Full wwPDB EM Validation Report (i)

Dec 12, 2022 – 05:48 am GMT

PDB ID	:	6XZ7
EMDB ID	:	EMD-10655
Title	:	E. coli 50S ribosomal subunit in complex with dirithromycin, fMet-Phe-tRNA(Phe) and deacylated tRNA(iMet).
Authors	:	Pichkur, E.B.; Polikanov, Y.S.; Myasnikov, A.G.; Konevega, A.L.
Deposited on	:	2020-02-03
Resolution	:	2.10 Å(reported)
Based on initial model	:	4YBB

This is a Full wwPDB EM 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/EMValidationReportHelp
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 (1)) were used in the production of this report:

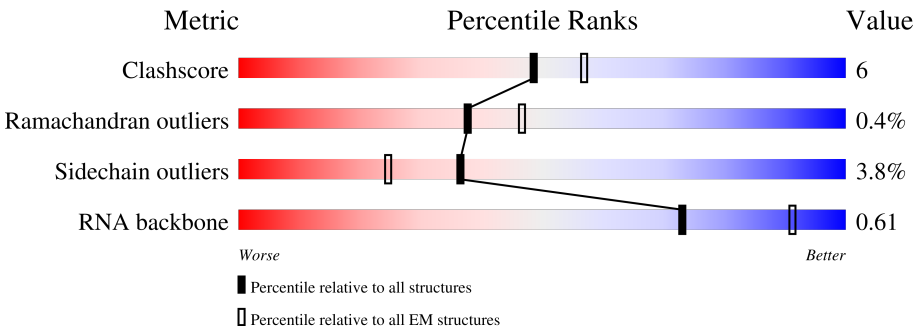
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2897	7%, 76%, 21%, •
2	B	120	•, 80%, 18%, •
3	C	271	85%, 15%
4	D	209	89%, 11%
5	E	201	•, 88%, 11%, •
6	F	177	40%, 54%, 40%, 6%, •
7	G	176	19%, 70%, 26%, •

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Mol	Chain	Length	Quality of chain
8	H	135	100%; 68%; 29%
9	I	134	100%; 77%; 21%
10	J	142	87%; 12%
11	K	123	85%; 15%
12	L	144	87%; 13%
13	M	136	88%; 11%
14	N	125	6%; 93%; 6%
15	O	117	80%; 19%
16	P	114	84%; 15%
17	Q	117	97%
18	R	103	90%; 7%
19	S	110	92%; 7%
20	T	93	85%; 14%
21	U	102	5%; 86%; 13%
22	V	94	81%; 18%
23	W	76	87%; 13%
24	X	77	88%; 12%
25	Y	62	6%; 89%; 11%
26	Z	58	90%; 9%
27	a	56	98%
28	b	51	98%
29	c	46	96%
30	d	64	94%; 6%
31	e	38	97%
32	f	76	70%; 24%; 55%; 21%

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Mol	Chain	Length	Quality of chain
33	g	76	62% 22% 47% 30%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 94915 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2897	62252	27778	11454	20121	2899	3	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2569	1144	468	837	120	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2083	1288	423	365	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	209	1566	980	288	294	4	1	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	177	1411	899	249	257	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	176	1323	832	243	246	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	135	1023	649	179	192	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	VAL	SER	conflict	UNP P0A7J3
H	86	THR	MET	conflict	UNP P0A7J3

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	134	979	619	169	185	6	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	142	1129	714	212	199	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	123	946	593	181	166	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	144	1053	654	207	190	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	136	1075	686	205	178	6	1	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	125	993	613	202	173	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	117	900	557	179	163	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	114	917	574	179	163	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	117	947	604	192	151	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	103	816	516	153	145	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	110	857	532	166	156	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	93	739	466	139	132	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	102	780	492	146	142	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	94	753	479	137	134	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	76	580	359	117	103	1	1	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	77	625	388	129	106	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	62	501	308	98	94	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	58	449	281	87	79	2	2	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	56	444	269	94	80	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	b	51	414	266	76	72	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	46	377	228	90	57	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	64	504	323	105	74	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	e	38	302	185	65	48	4	0	0

- Molecule 32 is a RNA chain called Deacylated tRNAi(Met).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
32	f	76	1625	725	294	529	76	1	0	0

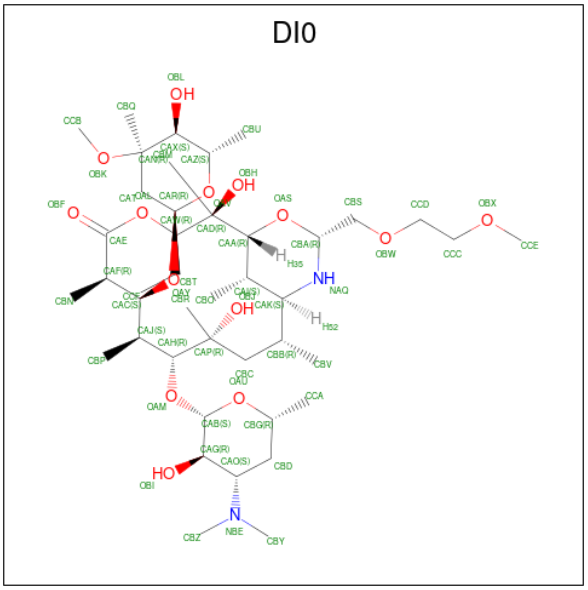
- Molecule 33 is a RNA chain called fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
33	g	76	1667	760	297	534	75	1	0	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	A	174	174	174	0
			Total	Mg	
34	B	3	3	3	0
			Total	Mg	
34	U	1	1	1	0

- Molecule 35 is Dirithromycin (three-letter code: DI0) (formula: $C_{42}H_{78}N_2O_{14}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
35	A	1	58	42	2	14	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	A	498	498	498	0
			Total	O	
36	B	9	9	9	0
			Total	O	
36	C	7	7	7	0
			Total	O	
36	D	1	1	1	0
			Total	O	
36	E	1	1	1	0

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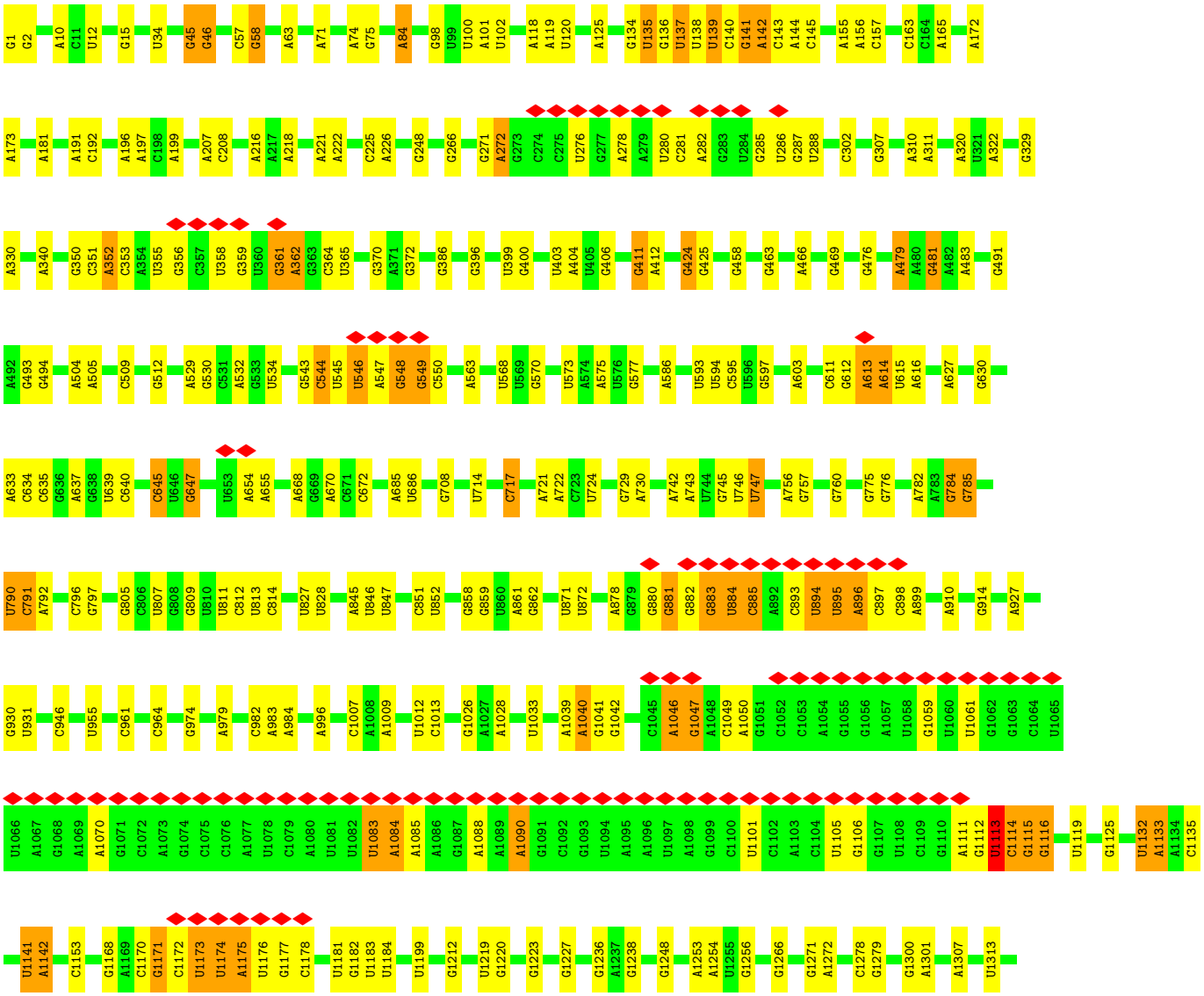
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	L	6	6	6	0
			Total	O	
36	N	1	1	1	0
			Total	O	
36	T	1	1	1	0
			Total	O	
36	d	4	4	4	0

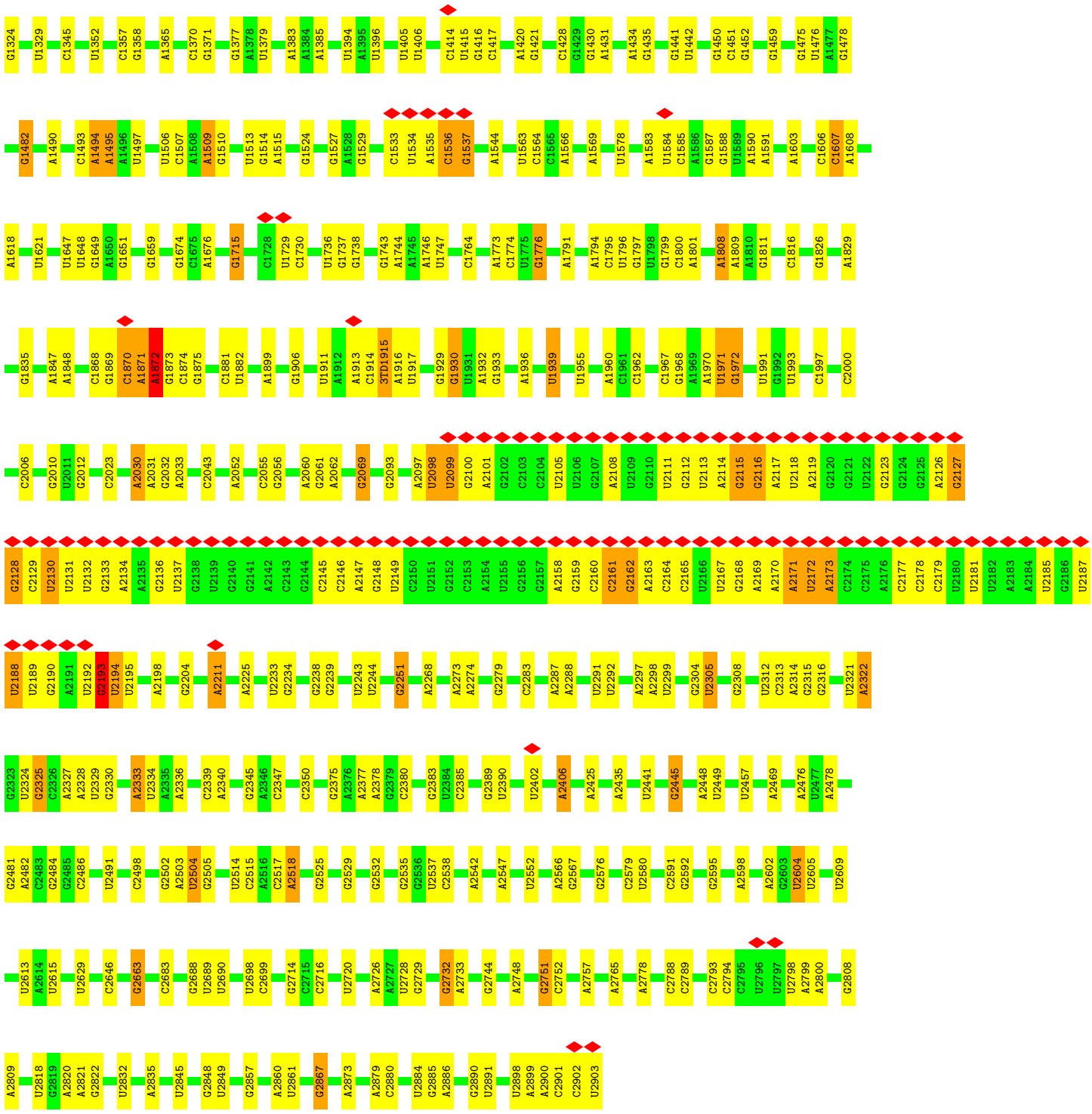
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 23S rRNA

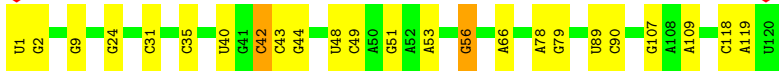
Chain A:





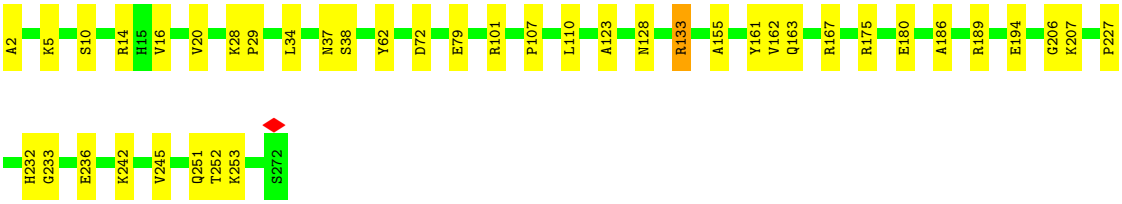
- Molecule 2: 5S rRNA

Chain B:



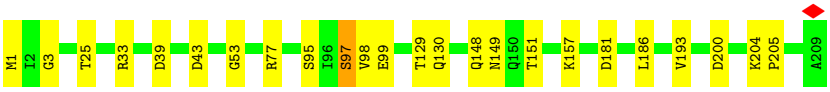
- Molecule 3: 50S ribosomal protein L2

Chain C:



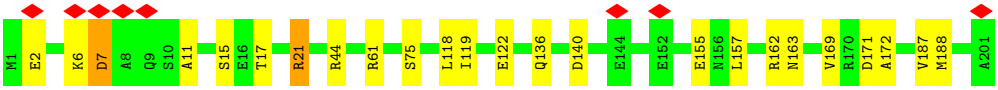
- Molecule 4: 50S ribosomal protein L3

Chain D:



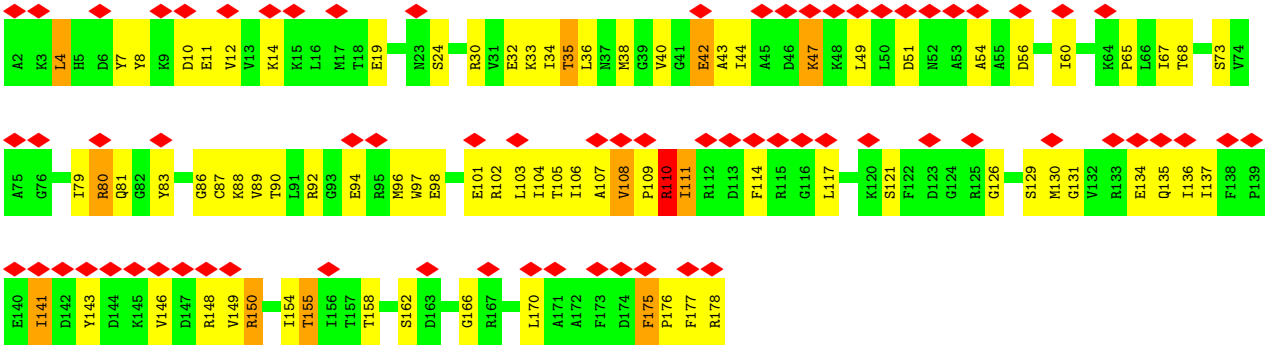
- Molecule 5: 50S ribosomal protein L4

Chain E:



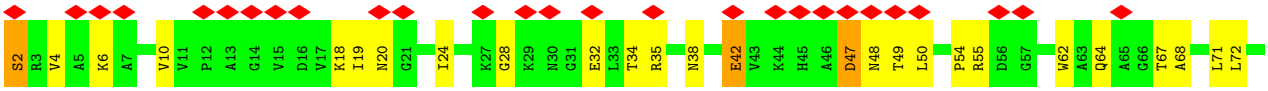
- Molecule 6: 50S ribosomal protein L5

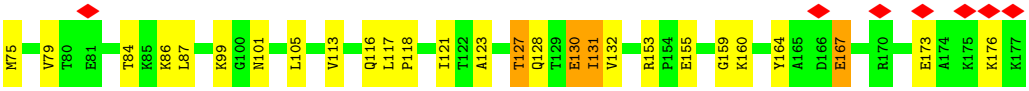
Chain F:



- Molecule 7: 50S ribosomal protein L6

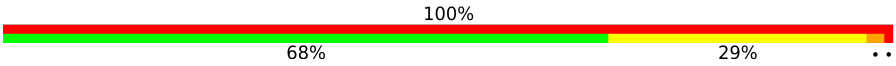
Chain G:

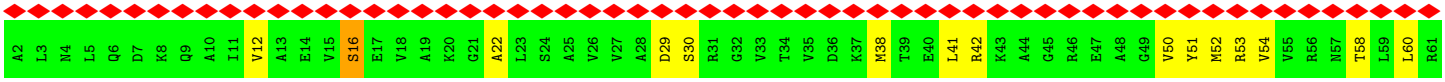


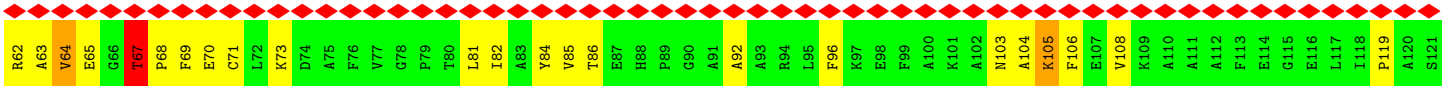


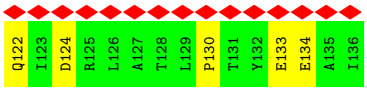
• Molecule 8: 50S ribosomal protein L10

Chain H:



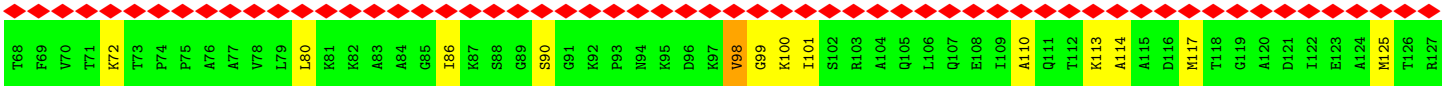


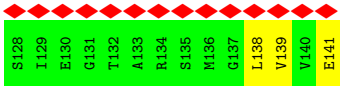




• Molecule 9: 50S ribosomal protein L11

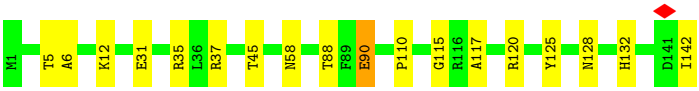
Chain I:





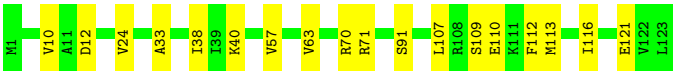
• Molecule 10: 50S ribosomal protein L13

Chain J:



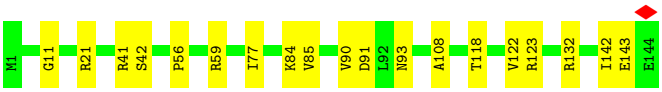
• Molecule 11: 50S ribosomal protein L14

Chain K:



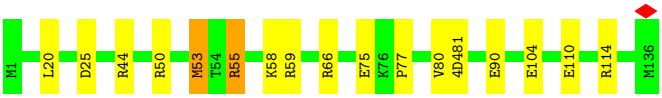
• Molecule 12: 50S ribosomal protein L15

Chain L:



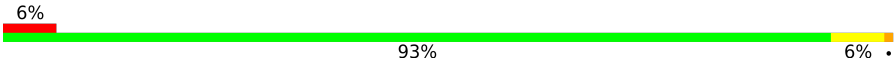
• Molecule 13: 50S ribosomal protein L16

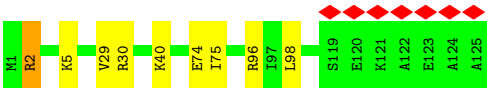
Chain M:



• Molecule 14: 50S ribosomal protein L17

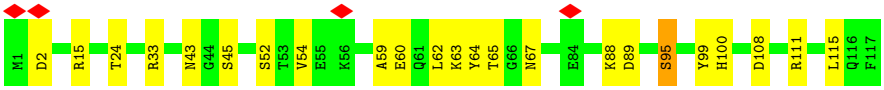
Chain N:





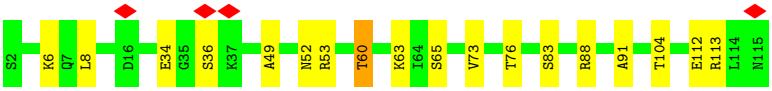
• Molecule 15: 50S ribosomal protein L18

Chain O:



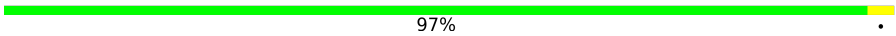
• Molecule 16: 50S ribosomal protein L19

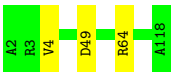
Chain P:



• Molecule 17: 50S ribosomal protein L20

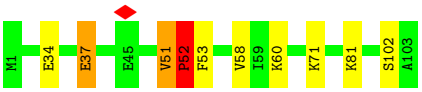
Chain Q:





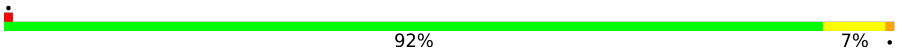
• Molecule 18: 50S ribosomal protein L21

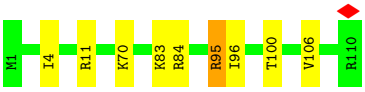
Chain R:



• Molecule 19: 50S ribosomal protein L22

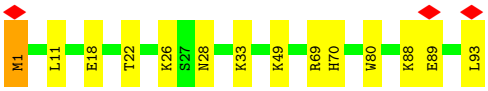
Chain S:





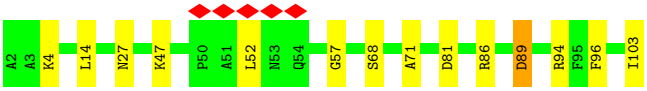
• Molecule 20: 50S ribosomal protein L23

Chain T:



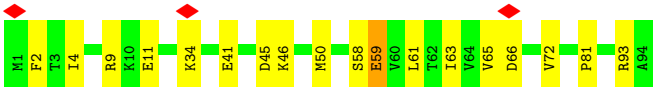
• Molecule 21: 50S ribosomal protein L24

Chain U:



• Molecule 22: 50S ribosomal protein L25

Chain V:

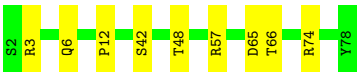


• Molecule 23: 50S ribosomal protein L27

Chain W:

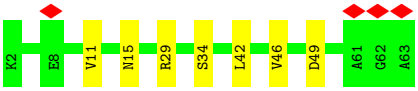
• Molecule 24: 50S ribosomal protein L28

Chain X:



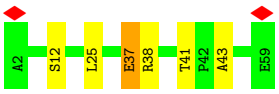
• Molecule 25: 50S ribosomal protein L29

Chain Y:

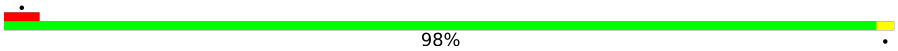


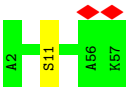
• Molecule 26: 50S ribosomal protein L30

Chain Z:

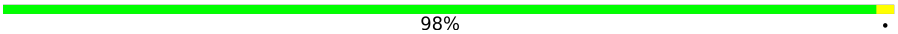


• Molecule 27: 50S ribosomal protein L32

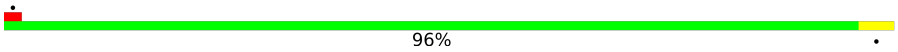
Chain a: 

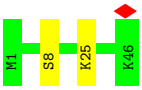


• Molecule 28: 50S ribosomal protein L33

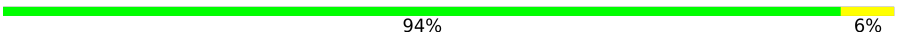
Chain b: 

• Molecule 29: 50S ribosomal protein L34

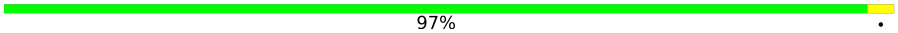
Chain c: 



• Molecule 30: 50S ribosomal protein L35

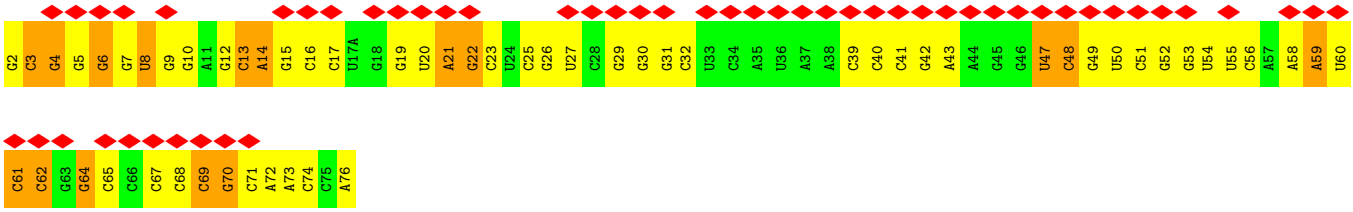
Chain d: 

• Molecule 31: 50S ribosomal protein L36

Chain e: 

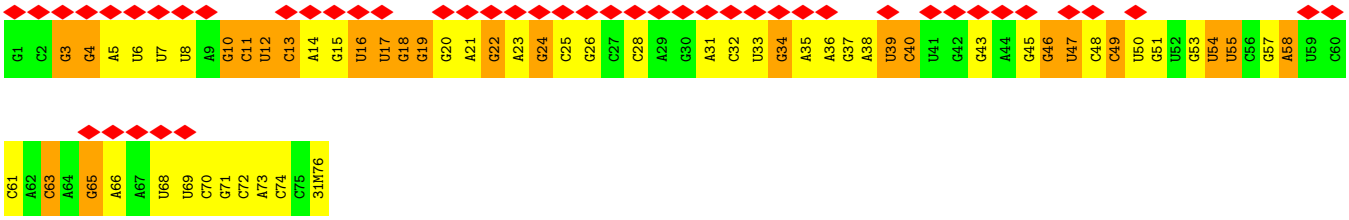
• Molecule 32: Deacylated tRNAi(Met)

Chain f: 70% 24% 55% 21%



- Molecule 33: fMet-Phe-tRNA(Phe)

Chain g: 62% 22% 47% 30%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	401905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.709	Depositor
Minimum map value	-1.212	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

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: DI0, PSU, OMG, 2MA, MEQ, G7M, 2MG, 4D4, MG, M2G, 4SU, 6MZ, H2U, 1MA, OMU, 1MG, 31M, YYG, 7MG, 5MC, 3TD, OMC, 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.72	1/69172 (0.0%)	0.74	7/107908 (0.0%)
2	B	0.56	0/2872	0.71	0/4478
3	C	0.37	0/2122	0.46	0/2852
4	D	0.36	0/1576	0.46	0/2119
5	E	0.34	0/1571	0.44	0/2113
6	F	0.29	0/1435	0.45	0/1926
7	G	0.30	0/1343	0.46	0/1816
8	H	0.42	0/1037	0.56	0/1402
9	I	0.47	0/993	0.64	0/1341
10	J	0.37	0/1152	0.43	0/1551
11	K	0.36	0/955	0.47	0/1279
12	L	0.34	0/1062	0.47	0/1413
13	M	0.36	0/1081	0.45	0/1443
14	N	0.35	0/1006	0.44	0/1345
15	O	0.31	0/910	0.44	0/1219
16	P	0.36	0/929	0.45	0/1242
17	Q	0.40	0/960	0.38	0/1278
18	R	0.41	0/829	0.54	1/1107 (0.1%)
19	S	0.36	0/864	0.45	0/1156
20	T	0.32	0/745	0.42	0/994
21	U	0.33	0/788	0.48	1/1051 (0.1%)
22	V	0.33	0/766	0.42	0/1025
23	W	0.37	0/587	0.44	0/776
24	X	0.37	0/635	0.46	0/848
25	Y	0.27	0/502	0.37	0/667
26	Z	0.31	0/453	0.44	0/605
27	a	0.35	0/450	0.45	0/599
28	b	0.32	0/421	0.44	0/561
29	c	0.34	0/380	0.43	0/498
30	d	0.38	0/513	0.46	0/676
31	e	0.35	0/303	0.44	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	f	0.80	4/1725 (0.2%)	1.72	77/2689 (2.9%)
33	g	0.68	1/1458 (0.1%)	1.38	33/2272 (1.5%)
All	All	0.64	6/101595 (0.0%)	0.73	119/152646 (0.1%)

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
18	R	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	59	A	O3'-P	-6.50	1.53	1.61
32	f	39	C	O3'-P	-6.25	1.53	1.61
32	f	12	G	O3'-P	-6.06	1.53	1.61
32	f	25	C	O3'-P	-6.00	1.53	1.61
1	A	1774	C	O3'-P	-5.19	1.54	1.61
33	g	63	C	O3'-P	-5.06	1.55	1.61

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	62	C	N1-C1'-C2'	-11.72	98.76	114.00
32	f	30	G	N9-C1'-C2'	-10.75	100.03	114.00
33	g	13	C	C4'-C3'-O3'	9.83	132.66	113.00
33	g	13	C	N1-C1'-C2'	-9.76	101.27	112.00
33	g	24	G	N9-C1'-C2'	-9.75	101.28	112.00
32	f	65	C	N1-C1'-C2'	-9.73	101.29	112.00
32	f	52	G	N9-C1'-C2'	-9.64	101.39	112.00
33	g	65	G	N9-C1'-C2'	-9.21	101.87	112.00
32	f	23	C	C4'-C3'-O3'	8.76	130.52	113.00
32	f	12	G	N9-C1'-C2'	-8.61	102.53	112.00
32	f	42	G	N9-C1'-C2'	-8.55	102.59	112.00
32	f	51	C	N1-C1'-C2'	-8.36	102.80	112.00
32	f	72	A	N9-C1'-C2'	-8.36	102.80	112.00
33	g	47	U	C4'-C3'-O3'	8.36	129.72	113.00
32	f	65	C	C4'-C3'-O3'	8.27	129.53	113.00
32	f	43	A	N9-C1'-C2'	-8.12	103.07	112.00
32	f	5	G	N9-C1'-C2'	-8.06	103.14	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	29	G	N9-C1'-C2'	-8.01	103.19	112.00
32	f	51	C	C1'-C2'-O2'	-7.87	86.98	110.60
33	g	22	G	C2'-C3'-O3'	7.83	126.72	109.50
32	f	29	G	C4'-C3'-O3'	7.81	128.61	113.00
33	g	51	G	N9-C1'-C2'	-7.71	103.51	112.00
32	f	72	A	C4'-C3'-O3'	7.66	128.31	113.00
33	g	22	G	P-O3'-C3'	7.64	128.87	119.70
33	g	68	U	N1-C1'-C2'	-7.62	103.62	112.00
33	g	50	U	N1-C1'-C2'	-7.62	103.62	112.00
32	f	73	A	N9-C1'-C2'	-7.57	103.68	112.00
32	f	21	A	O5'-P-OP2	-7.55	98.91	105.70
32	f	40	C	C1'-C2'-O2'	-7.54	87.97	110.60
33	g	5	A	N9-C1'-C2'	-7.50	103.75	112.00
32	f	6	G	N9-C1'-C2'	-7.49	103.76	112.00
32	f	2	G	N9-C1'-C2'	-7.42	103.84	112.00
32	f	13	C	N1-C1'-C2'	-7.38	103.88	112.00
32	f	12	G	C4'-C3'-O3'	7.35	127.69	113.00
32	f	42	G	C4'-C3'-O3'	7.26	127.52	113.00
32	f	14	A	N9-C1'-C2'	-7.24	104.03	112.00
33	g	11	C	N1-C1'-C2'	-7.24	104.04	112.00
32	f	23	C	C1'-C2'-O2'	-7.19	89.03	110.60
33	g	57	G	N9-C1'-C2'	-7.07	104.22	112.00
32	f	59	A	N9-C1'-C2'	-6.95	104.36	112.00
33	g	57	G	C1'-C2'-O2'	-6.94	89.79	110.60
32	f	64	G	C1'-C2'-O2'	-6.90	89.90	110.60
32	f	22	G	C1'-C2'-O2'	-6.88	89.97	110.60
32	f	71	C	C4'-C3'-O3'	6.84	126.68	113.00
32	f	47	U	P-O3'-C3'	6.81	127.87	119.70
32	f	64	G	C4'-C3'-O3'	6.77	126.54	113.00
33	g	69	U	N1-C1'-C2'	-6.76	104.56	112.00
33	g	51	G	C1'-C2'-O2'	-6.73	90.42	110.60
32	f	26	G	C1'-C2'-O2'	-6.72	90.45	110.60
32	f	23	C	N1-C1'-C2'	-6.68	104.66	112.00
32	f	40	C	N1-C1'-C2'	-6.67	104.66	112.00
1	A	2193	G	C2'-C3'-O3'	6.66	124.36	113.70
33	g	69	U	C4'-C3'-O3'	6.58	126.17	113.00
33	g	50	U	C4'-C3'-O3'	6.56	126.12	113.00
1	A	1113	U	C2'-C3'-O3'	6.55	124.17	113.70
32	f	71	C	N1-C1'-C2'	-6.44	104.92	112.00
32	f	2	G	C4'-C3'-O3'	6.41	125.83	113.00
33	g	12	U	N1-C1'-C2'	-6.41	104.95	112.00
33	g	50	U	C1'-C2'-O2'	-6.31	91.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	4	G	N9-C1'-C2'	-6.22	105.15	112.00
32	f	30	G	O5'-P-OP2	-6.20	100.12	105.70
32	f	53	G	N9-C1'-C2'	-6.20	105.18	112.00
32	f	61	C	N1-C1'-C2'	-6.12	105.27	112.00
33	g	70	C	N1-C1'-C2'	-6.12	105.27	112.00
32	f	27	U	N1-C1'-C2'	-6.09	105.30	112.00
33	g	18	G	C4'-C3'-O3'	-6.08	96.63	109.40
32	f	69	C	C4'-C3'-O3'	6.08	125.16	113.00
32	f	42	G	C1'-C2'-O2'	-6.07	92.40	110.60
32	f	52	G	C4'-C3'-O3'	6.01	125.02	113.00
32	f	40	C	C4'-C3'-O3'	5.99	124.98	113.00
1	A	1313	U	C2-N1-C1'	5.98	124.87	117.70
33	g	3	G	N9-C1'-C2'	-5.97	105.43	112.00
32	f	3	C	C1'-C2'-O2'	-5.94	92.77	110.60
32	f	70	G	N9-C1'-C2'	-5.94	105.47	112.00
33	g	13	C	C1'-C2'-O2'	-5.94	92.78	110.60
32	f	64	G	N9-C1'-C2'	-5.92	105.48	112.00
32	f	15	G	N9-C1'-C2'	-5.92	105.49	112.00
32	f	53	G	C4'-C3'-O3'	5.86	124.73	113.00
32	f	29	G	C1'-C2'-O2'	-5.86	93.03	110.60
32	f	13	C	C4'-C3'-O3'	5.85	124.70	113.00
33	g	5	A	C4'-C3'-O3'	5.82	124.63	113.00
32	f	27	U	C4'-C3'-O3'	5.79	124.58	113.00
33	g	19	G	C4'-C3'-O3'	-5.78	97.27	109.40
33	g	68	U	C4'-C3'-O3'	5.78	124.55	113.00
32	f	48	C	C4'-C3'-O3'	-5.74	97.35	109.40
32	f	74	C	O5'-P-OP1	-5.72	100.55	105.70
32	f	41	C	N1-C1'-C2'	-5.71	105.72	112.00
18	R	52	PRO	CA-N-CD	-5.64	103.61	111.50
32	f	62	C	C3'-C2'-C1'	5.59	105.97	101.50
33	g	65	G	O5'-P-OP2	-5.59	100.67	105.70
1	A	512	G	O4'-C1'-N9	5.58	112.66	108.20
32	f	74	C	C1'-C2'-O2'	-5.52	94.04	110.60
32	f	51	C	C4'-C3'-O3'	5.47	123.95	113.00
32	f	27	U	C1'-C2'-O2'	-5.44	94.27	110.60
32	f	43	A	C4'-C3'-O3'	5.44	123.88	113.00
32	f	22	G	N9-C1'-C2'	-5.43	106.03	112.00
32	f	69	C	N1-C1'-C2'	-5.41	106.05	112.00
32	f	43	A	P-O5'-C5'	-5.38	112.29	120.90
32	f	50	U	N1-C1'-C2'	-5.38	106.08	112.00
33	g	50	U	O5'-P-OP1	-5.35	100.89	105.70
32	f	70	G	O4'-C1'-N9	-5.30	103.96	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	74	C	C4'-C3'-O3'	5.28	123.55	113.00
1	A	404	A	O4'-C1'-C2'	-5.26	100.54	105.80
32	f	42	G	O5'-P-OP1	5.26	117.01	110.70
32	f	43	A	C1'-C2'-O2'	-5.23	94.90	110.60
32	f	62	C	O4'-C1'-N1	5.22	112.38	108.20
33	g	18	G	C1'-C2'-O2'	5.21	126.23	110.60
32	f	5	G	C4'-C3'-O3'	5.21	123.41	113.00
32	f	4	G	C4'-C3'-O3'	5.18	123.37	113.00
32	f	30	G	O5'-P-OP1	5.16	116.89	110.70
32	f	4	G	C1'-C2'-O2'	-5.13	95.22	110.60
32	f	50	U	C4'-C3'-O3'	5.10	123.20	113.00
33	g	47	U	P-O3'-C3'	5.08	125.80	119.70
33	g	70	C	C3'-C2'-C1'	5.08	105.56	101.50
1	A	12	U	N3-C2-O2	-5.04	118.67	122.20
21	U	52	LEU	CA-CB-CG	5.02	126.85	115.30
32	f	3	C	N1-C1'-C2'	-5.01	106.49	112.00
33	g	4	G	N9-C1'-C2'	-5.01	106.49	112.00
1	A	1872	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	51	VAL	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62252	0	31324	392	0
2	B	2569	0	1301	13	0
3	C	2083	0	2154	22	0
4	D	1566	0	1617	14	0
5	E	1552	0	1619	13	0
6	F	1411	0	1444	95	0
7	G	1323	0	1371	31	0
8	H	1023	0	1052	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	979	0	1028	30	0
10	J	1129	0	1162	10	0
11	K	946	0	1023	10	0
12	L	1053	0	1129	12	0
13	M	1075	0	1155	10	0
14	N	993	0	1034	6	0
15	O	900	0	935	18	0
16	P	917	0	962	10	0
17	Q	947	0	1019	3	0
18	R	816	0	839	7	0
19	S	857	0	922	5	0
20	T	739	0	807	14	0
21	U	780	0	830	7	0
22	V	753	0	780	11	0
23	W	580	0	593	5	0
24	X	625	0	652	4	0
25	Y	501	0	531	3	0
26	Z	449	0	487	3	0
27	a	444	0	458	0	0
28	b	414	0	442	0	0
29	c	377	0	418	0	0
30	d	504	0	572	0	0
31	e	302	0	343	0	0
32	f	1625	0	829	0	0
33	g	1667	0	880	0	0
34	A	174	0	0	0	0
34	B	3	0	0	0	0
34	U	1	0	0	0	0
35	A	58	0	0	1	0
36	A	498	0	0	13	0
36	B	9	0	0	0	0
36	C	7	0	0	1	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	L	6	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	d	4	0	0	0	0
All	All	94915	0	61712	730	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 6.

All (730) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:G:N2	1:A:894:U:O2	1.56	1.37
1:A:1:G:N2	1:A:2902:C:O2	1.64	1.30
9:I:98:VAL:O	9:I:138:LEU:HD23	1.22	1.25
1:A:1:G:N1	1:A:2902:C:N3	1.92	1.17
1:A:1050:A:N3	1:A:2751:G:C2	2.13	1.17
6:F:108:VAL:CG1	6:F:109:PRO:HD3	1.76	1.16
6:F:108:VAL:HG13	6:F:109:PRO:CD	1.78	1.14
8:H:67:THR:HG22	8:H:68:PRO:CD	1.76	1.14
6:F:103:LEU:HB2	6:F:107:ALA:CB	1.79	1.12
18:R:51:VAL:HG12	18:R:52:PRO:HD2	1.29	1.11
1:A:884:U:O4	1:A:893:C:C4	2.07	1.08
8:H:12:VAL:CG1	8:H:63:ALA:HB2	1.84	1.07
8:H:67:THR:HG22	8:H:68:PRO:HD3	1.04	1.03
1:A:2898:U:H2'	1:A:2899:A:C8	1.92	1.03
1:A:882:G:N1	1:A:895:U:O2	1.90	1.03
8:H:67:THR:HB	8:H:68:PRO:HD2	1.38	1.02
1:A:2898:U:H2'	1:A:2899:A:H8	1.24	1.00
6:F:103:LEU:HB2	6:F:107:ALA:HB3	1.38	1.00
1:A:884:U:O4	1:A:893:C:N3	1.96	0.99
9:I:100:LYS:HB2	9:I:141:GLU:HB2	1.46	0.98
1:A:1050:A:C4	1:A:2751:G:C2	2.51	0.98
8:H:67:THR:CG2	8:H:68:PRO:HD3	1.94	0.98
8:H:67:THR:CG2	8:H:68:PRO:CD	2.41	0.97
8:H:12:VAL:HG13	8:H:63:ALA:HB2	1.42	0.97
1:A:1050:A:H1'	1:A:2751:G:N2	1.79	0.96
1:A:894:U:O2'	1:A:895:U:OP1	1.82	0.95
1:A:1:G:N1	1:A:2902:C:C2	2.34	0.95
1:A:1050:A:C4	1:A:2751:G:N2	2.36	0.94
6:F:110:ARG:HB3	6:F:137:ILE:HG23	1.48	0.94
1:A:884:U:C4	1:A:893:C:N3	2.35	0.93
6:F:103:LEU:CB	6:F:107:ALA:HB3	1.98	0.92
1:A:2469:A:H4'	13:M:55:ARG:HD2	1.51	0.92
8:H:67:THR:CB	8:H:68:PRO:HD2	2.00	0.90
1:A:1:G:C2	1:A:2902:C:O2	2.24	0.90
1:A:1847:A:HO2'	1:A:1848:A:H8	0.98	0.90
1:A:1050:A:C2	1:A:2751:G:C2	2.59	0.90
6:F:103:LEU:CB	6:F:107:ALA:CB	2.50	0.89
1:A:883:G:H1	1:A:894:U:H3	0.89	0.89
1:A:2116:G:O6	1:A:2171:A:N6	2.06	0.89
6:F:103:LEU:CA	6:F:107:ALA:HB3	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:VAL:O	9:I:138:LEU:CD2	2.17	0.88
6:F:150:ARG:HG2	6:F:150:ARG:HH11	1.38	0.88
1:A:134:G:C6	1:A:135:U:C4	2.62	0.87
1:A:884:U:O4	1:A:893:C:N4	2.08	0.86
6:F:103:LEU:HA	6:F:107:ALA:CB	2.06	0.86
8:H:67:THR:CB	8:H:68:PRO:CD	2.53	0.85
6:F:103:LEU:CA	6:F:107:ALA:CB	2.54	0.85
1:A:1:G:C6	1:A:2902:C:N3	2.45	0.85
1:A:1049:C:H1'	1:A:1113:U:O2'	1.78	0.84
8:H:64:VAL:HG22	8:H:69:PHE:HB3	1.60	0.82
7:G:118:PRO:HG2	7:G:121:ILE:HD13	1.60	0.82
8:H:16:SER:OG	8:H:63:ALA:HB1	1.79	0.81
8:H:67:THR:CG2	8:H:68:PRO:HD2	2.11	0.81
8:H:67:THR:HB	8:H:68:PRO:CD	2.12	0.80
6:F:136:ILE:HG22	6:F:136:ILE:O	1.81	0.80
8:H:60:LEU:O	8:H:64:VAL:HB	1.82	0.80
1:A:884:U:H3'	1:A:885:C:H4'	1.64	0.80
1:A:2006:C:OP2	36:A:3201:HOH:O	1.98	0.80
1:A:894:U:H2'	1:A:895:U:H6	1.47	0.79
6:F:135:GLN:O	6:F:141:ILE:HG21	1.80	0.79
1:A:2099:U:H2'	1:A:2100:G:H8	1.47	0.78
1:A:1:G:O6	1:A:2902:C:N4	2.17	0.78
1:A:1050:A:H1'	1:A:2751:G:H21	1.47	0.78
1:A:1050:A:N3	1:A:2751:G:N2	2.31	0.78
1:A:883:G:C2	1:A:894:U:O2	2.36	0.78
6:F:104:ILE:O	6:F:108:VAL:HG11	1.84	0.78
8:H:12:VAL:HG12	8:H:63:ALA:HB2	1.65	0.77
1:A:2010:G:O6	36:A:3202:HOH:O	2.02	0.77
1:A:894:U:H2'	1:A:895:U:C6	2.19	0.77
6:F:103:LEU:HA	6:F:107:ALA:HB2	1.63	0.77
6:F:111:ILE:HG13	6:F:111:ILE:O	1.83	0.77
1:A:1:G:N1	1:A:2902:C:O2	2.18	0.76
1:A:1050:A:C1'	1:A:2751:G:N2	2.48	0.76
6:F:135:GLN:NE2	6:F:148:ARG:O	2.18	0.76
1:A:882:G:C6	1:A:883:G:N7	2.54	0.75
18:R:51:VAL:CG1	18:R:52:PRO:HD2	2.13	0.75
1:A:1050:A:C2	1:A:2751:G:C4	2.74	0.75
5:E:7:ASP:OD1	5:E:7:ASP:N	2.19	0.74
2:B:31:C:O2	2:B:53:A:N6	2.20	0.74
6:F:134:GLU:OE2	6:F:149:VAL:HG13	1.87	0.74
6:F:111:ILE:HD11	6:F:114:PHE:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2751:G:H2'	1:A:2751:G:N3	2.02	0.74
1:A:142:A:C2	1:A:143:C:C2	2.75	0.74
1:A:63:A:H2	20:T:70:HIS:CE1	2.05	0.74
6:F:134:GLU:CD	6:F:149:VAL:HG13	2.08	0.73
1:A:611:C:C4	1:A:612:G:C5	2.77	0.73
1:A:2683:C:O2	11:K:70:ARG:NH2	2.22	0.73
6:F:80:ARG:HB2	6:F:83:TYR:CZ	2.24	0.72
6:F:149:VAL:O	6:F:149:VAL:HG12	1.88	0.72
1:A:611:C:N4	1:A:612:G:C6	2.58	0.72
3:C:133:ARG:HB3	3:C:186:ALA:HB1	1.71	0.72
6:F:102:ARG:O	6:F:106:ILE:HB	1.90	0.72
1:A:883:G:N2	1:A:894:U:C2	2.56	0.72
9:I:113:LYS:O	9:I:117:MET:N	2.23	0.71
10:J:6:ALA:H	10:J:45:THR:HG21	1.55	0.71
1:A:611:C:C4	1:A:612:G:C6	2.77	0.71
1:A:884:U:H4'	1:A:884:U:OP1	1.91	0.71
1:A:1307:A:N6	1:A:1606:C:O2	2.19	0.71
1:A:1050:A:C2	1:A:2751:G:N3	2.58	0.71
6:F:80:ARG:NH1	6:F:80:ARG:HG3	2.05	0.71
6:F:80:ARG:HG3	6:F:80:ARG:HH11	1.56	0.70
1:A:760:G:H4'	1:A:1776:G:OP1	1.92	0.70
6:F:108:VAL:HG13	6:F:109:PRO:HD3	0.84	0.69
1:A:1869:G:H21	1:A:1872:A:H2	1.38	0.69
1:A:1478:G:H1	1:A:1513:U:H3	1.39	0.69
1:A:2099:U:H2'	1:A:2100:G:C8	2.27	0.69
1:A:881:G:H2'	1:A:882:G:C8	2.27	0.69
1:A:756:A:N7	36:A:3210:HOH:O	2.25	0.69
3:C:2:ALA:N	3:C:20:VAL:O	2.27	0.68
1:A:141:G:N3	1:A:141:G:H3'	2.09	0.68
6:F:111:ILE:HA	6:F:137:ILE:CD1	2.23	0.68
1:A:1324:G:N7	36:A:3214:HOH:O	2.28	0.67
6:F:103:LEU:O	6:F:107:ALA:N	2.26	0.67
12:L:85:VAL:HG11	12:L:90:VAL:HG12	1.77	0.67
12:L:56:PRO:HG2	12:L:59:ARG:HG3	1.76	0.67
1:A:139:U:C6	20:T:1:MET:SD	2.88	0.67
9:I:98:VAL:O	9:I:138:LEU:HA	1.95	0.66
1:A:136:G:C6	1:A:137:U:C5	2.83	0.66
1:A:894:U:C4	1:A:895:U:C4	2.83	0.66
1:A:1039:A:H2	1:A:1116:G:H22	1.42	0.66
1:A:1050:A:N9	1:A:2751:G:N2	2.43	0.66
1:A:611:C:C5	1:A:612:G:C5	2.83	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:C:O2	6:F:92:ARG:NH2	2.29	0.66
1:A:1113:U:O5'	1:A:1113:U:H6	1.79	0.66
8:H:12:VAL:HG13	8:H:63:ALA:CB	2.22	0.66
1:A:811:U:OP1	36:A:3204:HOH:O	2.14	0.66
1:A:2127:G:O2'	1:A:2128:G:O4'	2.13	0.66
1:A:1972:G:OP2	36:A:3203:HOH:O	2.13	0.65
10:J:88:THR:OG1	10:J:90:GLU:OE2	2.14	0.65
1:A:611:C:C5	1:A:612:G:C6	2.84	0.65
1:A:1377:G:N7	36:A:3216:HOH:O	2.29	0.65
6:F:134:GLU:OE1	6:F:149:VAL:CG1	2.45	0.64
1:A:1482:G:H1'	1:A:1509:A:H61	1.62	0.64
1:A:2127:G:O2'	1:A:2128:G:O5'	2.15	0.64
25:Y:11:VAL:O	25:Y:15:ASN:ND2	2.29	0.64
6:F:150:ARG:HG2	6:F:150:ARG:NH1	2.10	0.64
8:H:16:SER:CB	8:H:63:ALA:HB1	2.28	0.64
1:A:1871:A:O2'	1:A:1872:A:N3	2.25	0.64
6:F:47:LYS:H	6:F:47:LYS:HD2	1.62	0.64
1:A:881:G:H3'	1:A:882:G:C8	2.33	0.64
1:A:2900:A:O5'	1:A:2900:A:H8	1.80	0.64
3:C:236:GLU:OE2	36:C:301:HOH:O	2.15	0.64
6:F:104:ILE:O	6:F:108:VAL:CG1	2.46	0.64
1:A:1899:A:N7	36:A:3217:HOH:O	2.29	0.64
1:A:1061:U:OP2	9:I:10:LYS:NZ	2.31	0.63
1:A:1050:A:N3	1:A:2751:G:N3	2.46	0.63
1:A:882:G:H22	1:A:895:U:H2'	1.61	0.63
7:G:47:ASP:O	7:G:49:THR:N	2.29	0.63
1:A:134:G:C5	1:A:135:U:C4	2.86	0.63
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.81	0.62
1:A:790:U:O2'	1:A:791:C:C5	2.53	0.62
11:K:121:GLU:OE1	16:P:65:SER:OG	2.17	0.62
1:A:1:G:O6	1:A:2902:C:N3	2.32	0.62
1:A:1050:A:C4	1:A:2751:G:N1	2.67	0.62
1:A:1248:G:OP1	5:E:44:ARG:NH2	2.33	0.62
6:F:136:ILE:HD13	6:F:143:TYR:HD1	1.64	0.62
16:P:91:ALA:HB2	16:P:113:ARG:HA	1.80	0.62
6:F:4:LEU:HA	6:F:7:TYR:HB3	1.81	0.62
1:A:139:U:C5	20:T:1:MET:CE	2.83	0.62
1:A:881:G:C6	1:A:882:G:C6	2.87	0.62
18:R:37:GLU:OE2	18:R:37:GLU:HA	1.98	0.62
6:F:103:LEU:CA	6:F:107:ALA:HB2	2.28	0.61
1:A:1826:G:O2'	1:A:1971:U:OP2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:ARG:NH1	4:D:53:GLY:O	2.33	0.61
1:A:355:U:H2'	1:A:356:G:H8	1.65	0.61
1:A:881:G:H3'	1:A:882:G:H8	1.66	0.61
8:H:70:GLU:O	8:H:73:LYS:HG3	2.01	0.61
9:I:100:LYS:HA	9:I:139:VAL:O	1.99	0.61
6:F:103:LEU:CB	6:F:107:ALA:HB2	2.31	0.61
20:T:11:LEU:O	25:Y:29:ARG:NH1	2.31	0.61
1:A:862:G:N7	36:A:3222:HOH:O	2.31	0.60
1:A:84:A:N1	1:A:98:G:O2'	2.32	0.60
1:A:144:A:H2'	1:A:145:C:C6	2.36	0.60
6:F:80:ARG:HH11	6:F:80:ARG:CG	2.14	0.60
8:H:134:GLU:O	8:H:134:GLU:HG3	2.00	0.60
9:I:110:ALA:O	9:I:114:ALA:N	2.34	0.60
6:F:103:LEU:C	6:F:107:ALA:HB3	2.22	0.60
1:A:136:G:C5	1:A:137:U:C5	2.89	0.60
7:G:35:ARG:HD3	7:G:71:LEU:HD23	1.82	0.59
1:A:63:A:C2	20:T:70:HIS:CE1	2.90	0.59
1:A:2324:U:H3'	1:A:2325:G:C5'	2.32	0.59
6:F:101:GLU:HA	6:F:104:ILE:HG22	1.83	0.59
26:Z:41:THR:HG22	26:Z:43:ALA:H	1.67	0.59
7:G:87:LEU:HB2	7:G:131:ILE:HG23	1.85	0.59
14:N:29:VAL:HG21	14:N:75:ILE:HG23	1.84	0.59
22:V:4:ILE:HG12	22:V:50:MET:HE1	1.83	0.59
1:A:2752:C:H6	1:A:2752:C:O5'	1.86	0.59
3:C:29:PRO:HG2	3:C:34:LEU:HD11	1.85	0.59
6:F:136:ILE:O	6:F:136:ILE:CG2	2.48	0.59
1:A:45:G:H5'	1:A:46:G:H5'	1.85	0.59
1:A:894:U:N3	1:A:895:U:C4	2.70	0.59
7:G:127:THR:HG23	7:G:130:GLU:HB2	1.85	0.59
1:A:143:C:H6	1:A:143:C:O5'	1.86	0.59
1:A:1869:G:HO2'	1:A:1871:A:H2	1.49	0.59
7:G:127:THR:OG1	7:G:128:GLN:N	2.35	0.59
1:A:807:U:OP2	12:L:41:ARG:NH1	2.36	0.58
6:F:65:PRO:HA	6:F:89:VAL:HG22	1.85	0.58
1:A:134:G:C5	1:A:135:U:C5	2.92	0.58
1:A:884:U:N3	1:A:893:C:C2	2.68	0.58
6:F:134:GLU:CD	6:F:149:VAL:CG1	2.72	0.58
6:F:141:ILE:O	6:F:141:ILE:HG23	2.04	0.58
1:A:1527:G:N1	1:A:1544:A:OP2	2.32	0.58
1:A:894:U:C2	1:A:895:U:C5	2.92	0.58
1:A:320:A:N3	5:E:163:ASN:ND2	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:20:LEU:HD13	22:V:81:PRO:HG2	1.86	0.57
8:H:103:ASN:O	8:H:105:LYS:N	2.37	0.57
1:A:883:G:N1	1:A:894:U:N3	2.35	0.57
1:A:2518:A:H2'	1:A:2518:A:N3	2.20	0.57
7:G:19:ILE:HG13	7:G:24:ILE:HD12	1.87	0.57
6:F:134:GLU:OE2	6:F:149:VAL:CG1	2.52	0.57
1:A:139:U:C5	20:T:1:MET:HE1	2.40	0.57
22:V:58:SER:OG	22:V:59:GLU:OE1	2.20	0.57
1:A:2517:C:C6	1:A:2542:A:N7	2.73	0.57
1:A:757:G:O6	36:A:3205:HOH:O	2.14	0.56
1:A:2315:G:H2'	1:A:2316:G:H8	1.69	0.56
6:F:35:THR:HG23	6:F:155:THR:HG23	1.87	0.56
15:O:99:TYR:OH	15:O:111:ARG:NH1	2.38	0.56
6:F:117:LEU:HB2	6:F:176:PRO:O	2.05	0.56
7:G:42:GLU:HB3	7:G:55:ARG:HE	1.70	0.56
8:H:22:ALA:HA	8:H:86:THR:HA	1.88	0.56
1:A:271:G:O2'	1:A:272:A:O5'	2.22	0.56
3:C:227:PRO:HA	3:C:233:GLY:HA2	1.87	0.56
13:M:77:PRO:HG2	13:M:80:VAL:HG21	1.88	0.56
6:F:110:ARG:HB3	6:F:137:ILE:CG2	2.28	0.56
13:M:75:GLU:HB2	13:M:90:GLU:HG3	1.86	0.56
1:A:218:A:N7	36:A:3224:HOH:O	2.32	0.56
3:C:79:GLU:OE2	3:C:101:ARG:NE	2.39	0.56
7:G:155:GLU:OE1	7:G:160:LYS:N	2.33	0.56
9:I:19:ASN:HA	9:I:39:CYS:SG	2.46	0.56
5:E:136:GLN:NE2	5:E:140:ASP:OD1	2.38	0.56
1:A:1041:G:C2	1:A:1115:G:C2	2.93	0.56
9:I:99:GLY:HA3	9:I:138:LEU:HD22	1.87	0.56
1:A:2898:U:O2'	1:A:2899:A:H5'	2.06	0.55
19:S:4:ILE:HG12	19:S:106:VAL:HG22	1.89	0.55
19:S:83:LYS:HD2	19:S:95:ARG:HE	1.71	0.55
6:F:111:ILE:HA	6:F:137:ILE:HD12	1.87	0.55
26:Z:37:GLU:O	26:Z:38:ARG:NH1	2.39	0.55
6:F:126:GLY:O	6:F:158:THR:OG1	2.23	0.55
13:M:25:ASP:N	13:M:25:ASP:OD1	2.38	0.55
6:F:104:ILE:HG23	6:F:105:THR:HG23	1.88	0.55
13:M:66:ARG:NH1	13:M:104:GLU:OE1	2.39	0.55
11:K:110:GLU:HA	11:K:113:MET:HG2	1.89	0.55
1:A:597:G:O2'	12:L:11:GLY:O	2.24	0.55
1:A:134:G:C6	1:A:135:U:N3	2.76	0.54
1:A:2314:A:OP1	6:F:88:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:G:O2'	1:A:2012:G:O6	2.21	0.54
35:A:3175:DI0:CBN	35:A:3175:DI0:CAR	2.86	0.54
1:A:370:G:O2'	1:A:424:G:OP1	2.20	0.54
1:A:894:U:HO2'	1:A:895:U:P	2.29	0.54
1:A:2032:G:N2	4:D:151:THR:OG1	2.40	0.54
5:E:157:LEU:HG	5:E:169:VAL:HG11	1.89	0.54
1:A:790:U:O2'	1:A:791:C:C6	2.61	0.54
5:E:118:LEU:HD11	5:E:188:MET:HG3	1.90	0.54
1:A:141:G:N3	1:A:141:G:H5"	2.23	0.54
13:M:110:GLU:OE2	13:M:114:ARG:NH2	2.41	0.54
1:A:668:A:H2'	1:A:670:A:H62	1.73	0.54
10:J:45:THR:HG22	17:Q:64:ARG:HH21	1.73	0.54
1:A:1494:A:O2'	1:A:1495:A:OP1	2.26	0.54
1:A:2646:C:OP2	1:A:2732:G:O2'	2.25	0.54
5:E:17:THR:O	5:E:21:ARG:NH2	2.41	0.53
2:B:40:U:N3	2:B:44:G:OP2	2.29	0.53
1:A:1050:A:C1'	1:A:2751:G:H22	2.18	0.53
1:A:2172:U:H4'	1:A:2173:A:H5'	1.90	0.53
1:A:1871:A:O2'	1:A:1872:A:O5'	2.27	0.53
3:C:5:LYS:NZ	3:C:14:ARG:O	2.40	0.53
21:U:81:ASP:OD2	21:U:96:PHE:HB3	2.09	0.53
1:A:882:G:C6	1:A:883:G:C8	2.97	0.53
1:A:894:U:C4	1:A:895:U:O4	2.62	0.53
22:V:45:ASP:OD1	22:V:45:ASP:N	2.42	0.53
1:A:1007:C:OP1	10:J:37:ARG:NH2	2.42	0.53
16:P:63:LYS:HE2	16:P:65:SER:HB2	1.91	0.53
22:V:11:GLU:N	22:V:11:GLU:OE1	2.42	0.53
1:A:1:G:O6	1:A:2902:C:C4	2.62	0.52
1:A:881:G:C2'	1:A:882:G:C8	2.92	0.52
1:A:142:A:H2'	1:A:143:C:C6	2.44	0.52
20:T:89:GLU:H	20:T:89:GLU:CD	2.13	0.52
1:A:136:G:O5'	1:A:136:G:H8	1.91	0.52
1:A:155:A:H2'	1:A:156:A:C8	2.45	0.52
1:A:1141:U:H4'	1:A:1142:A:O4'	2.10	0.52
1:A:1105:U:H2'	1:A:1106:G:H8	1.75	0.52
1:A:1796:U:H2'	1:A:1797:G:C8	2.45	0.52
1:A:2291:U:OP1	1:A:2380:C:O2'	2.26	0.52
1:A:2751:G:N3	1:A:2751:G:C2'	2.73	0.52
3:C:107:PRO:HD2	3:C:110:LEU:HD22	1.91	0.52
7:G:123:ALA:HB1	7:G:131:ILE:HD11	1.92	0.52
18:R:37:GLU:HG3	18:R:53:PHE:CE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2857:G:N2	1:A:2860:A:OP2	2.35	0.52
23:W:65:GLY:HA2	23:W:85:GLU:HG2	1.92	0.52
1:A:141:G:N3	1:A:141:G:C3'	2.73	0.52
1:A:2788:C:O2'	1:A:2809:A:N3	2.38	0.52
1:A:2469:A:H4'	13:M:55:ARG:CD	2.33	0.52
1:A:881:G:C3'	1:A:882:G:C8	2.93	0.52
1:A:882:G:H22	1:A:895:U:C2'	2.23	0.52
6:F:34:ILE:HG12	6:F:96:MET:HG3	1.90	0.52
1:A:894:U:O2'	1:A:895:U:P	2.68	0.51
1:A:143:C:H2'	1:A:144:A:C8	2.45	0.51
1:A:2406:A:OP2	1:A:2406:A:H2'	2.10	0.51
1:A:1049:C:C1'	1:A:1113:U:O2'	2.55	0.51
2:B:51:G:OP1	15:O:63:LYS:NZ	2.37	0.51
1:A:1007:C:OP2	36:A:3206:HOH:O	2.19	0.51
1:A:2757:A:N1	7:G:67:THR:HG21	2.26	0.51
1:A:894:U:C2	1:A:895:U:C6	2.98	0.51
1:A:463:G:N2	1:A:466:A:OP2	2.37	0.51
1:A:2315:G:H2'	1:A:2316:G:C8	2.44	0.51
6:F:108:VAL:CG1	6:F:109:PRO:CD	2.61	0.51
20:T:28:ASN:ND2	20:T:88:LYS:O	2.43	0.51
1:A:612:G:H2'	1:A:614:A:C8	2.45	0.51
2:B:66:A:H61	2:B:107:G:H2'	1.76	0.51
1:A:743:A:O2'	1:A:1659:G:OP1	2.28	0.51
1:A:1046:A:H4'	8:H:58:THR:HG21	1.91	0.51
1:A:1172:C:C5	1:A:1173:U:H1'	2.46	0.51
12:L:91:ASP:OD1	12:L:93:ASN:N	2.43	0.51
11:K:107:LEU:HB2	11:K:116:ILE:HD11	1.93	0.50
1:A:1059:G:H4'	9:I:117:MET:HE2	1.93	0.50
1:A:1796:U:H2'	1:A:1797:G:H8	1.76	0.50
4:D:3:GLY:HA3	4:D:204:LYS:HG2	1.93	0.50
1:A:534:U:O2'	17:Q:49:ASP:OD2	2.25	0.50
1:A:1715:G:O2'	1:A:1743:G:O6	2.20	0.50
1:A:2469:A:N6	1:A:2481:G:O2'	2.44	0.50
3:C:133:ARG:O	3:C:167:ARG:NH2	2.45	0.50
3:C:245:VAL:HG12	3:C:251:GLN:HA	1.94	0.50
1:A:611:C:N4	1:A:612:G:N1	2.59	0.50
1:A:1808:A:H3'	1:A:1809:A:C8	2.47	0.50
1:A:2052:A:H4'	4:D:148:GLN:O	2.11	0.50
4:D:77:ARG:NH2	4:D:200:ASP:OD1	2.45	0.50
1:A:278:A:OP2	1:A:361:G:N1	2.45	0.50
1:A:613:A:H4'	1:A:614:A:H5"	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:G:H1'	1:A:1111:A:H61	1.76	0.50
1:A:1506:U:H2'	1:A:1507:C:C6	2.46	0.50
1:A:611:C:C6	1:A:612:G:N7	2.79	0.50
1:A:2848:G:O2'	1:A:2867:G:N2	2.33	0.50
1:A:2899:A:H2'	1:A:2900:A:C8	2.46	0.50
1:A:1090:A:N1	1:A:1101:U:O2	2.45	0.50
1:A:1587:G:H2'	1:A:1588:G:H8	1.77	0.50
6:F:73:SER:OG	6:F:81:GLN:N	2.39	0.50
1:A:2591:C:H2'	1:A:2592:G:C8	2.48	0.49
1:A:2898:U:C2	1:A:2899:A:N7	2.80	0.49
6:F:121:SER:OG	6:F:129:SER:O	2.29	0.49
1:A:784:G:H5'	1:A:785:G:OP1	2.12	0.49
16:P:49:ALA:HB3	16:P:60:THR:HG23	1.92	0.49
1:A:355:U:H2'	1:A:356:G:C8	2.47	0.49
22:V:9:ARG:HG2	22:V:41:GLU:HG3	1.94	0.49
3:C:72:ASP:OD2	3:C:189:ARG:NH1	2.33	0.49
1:A:136:G:C6	1:A:137:U:C4	3.01	0.49
1:A:191:A:H2'	1:A:192:C:C6	2.47	0.49
1:A:729:G:C6	3:C:207:LYS:HB2	2.47	0.49
1:A:1172:C:C6	1:A:1173:U:H1'	2.48	0.49
15:O:15:ARG:NH2	15:O:95:SER:HB2	2.27	0.49
1:A:1590:A:H2'	1:A:1591:A:C8	2.48	0.49
6:F:44:ILE:HG21	6:F:79:ILE:HG22	1.94	0.49
1:A:1794:A:H2'	1:A:1795:C:C6	2.48	0.49
1:A:2313:C:H5"	6:F:88:LYS:HD3	1.95	0.49
6:F:129:SER:HA	6:F:155:THR:HA	1.94	0.49
1:A:1170:C:H2'	1:A:1171:G:O4'	2.13	0.49
11:K:40:LYS:HE3	11:K:57:VAL:HG12	1.94	0.49
1:A:1046:A:C8	8:H:62:ARG:NH2	2.81	0.49
1:A:134:G:H2'	1:A:135:U:O4'	2.13	0.48
1:A:144:A:H2'	1:A:145:C:H6	1.77	0.48
1:A:141:G:N3	1:A:141:G:C5'	2.76	0.48
1:A:1870:C:O2'	1:A:1871:A:N3	2.36	0.48
1:A:1916:A:O5'	1:A:1916:A:H8	1.96	0.48
3:C:232:HIS:HA	3:C:242:LYS:HD2	1.95	0.48
6:F:4:LEU:HD13	6:F:97:TRP:HE3	1.79	0.48
6:F:108:VAL:N	6:F:109:PRO:CD	2.77	0.48
12:L:132:ARG:HG3	12:L:142:ILE:HD12	1.94	0.48
1:A:612:G:O5'	1:A:612:G:H8	1.96	0.48
1:A:896:A:C8	1:A:896:A:H3'	2.48	0.48
1:A:1590:A:H2'	1:A:1591:A:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:ALA:O	3:C:128:ASN:ND2	2.41	0.48
10:J:125:TYR:OH	10:J:132:HIS:NE2	2.45	0.48
22:V:72:VAL:HG12	22:V:93:ARG:HA	1.95	0.48
1:A:2000:C:OP1	14:N:5:LYS:NZ	2.35	0.48
1:A:1083:U:H4'	8:H:42:ARG:NH1	2.28	0.48
9:I:21:SER:HB3	9:I:22:PRO:HD3	1.96	0.48
1:A:1113:U:H2'	1:A:1114:C:C6	2.48	0.48
1:A:2514:U:H2'	1:A:2515:C:C6	2.48	0.48
6:F:136:ILE:HD11	6:F:146:VAL:HG21	1.95	0.48
7:G:101:ASN:ND2	7:G:116:GLN:OE1	2.47	0.48
1:A:1050:A:C5	1:A:2751:G:N1	2.82	0.48
6:F:79:ILE:HD12	6:F:79:ILE:O	2.14	0.48
1:A:546:U:O2'	1:A:548:G:OP2	2.27	0.47
1:A:1177:G:H2'	1:A:1178:C:C6	2.49	0.47
1:A:2243:U:H2'	1:A:2244:U:C6	2.49	0.47
24:X:6:GLN:O	24:X:74:ARG:NH1	2.47	0.47
1:A:630:G:N2	1:A:633:A:OP2	2.33	0.47
5:E:119:ILE:HB	5:E:187:VAL:HG22	1.97	0.47
6:F:108:VAL:N	6:F:109:PRO:HD2	2.29	0.47
22:V:2:PHE:HB2	22:V:61:LEU:HD22	1.95	0.47
23:W:26:PHE:N	23:W:29:GLU:OE1	2.36	0.47
1:A:1651:G:OP1	14:N:40:LYS:NZ	2.41	0.47
1:A:2162:G:H5"	1:A:2171:A:H2'	1.95	0.47
1:A:2751:G:H4'	7:G:4:VAL:CG2	2.45	0.47
9:I:22:PRO:HB2	9:I:23:PRO:HD3	1.96	0.47
1:A:2251:OMG:HM23	1:A:2251:OMG:H1'	1.70	0.47
20:T:33:LYS:HG2	20:T:80:TRP:CZ3	2.49	0.47
1:A:1113:U:H2'	1:A:1114:C:H6	1.80	0.47
5:E:171:ASP:OD1	5:E:172:ALA:N	2.45	0.47
1:A:307:G:N1	1:A:310:A:OP2	2.45	0.47
1:A:340:A:O2'	5:E:162:ARG:NH1	2.47	0.47
1:A:476:G:N1	1:A:479:A:OP2	2.48	0.47
1:A:611:C:C5	1:A:612:G:N7	2.82	0.47
1:A:896:A:H3'	1:A:896:A:H8	1.80	0.47
1:A:1105:U:H2'	1:A:1106:G:C8	2.49	0.47
1:A:2576:G:O2'	1:A:2579:C:OP2	2.25	0.47
3:C:163:GLN:OE1	3:C:175:ARG:NH1	2.40	0.47
4:D:129:THR:HG22	4:D:130:GLN:O	2.15	0.47
6:F:68:THR:N	6:F:86:GLY:O	2.37	0.47
6:F:103:LEU:O	6:F:107:ALA:HB3	2.14	0.47
9:I:20:PRO:HB2	9:I:23:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:100:LYS:O	9:I:100:LYS:HG3	2.15	0.47
9:I:113:LYS:O	9:I:117:MET:HG2	2.15	0.47
12:L:123:ARG:NE	12:L:143:GLU:OE2	2.46	0.47
24:X:3:ARG:O	24:X:12:PRO:HD3	2.15	0.47
1:A:400:G:N7	24:X:57:ARG:NH1	2.54	0.47
1:A:881:G:C3'	1:A:882:G:H8	2.26	0.47
1:A:1915:3TD:H6	1:A:1915:3TD:O5'	2.15	0.47
1:A:2099:U:O2'	1:A:2100:G:H5'	2.14	0.47
1:A:2532:G:N2	1:A:2663:G:O2'	2.48	0.47
1:A:881:G:C5	1:A:882:G:C6	3.02	0.47
1:A:2377:A:H2'	1:A:2378:A:C8	2.50	0.47
7:G:68:ALA:O	7:G:72:LEU:HD12	2.15	0.47
7:G:164:TYR:HB2	7:G:167:GLU:HG2	1.97	0.47
9:I:19:ASN:N	9:I:20:PRO:HD2	2.29	0.47
1:A:2305:U:H5"	6:F:131:GLY:HA3	1.97	0.47
9:I:12:GLN:HA	9:I:56:PRO:HA	1.96	0.46
1:A:2720:U:OP1	16:P:53:ARG:NH2	2.48	0.46
8:H:29:ASP:OD1	8:H:30:SER:N	2.48	0.46
1:A:281:C:H2'	1:A:282:A:C8	2.49	0.46
15:O:52:SER:OG	15:O:54:VAL:HG22	2.15	0.46
15:O:64:TYR:HB3	15:O:67:ASN:ND2	2.31	0.46
1:A:593:U:H2'	1:A:594:U:C6	2.51	0.46
1:A:1870:C:O2'	1:A:1871:A:O5'	2.34	0.46
1:A:882:G:C5	1:A:883:G:C8	3.03	0.46
4:D:181:ASP:HB3	4:D:186:LEU:HB2	1.98	0.46
6:F:166:GLY:O	6:F:170:LEU:HD12	2.15	0.46
8:H:54:VAL:HG22	8:H:81:LEU:HD13	1.96	0.46
10:J:58:ASN:HD21	10:J:128:ASN:ND2	2.13	0.46
22:V:65:VAL:HG22	22:V:66:ASP:OD1	2.15	0.46
1:A:287:G:H2'	1:A:288:U:C6	2.51	0.46
1:A:350:G:H2'	1:A:351:C:O4'	2.15	0.46
1:A:479:A:N3	1:A:481:G:H5"	2.30	0.46
1:A:577:G:O2'	1:A:1254:A:OP1	2.33	0.46
1:A:811:U:H2'	12:L:21:ARG:HA	1.98	0.46
1:A:1405:U:H2'	1:A:1406:U:C6	2.50	0.46
1:A:2314:A:H2'	1:A:2315:G:H8	1.81	0.46
7:G:2:SER:O	7:G:6:LYS:N	2.44	0.46
15:O:95:SER:O	15:O:95:SER:OG	2.26	0.46
1:A:144:A:O2'	1:A:145:C:H5'	2.14	0.46
1:A:1041:G:N1	1:A:1115:G:N1	2.63	0.46
1:A:1736:U:H2'	1:A:1737:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2097:A:C2'	1:A:2098:U:H5'	2.45	0.46
8:H:85:VAL:HG22	8:H:92:ALA:HB2	1.98	0.46
9:I:99:GLY:HA3	9:I:138:LEU:CD2	2.46	0.46
1:A:1183:U:H2'	1:A:1184:U:C6	2.51	0.46
1:A:1219:U:H2'	1:A:1220:G:C8	2.51	0.46
8:H:16:SER:HG	8:H:63:ALA:HB1	1.81	0.46
9:I:35:ILE:CG2	9:I:36:MET:N	2.79	0.46
1:A:1028:A:N3	1:A:2486:C:O2'	2.43	0.46
1:A:1874:C:H2'	1:A:1875:G:O4'	2.16	0.46
1:A:2291:U:H2'	1:A:2292:U:C6	2.51	0.46
6:F:104:ILE:C	6:F:108:VAL:HG12	2.36	0.46
6:F:150:ARG:NH1	6:F:150:ARG:CG	2.74	0.46
1:A:851:C:H2'	1:A:852:U:C6	2.51	0.46
1:A:964:C:O2'	1:A:2273:A:N3	2.42	0.46
3:C:252:THR:OG1	3:C:253:LYS:N	2.49	0.46
23:W:33:ALA:N	23:W:64:ASP:OD1	2.48	0.46
1:A:286:U:H2'	1:A:287:G:C8	2.51	0.45
1:A:1563:U:H2'	1:A:1564:C:C6	2.51	0.45
8:H:82:ILE:HD12	8:H:84:TYR:CE2	2.51	0.45
9:I:86:ILE:HD13	9:I:138:LEU:HD21	1.97	0.45
11:K:10:VAL:HG12	11:K:12:ASP:H	1.80	0.45
15:O:15:ARG:HH21	15:O:95:SER:HB2	1.81	0.45
1:A:2298:A:H2'	1:A:2299:U:O4'	2.16	0.45
1:A:896:A:C8	1:A:896:A:C3'	2.99	0.45
1:A:2799:A:O2'	1:A:2800:A:H5"	2.16	0.45
6:F:136:ILE:HD13	6:F:143:TYR:CD1	2.47	0.45
7:G:86:LYS:HG2	7:G:132:VAL:HG22	1.98	0.45
1:A:281:C:H2'	1:A:282:A:H8	1.81	0.45
1:A:570:G:H2'	1:A:2030:6MZ:N7	2.31	0.45
4:D:1:MET:HB3	4:D:205:PRO:HG2	1.99	0.45
1:A:930:G:H1'	26:Z:25:LEU:HD21	1.99	0.45
1:A:1009:A:N3	1:A:1153:C:O2'	2.48	0.45
6:F:40:VAL:HG11	6:F:43:ALA:HB2	1.99	0.45
19:S:83:LYS:HD2	19:S:95:ARG:HH11	1.81	0.45
1:A:280:U:H2'	1:A:281:C:C6	2.52	0.45
1:A:548:G:H5"	1:A:549:G:H5'	1.98	0.45
1:A:1607:C:N4	1:A:1621:U:OP2	2.50	0.45
21:U:89:ASP:OD1	21:U:89:ASP:N	2.49	0.45
1:A:1050:A:C2	1:A:2751:G:C5	3.04	0.45
6:F:43:ALA:HA	6:F:49:LEU:HD11	1.99	0.45
1:A:172:A:H2'	1:A:173:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:U:H2'	1:A:640:C:C6	2.52	0.45
1:A:2098:U:C2'	1:A:2099:U:H5'	2.47	0.45
1:A:2304:G:H22	1:A:2312:U:H3	1.65	0.45
9:I:18:ALA:C	9:I:20:PRO:HD2	2.37	0.45
15:O:88:LYS:HB2	15:O:88:LYS:HE2	1.71	0.45
1:A:1182:G:H2'	1:A:1183:U:O4'	2.17	0.45
1:A:2233:U:H2'	1:A:2234:G:C8	2.52	0.45
3:C:16:VAL:HG22	3:C:206:GLY:HA3	1.99	0.45
20:T:18:GLU:O	20:T:22:THR:HG22	2.17	0.45
1:A:1916:A:O5'	1:A:1916:A:C8	2.70	0.45
1:A:2788:C:H2'	1:A:2789:C:C6	2.52	0.45
19:S:84:ARG:O	19:S:96:ILE:N	2.44	0.45
1:A:1494:A:H2'	1:A:1495:A:C8	2.52	0.44
1:A:1868:C:H2'	1:A:1869:G:O4'	2.16	0.44
1:A:2537:U:H2'	1:A:2538:C:C6	2.52	0.44
1:A:2793:C:H2'	1:A:2794:C:C6	2.52	0.44
1:A:286:U:H2'	1:A:287:G:H8	1.82	0.44
1:A:568:U:O4	18:R:81:LYS:NZ	2.48	0.44
1:A:2193:G:H2'	1:A:2194:U:C6	2.51	0.44
1:A:2328:A:H2'	1:A:2329:U:C6	2.52	0.44
2:B:48:U:H4'	15:O:100:HIS:HD2	1.82	0.44
3:C:37:ASN:HB2	3:C:62:TYR:HB2	1.99	0.44
6:F:36:LEU:HD22	6:F:154:ILE:HG12	1.99	0.44
15:O:59:ALA:HA	15:O:62:LEU:HD12	1.98	0.44
1:A:883:G:C4	1:A:895:U:O2	2.70	0.44
1:A:1028:A:N6	1:A:1125:G:H2'	2.33	0.44
1:A:1050:A:C2	1:A:2751:G:N1	2.85	0.44
3:C:28:LYS:HA	3:C:28:LYS:HD2	1.82	0.44
7:G:28:GLY:HA3	7:G:79:VAL:HB	2.00	0.44
8:H:50:VAL:HG22	8:H:85:VAL:HG13	1.98	0.44
15:O:33:ARG:O	15:O:65:THR:HG23	2.18	0.44
1:A:351:C:H2'	1:A:352:A:O4'	2.17	0.44
1:A:543:G:H2'	1:A:544:C:O4'	2.18	0.44
6:F:103:LEU:C	6:F:107:ALA:H	2.20	0.44
16:P:60:THR:HB	16:P:73:VAL:HG22	1.98	0.44
1:A:134:G:C2	1:A:135:U:C2	3.05	0.44
1:A:137:U:O2	1:A:137:U:H2'	2.18	0.44
1:A:2822:G:O6	14:N:2:ARG:NH1	2.50	0.44
8:H:119:PRO:HG2	8:H:122:GLN:HB2	1.98	0.44
1:A:411:G:OP2	1:A:2406:A:O2'	2.30	0.44
1:A:1746:A:H2'	1:A:1747:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:ARG:HG3	6:F:30:ARG:HH11	1.83	0.44
20:T:69:ARG:O	20:T:69:ARG:HG2	2.18	0.44
1:A:2161:C:H4'	1:A:2173:A:P	2.58	0.44
1:A:2845:U:H5"	16:P:52:ASN:O	2.18	0.44
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.99	0.44
14:N:30:ARG:NH2	14:N:74:GLU:OE1	2.40	0.44
15:O:2:ASP:OD1	15:O:2:ASP:N	2.51	0.44
1:A:796:C:H2'	1:A:797:G:C8	2.53	0.44
1:A:871:U:H2'	1:A:872:U:C6	2.53	0.44
9:I:80:LEU:CD2	9:I:101:ILE:HD13	2.48	0.44
18:R:34:GLU:OE1	18:R:60:LYS:HG2	2.17	0.44
16:P:34:GLU:N	16:P:34:GLU:OE1	2.50	0.43
1:A:1181:U:H2'	1:A:1182:G:C8	2.54	0.43
3:C:161:TYR:HB3	3:C:194:GLU:HB2	1.98	0.43
9:I:20:PRO:HB2	9:I:23:PRO:CG	2.47	0.43
14:N:96:ARG:HD3	14:N:98:LEU:HD21	2.00	0.43
1:A:898:C:H2'	1:A:899:A:O4'	2.18	0.43
1:A:1847:A:O2'	1:A:1848:A:H8	1.79	0.43
1:A:2595:G:N2	1:A:2598:A:OP2	2.40	0.43
4:D:39:ASP:N	4:D:39:ASP:OD1	2.51	0.43
12:L:90:VAL:HG22	12:L:122:VAL:HA	1.99	0.43
21:U:96:PHE:CE2	21:U:103:ILE:HG12	2.53	0.43
1:A:672:C:OP2	12:L:42:SER:OG	2.29	0.43
1:A:1536:C:H4'	1:A:1537:G:C4	2.54	0.43
1:A:2688:G:N1	1:A:2720:U:OP2	2.32	0.43
1:A:2329:U:H2'	1:A:2330:G:C8	2.53	0.43
2:B:24:G:N7	2:B:56:G:H2'	2.33	0.43
16:P:88:ARG:HH21	16:P:112:GLU:HB2	1.82	0.43
1:A:1939:5MU:OP1	1:A:2604:PSU:O2'	2.37	0.43
4:D:97:SER:OG	4:D:98:VAL:N	2.51	0.43
9:I:18:ALA:O	9:I:19:ASN:CB	2.67	0.43
1:A:813:U:H2'	1:A:814:C:C6	2.54	0.43
6:F:104:ILE:HD11	6:F:176:PRO:HD3	2.00	0.43
7:G:155:GLU:OE1	7:G:159:GLY:N	2.52	0.43
11:K:71:ARG:HD3	11:K:71:ARG:HA	1.85	0.43
1:A:136:G:O5'	1:A:136:G:C8	2.70	0.43
1:A:143:C:O5'	1:A:143:C:C6	2.70	0.43
1:A:586:A:N1	1:A:809:G:O2'	2.46	0.43
1:A:1050:A:C6	1:A:2751:G:C6	3.06	0.43
1:A:2188:U:H2'	1:A:2189:U:O4'	2.19	0.43
1:A:2273:A:H2'	1:A:2274:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:35:THR:HA	6:F:90:THR:HA	2.01	0.43
11:K:24:VAL:HG13	11:K:33:ALA:HB2	2.01	0.43
19:S:11:ARG:HD2	19:S:100:THR:HG22	2.00	0.43
1:A:134:G:O6	1:A:135:U:O4	2.36	0.43
1:A:1676:A:N7	36:A:3236:HOH:O	2.37	0.43
1:A:2339:C:H2'	1:A:2340:A:C8	2.53	0.43
2:B:1:U:H2'	2:B:2:G:H8	1.83	0.43
2:B:48:U:H4'	15:O:100:HIS:CD2	2.54	0.43
6:F:54:ALA:HB1	6:F:65:PRO:HG2	2.01	0.43
15:O:108:ASP:HA	15:O:111:ARG:HB2	2.00	0.43
2:B:42:C:N3	6:F:90:THR:HG22	2.33	0.43
9:I:56:PRO:HG2	9:I:72:LYS:HB2	2.01	0.43
15:O:115:LEU:HD12	15:O:115:LEU:HA	1.85	0.43
25:Y:42:LEU:O	25:Y:46:VAL:HG12	2.19	0.43
1:A:278:A:N1	1:A:361:G:O2'	2.49	0.42
1:A:594:U:H2'	1:A:595:C:C6	2.54	0.42
1:A:1040:A:N1	1:A:1115:G:N2	2.66	0.42
1:A:1199:U:H1'	17:Q:4:VAL:HG22	2.01	0.42
1:A:1441:G:H2'	1:A:1442:U:C6	2.54	0.42
6:F:150:ARG:H	6:F:150:ARG:HG3	1.46	0.42
7:G:105:LEU:HB2	7:G:113:VAL:HG13	2.01	0.42
1:A:57:C:H2'	1:A:58:G:O4'	2.19	0.42
1:A:708:G:N2	1:A:724:U:H1'	2.34	0.42
1:A:1041:G:C2	1:A:1115:G:N1	2.87	0.42
1:A:2314:A:H2'	1:A:2315:G:C8	2.53	0.42
1:A:2808:G:O2'	1:A:2890:G:O6	2.29	0.42
9:I:20:PRO:HB2	9:I:23:PRO:HG2	2.01	0.42
9:I:86:ILE:CD1	9:I:138:LEU:HD21	2.49	0.42
9:I:114:ALA:CB	9:I:125:MET:SD	3.07	0.42
1:A:544:C:H2'	1:A:545:U:O4'	2.19	0.42
1:A:1420:A:C5	1:A:2211:A:C6	3.07	0.42
1:A:1915:3TD:H2'	1:A:1916:A:H8	1.84	0.42
1:A:2333:A:P	23:W:77:ARG:HH22	2.42	0.42
1:A:2389:G:H5"	1:A:2390:U:O4'	2.19	0.42
7:G:153:ARG:HB2	7:G:153:ARG:CZ	2.49	0.42
21:U:14:LEU:HD11	21:U:71:ALA:HB2	2.01	0.42
24:X:65:ASP:OD1	24:X:66:THR:N	2.53	0.42
1:A:207:A:H2'	1:A:208:C:O4'	2.18	0.42
1:A:1172:C:H3'	1:A:1173:U:C4'	2.49	0.42
1:A:2728:U:O2'	1:A:2729:G:H8	2.03	0.42
6:F:38:MET:HE2	6:F:87:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:GLU:O	8:H:65:GLU:HG3	2.20	0.42
21:U:47:LYS:HE2	21:U:47:LYS:HB3	1.88	0.42
1:A:2698:U:H2'	1:A:2699:C:C6	2.54	0.42
2:B:48:U:H2'	2:B:49:C:C6	2.54	0.42
6:F:175:PHE:HB3	6:F:177:PHE:CE1	2.55	0.42
1:A:483:A:O2'	21:U:57:GLY:N	2.49	0.42
1:A:721:A:H2'	1:A:722:A:C8	2.55	0.42
1:A:1915:3TD:H2'	1:A:1916:A:C8	2.55	0.42
7:G:72:LEU:HA	7:G:75:MET:HB2	2.01	0.42
12:L:77:ILE:HD13	12:L:108:ALA:HB1	2.02	0.42
23:W:17:GLU:O	23:W:19:LYS:NZ	2.52	0.42
1:A:139:U:C5	20:T:1:MET:SD	3.13	0.42
1:A:612:G:H1'	1:A:616:A:H61	1.84	0.42
6:F:121:SER:OG	6:F:121:SER:O	2.35	0.42
7:G:155:GLU:H	7:G:155:GLU:HG3	1.68	0.42
1:A:2481:G:HO2'	1:A:2482:A:H8	1.65	0.42
7:G:38:ASN:HD22	7:G:64:GLN:CD	2.23	0.42
22:V:46:LYS:HE3	22:V:46:LYS:HB2	1.79	0.42
1:A:225:C:H2'	1:A:226:A:O4'	2.20	0.42
1:A:1930:G:O2'	1:A:1968:G:O6	2.33	0.42
6:F:56:ASP:O	6:F:60:ILE:HG12	2.20	0.42
7:G:50:LEU:HA	7:G:50:LEU:HD23	1.87	0.42
10:J:117:ALA:HA	10:J:120:ARG:HH21	1.85	0.42
22:V:63:ILE:HD12	22:V:72:VAL:HG21	2.01	0.42
7:G:54:PRO:HG3	7:G:62:TRP:CE2	2.54	0.41
8:H:38:MET:O	8:H:41:LEU:N	2.53	0.41
18:R:58:VAL:HB	18:R:102:SER:OG	2.19	0.41
1:A:714:U:H1'	1:A:717:C:H5	1.86	0.41
1:A:1047:G:H1'	1:A:1111:A:N6	2.35	0.41
1:A:2375:G:N2	1:A:2378:A:OP2	2.47	0.41
7:G:10:VAL:HA	7:G:49:THR:HA	2.02	0.41
1:A:364:C:H2'	1:A:365:U:C6	2.56	0.41
1:A:2162:G:OP1	1:A:2171:A:H2'	2.20	0.41
8:H:51:TYR:OH	8:H:53:ARG:NH1	2.53	0.41
11:K:38:ILE:HD11	11:K:112:PHE:HZ	1.85	0.41
1:A:358:U:H2'	1:A:359:G:C8	2.55	0.41
1:A:1084:A:C6	1:A:1085:A:C6	3.08	0.41
1:A:1385:A:O2'	1:A:1396:U:O2	2.39	0.41
1:A:1475:G:O2'	1:A:1514:G:O6	2.34	0.41
1:A:2129:C:N4	1:A:2130:U:O4	2.54	0.41
6:F:8:TYR:HA	6:F:12:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:175:PHE:HB3	6:F:177:PHE:HE1	1.85	0.41
8:H:52:MET:HE1	8:H:96:PHE:HZ	1.85	0.41
10:J:31:GLU:OE2	10:J:35:ARG:NE	2.51	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.56	0.41
1:A:984:A:N3	1:A:984:A:H2'	2.35	0.41
1:A:1042:G:N2	1:A:1114:C:H1'	2.35	0.41
6:F:80:ARG:HB2	6:F:83:TYR:CE2	2.55	0.41
13:M:50:ARG:O	13:M:53:MET:HG2	2.20	0.41
1:A:1174:U:H5'	1:A:1175:A:OP2	2.20	0.41
1:A:1278:C:H2'	1:A:1279:G:C8	2.56	0.41
1:A:1482:G:H1'	1:A:1509:A:N6	2.32	0.41
1:A:2321:U:H5'	1:A:2322:A:OP2	2.21	0.41
15:O:43:ASN:OD1	15:O:45:SER:OG	2.29	0.41
15:O:60:GLU:H	15:O:60:GLU:HG2	1.72	0.41
1:A:287:G:H2'	1:A:288:U:H6	1.85	0.41
6:F:67:ILE:HD13	6:F:87:CYS:HB3	2.02	0.41
6:F:94:GLU:HA	6:F:97:TRP:HD1	1.85	0.41
10:J:110:PRO:O	10:J:115:GLY:HA3	2.21	0.41
1:A:278:A:N6	1:A:362:A:N7	2.69	0.41
1:A:322:A:OP2	5:E:163:ASN:HB2	2.21	0.41
1:A:1223:G:C6	1:A:1227:G:C6	3.08	0.41
1:A:1799:G:O2'	3:C:180:GLU:OE2	2.24	0.41
1:A:2114:A:OP2	1:A:2115:G:C6	2.73	0.41
7:G:18:LYS:NZ	7:G:20:ASN:HB2	2.36	0.41
1:A:882:G:C2	1:A:883:G:C8	3.08	0.41
1:A:1050:A:N1	1:A:2751:G:C6	2.88	0.41
1:A:1278:C:H2'	1:A:1279:G:H8	1.86	0.41
1:A:1932:A:H2'	1:A:1933:G:O4'	2.21	0.41
2:B:78:A:H2'	2:B:79:G:O4'	2.21	0.41
2:B:118:C:H2'	2:B:119:A:C8	2.56	0.41
3:C:155:ALA:HB2	3:C:162:VAL:HG23	2.03	0.41
5:E:2:GLU:HB3	5:E:11:ALA:HB1	2.03	0.41
5:E:6:LYS:HE2	5:E:6:LYS:HA	2.02	0.41
6:F:32:GLU:OE2	6:F:32:GLU:N	2.53	0.41
6:F:42:GLU:H	6:F:42:GLU:HG3	1.72	0.41
6:F:103:LEU:HA	6:F:107:ALA:H	1.85	0.41
7:G:117:LEU:HD13	7:G:117:LEU:HA	1.88	0.41
8:H:103:ASN:C	8:H:105:LYS:H	2.24	0.41
20:T:33:LYS:HE2	20:T:80:TRP:CE3	2.56	0.41
1:A:458:G:O2'	1:A:469:G:O6	2.32	0.41
1:A:634:C:H2'	1:A:635:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:G:C2	1:A:881:G:H1'	2.56	0.41
1:A:979:A:H2'	1:A:982:C:H42	1.85	0.41
1:A:1049:C:HO2'	1:A:1114:C:P	2.43	0.41
1:A:1394:U:H4'	1:A:1603:A:H4'	2.03	0.41
1:A:2484:G:OP1	13:M:44:ARG:NH2	2.49	0.41
6:F:103:LEU:O	6:F:108:VAL:N	2.54	0.41
12:L:77:ILE:CD1	12:L:108:ALA:HB1	2.51	0.41
20:T:26:LYS:HE2	20:T:26:LYS:HA	2.02	0.41
1:A:861:A:H2'	1:A:862:G:O4'	2.20	0.40
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.40
1:A:1871:A:H1'	1:A:1872:A:H5'	2.02	0.40
1:A:1881:C:H2'	1:A:1882:U:O4'	2.21	0.40
1:A:2116:G:C6	1:A:2171:A:N6	2.84	0.40
4:D:99:GLU:H	4:D:99:GLU:HG3	1.74	0.40
4:D:157:LYS:HE3	4:D:157:LYS:HB2	1.85	0.40
11:K:63:VAL:HG12	11:K:107:LEU:HD11	2.03	0.40
1:A:493:G:H2'	1:A:494:G:O4'	2.21	0.40
1:A:1370:C:H2'	1:A:1371:G:O4'	2.22	0.40
1:A:1430:G:H2'	1:A:1431:A:O4'	2.21	0.40
1:A:1450:G:C6	1:A:1451:C:N4	2.89	0.40
4:D:186:LEU:HD13	16:P:8:LEU:HD11	2.04	0.40
9:I:90:SER:HB2	9:I:98:VAL:CG2	2.51	0.40
10:J:58:ASN:HD21	10:J:128:ASN:HD22	1.69	0.40
1:A:1414:C:H2'	1:A:1415:U:O4'	2.21	0.40
6:F:10:ASP:OD1	6:F:11:GLU:N	2.54	0.40
1:A:1:G:H2'	1:A:2:G:H8	1.85	0.40
1:A:882:G:C6	1:A:883:G:C5	3.10	0.40
7:G:48:ASN:O	7:G:48:ASN:ND2	2.54	0.40
15:O:89:ASP:OD1	15:O:89:ASP:N	2.54	0.40
1:A:645:C:H2'	1:A:647:G:C8	2.57	0.40
1:A:1132:U:H3'	1:A:1133:A:H5"	2.04	0.40
7:G:121:ILE:N	7:G:121:ILE:HD12	2.35	0.40
21:U:4:LYS:O	21:U:94:ARG:NH2	2.50	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	C	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
4	D	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29	26
5	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
6	F	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	25	21
7	G	174/176 (99%)	168 (97%)	5 (3%)	1 (1%)	25	21
8	H	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	2	0
9	I	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	4	1
10	J	140/142 (99%)	140 (100%)	0	0	100	100
11	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
12	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
13	M	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
14	N	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
15	O	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
16	P	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
17	Q	115/117 (98%)	115 (100%)	0	0	100	100
18	R	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	11
19	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
21	U	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
24	X	75/77 (97%)	75 (100%)	0	0	100	100
25	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Z	56/58 (97%)	56 (100%)	0	0	100	100
27	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	49/51 (96%)	49 (100%)	0	0	100	100
29	c	44/46 (96%)	44 (100%)	0	0	100	100
30	d	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	e	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3291/3351 (98%)	3184 (97%)	93 (3%)	14 (0%)	38	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	104	ALA
8	H	106	PHE
9	I	15	ALA
9	I	19	ASN
18	R	52	PRO
4	D	149	ASN
8	H	67	THR
8	H	108	VAL
9	I	25	GLY
8	H	124	ASP
9	I	23	PRO
8	H	130	PRO
7	G	47	ASP
6	F	110	ARG

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	C	216/216 (100%)	213 (99%)	3 (1%)	67	73
4	D	163/163 (100%)	160 (98%)	3 (2%)	59	65
5	E	165/165 (100%)	158 (96%)	7 (4%)	30	30
6	F	148/148 (100%)	127 (86%)	21 (14%)	3	1
7	G	137/137 (100%)	125 (91%)	12 (9%)	10	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	103/103 (100%)	97 (94%)	6 (6%)	20	17
9	I	104/104 (100%)	102 (98%)	2 (2%)	57	63
10	J	116/116 (100%)	112 (97%)	4 (3%)	37	39
11	K	104/104 (100%)	102 (98%)	2 (2%)	57	63
12	L	103/103 (100%)	101 (98%)	2 (2%)	57	63
13	M	108/108 (100%)	104 (96%)	4 (4%)	34	35
14	N	102/102 (100%)	101 (99%)	1 (1%)	76	82
15	O	87/87 (100%)	85 (98%)	2 (2%)	50	55
16	P	99/99 (100%)	93 (94%)	6 (6%)	18	16
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	82 (98%)	2 (2%)	49	53
19	S	93/93 (100%)	91 (98%)	2 (2%)	52	57
20	T	80/80 (100%)	77 (96%)	3 (4%)	33	34
21	U	83/83 (100%)	79 (95%)	4 (5%)	25	24
22	V	78/78 (100%)	76 (97%)	2 (3%)	46	50
23	W	57/58 (98%)	56 (98%)	1 (2%)	59	65
24	X	67/67 (100%)	65 (97%)	2 (3%)	41	44
25	Y	54/54 (100%)	52 (96%)	2 (4%)	34	35
26	Z	48/48 (100%)	46 (96%)	2 (4%)	30	30
27	a	47/47 (100%)	46 (98%)	1 (2%)	53	59
28	b	45/46 (98%)	44 (98%)	1 (2%)	52	57
29	c	38/38 (100%)	36 (95%)	2 (5%)	22	20
30	d	51/51 (100%)	47 (92%)	4 (8%)	12	9
31	e	34/34 (100%)	33 (97%)	1 (3%)	42	46
All	All	2703/2705 (100%)	2599 (96%)	104 (4%)	36	34

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	10	SER
3	C	38	SER
3	C	133	ARG
4	D	43	ASP
4	D	95	SER

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Mol	Chain	Res	Type
4	D	97	SER
5	E	7	ASP
5	E	15	SER
5	E	21	ARG
5	E	61	ARG
5	E	75	SER
5	E	122	GLU
5	E	155	GLU
6	F	4	LEU
6	F	14	LYS
6	F	19	GLU
6	F	24	SER
6	F	33	LYS
6	F	35	THR
6	F	42	GLU
6	F	47	LYS
6	F	51	ASP
6	F	80	ARG
6	F	98	GLU
6	F	108	VAL
6	F	110	ARG
6	F	111	ILE
6	F	130	MET
6	F	141	ILE
6	F	150	ARG
6	F	155	THR
6	F	162	SER
6	F	175	PHE
6	F	178	ARG
7	G	2	SER
7	G	32	GLU
7	G	34	THR
7	G	42	GLU
7	G	84	THR
7	G	99	LYS
7	G	127	THR
7	G	130	GLU
7	G	131	ILE
7	G	167	GLU
7	G	173	GLU
7	G	176	LYS
8	H	16	SER

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Mol	Chain	Res	Type
8	H	64	VAL
8	H	67	THR
8	H	71	CYS
8	H	105	LYS
8	H	133	GLU
9	I	59	ILE
9	I	98	VAL
10	J	5	THR
10	J	12	LYS
10	J	90	GLU
10	J	142	ILE
11	K	91	SER
11	K	109	SER
12	L	84	LYS
12	L	118	THR
13	M	53	MET
13	M	55	ARG
13	M	58	LYS
13	M	59	ARG
14	N	2	ARG
15	O	24	THR
15	O	95	SER
16	P	6	LYS
16	P	36	SER
16	P	60	THR
16	P	76	THR
16	P	83	SER
16	P	104	THR
18	R	37	GLU
18	R	71	LYS
19	S	70	LYS
19	S	95	ARG
20	T	1	MET
20	T	49	LYS
20	T	93	LEU
21	U	27	ASN
21	U	68	SER
21	U	86	ARG
21	U	89	ASP
22	V	34	LYS
22	V	59	GLU
23	W	11	ARG

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Mol	Chain	Res	Type
24	X	42	SER
24	X	48	THR
25	Y	34	SER
25	Y	49	ASP
26	Z	12	SER
26	Z	37	GLU
27	a	11	SER
28	b	17	THR
29	c	8	SER
29	c	25	LYS
30	d	15	LYS
30	d	31	HIS
30	d	33	LEU
30	d	52	LYS
31	e	20	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	134	ASN
5	E	9	GLN
5	E	90	GLN
7	G	104	ASN
7	G	111	HIS
7	G	115	HIS
10	J	128	ASN
13	M	3	GLN
15	O	100	HIS
16	P	41	GLN
16	P	66	ASN
17	Q	81	ASN
20	T	70	HIS
21	U	27	ASN
21	U	46	GLN
22	V	87	GLN
25	Y	58	ASN
29	c	29	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2888/2897 (99%)	382 (13%)	16 (0%)
2	B	119/120 (99%)	7 (5%)	0
32	f	75/76 (98%)	31 (41%)	0
33	g	74/76 (97%)	48 (64%)	0
All	All	3156/3169 (99%)	468 (14%)	16 (0%)

All (468) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	15	G
1	A	34	U
1	A	45	G
1	A	46	G
1	A	58	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	101	A
1	A	102	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	135	U
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	157	C
1	A	163	C
1	A	165	A
1	A	181	A
1	A	196	A
1	A	199	A
1	A	216	A
1	A	221	A
1	A	222	A
1	A	248	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	272	A
1	A	276	U
1	A	285	G
1	A	302	C
1	A	311	A
1	A	329	G
1	A	330	A
1	A	352	A
1	A	353	C
1	A	361	G
1	A	362	A
1	A	372	G
1	A	386	G
1	A	396	G
1	A	399	U
1	A	403	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	424	G
1	A	425	G
1	A	479	A
1	A	481	G
1	A	491	G
1	A	504	A
1	A	505	A
1	A	509	C
1	A	529	A
1	A	530	G
1	A	532	A
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	563	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	613	A
1	A	614	A

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Mol	Chain	Res	Type
1	A	615	U
1	A	627	A
1	A	637	A
1	A	645	C
1	A	647	G
1	A	654	A
1	A	655	A
1	A	685	A
1	A	686	U
1	A	717	C
1	A	730	A
1	A	747	5MU
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	790	U
1	A	791	C
1	A	792	A
1	A	805	G
1	A	812	C
1	A	827	U
1	A	828	U
1	A	845	A
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	878	A
1	A	881	G
1	A	883	G
1	A	884	U
1	A	885	C
1	A	895	U
1	A	896	A
1	A	897	C
1	A	910	A
1	A	914	G
1	A	927	A
1	A	931	U
1	A	946	C

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Mol	Chain	Res	Type
1	A	961	C
1	A	974	G
1	A	983	A
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1026	G
1	A	1033	U
1	A	1040	A
1	A	1046	A
1	A	1047	G
1	A	1070	A
1	A	1083	U
1	A	1084	A
1	A	1088	A
1	A	1090	A
1	A	1112	G
1	A	1114	C
1	A	1115	G
1	A	1116	G
1	A	1119	U
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1141	U
1	A	1142	A
1	A	1168	G
1	A	1171	G
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1212	G
1	A	1236	G
1	A	1238	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1300	G
1	A	1301	A
1	A	1329	U

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Mol	Chain	Res	Type
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1379	U
1	A	1383	A
1	A	1416	G
1	A	1417	C
1	A	1421	G
1	A	1428	C
1	A	1434	A
1	A	1435	G
1	A	1452	G
1	A	1459	G
1	A	1476	U
1	A	1482	G
1	A	1490	A
1	A	1493	C
1	A	1494	A
1	A	1495	A
1	A	1497	U
1	A	1509	A
1	A	1510	G
1	A	1515	A
1	A	1524	G
1	A	1529	G
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1607	C
1	A	1608	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1674	G

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Mol	Chain	Res	Type
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1738	G
1	A	1744	A
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1955	U
1	A	1960	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G

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Mol	Chain	Res	Type
1	A	2062	A
1	A	2069	G7M
1	A	2093	G
1	A	2098	U
1	A	2099	U
1	A	2101	A
1	A	2105	U
1	A	2108	A
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2123	G
1	A	2126	A
1	A	2127	G
1	A	2128	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2136	G
1	A	2137	U
1	A	2145	C
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2149	U
1	A	2159	G
1	A	2160	C
1	A	2161	C
1	A	2162	G
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2170	A

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Mol	Chain	Res	Type
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2177	C
1	A	2178	C
1	A	2179	C
1	A	2181	U
1	A	2185	U
1	A	2187	U
1	A	2188	U
1	A	2190	G
1	A	2192	U
1	A	2193	G
1	A	2194	U
1	A	2195	U
1	A	2198	A
1	A	2204	G
1	A	2211	A
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2268	A
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2297	A
1	A	2305	U
1	A	2308	G
1	A	2322	A
1	A	2325	G
1	A	2327	A
1	A	2333	A
1	A	2334	U
1	A	2336	A
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2383	G
1	A	2385	C
1	A	2402	U
1	A	2406	A

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Mol	Chain	Res	Type
1	A	2425	A
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2448	A
1	A	2476	A
1	A	2478	A
1	A	2491	U
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2518	A
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2547	A
1	A	2566	A
1	A	2567	G
1	A	2602	A
1	A	2609	U
1	A	2613	U
1	A	2615	U
1	A	2629	U
1	A	2663	G
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2716	C
1	A	2726	A
1	A	2732	G
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2751	G
1	A	2765	A
1	A	2778	A
1	A	2798	U
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2832	U
1	A	2835	A

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Mol	Chain	Res	Type
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2873	A
1	A	2879	A
1	A	2880	C
1	A	2884	U
1	A	2885	G
1	A	2886	A
1	A	2891	U
1	A	2901	C
1	A	2903	U
2	B	9	G
2	B	35	C
2	B	42	C
2	B	56	G
2	B	89	U
2	B	90	C
2	B	109	A
32	f	3	C
32	f	4	G
32	f	6	G
32	f	7	G
32	f	8	4SU
32	f	9	G
32	f	10	G
32	f	13	C
32	f	14	A
32	f	16	C
32	f	17	C
32	f	19	G
32	f	20	U
32	f	21	A
32	f	22	G
32	f	31	G
32	f	47	U
32	f	48	C
32	f	49	G
32	f	56	C
32	f	58	A
32	f	59	A
32	f	60	U

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Mol	Chain	Res	Type
32	f	61	C
32	f	62	C
32	f	64	G
32	f	67	C
32	f	68	C
32	f	69	C
32	f	70	G
32	f	76	A
33	g	3	G
33	g	4	G
33	g	6	U
33	g	7	U
33	g	8	U
33	g	10	2MG
33	g	11	C
33	g	12	U
33	g	13	C
33	g	14	A
33	g	15	G
33	g	16	H2U
33	g	17	H2U
33	g	18	G
33	g	19	G
33	g	20	G
33	g	21	A
33	g	22	G
33	g	23	A
33	g	24	G
33	g	25	C
33	g	28	C
33	g	31	A
33	g	33	U
33	g	34	OMG
33	g	35	A
33	g	36	A
33	g	38	A
33	g	39	PSU
33	g	40	5MC
33	g	43	G
33	g	45	G
33	g	46	7MG
33	g	47	U

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Mol	Chain	Res	Type
33	g	48	C
33	g	49	5MC
33	g	53	G
33	g	54	5MU
33	g	55	PSU
33	g	58	1MA
33	g	61	C
33	g	63	C
33	g	65	G
33	g	66	A
33	g	71	G
33	g	72	C
33	g	73	A
33	g	74	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	100	U
1	A	549	G
1	A	784	G
1	A	790	U
1	A	894	U
1	A	1046	A
1	A	1113	U
1	A	1494	A
1	A	1535	A
1	A	2099	U
1	A	2118	U
1	A	2127	G
1	A	2130	U
1	A	2158	A
1	A	2193	G
1	A	2406	A

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

45 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	$\#\|Z\| > 2$
33	5MU	g	54	33	19,22,23	1.54	3 (15%)	28,32,35	2.42	7 (25%)
33	1MA	g	58	33	16,25,26	1.65	5 (31%)	18,37,40	2.30	5 (27%)
1	PSU	A	2457	1	18,21,22	2.46	8 (44%)	22,30,33	1.90	4 (18%)
1	PSU	A	955	1	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
1	5MC	A	1962	1	18,22,23	2.01	6 (33%)	26,32,35	1.16	2 (7%)
33	H2U	g	17	33	18,21,22	1.01	2 (11%)	21,30,33	3.29	5 (23%)
33	M2G	g	26	33	20,27,28	1.57	3 (15%)	22,40,43	1.06	2 (9%)
33	5MC	g	40	33	18,22,23	1.27	1 (5%)	26,32,35	2.12	10 (38%)
1	2MA	A	2503	1,34	17,25,26	1.59	3 (17%)	17,37,40	1.04	2 (11%)
33	H2U	g	16	33	18,21,22	0.99	2 (11%)	21,30,33	1.90	2 (9%)
1	5MU	A	1939	1	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
33	7MG	g	46	33	22,26,27	2.13	4 (18%)	29,39,42	3.15	10 (34%)
1	H2U	A	2449	1	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
33	31M	g	76	1	38,44,45	4.34	18 (47%)	38,61,64	2.23	13 (34%)
1	PSU	A	1917	1	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)
1	5MU	A	747	1	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
1	OMG	A	2251	32,1	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
33	OMC	g	32	33	19,22,23	1.39	3 (15%)	26,31,34	2.13	2 (7%)
32	5MU	f	54	32	19,22,23	1.65	3 (15%)	28,32,35	2.93	11 (39%)
1	PSU	A	2504	1	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
1	PSU	A	2604	1	18,21,22	2.40	8 (44%)	22,30,33	1.87	4 (18%)
1	6MZ	A	2030	1	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)
13	4D4	M	81	13	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
1	PSU	A	2580	1	18,21,22	2.47	10 (55%)	22,30,33	1.90	5 (22%)
32	5MC	f	32	32	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
1	2MG	A	1835	1	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)
32	PSU	f	55	32	18,21,22	1.31	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A	1911	1	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
33	2MG	g	10	33	18,26,27	1.53	3 (16%)	16,38,41	1.64	4 (25%)
33	PSU	g	39	33	18,21,22	1.84	5 (27%)	22,30,33	2.49	7 (31%)
1	G7M	A	2069	1	20,26,27	2.24	5 (25%)	17,39,42	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	YYG	g	37	33	31,42,43	2.16	7 (22%)	33,62,65	2.03	10 (30%)
4	MEQ	D	150[A]	4	8,9,10	0.95	0	5,10,12	0.66	0
33	OMG	g	34	33	18,26,27	1.57	3 (16%)	19,38,41	1.52	4 (21%)
1	OMU	A	2552	1	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
33	PSU	g	55	33	18,21,22	2.22	6 (33%)	22,30,33	2.47	8 (36%)
1	3TD	A	1915	1	18,22,23	6.42	12 (66%)	22,32,35	1.93	4 (18%)
32	4SU	f	8	32	18,21,22	3.20	5 (27%)	26,30,33	3.64	10 (38%)
1	2MG	A	2445	1	18,26,27	3.39	7 (38%)	16,38,41	1.30	3 (18%)
33	5MC	g	49	33	18,22,23	1.07	2 (11%)	26,32,35	1.72	4 (15%)
1	PSU	A	2605	1	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
1	1MG	A	745	1	18,26,27	2.80	4 (22%)	19,39,42	1.28	3 (15%)
1	OMC	A	2498	1,34	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)
1	PSU	A	746	1,34	18,21,22	2.37	9 (50%)	22,30,33	1.80	4 (18%)
1	6MZ	A	1618	1	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)

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
33	5MU	g	54	33	-	2/7/25/26	0/2/2/2
33	1MA	g	58	33	-	2/3/25/26	0/3/3/3
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
33	H2U	g	17	33	-	5/7/38/39	0/2/2/2
33	M2G	g	26	33	-	0/7/29/30	0/3/3/3
33	5MC	g	40	33	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1,34	-	1/3/25/26	0/3/3/3
33	H2U	g	16	33	-	3/7/38/39	0/2/2/2
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
33	7MG	g	46	33	-	3/7/37/38	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
33	31M	g	76	1	-	6/27/49/50	0/4/4/4
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	32,1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	OMC	g	32	33	-	0/9/27/28	0/2/2/2
32	5MU	f	54	32	-	1/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	2/5/27/28	0/3/3/3
13	4D4	M	81	13	-	3/11/12/14	-
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
32	5MC	f	32	32	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
32	PSU	f	55	32	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
33	2MG	g	10	33	-	0/5/27/28	0/3/3/3
33	PSU	g	39	33	-	3/7/25/26	0/2/2/2
1	G7M	A	2069	1	-	1/3/25/26	0/3/3/3
33	YYG	g	37	33	-	16/20/42/43	0/3/4/4
4	MEQ	D	150[A]	4	-	4/8/9/11	-
33	OMG	g	34	33	-	3/5/27/28	0/3/3/3
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
33	PSU	g	55	33	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	0/7/25/26	0/2/2/2
32	4SU	f	8	32	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
33	5MC	g	49	33	-	3/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	OMC	A	2498	1,34	-	0/9/27/28	0/2/2/2
1	PSU	A	746	1,34	-	2/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3

All (239) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C2'-C1'	-18.07	1.30	1.53
33	g	76	31M	C2'-C1'	-16.92	1.28	1.53
1	A	1915	3TD	O4'-C1'	14.21	1.63	1.43
33	g	76	31M	O4'-C1'	12.06	1.57	1.41
1	A	2449	H2U	O4-C4	10.10	1.43	1.23
33	g	76	31M	O4'-C4'	-9.47	1.23	1.45
1	A	1835	2MG	O6-C6	9.24	1.42	1.23
1	A	2445	2MG	O6-C6	9.16	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	1MG	O6-C6	9.03	1.40	1.22
1	A	1915	3TD	O4-C4	8.29	1.40	1.23
32	f	8	4SU	C4-S4	-8.15	1.53	1.68
1	A	2449	H2U	C2-N1	8.08	1.47	1.35
1	A	2449	H2U	O2-C2	8.07	1.37	1.23
1	A	2552	OMU	O4-C4	7.89	1.39	1.24
1	A	1618	6MZ	C6-N6	7.88	1.47	1.35
1	A	2030	6MZ	C6-N6	7.75	1.47	1.35
1	A	1915	3TD	O4'-C4'	-7.63	1.28	1.45
32	f	8	4SU	C4-N3	-6.86	1.30	1.37
33	g	37	YYG	O23-C21	6.69	1.46	1.34
1	A	1939	5MU	C2-N1	-6.47	1.28	1.38
33	g	46	7MG	C5-N7	-6.47	1.28	1.35
1	A	2251	OMG	O6-C6	6.41	1.36	1.23
1	A	2069	G7M	O6-C6	6.32	1.36	1.23
1	A	2449	H2U	C2-N3	6.14	1.48	1.38
1	A	747	5MU	C2-N1	-6.10	1.28	1.38
1	A	1835	2MG	C2-N2	5.69	1.46	1.33
1	A	2445	2MG	C2-N2	5.64	1.45	1.33
32	f	8	4SU	C5-C4	-5.44	1.35	1.42
1	A	1835	2MG	CM2-N2	5.35	1.55	1.45
33	g	37	YYG	O18-C16	5.25	1.46	1.33
1	A	2445	2MG	CM2-N2	5.22	1.54	1.45
33	g	76	31M	O-C	-5.10	1.13	1.23
1	A	745	1MG	C2-N2	5.06	1.43	1.34
1	A	2251	OMG	C6-N1	-5.05	1.30	1.37
33	g	76	31M	O5'-C5'	-4.93	1.32	1.44
1	A	2580	PSU	C1'-C5	-4.84	1.39	1.50
1	A	2604	PSU	C1'-C5	-4.81	1.39	1.50
1	A	2457	PSU	C1'-C5	-4.80	1.39	1.50
1	A	2445	2MG	C6-N1	-4.80	1.30	1.37
33	g	34	OMG	C6-N1	-4.78	1.30	1.37
1	A	2069	G7M	C2-N2	4.76	1.45	1.34
13	M	81	4D4	CZ-NE	4.74	1.42	1.33
1	A	1939	5MU	C2-N3	-4.73	1.29	1.38
1	A	2449	H2U	C4-N3	4.73	1.45	1.37
33	g	55	PSU	C4-N3	-4.73	1.30	1.38
1	A	1917	PSU	C1'-C5	-4.71	1.39	1.50
1	A	955	PSU	C1'-C5	-4.70	1.39	1.50
1	A	2605	PSU	C1'-C5	-4.69	1.39	1.50
1	A	746	PSU	C1'-C5	-4.68	1.39	1.50
1	A	2504	PSU	C1'-C5	-4.67	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1911	PSU	C1'-C5	-4.66	1.39	1.50
32	f	8	4SU	C2-N3	-4.66	1.29	1.38
33	g	26	M2G	C2-N3	4.65	1.36	1.30
33	g	37	YYG	C4-N3	-4.65	1.31	1.40
1	A	2498	OMC	C4-N4	4.65	1.44	1.33
1	A	1939	5MU	C6-N1	-4.62	1.30	1.38
1	A	2503	2MA	C6-N6	4.61	1.47	1.28
1	A	1835	2MG	C6-N1	-4.60	1.31	1.37
1	A	747	5MU	C2-N3	-4.58	1.29	1.38
1	A	2552	OMU	C2-N1	-4.55	1.31	1.38
1	A	2251	OMG	C2-N2	4.53	1.45	1.34
1	A	747	5MU	C6-N1	-4.46	1.30	1.38
33	g	76	31M	CTM-N	4.38	1.43	1.34
33	g	46	7MG	C4-N9	-4.33	1.32	1.37
33	g	55	PSU	C2-N3	-4.23	1.30	1.37
1	A	1962	5MC	C4-N4	4.17	1.45	1.34
1	A	2069	G7M	C6-N1	-4.16	1.31	1.37
32	f	54	5MU	C6-N1	-4.15	1.31	1.38
33	g	39	PSU	C2-N1	-4.13	1.31	1.36
33	g	46	7MG	C6-N1	-4.08	1.31	1.38
33	g	76	31M	C3'-N3'	-4.08	1.39	1.45
33	g	76	31M	C8-N7	-4.06	1.27	1.34
1	A	2457	PSU	C4-N3	-4.03	1.31	1.38
1	A	2580	PSU	C4-N3	-4.03	1.31	1.38
1	A	1962	5MC	C2-N1	-4.02	1.31	1.40
1	A	955	PSU	C2-N1	-4.01	1.31	1.36
1	A	2457	PSU	C2-N1	-3.96	1.31	1.36
1	A	955	PSU	C4-N3	-3.96	1.31	1.38
1	A	2605	PSU	C4-N3	-3.93	1.31	1.38
1	A	2504	PSU	C4-N3	-3.89	1.31	1.38
1	A	2580	PSU	C2-N1	-3.89	1.31	1.36
1	A	2445	2MG	C5-C6	-3.89	1.39	1.47
33	g	40	5MC	C6-N1	-3.88	1.31	1.38
1	A	2604	PSU	C4-N3	-3.86	1.31	1.38
1	A	2552	OMU	C4-N3	-3.83	1.31	1.38
1	A	1962	5MC	C6-N1	-3.83	1.31	1.38
1	A	2504	PSU	C2-N1	-3.82	1.31	1.36
1	A	1835	2MG	C5-C6	-3.81	1.39	1.47
33	g	10	2MG	C6-N1	-3.80	1.32	1.37
1	A	2604	PSU	C2-N1	-3.80	1.31	1.36
1	A	2605	PSU	C2-N1	-3.79	1.31	1.36
1	A	746	PSU	C4-N3	-3.77	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2457	PSU	C2-N3	-3.75	1.31	1.37
1	A	1911	PSU	C4-N3	-3.75	1.31	1.38
1	A	745	1MG	C6-N1	-3.75	1.32	1.39
1	A	2605	PSU	C2-N3	-3.74	1.31	1.37
1	A	2552	OMU	C2-N3	-3.73	1.31	1.38
1	A	2498	OMC	C2-N1	-3.72	1.31	1.40
1	A	1917	PSU	C4-N3	-3.72	1.31	1.38
1	A	1915	3TD	O2'-C2'	3.71	1.51	1.43
1	A	746	PSU	C2-N1	-3.70	1.31	1.36
1	A	955	PSU	C2-N3	-3.69	1.31	1.37
33	g	76	31M	C4-N3	-3.69	1.30	1.35
1	A	2580	PSU	C2-N3	-3.66	1.31	1.37
1	A	1915	3TD	C4-N3	-3.66	1.32	1.40
1	A	2604	PSU	C2-N3	-3.65	1.31	1.37
1	A	1911	PSU	C2-N1	-3.64	1.31	1.36
1	A	2504	PSU	C2-N3	-3.63	1.31	1.37
1	A	1917	PSU	C2-N1	-3.63	1.31	1.36
1	A	1915	3TD	C2-N1	-3.60	1.32	1.37
1	A	1939	5MU	C4-N3	-3.59	1.32	1.38
1	A	746	PSU	C2-N3	-3.53	1.31	1.37
1	A	747	5MU	C6-C5	3.52	1.40	1.34
32	f	54	5MU	C4-N3	-3.52	1.32	1.38
1	A	1939	5MU	C6-C5	3.51	1.40	1.34
1	A	1917	PSU	C2-N3	-3.48	1.31	1.37
1	A	747	5MU	C4-N3	-3.47	1.32	1.38
1	A	2445	2MG	C2-N1	-3.46	1.31	1.36
33	g	58	1MA	C2-N3	3.45	1.33	1.29
33	g	55	PSU	C2-N1	-3.43	1.32	1.36
1	A	1911	PSU	C2-N3	-3.42	1.31	1.37
33	g	39	PSU	C4-N3	-3.40	1.32	1.38
1	A	1915	3TD	C6-C5	3.34	1.39	1.35
32	f	54	5MU	C2-N3	-3.31	1.32	1.38
33	g	54	5MU	C4-N3	-3.28	1.32	1.38
1	A	1835	2MG	C2-N1	-3.27	1.31	1.36
33	g	76	31M	C-N3'	3.25	1.41	1.34
33	g	10	2MG	C2'-C1'	-3.10	1.49	1.53
33	g	55	PSU	C6-N1	-3.08	1.31	1.36
33	g	37	YYG	C2-N1	-3.08	1.31	1.37
33	g	54	5MU	C6-N1	-3.07	1.32	1.38
33	g	54	5MU	C2-N3	-3.04	1.32	1.38
13	M	81	4D4	CZ-NH2	3.03	1.44	1.32
1	A	1962	5MC	O2-C2	-3.02	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	5MU	O4-C4	-3.00	1.17	1.23
1	A	1939	5MU	O2-C2	-3.00	1.17	1.23
1	A	2498	OMC	O2-C2	-2.99	1.18	1.23
1	A	2605	PSU	O4-C4	-2.99	1.17	1.23
33	g	32	OMC	C6-N1	-2.98	1.30	1.38
1	A	2457	PSU	O4-C4	-2.98	1.17	1.23
33	g	37	YYG	C12-N1	-2.98	1.31	1.36
33	g	46	7MG	C8-N9	-2.97	1.44	1.46
1	A	955	PSU	O4-C4	-2.97	1.17	1.23
1	A	747	5MU	O4-C4	-2.97	1.17	1.23
1	A	1911	PSU	C6-C5	2.95	1.38	1.35
33	g	55	PSU	C2'-C1'	-2.95	1.49	1.53
1	A	2580	PSU	O4-C4	-2.93	1.18	1.23
1	A	1917	PSU	C6-C5	2.90	1.38	1.35
1	A	2504	PSU	C6-C5	2.90	1.38	1.35
1	A	747	5MU	O2-C2	-2.89	1.17	1.23
1	A	2604	PSU	O4-C4	-2.89	1.18	1.23
1	A	746	PSU	C6-C5	2.89	1.38	1.35
1	A	2504	PSU	O4-C4	-2.88	1.18	1.23
32	f	55	PSU	C6-C5	2.87	1.38	1.35
1	A	746	PSU	O4-C4	-2.85	1.18	1.23
33	g	76	31M	C2'-C3'	-2.84	1.48	1.53
1	A	2604	PSU	C6-C5	2.81	1.38	1.35
1	A	2069	G7M	C2-N1	-2.78	1.30	1.37
33	g	26	M2G	C6-N1	-2.78	1.33	1.37
1	A	955	PSU	C6-C5	2.77	1.38	1.35
1	A	1915	3TD	O3'-C3'	-2.75	1.36	1.43
1	A	1911	PSU	O4-C4	-2.75	1.18	1.23
1	A	2580	PSU	C6-N1	-2.75	1.31	1.36
1	A	1915	3TD	C2-N3	-2.75	1.32	1.38
1	A	2580	PSU	C6-C5	2.74	1.38	1.35
1	A	2457	PSU	C6-C5	2.74	1.38	1.35
1	A	2503	2MA	C6-N1	-2.73	1.31	1.38
33	g	76	31M	C5-N7	-2.72	1.29	1.39
1	A	2552	OMU	O2-C2	-2.72	1.18	1.23
1	A	2605	PSU	C6-C5	2.72	1.38	1.35
1	A	955	PSU	C6-N1	-2.72	1.31	1.36
33	g	10	2MG	C2-N1	-2.71	1.32	1.36
32	f	32	5MC	C6-N1	-2.70	1.33	1.38
1	A	745	1MG	C5-C6	-2.69	1.39	1.47
33	g	37	YYG	C2'-C1'	-2.67	1.49	1.53
33	g	49	5MC	C6-N1	-2.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2457	PSU	C6-N1	-2.65	1.31	1.36
1	A	1917	PSU	O4-C4	-2.64	1.18	1.23
33	g	17	H2U	C4-N3	-2.63	1.33	1.37
1	A	2605	PSU	C6-N1	-2.61	1.31	1.36
1	A	2604	PSU	C6-N1	-2.60	1.31	1.36
1	A	2457	PSU	O2-C2	-2.59	1.18	1.23
1	A	2504	PSU	C6-N1	-2.59	1.31	1.36
33	g	26	M2G	C2-N2	2.58	1.40	1.35
32	f	8	4SU	C6-N1	-2.58	1.31	1.38
33	g	39	PSU	C2-N3	-2.58	1.33	1.37
33	g	32	OMC	C5-C4	-2.58	1.37	1.42
33	g	37	YYG	C4-N9	-2.57	1.31	1.37
33	g	58	1MA	C2-N1	-2.57	1.31	1.35
1	A	2580	PSU	O2-C2	-2.56	1.18	1.23
1	A	2552	OMU	C6-N1	-2.55	1.31	1.38
1	A	955	PSU	O2-C2	-2.55	1.18	1.23
1	A	2251	OMG	C5-C6	-2.55	1.42	1.47
1	A	1917	PSU	C6-N1	-2.54	1.32	1.36
33	g	76	31M	C5-C4	-2.54	1.34	1.40
33	g	16	H2U	C2-N3	-2.52	1.33	1.38
1	A	2498	OMC	C6-N1	-2.51	1.31	1.38
33	g	39	PSU	C6-N1	-2.49	1.32	1.36
1	A	1911	PSU	C6-N1	-2.49	1.32	1.36
33	g	39	PSU	C2'-C1'	-2.47	1.50	1.53
32	f	55	PSU	C4-N3	-2.47	1.34	1.38
33	g	16	H2U	C4-N3	-2.47	1.33	1.37
1	A	2605	PSU	O2-C2	-2.47	1.18	1.23
1	A	2504	PSU	O2-C2	-2.45	1.18	1.23
1	A	1962	5MC	C2-N3	-2.44	1.31	1.36
1	A	2604	PSU	O2-C2	-2.44	1.18	1.23
1	A	2498	OMC	C2-N3	-2.42	1.31	1.36
1	A	746	PSU	C6-N1	-2.41	1.32	1.36
1	A	2552	OMU	C5-C4	-2.41	1.38	1.43
33	g	58	1MA	C6-N6	2.40	1.33	1.27
33	g	76	31M	OTM-CTM	-2.40	1.18	1.23
1	A	1917	PSU	O2-C2	-2.38	1.18	1.23
32	f	32	5MC	C6-C5	2.35	1.38	1.34
1	A	1911	PSU	O2-C2	-2.34	1.18	1.23
33	g	17	H2U	C2-N3	-2.34	1.33	1.38
1	A	746	PSU	O2-C2	-2.34	1.18	1.23
1	A	2580	PSU	O4'-C1'	-2.30	1.40	1.43
33	g	76	31M	C2-N3	-2.30	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	34	OMG	C2-N1	-2.28	1.32	1.37
33	g	58	1MA	C5-C4	2.27	1.48	1.43
1	A	1915	3TD	C6-N1	-2.25	1.32	1.36
1	A	2251	OMG	C5-C4	-2.25	1.37	1.43
33	g	55	PSU	C1'-C5	-2.23	1.45	1.50
1	A	1962	5MC	C6-C5	2.22	1.38	1.34
1	A	1915	3TD	O2-C2	-2.22	1.19	1.23
33	g	32	OMC	C2-N3	-2.21	1.31	1.36
1	A	746	PSU	O4'-C1'	-2.18	1.40	1.43
1	A	2503	2MA	C5-C4	-2.17	1.37	1.43
1	A	2445	2MG	C4-N3	-2.12	1.32	1.37
33	g	76	31M	CE1-CD1	-2.11	1.34	1.38
33	g	49	5MC	C6-C5	2.11	1.38	1.34
33	g	76	31M	O2'-C2'	2.09	1.47	1.43
1	A	2069	G7M	C5-C6	-2.09	1.40	1.45
33	g	76	31M	C2-N1	-2.08	1.30	1.33
33	g	58	1MA	C4-N3	-2.07	1.31	1.37
33	g	34	OMG	C4-N3	-2.05	1.32	1.37
1	A	1835	2MG	C4-N3	-2.03	1.32	1.37
1	A	2580	PSU	C4-C5	-2.01	1.38	1.44
1	A	2498	OMC	C5-C4	-2.00	1.38	1.42

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2449	H2U	C4-N3-C2	-15.23	113.16	125.79
33	g	17	H2U	C4-N3-C2	-13.77	114.37	125.79
1	A	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
33	g	46	7MG	N9-C4-N3	10.82	141.66	125.47
32	f	8	4SU	C4-N3-C2	-10.44	117.20	127.34
32	f	8	4SU	C5-C4-N3	10.31	124.25	114.69
33	g	32	OMC	C2'-C1'-N1	-9.28	96.21	114.22
1	A	1939	5MU	C4-N3-C2	-9.13	115.53	127.35
32	f	54	5MU	O4-C4-C5	-8.97	114.50	124.90
1	A	747	5MU	C4-N3-C2	-8.56	116.27	127.35
1	A	747	5MU	C5M-C5-C4	8.48	128.10	118.77
1	A	1939	5MU	N3-C2-N1	8.44	126.09	114.89
1	A	1939	5MU	C5-C6-N1	-8.33	114.77	123.34
1	A	747	5MU	N3-C2-N1	8.22	125.80	114.89
1	A	1939	5MU	C5M-C5-C4	8.09	127.67	118.77
1	A	2449	H2U	O4-C4-N3	-7.92	107.72	120.28
33	g	55	PSU	N1-C2-N3	7.43	123.55	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	747	5MU	C5-C6-N1	-7.32	115.81	123.34
1	A	2449	H2U	O2-C2-N3	-7.19	108.11	121.50
33	g	16	H2U	C4-N3-C2	-6.92	120.05	125.79
1	A	1939	5MU	C5-C4-N3	6.87	121.18	115.31
1	A	1915	3TD	N1-C2-N3	6.71	121.43	116.14
33	g	46	7MG	N9-C8-N7	-6.57	93.97	103.38
1	A	747	5MU	C5M-C5-C6	-6.57	114.07	122.85
1	A	2449	H2U	O4-C4-C5	-6.54	108.19	122.17
1	A	1939	5MU	C5M-C5-C6	-6.51	114.16	122.85
1	A	2030	6MZ	C9-N6-C6	-6.46	117.30	122.87
1	A	747	5MU	C5-C4-N3	6.46	120.83	115.31
33	g	58	1MA	O4'-C1'-C2'	-6.40	97.57	106.93
33	g	46	7MG	C5-C4-N3	-6.33	116.07	128.13
32	f	8	4SU	C5-C4-S4	-6.21	116.46	124.47
32	f	54	5MU	C4-N3-C2	-6.08	119.48	127.35
1	A	2449	H2U	N3-C2-N1	-6.07	110.24	116.65
33	g	54	5MU	C5-C4-N3	5.97	120.40	115.31
33	g	54	5MU	C4-N3-C2	-5.93	119.68	127.35
32	f	55	PSU	N1-C2-N3	5.78	121.68	115.13
1	A	2580	PSU	N1-C2-N3	5.74	121.64	115.13
1	A	2504	PSU	N1-C2-N3	5.72	121.61	115.13
1	A	2457	PSU	N1-C2-N3	5.71	121.60	115.13
32	f	54	5MU	N3-C2-N1	5.67	122.42	114.89
1	A	2604	PSU	N1-C2-N3	5.62	121.50	115.13
1	A	955	PSU	N1-C2-N3	5.57	121.44	115.13
1	A	1917	PSU	N1-C2-N3	5.56	121.44	115.13
1	A	2605	PSU	N1-C2-N3	5.56	121.42	115.13
1	A	2552	OMU	N3-C2-N1	5.51	122.21	114.89
1	A	1911	PSU	N1-C2-N3	5.51	121.37	115.13
33	g	76	31M	N3-C2-N1	-5.46	120.15	128.68
33	g	39	PSU	N1-C2-N3	5.44	121.29	115.13
32	f	8	4SU	N3-C2-N1	5.43	122.10	114.89
1	A	746	PSU	N1-C2-N3	5.43	121.28	115.13
32	f	54	5MU	C5-C4-N3	5.40	119.92	115.31
1	A	2030	6MZ	C2-N1-C6	5.24	121.08	116.59
33	g	76	31M	C4-C5-N7	-5.15	104.03	109.40
33	g	54	5MU	N3-C2-N1	5.05	121.60	114.89
33	g	40	5MC	O2-C2-N3	-5.02	114.16	122.33
1	A	2030	6MZ	N3-C2-N1	-4.92	120.99	128.68
33	g	54	5MU	O4-C4-C5	-4.90	119.23	124.90
33	g	39	PSU	O2-C2-N1	-4.88	117.41	122.79
1	A	1618	6MZ	C2-N1-C6	4.81	120.71	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	55	PSU	C4-N3-C2	-4.76	119.48	126.34
1	A	2552	OMU	C4-N3-C2	-4.76	120.31	126.58
1	A	1618	6MZ	C9-N6-C6	-4.75	118.78	122.87
1	A	1618	6MZ	N3-C2-N1	-4.71	121.31	128.68
33	g	49	5MC	C5-C6-N1	-4.69	118.51	123.34
33	g	76	31M	C5-C6-N6	4.67	127.45	120.35
33	g	39	PSU	C4-N3-C2	-4.66	119.63	126.34
33	g	58	1MA	N1-C2-N3	4.53	131.30	126.02
33	g	39	PSU	C6-C5-C4	-4.53	115.03	118.20
33	g	76	31M	CB-CA-C	-4.38	98.88	110.25
33	g	46	7MG	C2-N3-C4	4.32	120.00	112.30
32	f	32	5MC	C5-C6-N1	-4.29	118.92	123.34
33	g	37	YYG	O4'-C1'-C2'	-4.28	100.67	106.93
1	A	1939	5MU	O2-C2-N1	-4.24	117.15	122.79
1	A	1962	5MC	C5-C6-N1	-4.23	118.99	123.34
1	A	2605	PSU	C4-N3-C2	-4.12	120.40	126.34
1	A	2457	PSU	C4-N3-C2	-4.09	120.44	126.34
1	A	746	PSU	C4-N3-C2	-4.06	120.50	126.34
1	A	2604	PSU	C4-N3-C2	-4.05	120.50	126.34
1	A	2504	PSU	C4-N3-C2	-4.04	120.51	126.34
32	f	55	PSU	C4-N3-C2	-4.02	120.54	126.34
1	A	1939	5MU	O4-C4-N3	-4.00	112.44	120.12
1	A	955	PSU	C4-N3-C2	-3.92	120.68	126.34
1	A	1911	PSU	C4-N3-C2	-3.92	120.69	126.34
1	A	1917	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A	2580	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A	747	5MU	O4-C4-N3	-3.87	112.69	120.12
33	g	49	5MC	O2-C2-N3	-3.72	116.28	122.33
33	g	49	5MC	C2'-C1'-N1	-3.68	102.80	113.22
33	g	76	31M	CA-C-N3'	3.67	124.74	116.70
33	g	54	5MU	C5-C6-N1	-3.65	119.58	123.34
1	A	1915	3TD	C4-N3-C2	-3.63	120.67	124.61
13	M	81	4D4	NE-CZ-NH2	-3.60	114.37	120.70
32	f	54	5MU	O2-C2-N1	-3.60	118.01	122.79
33	g	58	1MA	C2'-C3'-C4'	-3.52	95.80	102.64
33	g	37	YYG	C3'-C2'-C1'	3.52	106.28	100.98
33	g	37	YYG	C24-O23-C21	3.52	119.82	115.66
33	g	46	7MG	C5-C6-N1	3.48	117.12	110.99
1	A	747	5MU	O2-C2-N1	-3.46	118.19	122.79
33	g	76	31M	O-C-N3'	-3.42	116.60	122.93
32	f	55	PSU	O2-C2-N1	-3.42	119.03	122.79
33	g	37	YYG	C2'-C3'-C4'	-3.40	96.04	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	55	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A	745	1MG	C5-C6-N1	3.38	118.98	113.90
33	g	37	YYG	O18-C16-C15	3.35	120.09	111.52
33	g	17	H2U	C5-C4-N3	-3.31	112.93	116.65
33	g	55	PSU	C3'-C2'-C1'	3.30	105.48	101.64
1	A	2504	PSU	O2-C2-N1	-3.29	119.17	122.79
33	g	39	PSU	O4-C4-C5	-3.25	115.53	124.05
1	A	955	PSU	O2-C2-N1	-3.24	119.23	122.79
33	g	40	5MC	O4'-C1'-N1	3.23	115.75	108.36
33	g	10	2MG	O2'-C2'-C3'	-3.18	101.54	111.82
1	A	1835	2MG	C5-C6-N1	3.17	119.56	113.95
1	A	2580	PSU	O2-C2-N1	-3.17	119.30	122.79
33	g	37	YYG	C19-O18-C16	3.17	123.11	115.94
13	M	81	4D4	NH1-CZ-NE	3.16	126.48	119.19
33	g	46	7MG	C5-C4-N9	-3.15	102.26	106.35
1	A	2457	PSU	O2-C2-N1	-3.14	119.34	122.79
32	f	8	4SU	O2'-C2'-C1'	-3.09	99.69	110.02
33	g	40	5MC	C5-C6-N1	-3.07	120.18	123.34
33	g	37	YYG	C5-C6-N1	3.06	118.52	113.96
1	A	1911	PSU	O2-C2-N1	-3.05	119.44	122.79
1	A	2552	OMU	O2-C2-N1	-3.04	118.74	122.79
1	A	746	PSU	O2-C2-N1	-3.03	119.45	122.79
1	A	1917	PSU	O2-C2-N1	-3.01	119.48	122.79
33	g	76	31M	O4'-C1'-C2'	-3.00	102.55	106.93
1	A	2445	2MG	C5-C6-N1	3.00	119.24	113.95
1	A	747	5MU	C1'-N1-C6	-2.98	116.17	121.12
1	A	747	5MU	O2-C2-N3	-2.95	116.01	121.50
33	g	55	PSU	C5-C6-N1	-2.94	117.70	122.11
1	A	1939	5MU	C6-N1-C2	2.93	124.27	121.30
32	f	8	4SU	C3'-C2'-C1'	2.92	106.98	101.43
1	A	2604	PSU	O2-C2-N1	-2.92	119.58	122.79
33	g	46	7MG	C2-N1-C6	-2.89	119.82	125.10
1	A	2498	OMC	O2-C2-N3	-2.89	117.62	122.33
33	g	46	7MG	O6-C6-C5	-2.89	120.45	127.54
33	g	10	2MG	C8-N7-C5	2.86	108.44	102.99
1	A	2503	2MA	C5-C6-N1	2.86	118.95	114.02
32	f	54	5MU	O4-C4-N3	2.85	125.57	120.12
1	A	2251	OMG	C8-N7-C5	2.84	108.40	102.99
1	A	1915	3TD	C3'-C2'-C1'	2.84	104.94	101.64
33	g	40	5MC	C1'-N1-C2	2.83	124.74	118.42
33	g	40	5MC	C1'-N1-C6	-2.82	116.42	121.12
32	f	54	5MU	O3'-C3'-C2'	2.82	120.96	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2605	PSU	O2-C2-N1	-2.81	119.69	122.79
33	g	55	PSU	O2'-C2'-C1'	-2.75	104.68	111.23
33	g	32	OMC	C5-C6-N1	-2.74	117.22	121.81
33	g	49	5MC	C5'-C4'-C3'	-2.74	104.93	115.18
1	A	1835	2MG	C8-N7-C5	2.73	108.19	102.99
33	g	46	7MG	O4'-C1'-N9	2.73	113.01	109.30
1	A	745	1MG	C8-N7-C5	2.73	108.19	102.99
32	f	8	4SU	C6-C5-C4	-2.71	117.60	119.95
1	A	2445	2MG	C8-N7-C5	2.71	108.14	102.99
1	A	2552	OMU	C5-C6-N1	-2.67	117.33	121.81
1	A	2030	6MZ	C4-C5-N7	-2.66	106.62	109.40
33	g	10	2MG	O3'-C3'-C4'	2.65	118.72	111.05
33	g	76	31M	CEM-SDM-CGM	2.64	109.48	100.40
33	g	17	H2U	C2'-C3'-C4'	2.64	107.77	102.64
32	f	8	4SU	O2-C2-N3	-2.63	116.60	121.50
33	g	10	2MG	C5-C6-N1	2.63	118.59	113.95
1	A	2552	OMU	C5-C4-N3	2.62	118.76	114.84
33	g	34	OMG	C5-C6-N1	2.62	118.57	113.95
33	g	39	PSU	C5'-C4'-C3'	-2.62	105.38	115.18
32	f	32	5MC	C5-C4-N3	-2.61	118.86	121.67
33	g	34	OMG	C3'-C2'-C1'	2.60	107.77	102.89
1	A	1939	5MU	O2-C2-N3	-2.55	116.75	121.50
33	g	76	31M	CB-CA-N	-2.53	105.46	110.79
1	A	2552	OMU	O4-C4-C5	-2.51	120.75	125.16
1	A	2457	PSU	C5-C6-N1	-2.51	118.35	122.11
33	g	16	H2U	C3'-C2'-C1'	2.50	106.17	101.43
33	g	17	H2U	O4-C4-N3	2.49	124.23	120.28
33	g	34	OMG	O4'-C1'-C2'	-2.47	102.31	106.59
1	A	2604	PSU	C5-C6-N1	-2.47	118.41	122.11
1	A	746	PSU	C5-C6-N1	-2.46	118.42	122.11
1	A	2605	PSU	C5-C6-N1	-2.46	118.42	122.11
13	M	81	4D4	CB-CA-C	-2.45	107.85	111.77
33	g	37	YYG	O23-C21-N20	2.44	115.08	110.80
33	g	40	5MC	C5-C4-N3	-2.41	119.08	121.67
33	g	40	5MC	O4'-C4'-C5'	2.40	117.27	109.37
1	A	2251	OMG	C5-C6-N1	2.38	118.16	113.95
33	g	37	YYG	O18-C16-O17	-2.37	119.20	123.84
33	g	34	OMG	C2-N1-C6	-2.36	120.75	125.10
33	g	55	PSU	O2-C2-N3	-2.35	117.39	121.82
1	A	1911	PSU	C5-C6-N1	-2.33	118.61	122.11
33	g	26	M2G	C8-N7-C5	2.33	107.43	102.99
1	A	2449	H2U	C5-C4-N3	-2.33	114.03	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	40	5MC	O2'-C2'-C1'	-2.33	102.24	110.02
33	g	39	PSU	O5'-C5'-C4'	2.32	116.90	108.99
1	A	2504	PSU	C5-C6-N1	-2.30	118.65	122.11
33	g	40	5MC	N1-C2-N3	2.28	122.96	118.81
33	g	58	1MA	C3'-C2'-C1'	-2.28	97.55	100.98
1	A	745	1MG	O6-C6-C5	-2.26	120.18	124.19
1	A	1917	PSU	C5-C6-N1	-2.25	118.73	122.11
32	f	54	5MU	C5-C6-N1	-2.25	121.03	123.34
32	f	32	5MC	CM5-C5-C6	-2.25	119.85	122.85
1	A	2445	2MG	CM2-N2-C2	-2.24	118.91	123.86
32	f	54	5MU	C6-N1-C2	-2.24	119.03	121.30
33	g	58	1MA	O2'-C2'-C3'	-2.23	104.61	111.82
1	A	2580	PSU	C5-C6-N1	-2.21	118.79	122.11
33	g	40	5MC	O4'-C4'-C3'	-2.21	100.74	105.11
33	g	26	M2G	C5-C6-N1	2.21	117.85	113.95
1	A	955	PSU	C5-C6-N1	-2.21	118.80	122.11
1	A	1835	2MG	CM2-N2-C2	-2.20	119.00	123.86
1	A	2580	PSU	O4'-C1'-C2'	2.19	108.23	105.14
33	g	76	31M	C2-N1-C6	2.16	122.46	118.75
33	g	76	31M	OTM-CTM-N	-2.15	118.94	122.93
1	A	1618	6MZ	C4-C5-N7	-2.15	107.16	109.40
1	A	2503	2MA	C8-N7-C5	2.15	107.08	102.99
32	f	55	PSU	C5-C6-N1	-2.14	118.90	122.11
1	A	747	5MU	C6-N1-C2	2.13	123.45	121.30
33	g	55	PSU	O4'-C4'-C3'	-2.13	100.91	105.11
33	g	46	7MG	C5'-C4'-C3'	-2.12	107.25	115.18
33	g	54	5MU	O2-C2-N1	-2.12	119.97	122.79
33	g	37	YYG	O23-C21-O22	-2.10	121.49	124.58
13	M	81	4D4	O-C-CA	-2.10	119.27	124.78
32	f	54	5MU	C1'-N1-C2	2.10	121.38	117.57
33	g	76	31M	CBM-CAM-CTM	2.08	115.35	110.85
33	g	17	H2U	C4'-O4'-C1'	2.08	114.06	109.47
32	f	8	4SU	C2'-C1'-N1	-2.05	107.41	113.22
1	A	1915	3TD	C5-C6-N1	-2.03	119.06	122.11
32	f	54	5MU	O2'-C2'-C1'	-2.03	103.24	110.02
32	f	8	4SU	O5'-C5'-C4'	2.03	115.89	108.99
1	A	1962	5MC	C5-C4-N3	-2.02	119.50	121.67
33	g	54	5MU	C2'-C1'-N1	-2.01	107.51	113.22
1	A	2251	OMG	C2-N1-C6	-2.01	121.40	125.10
33	g	76	31M	C-CA-N	2.01	116.63	111.16

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	150[A]	MEQ	N-CA-CB-CG
13	M	81	4D4	NE-CD-CG-CB
1	A	746	PSU	C2'-C1'-C5-C4
1	A	2251	OMG	C1'-C2'-O2'-CM2
33	g	17	H2U	O4'-C1'-N1-C6
33	g	34	OMG	O4'-C4'-C5'-O5'
33	g	34	OMG	C1'-C2'-O2'-CM2
33	g	37	YYG	N1-C12-C13-C14
33	g	37	YYG	C12-C13-C14-C15
33	g	37	YYG	C13-C14-C15-N20
33	g	37	YYG	C15-C16-O18-C19
33	g	37	YYG	O23-C21-N20-C15
33	g	37	YYG	N20-C21-O23-C24
33	g	37	YYG	O22-C21-O23-C24
33	g	39	PSU	C3'-C4'-C5'-O5'
33	g	46	7MG	O4'-C4'-C5'-O5'
33	g	49	5MC	O4'-C4'-C5'-O5'
33	g	49	5MC	C3'-C4'-C5'-O5'
33	g	54	5MU	C3'-C4'-C5'-O5'
33	g	54	5MU	O4'-C4'-C5'-O5'
33	g	76	31M	CTM-CAM-CBM-CGM
33	g	76	31M	NM-CAM-CBM-CGM
33	g	37	YYG	O17-C16-O18-C19
33	g	37	YYG	O22-C21-N20-C15
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
33	g	16	H2U	C3'-C4'-C5'-O5'
33	g	34	OMG	C3'-C4'-C5'-O5'
33	g	46	7MG	C3'-C4'-C5'-O5'
33	g	58	1MA	O4'-C4'-C5'-O5'
33	g	76	31M	CBM-CGM-SDM-CEM
1	A	2504	PSU	C3'-C4'-C5'-O5'
33	g	39	PSU	O4'-C4'-C5'-O5'
33	g	58	1MA	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
33	g	37	YYG	O4'-C4'-C5'-O5'
13	M	81	4D4	OB-CB-CG-CD
33	g	37	YYG	C13-C14-C15-C16
4	D	150[A]	MEQ	C-CA-CB-CG
13	M	81	4D4	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
33	g	37	YYG	C11-C12-C13-C14
33	g	37	YYG	N20-C15-C16-O17
33	g	37	YYG	C16-C15-N20-C21
33	g	16	H2U	O4'-C4'-C5'-O5'
33	g	37	YYG	C3'-C4'-C5'-O5'
4	D	150[A]	MEQ	OE1-CD-CG-CB
33	g	37	YYG	N20-C15-C16-O18
33	g	17	H2U	C4'-C5'-O5'-P
4	D	150[A]	MEQ	NE2-CD-CG-CB
33	g	46	7MG	C2'-C1'-N9-C8
33	g	16	H2U	C4'-C5'-O5'-P
33	g	39	PSU	C4'-C5'-O5'-P
33	g	76	31M	CAM-CBM-CGM-SDM
33	g	76	31M	CA-CB-CG-CD1
33	g	17	H2U	O4'-C1'-N1-C2
1	A	1962	5MC	C2'-C1'-N1-C6
1	A	2503	2MA	O4'-C4'-C5'-O5'
1	A	1962	5MC	O4'-C1'-N1-C6
32	f	54	5MU	O4'-C4'-C5'-O5'
33	g	17	H2U	C3'-C4'-C5'-O5'
33	g	76	31M	CA-CB-CG-CD2
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2069	G7M	O4'-C4'-C5'-O5'
33	g	17	H2U	C2'-C1'-N1-C2
33	g	49	5MC	C2'-C1'-N1-C2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1939	5MU	1	0
1	A	2251	OMG	1	0
1	A	2604	PSU	1	0
1	A	2030	6MZ	2	0
1	A	1915	3TD	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 179 ligands modelled in this entry, 178 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
35	DI0	A	3175	-	58,61,61	1.62	11 (18%)	77,92,92	1.65	20 (25%)

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
35	DI0	A	3175	-	-	10/70/121/121	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3175	DI0	CAF-CAE	-5.60	1.39	1.51
35	A	3175	DI0	OBI-CAG	-4.12	1.33	1.43
35	A	3175	DI0	OAU-CBG	-3.41	1.38	1.44
35	A	3175	DI0	OAY-CAC	-3.13	1.35	1.43
35	A	3175	DI0	CBC-CBB	2.86	1.58	1.54
35	A	3175	DI0	OAU-CAB	-2.79	1.34	1.41
35	A	3175	DI0	CAP-CAH	2.66	1.60	1.55
35	A	3175	DI0	CAI-CAK	2.49	1.57	1.54
35	A	3175	DI0	CAD-CAW	-2.49	1.50	1.54
35	A	3175	DI0	OBJ-CAP	-2.28	1.40	1.44
35	A	3175	DI0	OBL-CAX	-2.25	1.38	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	3175	DI0	OAL-CAW-CBT	4.88	116.70	107.40
35	A	3175	DI0	CBT-CAW-CAD	-4.69	106.31	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	3175	DI0	OBK-CAN-CAX	4.22	110.07	103.81
35	A	3175	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
35	A	3175	DI0	CBR-CAP-CBC	-2.75	106.45	111.09
35	A	3175	DI0	CCB-OBK-CAN	-2.68	111.95	117.55
35	A	3175	DI0	CBV-CBB-CBC	-2.64	106.45	112.45
35	A	3175	DI0	CBP-CAJ-CAC	-2.51	106.89	111.40
35	A	3175	DI0	CAF-CAC-CAJ	-2.37	106.20	113.05
35	A	3175	DI0	OBI-CAG-CAO	-2.35	105.59	109.77
35	A	3175	DI0	OBJ-CAP-CAH	2.22	111.80	107.59
35	A	3175	DI0	OBK-CAN-CAT	-2.22	109.41	112.96
35	A	3175	DI0	OAY-CAR-CAT	2.13	112.68	109.01
35	A	3175	DI0	CBO-CAI-CAA	-2.12	107.97	112.94
35	A	3175	DI0	CBO-CAI-CAK	-2.11	109.52	112.02
35	A	3175	DI0	OAU-CAB-CAG	-2.08	105.95	110.35
35	A	3175	DI0	OBK-CAN-CBQ	-2.07	107.48	110.92
35	A	3175	DI0	CAN-CAX-CAZ	-2.06	107.98	111.14
35	A	3175	DI0	OAM-CAH-CAJ	-2.04	108.48	111.54
35	A	3175	DI0	OAM-CAB-OAU	-2.03	105.02	110.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	3175	DI0	NAQ-CBA-CBS-OBW
35	A	3175	DI0	NAQ-CAK-CBB-CBC
35	A	3175	DI0	CAJ-CAH-CAP-OBJ
35	A	3175	DI0	OBX-CCC-CCD-OBW
35	A	3175	DI0	OAL-CAW-CBT-CCF
35	A	3175	DI0	CAD-CAW-OAL-CAE
35	A	3175	DI0	CBA-CBS-OBW-CCD
35	A	3175	DI0	CAJ-CAC-CAF-CBN
35	A	3175	DI0	CAD-CAW-CBT-CCF
35	A	3175	DI0	NAQ-CAK-CBB-CBV

There are no ring outliers.

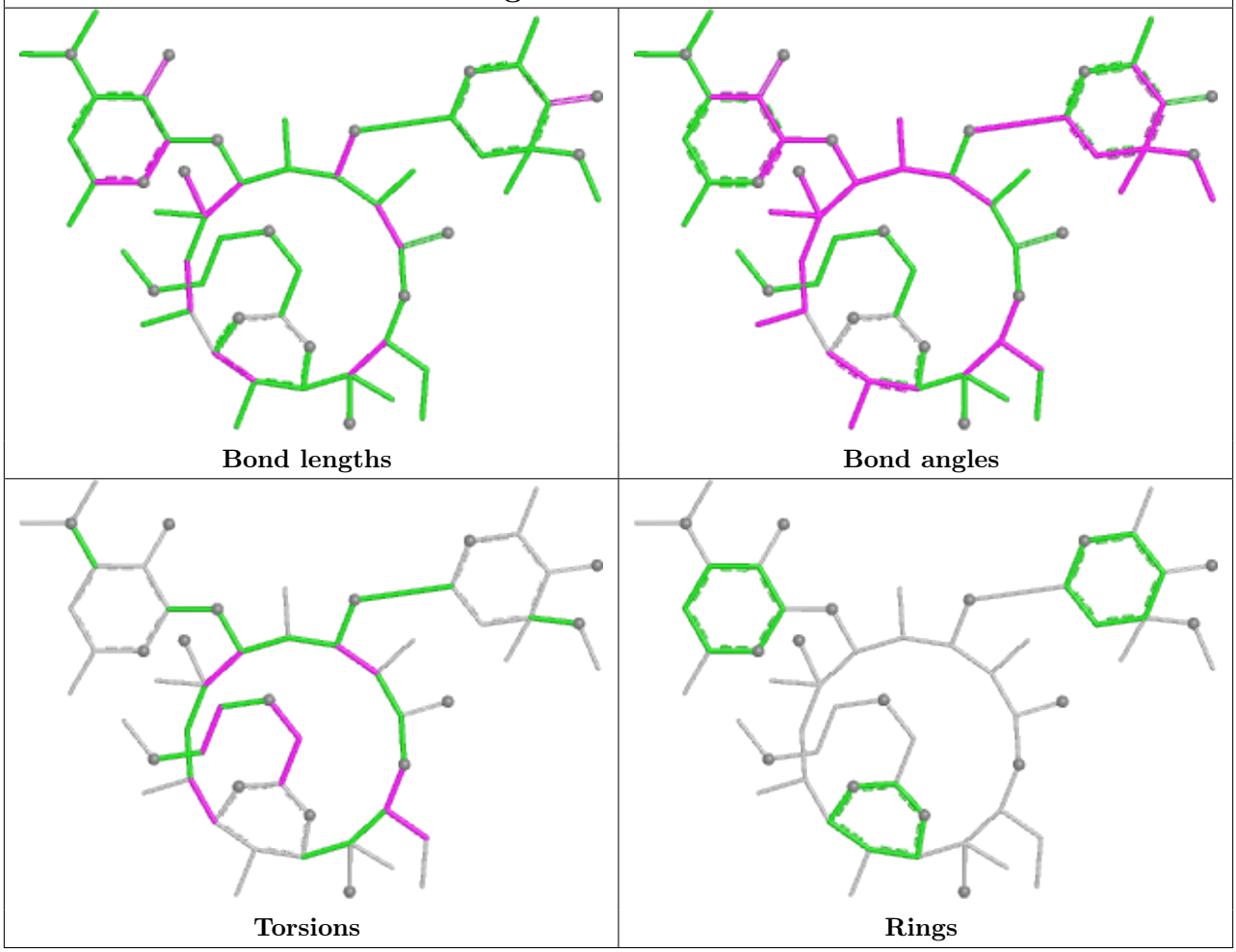
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	3175	DI0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DI0 A 3175



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	A	2
33	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	885:C	O3'	892:A	P	11.25
1	A	1915:3TD	O3'	1916:A	P	1.31
1	g	75:C	O3'	76:31M	P	1.09

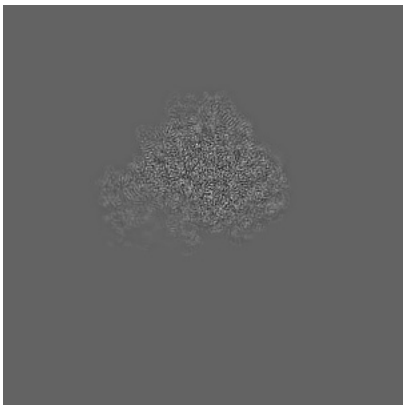
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10655. These allow visual inspection of the internal detail of the map and identification of artifacts.

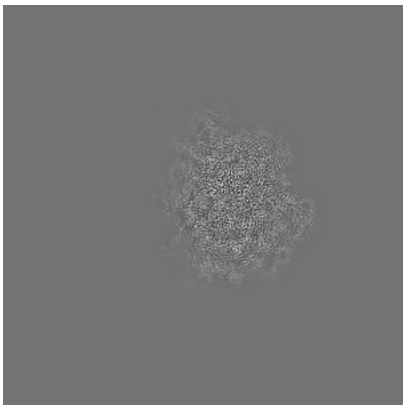
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

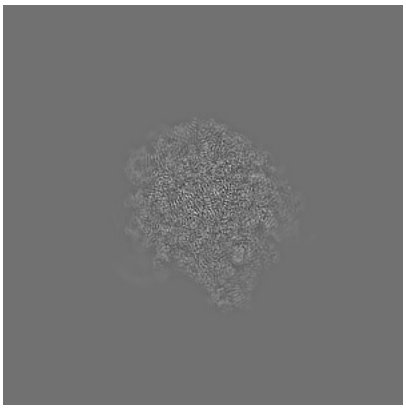
6.1.1 Primary map



X

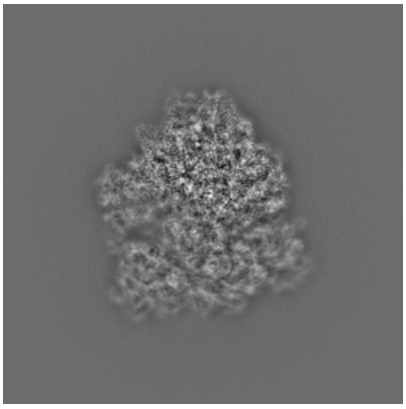


Y

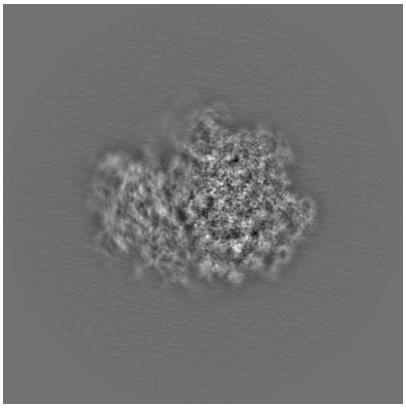


Z

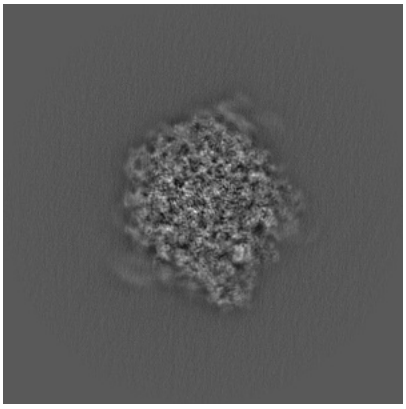
6.1.2 Raw map



X



Y



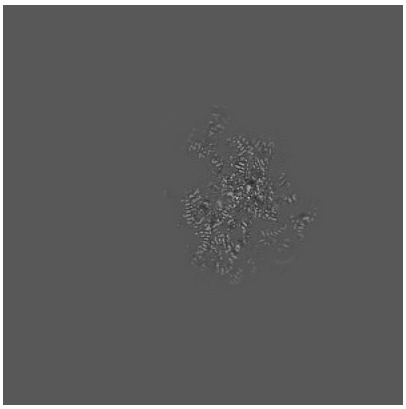
Z

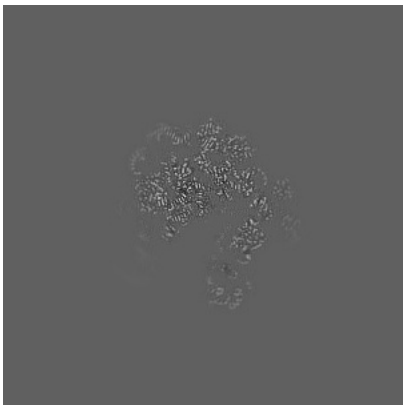
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

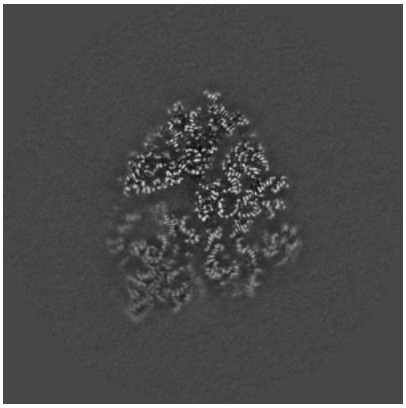
6.2.1 Primary map

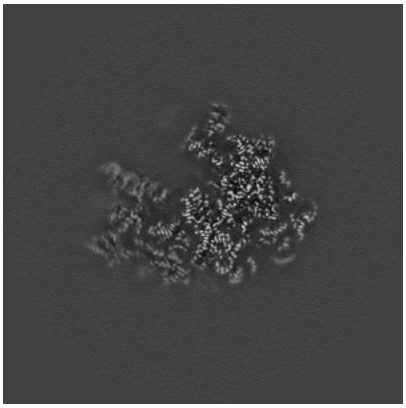
X Index: 256

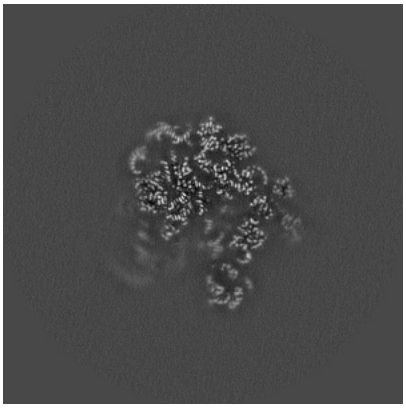

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256


Y Index: 256

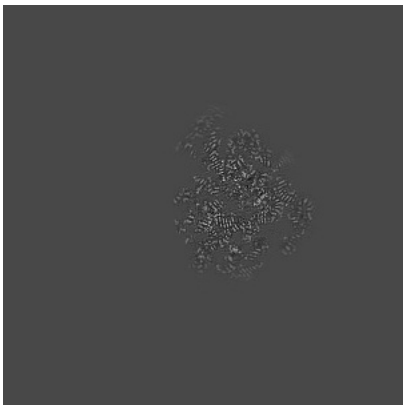

Z Index: 256

The images above show central slices of the map in three orthogonal directions.

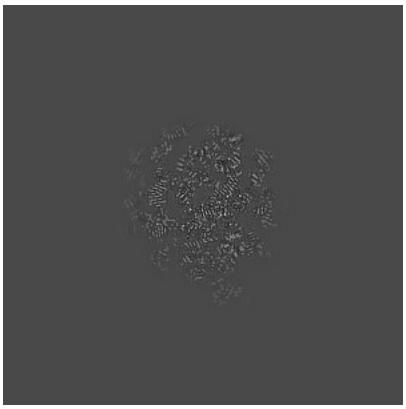
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 274

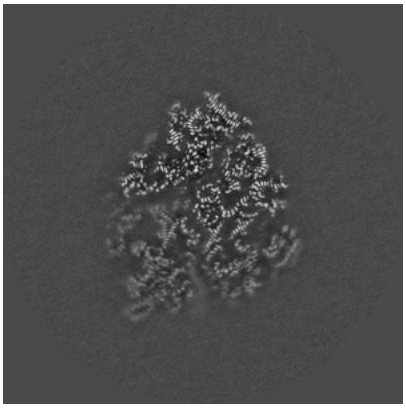


Y Index: 267

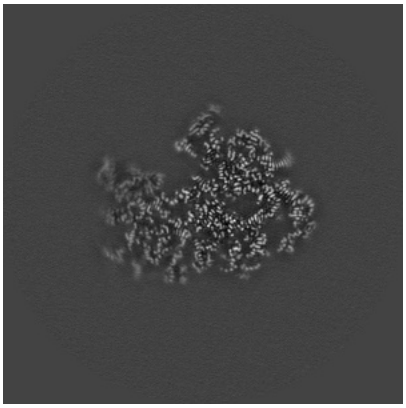


Z Index: 297

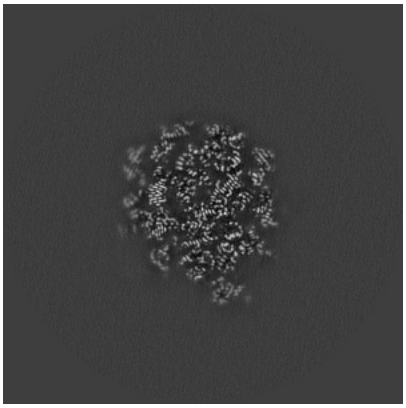
6.3.2 Raw map



X Index: 259



Y Index: 271



Z Index: 297

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

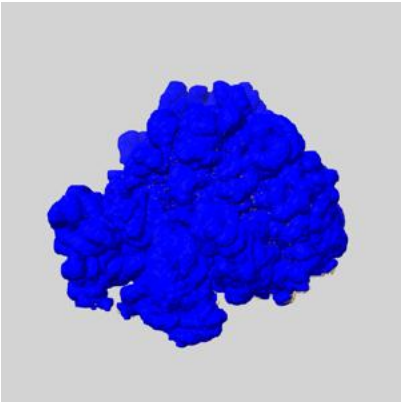
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

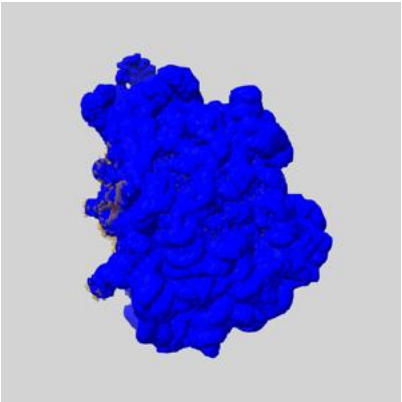
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

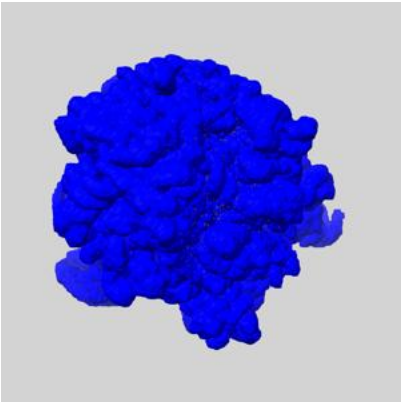
6.5.1 emd_10655_msk_1.map (i)



X



Y

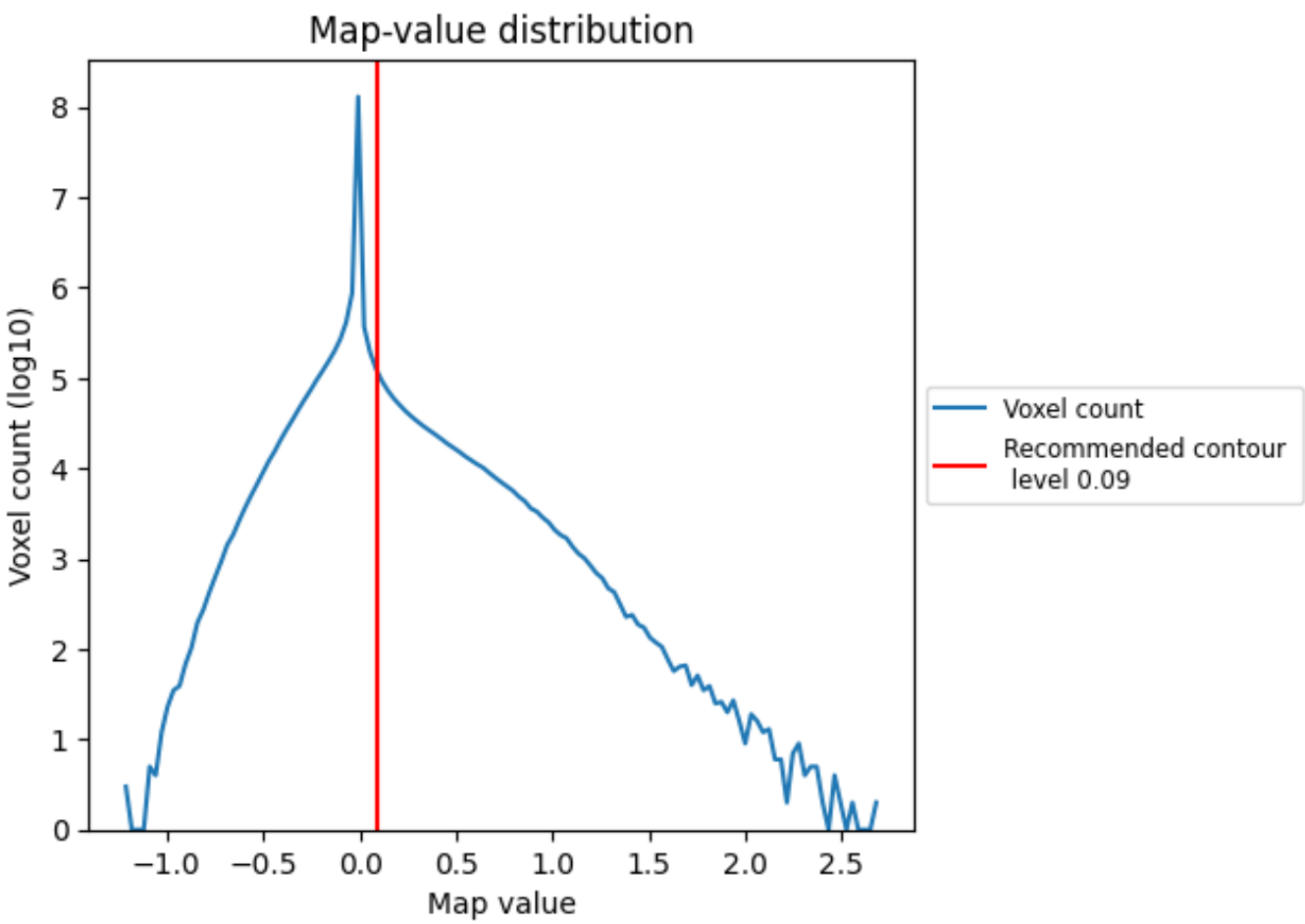


Z

7 Map analysis (i)

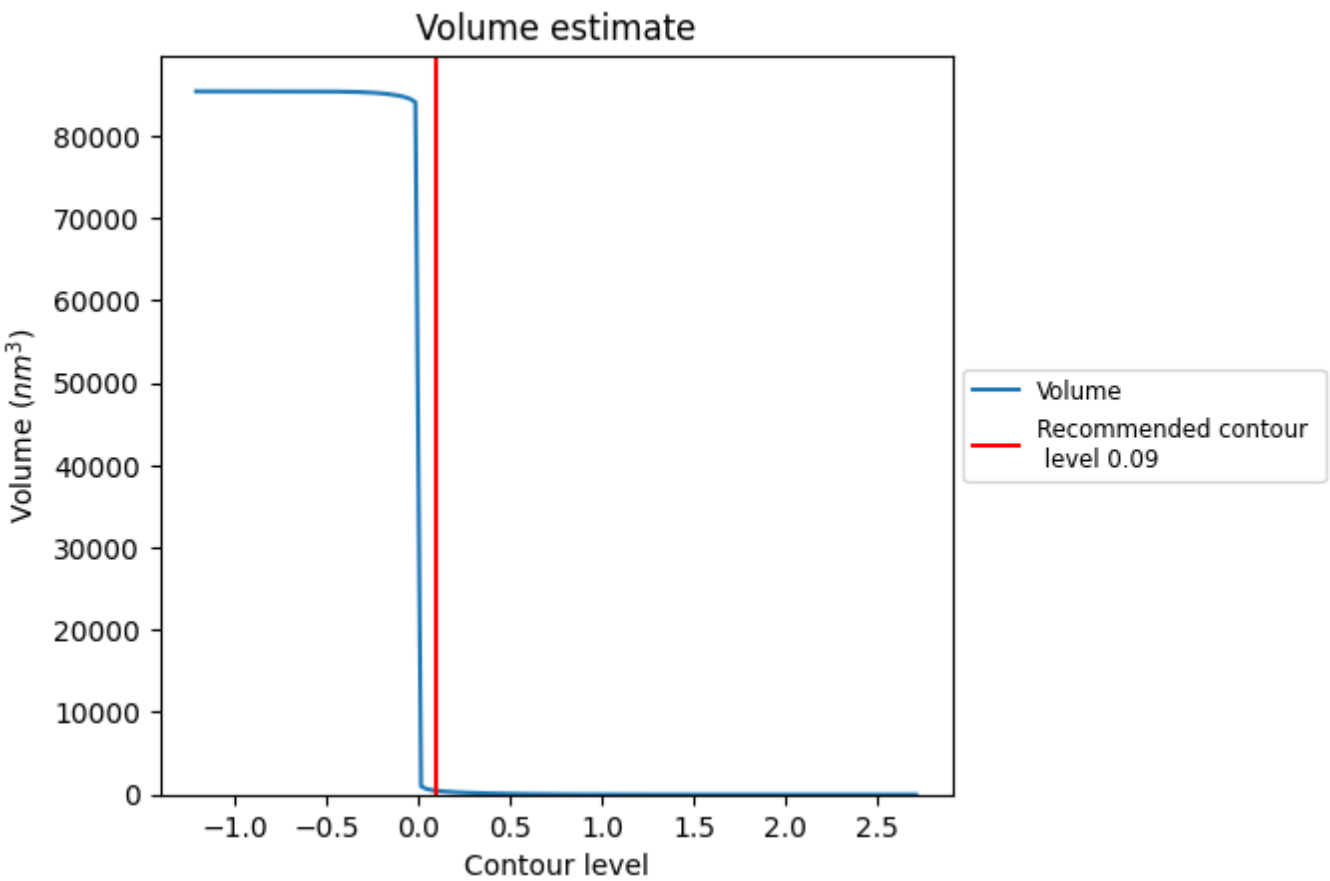
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

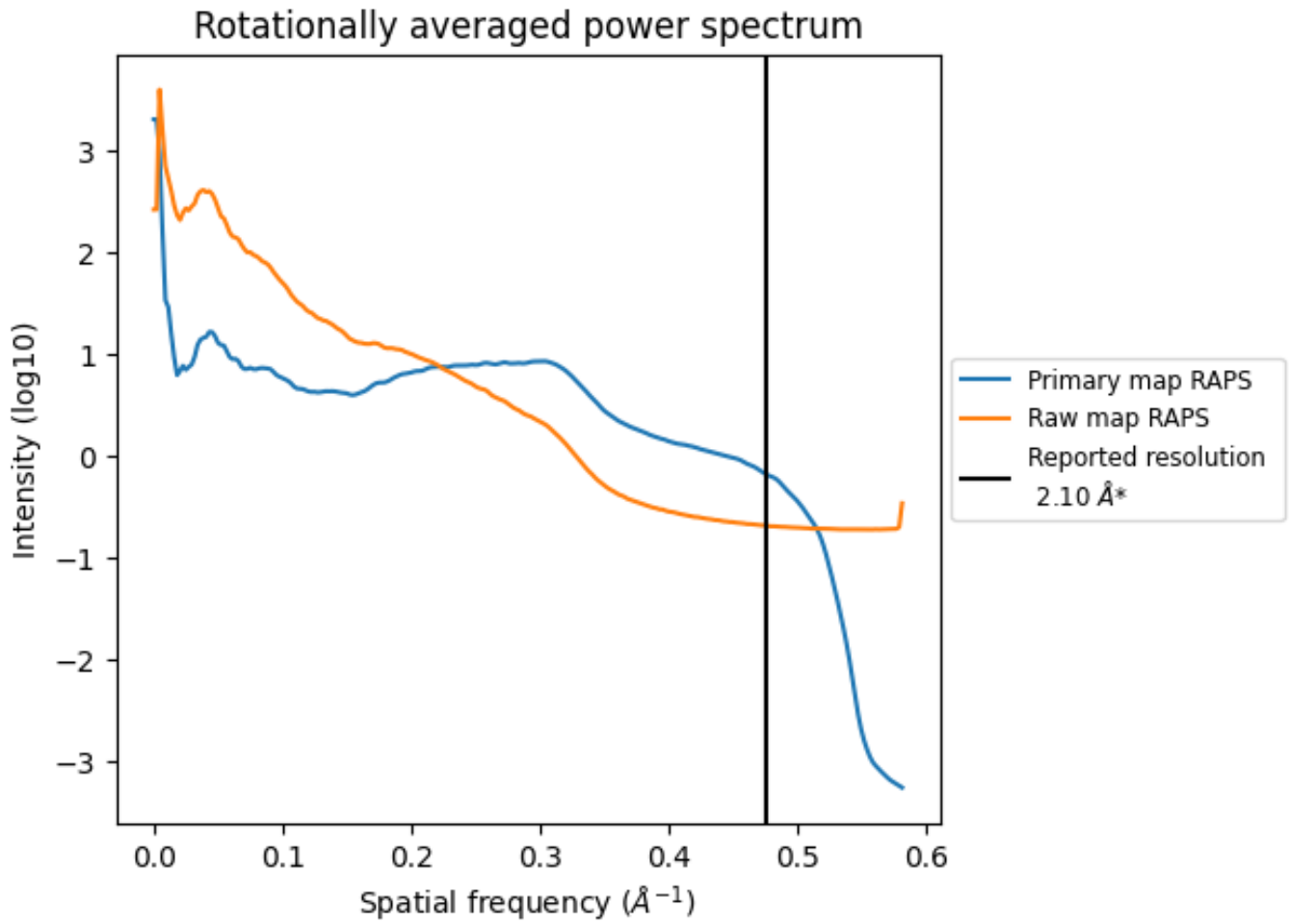
7.2 Volume estimate (i)



The volume at the recommended contour level is 487 nm^3; this corresponds to an approximate mass of 440 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

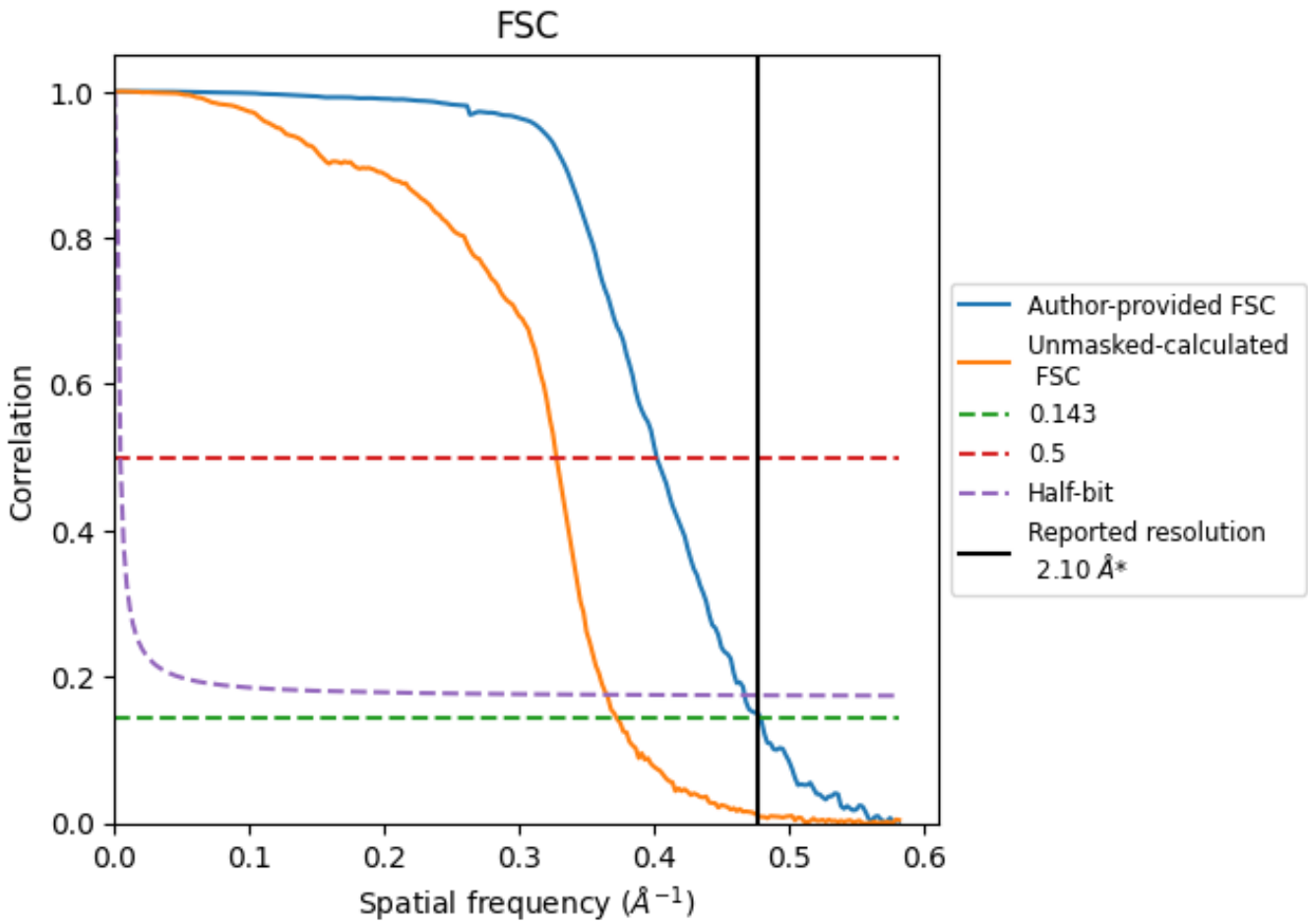


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8.2 Resolution estimates (i)

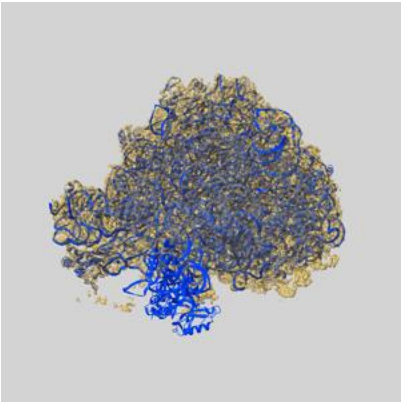
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.09	2.49	2.14
Unmasked-calculated*	2.69	3.05	2.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.69 differs from the reported value 2.1 by more than 10 %

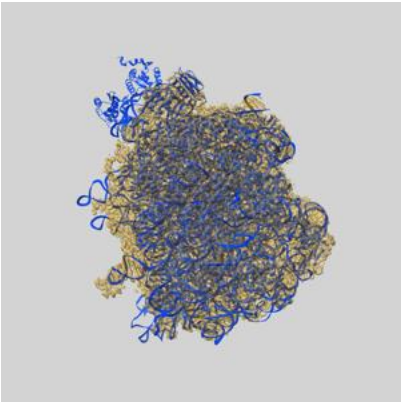
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10655 and PDB model 6XZ7. Per-residue inclusion information can be found in section 3 on page 12.

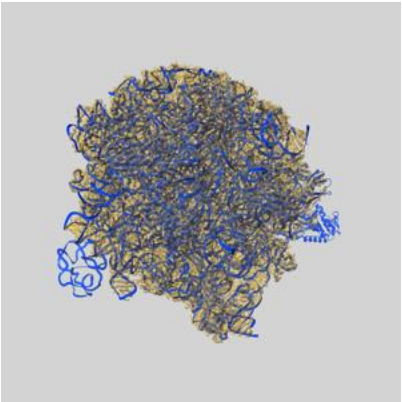
9.1 Map-model overlay (i)



X



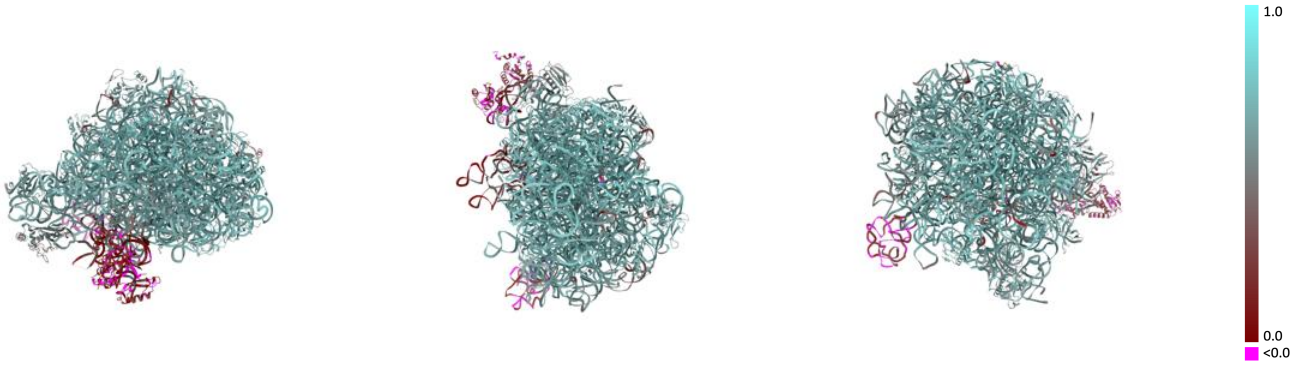
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

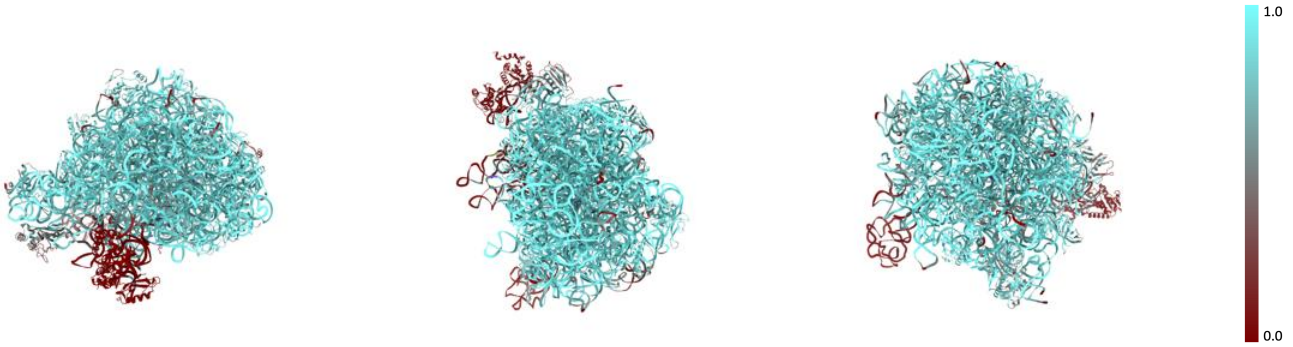
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

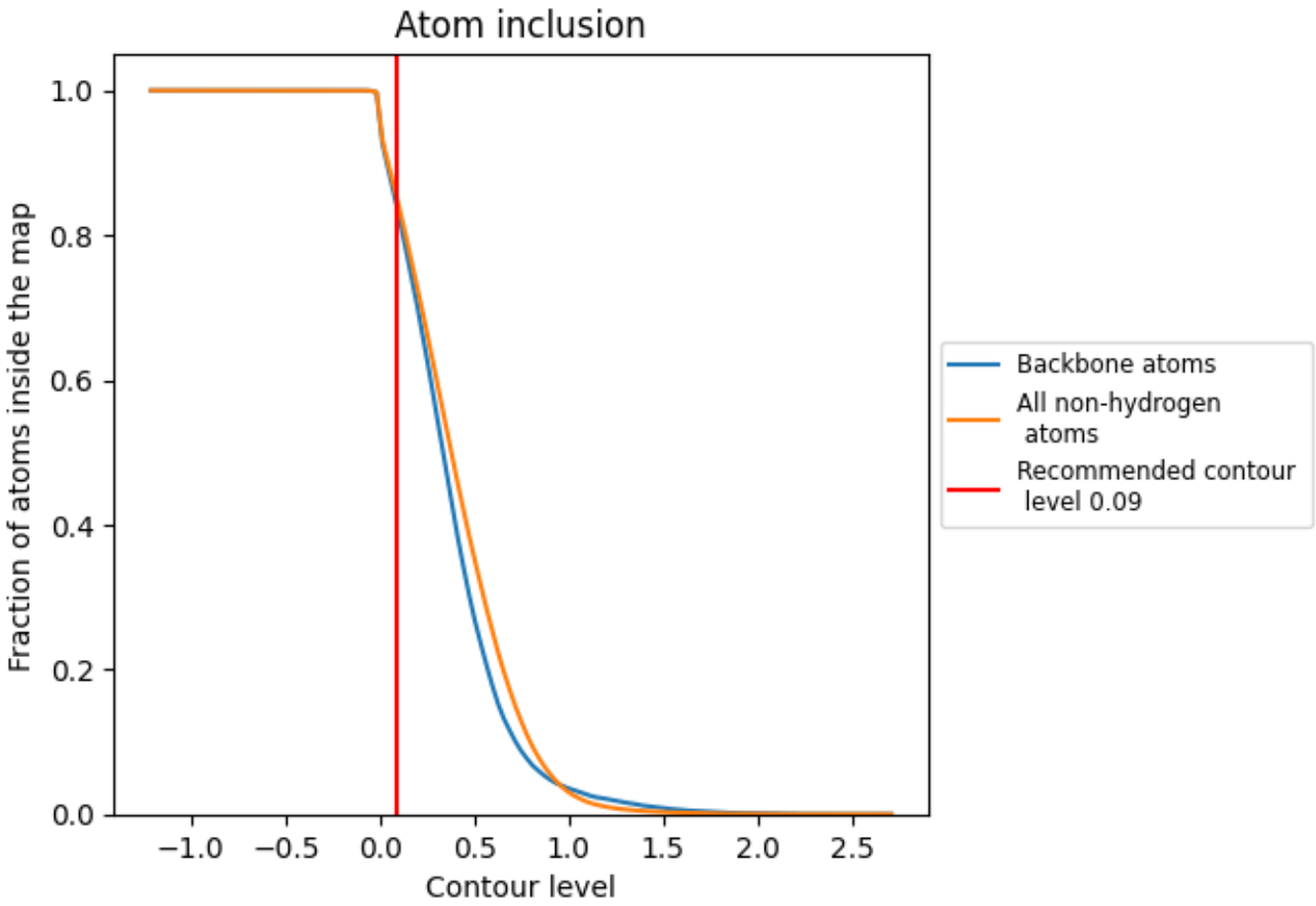
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8517	0.6430
A	0.9028	0.6720
B	0.9086	0.6460
C	0.9499	0.7170
D	0.9344	0.7080
E	0.8783	0.6770
F	0.4672	0.4930
G	0.6222	0.5550
H	0.0000	0.1280
I	0.0000	0.0590
J	0.9373	0.7070
K	0.9338	0.7020
L	0.9277	0.6990
M	0.9406	0.7050
N	0.9257	0.7040
O	0.8060	0.6160
P	0.8930	0.6750
Q	0.9659	0.7490
R	0.8821	0.6700
S	0.9222	0.7070
T	0.8728	0.6540
U	0.8440	0.6310
V	0.8442	0.6340
W	0.9220	0.6990
X	0.9351	0.6880
Y	0.7975	0.6110
Z	0.8970	0.6860
a	0.9182	0.7040
b	0.8448	0.6480
c	0.9577	0.7370
d	0.9776	0.7360
e	0.9486	0.6900
f	0.2320	0.2270
g	0.2573	0.2550