3.90)
Ramachandran outliers	138981	1004 (8.50-3.88)
Sidechain outliers	138945	1003 (8.50-3.84)
RSRZ outliers	127900	1017 (8.50-3.78)
RNA backbone	3102	1076 (8.70-3.00)

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 <=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	18%; 37%, 37%, 21%, 5%
1	F	76	16%; 38%, 38%, 18%, 5%
2	A	437	81%, 16%, •
2	B	437	81%, 16%, •

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	17	-	-	-	X
1	OMG	E	34	-	-	-	X
1	YG	E	37	-	-	-	X
1	H2U	F	17	-	-	-	X
1	OMG	F	34	-	-	-	X
1	YG	F	37	-	-	-	X
1	PSU	F	39	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	P			
1	E	76	1648	746	294	533	75	0	0	0
1	F	76	1648	746	294	533	75	0	0	0

- Molecule 2 is a protein called tRNA nucleotidyltransferase.

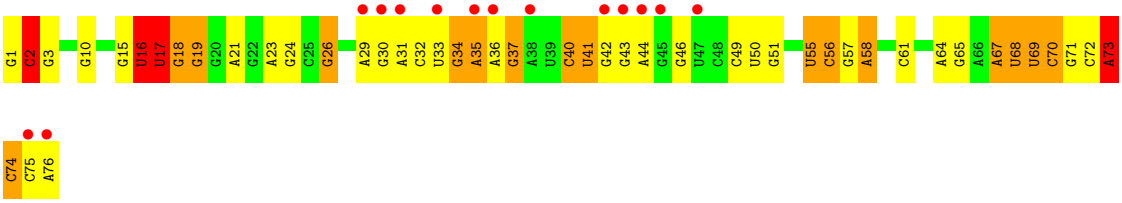
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	437	3630	2333	632	652	13	0	0	0
2	B	437	3630	2333	632	652	13	0	0	0

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.

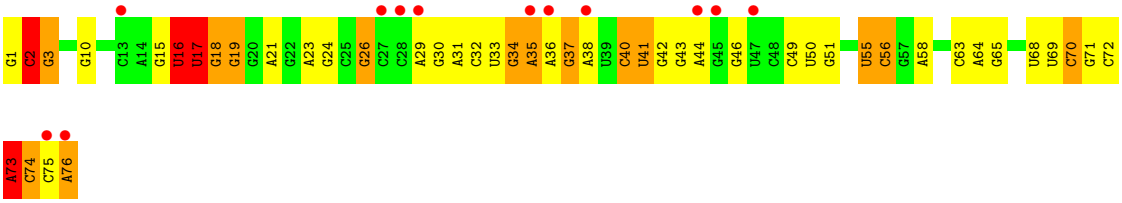
- Molecule 1: T-RNA (76-MER)

Chain E:



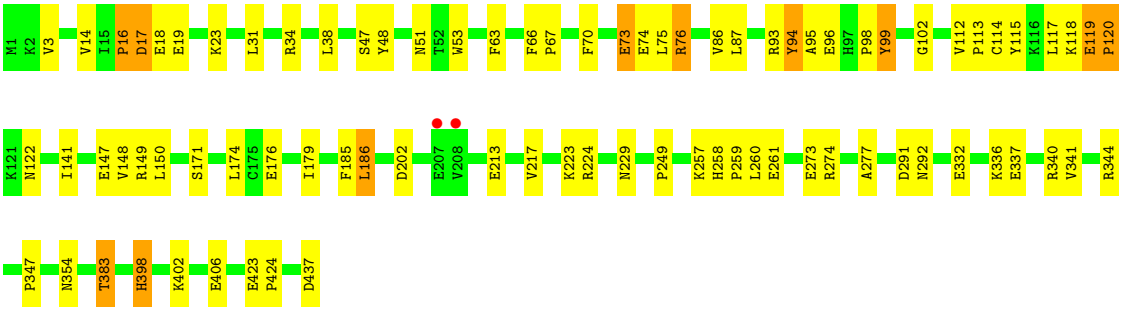
- Molecule 1: T-RNA (76-MER)

Chain F:



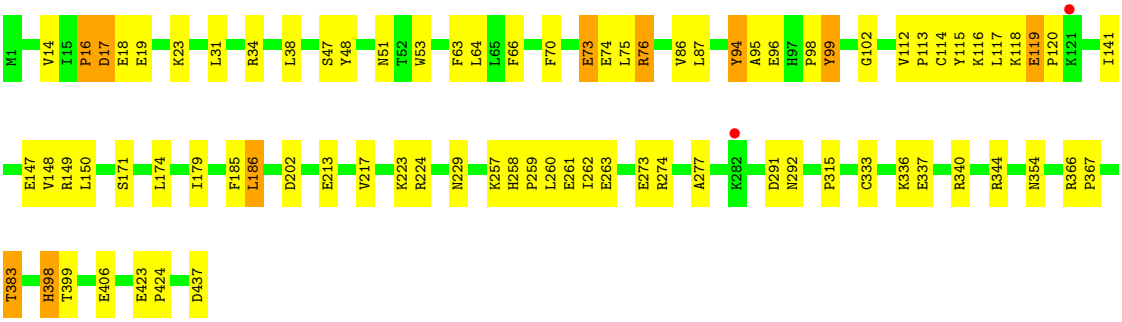
- Molecule 2: tRNA nucleotidyltransferase

Chain A:



- Molecule 2: tRNA nucleotidyltransferase

Chain B:


M1
V14
I15
P16
D17
E18
E19
K23
L31
R34
L38
S47
Y48
N51
T52
W53
F63
L64
L65
F66
F70
E73
E74
L75
R76
V86
L87
Y94
A95
E96
H97
P98
Y99
G102
V112
P113
C114
Y115
K116
L117
K118
E119
P120
K121
I141
E147
V148
R149
L150
S171
L174
I179
F185
L186
D202
E213
V217
K223
R224
N229
K257
H258
P259
L260
E261
I262
E263
E273
R274
A277
K282
D291
N292
P315
C333
K336
E337
R340
R344
N354
R366
P367
T383
H398
T399
E406
E423
P424
D437

4 Data and refinement statistics (i)

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 44.66 – 6.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.72-6.21) 98.4 (44.66-6.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [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)	0.24 , -6.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, OMC, 5MC, 7MG, H2U, OMG, YG, 1MA, 2MG, M2G

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	0.97	5/1483 (0.3%)	1.16	16/2311 (0.7%)
1	F	0.99	5/1483 (0.3%)	1.26	19/2311 (0.8%)
2	A	0.37	0/3713	0.53	0/4987
2	B	0.37	0/3713	0.51	0/4987
All	All	0.61	10/10392 (0.1%)	0.80	35/14596 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	56	C	O3'-P	-13.20	1.45	1.61
1	E	58	1MA	O3'-P	-11.84	1.47	1.61
1	F	58	1MA	O3'-P	8.15	1.71	1.61
1	E	56	C	O3'-P	6.77	1.69	1.61
1	F	70	C	N1-C2	-6.63	1.33	1.40
1	E	55	PSU	O3'-P	-6.46	1.53	1.61
1	E	46	7MG	O3'-P	5.59	1.67	1.61
1	F	46	7MG	O3'-P	5.52	1.67	1.61
1	F	34	OMG	O3'-P	5.40	1.67	1.61
1	E	34	OMG	O3'-P	5.35	1.67	1.61

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	58	1MA	P-O3'-C3'	21.66	145.69	119.70
1	F	58	1MA	O3'-P-O5'	10.34	123.64	104.00
1	F	58	1MA	OP2-P-O3'	-10.19	82.78	105.20
1	E	56	C	P-O3'-C3'	-9.78	107.97	119.70
1	F	2	C	C3'-C2'-C1'	-8.41	94.77	101.50
1	E	68	U	P-O3'-C3'	-8.30	109.74	119.70
1	F	18	G	C5'-C4'-O4'	-8.13	99.35	109.10
1	E	18	G	C5'-C4'-O4'	-8.07	99.42	109.10
1	E	58	1MA	P-O3'-C3'	7.58	128.79	119.70
1	F	56	C	P-O3'-C3'	-7.11	111.16	119.70
1	F	70	C	N3-C4-C5	-7.08	119.07	121.90
1	E	69	U	OP1-P-OP2	-6.62	109.67	119.60
1	E	68	U	OP1-P-OP2	-6.36	110.06	119.60
1	F	70	C	OP1-P-OP2	-6.34	110.09	119.60
1	E	67	A	P-O3'-C3'	6.30	127.27	119.70
1	F	2	C	O4'-C4'-C3'	-6.29	97.71	104.00
1	F	69	U	OP1-P-OP2	-6.09	110.46	119.60
1	F	55	PSU	P-O3'-C3'	-5.91	112.60	119.70
1	E	15	G	N9-C1'-C2'	-5.79	105.63	112.00
1	E	70	C	OP1-P-OP2	-5.76	110.96	119.60
1	F	2	C	O3'-P-O5'	-5.75	93.06	104.00
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	F	58	1MA	OP1-P-O3'	5.71	117.76	105.20
1	F	15	G	N9-C1'-C2'	-5.70	105.73	112.00
1	E	68	U	C4'-C3'-C2'	5.64	108.24	102.60
1	E	56	C	OP2-P-O3'	5.55	117.41	105.20
1	F	2	C	C5'-C4'-C3'	-5.48	107.23	116.00
1	E	58	1MA	O3'-P-O5'	5.47	114.40	104.00
1	E	55	PSU	P-O3'-C3'	-5.47	113.14	119.70
1	E	55	PSU	OP2-P-O3'	5.29	116.84	105.20
1	E	2	C	C3'-C2'-C1'	-5.27	97.29	101.50
1	F	70	C	C2-N3-C4	5.20	122.50	119.90
1	F	68	U	P-O3'-C3'	-5.15	113.52	119.70
1	F	69	U	P-O3'-C3'	5.13	125.86	119.70

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	67	0
1	F	1648	0	862	75	0
2	A	3630	0	3633	67	0
2	B	3630	0	3633	66	0
All	All	10556	0	8990	234	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 (234) 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:16:H2U:H1'	1:F:17:H2U:OP2	1.61	1.01
1:F:1:G:H2'	1:F:2:C:H5'	1.50	0.94
1:F:16:H2U:C1'	1:F:17:H2U:OP2	2.19	0.90
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:F:16:H2U:O2'	1:F:17:H2U:OP2	1.92	0.88
1:E:1:G:C2'	1:E:2:C:H5'	2.06	0.85
1:F:16:H2U:C2'	1:F:17:H2U:OP2	2.23	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: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:F:2:C:H5"	2:B:292:ASN:CG	2.06	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:C:H42	2:B:95:ALA:HB1	1.52	0.74
1:F:2:C:H5"	2:B:292:ASN:OD1	1.87	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
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:37:YG:H31	1:F:37:YG:C1'	2.21	0.70
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:37:YG:C1'	1:E:37:YG:H31	2.21	0.70
1:E:34:OMG:H8	1:E:34:OMG:OP1	1.74	0.70
1:E:37:YG:H31	1:E:37:YG:C2'	2.22	0.70
1:F:37:YG:H31	1:F:37:YG:C2'	2.21	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:E:37:YG:N20	1:E:37:YG:H101	2.08	0.68
1:F:37:YG:N20	1:F:37:YG:H101	2.08	0.68
1:F:70:C:H2'	1:F:71:G:O4'	1.93	0.67
2:A:76:ARG:HA	2:A:76:ARG:CZ	2.24	0.67
1:F:37:YG:H31	1:F:37:YG:H1'	1.77	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
1:E:37:YG:H31	1:E:37:YG:H1'	1.76	0.65
2:B:260:LEU:HD11	2:B:437:ASP:HB3	1.77	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:YG:H101	1:F:37:YG:C21	2.31	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:37:YG:H101	1:E:37:YG:C21	2.31	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
2:B:17:ASP:C	2:B:19:GLU:H	2.03	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
1:E:16:H2U:O2'	1:E:17:H2U:OP2	2.16	0.59
2:A:17:ASP:C	2:A:19:GLU:H	2.05	0.58
1:F:64:A:OP1	2:B:398:HIS:C	2.41	0.58
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:58:1MA:HM12	1:E:61:C:C1'	2.34	0.57
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:E:72:C:H2'	1:E:73:A:O4'	2.11	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
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
2:B:115:TYR:C	2:B:117:LEU:H	2.17	0.48
1:F:2:C:H3'	1:F:2:C:C6	2.49	0.48
1:E:64:A:OP1	2:A:398:HIS:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:37:YG:H31	1:F:37:YG:O2'	2.16	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:115:TYR:C	2:A:117:LEU:H	2.19	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:E:37:YG:H31	1:E:37:YG:O2'	2.16	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
2:B:66:PHE:HB3	2:B:75:LEU:HD22	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:32:OMC:H6	1:E:32:OMC:O5'	2.02	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
1:E:71:G:H2'	1:E:72:C:O5'	2.20	0.41
1:F:37:YG:H32	1:F:38:A:O4'	2.20	0.41
2:A:120:PRO:C	2:A:122:ASN:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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%)	11 46
2	B	435/437 (100%)	397 (91%)	31 (7%)	7 (2%)	9 44
All	All	870/874 (100%)	794 (91%)	63 (7%)	13 (2%)	10 45

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

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Mol	Chain	Res	Type
2	B	120	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	
2	A	387/387 (100%)	371 (96%)	16 (4%)	30	55
2	B	387/387 (100%)	371 (96%)	16 (4%)	30	55
All	All	774/774 (100%)	742 (96%)	32 (4%)	30	55

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	23	LYS
2	A	38	LEU
2	A	73	GLU
2	A	76	ARG
2	A	94	TYR
2	A	96	GLU
2	A	99	TYR
2	A	213	GLU
2	A	223	LYS
2	A	257	LYS
2	A	273	GLU
2	A	291	ASP
2	A	340	ARG
2	A	383	THR
2	A	398	HIS
2	A	406	GLU
2	B	23	LYS
2	B	38	LEU
2	B	73	GLU
2	B	76	ARG
2	B	94	TYR
2	B	96	GLU

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Mol	Chain	Res	Type
2	B	99	TYR
2	B	213	GLU
2	B	223	LYS
2	B	257	LYS
2	B	273	GLU
2	B	291	ASP
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	229	ASN
2	A	292	ASN
2	B	229	ASN
2	B	292	ASN
2	B	354	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	75/76 (98%)	10 (13%)	2 (2%)
1	F	75/76 (98%)	11 (14%)	3 (4%)
All	All	150/152 (98%)	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

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Mol	Chain	Res	Type
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	OMG	E	34	1	18,26,27	1.05	2 (11%)	19,38,41	0.86	2 (10%)
1	PSU	E	39	1	18,21,22	0.60	0	22,30,33	0.61	0
1	5MC	E	49	1	18,22,23	0.71	0	26,32,35	0.70	1 (3%)
1	7MG	F	46	1	22,26,27	1.13	3 (13%)	29,39,42	1.17	3 (10%)
1	7MG	E	46	1	22,26,27	1.15	3 (13%)	29,39,42	1.19	3 (10%)
1	H2U	E	17	1	18,21,22	1.09	2 (11%)	21,30,33	0.94	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	H2U	F	16	1	18,21,22	1.09	2 (11%)	21,30,33	1.01	1 (4%)
1	5MU	E	54	1	19,22,23	0.53	0	28,32,35	0.61	0
1	PSU	E	55	1	18,21,22	0.67	0	22,30,33	0.79	0
1	1MA	E	58	1	16,25,26	2.68	4 (25%)	18,37,40	1.90	5 (27%)
1	OMC	E	32	1	19,22,23	0.43	0	26,31,34	0.57	0
1	M2G	E	26	1	20,27,28	1.19	2 (10%)	22,40,43	0.76	0
1	1MA	F	58	1	16,25,26	2.70	4 (25%)	18,37,40	1.89	5 (27%)
1	YG	E	37	1	31,42,43	0.90	0	33,62,65	2.46	9 (27%)
1	2MG	F	10	1	18,26,27	1.09	1 (5%)	16,38,41	0.72	0
1	PSU	F	39	1	18,21,22	0.61	0	22,30,33	0.61	0
1	5MC	E	40	1	18,22,23	0.44	0	26,32,35	0.67	1 (3%)
1	2MG	E	10	1	18,26,27	1.08	1 (5%)	16,38,41	0.72	0
1	H2U	F	17	1	18,21,22	1.39	2 (11%)	21,30,33	0.95	1 (4%)
1	5MC	F	40	1	18,22,23	0.43	0	26,32,35	0.66	1 (3%)
1	5MC	F	49	1	18,22,23	0.71	0	26,32,35	0.70	1 (3%)
1	OMG	F	34	1	18,26,27	1.05	2 (11%)	19,38,41	0.87	1 (5%)
1	5MU	F	54	1	19,22,23	0.51	0	28,32,35	0.62	0
1	H2U	E	16	1	18,21,22	1.11	2 (11%)	21,30,33	1.01	1 (4%)
1	M2G	F	26	1	20,27,28	1.21	2 (10%)	22,40,43	0.76	0
1	OMC	F	32	1	19,22,23	0.42	0	26,31,34	0.58	0
1	PSU	F	55	1	18,21,22	0.67	0	22,30,33	0.80	0
1	YG	F	37	1	31,42,43	0.91	0	33,62,65	2.44	8 (24%)

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	OMG	E	34	1	-	1/5/27/28	0/3/3/3
1	PSU	E	39	1	-	0/7/25/26	0/2/2/2
1	5MC	E	49	1	-	0/7/25/26	0/2/2/2
1	7MG	F	46	1	-	2/7/37/38	0/3/3/3
1	7MG	E	46	1	-	2/7/37/38	0/3/3/3
1	H2U	E	17	1	-	0/7/38/39	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	PSU	E	55	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	E	58	1	-	0/3/25/26	0/3/3/3
1	OMC	E	32	1	-	0/9/27/28	0/2/2/2
1	M2G	E	26	1	-	0/7/29/30	0/3/3/3
1	1MA	F	58	1	-	0/3/25/26	0/3/3/3
1	YG	E	37	1	-	7/20/42/43	0/3/4/4
1	2MG	F	10	1	-	0/5/27/28	0/3/3/3
1	PSU	F	39	1	-	0/7/25/26	0/2/2/2
1	5MC	E	40	1	-	1/7/25/26	0/2/2/2
1	2MG	E	10	1	-	0/5/27/28	0/3/3/3
1	H2U	F	17	1	-	2/7/38/39	0/2/2/2
1	5MC	F	40	1	-	1/7/25/26	0/2/2/2
1	5MC	F	49	1	-	0/7/25/26	0/2/2/2
1	OMG	F	34	1	-	1/5/27/28	0/3/3/3
1	5MU	F	54	1	-	0/7/25/26	0/2/2/2
1	H2U	E	16	1	-	4/7/38/39	0/2/2/2
1	M2G	F	26	1	-	0/7/29/30	0/3/3/3
1	OMC	F	32	1	-	0/9/27/28	0/2/2/2
1	PSU	F	55	1	-	1/7/25/26	0/2/2/2
1	YG	F	37	1	-	7/20/42/43	0/3/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	1MA	C6-N6	7.44	1.46	1.27
1	E	58	1MA	C6-N6	7.36	1.46	1.27
1	F	58	1MA	C2-N3	6.81	1.37	1.29
1	E	58	1MA	C2-N3	6.80	1.37	1.29
1	F	17	H2U	C1'-N1	4.98	1.56	1.46
1	E	17	H2U	C6-C5	-3.27	1.43	1.52
1	E	16	H2U	C6-C5	-3.07	1.44	1.52
1	F	26	M2G	C5-C6	-3.06	1.41	1.47
1	F	16	H2U	C6-C5	-3.01	1.44	1.52
1	E	26	M2G	C5-C6	-3.00	1.41	1.47
1	F	46	7MG	C5-N7	2.99	1.39	1.35
1	F	10	2MG	C5-C6	-2.97	1.41	1.47
1	E	46	7MG	C5-N7	2.93	1.39	1.35
1	E	10	2MG	C5-C6	-2.89	1.41	1.47
1	E	46	7MG	C4-N9	2.62	1.40	1.37
1	E	16	H2U	C2-N1	2.62	1.39	1.35
1	F	46	7MG	C4-N9	2.60	1.40	1.37
1	F	17	H2U	C2-N1	2.60	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	16	H2U	C2-N1	2.59	1.39	1.35
1	E	46	7MG	C8-N9	-2.57	1.44	1.46
1	F	26	M2G	C8-N7	-2.57	1.30	1.35
1	E	17	H2U	C2-N1	2.51	1.39	1.35
1	E	26	M2G	C8-N7	-2.49	1.30	1.35
1	F	34	OMG	C8-N7	-2.37	1.31	1.35
1	E	34	OMG	C8-N7	-2.37	1.31	1.35
1	F	58	1MA	C8-N7	-2.37	1.31	1.35
1	E	58	1MA	C8-N7	-2.26	1.31	1.35
1	F	46	7MG	C8-N9	-2.26	1.44	1.46
1	E	58	1MA	C5-C4	-2.12	1.37	1.43
1	F	58	1MA	C5-C4	-2.12	1.37	1.43
1	F	34	OMG	C5-C6	-2.08	1.43	1.47
1	E	34	OMG	C5-C6	-2.06	1.43	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	37	YG	C11-C12-N1	7.61	110.82	106.53
1	F	37	YG	C11-C12-N1	7.55	110.79	106.53
1	E	37	YG	C24-O23-C21	6.25	123.04	115.66
1	F	37	YG	C24-O23-C21	6.13	122.91	115.66
1	F	37	YG	C3-N3-C4	4.99	125.57	116.71
1	E	37	YG	C3-N3-C4	4.98	125.56	116.71
1	E	37	YG	O23-C21-N20	4.43	118.58	110.80
1	F	37	YG	O23-C21-N20	4.35	118.43	110.80
1	F	58	1MA	N1-C2-N3	4.05	130.75	126.02
1	E	58	1MA	N1-C2-N3	4.04	130.73	126.02
1	F	58	1MA	CM1-N1-C6	-3.99	114.23	120.27
1	E	58	1MA	CM1-N1-C6	-3.97	114.26	120.27
1	E	46	7MG	C4-C5-N7	3.87	110.90	105.53
1	F	46	7MG	C4-C5-N7	3.79	110.79	105.53
1	F	58	1MA	CM1-N1-C2	3.66	128.24	120.55
1	E	58	1MA	CM1-N1-C2	3.63	128.19	120.55
1	E	37	YG	O23-C21-O22	-3.49	119.44	124.58
1	F	37	YG	O23-C21-O22	-3.42	119.56	124.58
1	E	37	YG	C4-N3-C2	-3.21	112.42	122.15
1	F	37	YG	C4-N3-C2	-3.20	112.44	122.15
1	E	46	7MG	N9-C8-N7	3.10	107.81	103.38
1	F	46	7MG	N9-C8-N7	3.08	107.78	103.38
1	F	17	H2U	C4-N3-C2	2.88	128.18	125.79
1	F	37	YG	C19-O18-C16	2.77	122.21	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	37	YG	C19-O18-C16	2.70	122.04	115.94
1	E	49	5MC	C5-C6-N1	-2.59	120.67	123.34
1	F	16	H2U	C4-N3-C2	2.59	127.94	125.79
1	F	49	5MC	C5-C6-N1	-2.58	120.68	123.34
1	E	16	H2U	C4-N3-C2	2.58	127.93	125.79
1	F	46	7MG	CM7-N7-C5	2.49	132.81	126.40
1	E	46	7MG	CM7-N7-C5	2.47	132.77	126.40
1	F	37	YG	O18-C16-C15	2.46	117.81	111.52
1	E	37	YG	O18-C16-C15	2.45	117.78	111.52
1	E	40	5MC	C5-C6-N1	-2.42	120.85	123.34
1	E	58	1MA	N1-C6-N6	2.41	125.91	119.77
1	F	58	1MA	N1-C6-N6	2.41	125.91	119.77
1	F	40	5MC	C5-C6-N1	-2.40	120.87	123.34
1	E	17	H2U	C4-N3-C2	2.28	127.69	125.79
1	E	58	1MA	O4'-C1'-C2'	-2.28	103.60	106.93
1	F	34	OMG	O6-C6-C5	2.23	128.73	124.37
1	E	34	OMG	O6-C6-C5	2.14	128.56	124.37
1	F	58	1MA	O4'-C1'-C2'	-2.13	103.81	106.93
1	E	34	OMG	CM2-O2'-C2'	2.03	119.85	114.52
1	E	37	YG	C3-N3-C2	2.02	122.02	120.13

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
1	E	16	H2U	O4'-C1'-N1-C6
1	E	37	YG	C12-C13-C14-C15
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	C12-C13-C14-C15
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	F	16	H2U	C2'-C1'-N1-C6
1	E	16	H2U	C2'-C1'-N1-C2
1	F	16	H2U	C2'-C1'-N1-C2
1	E	37	YG	C13-C14-C15-C16

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

There are no ring outliers.

17 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	34	OMG	5	0
1	E	17	H2U	2	0
1	F	16	H2U	5	0
1	E	55	PSU	2	0
1	E	58	1MA	1	0
1	E	32	OMC	1	0
1	E	26	M2G	1	0
1	E	37	YG	7	0
1	E	40	5MC	2	0
1	F	17	H2U	5	0
1	F	40	5MC	2	0
1	F	34	OMG	5	0
1	E	16	H2U	2	0
1	F	26	M2G	1	0
1	F	32	OMC	1	0
1	F	55	PSU	3	0
1	F	37	YG	8	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	1.18	14 (22%)	0	2	101, 102, 102, 102	0
1	F	62/76 (81%)	0.98	12 (19%)	1	3	101, 102, 102, 102	0
2	A	437/437 (100%)	0.10	2 (0%)	91	86	102, 102, 102, 107	0
2	B	437/437 (100%)	0.10	2 (0%)	91	86	102, 102, 102, 107	0
All	All	998/1026 (97%)	0.22	30 (3%)	50	43	101, 102, 102, 107	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	44	A	3.5
1	E	35	A	3.4
1	E	76	A	3.3
1	F	28	C	3.3
2	B	282	LYS	3.3
1	E	36	A	3.2
1	E	43	G	3.1
2	A	207	GLU	3.0
1	F	76	A	3.0
1	E	30	G	2.7
1	E	38	A	2.7
1	F	47	U	2.6
1	F	35	A	2.6
1	E	42	G	2.6
1	F	29	A	2.6
1	E	75	C	2.5
1	F	38	A	2.5
2	A	208	VAL	2.5
1	F	27	C	2.5
1	F	75	C	2.4
1	E	47	U	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	29	A	2.3
1	F	36	A	2.3
1	E	31	A	2.2
1	E	45	G	2.2
1	F	13	C	2.2
1	F	45	G	2.2
1	E	33	U	2.1
1	F	44	A	2.0
2	B	121	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	H2U	E	17	20/21	0.57	0.49	101,101,101,101	4
1	OMG	F	34	24/25	0.67	0.47	102,102,102,102	0
1	H2U	F	17	20/21	0.68	0.47	101,101,101,101	10
1	7MG	F	46	24/25	0.70	0.30	101,101,102,102	0
1	YG	E	37	39/40	0.71	0.60	101,102,102,102	0
1	OMC	F	32	21/22	0.75	0.37	101,102,102,102	0
1	PSU	F	39	20/21	0.77	0.42	101,101,101,101	0
1	OMC	E	32	21/22	0.77	0.39	101,102,102,102	0
1	YG	F	37	39/40	0.79	0.48	101,102,102,102	0
1	H2U	F	16	20/21	0.79	0.37	101,101,101,101	13
1	H2U	E	16	20/21	0.79	0.35	101,101,101,101	13
1	7MG	E	46	24/25	0.80	0.26	101,102,102,102	0
1	OMG	E	34	24/25	0.80	0.61	101,102,102,102	0
1	5MC	F	40	21/22	0.82	0.47	102,102,102,102	0
1	M2G	E	26	25/26	0.82	0.24	101,101,101,101	0
1	2MG	F	10	24/25	0.86	0.32	101,102,102,102	0
1	PSU	E	39	20/21	0.87	0.30	101,101,101,101	0
1	5MC	E	49	21/22	0.88	0.30	101,101,102,102	0
1	5MC	E	40	21/22	0.88	0.33	101,101,102,102	0
1	M2G	F	26	25/26	0.88	0.29	101,102,102,102	0
1	PSU	F	55	20/21	0.88	0.20	101,101,101,101	0
1	1MA	E	58	23/24	0.90	0.20	101,101,101,101	0
1	2MG	E	10	24/25	0.90	0.24	101,102,102,102	0
1	PSU	E	55	20/21	0.91	0.22	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	F	49	21/22	0.92	0.16	101,101,102,102	0
1	5MU	E	54	21/22	0.92	0.24	101,101,101,101	0
1	1MA	F	58	23/24	0.93	0.13	101,101,101,101	0
1	5MU	F	54	21/22	0.95	0.15	101,101,101,101	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.