wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:05 PM BST

PDB ID	:	4CXG
EMDB ID:	:	EMD-2623
Title	:	Regulation of the mammalian elongation cycle by 40S subunit rolling: a eukaryotic-specific ribosome rearrangement
Authors	:	Budkevich, T.V.; Giesebrecht, J.; Behrmann, E.; Loerke, J.; Ramrath, D.J.F.; Mielke, T.; Ismer, J.; Hildebrand, P.; Tung, C.-S.; Nierhaus, K.H.; Sanbonmatsu, K.Y.; Spahn, C.M.T.
Deposited on	:	2014-04-07
Resolution	:	8.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

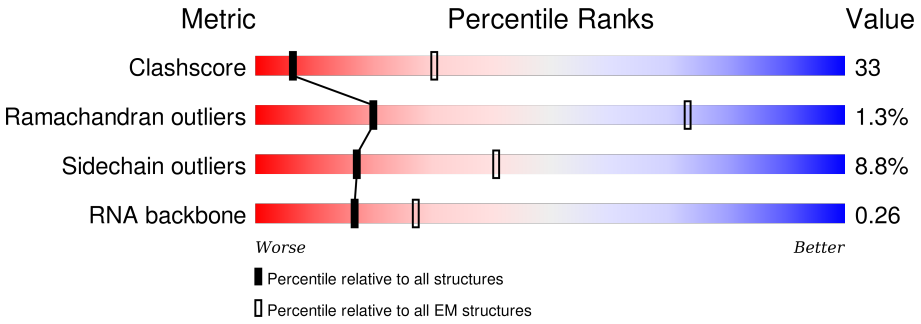
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	1	135	17% 52% 30% •
2	2	50	18% 30% 52%
3	A	437	75% 19% • •
4	X	143	54% 36% • 6%
5	Y	76	14% 22% 54% 9%
6	a	48	33% 65% •
7	b	17	41% 59%
8	c	19	42% 53% 5%

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Mol	Chain	Length	Quality of chain
9	x	28	36% 64%

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
5	2MG	Y	10	-	-	X	-
5	M2G	Y	26	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12269 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 18S RRNA - H44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	135	2890	1288	527	940	135	0	0

- Molecule 2 is a RNA chain called 28S RRNA - H89.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	50	1057	471	176	360	50	0	0

- Molecule 3 is a protein called ELONGATION FACTOR 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	427	3272	2104	570	585	13	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	134	1046	663	205	176	2	0	0

- Molecule 5 is a RNA chain called TRANSFER RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	Y	76	1636	737	290	532	76	1	0	0

- Molecule 6 is a RNA chain called 18S RRNA - H5-H14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	a	48	1024	458	192	326	48	0	0

- Molecule 7 is a RNA chain called 18S RRNA - H8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	17	Total	C	N	O	P	0	0
			363	162	63	121	17		

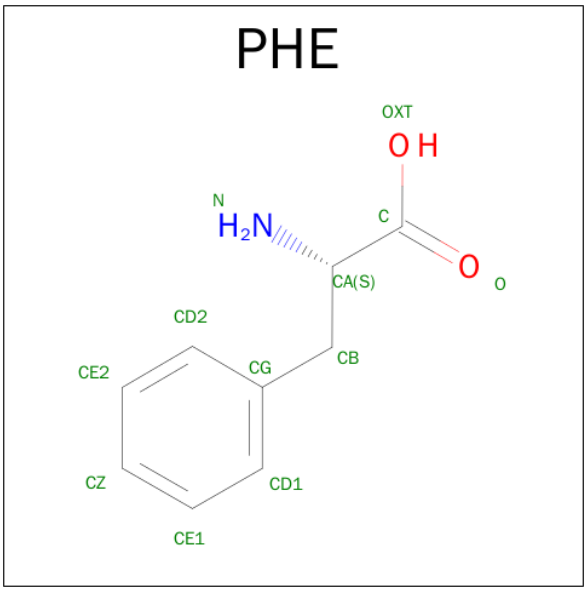
- Molecule 8 is a RNA chain called 28S RRNA - H95.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	19	Total	C	N	O	P	0	0
			410	183	78	130	19		

- Molecule 9 is a RNA chain called MESSENGER RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	x	28	Total	C	N	O	P	0	0
			560	252	56	224	28		

- Molecule 10 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



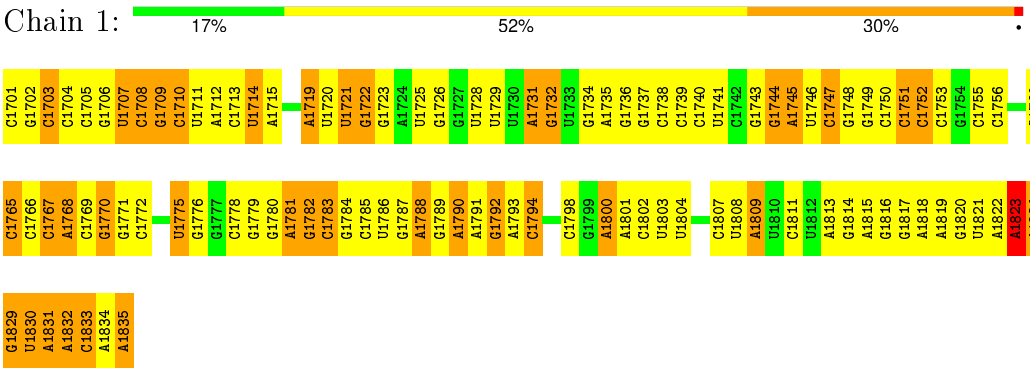
Mol	Chain	Residues	Atoms				AltConf
10	Y	1	Total	C	N	O	0
			11	9	1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

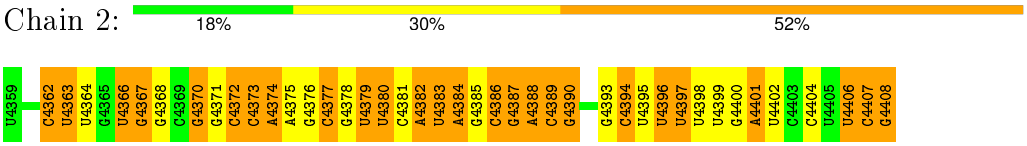
- Molecule 1: 18S RRNA - H44

Chain 1:



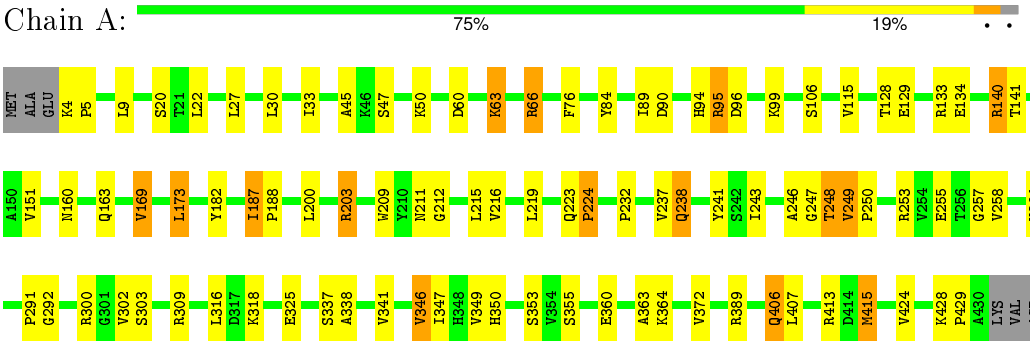
- Molecule 2: 28S RRNA - H89

Chain 2:



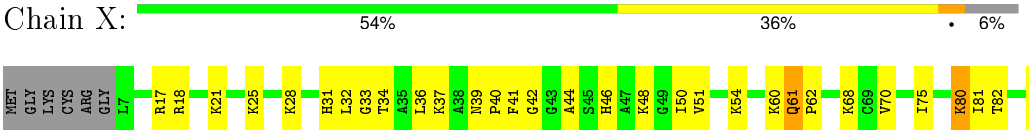
- Molecule 3: ELONGATION FACTOR 1A

Chain A:



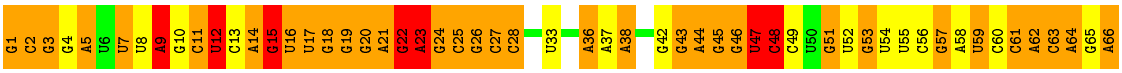
- Molecule 4: 40S RIBOSOMAL PROTEIN US12

Chain X:



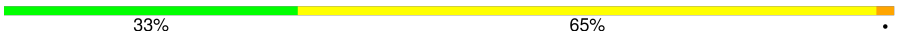
- Molecule 5: TRANSFER RNA

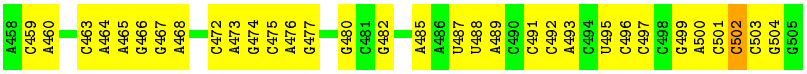
Chain Y:



- Molecule 6: 18S RRNA - H5-H14

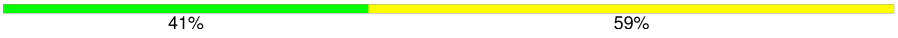
Chain a:

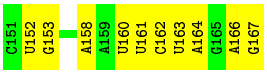




- Molecule 7: 18S RRNA - H8

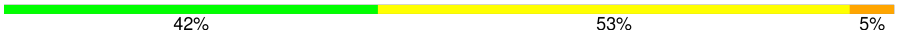
Chain b:

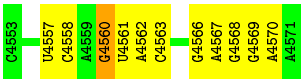




- Molecule 8: 28S RRNA - H95

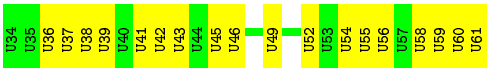
Chain c:





- Molecule 9: MESSENGER RNA

Chain x:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP, Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, H2U, MIA, 2MG, 5MC, 1MA, M2G, 7MG, 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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	1	0.33	0/3232	0.77	0/5039
2	2	0.34	0/1177	0.81	0/1831
3	A	0.44	0/3346	0.62	0/4542
4	X	0.46	0/1063	0.70	0/1421
5	Y	0.48	1/1550 (0.1%)	1.94	65/2410 (2.7%)
6	a	0.37	0/1145	0.83	1/1782 (0.1%)
7	b	0.35	0/405	0.78	0/629
8	c	0.35	0/459	0.86	1/714 (0.1%)
9	x	0.42	1/615 (0.2%)	1.25	11/948 (1.2%)
All	All	0.40	2/12992 (0.0%)	1.00	78/19316 (0.4%)

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	1	0	1
5	Y	1	1
9	x	1	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	1	G	OP3-P	-5.77	1.54	1.61
9	x	60	U	O3'-P	5.07	1.67	1.61

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	22	G	O4'-C1'-N9	29.56	131.85	108.20
5	Y	21	A	N9-C1'-C2'	-20.07	87.90	114.00
5	Y	22	G	N9-C1'-C2'	-18.97	89.33	114.00
5	Y	71	G	O4'-C1'-N9	-17.30	94.36	108.20
5	Y	48	C	O4'-C1'-N1	15.16	120.33	108.20
5	Y	18	G	O4'-C1'-N9	14.46	119.77	108.20
5	Y	47	U	N1-C1'-C2'	13.15	131.10	114.00
5	Y	19	G	O5'-P-OP2	-12.69	94.28	105.70
5	Y	47	U	O4'-C1'-N1	12.69	118.35	108.20
9	x	58	U	P-O5'-C5'	12.68	141.18	120.90
5	Y	19	G	N9-C1'-C2'	-12.49	97.77	114.00
5	Y	59	U	O4'-C1'-N1	11.24	117.19	108.20
5	Y	7	U	N1-C1'-C2'	-11.16	99.49	114.00
5	Y	61	C	O4'-C1'-N1	11.03	117.02	108.20
5	Y	3	G	N9-C1'-C2'	-10.69	100.10	114.00
5	Y	23	A	O4'-C1'-N9	10.39	116.52	108.20
9	x	59	U	P-O5'-C5'	10.22	137.25	120.90
5	Y	23	A	N9-C1'-C2'	9.70	126.62	114.00
5	Y	73	A	N9-C1'-C2'	-9.40	101.66	112.00
9	x	58	U	C4'-C3'-O3'	9.33	131.65	113.00
5	Y	66	A	O4'-C1'-N9	-9.24	100.81	108.20
5	Y	56	C	O4'-C1'-N1	-9.13	100.89	108.20
5	Y	18	G	N9-C1'-C2'	-8.86	102.26	112.00
5	Y	36	A	C2'-C3'-O3'	8.83	128.93	109.50
9	x	60	U	C5'-C4'-C3'	8.38	129.40	116.00
5	Y	74	C	O4'-C1'-N1	-8.21	101.64	108.20
5	Y	21	A	C3'-C2'-O2'	-7.92	90.33	113.30
5	Y	5	A	O4'-C1'-N9	7.70	114.36	108.20
5	Y	3	G	O4'-C1'-N9	7.63	114.31	108.20
5	Y	1	G	O4'-C1'-N9	-7.41	102.27	108.20
5	Y	7	U	O4'-C1'-N1	7.29	114.03	108.20
5	Y	63	C	OP2-P-O3'	-7.12	89.53	105.20
5	Y	53	G	O4'-C1'-N9	-7.11	102.51	108.20
5	Y	62	A	O4'-C1'-N9	-7.07	102.54	108.20
5	Y	9	A	O4'-C1'-N9	7.05	113.84	108.20
5	Y	64	A	OP1-P-OP2	7.00	130.10	119.60
5	Y	15	G	O4'-C1'-N9	-6.84	102.73	108.20
5	Y	65	G	O5'-P-OP1	-6.83	99.55	105.70
5	Y	68	U	O4'-C1'-N1	6.78	113.62	108.20
5	Y	22	G	C4'-C3'-O3'	6.77	126.54	113.00
5	Y	69	U	C2'-C3'-O3'	6.71	124.44	113.70
5	Y	21	A	P-O5'-C5'	-6.70	110.19	120.90
5	Y	3	G	O3'-P-O5'	6.69	116.71	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	15	G	N9-C1'-C2'	6.59	122.57	114.00
5	Y	62	A	OP1-P-O3'	6.53	119.57	105.20
5	Y	2	C	OP1-P-O3'	6.49	119.48	105.20
5	Y	75	C	O5'-P-OP2	6.48	118.48	110.70
9	x	60	U	O5'-C5'-C4'	6.48	124.01	111.70
9	x	59	U	O3'-P-O5'	-6.42	91.80	104.00
5	Y	7	U	O5'-P-OP1	6.33	118.29	110.70
5	Y	18	G	OP2-P-O3'	6.31	119.09	105.20
5	Y	20	G	N9-C1'-C2'	-6.30	105.07	112.00
5	Y	63	C	N1-C1'-C2'	-6.17	105.21	112.00
5	Y	64	A	OP1-P-O3'	6.17	118.78	105.20
5	Y	69	U	O5'-P-OP1	6.16	118.10	110.70
5	Y	51	G	N9-C1'-C2'	6.16	122.01	114.00
9	x	59	U	C4'-C3'-O3'	6.15	125.30	113.00
9	x	58	U	O3'-P-O5'	6.14	115.66	104.00
6	a	502	C	C3'-C2'-C1'	-6.07	96.64	101.50
8	c	4560	G	C3'-C2'-C1'	-6.06	96.66	101.50
5	Y	3	G	O5'-P-OP1	-6.04	100.26	105.70
5	Y	24	G	N9-C1'-C2'	-5.97	105.44	112.00
5	Y	61	C	O5'-P-OP2	-5.90	100.39	105.70
5	Y	57	G	O4'-C1'-N9	-5.82	103.55	108.20
5	Y	11	C	N1-C1'-C2'	-5.76	105.66	112.00
5	Y	69	U	O3'-P-O5'	-5.76	93.06	104.00
9	x	60	U	P-O5'-C5'	-5.75	111.70	120.90
5	Y	22	G	O5'-P-OP1	-5.74	100.53	105.70
5	Y	23	A	OP1-P-O3'	5.62	117.58	105.20
9	x	58	U	C2'-C3'-O3'	5.53	122.54	113.70
5	Y	71	G	C2'-C3'-O3'	5.52	122.53	113.70
5	Y	69	U	P-O3'-C3'	-5.51	113.08	119.70
5	Y	70	C	N1-C1'-C2'	-5.51	105.94	112.00
5	Y	52	U	O5'-P-OP1	-5.44	100.80	105.70
5	Y	12	U	O4'-C1'-N1	-5.31	103.95	108.20
5	Y	23	A	O5'-P-OP1	-5.26	100.97	105.70
9	x	58	U	N1-C1'-C2'	5.26	120.83	114.00
5	Y	22	G	OP2-P-O3'	5.21	116.65	105.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	Y	36	A	C3'
9	x	58	U	C3'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1823	A	Sidechain
5	Y	33	U	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	1	2890	0	1462	156	0
2	2	1057	0	535	67	0
3	A	3272	0	3292	88	0
4	X	1046	0	1110	48	0
5	Y	1636	0	848	145	0
6	a	1024	0	525	0	0
7	b	363	0	182	0	0
8	c	410	0	207	0	0
9	x	560	0	281	0	0
10	Y	11	0	8	0	0
All	All	12269	0	8450	464	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 33.

All (464) 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)
3:A:249:VAL:CG1	5:Y:76:A:N3	1.70	1.51
3:A:249:VAL:HG11	5:Y:76:A:C2	1.58	1.38
3:A:249:VAL:CG1	5:Y:76:A:C2	2.08	1.37
3:A:243:ILE:O	5:Y:76:A:N6	1.62	1.29
3:A:415:MET:CE	5:Y:51:G:H21	1.46	1.28
3:A:249:VAL:HG11	5:Y:76:A:N3	0.92	1.24
3:A:241:TYR:CG	5:Y:76:A:H4'	1.72	1.22
3:A:247:GLY:H	5:Y:76:A:N6	1.37	1.19
3:A:415:MET:CE	5:Y:51:G:N2	2.05	1.17
3:A:247:GLY:N	5:Y:76:A:N6	1.94	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:415:MET:HE3	5:Y:51:G:H21	1.05	1.08
3:A:249:VAL:HG12	5:Y:76:A:C2	1.86	1.07
3:A:241:TYR:CD1	5:Y:76:A:H4'	1.90	1.07
1:1:1833:C:H5'	1:1:1833:C:H6	1.18	1.05
1:1:1768:A:H2'	1:1:1769:C:H5'	1.38	1.04
5:Y:45:G:H5'	5:Y:45:G:H8	1.24	1.03
3:A:415:MET:CE	5:Y:64:A:H1'	1.91	1.01
5:Y:42:G:C2'	5:Y:43:G:H5'	1.97	0.95
1:1:1750:C:H2'	1:1:1751:C:H5'	1.48	0.95
1:1:1832:A:H2'	1:1:1833:C:H5"	1.46	0.94
1:1:1766:C:H3'	1:1:1767:C:C5	2.04	0.93
3:A:415:MET:HE1	5:Y:51:G:N2	1.83	0.93
5:Y:27:C:H2'	5:Y:28:C:C6	2.04	0.92
3:A:415:MET:SD	5:Y:64:A:H1'	2.10	0.91
3:A:241:TYR:HB3	5:Y:76:A:O4'	1.70	0.91
3:A:337:SER:HB3	5:Y:53:G:OP2	1.72	0.90
5:Y:42:G:H2'	5:Y:43:G:H5'	1.53	0.89
5:Y:11:C:H2'	5:Y:12:U:H6	1.37	0.89
5:Y:26:M2G:H2'	5:Y:27:C:N1	1.89	0.88
3:A:241:TYR:HB3	5:Y:76:A:C4'	2.03	0.87
1:1:1765:C:H2'	1:1:1766:C:O4'	1.74	0.86
1:1:1768:A:C2'	1:1:1769:C:H5'	2.05	0.86
1:1:1781:A:H1'	1:1:1782:G:OP2	1.76	0.85
3:A:243:ILE:O	5:Y:76:A:C6	2.21	0.85
5:Y:25:C:H2'	5:Y:26:M2G:O4'	1.76	0.85
5:Y:11:C:H2'	5:Y:12:U:C6	2.11	0.85
1:1:1825:A:H2'	1:1:1826:G:H5"	1.59	0.84
1:1:1832:A:C2'	1:1:1833:C:H5"	2.06	0.84
5:Y:15:G:C2'	5:Y:16:H2U:H5'	2.08	0.84
1:1:1775:U:H2'	1:1:1776:G:H8	1.42	0.84
1:1:1833:C:C6	1:1:1833:C:H5'	2.11	0.83
1:1:1766:C:H3'	1:1:1767:C:C6	2.12	0.83
4:X:87:ASN:HB2	4:X:90:CYS:SG	2.19	0.83
3:A:415:MET:HE1	5:Y:64:A:H1'	1.57	0.82
5:Y:23:A:H2'	5:Y:24:G:H8	1.43	0.82
5:Y:13:C:H2'	5:Y:14:A:H8	1.43	0.82
3:A:241:TYR:CB	5:Y:76:A:H4'	2.10	0.81
5:Y:24:G:H2'	5:Y:25:C:H6	1.46	0.81
3:A:415:MET:SD	5:Y:64:A:C1'	2.69	0.80
5:Y:26:M2G:H2'	5:Y:27:C:C6	2.16	0.80
5:Y:23:A:H2'	5:Y:24:G:C8	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1743:G:H1'	1:1:1792:G:N2	1.97	0.80
3:A:241:TYR:CB	5:Y:76:A:C4'	2.60	0.79
1:1:1769:C:H2'	1:1:1770:G:H8	1.47	0.79
5:Y:26:M2G:H2'	5:Y:27:C:C1'	2.13	0.79
5:Y:27:C:H2'	5:Y:28:C:H6	1.45	0.79
1:1:1769:C:H2'	1:1:1770:G:C8	2.17	0.78
5:Y:25:C:H2'	5:Y:26:M2G:C4'	2.13	0.78
3:A:247:GLY:N	5:Y:76:A:C6	2.51	0.78
3:A:241:TYR:CG	5:Y:76:A:C4'	2.64	0.78
4:X:61:GLN:HB3	4:X:62:PRO:CD	2.13	0.78
5:Y:45:G:C8	5:Y:45:G:H5'	2.16	0.78
3:A:249:VAL:CG1	5:Y:76:A:C4	2.67	0.77
1:1:1833:C:C5'	1:1:1833:C:H6	1.97	0.77
1:1:1787:G:H2'	1:1:1788:A:C8	2.19	0.76
1:1:1725:U:H2'	1:1:1726:G:C8	2.20	0.76
5:Y:15:G:O2'	5:Y:16:H2U:H5'	1.86	0.75
3:A:241:TYR:CD1	5:Y:76:A:C4'	2.69	0.75
3:A:337:SER:CB	5:Y:53:G:OP2	2.34	0.74
1:1:1755:C:H2'	1:1:1756:C:C6	2.21	0.74
1:1:1825:A:H8	1:1:1825:A:O5'	1.70	0.74
2:2:4374:A:H2'	2:2:4382:A:C2	2.21	0.74
3:A:415:MET:SD	5:Y:51:G:N2	2.60	0.74
1:1:1771:G:H2'	1:1:1772:C:C6	2.23	0.73
1:1:1787:G:H2'	1:1:1788:A:H8	1.53	0.73
3:A:241:TYR:CD1	5:Y:76:A:C5'	2.71	0.73
1:1:1807:C:H2'	1:1:1808:U:C6	2.24	0.73
2:2:4374:A:H2'	2:2:4382:A:N1	2.04	0.73
2:2:4399:U:C2'	2:2:4400:G:H5'	2.20	0.72
2:2:4373:C:H3'	2:2:4373:C:O2	1.90	0.72
1:1:1731:A:H2'	1:1:1732:G:C8	2.24	0.71
1:1:1704:C:H1'	1:1:1832:A:N1	2.05	0.71
1:1:1815:A:H3'	1:1:1816:G:H8	1.54	0.71
4:X:51:VAL:HG13	4:X:70:VAL:HG13	1.73	0.71
5:Y:45:G:C5'	5:Y:45:G:H8	2.02	0.71
2:2:4367:G:H2'	2:2:4368:G:H8	1.55	0.71
2:2:4400:G:H2'	2:2:4401:A:C8	2.26	0.70
1:1:1784:G:H2'	1:1:1785:C:C6	2.26	0.70
5:Y:43:G:O3'	5:Y:44:A:O4'	2.09	0.70
1:1:1736:G:H2'	1:1:1737:G:C8	2.27	0.70
2:2:4384:A:N3	2:2:4384:A:H2'	2.08	0.69
1:1:1780:G:P	1:1:1781:A:H5"	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1814:G:O5'	1:1:1814:G:H8	1.75	0.69
1:1:1764:G:N3	1:1:1764:G:H3'	2.07	0.69
5:Y:10:2MG:N2	5:Y:26:M2G:H1'	2.08	0.69
1:1:1721:U:H4'	1:1:1722:G:O5'	1.93	0.69
1:1:1750:C:C2'	1:1:1751:C:H5'	2.23	0.68
2:2:4399:U:H2'	2:2:4400:G:H5'	1.75	0.68
5:Y:1:G:C2'	5:Y:2:C:H5'	2.23	0.68
5:Y:44:A:O2'	5:Y:45:G:H5'	1.93	0.68
4:X:100:VAL:CG1	4:X:122:VAL:HG13	2.24	0.68
5:Y:42:G:O2'	5:Y:43:G:H5'	1.93	0.68
1:1:1750:C:H2'	1:1:1751:C:C5'	2.23	0.68
5:Y:24:G:H2'	5:Y:25:C:C6	2.29	0.68
1:1:1746:U:H2'	1:1:1747:C:C6	2.30	0.67
5:Y:17:H2U:H4'	5:Y:18:G:H5"	1.75	0.67
2:2:4373:C:H2'	2:2:4374:A:O4'	1.95	0.67
5:Y:1:G:O2'	5:Y:2:C:H5'	1.95	0.67
2:2:4383:U:H3'	2:2:4383:U:H6	1.60	0.66
1:1:1778:C:H2'	1:1:1779:G:C8	2.31	0.66
3:A:20:SER:OG	3:A:90:ASP:OD2	2.13	0.65
1:1:1743:G:H1'	1:1:1792:G:H22	1.61	0.65
1:1:1721:U:H1'	1:1:1722:G:OP2	1.96	0.65
4:X:46:HIS:HB3	4:X:101:LEU:HD11	1.77	0.65
5:Y:19:G:H4'	5:Y:20:G:C4	2.30	0.65
5:Y:25:C:N3	5:Y:26:M2G:C8	2.65	0.65
5:Y:16:H2U:H4'	5:Y:17:H2U:OP1	1.96	0.65
3:A:255:GLU:HB3	3:A:406:GLN:HG3	1.79	0.65
4:X:112:VAL:HB	4:X:115:ILE:HD13	1.78	0.65
3:A:241:TYR:CB	5:Y:76:A:O4'	2.44	0.64
1:1:1767:C:C2'	1:1:1768:A:H5'	2.27	0.64
1:1:1778:C:H2'	1:1:1779:G:H8	1.62	0.64
4:X:51:VAL:HG22	4:X:70:VAL:HG11	1.79	0.63
5:Y:7:U:H4'	5:Y:8:U:OP1	1.97	0.63
1:1:1767:C:O2'	1:1:1768:A:H5'	1.98	0.63
3:A:415:MET:HE3	5:Y:51:G:N2	1.87	0.63
1:1:1734:G:H8	1:1:1734:G:O5'	1.81	0.63
5:Y:25:C:C2	5:Y:26:M2G:C8	2.86	0.63
4:X:132:ALA:O	4:X:138:LYS:HB2	1.99	0.63
1:1:1775:U:H2'	1:1:1776:G:C8	2.30	0.63
1:1:1768:A:H2'	1:1:1769:C:C5'	2.23	0.63
1:1:1825:A:C8	1:1:1825:A:O5'	2.52	0.62
3:A:241:TYR:HD1	5:Y:76:A:H5'	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:415:MET:SD	5:Y:64:A:O4'	2.57	0.62
1:1:1832:A:C3'	1:1:1833:C:H5"	2.29	0.62
4:X:61:GLN:HB3	4:X:62:PRO:HD3	1.80	0.62
1:1:1714:U:H3'	1:1:1715:A:C8	2.34	0.62
2:2:4384:A:H5'	2:2:4385:G:OP2	1.99	0.62
1:1:1835:A:N3	1:1:1835:A:H2'	2.14	0.62
5:Y:10:2MG:HM22	5:Y:26:M2G:O2'	2.00	0.62
3:A:169:VAL:HG23	3:A:173:LEU:HD22	1.81	0.62
2:2:4400:G:H2'	2:2:4401:A:H8	1.64	0.62
1:1:1808:U:H2'	1:1:1809:A:C8	2.35	0.61
1:1:1741:U:O4	1:1:1793:A:C2	2.54	0.61
2:2:4383:U:C6	2:2:4383:U:H3'	2.34	0.61
1:1:1820:G:H2'	1:1:1821:U:C6	2.36	0.61
2:2:4377:C:H3'	2:2:4378:G:H8	1.66	0.61
5:Y:10:2MG:N2	5:Y:26:M2G:O2'	2.33	0.60
1:1:1714:U:H3'	1:1:1715:A:H8	1.66	0.60
2:2:4387:G:H4'	2:2:4387:G:OP1	2.00	0.60
2:2:4394:C:H2'	2:2:4395:U:O4'	2.02	0.60
1:1:1751:C:C2'	1:1:1752:C:H5'	2.32	0.60
3:A:203:ARG:NH2	3:A:212:GLY:O	2.30	0.60
4:X:105:PHE:CZ	4:X:121:LYS:HD2	2.37	0.60
5:Y:18:G:OP2	5:Y:58:1MA:HM11	2.02	0.60
5:Y:10:2MG:HN2	5:Y:26:M2G:H1'	1.66	0.59
1:1:1782:G:N3	1:1:1783:C:N4	2.49	0.59
1:1:1771:G:H2'	1:1:1772:C:H6	1.66	0.59
5:Y:26:M2G:C2'	5:Y:27:C:C6	2.85	0.59
3:A:253:ARG:HE	3:A:292:GLY:HA2	1.68	0.59
2:2:4370:G:H2'	2:2:4371:G:H5'	1.83	0.59
2:2:4372:C:H42	2:2:4390:G:H1	1.49	0.58
5:Y:10:2MG:CM2	5:Y:26:M2G:O2'	2.51	0.58
1:1:1784:G:H2'	1:1:1785:C:H6	1.68	0.58
2:2:4363:U:O2'	2:2:4364:U:H5'	2.03	0.58
5:Y:25:C:O2'	5:Y:26:M2G:H5'	2.03	0.58
4:X:41:PHE:HE1	4:X:120:PHE:CE1	2.21	0.58
1:1:1828:C:H3'	1:1:1829:G:H8	1.68	0.58
1:1:1701:C:OP2	1:1:1701:C:H4'	2.02	0.58
2:2:4381:C:C2'	2:2:4382:A:H5'	2.33	0.58
2:2:4384:A:H3'	2:2:4385:G:H8	1.68	0.58
1:1:1800:A:H3'	1:1:1801:A:H8	1.66	0.57
1:1:1800:A:H5"	1:1:1801:A:OP2	2.04	0.57
1:1:1828:C:H3'	1:1:1829:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4379:U:O2	2:2:4379:U:H2'	2.03	0.57
5:Y:25:C:C4	5:Y:26:M2G:C8	2.92	0.57
1:1:1790:A:C2'	1:1:1791:A:H5'	2.35	0.57
4:X:123:VAL:O	4:X:130:LEU:HG	2.04	0.56
1:1:1802:C:H2'	1:1:1803:U:O4'	2.05	0.56
3:A:63:LYS:NZ	5:Y:74:C:OP2	2.37	0.56
3:A:94:HIS:HD2	3:A:96:ASP:HB2	1.69	0.56
2:2:4406:U:O2	2:2:4406:U:H2'	2.05	0.56
5:Y:43:G:H2'	5:Y:44:A:C4	2.41	0.56
3:A:248:THR:HG21	3:A:302:VAL:O	2.06	0.56
1:1:1746:U:H2'	1:1:1747:C:H6	1.70	0.56
1:1:1830:U:H1'	1:1:1831:A:OP2	2.06	0.56
1:1:1783:C:H2'	1:1:1783:C:O2	2.05	0.56
1:1:1791:A:H2'	1:1:1792:G:O4'	2.06	0.55
1:1:1821:U:H2'	1:1:1822:A:C8	2.41	0.55
3:A:360:GLU:HG2	3:A:389:ARG:HE	1.71	0.55
1:1:1739:C:H6	1:1:1739:C:O5'	1.89	0.55
2:2:4396:U:H4'	2:2:4397:U:OP1	2.05	0.55
4:X:68:LYS:HB2	4:X:85:VAL:HB	1.87	0.55
5:Y:16:H2U:O2'	5:Y:16:H2U:H62	2.02	0.55
1:1:1755:C:H2'	1:1:1756:C:H6	1.67	0.55
5:Y:10:2MG:CM2	5:Y:26:M2G:O3'	2.54	0.55
1:1:1835:A:N3	1:1:1835:A:C2'	2.69	0.54
5:Y:45:G:C5'	5:Y:45:G:C8	2.85	0.54
2:2:4367:G:H2'	2:2:4368:G:C8	2.40	0.54
4:X:32:LEU:HD22	4:X:34:THR:HB	1.89	0.54
2:2:4379:U:O2	2:2:4379:U:C2'	2.55	0.54
1:1:1815:A:H3'	1:1:1816:G:C8	2.40	0.54
3:A:94:HIS:CD2	3:A:96:ASP:H	2.25	0.54
2:2:4388:A:H3'	2:2:4389:C:O4'	2.07	0.54
5:Y:10:2MG:HM21	5:Y:26:M2G:O3'	2.07	0.54
4:X:90:CYS:O	4:X:94:ILE:HG13	2.07	0.54
4:X:61:GLN:HB3	4:X:62:PRO:HD2	1.90	0.53
2:2:4383:U:C3'	2:2:4383:U:C6	2.89	0.53
3:A:95:ARG:HH21	3:A:129:GLU:HB3	1.73	0.53
5:Y:46:7MG:H4'	5:Y:47:U:OP1	2.07	0.53
4:X:39:ASN:OD1	4:X:41:PHE:HB2	2.07	0.53
1:1:1752:C:C2'	1:1:1753:C:H5'	2.39	0.53
3:A:363:ALA:HB1	3:A:372:VAL:HG13	1.90	0.53
4:X:95:GLU:HB2	4:X:98:ASP:OD2	2.09	0.53
3:A:94:HIS:CD2	3:A:96:ASP:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1825:A:H2'	1:1:1826:G:C5'	2.34	0.53
3:A:337:SER:OG	5:Y:53:G:OP2	2.27	0.53
2:2:4364:U:O2	2:2:4364:U:H2'	2.08	0.53
5:Y:10:2MG:C2	5:Y:26:M2G:O2'	2.61	0.52
4:X:36:LEU:O	4:X:42:GLY:HA2	2.09	0.52
2:2:4374:A:C8	2:2:4382:A:C2	2.97	0.52
3:A:94:HIS:HD2	3:A:96:ASP:H	1.55	0.52
1:1:1714:U:O5'	1:1:1714:U:H6	1.91	0.52
5:Y:9:A:H5'	5:Y:46:7MG:H1'	1.90	0.52
1:1:1822:A:C6	1:1:1823:A:C6	2.97	0.52
5:Y:14:A:C2'	5:Y:15:G:H5'	2.40	0.52
5:Y:13:C:C2	5:Y:14:A:C8	2.98	0.52
5:Y:25:C:C2'	5:Y:26:M2G:H5'	2.40	0.52
5:Y:44:A:O2'	5:Y:45:G:C8	2.62	0.52
1:1:1747:C:H2'	1:1:1748:G:C8	2.44	0.52
4:X:82:THR:OG1	4:X:118:VAL:HG22	2.09	0.52
5:Y:11:C:C6	5:Y:12:U:H5	2.27	0.52
5:Y:11:C:O5'	5:Y:11:C:H6	1.93	0.52
5:Y:14:A:C5	5:Y:22:G:C2	2.98	0.52
1:1:1743:G:H21	1:1:1791:A:H62	1.56	0.52
1:1:1705:C:H2'	1:1:1706:G:C8	2.45	0.52
4:X:32:LEU:C	4:X:34:THR:H	2.14	0.51
1:1:1767:C:H3'	1:1:1767:C:C6	2.46	0.51
2:2:4402:U:H6	2:2:4402:U:O5'	1.92	0.51
3:A:241:TYR:CD1	5:Y:76:A:H5'	2.40	0.51
1:1:1782:G:P	1:1:1782:G:O4'	2.68	0.51
1:1:1761:U:H3	1:1:1771:G:H1	1.58	0.51
2:2:4387:G:H5"	2:2:4387:G:C8	2.45	0.51
4:X:50:ILE:HG23	4:X:97:ASN:HA	1.92	0.51
5:Y:10:2MG:C6	5:Y:11:C:C4	2.99	0.51
4:X:18:ARG:O	4:X:21:LYS:HB3	2.10	0.51
5:Y:37:MIA:H121	5:Y:38:A:N1	2.26	0.51
1:1:1790:A:O2'	1:1:1791:A:H5'	2.11	0.51
3:A:257:GLY:O	3:A:291:PRO:HD3	2.11	0.51
5:Y:66:A:O2'	5:Y:67:A:H5'	2.11	0.51
2:2:4362:C:H5'	2:2:4363:U:OP2	2.11	0.51
3:A:249:VAL:HG13	5:Y:76:A:N3	2.07	0.51
2:2:4373:C:O2	2:2:4373:C:C3'	2.58	0.51
4:X:122:VAL:O	4:X:130:LEU:HD11	2.11	0.50
5:Y:14:A:C6	5:Y:22:G:C2	2.99	0.50
5:Y:25:C:C4	5:Y:26:M2G:N7	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1814:G:O5'	1:1:1814:G:C8	2.62	0.50
1:1:1823:A:H4'	1:1:1824:A:O5'	2.11	0.50
2:2:4397:U:H2'	2:2:4398:U:H5'	1.93	0.50
1:1:1818:A:H8	1:1:1818:A:O5'	1.94	0.50
5:Y:48:C:N4	5:Y:59:U:C5	2.79	0.50
3:A:146:GLN:NE2	3:A:223:GLN:O	2.42	0.50
4:X:100:VAL:HG11	4:X:122:VAL:HG13	1.94	0.50
2:2:4374:A:C8	2:2:4382:A:N1	2.79	0.50
4:X:54:LYS:HD2	4:X:91:LEU:HD11	1.94	0.50
2:2:4371:G:H2'	2:2:4372:C:C6	2.47	0.50
1:1:1704:C:C1'	1:1:1832:A:N1	2.75	0.49
5:Y:48:C:N4	5:Y:59:U:C4	2.80	0.49
5:Y:11:C:C2	5:Y:12:U:C5	3.00	0.49
1:1:1709:G:H8	1:1:1709:G:OP2	1.94	0.49
1:1:1788:A:H2'	1:1:1788:A:N3	2.27	0.49
4:X:123:VAL:HA	4:X:130:LEU:CD1	2.42	0.49
1:1:1781:A:C4	1:1:1782:G:N2	2.81	0.49
1:1:1704:C:H1'	1:1:1832:A:C6	2.48	0.49
1:1:1707:U:C2'	1:1:1708:C:H5'	2.42	0.49
2:2:4399:U:O2'	2:2:4400:G:H5'	2.13	0.49
2:2:4367:G:C4	2:2:4368:G:C8	3.01	0.49
3:A:232:PRO:HB3	3:A:318:LYS:HD2	1.94	0.49
5:Y:24:G:C5	5:Y:25:C:C5	3.00	0.49
5:Y:24:G:C4	5:Y:25:C:C6	3.01	0.49
2:2:4386:C:H2'	2:2:4386:C:O2	2.12	0.49
5:Y:14:A:H2'	5:Y:14:A:N3	2.28	0.48
5:Y:14:A:C4	5:Y:22:G:N2	2.81	0.48
5:Y:23:A:C2	5:Y:24:G:C5	3.00	0.48
2:2:4408:G:H8	2:2:4408:G:H5"	1.78	0.48
5:Y:10:2MG:C2	5:Y:26:M2G:H1'	2.48	0.48
5:Y:14:A:H2'	5:Y:15:G:H5'	1.95	0.48
5:Y:22:G:C6	5:Y:23:A:N7	2.81	0.48
1:1:1731:A:H2'	1:1:1732:G:H8	1.75	0.48
1:1:1714:U:C3'	1:1:1715:A:H8	2.27	0.48
4:X:86:PRO:HB3	4:X:121:LYS:NZ	2.29	0.48
3:A:347:ILE:O	3:A:353:SER:HA	2.14	0.48
1:1:1769:C:C6	1:1:1769:C:O5'	2.67	0.48
3:A:238:GLN:O	3:A:309:ARG:NE	2.41	0.48
1:1:1762:C:H2'	1:1:1763:G:C8	2.48	0.48
5:Y:26:M2G:H3'	5:Y:27:C:H6	1.79	0.48
3:A:140:ARG:HG2	3:A:182:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:14:A:N6	5:Y:22:G:C6	2.82	0.48
4:X:48:LYS:HD3	4:X:99:GLU:OE2	2.14	0.48
5:Y:25:C:H2'	5:Y:26:M2G:C5'	2.43	0.48
5:Y:27:C:O2'	5:Y:28:C:H5'	2.13	0.48
4:X:100:VAL:HA	4:X:124:LYS:O	2.12	0.48
4:X:100:VAL:HG13	4:X:122:VAL:HG13	1.95	0.48
2:2:4371:G:H2'	2:2:4372:C:H6	1.79	0.48
1:1:1825:A:C8	1:1:1825:A:H3'	2.49	0.47
5:Y:59:U:C5	5:Y:60:C:N4	2.82	0.47
3:A:215:LEU:O	3:A:219:LEU:HG	2.14	0.47
4:X:51:VAL:HG13	4:X:70:VAL:CG1	2.43	0.47
1:1:1829:G:O5'	1:1:1829:G:C8	2.68	0.47
1:1:1712:A:H2'	1:1:1713:C:C6	2.50	0.47
1:1:1743:G:O2'	1:1:1744:G:H5'	2.14	0.47
2:2:4401:A:H8	2:2:4401:A:OP2	1.96	0.47
2:2:4393:G:O2'	2:2:4394:C:H5'	2.15	0.47
4:X:25:LYS:O	4:X:28:LYS:HB3	2.14	0.47
3:A:277:ARG:NH2	3:A:300:ARG:HG3	2.28	0.47
1:1:1822:A:N1	1:1:1823:A:C6	2.82	0.47
1:1:1771:G:O2'	1:1:1772:C:H5'	2.14	0.47
1:1:1824:A:N3	1:1:1824:A:H5"	2.29	0.47
2:2:4398:U:H6	2:2:4398:U:OP2	1.98	0.47
1:1:1803:U:H2'	1:1:1804:U:C6	2.50	0.47
2:2:4407:C:O2'	2:2:4408:G:P	2.73	0.47
1:1:1751:C:H2'	1:1:1752:C:H5'	1.96	0.47
3:A:140:ARG:HG2	3:A:182:TYR:CE2	2.50	0.47
4:X:106:GLY:O	4:X:107:ARG:O	2.33	0.47
1:1:1767:C:H6	1:1:1767:C:H3'	1.80	0.47
5:Y:18:G:O6	5:Y:55:PSU:H1'	2.15	0.46
2:2:4393:G:H2'	2:2:4394:C:C6	2.50	0.46
1:1:1752:C:O2'	1:1:1753:C:H5'	2.15	0.46
5:Y:26:M2G:H3'	5:Y:27:C:C6	2.50	0.46
2:2:4374:A:H2'	2:2:4382:A:C6	2.49	0.46
1:1:1767:C:C3'	1:1:1767:C:C6	2.99	0.46
3:A:187:ILE:HA	3:A:188:PRO:HD3	1.73	0.46
2:2:4388:A:H3'	2:2:4389:C:C5'	2.46	0.46
4:X:61:GLN:CB	4:X:62:PRO:CD	2.89	0.46
2:2:4383:U:C3'	2:2:4383:U:H6	2.27	0.46
1:1:1778:C:O5'	1:1:1778:C:H6	1.99	0.46
1:1:1766:C:O2	1:1:1766:C:H2'	2.15	0.46
5:Y:24:G:C6	5:Y:25:C:C4	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1780:G:OP2	1:1:1781:A:C8	2.69	0.46
4:X:98:ASP:O	4:X:100:VAL:HG23	2.16	0.46
3:A:246:ALA:C	5:Y:76:A:C6	2.75	0.46
1:1:1704:C:H6	1:1:1704:C:O5'	1.98	0.46
1:1:1709:G:H2'	1:1:1710:C:H5"	1.97	0.46
5:Y:22:G:N1	5:Y:23:A:N7	2.64	0.46
5:Y:58:1MA:HM12	5:Y:61:C:H1'	1.97	0.46
4:X:68:LYS:CB	4:X:85:VAL:HB	2.45	0.45
1:1:1738:C:O5'	1:1:1738:C:H6	1.99	0.45
1:1:1782:G:C2	1:1:1783:C:N4	2.84	0.45
1:1:1808:U:H6	1:1:1808:U:O5'	1.99	0.45
2:2:4388:A:H5"	2:2:4388:A:C8	2.51	0.45
1:1:1781:A:HO2'	1:1:1782:G:P	2.38	0.45
3:A:60:ASP:O	3:A:66:ARG:HD3	2.15	0.45
5:Y:15:G:H2'	5:Y:16:H2U:H5'	1.92	0.45
5:Y:44:A:O2'	5:Y:45:G:H8	1.99	0.45
4:X:41:PHE:HB3	4:X:44:ALA:HB3	1.99	0.45
2:2:4381:C:C3'	2:2:4382:A:H5'	2.47	0.45
2:2:4388:A:H3'	2:2:4389:C:C4'	2.47	0.45
5:Y:59:U:C2'	5:Y:60:C:H5'	2.47	0.45
1:1:1750:C:C6	1:1:1750:C:O5'	2.70	0.45
5:Y:71:G:C2'	5:Y:72:C:H5'	2.47	0.45
5:Y:14:A:C6	5:Y:22:G:N1	2.85	0.44
5:Y:25:C:C2'	5:Y:26:M2G:C5'	2.95	0.44
1:1:1815:A:O5'	1:1:1815:A:H8	2.01	0.44
1:1:1747:C:H2'	1:1:1748:G:H8	1.82	0.44
2:2:4397:U:H4'	2:2:4397:U:OP2	2.17	0.44
5:Y:59:U:O2'	5:Y:60:C:H5'	2.16	0.44
3:A:216:VAL:HA	3:A:219:LEU:HD12	1.99	0.44
2:2:4366:U:C2'	2:2:4367:G:H5'	2.47	0.44
5:Y:28:C:OP2	5:Y:28:C:C6	2.70	0.44
1:1:1745:A:N3	1:1:1745:A:H3'	2.32	0.44
5:Y:44:A:C8	5:Y:44:A:OP2	2.70	0.44
1:1:1721:U:C4'	1:1:1722:G:O5'	2.64	0.44
5:Y:62:A:C2'	5:Y:63:C:H5'	2.47	0.44
1:1:1794:C:H6	1:1:1794:C:O5'	2.00	0.44
3:A:200:LEU:O	3:A:216:VAL:HG23	2.18	0.44
5:Y:17:H2U:C4'	5:Y:18:G:H5"	2.43	0.44
3:A:325:GLU:OE2	3:A:389:ARG:HD2	2.17	0.44
4:X:32:LEU:O	4:X:34:THR:N	2.51	0.44
2:2:4377:C:C5'	2:2:4377:C:C6	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1762:C:H2'	1:1:1763:G:H8	1.82	0.44
1:1:1829:G:H8	1:1:1829:G:O5'	2.01	0.44
1:1:1831:A:C2'	1:1:1832:A:H5'	2.48	0.44
3:A:341:VAL:HG22	3:A:360:GLU:HA	1.99	0.44
1:1:1833:C:C5'	1:1:1833:C:C6	2.85	0.43
5:Y:13:C:C2	5:Y:14:A:N7	2.86	0.43
3:A:84:TYR:HE1	3:A:224:PRO:HG3	1.83	0.43
1:1:1766:C:H5'	1:1:1767:C:OP2	2.18	0.43
1:1:1769:C:O5'	1:1:1769:C:H6	2.00	0.43
4:X:87:ASN:HB2	4:X:90:CYS:HG	1.81	0.43
5:Y:62:A:H2'	5:Y:63:C:O4'	2.18	0.43
1:1:1739:C:O5'	1:1:1739:C:C6	2.70	0.43
3:A:45:ALA:HB1	3:A:50:LYS:O	2.19	0.43
1:1:1830:U:O5'	1:1:1830:U:C6	2.71	0.43
1:1:1765:C:H2'	1:1:1766:C:C1'	2.46	0.43
5:Y:8:U:O2	5:Y:15:G:O6	2.36	0.43
3:A:163:GLN:HB2	3:A:209:TRP:CD2	2.53	0.43
3:A:346:VAL:HA	3:A:355:SER:HA	2.01	0.43
4:X:123:VAL:HA	4:X:130:LEU:HD12	2.00	0.43
2:2:4377:C:H6	2:2:4377:C:H5"	1.83	0.43
3:A:76:PHE:CD2	3:A:89:ILE:HG12	2.53	0.43
3:A:337:SER:OG	3:A:338:ALA:N	2.51	0.43
1:1:1781:A:O2'	1:1:1782:G:P	2.76	0.43
2:2:4401:A:OP2	2:2:4401:A:C8	2.71	0.43
2:2:4384:A:H3'	2:2:4385:G:C8	2.53	0.43
1:1:1748:G:H1	1:1:1786:U:H3	1.67	0.43
4:X:60:LYS:O	4:X:61:GLN:HB2	2.19	0.43
3:A:163:GLN:HB2	3:A:209:TRP:CE2	2.54	0.43
1:1:1719:A:H8	1:1:1719:A:O5'	2.02	0.43
3:A:115:VAL:HG13	3:A:151:VAL:HA	2.00	0.43
1:1:1703:C:H3'	1:1:1704:C:C5	2.54	0.43
4:X:32:LEU:CD2	4:X:34:THR:HB	2.49	0.43
1:1:1739:C:H2'	1:1:1740:C:O4'	2.19	0.43
1:1:1703:C:C4	1:1:1704:C:C4	3.06	0.42
4:X:80:LYS:H	4:X:80:LYS:HG3	1.71	0.42
3:A:4:LYS:HA	3:A:5:PRO:HD3	1.90	0.42
3:A:264:LYS:HB2	3:A:264:LYS:HE3	1.71	0.42
2:2:4399:U:H2'	2:2:4400:G:C5'	2.45	0.42
2:2:4396:U:P	2:2:4396:U:H6	2.43	0.42
3:A:264:LYS:HG2	3:A:316:LEU:HD21	2.00	0.42
1:1:1829:G:C4	1:1:1830:U:H5	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:187:ILE:O	3:A:187:ILE:HG12	2.18	0.42
1:1:1766:C:C5	1:1:1767:C:N4	2.88	0.42
1:1:1782:G:H1'	1:1:1783:C:C5	2.54	0.42
1:1:1782:G:O2'	1:1:1783:C:C6	2.68	0.42
1:1:1746:U:O5'	1:1:1746:U:H6	2.02	0.42
3:A:134:GLU:OE2	3:A:413:ARG:NH2	2.50	0.42
1:1:1822:A:C3'	1:1:1823:A:H5"	2.50	0.42
1:1:1829:G:H2'	1:1:1829:G:N3	2.35	0.41
5:Y:53:G:H2'	5:Y:54:5MU:O4'	2.20	0.41
3:A:169:VAL:O	3:A:173:LEU:HB2	2.19	0.41
1:1:1764:G:N3	1:1:1764:G:C3'	2.80	0.41
3:A:428:LYS:HA	3:A:429:PRO:HD3	1.91	0.41
2:2:4395:U:H3'	2:2:4396:U:C5	2.55	0.41
5:Y:8:U:H5'	5:Y:49:5MC:OP1	2.20	0.41
4:X:39:ASN:HB2	4:X:40:PRO:HD2	2.02	0.41
1:1:1711:U:H2'	1:1:1712:A:C8	2.55	0.41
5:Y:26:M2G:C2'	5:Y:27:C:C1'	2.94	0.41
4:X:41:PHE:HE1	4:X:120:PHE:CD1	2.38	0.41
3:A:223:GLN:HA	3:A:224:PRO:HD3	1.92	0.41
1:1:1790:A:H2'	1:1:1791:A:H5'	2.03	0.41
1:1:1745:A:C2	1:1:1746:U:C5	3.08	0.41
4:X:132:ALA:HA	4:X:138:LYS:HG3	2.03	0.41
3:A:349:VAL:HG22	3:A:350:HIS:CD2	2.55	0.41
5:Y:11:C:H2'	5:Y:12:U:C5	2.50	0.41
1:1:1743:G:C2'	1:1:1744:G:H5'	2.51	0.41
1:1:1731:A:C6	1:1:1732:G:C6	3.09	0.41
2:2:4397:U:H5'	2:2:4397:U:C6	2.56	0.41
3:A:27:LEU:HB3	3:A:33:ILE:HD13	2.02	0.41
5:Y:60:C:H2'	5:Y:60:C:H6	1.50	0.41
3:A:277:ARG:HH21	3:A:300:ARG:HG3	1.86	0.40
2:2:4380:U:OP2	2:2:4381:C:C5	2.74	0.40
5:Y:44:A:O4'	5:Y:44:A:P	2.79	0.40
5:Y:14:A:C5	5:Y:22:G:N2	2.89	0.40
1:1:1781:A:C2	1:1:1782:G:N2	2.89	0.40
2:2:4381:C:H2'	2:2:4382:A:H5'	2.03	0.40
1:1:1721:U:H4'	1:1:1721:U:OP1	2.21	0.40
3:A:249:VAL:HA	3:A:250:PRO:HD2	1.84	0.40
2:2:4377:C:H3'	2:2:4378:G:C8	2.51	0.40
4:X:86:PRO:HB3	4:X:121:LYS:HZ2	1.86	0.40
2:2:4406:U:O2	2:2:4406:U:C2'	2.70	0.40
1:1:1787:G:C2'	1:1:1788:A:H8	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1825:A:C8	1:1:1825:A:C3'	3.03	0.40
5:Y:43:G:C5'	5:Y:44:A:OP1	2.70	0.40
5:Y:24:G:H2'	5:Y:25:C:O5'	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 PDB entries followed by that with respect to all EM entries.

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
3	A	425/437 (97%)	413 (97%)	12 (3%)	0	100 100
4	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2 29
All	All	557/580 (96%)	533 (96%)	17 (3%)	7 (1%)	20 60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	61	GLN
4	X	106	GLY
4	X	107	ARG
4	X	116	PRO
4	X	33	GLY
4	X	86	PRO
4	X	75	ILE

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 PDB entries followed by that with respect to all EM entries.

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
3	A	344/372 (92%)	309 (90%)	35 (10%)	9 37
4	X	108/115 (94%)	103 (95%)	5 (5%)	33 68
All	All	452/487 (93%)	412 (91%)	40 (9%)	17 45

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	9	LEU
3	A	22	LEU
3	A	30	LEU
3	A	47	SER
3	A	63	LYS
3	A	66	ARG
3	A	95	ARG
3	A	99	LYS
3	A	106	SER
3	A	128	THR
3	A	133	ARG
3	A	140	ARG
3	A	141	THR
3	A	147	ILE
3	A	149	VAL
3	A	160	ASN
3	A	169	VAL
3	A	173	LEU
3	A	187	ILE
3	A	203	ARG
3	A	211	ASN
3	A	224	PRO
3	A	237	VAL
3	A	238	GLN
3	A	248	THR
3	A	249	VAL
3	A	258	VAL
3	A	288	GLN
3	A	303	SER
3	A	346	VAL
3	A	364	LYS
3	A	406	GLN
3	A	407	LEU
3	A	415	MET

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Mol	Chain	Res	Type
3	A	424	VAL
4	X	17	ARG
4	X	31	HIS
4	X	37	LYS
4	X	80	LYS
4	X	81	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	94	HIS
3	A	287	GLN
3	A	315	HIS
3	A	348	HIS
4	X	31	HIS
4	X	61	GLN
4	X	73	GLN
4	X	77	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	134/135 (99%)	57 (42%)	7 (5%)
2	2	49/50 (98%)	28 (57%)	4 (8%)
5	Y	74/76 (97%)	29 (39%)	7 (9%)
6	a	47/48 (97%)	32 (68%)	0
7	b	16/17 (94%)	10 (62%)	0
8	c	18/19 (94%)	11 (61%)	0
9	x	27/28 (96%)	15 (55%)	0
All	All	365/373 (97%)	182 (49%)	18 (4%)

All (182) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	1702	G
1	1	1703	C
1	1	1707	U
1	1	1708	C
1	1	1709	G
1	1	1710	C

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Mol	Chain	Res	Type
1	1	1714	U
1	1	1719	A
1	1	1720	U
1	1	1721	U
1	1	1722	G
1	1	1723	G
1	1	1728	U
1	1	1729	U
1	1	1731	A
1	1	1732	G
1	1	1735	A
1	1	1744	G
1	1	1745	A
1	1	1747	C
1	1	1749	G
1	1	1751	C
1	1	1752	C
1	1	1760	G
1	1	1761	U
1	1	1764	G
1	1	1765	C
1	1	1767	C
1	1	1768	A
1	1	1770	G
1	1	1775	U
1	1	1781	A
1	1	1782	G
1	1	1783	C
1	1	1788	A
1	1	1789	G
1	1	1790	A
1	1	1792	G
1	1	1794	C
1	1	1798	C
1	1	1800	A
1	1	1809	A
1	1	1811	C
1	1	1813	A
1	1	1817	G
1	1	1819	A
1	1	1823	A
1	1	1824	A

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Mol	Chain	Res	Type
1	1	1825	A
1	1	1826	G
1	1	1827	U
1	1	1829	G
1	1	1831	A
1	1	1832	A
1	1	1833	C
1	1	1834	A
1	1	1835	A
2	2	4362	C
2	2	4363	U
2	2	4366	U
2	2	4367	G
2	2	4370	G
2	2	4372	C
2	2	4373	C
2	2	4375	A
2	2	4376	G
2	2	4377	C
2	2	4379	U
2	2	4380	U
2	2	4382	A
2	2	4383	U
2	2	4384	A
2	2	4386	C
2	2	4387	G
2	2	4388	A
2	2	4389	C
2	2	4390	G
2	2	4394	C
2	2	4396	U
2	2	4397	U
2	2	4401	A
2	2	4404	C
2	2	4406	U
2	2	4407	C
2	2	4408	G
5	Y	4	G
5	Y	5	A
5	Y	9	A
5	Y	12	U
5	Y	14	A

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Mol	Chain	Res	Type
5	Y	15	G
5	Y	16	H2U
5	Y	17	H2U
5	Y	21	A
5	Y	22	G
5	Y	23	A
5	Y	25	C
5	Y	27	C
5	Y	28	C
5	Y	36	A
5	Y	38	A
5	Y	43	G
5	Y	44	A
5	Y	45	G
5	Y	46	7MG
5	Y	47	U
5	Y	48	C
5	Y	57	G
5	Y	67	A
5	Y	68	U
5	Y	69	U
5	Y	73	A
5	Y	75	C
5	Y	76	A
6	a	459	C
6	a	460	A
6	a	463	C
6	a	464	A
6	a	465	A
6	a	466	G
6	a	467	G
6	a	468	A
6	a	472	C
6	a	473	A
6	a	474	G
6	a	475	C
6	a	476	A
6	a	477	G
6	a	480	G
6	a	482	G
6	a	485	A
6	a	487	U

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Mol	Chain	Res	Type
6	a	488	U
6	a	489	A
6	a	491	C
6	a	492	C
6	a	493	A
6	a	495	U
6	a	496	C
6	a	497	C
6	a	499	G
6	a	500	A
6	a	501	C
6	a	502	C
6	a	503	C
6	a	504	G
7	b	152	U
7	b	153	G
7	b	158	A
7	b	160	U
7	b	161	U
7	b	162	C
7	b	163	U
7	b	164	A
7	b	166	A
7	b	167	G
8	c	4557	U
8	c	4558	C
8	c	4560	G
8	c	4561	U
8	c	4562	A
8	c	4563	C
8	c	4566	G
8	c	4567	A
8	c	4568	G
8	c	4569	G
8	c	4570	A
9	x	36	U
9	x	37	U
9	x	38	U
9	x	39	U
9	x	41	U
9	x	42	U
9	x	43	U

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Mol	Chain	Res	Type
9	x	45	U
9	x	46	U
9	x	49	U
9	x	52	U
9	x	54	U
9	x	55	U
9	x	56	U
9	x	61	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1721	U
1	1	1781	A
1	1	1823	A
1	1	1824	A
1	1	1830	U
1	1	1833	C
1	1	1834	A
2	2	4374	A
2	2	4387	G
2	2	4388	A
2	2	4396	U
5	Y	3	G
5	Y	16	H2U
5	Y	21	A
5	Y	22	G
5	Y	26	M2G
5	Y	45	G
5	Y	46	7MG

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

11 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	$\#\|Z\|>2$
5	2MG	Y	10	5	18,26,27	1.06	1 (5%)	21,38,41	2.94	5 (23%)
5	H2U	Y	16	5	17,21,22	0.90	0	23,30,33	2.60	7 (30%)
5	H2U	Y	17	5	17,21,22	0.74	1 (5%)	23,30,33	1.96	5 (21%)
5	M2G	Y	26	5	18,27,28	1.51	5 (27%)	22,40,43	2.78	7 (31%)
5	OMC	Y	32	5	15,22,23	0.75	0	20,31,34	0.67	1 (5%)
5	MIA	Y	37	5	22,31,32	1.10	3 (13%)	26,44,47	1.71	5 (19%)
5	7MG	Y	46	5	20,26,27	2.26	4 (20%)	23,39,42	2.55	5 (21%)
5	5MC	Y	49	5	14,22,23	1.04	2 (14%)	17,32,35	3.22	5 (29%)
5	5MU	Y	54	5	13,22,23	7.20	3 (23%)	16,32,35	5.98	6 (37%)
5	PSU	Y	55	5	15,21,22	1.67	3 (20%)	16,30,33	4.10	5 (31%)
5	1MA	Y	58	5	15,25,26	1.04	1 (6%)	15,37,40	1.33	2 (13%)

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
5	2MG	Y	10	5	-	0/5/27/28	0/3/3/3
5	H2U	Y	16	5	-	0/7/38/39	0/2/2/2
5	H2U	Y	17	5	-	0/7/38/39	0/2/2/2
5	M2G	Y	26	5	-	0/7/29/30	0/3/3/3
5	OMC	Y	32	5	-	0/5/27/28	0/2/2/2
5	MIA	Y	37	5	-	0/11/33/34	0/3/3/3
5	7MG	Y	46	5	-	0/7/37/38	0/3/3/3
5	5MC	Y	49	5	-	0/3/25/26	0/2/2/2
5	5MU	Y	54	5	-	0/3/25/26	0/2/2/2
5	PSU	Y	55	5	-	0/7/25/26	0/2/2/2
5	1MA	Y	58	5	-	0/3/25/26	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	54	5MU	C5M-C5	-25.66	1.02	1.51
5	Y	46	7MG	C8-N9	-5.56	1.37	1.45
5	Y	55	PSU	C5-C1'	-4.24	1.48	1.52
5	Y	55	PSU	C6-C5	-3.13	1.34	1.38
5	Y	46	7MG	C8-N7	-2.79	1.30	1.43
5	Y	49	5MC	CM5-C5	-2.70	1.45	1.51
5	Y	37	MIA	C12-N6	-2.26	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	54	5MU	C6-C5	-2.20	1.34	1.40
5	Y	26	M2G	C4-N3	-2.07	1.32	1.35
5	Y	49	5MC	C6-C5	-2.06	1.34	1.40
5	Y	37	MIA	C13-C14	-2.04	1.36	1.51
5	Y	37	MIA	C2-S10	2.01	1.77	1.75
5	Y	17	H2U	C2-N1	2.12	1.38	1.35
5	Y	26	M2G	C5-C4	2.16	1.45	1.40
5	Y	26	M2G	C6-N1	2.17	1.36	1.33
5	Y	26	M2G	O4'-C1'	2.64	1.45	1.41
5	Y	55	PSU	C4-N3	2.66	1.37	1.33
5	Y	54	5MU	C4-N3	2.91	1.38	1.33
5	Y	46	7MG	C6-N1	2.94	1.38	1.33
5	Y	58	1MA	C6-N6	2.95	1.34	1.29
5	Y	26	M2G	C2-N2	3.33	1.40	1.34
5	Y	10	2MG	C6-N1	3.51	1.39	1.33
5	Y	46	7MG	CM7-N7	7.01	1.58	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	54	5MU	C5-C4-N3	-12.79	114.62	125.35
5	Y	49	5MC	CM5-C5-C4	-10.69	110.16	121.47
5	Y	10	2MG	C5-C6-N1	-9.18	111.53	123.52
5	Y	46	7MG	C5-C6-N1	-7.75	111.85	123.39
5	Y	16	H2U	C6-N1-C2	-7.27	110.93	122.16
5	Y	26	M2G	C5-C6-N1	-7.01	114.35	123.52
5	Y	55	PSU	C5-C1'-C2'	-6.34	104.67	115.44
5	Y	17	H2U	C4-N3-C2	-6.27	120.08	125.77
5	Y	26	M2G	C6-C5-C4	-6.18	113.80	120.86
5	Y	54	5MU	O2'-C2'-C3'	-5.69	93.45	111.86
5	Y	54	5MU	C5M-C5-C6	-5.44	107.58	118.63
5	Y	16	H2U	C5-C6-N1	-5.11	105.17	110.76
5	Y	16	H2U	O2-C2-N1	-4.45	117.34	123.17
5	Y	16	H2U	C4-N3-C2	-4.19	121.97	125.77
5	Y	10	2MG	CM2-N2-C2	-4.10	118.42	123.03
5	Y	58	1MA	C2-N3-C4	-3.68	110.86	116.44
5	Y	54	5MU	O4'-C1'-N1	-3.52	101.42	108.10
5	Y	37	MIA	C5-C6-N1	-3.16	117.38	120.58
5	Y	17	H2U	O2-C2-N1	-2.86	119.42	123.17
5	Y	55	PSU	C4-C5-C1'	-2.85	116.42	121.22
5	Y	10	2MG	C2-N3-C4	-2.83	111.89	114.99
5	Y	26	M2G	N3-C2-N1	-2.68	121.80	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	16	H2U	O4-C4-C5	-2.58	116.76	122.29
5	Y	46	7MG	O3'-C3'-C2'	-2.50	103.76	111.86
5	Y	17	H2U	O3'-C3'-C4'	-2.50	103.55	111.01
5	Y	16	H2U	C6-C5-C4	-2.26	103.85	115.77
5	Y	32	OMC	CM2-O2'-C2'	-2.21	108.39	114.58
5	Y	17	H2U	O4-C4-C5	-2.16	117.67	122.29
5	Y	55	PSU	O2'-C2'-C1'	-2.09	107.38	111.93
5	Y	49	5MC	O2'-C2'-C3'	2.02	118.39	111.86
5	Y	49	5MC	O3'-C3'-C4'	2.07	117.19	111.01
5	Y	49	5MC	O4'-C1'-N1	2.18	112.24	108.10
5	Y	37	MIA	C2-N1-C6	2.18	119.12	113.13
5	Y	37	MIA	C5-C6-N6	2.26	124.16	120.61
5	Y	46	7MG	O2'-C2'-C1'	2.35	118.13	109.98
5	Y	26	M2G	O4'-C1'-N9	2.44	112.71	108.11
5	Y	46	7MG	O3'-C3'-C4'	2.65	118.93	111.01
5	Y	10	2MG	N2-C2-N3	2.69	120.07	116.94
5	Y	26	M2G	C2'-C3'-C4'	2.82	108.42	102.64
5	Y	58	1MA	C2'-C1'-N9	2.84	121.08	113.47
5	Y	55	PSU	O4'-C1'-C2'	2.88	107.81	104.69
5	Y	16	H2U	C1'-N1-C2	3.70	123.37	118.19
5	Y	17	H2U	N3-C2-N1	3.78	120.14	116.64
5	Y	26	M2G	C2'-C1'-N9	3.79	123.61	113.47
5	Y	37	MIA	C12-N6-C6	4.18	128.30	123.46
5	Y	37	MIA	C11-S10-C2	5.04	105.87	102.31
5	Y	26	M2G	C1'-N9-C4	5.74	133.21	126.81
5	Y	49	5MC	CM5-C5-C6	6.76	132.33	118.63
5	Y	10	2MG	C6-N1-C2	6.84	125.04	115.24
5	Y	46	7MG	C6-N1-C2	7.66	124.85	115.88
5	Y	54	5MU	C5M-C5-C4	11.46	132.67	119.97
5	Y	54	5MU	C4-N3-C2	14.02	126.86	115.16
5	Y	55	PSU	C4-N3-C2	14.23	127.03	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	10	2MG	10	0
5	Y	16	H2U	5	0
5	Y	17	H2U	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	26	M2G	26	0
5	Y	37	MIA	1	0
5	Y	46	7MG	2	0
5	Y	49	5MC	1	0
5	Y	54	5MU	1	0
5	Y	55	PSU	1	0
5	Y	58	1MA	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
10	PHE	Y	77	5	9,11,12	0.59	0	11,13,15	2.03	2 (18%)

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
10	PHE	Y	77	5	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Y	77	PHE	CG-CB-CA	-4.86	102.92	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Y	77	PHE	O-C-CA	-4.45	113.79	125.72

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.