



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:52 AM UTC

PDB ID : 9FRA / pdb_00009fra
EMDB ID : EMD-50709
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to Ss-MAP leaderless mRNA
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-06-18
Resolution : 2.80 Å(reported)

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

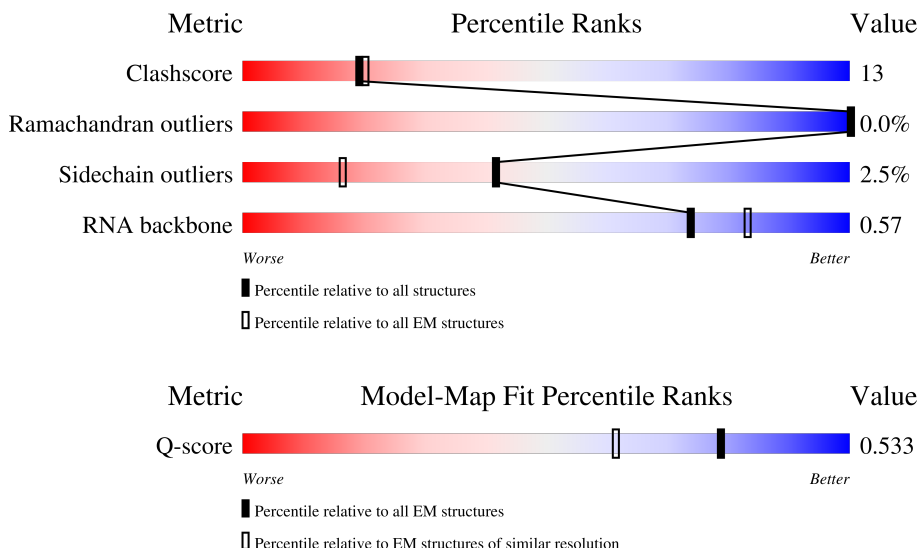
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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 $\leq 5\%$. 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	2	1497	
2	A	208	
3	B	231	

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Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	E	239	
7	F	211	
8	G	214	
9	H	193	
10	I	133	
11	J	133	
12	K	137	
13	L	102	
14	M	132	
15	N	147	
16	O	165	
17	P	54	
18	Q	152	
19	R	114	
20	S	79	
21	T	140	
22	U	158	
23	V	120	
24	W	66	
25	X	83	
26	Y	75	
27	Z	229	
28	3	127	

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Mol	Chain	Length	Quality of chain
29	a	72	
30	c	110	
31	d	72	
32	e	52	
33	5	15	
34	4	77	
35	s	15	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 66665 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 rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1496	Total	C	N	O	P	0	0
			32178	14348	5942	10392	1496		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	930	C4J	U	conflict	GB AE006641.1
2	1466	4AC	C	conflict	GB AE006641.1
2	1467	4AC	C	conflict	GB AE006641.1
2	1477	4AC	C	conflict	GB AE006641.1
2	1478	4AC	C	conflict	GB AE006641.1
2	1496	C	A	conflict	GB AE006641.1

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	186	Total	C	N	O	S	0	0
			1515	974	261	278	2		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1698	1092	291	312	3		

- Molecule 4 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	58	Total	C	N	O	S	0	0
			455	282	84	81	8		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	166	Total	C	N	O	S	0	0
			1354	864	249	240	1		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	238	Total	C	N	O	S	0	0
			1930	1238	342	344	6		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	210	Total	C	N	O	S	0	0
			1625	1041	275	303	6		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	213	Total	C	N	O	S	0	0
			1661	1052	292	315	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	192	Total	C	N	O	S	0	0
			1543	983	283	274	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	132	Total	C	N	O	S	0	0
			1050	675	187	182	6		

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	127	Total	C	N	O		0	0
			982	617	186	179			

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	133	Total	C	N	O	S	0	0
			1068	675	201	185	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			840	536	157	142	5		

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	127	Total	C	N	O	S	0	0
			944	587	184	170	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1140	723	220	193	4		

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	140	Total	C	N	O	S	0	0
			1124	708	210	202	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	53	Total	C	N	O	S	0	0
			440	282	80	74	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	145	Total	C	N	O	S	0	0
			1185	753	224	205	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	113	Total	C	N	O	S	0	0
			901	570	166	161	4		

- Molecule 20 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			571	364	101	105	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	128	Total	C	N	O	S	0	0
			1064	684	192	184	4		

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	154	Total	C	N	O	S	0	0
			1247	805	223	217	2		

- Molecule 23 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	107	Total	C	N	O	S	0	0
			836	524	154	156	2		

- Molecule 24 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	65	Total	C	N	O	S	0	0
			503	319	93	84	7		

- Molecule 25 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	67	Total	C	N	O	0	0
			535	335	103	97		

- Molecule 26 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	49	Total	C	N	O	S	0	0
			395	252	73	65	5		

- Molecule 27 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	196	Total	C	N	O	S	0	0
			1561	1009	274	272	6		

- Molecule 28 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 29 is a protein called aS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	71	Total	C	N	O	S	0	0
			562	361	98	96	7		

- Molecule 30 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	109	Total	C	N	O	S	0	0
			856	539	152	164	1		

- Molecule 31 is a protein called VapB-type antitoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	70	Total	C	N	O	S	0	0
			570	370	92	105	3		

- Molecule 32 is a protein called LSU ribosomal protein S30E (Rps30E).

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	43	Total	C	N	O	0	0
			354	220	74	60		

- Molecule 33 is a RNA chain called mRNA_Map.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	14	Total	C	N	O	P	1	0
			345	146	64	116	19		

- Molecule 34 is a RNA chain called tRNA initiator Met.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	4	77	Total	C	N	O	P	S	0	0
			1645	734	296	537	77	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	C	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

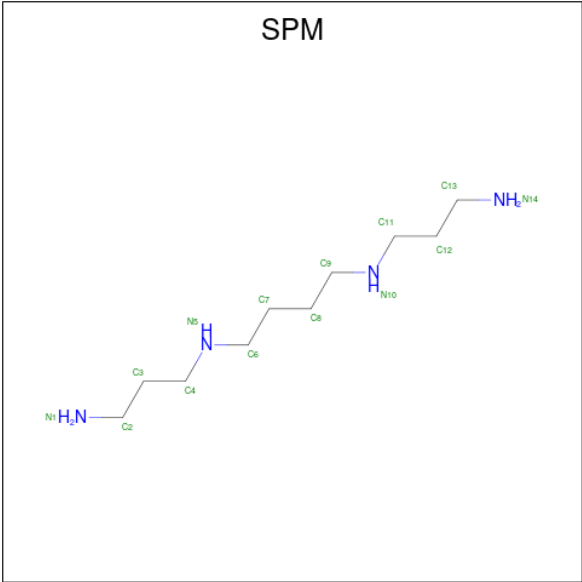
- Molecule 35 is a RNA chain called mRNA_Map.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	s	10	Total	C	N	O	P	0	0
			220	98	44	68	10		

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	53	Total	Mg	0
			53	53	
36	F	2	Total	Mg	0
			2	2	
36	P	1	Total	Mg	0
			1	1	
36	R	1	Total	Mg	0
			1	1	
36	5	1	Total	Mg	0
			1	1	

- Molecule 37 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	C	2	Total	Zn	0
			2	2	
38	F	1	Total	Zn	0
			1	1	
38	P	1	Total	Zn	0
			1	1	
38	R	1	Total	Zn	0
			1	1	
38	W	1	Total	Zn	0
			1	1	
38	a	2	Total	Zn	0
			2	2	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	2	199	Total	O	0
			199	199	
39	D	1	Total	O	0
			1	1	
39	E	1	Total	O	0
			1	1	
39	H	1	Total	O	0
			1	1	

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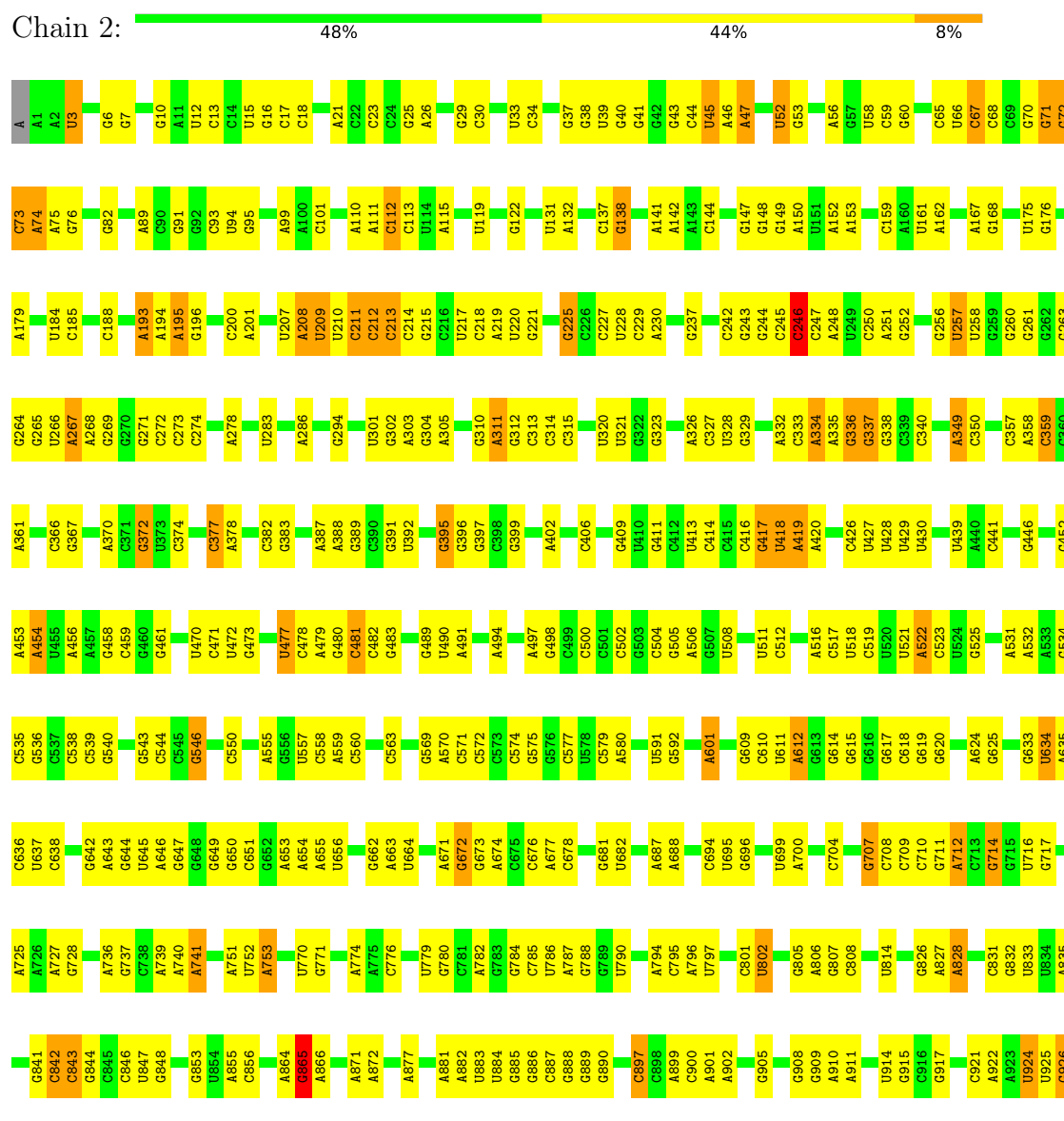
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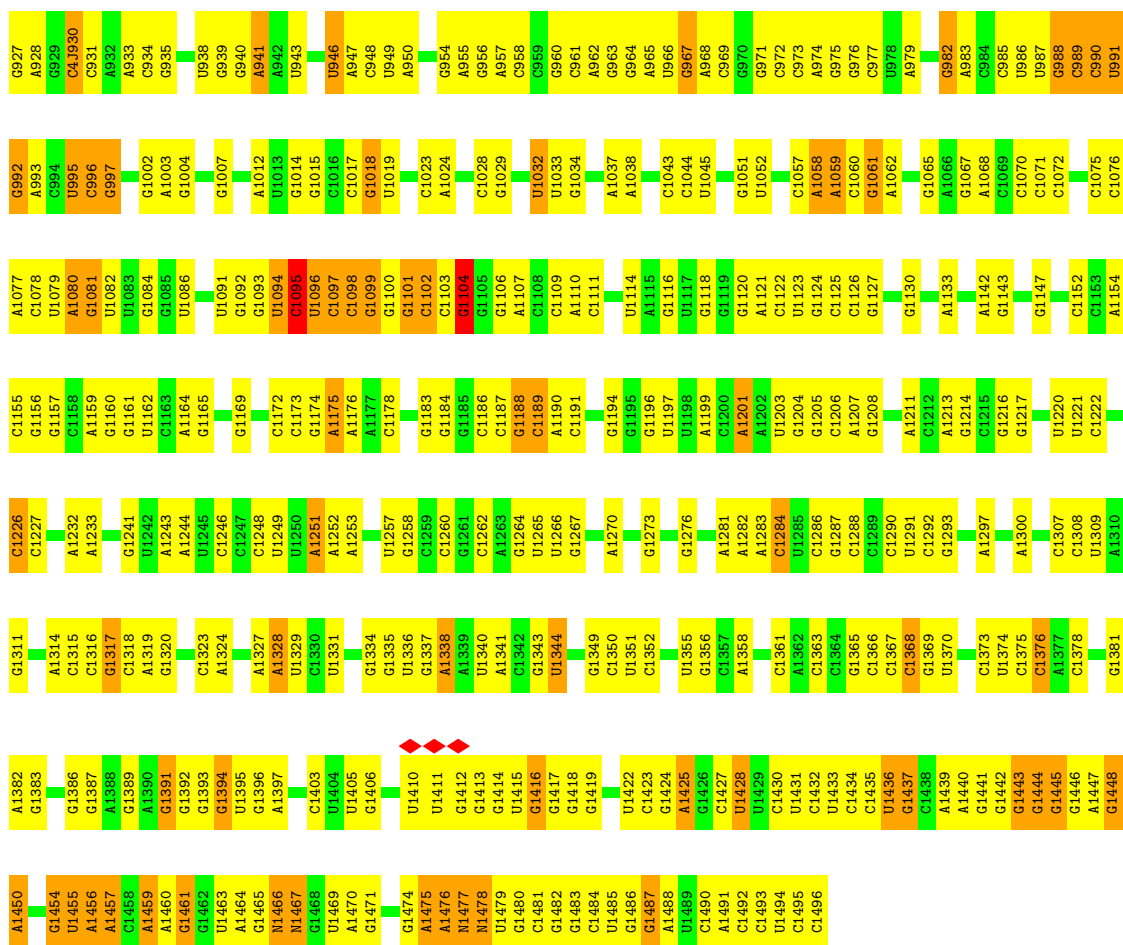
Mol	Chain	Residues	Atoms		AltConf
39	I	2	Total 2	O 2	0
39	K	2	Total 2	O 2	0
39	P	1	Total 1	O 1	0
39	Q	1	Total 1	O 1	0
39	R	2	Total 2	O 2	0
39	5	8	Total 8	O 8	0
39	4	3	Total 3	O 3	0

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.

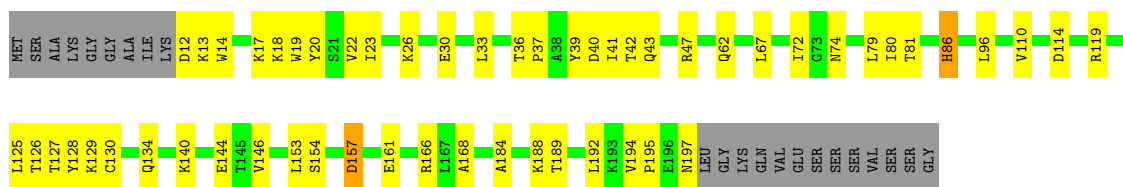
• Molecule 1: rRNA 16S





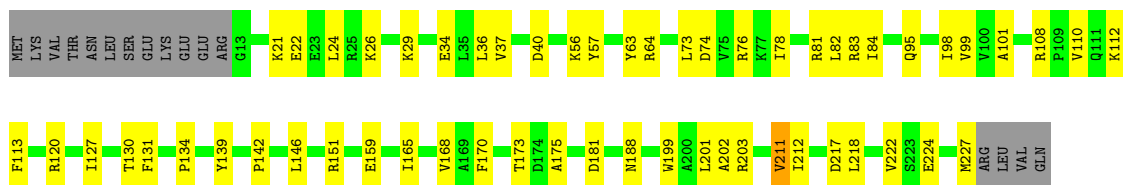
• Molecule 2: Small ribosomal subunit protein eS1

Chain A: 63% 25% 11%



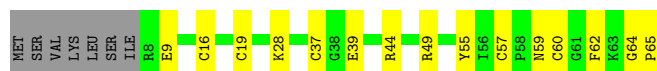
• Molecule 3: Small ribosomal subunit protein uS2

Chain B: 68% 24% 7%



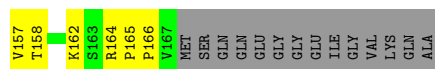
• Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein

Chain C:  66% 23% 11%




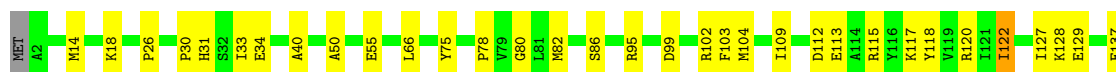
- Molecule 5: Small ribosomal subunit protein uS4

Chain D:  70% 21% 8%




- Molecule 6: Small ribosomal subunit protein eS4

Chain E:  76% 23%



- Molecule 7: Small ribosomal subunit protein uS5

Chain F:  82% 17%



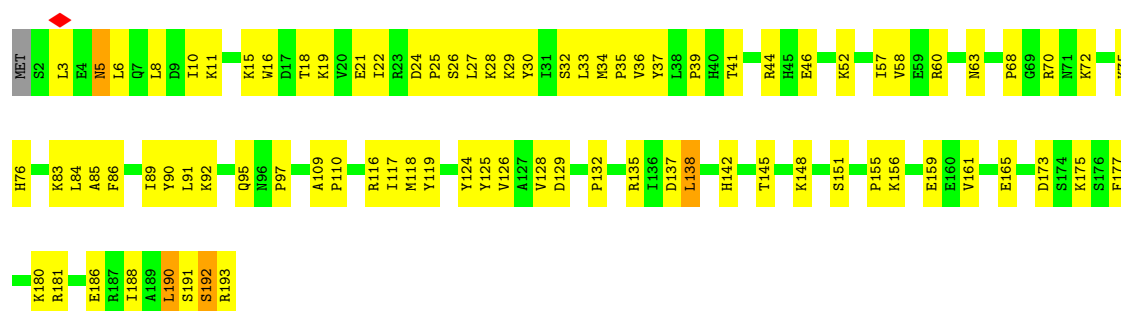
- Molecule 8: Small ribosomal subunit protein eS6

Chain G:  72% 26%



- Molecule 9: Small ribosomal subunit protein uS7

Chain H:  56% 41%



- Molecule 10: Small ribosomal subunit protein uS8

Chain I: 81% 17% ..



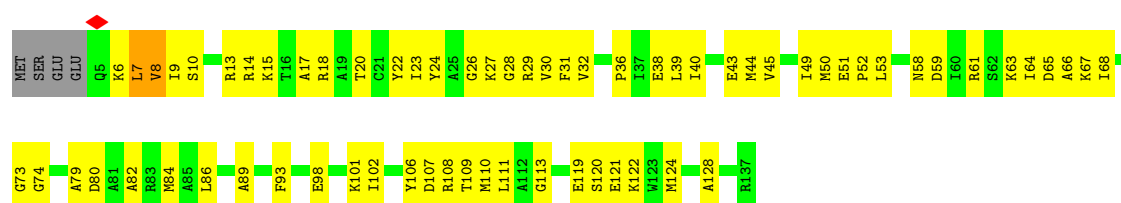
- Molecule 11: Small ribosomal subunit protein eS8

Chain J: 72% 23% 5%



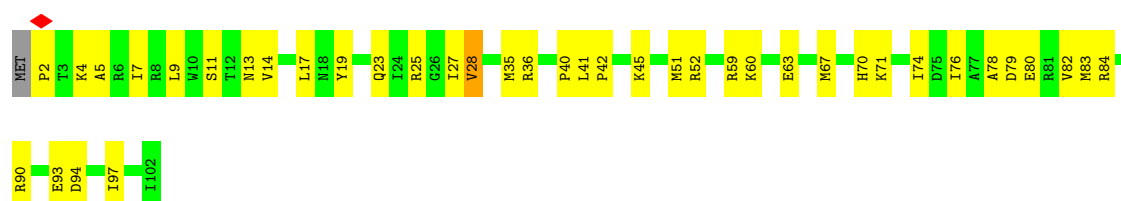
- Molecule 12: Small ribosomal subunit protein uS9

Chain K: 48% 47% ..



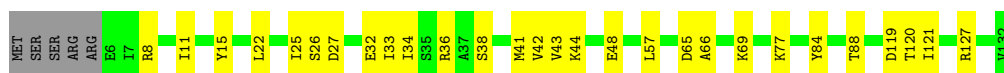
- Molecule 13: Small ribosomal subunit protein uS10

Chain L: 60% 38% ..



- Molecule 14: Small ribosomal subunit protein uS11

Chain M: 75% 21% .



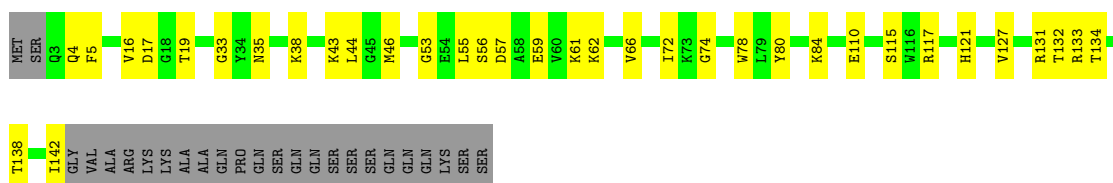
- Molecule 15: Small ribosomal subunit protein uS12

Chain N: 74% 25%



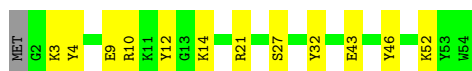
- Molecule 16: Small ribosomal subunit protein uS13

Chain O: 64% 21% 15%



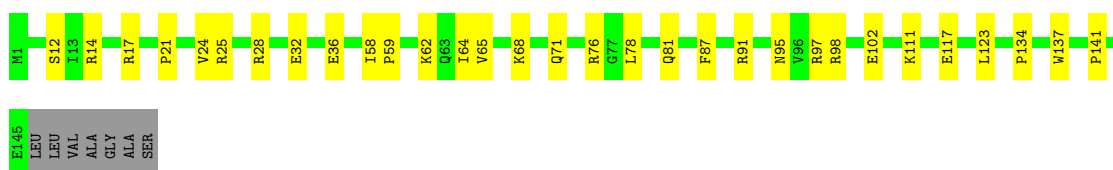
- Molecule 17: Small ribosomal subunit protein uS14

Chain P: 76% 22%



- Molecule 18: Small ribosomal subunit protein uS15

Chain Q: 75% 20% 5%



- Molecule 19: Small ribosomal subunit protein uS17

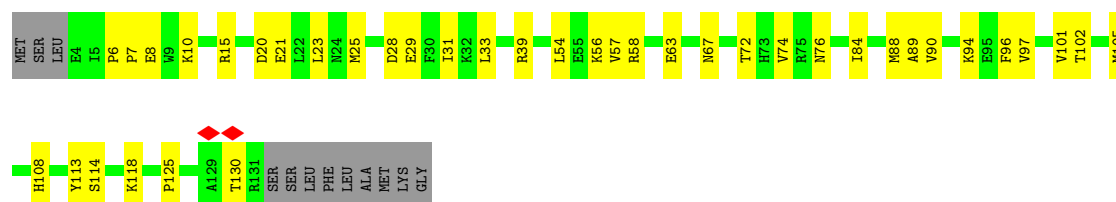
Chain R: 86% 12%



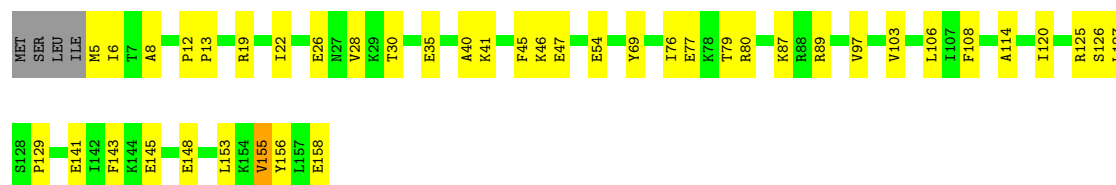
- Molecule 20: Small ribosomal subunit protein eS17



- Molecule 21: Small ribosomal subunit protein uS19



- Molecule 22: Small ribosomal subunit protein eS19



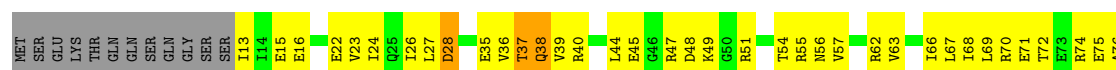
- Molecule 23: Small ribosomal subunit protein eS24

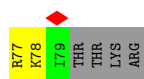


- Molecule 24: Small ribosomal subunit protein eS27

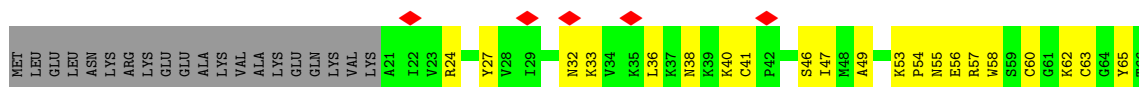


- Molecule 25: Small ribosomal subunit protein eS28





- Molecule 26: Small ribosomal subunit protein eS31

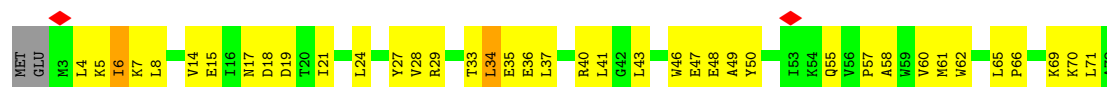


- Molecule 27: Small ribosomal subunit protein uS3





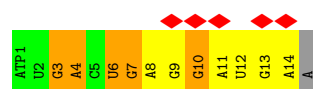
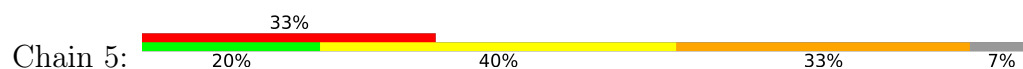
- Molecule 31: VapB-type antitoxin



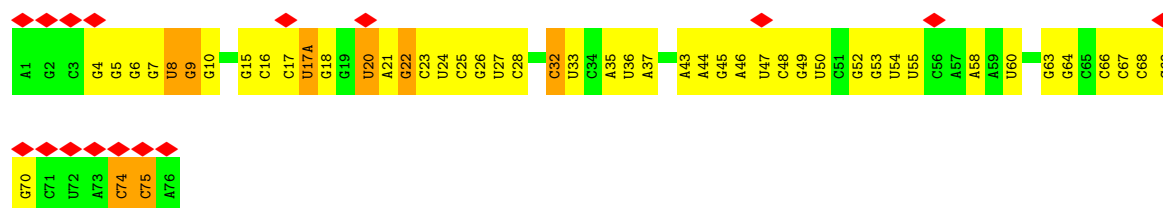
- Molecule 32: LSU ribosomal protein S30E (Rps30E)



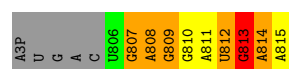
- Molecule 33: mRNA_Map



- Molecule 34: tRNA initiator Met



- Molecule 35: mRNA_Map



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	365.292, 365.292, 365.292	wwPDB
Map dimensions	438, 438, 438	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, SPM, H2U, ATP, 5MC, A2M, OMC, PSU, MG, C4J, 4SU, ZN, MA6, 4AC, 6MZ, OMG, OMU

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	2	0.25	5/35206 (0.0%)	0.29	5/54930 (0.0%)
2	A	0.19	0/1543	0.37	0/2077
3	B	0.18	0/1731	0.37	0/2349
4	C	0.20	0/466	0.39	0/625
5	D	0.20	0/1380	0.28	0/1859
6	E	0.21	0/1965	0.37	0/2644
7	F	0.23	0/1654	0.38	0/2240
8	G	0.16	0/1684	0.36	0/2265
9	H	0.20	0/1571	0.45	0/2116
10	I	0.23	0/1070	0.31	0/1444
11	J	0.22	0/994	0.37	0/1337
12	K	0.20	0/1084	0.47	0/1450
13	L	0.23	0/856	0.52	0/1154
14	M	0.22	0/960	0.50	0/1294
15	N	0.22	0/1155	0.39	0/1540
16	O	0.17	0/1142	0.40	0/1532
17	P	0.21	0/451	0.33	0/600
18	Q	0.20	0/1206	0.35	0/1618
19	R	0.24	0/918	0.35	0/1236
20	S	0.22	0/578	0.51	0/770
21	T	0.16	0/1087	0.30	0/1456
22	U	0.18	0/1270	0.37	0/1710
23	V	0.19	0/843	0.39	0/1124
24	W	0.23	0/511	0.48	0/684
25	X	0.18	0/538	0.48	0/722
26	Y	0.19	0/404	0.55	0/540
27	Z	0.20	0/1584	0.37	1/2124 (0.0%)
28	3	0.18	0/902	0.46	0/1216
29	a	0.20	0/574	0.44	0/770
30	c	0.18	0/861	0.49	0/1143
31	d	0.21	0/581	0.54	0/786

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.20	0/360	0.47	0/477
33	5	0.29	0/317	0.40	0/493
34	4	0.17	1/1725 (0.1%)	0.21	0/2687
35	s	0.38	0/247	0.75	1/384 (0.3%)
All	All	0.23	6/69418 (0.0%)	0.34	7/101396 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1095	C	C4'-O4'	12.46	1.64	1.45
1	2	843	C	O3'-P	-11.38	1.44	1.61
1	2	843	C	C1'-N1	6.52	1.58	1.48
1	2	678	C	O3'-P	5.85	1.70	1.61
1	2	842	C	O3'-P	-5.43	1.53	1.61
34	4	8	4SU	O3'-P	5.13	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1095	C	C1'-O4'-C4'	-10.02	99.68	109.70
1	2	843	C	O3'-P-O5'	9.48	118.23	104.00
1	2	842	C	O3'-P-O5'	-7.62	92.58	104.00
1	2	843	C	P-O3'-C3'	-7.56	108.86	120.20
1	2	1104	G	C5'-C4'-O4'	-5.60	101.40	109.80
27	Z	25	GLN	N-CA-C	5.27	119.84	113.41
35	s	813	G	C4'-C3'-O3'	5.20	117.20	109.40

There are no chirality outliers.

There are no planarity outliers.

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	2	32178	0	16275	617	0
2	A	1515	0	1565	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1698	0	1753	39	0
4	C	455	0	437	15	0
5	D	1354	0	1419	26	0
6	E	1930	0	2013	42	0
7	F	1625	0	1689	25	0
8	G	1661	0	1737	48	0
9	H	1543	0	1611	96	0
10	I	1050	0	1100	16	0
11	J	982	0	1046	21	0
12	K	1068	0	1125	65	0
13	L	840	0	893	35	0
14	M	944	0	978	33	0
15	N	1140	0	1244	27	0
16	O	1124	0	1162	26	0
17	P	440	0	435	12	0
18	Q	1185	0	1260	21	0
19	R	901	0	935	11	0
20	S	571	0	598	21	0
21	T	1064	0	1107	32	0
22	U	1247	0	1329	39	0
23	V	836	0	894	24	0
24	W	503	0	532	17	0
25	X	535	0	572	38	0
26	Y	395	0	405	23	0
27	Z	1561	0	1667	45	0
28	3	893	0	940	68	0
29	a	562	0	574	18	0
30	c	856	0	941	31	0
31	d	570	0	590	37	0
32	e	354	0	386	9	0
33	5	345	0	163	10	0
34	4	1645	0	840	34	0
35	s	220	0	109	7	0
36	2	53	0	0	0	0
36	5	1	0	0	0	0
36	F	2	0	0	0	0
36	P	1	0	0	0	0
36	R	1	0	0	0	0
37	2	588	0	1091	58	0
38	C	2	0	0	0	0
38	F	1	0	0	0	0
38	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	R	1	0	0	0	0
38	W	1	0	0	0	0
38	a	2	0	0	0	0
39	2	199	0	0	8	0
39	4	3	0	0	0	0
39	5	8	0	0	0	0
39	D	1	0	0	0	0
39	E	1	0	0	0	0
39	H	1	0	0	0	0
39	I	2	0	0	0	0
39	K	2	0	0	0	0
39	P	1	0	0	0	0
39	Q	1	0	0	0	0
39	R	2	0	0	0	0
All	All	66665	0	51415	1483	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 13.

All (1483) 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)
1:2:1095:C:O4'	1:2:1095:C:C4'	1.64	1.37
9:H:6:LEU:HD21	9:H:8:LEU:HD23	1.35	1.08
1:2:677:A:H5'	14:M:119:ASP:CG	1.79	1.06
1:2:677:A:H5'	14:M:119:ASP:OD2	1.63	0.97
1:2:1096:U:C2	1:2:1098:C:N3	2.35	0.95
13:L:79:ASP:OD1	13:L:82:VAL:HG13	1.67	0.94
28:3:55:GLU:O	28:3:60:GLU:OE2	1.84	0.94
1:2:949:U:H3	1:2:1183:G:H1	1.00	0.93
28:3:56:ASP:HA	28:3:60:GLU:OE2	1.68	0.92
28:3:32:ILE:O	28:3:33:LYS:HG3	1.72	0.90
9:H:11:LYS:NZ	9:H:15:LYS:C	2.29	0.90
9:H:11:LYS:NZ	9:H:15:LYS:O	2.08	0.87
9:H:11:LYS:HZ1	9:H:15:LYS:C	1.82	0.87
4:C:16:CYS:HB3	4:C:19:CYS:SG	2.14	0.86
1:2:1096:U:H2'	1:2:1098:C:C5	2.09	0.85
1:2:1406:G:H1	1:2:1415:U:H3	1.22	0.84
1:2:500:C:OP2	32:e:25:LYS:NZ	2.12	0.83
34:4:50:U:H3	34:4:64:G:H1	0.84	0.82
1:2:1189:C:HO2'	30:c:2:GLY:N	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:71:G:N1	1:2:213:C:N3	2.28	0.81
28:3:18:LYS:NZ	28:3:110:LEU:O	2.13	0.80
1:2:677:A:H5'	14:M:119:ASP:OD1	1.81	0.79
9:H:8:LEU:HD12	9:H:8:LEU:O	1.81	0.79
1:2:1096:U:H2'	1:2:1098:C:C4	2.18	0.79
13:L:19:TYR:OH	13:L:90:ARG:NH1	2.16	0.79
1:2:71:G:N2	1:2:213:C:O2	2.16	0.78
1:2:1095:C:H1'	1:2:1096:U:H5'	1.64	0.78
12:K:27:LYS:NZ	22:U:155:VAL:O	2.17	0.78
1:2:6:G:OP1	37:2:1581:SPM:H42	1.84	0.77
8:G:203:GLN:N	8:G:203:GLN:OE1	2.18	0.77
9:H:6:LEU:CD2	9:H:8:LEU:HD23	2.14	0.77
28:3:57:VAL:O	28:3:60:GLU:CG	2.32	0.77
5:D:164:ARG:O	5:D:164:ARG:NH1	2.18	0.77
28:3:49:LYS:HZ1	28:3:103:GLU:H	1.31	0.77
9:H:6:LEU:HD21	9:H:8:LEU:CD2	2.15	0.76
9:H:22:ILE:O	9:H:28:LYS:NZ	2.19	0.76
28:3:55:GLU:O	28:3:60:GLU:CD	2.28	0.76
13:L:11:SER:HB3	13:L:17:LEU:HG	1.66	0.75
1:2:1091:U:H3	1:2:1104:G:H1	1.35	0.75
5:D:116:SER:HB2	5:D:121:GLN:HG2	1.69	0.74
12:K:124:MET:HE2	13:L:60:LYS:H	1.53	0.74
15:N:99:GLU:OE1	15:N:99:GLU:N	2.20	0.74
1:2:965:A:H2'	28:3:94:VAL:HG11	1.70	0.74
1:2:1082:U:C2	1:2:1084:G:C8	2.76	0.74
14:M:48:GLU:OE1	14:M:48:GLU:N	2.19	0.74
9:H:90:TYR:HB2	9:H:97:PRO:HG3	1.69	0.73
28:3:19:VAL:HG12	28:3:114:ILE:HG12	1.69	0.73
18:Q:134:PRO:HG2	18:Q:137:TRP:HB2	1.70	0.73
9:H:29:LYS:NZ	31:d:27:TYR:O	2.22	0.73
11:J:33:THR:HG21	11:J:56:ARG:HD3	1.71	0.73
22:U:45:PHE:HB2	22:U:87:LYS:HB2	1.70	0.73
28:3:110:LEU:C	28:3:110:LEU:HD13	2.14	0.73
1:2:1096:U:C2	1:2:1098:C:C2	2.77	0.73
1:2:1096:U:N3	1:2:1098:C:N3	2.37	0.72
1:2:619:G:H2'	1:2:620:G:C8	2.25	0.72
4:C:57:CYS:CB	4:C:60:CYS:SG	2.77	0.72
21:T:25:MET:HE2	21:T:29:GLU:HG3	1.70	0.72
1:2:967:G:N7	28:3:37:ASN:ND2	2.38	0.72
1:2:550:C:OP1	10:I:32:LYS:NZ	2.23	0.72
9:H:26:SER:HA	25:X:66:ILE:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:29:ARG:NH2	22:U:156:TYR:O	2.22	0.71
9:H:41:THR:O	9:H:44:ARG:NH1	2.23	0.71
1:2:644:G:N3	14:M:36:ARG:NH2	2.35	0.71
4:C:59:ASN:OD1	4:C:60:CYS:N	2.23	0.71
27:Z:58:ARG:O	27:Z:58:ARG:NH1	2.22	0.71
25:X:35:GLU:N	25:X:35:GLU:OE1	2.22	0.71
28:3:57:VAL:O	28:3:60:GLU:HG3	1.90	0.71
8:G:142:GLN:H	8:G:142:GLN:CD	1.99	0.71
1:2:481:OMC:HM22	1:2:482:C:H5'	1.72	0.70
9:H:89:ILE:HD11	9:H:97:PRO:HA	1.73	0.70
18:Q:97:ARG:NH2	18:Q:117:GLU:OE2	2.24	0.70
1:2:310:G:HO2'	5:D:2:GLY:N	1.88	0.70
31:d:18:ASP:OD1	31:d:19:ASP:N	2.24	0.70
19:R:23:CYS:HB2	19:R:83:PRO:HG2	1.74	0.70
23:V:59:GLN:OE1	23:V:59:GLN:N	2.25	0.70
5:D:154:ASP:OD1	5:D:155:TYR:N	2.24	0.70
29:a:22:ARG:NH1	29:a:45:TYR:O	2.24	0.70
12:K:14:ARG:HG2	12:K:80:ASP:HB3	1.74	0.70
28:3:50:LEU:HD11	28:3:115:ILE:HD11	1.74	0.70
1:2:39:U:O4	6:E:18:LYS:NZ	2.25	0.70
34:4:9:G:O2'	34:4:10:G:N7	2.24	0.70
1:2:1188:G:H3'	1:2:1188:G:N3	2.07	0.69
1:2:1490:C:H2'	1:2:1491:A:H8	1.58	0.69
9:H:26:SER:HB3	25:X:68:ILE:HD11	1.74	0.69
18:Q:81:GLN:OE1	18:Q:81:GLN:N	2.20	0.69
1:2:71:G:O6	1:2:213:C:N4	2.25	0.69
1:2:676:C:H4'	14:M:119:ASP:OD2	1.92	0.69
1:2:921:C:O3'	21:T:118:LYS:NZ	2.26	0.69
13:L:93:GLU:OE2	27:Z:37:LEU:HA	1.93	0.69
18:Q:98:ARG:NH1	18:Q:102:GLU:OE2	2.24	0.69
23:V:44:SER:OG	23:V:47:ASP:OD2	2.10	0.69
1:2:1203:U:H5'	30:c:102:ARG:HD3	1.74	0.68
1:2:1251:A:H2'	1:2:1252:A:C8	2.27	0.68
1:2:786:U:OP2	24:W:6:ARG:NH2	2.26	0.68
3:B:95:GLN:OE1	3:B:95:GLN:N	2.19	0.68
12:K:102:ILE:HD13	31:d:66:PRO:HB2	1.74	0.68
27:Z:80:GLN:OE1	27:Z:80:GLN:N	2.26	0.68
1:2:900:C:H2'	1:2:901:A:H8	1.58	0.68
1:2:910:A:H2'	1:2:911:A:C8	2.29	0.68
1:2:1081:G:N2	1:2:1082:U:O4	2.26	0.68
1:2:1391:G:H2'	1:2:1392:G:H8	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:45:LYS:HB2	8:G:93:TRP:HB2	1.76	0.68
1:2:885:G:H2'	1:2:886:G:C8	2.29	0.68
22:U:77:GLU:OE1	22:U:77:GLU:N	2.26	0.68
1:2:973:C:N4	1:2:982:G:O6	2.19	0.68
27:Z:35:GLU:HG3	27:Z:48:TYR:HE1	1.59	0.68
1:2:337:OMG:HM22	1:2:338:G:H5'	1.76	0.68
8:G:167:VAL:HG21	8:G:196:ILE:HD11	1.74	0.67
6:E:161:GLU:OE1	6:E:164:SER:OG	2.12	0.67
19:R:20:GLU:OE1	19:R:20:GLU:N	2.26	0.67
34:4:32:OMC:HM22	34:4:33:U:H5'	1.76	0.67
11:J:81:ILE:HD11	11:J:96:ILE:HG12	1.76	0.67
28:3:57:VAL:O	28:3:60:GLU:HG2	1.95	0.67
22:U:76:ILE:O	22:U:79:THR:OG1	2.12	0.67
9:H:3:LEU:O	31:d:70:LYS:NZ	2.28	0.67
1:2:610:C:N4	1:2:712:A:OP2	2.27	0.67
1:2:1032:OMU:HM22	1:2:1033:U:H5'	1.76	0.67
28:3:51:VAL:HB	28:3:66:LEU:HD21	1.77	0.67
2:A:119:ARG:HB2	2:A:192:LEU:HD21	1.77	0.67
13:L:94:ASP:OD1	13:L:94:ASP:N	2.28	0.67
12:K:32:VAL:HG21	12:K:40:ILE:HD11	1.77	0.66
1:2:1102:C:H5''	1:2:1102:C:C6	2.30	0.66
1:2:150:A:N7	37:2:1585:SPM:N14	2.43	0.66
1:2:843:C:H5	15:N:6:SER:HG	1.41	0.66
30:c:5:SER:OG	30:c:7:LYS:NZ	2.28	0.66
31:d:5:LYS:HA	31:d:5:LYS:HE2	1.78	0.66
2:A:161:GLU:OE2	2:A:166:ARG:NH1	2.27	0.66
16:O:43:LYS:HZ1	16:O:74:GLY:H	1.43	0.66
16:O:72:ILE:O	16:O:80:TYR:OH	2.13	0.66
15:N:49:MET:HB3	15:N:106:THR:HG22	1.78	0.66
30:c:39:GLU:HB2	30:c:76:ILE:HA	1.78	0.66
1:2:1034:G:N2	1:2:1037:A:OP2	2.25	0.66
3:B:98:ILE:HG12	3:B:142:PRO:HB3	1.76	0.66
16:O:84:LYS:O	21:T:15:ARG:NH1	2.28	0.66
7:F:198:LEU:O	7:F:201:THR:OG1	2.13	0.66
12:K:38:GLU:OE2	12:K:61:ARG:NH2	2.29	0.66
1:2:672:OMG:H2'	1:2:673:G:C8	2.31	0.66
1:2:1165:G:N2	17:P:43:GLU:OE1	2.28	0.66
3:B:84:ILE:HD13	4:C:62:PHE:CE1	2.30	0.66
9:H:117:ILE:HD13	9:H:126:VAL:HB	1.78	0.66
27:Z:130:GLU:HG3	27:Z:148:LYS:HB2	1.78	0.66
11:J:63:ALA:HB2	11:J:78:ILE:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:32:ILE:O	28:3:33:LYS:CG	2.43	0.66
33:5:9:G:O6	33:5:10:G:N2	2.29	0.65
9:H:193:ARG:HD2	25:X:74:ARG:HH21	1.61	0.65
18:Q:36:GLU:OE1	18:Q:76:ARG:NH1	2.29	0.65
1:2:1216:G:OP1	13:L:45:LYS:NZ	2.30	0.65
1:2:1491:A:H2'	1:2:1492:C:H6	1.62	0.65
9:H:118:MET:HA	9:H:118:MET:HE2	1.78	0.65
1:2:634:U:OP1	2:A:188:LYS:NZ	2.30	0.65
21:T:20:ASP:OD1	21:T:21:GLU:N	2.30	0.65
24:W:18:ARG:HB3	24:W:62:VAL:HG22	1.78	0.65
35:s:812:U:C6	35:s:812:U:OP1	2.50	0.65
1:2:1318:C:H2'	1:2:1319:A:H8	1.62	0.64
13:L:9:LEU:HD23	13:L:97:ILE:HD13	1.79	0.64
1:2:418:U:H1'	1:2:419:A:C5	2.32	0.64
1:2:962:A:H2'	1:2:963:G:C8	2.32	0.64
12:K:7:LEU:HD12	12:K:24:TYR:HD2	1.61	0.64
16:O:4:GLN:N	16:O:4:GLN:OE1	2.29	0.64
1:2:790:U:O2'	1:2:1496:C:OP1	2.14	0.64
1:2:1122:C:H6	20:S:28:TYR:CZ	2.16	0.64
11:J:40:GLU:N	11:J:40:GLU:OE1	2.30	0.64
1:2:1352:C:H4'	37:2:1593:SPM:H42	1.77	0.64
8:G:164:ARG:NH1	8:G:181:PRO:O	2.30	0.64
5:D:19:ILE:HG22	5:D:22:ARG:H	1.61	0.64
24:W:38:VAL:H	24:W:48:VAL:HG22	1.63	0.64
12:K:84:MET:HE3	12:K:113:GLY:HA2	1.79	0.64
1:2:21:A:OP2	37:2:1583:SPM:N1	2.31	0.64
1:2:645:U:O4	1:2:662:G:O2'	2.14	0.64
1:2:1447:A:H2'	1:2:1448:G:H8	1.63	0.63
12:K:8:VAL:HG22	12:K:23:ILE:HG22	1.80	0.63
27:Z:36:VAL:HG12	27:Z:45:VAL:HG22	1.81	0.63
1:2:962:A:H2'	1:2:963:G:H8	1.64	0.63
1:2:1095:C:O4'	1:2:1095:C:C5'	2.45	0.63
1:2:1491:A:H2'	1:2:1492:C:C6	2.32	0.63
2:A:157:ASP:N	2:A:157:ASP:OD1	2.31	0.63
9:H:193:ARG:NH2	25:X:71:GLU:OE1	2.32	0.63
12:K:13:ARG:HG2	12:K:18:ARG:HD3	1.79	0.63
1:2:502:C:OP1	32:e:41:ARG:NH1	2.31	0.62
6:E:122:ILE:HD11	6:E:137:GLU:HG3	1.80	0.62
17:P:46:TYR:OH	27:Z:160:GLU:OE2	2.12	0.62
28:3:61:GLU:N	28:3:61:GLU:OE1	2.32	0.62
1:2:12:U:H2'	1:2:13:C:C6	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:479:A:OP1	15:N:71:LYS:NZ	2.32	0.62
1:2:483:G:H1'	37:2:1555:SPM:H121	1.81	0.62
6:E:234:SER:OG	6:E:236:LEU:O	2.17	0.62
7:F:79:LEU:HD11	7:F:188:GLU:HA	1.80	0.62
5:D:30:LEU:HD23	5:D:35:LEU:HB2	1.81	0.62
1:2:1465:G:OP1	37:2:1576:SPM:N14	2.28	0.62
34:4:69:C:H2'	34:4:70:G:H8	1.64	0.62
1:2:237:G:OP2	37:2:1586:SPM:N1	2.33	0.62
22:U:30:THR:HG21	22:U:114:ALA:HB2	1.81	0.62
12:K:101:LYS:HE3	31:d:66:PRO:HB3	1.81	0.61
29:a:64:CYS:SG	29:a:66:THR:OG1	2.53	0.61
25:X:47:ARG:O	25:X:47:ARG:NH1	2.33	0.61
28:3:112:ASP:HA	28:3:115:ILE:HD12	1.81	0.61
1:2:349:A:H5''	1:2:350:C:H5	1.64	0.61
1:2:1405:U:H2'	1:2:1406:G:H8	1.65	0.61
1:2:636:C:H2'	1:2:637:U:C6	2.35	0.61
8:G:80:LYS:NZ	8:G:145:GLY:O	2.33	0.61
1:2:646:A:H4'	14:M:41:MET:HE1	1.83	0.61
27:Z:56:ILE:HG23	27:Z:63:ILE:HD11	1.82	0.61
1:2:218:C:H2'	1:2:219:A:H8	1.65	0.61
6:E:95:ARG:NH2	6:E:113:GLU:O	2.34	0.61
25:X:27:LEU:HB2	25:X:38:GLN:HB3	1.81	0.61
1:2:1188:G:H4'	1:2:1189:C:OP2	1.99	0.61
3:B:112:LYS:NZ	3:B:224:GLU:O	2.33	0.61
9:H:11:LYS:HZ2	9:H:16:TRP:N	1.99	0.61
1:2:1162:U:O4	37:2:1568:SPM:N1	2.33	0.61
1:2:1391:G:H2'	1:2:1392:G:C8	2.35	0.61
8:G:41:VAL:HG11	8:G:146:LEU:HD21	1.81	0.61
21:T:15:ARG:HG3	21:T:33:LEU:HB3	1.82	0.61
12:K:17:ALA:HB2	12:K:73:GLY:HA3	1.83	0.61
1:2:1012:A:O2'	27:Z:140:GLU:OE1	2.19	0.60
23:V:66:ARG:NH1	23:V:94:GLU:OE1	2.34	0.60
26:Y:32:ASN:HA	28:3:68:LEU:HB2	1.82	0.60
14:M:25:ILE:HG22	14:M:34:ILE:HB	1.83	0.60
1:2:1324:A:C8	17:P:12:TYR:HB3	2.37	0.60
6:E:109:ILE:HB	6:E:113:GLU:HG3	1.82	0.60
23:V:19:ARG:HB2	23:V:32:SER:HB3	1.82	0.60
1:2:1490:C:H2'	1:2:1491:A:C8	2.36	0.60
23:V:11:ASP:OD1	23:V:11:ASP:N	2.34	0.60
1:2:1328:A:OP2	22:U:89:ARG:NH2	2.30	0.60
7:F:160:VAL:HG12	7:F:178:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:10:ILE:HA	9:H:37:TYR:CZ	2.35	0.60
12:K:26:GLY:HA3	12:K:65:ASP:HB2	1.82	0.60
27:Z:58:ARG:HH11	27:Z:58:ARG:C	2.09	0.60
34:4:58:A:O2'	34:4:60:U:OP2	2.16	0.60
9:H:119:TYR:HB2	9:H:124:TYR:CE2	2.37	0.60
12:K:66:ALA:O	12:K:67:LYS:NZ	2.32	0.60
12:K:50:MET:HA	12:K:50:MET:HE2	1.82	0.60
26:Y:24:ARG:HD3	28:3:37:ASN:HB3	1.84	0.60
1:2:1292:C:OP1	16:O:35:ASN:ND2	2.33	0.60
1:2:1188:G:H5'	1:2:1189:C:H5	1.66	0.59
24:W:26:ASN:OD1	24:W:27:GLU:N	2.35	0.59
1:2:886:G:O2'	1:2:1363:C:OP2	2.18	0.59
1:2:1318:C:H2'	1:2:1319:A:C8	2.37	0.59
27:Z:55:ILE:HG22	27:Z:83:ILE:HD13	1.84	0.59
1:2:217:U:H2'	1:2:218:C:H6	1.67	0.59
1:2:1213:A:H2'	1:2:1214:G:C8	2.37	0.59
2:A:126:THR:OG1	2:A:128:TYR:O	2.19	0.59
9:H:6:LEU:CD2	9:H:8:LEU:CD2	2.79	0.59
5:D:158:THR:HG21	23:V:39:GLY:HA3	1.83	0.59
8:G:20:LYS:O	8:G:90:ASN:ND2	2.30	0.59
30:c:97:TYR:CE1	30:c:105:ILE:HD13	2.37	0.59
1:2:704:C:OP1	1:2:814:U:O2'	2.19	0.59
8:G:42:PRO:HB2	8:G:79:PHE:HD2	1.66	0.59
25:X:22:GLU:OE2	31:d:33:THR:OG1	2.21	0.59
23:V:107:GLN:C	23:V:108:LYS:HD3	2.27	0.59
1:2:902:A:N3	1:2:1340:U:O2'	2.32	0.59
23:V:19:ARG:HB3	23:V:19:ARG:NH1	2.18	0.59
32:e:43:VAL:HG23	32:e:44:LYS:HE2	1.85	0.59
15:N:70:ARG:HG3	15:N:119:LEU:HD13	1.85	0.59
17:P:21:ARG:NE	27:Z:20:GLU:OE2	2.29	0.59
17:P:43:GLU:HB3	29:a:9:ASN:OD1	2.02	0.59
1:2:7:G:H5''	37:2:1582:SPM:H122	1.85	0.58
1:2:1081:G:N7	1:2:1109:C:O2'	2.35	0.58
5:D:31:GLY:HA3	32:e:38:TYR:CD1	2.38	0.58
9:H:10:ILE:CG2	9:H:35:PRO:O	2.51	0.58
28:3:55:GLU:HB2	28:3:80:VAL:HG21	1.85	0.58
1:2:1405:U:H2'	1:2:1406:G:C8	2.38	0.58
9:H:16:TRP:CZ3	9:H:86:PHE:HB3	2.38	0.58
12:K:29:ARG:N	12:K:65:ASP:OD1	2.34	0.58
1:2:975:G:H2'	1:2:976:G:H8	1.68	0.58
1:2:987:U:H2'	1:2:988:G:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:62:GLN:OE1	2:A:62:GLN:N	2.36	0.58
7:F:141:LYS:NZ	7:F:143:GLY:O	2.36	0.58
9:H:92:LYS:HD3	30:c:62:GLU:OE2	2.04	0.58
25:X:40:ARG:HG3	25:X:54:THR:HG22	1.86	0.58
4:C:9:GLU:OE1	4:C:9:GLU:N	2.27	0.58
12:K:52:PRO:HG2	12:K:86:LEU:HD22	1.85	0.58
18:Q:95:ASN:OD1	18:Q:98:ARG:NH2	2.29	0.58
23:V:19:ARG:HB3	23:V:19:ARG:HH11	1.69	0.58
1:2:673:G:H2'	1:2:674:A:H8	1.68	0.58
26:Y:41:CYS:HB3	26:Y:46:SER:H	1.67	0.58
1:2:16:G:H2'	1:2:17:C:C6	2.39	0.58
1:2:246:OMC:HM22	1:2:247:C:H5'	1.85	0.58
3:B:95:GLN:O	3:B:120:ARG:NH2	2.37	0.58
21:T:101:VAL:HA	21:T:105:MET:HE2	1.86	0.58
26:Y:56:GLU:HB3	26:Y:69:ILE:HB	1.86	0.58
27:Z:165:ARG:NH1	29:a:6:ARG:O	2.37	0.58
1:2:1076:C:H2'	1:2:1077:A:H8	1.69	0.58
12:K:30:VAL:HG12	12:K:66:ALA:HB3	1.84	0.58
1:2:965:A:O4'	1:2:993:A:N6	2.37	0.58
1:2:1260:C:H4'	1:2:1266:U:O4	2.03	0.58
3:B:101:ALA:HB2	3:B:110:VAL:HG21	1.85	0.58
23:V:88:GLU:OE1	23:V:88:GLU:N	2.20	0.58
27:Z:70:PHE:HB3	27:Z:76:LEU:HD12	1.85	0.58
1:2:1355:U:H2'	1:2:1356:G:C8	2.39	0.57
34:4:17:C:OP2	34:4:17(A):U:O2'	2.20	0.57
28:3:35:GLY:O	28:3:39:THR:OG1	2.19	0.57
9:H:10:ILE:HA	9:H:37:TYR:CE2	2.39	0.57
15:N:119:LEU:HD12	15:N:120:PRO:HD2	1.86	0.57
1:2:843:C:O2'	1:2:844:G:H5'	2.04	0.57
2:A:19:TRP:CG	14:M:8:ARG:HH21	2.22	0.57
6:E:117:LYS:HB2	6:E:162:LEU:HD11	1.84	0.57
9:H:10:ILE:HG23	9:H:37:TYR:CD1	2.40	0.57
35:s:812:U:OP1	35:s:812:U:C5	2.57	0.57
1:2:1015:G:H5''	27:Z:167:ILE:HD13	1.85	0.57
3:B:170:PHE:O	3:B:188:ASN:ND2	2.37	0.57
28:3:15:LEU:HD22	28:3:117:ARG:HE	1.70	0.57
9:H:30:TYR:OH	25:X:62:ARG:NH1	2.37	0.57
9:H:156:LYS:HD3	9:H:161:VAL:HG12	1.85	0.57
1:2:611:U:O4	1:2:711:G:O2'	2.21	0.57
1:2:796:A:OP1	39:2:1601:HOH:O	2.18	0.57
1:2:458:G:H2'	1:2:459:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:127:ILE:HG13	6:E:128:LYS:N	2.19	0.57
1:2:37:G:H3'	37:2:1584:SPM:H21	1.86	0.57
1:2:361:A:O2'	1:2:372:G:O2'	2.22	0.57
1:2:677:A:C5'	14:M:119:ASP:OD1	2.50	0.57
1:2:885:G:H2'	1:2:886:G:H8	1.70	0.57
1:2:943:U:H4'	37:2:1567:SPM:H112	1.86	0.57
37:2:1573:SPM:H111	37:2:1584:SPM:HN11	1.69	0.57
1:2:617:G:H2'	1:2:618:C:C6	2.40	0.56
1:2:985:C:C2	1:2:986:U:H5	2.23	0.56
1:2:1043:C:H2'	1:2:1044:C:H6	1.70	0.56
1:2:1188:G:O2'	1:2:1189:C:OP1	2.20	0.56
1:2:1375:C:O2'	1:2:1376:C:O5'	2.16	0.56
20:S:36:ILE:HG12	20:S:47:ARG:HD2	1.85	0.56
1:2:714:G:H21	10:I:3:PHE:HZ	1.52	0.56
1:2:770:U:O2'	1:2:864:A:N1	2.37	0.56
1:2:842:C:H2'	1:2:843:C:C6	2.39	0.56
4:C:16:CYS:CB	4:C:19:CYS:SG	2.82	0.56
28:3:18:LYS:NZ	28:3:113:GLU:HB3	2.20	0.56
1:2:263:G:H2'	1:2:264:G:H8	1.70	0.56
1:2:461:G:H5'	37:2:1555:SPM:H21	1.87	0.56
1:2:1436:U:H2'	1:2:1437:G:C8	2.40	0.56
21:T:31:ILE:HG23	21:T:39:ARG:HG2	1.87	0.56
30:c:35:LYS:HZ3	30:c:39:GLU:HG3	1.70	0.56
31:d:7:LYS:NZ	31:d:8:LEU:H	2.03	0.56
31:d:65:LEU:O	31:d:69:LYS:HG2	2.05	0.56
1:2:12:U:OP1	7:F:62:LYS:NZ	2.31	0.56
1:2:989:C:OP1	26:Y:49:ALA:HA	2.06	0.56
8:G:47:ASN:HB3	8:G:49:LYS:HZ2	1.71	0.56
31:d:4:LEU:HD11	31:d:15:GLU:HG2	1.87	0.56
3:B:57:TYR:OH	4:C:65:PRO:O	2.23	0.56
26:Y:57:ARG:HA	26:Y:68:PHE:HA	1.86	0.56
6:E:210:THR:HG23	6:E:220:GLN:HG2	1.87	0.56
28:3:20:LEU:O	28:3:24:ARG:NH1	2.38	0.56
28:3:81:SER:HB2	28:3:86:LEU:HD23	1.88	0.56
1:2:1143:G:OP1	12:K:108:ARG:NH2	2.39	0.56
5:D:143:TYR:OH	5:D:149:GLU:OE2	2.18	0.56
34:4:50:U:O2	34:4:64:G:N2	2.24	0.56
1:2:1024:A:N1	1:2:1065:G:O2'	2.35	0.56
1:2:1096:U:O2	1:2:1098:C:C2	2.59	0.56
1:2:1184:G:OP2	37:2:1567:SPM:H122	2.06	0.56
10:I:83:TYR:OH	10:I:123:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:4:LEU:HD22	31:d:5:LYS:H	1.70	0.56
33:5:3:G:H8	33:5:3:G:OP2	1.89	0.56
1:2:1450:A:N1	33:5:4:A:C8	2.74	0.56
3:B:82:LEU:HD23	3:B:201:LEU:HD23	1.87	0.56
5:D:164:ARG:HH22	5:D:166:PRO:HA	1.71	0.56
9:H:25:PRO:HA	9:H:28:LYS:HE2	1.87	0.56
11:J:93:ARG:HB2	11:J:95:ILE:HD13	1.88	0.56
27:Z:189:ILE:HG22	27:Z:192:LYS:H	1.70	0.56
9:H:132:PRO:HA	9:H:135:ARG:HD3	1.89	0.55
21:T:6:PRO:HB2	21:T:8:GLU:OE1	2.05	0.55
1:2:1204:G:H2'	1:2:1205:G:C8	2.41	0.55
1:2:643:A:O2'	14:M:32:GLU:OE1	2.22	0.55
1:2:1204:G:H2'	1:2:1205:G:H8	1.71	0.55
1:2:1494:U:H2'	1:2:1495:C:C6	2.40	0.55
2:A:18:LYS:NZ	2:A:39:TYR:O	2.40	0.55
28:3:22:ALA:HB1	28:3:111:VAL:HG23	1.88	0.55
34:4:74:C:H4'	34:4:75:C:O5'	2.06	0.55
18:Q:28:ARG:HG3	18:Q:65:VAL:HA	1.89	0.55
20:S:60:ILE:HD12	20:S:61:MET:HG2	1.88	0.55
1:2:1481:C:H2'	1:2:1482:G:H8	1.72	0.55
8:G:94:ILE:HD12	8:G:98:MET:HB2	1.88	0.55
27:Z:165:ARG:HB2	27:Z:182:VAL:HG22	1.88	0.55
1:2:1012:A:O2'	27:Z:140:GLU:O	2.19	0.55
1:2:1393:G:H2'	1:2:1394:G:H8	1.72	0.55
5:D:31:GLY:HA3	32:e:38:TYR:CG	2.42	0.55
9:H:83:LYS:NZ	12:K:43:GLU:OE2	2.36	0.55
20:S:32:LYS:O	20:S:36:ILE:HG13	2.07	0.55
1:2:93:C:H1'	1:2:359:C:H5'	1.88	0.55
1:2:612:A:H5''	10:I:57:ARG:HE	1.71	0.55
1:2:1028:C:H2'	1:2:1029:G:H8	1.72	0.55
6:E:26:PRO:HG2	6:E:33:ILE:HG12	1.88	0.55
1:2:406:C:O2'	1:2:580:A:N3	2.35	0.55
1:2:1479:U:H2'	1:2:1480:G:H8	1.72	0.55
6:E:66:LEU:HB2	6:E:86:SER:HB2	1.87	0.55
1:2:1368:5MC:H2'	1:2:1369:G:C8	2.42	0.55
1:2:1457:6MZ:O1P	37:2:1576:SPM:N14	2.40	0.55
10:I:37:VAL:O	10:I:41:MET:HG3	2.07	0.55
10:I:81:LEU:HB2	10:I:86:MET:HE2	1.88	0.55
26:Y:60:CYS:HB3	26:Y:63:CYS:HB3	1.87	0.55
1:2:17:C:H2'	1:2:18:C:C6	2.42	0.54
1:2:897:C:O2'	1:2:1308:C:OP2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:81:GLY:O	5:D:84:LYS:NZ	2.40	0.54
11:J:43:ARG:NE	11:J:119:GLY:O	2.36	0.54
14:M:65:ASP:O	14:M:69:LYS:HG2	2.08	0.54
27:Z:90:GLU:OE2	27:Z:120:ARG:NH2	2.40	0.54
1:2:1191:C:OP2	30:c:2:GLY:N	2.40	0.54
1:2:1316:C:H2'	1:2:1317:G:C8	2.43	0.54
16:O:62:LYS:O	16:O:66:VAL:HG23	2.07	0.54
27:Z:25:GLN:C	27:Z:26:TYR:HD1	2.16	0.54
1:2:1373:C:N4	1:2:1374:U:O4	2.41	0.54
15:N:39:GLU:CD	15:N:39:GLU:H	2.15	0.54
23:V:100:ASP:OD2	23:V:107:GLN:NE2	2.41	0.54
9:H:10:ILE:HD12	9:H:35:PRO:HB2	1.87	0.54
12:K:45:VAL:O	12:K:49:ILE:HG12	2.07	0.54
15:N:143:GLN:OE1	15:N:143:GLN:N	2.40	0.54
34:4:52:G:H2'	34:4:53:G:H8	1.72	0.54
1:2:95:G:OP2	37:2:1560:SPM:N5	2.41	0.54
1:2:257:U:H2'	1:2:258:U:C6	2.43	0.54
1:2:428:U:O2'	1:2:430:U:O4	2.16	0.54
29:a:20:TYR:HD2	29:a:25:ASN:ND2	2.05	0.54
1:2:617:G:H2'	1:2:618:C:H6	1.73	0.54
1:2:1395:U:H2'	1:2:1396:G:O4'	2.08	0.54
1:2:642:G:H2'	1:2:643:A:C8	2.42	0.54
1:2:687:A:H2'	1:2:688:A:C8	2.42	0.54
1:2:964:G:N2	1:2:965:A:N1	2.55	0.54
30:c:96:LEU:HB2	30:c:106:TYR:CE1	2.43	0.54
33:5:6:U:H2'	33:5:6:U:O2	2.07	0.54
37:2:1569:SPM:N14	12:K:122:LYS:O	2.41	0.53
1:2:71:G:H2'	1:2:72:G:C8	2.44	0.53
1:2:1396:G:O2'	1:2:1425:A:N6	2.36	0.53
1:2:1481:C:H2'	1:2:1482:G:C8	2.43	0.53
8:G:3:ASP:OD1	8:G:3:ASP:N	2.40	0.53
22:U:108:PHE:CD2	22:U:125:ARG:HD3	2.43	0.53
1:2:93:C:H2'	1:2:94:U:C6	2.43	0.53
37:2:1585:SPM:H61	37:2:1585:SPM:HN0	1.74	0.53
2:A:14:TRP:HE1	2:A:17:LYS:HD2	1.72	0.53
3:B:29:LYS:HB2	3:B:76:ARG:HH11	1.73	0.53
9:H:192:SER:OG	9:H:192:SER:O	2.26	0.53
1:2:909:G:C2	1:2:910:A:C8	2.97	0.53
16:O:110:GLU:OE1	16:O:115:SER:OG	2.19	0.53
19:R:23:CYS:HB3	19:R:84:CYS:HB3	1.89	0.53
24:W:39:ARG:NH1	24:W:44:GLY:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:4:43:A:H2'	34:4:44:A:C8	2.44	0.53
1:2:251:A:N1	1:2:283:U:O2'	2.37	0.53
1:2:534:G:O6	15:N:3:LYS:NZ	2.40	0.53
1:2:924:U:H2'	1:2:1188:G:O6	2.09	0.53
2:A:14:TRP:CH2	14:M:69:LYS:HE3	2.44	0.53
8:G:49:LYS:NZ	8:G:89:ASP:HA	2.23	0.53
24:W:47:LEU:HA	24:W:58:VAL:HG22	1.91	0.53
1:2:1470:A:OP1	37:2:1595:SPM:N1	2.42	0.53
3:B:227:MET:SD	3:B:227:MET:N	2.82	0.53
9:H:6:LEU:CD2	9:H:8:LEU:HG	2.38	0.53
9:H:159:GLU:OE2	30:c:100:ASN:ND2	2.40	0.53
12:K:28:GLY:N	12:K:64:ILE:O	2.42	0.53
28:3:20:LEU:O	28:3:24:ARG:HD2	2.09	0.53
29:a:36:TYR:CE2	29:a:54:LYS:HD3	2.44	0.53
8:G:43:GLN:NE2	8:G:82:ASP:OD2	2.42	0.53
10:I:114:MET:HE2	10:I:118:GLU:HG3	1.90	0.53
25:X:13:ILE:O	25:X:16:GLU:HG3	2.09	0.53
28:3:114:ILE:O	28:3:118:VAL:HG23	2.09	0.53
1:2:673:G:H2'	1:2:674:A:C8	2.44	0.53
9:H:11:LYS:CE	9:H:15:LYS:C	2.82	0.53
9:H:52:LYS:NZ	9:H:137:ASP:OD2	2.41	0.53
11:J:38:SER:OG	11:J:39:ALA:N	2.34	0.53
12:K:49:ILE:HD12	12:K:82:ALA:HB3	1.91	0.53
22:U:120:ILE:HD13	22:U:126:SER:HB3	1.90	0.53
31:d:46:TRP:HA	31:d:49:ALA:HB3	1.91	0.53
1:2:990:C:H4'	26:Y:62:LYS:HE2	1.90	0.53
6:E:215:ASP:OD2	6:E:217:ASN:ND2	2.42	0.53
13:L:28:VAL:HG21	13:L:35:MET:HB3	1.90	0.53
34:4:69:C:H2'	34:4:70:G:C8	2.44	0.53
1:2:263:G:H2'	1:2:264:G:C8	2.44	0.52
9:H:6:LEU:CD2	9:H:8:LEU:CG	2.87	0.52
28:3:53:ILE:HD13	28:3:67:PRO:HD3	1.91	0.52
1:2:242:C:OP1	19:R:75:SER:HB2	2.10	0.52
1:2:246:OMC:HM21	15:N:34:ILE:HA	1.91	0.52
1:2:633:G:H2'	1:2:634:U:C6	2.44	0.52
8:G:157:ASP:HA	8:G:205:ILE:HA	1.90	0.52
12:K:107:ASP:HB3	12:K:110:MET:HE2	1.92	0.52
1:2:917:G:N7	16:O:133:ARG:NH2	2.51	0.52
1:2:1188:G:N3	1:2:1188:G:C2'	2.72	0.52
2:A:86:HIS:ND1	2:A:189:THR:HG22	2.25	0.52
5:D:16:HIS:HB3	5:D:19:ILE:HD13	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:79:ASP:O	13:L:82:VAL:HG22	2.09	0.52
18:Q:87:PHE:CE2	18:Q:91:ARG:HD3	2.45	0.52
20:S:8:ASP:OD1	20:S:8:ASP:N	2.41	0.52
21:T:20:ASP:HA	21:T:23:LEU:HD12	1.91	0.52
21:T:89:ALA:HB1	21:T:96:PHE:HB3	1.91	0.52
27:Z:63:ILE:H	27:Z:63:ILE:HD12	1.75	0.52
1:2:1188:G:N3	1:2:1188:G:C3'	2.73	0.52
2:A:14:TRP:NE1	2:A:17:LYS:HD2	2.24	0.52
25:X:26:ILE:HD12	25:X:63:VAL:HG13	1.91	0.52
1:2:707:G:C8	18:Q:59:PRO:HB2	2.44	0.52
31:d:7:LYS:HZ3	31:d:8:LEU:H	1.56	0.52
1:2:910:A:O2'	1:2:1297:A:N3	2.39	0.52
2:A:26:LYS:NZ	2:A:30:GLU:OE2	2.41	0.52
1:2:266:U:OP1	11:J:56:ARG:NH2	2.42	0.52
1:2:699:U:H2'	1:2:700:A:H8	1.73	0.52
1:2:947:A:O2'	1:2:1007:G:OP2	2.24	0.52
25:X:55:ARG:NH1	25:X:74:ARG:HB2	2.24	0.52
28:3:24:ARG:HG3	28:3:89:ALA:HB1	1.92	0.52
1:2:1095:C:OP1	22:U:129:PRO:CB	2.58	0.52
12:K:24:TYR:HE1	12:K:65:ASP:HB3	1.74	0.52
10:I:108:SER:HB2	10:I:129:LEU:HD11	1.91	0.51
1:2:25:G:H2'	1:2:26:A:C8	2.45	0.51
1:2:119:U:O2	6:E:141:ASN:ND2	2.38	0.51
1:2:152:A:H2'	1:2:153:A:C8	2.44	0.51
1:2:195:A:N1	1:2:225:G:O2'	2.42	0.51
1:2:1082:U:N3	1:2:1084:G:C8	2.78	0.51
1:2:1152:C:OP1	17:P:52:LYS:NZ	2.43	0.51
1:2:1343:G:H2'	1:2:1344:OMU:H6	1.91	0.51
23:V:45:ARG:NH1	23:V:65:VAL:O	2.41	0.51
1:2:900:C:C2	1:2:901:A:C8	2.98	0.51
6:E:232:GLU:OE1	6:E:232:GLU:N	2.44	0.51
22:U:158:GLU:OE1	22:U:158:GLU:N	2.37	0.51
9:H:11:LYS:NZ	9:H:16:TRP:N	2.56	0.51
12:K:31:PHE:HB2	12:K:67:LYS:HD3	1.93	0.51
1:2:418:U:O2	1:2:419:A:N6	2.44	0.51
1:2:922:A:N3	1:2:949:U:O2'	2.41	0.51
1:2:949:U:H2'	1:2:950:A:C8	2.45	0.51
1:2:1314:A:H1'	9:H:72:LYS:HG2	1.92	0.51
9:H:10:ILE:HG22	9:H:35:PRO:O	2.10	0.51
11:J:109:ALA:HB1	11:J:123:ALA:HB1	1.91	0.51
21:T:54:LEU:O	21:T:58:ARG:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:521:U:C4	15:N:27:GLN:HG2	2.46	0.51
1:2:739:A:OP1	37:2:1565:SPM:N14	2.43	0.51
1:2:940:G:OP1	39:2:1602:HOH:O	2.19	0.51
34:4:4:G:H2'	34:4:5:G:H8	1.76	0.51
1:2:392:U:O4	37:2:1570:SPM:N14	2.43	0.51
1:2:965:A:H8	28:3:34:LYS:HE2	1.76	0.51
3:B:181:ASP:OD1	4:C:44:ARG:NH1	2.40	0.51
11:J:65:VAL:HG22	11:J:123:ALA:HB3	1.93	0.51
30:c:22:LYS:HA	30:c:25:LYS:HB2	1.92	0.51
1:2:871:A:H2'	1:2:872:A:H8	1.76	0.51
3:B:36:LEU:O	3:B:203:ARG:NH2	2.44	0.51
4:C:39:GLU:OE1	4:C:59:ASN:ND2	2.44	0.51
10:I:49:GLU:OE1	10:I:49:GLU:HA	2.11	0.51
1:2:1096:U:O2	1:2:1100:G:O6	2.29	0.51
3:B:151:ARG:HD3	3:B:175:ALA:HA	1.93	0.51
4:C:37:CYS:HB3	4:C:60:CYS:HB3	1.92	0.51
30:c:56:LEU:HA	30:c:59:ILE:HG22	1.93	0.51
1:2:397:G:O6	37:2:1561:SPM:N1	2.44	0.50
1:2:677:A:C4'	14:M:119:ASP:OD1	2.59	0.50
1:2:1491:A:C6	35:s:813:G:N1	2.79	0.50
1:2:557:U:OP1	19:R:70:TYR:OH	2.28	0.50
6:E:99:ASP:O	6:E:103:PHE:HA	2.11	0.50
8:G:79:PHE:HE2	8:G:98:MET:HG3	1.74	0.50
9:H:76:HIS:CD2	12:K:44:MET:HG3	2.45	0.50
12:K:58:ASN:OD1	12:K:58:ASN:N	2.44	0.50
18:Q:21:PRO:HG2	18:Q:24:VAL:HG23	1.93	0.50
24:W:40:CYS:HB3	24:W:44:GLY:H	1.76	0.50
26:Y:65:TYR:O	26:Y:65:TYR:CG	2.64	0.50
1:2:29:G:H2'	1:2:30:C:C6	2.46	0.50
1:2:439:U:OP2	23:V:101:ARG:NH1	2.40	0.50
1:2:1097:C:O2'	1:2:1099:G:N1	2.43	0.50
9:H:19:LYS:NZ	31:d:71:LEU:HD21	2.27	0.50
15:N:28:ARG:O	15:N:32:THR:HG23	2.11	0.50
23:V:65:VAL:HG22	23:V:81:LEU:HD12	1.92	0.50
29:a:43:LYS:HD3	29:a:44:LYS:N	2.26	0.50
1:2:167:A:H2'	1:2:168:G:H8	1.77	0.50
1:2:263:G:H5''	11:J:98:ARG:HB3	1.93	0.50
1:2:1450:A:C6	33:5:4:A:C8	2.99	0.50
24:W:3:ARG:HB2	24:W:6:ARG:HG2	1.92	0.50
26:Y:53:LYS:HG3	26:Y:54:PRO:HD3	1.94	0.50
1:2:200:C:H2'	1:2:201:A:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:129:ASP:OD2	25:X:67:LEU:HD23	2.11	0.50
12:K:53:LEU:HD21	12:K:61:ARG:HD2	1.93	0.50
19:R:24:GLU:OE1	19:R:24:GLU:HA	2.11	0.50
27:Z:159:LEU:HD22	27:Z:163:ILE:HG12	1.93	0.50
33:5:8:A:H2'	33:5:9:G:C8	2.46	0.50
1:2:74:A:N1	1:2:213:C:O2'	2.41	0.50
1:2:1328:A:P	22:U:89:ARG:HH22	2.35	0.50
1:2:1470:A:H2'	1:2:1471:G:C8	2.46	0.50
1:2:243:G:OP1	19:R:73:ARG:NH1	2.42	0.50
1:2:1095:C:OP1	22:U:129:PRO:HB3	2.11	0.50
1:2:1291:U:OP1	22:U:41:LYS:NZ	2.27	0.50
1:2:1393:G:O2'	1:2:1394:G:H5'	2.12	0.50
8:G:49:LYS:HD2	8:G:50:THR:N	2.26	0.50
1:2:176:G:N1	1:2:179:A:OP2	2.43	0.50
1:2:843:C:H2'	1:2:844:G:H8	1.77	0.50
5:D:107:GLN:HE21	5:D:119:ILE:HG13	1.77	0.50
25:X:23:VAL:HG23	25:X:63:VAL:HA	1.93	0.50
31:d:40:ARG:NH1	31:d:40:ARG:HB2	2.27	0.50
1:2:1034:G:H4'	37:2:1566:SPM:H42	1.94	0.50
1:2:1082:U:C2	1:2:1084:G:N7	2.80	0.50
1:2:1311:G:N2	1:2:1338:A:OP2	2.31	0.50
7:F:90:SER:HB3	7:F:114:ILE:HA	1.94	0.50
12:K:59:ASP:OD1	12:K:59:ASP:N	2.44	0.50
12:K:68:ILE:HD11	12:K:86:LEU:HD12	1.94	0.50
22:U:35:GLU:OE1	22:U:35:GLU:N	2.39	0.50
1:2:131:U:H2'	1:2:132:A:H8	1.76	0.49
1:2:137:C:O2'	8:G:118:GLN:HB2	2.11	0.49
1:2:949:U:H2'	1:2:950:A:H8	1.77	0.49
8:G:180:PRO:O	8:G:182:GLY:N	2.45	0.49
15:N:57:LYS:HD2	15:N:94:VAL:HG22	1.94	0.49
27:Z:29:ALA:HB2	27:Z:54:MET:HG3	1.94	0.49
1:2:218:C:H2'	1:2:219:A:C8	2.46	0.49
1:2:334:A:OP2	37:2:1562:SPM:N5	2.40	0.49
1:2:636:C:H2'	1:2:637:U:H6	1.78	0.49
3:B:22:GLU:O	3:B:26:LYS:HD2	2.12	0.49
20:S:11:ARG:HG2	20:S:11:ARG:HH11	1.77	0.49
20:S:18:ASP:OD1	20:S:19:ARG:N	2.45	0.49
28:3:24:ARG:NH2	28:3:85:ALA:O	2.45	0.49
1:2:229:C:H2'	1:2:230:A:H8	1.75	0.49
1:2:1122:C:OP2	20:S:45:LYS:HG3	2.11	0.49
1:2:1154:A:H4'	27:Z:154:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1282:A:O2'	21:T:76:ASN:ND2	2.43	0.49
2:A:19:TRP:CD1	14:M:8:ARG:HH21	2.31	0.49
7:F:59:VAL:HG11	7:F:81:ILE:HD12	1.93	0.49
11:J:66:LEU:HA	11:J:73:ALA:HA	1.94	0.49
13:L:4:LYS:HE2	13:L:4:LYS:H	1.76	0.49
24:W:19:VAL:HG21	24:W:30:ILE:HD12	1.94	0.49
30:c:19:GLU:O	30:c:23:GLN:N	2.44	0.49
1:2:558:C:H2'	1:2:559:A:H8	1.77	0.49
1:2:784:G:O2'	10:I:9:ASN:OD1	2.28	0.49
1:2:964:G:O2'	1:2:967:G:O2'	2.30	0.49
20:S:60:ILE:O	20:S:64:LYS:HG2	2.13	0.49
27:Z:17:LYS:HG3	29:a:16:TRP:CD2	2.48	0.49
34:4:15:G:N2	34:4:48:C:C2	2.78	0.49
1:2:910:A:H2'	1:2:911:A:H8	1.75	0.49
1:2:996:C:O2'	1:2:997:G:H8	1.96	0.49
1:2:1102:C:H5''	1:2:1102:C:H6	1.77	0.49
3:B:84:ILE:HD13	4:C:62:PHE:HE1	1.78	0.49
3:B:108:ARG:NH1	3:B:227:MET:O	2.45	0.49
9:H:5:ASN:OD1	9:H:5:ASN:N	2.40	0.49
1:2:374:C:OP1	37:2:1587:SPM:N14	2.46	0.49
1:2:865:OMG:HM22	1:2:866:A:O4'	2.13	0.49
1:2:1092:G:C6	1:2:1104:G:C6	3.00	0.49
1:2:1116:G:OP1	13:L:70:HIS:ND1	2.45	0.49
1:2:1201:A:H2	1:2:1204:G:N3	2.11	0.49
13:L:41:LEU:HB2	13:L:71:LYS:HB3	1.95	0.49
26:Y:57:ARG:HB3	26:Y:68:PHE:HD1	1.76	0.49
1:2:956:G:H22	1:2:1175:A:P	2.34	0.49
1:2:991:U:H2'	1:2:992:G:C4	2.47	0.49
1:2:1043:C:H2'	1:2:1044:C:C6	2.48	0.49
1:2:17:C:H4'	1:2:848:G:C8	2.48	0.49
1:2:842:C:H2'	1:2:843:C:H6	1.76	0.49
5:D:44:ALA:HA	5:D:101:LEU:HD23	1.94	0.49
7:F:12:GLU:OE1	7:F:12:GLU:N	2.45	0.49
12:K:53:LEU:HB2	12:K:86:LEU:HD21	1.95	0.49
14:M:27:ASP:OD1	14:M:27:ASP:N	2.46	0.49
27:Z:20:GLU:HG3	29:a:12:GLY:HA2	1.94	0.49
27:Z:141:ARG:NH1	33:5:8:A:H5''	2.27	0.49
1:2:655:A:H2'	1:2:656:U:H6	1.77	0.49
1:2:727:A:H4'	1:2:1480:G:N2	2.28	0.49
1:2:1067:G:N1	27:Z:191:ASP:OD2	2.46	0.49
1:2:1077:A:H2'	1:2:1078:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1483:G:OP2	14:M:127:ARG:NH2	2.45	0.49
14:M:42:VAL:HG23	14:M:43:VAL:HG13	1.95	0.49
19:R:49:ARG:NH1	19:R:89:GLU:OE2	2.46	0.49
27:Z:37:LEU:O	27:Z:43:THR:HA	2.13	0.49
1:2:1130:G:N2	1:2:1133:A:OP2	2.44	0.49
9:H:15:LYS:HG2	9:H:16:TRP:CE2	2.48	0.49
14:M:44:LYS:HE2	14:M:44:LYS:N	2.28	0.49
31:d:5:LYS:HD3	31:d:6:ILE:O	2.13	0.49
1:2:643:A:H2'	1:2:644:G:O4'	2.13	0.48
1:2:699:U:H2'	1:2:700:A:C8	2.47	0.48
1:2:1495:C:H2'	1:2:1496:C:C6	2.48	0.48
6:E:120:ARG:NH1	6:E:226:VAL:O	2.46	0.48
14:M:15:TYR:HB3	14:M:22:LEU:HB2	1.94	0.48
23:V:86:SER:HB3	23:V:89:ILE:HD12	1.95	0.48
25:X:49:LYS:NZ	31:d:47:GLU:OE1	2.46	0.48
1:2:426:C:H2'	1:2:427:U:C6	2.48	0.48
1:2:601:A:N7	10:I:110:SER:HA	2.28	0.48
1:2:1217:G:OP1	17:P:32:TYR:OH	2.17	0.48
2:A:14:TRP:CD1	2:A:17:LYS:HD2	2.48	0.48
6:E:50:ALA:HB1	6:E:55:GLU:HB2	1.95	0.48
7:F:128:CYS:SG	7:F:132:HIS:HD2	2.21	0.48
18:Q:68:LYS:HB2	18:Q:71:GLN:HG3	1.94	0.48
30:c:85:LEU:HD23	30:c:106:TYR:CD2	2.48	0.48
31:d:17:ASN:ND2	31:d:19:ASP:HB3	2.28	0.48
1:2:521:U:H4'	1:2:522:A:H5'	1.96	0.48
1:2:637:U:H2'	1:2:638:C:H6	1.79	0.48
1:2:843:C:H5	15:N:6:SER:OG	1.96	0.48
1:2:1461:G:OP1	1:2:1464:A:H4'	2.13	0.48
14:M:32:GLU:OE1	14:M:32:GLU:HA	2.13	0.48
16:O:46:MET:HE1	16:O:55:LEU:HD21	1.95	0.48
28:3:43:VAL:HG12	28:3:73:LYS:HE3	1.94	0.48
1:2:131:U:H2'	1:2:132:A:C8	2.48	0.48
1:2:227:C:H2'	1:2:228:U:H6	1.78	0.48
1:2:828:A:H8	1:2:828:A:OP2	1.96	0.48
1:2:899:A:H2'	1:2:900:C:C6	2.48	0.48
1:2:968:A:H62	1:2:992:G:H21	1.61	0.48
1:2:1188:G:H5'	1:2:1189:C:C5	2.47	0.48
1:2:1369:G:H2'	1:2:1370:U:H6	1.79	0.48
8:G:45:LYS:NZ	8:G:82:ASP:OD1	2.43	0.48
12:K:31:PHE:HE1	22:U:156:TYR:CE1	2.31	0.48
16:O:44:LEU:HD21	16:O:66:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:19:ARG:HH12	22:U:141:GLU:CD	2.21	0.48
1:2:871:A:H2'	1:2:872:A:C8	2.49	0.48
1:2:975:G:H2'	1:2:976:G:C8	2.49	0.48
1:2:1004:G:O2'	1:2:1178:C:O2'	2.26	0.48
1:2:1169:G:H5'	27:Z:171:MET:HE1	1.95	0.48
1:2:1349:G:H2'	1:2:1350:C:H6	1.78	0.48
4:C:57:CYS:HB3	4:C:60:CYS:SG	2.49	0.48
6:E:34:GLU:OE1	6:E:34:GLU:N	2.31	0.48
20:S:56:ARG:O	20:S:60:ILE:HG13	2.13	0.48
25:X:37:THR:HG23	25:X:57:VAL:HG13	1.96	0.48
1:2:302:G:N2	1:2:305:A:OP2	2.39	0.48
1:2:725:A:OP2	1:2:771:G:N2	2.47	0.48
1:2:881:A:H2'	1:2:882:A:C8	2.49	0.48
1:2:1287:G:OP2	39:2:1603:HOH:O	2.19	0.48
1:2:1475:MA6:H2'	1:2:1476:A:C8	2.48	0.48
13:L:23:GLN:OE1	13:L:90:ARG:NH2	2.46	0.48
14:M:38:SER:H	14:M:41:MET:HG3	1.78	0.48
23:V:84:TYR:OH	23:V:94:GLU:OE2	2.27	0.48
25:X:35:GLU:H	25:X:35:GLU:CD	2.19	0.48
30:c:85:LEU:HB3	30:c:106:TYR:CE2	2.48	0.48
1:2:217:U:H2'	1:2:218:C:C6	2.47	0.48
1:2:220:U:H2'	1:2:221:G:H8	1.79	0.48
1:2:1101:G:H2'	1:2:1102:C:C6	2.48	0.48
1:2:1319:A:H2'	1:2:1320:G:H8	1.79	0.48
1:2:1382:A:N7	1:2:1439:A:H2	2.12	0.48
1:2:1392:G:H2'	1:2:1393:G:O4'	2.14	0.48
1:2:1393:G:H22	1:2:1428:U:H3	1.62	0.48
1:2:1469:U:H5''	37:2:1595:SPM:H22	1.95	0.48
3:B:34:GLU:OE1	3:B:83:ARG:NH2	2.46	0.48
3:B:113:PHE:HD1	3:B:202:ALA:HB2	1.79	0.48
9:H:10:ILE:HG21	9:H:35:PRO:O	2.13	0.48
9:H:39:PRO:HB3	9:H:58:VAL:HG23	1.96	0.48
15:N:136:ALA:HB1	15:N:142:LYS:HB2	1.95	0.48
21:T:56:LYS:HE2	21:T:56:LYS:HB2	1.74	0.48
21:T:89:ALA:HA	21:T:97:VAL:O	2.13	0.48
1:2:25:G:H2'	1:2:26:A:H8	1.79	0.48
1:2:614:G:H2'	1:2:615:G:H8	1.78	0.48
1:2:965:A:C8	28:3:34:LYS:HE2	2.48	0.48
1:2:1017:C:H2'	1:2:1018:OMG:H8	1.78	0.48
2:A:23:ILE:HD11	2:A:80:ILE:HG22	1.95	0.48
12:K:59:ASP:O	12:K:63:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:7:PRO:HA	21:T:10:LYS:HD3	1.95	0.48
27:Z:73:VAL:HG11	29:a:17:LEU:HD22	1.94	0.48
1:2:452:G:O2'	1:2:454:A:H1'	2.12	0.48
1:2:826:G:O6	37:2:1566:SPM:H81	2.13	0.48
1:2:1466:4AC:HM73	1:2:1467:4AC:HM72	1.95	0.48
1:2:91:G:O6	37:2:1558:SPM:N1	2.47	0.48
1:2:382:C:H2'	1:2:383:G:H8	1.79	0.48
1:2:417:G:H21	1:2:419:A:H1'	1.78	0.48
8:G:146:LEU:HB2	8:G:148:VAL:HG22	1.96	0.48
28:3:86:LEU:HD12	28:3:87:GLY:N	2.28	0.48
33:5:6:U:H3'	33:5:7:G:H5'	1.96	0.48
34:4:4:G:H2'	34:4:5:G:C8	2.49	0.48
1:2:1253:A:N1	1:2:1335:G:O2'	2.39	0.47
1:2:1284:C:OP2	39:2:1606:HOH:O	2.20	0.47
2:A:20:TYR:CE2	2:A:41:ILE:HD12	2.49	0.47
8:G:142:GLN:HG2	8:G:143:LEU:HD22	1.95	0.47
12:K:8:VAL:HG22	12:K:23:ILE:CG2	2.44	0.47
16:O:5:PHE:CE2	16:O:53:GLY:HA3	2.49	0.47
1:2:741:A:H4'	1:2:1471:G:O2'	2.13	0.47
1:2:1070:C:H2'	1:2:1071:C:H6	1.78	0.47
1:2:1124:G:C2	1:2:1125:C:C6	3.02	0.47
1:2:1175:A:O2'	1:2:1176:A:OP2	2.30	0.47
9:H:27:LEU:HD21	9:H:135:ARG:HE	1.79	0.47
14:M:43:VAL:C	14:M:44:LYS:HE2	2.38	0.47
21:T:90:VAL:HG23	21:T:114:SER:HB2	1.96	0.47
23:V:61:ASN:O	23:V:87:ARG:NH1	2.39	0.47
1:2:826:G:N7	37:2:1566:SPM:H111	2.30	0.47
1:2:1343:G:H2'	1:2:1344:OMU:C6	2.43	0.47
3:B:199:TRP:CD2	3:B:222:VAL:HG22	2.49	0.47
12:K:9:ILE:HD12	12:K:22:TYR:CD2	2.49	0.47
27:Z:157:GLN:NE2	27:Z:160:GLU:OE1	2.47	0.47
28:3:78:VAL:HG13	28:3:114:ILE:HG21	1.96	0.47
1:2:3:U:H5'	7:F:159:VAL:HG12	1.97	0.47
1:2:961:C:H2'	1:2:962:A:H8	1.80	0.47
1:2:1206:C:H5''	22:U:47:GLU:OE2	2.14	0.47
1:2:1455:U:H1'	1:2:1456:A:N7	2.29	0.47
1:2:1484:C:H2'	1:2:1485:U:C6	2.49	0.47
3:B:56:LYS:HA	3:B:56:LYS:HD3	1.61	0.47
3:B:217:ASP:N	3:B:217:ASP:OD1	2.48	0.47
8:G:42:PRO:HB2	8:G:79:PHE:CD2	2.48	0.47
9:H:116:ARG:C	9:H:117:ILE:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:128:VAL:HG23	25:X:56:ASN:HB2	1.96	0.47
9:H:193:ARG:HH11	25:X:74:ARG:HE	1.63	0.47
14:M:11:ILE:HD13	14:M:77:LYS:HE3	1.96	0.47
18:Q:62:LYS:HD3	18:Q:68:LYS:HG3	1.96	0.47
30:c:87:GLU:O	30:c:91:GLN:HG3	2.13	0.47
1:2:577:C:OP2	37:2:1590:SPM:N14	2.31	0.47
1:2:1226:C:H2'	1:2:1227:C:C6	2.49	0.47
7:F:187:THR:O	7:F:191:VAL:HG23	2.15	0.47
12:K:36:PRO:HB2	12:K:39:LEU:HD23	1.95	0.47
12:K:98:GLU:OE1	12:K:98:GLU:N	2.24	0.47
22:U:28:VAL:HG12	22:U:30:THR:HG22	1.96	0.47
1:2:220:U:C2	1:2:221:G:C8	3.03	0.47
1:2:979:A:H4'	21:T:72:THR:HA	1.96	0.47
2:A:14:TRP:HH2	14:M:69:LYS:O	1.97	0.47
6:E:120:ARG:NE	6:E:137:GLU:OE2	2.34	0.47
25:X:26:ILE:HA	25:X:39:VAL:HG23	1.97	0.47
28:3:27:LYS:HA	28:3:32:ILE:HG22	1.96	0.47
1:2:268:A:H2'	1:2:269:G:C8	2.50	0.47
1:2:472:U:H2'	1:2:473:G:H8	1.79	0.47
1:2:489:G:N3	1:2:489:G:H2'	2.30	0.47
1:2:539:C:H2'	1:2:540:G:O4'	2.15	0.47
1:2:646:A:C2	1:2:663:A:C5	3.02	0.47
1:2:654:A:H2'	1:2:655:A:C8	2.50	0.47
1:2:1122:C:O2	1:2:1122:C:H3'	2.15	0.47
1:2:1226:C:H2'	1:2:1227:C:H6	1.80	0.47
1:2:1335:G:O3'	12:K:74:GLY:HA3	2.14	0.47
1:2:1465:G:H2'	1:2:1466:4AC:H6	1.97	0.47
1:2:1470:A:H2'	1:2:1471:G:H8	1.80	0.47
5:D:117:ASN:H	5:D:121:GLN:HE21	1.63	0.47
8:G:16:PRO:HB2	8:G:112:TYR:HB2	1.95	0.47
12:K:107:ASP:OD1	12:K:109:THR:OG1	2.30	0.47
13:L:13:ASN:HB3	13:L:94:ASP:OD2	2.14	0.47
13:L:23:GLN:O	13:L:27:ILE:HG12	2.15	0.47
13:L:25:ARG:O	13:L:28:VAL:HG12	2.15	0.47
13:L:79:ASP:O	13:L:83:MET:HE2	2.14	0.47
21:T:63:GLU:N	21:T:63:GLU:OE1	2.48	0.47
28:3:20:LEU:HG	28:3:24:ARG:NH2	2.29	0.47
28:3:114:ILE:HD12	28:3:114:ILE:H	1.79	0.47
9:H:32:SER:HA	31:d:62:TRP:CE2	2.49	0.47
28:3:43:VAL:HG22	28:3:48:ALA:HB3	1.96	0.47
31:d:7:LYS:HB3	31:d:14:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:37:G:H3'	37:2:1584:SPM:C2	2.44	0.47
5:D:145:VAL:HG11	5:D:153:ILE:HD11	1.96	0.47
6:E:30:PRO:HD2	6:E:78:PRO:HG2	1.97	0.47
15:N:140:GLY:O	15:N:141:LYS:HG2	2.14	0.47
20:S:44:LYS:HG3	20:S:47:ARG:NH2	2.30	0.47
31:d:37:LEU:HD11	31:d:49:ALA:HB1	1.97	0.47
1:2:716:U:H2'	1:2:717:G:O4'	2.15	0.47
1:2:728:G:H4'	1:2:1470:A:H4'	1.97	0.47
3:B:63:TYR:CE2	3:B:64:ARG:HD3	2.50	0.47
9:H:193:ARG:NH1	25:X:74:ARG:HE	2.12	0.47
21:T:88:MET:HE2	21:T:88:MET:HB2	1.82	0.47
1:2:1101:G:H2'	1:2:1102:C:H6	1.80	0.46
25:X:54:THR:OG1	25:X:75:GLU:OE2	2.31	0.46
30:c:59:ILE:HG23	30:c:60:LYS:HE3	1.97	0.46
1:2:637:U:H2'	1:2:638:C:C6	2.50	0.46
1:2:961:C:C2	1:2:962:A:C8	3.03	0.46
1:2:1096:U:C2	1:2:1100:G:O6	2.68	0.46
1:2:1494:U:C2	35:s:809:G:N2	2.83	0.46
10:I:118:GLU:OE2	10:I:121:ARG:NH2	2.29	0.46
22:U:8:ALA:HB3	22:U:69:TYR:CE1	2.50	0.46
26:Y:58:TRP:N	26:Y:67:GLU:O	2.47	0.46
28:3:18:LYS:HZ1	28:3:113:GLU:HB3	1.81	0.46
30:c:70:LEU:H	30:c:70:LEU:HD12	1.81	0.46
1:2:395:G:H2'	1:2:396:G:C8	2.50	0.46
1:2:827:A:H2'	1:2:828:A:C8	2.49	0.46
1:2:1416:G:C2	1:2:1417:G:C8	3.03	0.46
9:H:186:GLU:HB3	25:X:70:ARG:HH22	1.80	0.46
18:Q:17:ARG:HH21	18:Q:21:PRO:HD3	1.80	0.46
1:2:954:G:H2'	1:2:955:A:C8	2.49	0.46
1:2:1174:G:H5'	1:2:1176:A:H1'	1.97	0.46
1:2:1329:U:OP1	37:2:1579:SPM:N14	2.49	0.46
1:2:207:U:H2'	1:2:208:A:C8	2.50	0.46
1:2:210:U:H5''	1:2:211:C:H5'	1.98	0.46
1:2:505:G:C4	32:e:30:PRO:HG3	2.49	0.46
1:2:888:G:C2	1:2:890:G:C8	3.03	0.46
1:2:1443:G:O2'	1:2:1444:G:OP1	2.32	0.46
7:F:33:GLU:OE2	7:F:37:ARG:NH1	2.48	0.46
9:H:95:GLN:OE1	9:H:95:GLN:N	2.43	0.46
13:L:5:ALA:HB3	13:L:76:ILE:HG13	1.97	0.46
13:L:7:ILE:HB	13:L:74:ILE:HB	1.96	0.46
22:U:145:GLU:O	22:U:148:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:4:44:A:H2'	34:4:45:G:O4'	2.15	0.46
1:2:260:G:H2'	1:2:261:G:H8	1.79	0.46
1:2:612:A:C6	24:W:10:PRO:HG3	2.51	0.46
1:2:955:A:OP1	17:P:3:LYS:NZ	2.31	0.46
1:2:1350:C:H2'	1:2:1351:U:H6	1.80	0.46
1:2:1430:C:H2'	1:2:1431:U:C6	2.50	0.46
3:B:98:ILE:CG1	3:B:142:PRO:HB3	2.45	0.46
6:E:112:ASP:HA	6:E:115:ARG:NH2	2.31	0.46
6:E:128:LYS:HG3	6:E:129:GLU:OE1	2.14	0.46
13:L:2:PRO:O	13:L:78:ALA:HB3	2.15	0.46
21:T:118:LYS:CD	21:T:118:LYS:H	2.29	0.46
34:4:10:G:N2	34:4:26:G:H1'	2.30	0.46
1:2:40:G:H2'	1:2:41:G:C8	2.51	0.46
1:2:243:G:H2'	1:2:244:G:C8	2.51	0.46
1:2:1252:A:H2'	1:2:1253:A:C8	2.51	0.46
6:E:176:ARG:HB2	6:E:176:ARG:NH1	2.31	0.46
8:G:157:ASP:OD1	8:G:161:PHE:N	2.48	0.46
20:S:34:ILE:HG23	20:S:38:TYR:HD2	1.79	0.46
23:V:107:GLN:O	23:V:108:LYS:HD3	2.15	0.46
28:3:82:SER:O	28:3:82:SER:OG	2.34	0.46
28:3:86:LEU:HD12	28:3:87:GLY:H	1.80	0.46
28:3:110:LEU:O	28:3:110:LEU:HD13	2.15	0.46
34:4:15:G:N2	34:4:48:C:O2	2.38	0.46
1:2:212:C:H2'	1:2:213:C:C6	2.51	0.46
1:2:382:C:H2'	1:2:383:G:C8	2.50	0.46
1:2:413:U:H2'	1:2:414:C:C6	2.50	0.46
1:2:1188:G:N3	1:2:1188:G:H2'	2.31	0.46
1:2:1287:G:H2'	1:2:1288:C:C6	2.50	0.46
3:B:165:ILE:O	4:C:49:ARG:NH2	2.48	0.46
8:G:157:ASP:HB3	8:G:197:ARG:HD3	1.96	0.46
9:H:15:LYS:HE3	9:H:15:LYS:HB2	1.59	0.46
1:2:21:A:OP1	37:2:1583:SPM:H71	2.15	0.46
1:2:149:G:H2'	1:2:150:A:H8	1.81	0.46
1:2:200:C:H2'	1:2:201:A:C8	2.51	0.46
1:2:538:OMC:HM21	18:Q:111:LYS:HE2	1.98	0.46
1:2:1155:C:H2'	1:2:1156:G:O4'	2.16	0.46
3:B:73:LEU:HD21	3:B:173:THR:HG22	1.98	0.46
6:E:14:MET:SD	6:E:102:ARG:HG3	2.56	0.46
9:H:21:GLU:OE1	31:d:58:ALA:N	2.45	0.46
9:H:142:HIS:CD2	9:H:181:ARG:HG2	2.51	0.46
20:S:20:TYR:O	20:S:24:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:6:ILE:HD12	22:U:143:PHE:CD2	2.51	0.46
22:U:54:GLU:OE1	22:U:54:GLU:N	2.34	0.46
28:3:66:LEU:O	28:3:70:CYS:N	2.48	0.46
1:2:477:U:H2'	1:2:489:G:C8	2.51	0.46
1:2:1435:C:H2'	1:2:1436:U:C6	2.51	0.46
9:H:11:LYS:HZ2	9:H:16:TRP:CA	2.28	0.46
15:N:51:ARG:HD2	15:N:102:GLU:OE1	2.15	0.46
1:2:219:A:H2'	1:2:220:U:H6	1.81	0.45
1:2:985:C:C2	1:2:986:U:C5	3.04	0.45
1:2:1094:U:O2	1:2:1094:U:H2'	2.15	0.45
1:2:1186:C:OP1	1:2:1188:G:C8	2.69	0.45
1:2:1445:G:H2'	1:2:1446:G:C8	2.51	0.45
2:A:17:LYS:HD3	2:A:37:PRO:HB2	1.99	0.45
12:K:6:LYS:HG3	12:K:93:PHE:CE1	2.51	0.45
13:L:83:MET:SD	13:L:83:MET:N	2.89	0.45
1:2:175:U:H2'	1:2:176:G:O4'	2.16	0.45
1:2:188:C:O2'	11:J:64:ASN:OD1	2.32	0.45
1:2:546:OMG:C2	1:2:714:G:C6	3.05	0.45
1:2:883:U:H2'	1:2:884:U:C6	2.52	0.45
1:2:975:G:H1'	26:Y:53:LYS:NZ	2.31	0.45
7:F:141:LYS:HG3	7:F:146:GLU:OE2	2.15	0.45
12:K:27:LYS:HD3	22:U:155:VAL:HG22	1.97	0.45
12:K:49:ILE:HD11	12:K:79:ALA:HA	1.99	0.45
12:K:64:ILE:HD12	12:K:64:ILE:HA	1.82	0.45
1:2:954:G:H2'	1:2:955:A:H8	1.81	0.45
1:2:1188:G:OP1	16:O:132:THR:N	2.49	0.45
20:S:29:ASN:O	20:S:33:GLN:HG2	2.16	0.45
26:Y:32:ASN:O	26:Y:33:LYS:HD2	2.16	0.45
1:2:1078:C:H2'	1:2:1079:U:C6	2.51	0.45
1:2:1081:G:H5''	13:L:36:ARG:HB3	1.98	0.45
1:2:1208:G:OP2	22:U:46:LYS:NZ	2.41	0.45
1:2:1487:G:H2'	1:2:1488:A:H8	1.82	0.45
6:E:177:SER:HA	6:E:231:ARG:O	2.16	0.45
7:F:121:CYS:SG	7:F:126:CYS:HB3	2.56	0.45
9:H:173:ASP:OD1	9:H:175:LYS:NZ	2.49	0.45
22:U:45:PHE:HB3	22:U:97:VAL:HB	1.97	0.45
24:W:40:CYS:C	24:W:42:SER:H	2.24	0.45
25:X:48:ASP:OD1	25:X:51:ARG:NE	2.50	0.45
30:c:59:ILE:HG23	30:c:60:LYS:CE	2.46	0.45
1:2:220:U:H2'	1:2:221:G:C8	2.52	0.45
1:2:644:G:H1'	14:M:33:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:928:A:H62	37:2:1578:SPM:H111	1.80	0.45
1:2:1019:U:OP1	13:L:59:ARG:NE	2.39	0.45
2:A:39:TYR:N	2:A:43:GLN:OE1	2.49	0.45
6:E:118:TYR:OH	6:E:235:ASP:OD2	2.26	0.45
9:H:109:ALA:HB1	9:H:135:ARG:HB3	1.98	0.45
12:K:119:GLU:HG2	12:K:128:ALA:HB1	1.98	0.45
22:U:5:MET:O	22:U:6:ILE:HD13	2.15	0.45
30:c:39:GLU:OE1	30:c:39:GLU:N	2.38	0.45
35:s:807:G:H2'	35:s:808:A:C8	2.51	0.45
1:2:269:G:O2'	19:R:100:PRO:O	2.31	0.45
1:2:938:U:OP2	17:P:27:SER:OG	2.29	0.45
5:D:134:ASN:C	5:D:134:ASN:HD22	2.24	0.45
8:G:10:ASP:OD2	8:G:113:ARG:NH1	2.49	0.45
17:P:3:LYS:HD3	17:P:4:TYR:CZ	2.52	0.45
25:X:36:VAL:HG11	25:X:56:ASN:HB3	1.98	0.45
28:3:93:GLN:OE1	28:3:93:GLN:N	2.50	0.45
28:3:105:GLY:C	28:3:106:GLU:HG3	2.42	0.45
28:3:120:GLU:OE1	28:3:120:GLU:N	2.50	0.45
1:2:538:OMC:HM22	1:2:539:C:O4'	2.17	0.45
1:2:563:C:OP1	6:E:184:GLY:HA3	2.17	0.45
1:2:612:A:N6	24:W:10:PRO:HG3	2.31	0.45
1:2:1161:G:O6	37:2:1568:SPM:N1	2.50	0.45
1:2:1337:G:N7	12:K:15:LYS:NZ	2.65	0.45
37:2:1569:SPM:H91	12:K:121:GLU:OE1	2.17	0.45
3:B:113:PHE:CD1	3:B:202:ALA:HB2	2.51	0.45
8:G:23:VAL:HG22	8:G:92:VAL:HB	1.98	0.45
8:G:49:LYS:HZ1	8:G:89:ASP:HA	1.82	0.45
16:O:38:LYS:HE3	16:O:38:LYS:HB3	1.70	0.45
24:W:39:ARG:HH11	24:W:39:ARG:HG2	1.82	0.45
25:X:26:ILE:HD11	25:X:62:ARG:HA	1.98	0.45
31:d:57:PRO:O	31:d:60:VAL:HG22	2.17	0.45
1:2:47:A:OP2	39:2:1605:HOH:O	2.20	0.45
1:2:71:G:H2'	1:2:72:G:H8	1.81	0.45
1:2:328:U:H2'	1:2:329:G:O4'	2.17	0.45
1:2:801:C:H2'	1:2:802:U:O4'	2.17	0.45
1:2:1075:C:H1'	1:2:1142:A:C4	2.52	0.45
1:2:1096:U:O2	1:2:1100:G:C6	2.70	0.45
2:A:22:VAL:HG12	2:A:79:LEU:HB2	1.98	0.45
2:A:23:ILE:O	2:A:81:THR:HG22	2.17	0.45
6:E:30:PRO:HB2	6:E:31:HIS:CD2	2.52	0.45
13:L:45:LYS:HA	13:L:67:MET:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:80:VAL:HG22	28:3:81:SER:O	2.17	0.45
31:d:7:LYS:HE3	31:d:55:GLN:CD	2.42	0.45
1:2:1028:C:H2'	1:2:1029:G:C8	2.50	0.45
1:2:1057:C:N4	1:2:1060:OMC:OP2	2.50	0.45
8:G:148:VAL:HB	8:G:212:ILE:HG23	1.99	0.45
26:Y:41:CYS:HA	26:Y:65:TYR:HH	1.82	0.45
28:3:16:ALA:O	28:3:19:VAL:HG22	2.16	0.45
34:4:63:G:H2'	34:4:64:G:H8	1.82	0.45
1:2:257:U:H5''	11:J:10:ARG:HG2	1.98	0.45
1:2:1059:A:H2'	1:2:1060:OMC:C6	2.52	0.45
1:2:1340:U:H2'	1:2:1341:A:C8	2.52	0.45
2:A:110:VAL:HG11	2:A:146:VAL:HG12	1.99	0.45
8:G:46:VAL:HG13	8:G:50:THR:OG1	2.18	0.45
14:M:26:SER:HB2	14:M:33:ILE:HG22	1.98	0.45
22:U:77:GLU:HA	22:U:80:ARG:HG3	1.98	0.45
27:Z:165:ARG:HD3	29:a:6:ARG:HB3	1.99	0.45
1:2:504:C:O2'	1:2:508:U:OP1	2.35	0.44
1:2:614:G:H2'	1:2:615:G:C8	2.52	0.44
1:2:681:G:N7	2:A:129:LYS:NZ	2.65	0.44
1:2:1319:A:H2'	1:2:1320:G:C8	2.52	0.44
2:A:36:THR:OG1	2:A:47:ARG:NH1	2.50	0.44
5:D:145:VAL:HG13	5:D:149:GLU:HG3	1.99	0.44
8:G:47:ASN:O	8:G:50:THR:OG1	2.29	0.44
9:H:26:SER:HB2	25:X:66:ILE:O	2.16	0.44
18:Q:25:ARG:CZ	18:Q:25:ARG:HA	2.47	0.44
23:V:52:ILE:HD13	23:V:52:ILE:HA	1.89	0.44
27:Z:25:GLN:O	27:Z:26:TYR:HD1	2.00	0.44
1:2:23:C:O2'	1:2:301:U:OP1	2.33	0.44
1:2:1276:G:P	21:T:39:ARG:HH22	2.41	0.44
1:2:40:G:H2'	1:2:41:G:H8	1.82	0.44
1:2:147:G:H2'	1:2:148:G:H8	1.82	0.44
1:2:1477:4AC:O7	1:2:1477:4AC:H5	2.16	0.44
37:2:1559:SPM:H62	37:2:1559:SPM:H31	1.69	0.44
2:A:40:ASP:OD1	2:A:40:ASP:C	2.61	0.44
3:B:131:PHE:HB2	3:B:159:GLU:HB3	1.99	0.44
7:F:207:LEU:HD22	7:F:210:TRP:CZ2	2.52	0.44
12:K:121:GLU:HA	12:K:128:ALA:HA	2.00	0.44
27:Z:17:LYS:HD2	27:Z:74:PHE:CE1	2.53	0.44
28:3:41:LYS:HB3	28:3:41:LYS:HE3	1.80	0.44
1:2:229:C:H2'	1:2:230:A:C8	2.52	0.44
1:2:413:U:H2'	1:2:414:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:418:U:H4'	1:2:419:A:H5'	1.99	0.44
1:2:807:G:H2'	1:2:808:C:H6	1.83	0.44
1:2:1038:A:OP2	7:F:95:LYS:NZ	2.51	0.44
6:E:176:ARG:HB2	6:E:176:ARG:HH11	1.82	0.44
8:G:95:SER:OG	8:G:97:THR:OG1	2.35	0.44
9:H:36:VAL:HG23	12:K:106:TYR:CZ	2.53	0.44
13:L:80:GLU:O	13:L:84:ARG:HG3	2.18	0.44
21:T:54:LEU:HA	21:T:57:VAL:HG12	1.99	0.44
25:X:55:ARG:CZ	25:X:69:LEU:HD12	2.47	0.44
31:d:43:LEU:HD21	31:d:48:GLU:HG2	2.00	0.44
34:4:67:C:H2'	34:4:68:C:C6	2.53	0.44
1:2:1241:G:O2'	1:2:1243:A:N3	2.47	0.44
1:2:1427:C:H2'	1:2:1428:U:O4'	2.17	0.44
6:E:210:THR:HG23	6:E:220:GLN:CG	2.47	0.44
9:H:138:LEU:HD23	9:H:142:HIS:NE2	2.32	0.44
28:3:6:TYR:CZ	28:3:8:LYS:HD2	2.52	0.44
31:d:37:LEU:O	31:d:41:LEU:HG	2.18	0.44
1:2:44:C:H3'	1:2:45:U:H5''	1.99	0.44
1:2:349:A:H5''	1:2:350:C:C5	2.50	0.44
1:2:377:C:O2'	37:2:1570:SPM:N14	2.50	0.44
1:2:409:G:O2'	1:2:456:A:N1	2.47	0.44
1:2:784:G:H2'	1:2:785:C:H6	1.81	0.44
1:2:1323:C:H5''	17:P:14:LYS:HA	1.99	0.44
6:E:34:GLU:H	6:E:34:GLU:CD	2.17	0.44
9:H:34:MET:HA	9:H:35:PRO:HD3	1.76	0.44
10:I:14:ILE:HD11	10:I:38:LEU:HD21	1.99	0.44
20:S:34:ILE:HA	20:S:37:ARG:HG2	1.98	0.44
28:3:52:ILE:HG12	28:3:78:VAL:HB	2.00	0.44
34:4:27:U:H2'	34:4:28:C:C6	2.53	0.44
35:s:814:A:OP1	35:s:814:A:C8	2.71	0.44
1:2:167:A:H2'	1:2:168:G:C8	2.53	0.44
1:2:395:G:H2'	1:2:396:G:H8	1.83	0.44
1:2:1079:U:H2'	1:2:1080:A:O4'	2.18	0.44
1:2:1257:U:OP1	30:c:99:LYS:NZ	2.51	0.44
2:A:168:ALA:HB1	2:A:184:ALA:O	2.17	0.44
6:E:147:GLU:OE1	6:E:147:GLU:HA	2.18	0.44
12:K:101:LYS:CE	31:d:66:PRO:HB3	2.45	0.44
19:R:30:TYR:OH	19:R:110:LEU:O	2.33	0.44
24:W:40:CYS:CB	24:W:43:CYS:SG	3.05	0.44
27:Z:127:LEU:HG	27:Z:186:PRO:HA	2.00	0.44
1:2:82:G:O2'	1:2:132:A:N3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:391:G:OP2	37:2:1570:SPM:H42	2.18	0.44
1:2:831:C:H2'	1:2:832:G:O4'	2.18	0.44
1:2:909:G:OP2	39:2:1607:HOH:O	2.21	0.44
1:2:1207:A:H2'	1:2:1208:G:H8	1.83	0.44
1:2:1341:A:N6	9:H:46:GLU:OE2	2.42	0.44
1:2:1422:U:H2'	1:2:1423:C:H6	1.83	0.44
8:G:47:ASN:OD1	8:G:85:ASN:HA	2.18	0.44
12:K:30:VAL:HA	12:K:66:ALA:O	2.18	0.44
18:Q:76:ARG:HB2	18:Q:78:LEU:HD12	1.99	0.44
25:X:22:GLU:HB2	25:X:44:LEU:HD21	2.00	0.44
25:X:47:ARG:HG2	25:X:47:ARG:HH11	1.82	0.44
29:a:22:ARG:N	29:a:48:TYR:O	2.47	0.44
33:5:6:U:H3'	33:5:7:G:C5'	2.46	0.44
1:2:66:U:H2'	1:2:67:C:O4'	2.18	0.44
1:2:1344:OMU:HM23	1:2:1344:OMU:H1'	1.81	0.44
1:2:1464:A:H2'	1:2:1465:G:C8	2.53	0.44
37:2:1571:SPM:H72	37:2:1571:SPM:H41	1.69	0.44
8:G:89:ASP:OD1	8:G:90:ASN:N	2.51	0.44
15:N:91:ASP:N	15:N:138:TYR:OH	2.47	0.44
16:O:56:SER:OG	16:O:59:GLU:OE1	2.24	0.44
20:S:16:ILE:HD11	20:S:39:VAL:CG2	2.48	0.44
34:4:23:C:H2'	34:4:24:U:C6	2.53	0.44
1:2:45:U:O2'	1:2:46:A:H2'	2.18	0.43
1:2:112:C:H2'	1:2:113:OMC:C6	2.53	0.43
1:2:498:G:H5''	32:e:22:PRO:HB3	2.00	0.43
1:2:651:C:O2'	1:2:653:A:N7	2.46	0.43
1:2:1093:G:H3'	1:2:1094:U:H6	1.83	0.43
2:A:19:TRP:CZ2	2:A:37:PRO:HG3	2.53	0.43
2:A:67:LEU:HD23	2:A:86:HIS:HB2	2.00	0.43
8:G:72:LYS:HD2	8:G:72:LYS:HA	1.73	0.43
9:H:24:ASP:OD1	9:H:26:SER:N	2.51	0.43
9:H:110:PRO:O	9:H:135:ARG:HG2	2.18	0.43
31:d:61:MET:HE3	31:d:61:MET:HB2	1.90	0.43
1:2:387:A:H2'	1:2:388:A:C8	2.52	0.43
1:2:518:U:OP2	37:2:1554:SPM:N5	2.52	0.43
1:2:779:U:H4'	1:2:780:G:OP2	2.18	0.43
1:2:934:C:OP1	13:L:60:LYS:NZ	2.47	0.43
1:2:1058:A:H4'	1:2:1059:A:H5'	1.99	0.43
1:2:1363:C:O2	1:2:1459:A:N6	2.51	0.43
1:2:1422:U:H2'	1:2:1423:C:C6	2.53	0.43
6:E:40:ALA:HB2	6:E:75:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:194:LYS:NZ	6:E:194:LYS:HB3	2.33	0.43
9:H:6:LEU:HD22	9:H:8:LEU:HG	1.98	0.43
11:J:11:LYS:HG2	11:J:17:LYS:HD3	2.00	0.43
11:J:58:LYS:HA	11:J:58:LYS:HD2	1.67	0.43
12:K:9:ILE:HD12	12:K:22:TYR:HD2	1.83	0.43
14:M:42:VAL:HG21	14:M:57:LEU:HB2	2.00	0.43
22:U:127:LEU:HD23	22:U:127:LEU:HA	1.87	0.43
24:W:18:ARG:NH1	24:W:27:GLU:HG3	2.32	0.43
27:Z:112:ARG:HG3	33:5:14:A:OP1	2.19	0.43
31:d:33:THR:HG22	31:d:36:GLU:OE2	2.18	0.43
1:2:1336:U:H2'	1:2:1337:G:O4'	2.18	0.43
1:2:1375:C:HO2'	1:2:1376:C:P	2.40	0.43
34:4:22:G:H2'	34:4:23:C:C6	2.52	0.43
34:4:68:C:H2'	34:4:69:C:C6	2.53	0.43
1:2:268:A:H2'	1:2:269:G:H8	1.84	0.43
1:2:441:C:P	23:V:101:ARG:HH21	2.42	0.43
1:2:1262:C:C4	9:H:155:PRO:HA	2.52	0.43
1:2:1290:C:H2'	1:2:1291:U:H6	1.84	0.43
2:A:22:VAL:O	2:A:33:LEU:N	2.36	0.43
14:M:25:ILE:O	14:M:34:ILE:N	2.38	0.43
18:Q:58:ILE:HG23	18:Q:64:ILE:HD12	2.00	0.43
28:3:27:LYS:HG3	28:3:32:ILE:HG21	2.00	0.43
32:e:28:GLU:HB2	32:e:33:ARG:HB2	2.00	0.43
1:2:72:G:N1	1:2:209:U:O2'	2.48	0.43
1:2:511:U:H2'	1:2:512:OMC:C6	2.53	0.43
1:2:784:G:H2'	1:2:785:C:C6	2.54	0.43
1:2:1114:U:O2'	13:L:40:PRO:O	2.35	0.43
1:2:1307:C:H2'	1:2:1308:C:C6	2.54	0.43
7:F:118:ARG:HH22	7:F:209:ASP:CG	2.25	0.43
9:H:11:LYS:HE3	9:H:15:LYS:CA	2.48	0.43
9:H:91:LEU:HD12	30:c:97:TYR:OH	2.17	0.43
16:O:17:ASP:OD1	16:O:19:THR:HG22	2.19	0.43
31:d:4:LEU:HD22	31:d:5:LYS:N	2.34	0.43
35:s:812:U:OP1	35:s:812:U:H6	2.00	0.43
1:2:843:C:C5	15:N:6:SER:OG	2.66	0.43
1:2:1110:A:H5'	1:2:1111:C:OP2	2.18	0.43
1:2:1189:C:O2'	30:c:2:GLY:N	2.46	0.43
1:2:1207:A:H2'	1:2:1208:G:C8	2.54	0.43
1:2:1394:G:H2'	1:2:1395:U:O4'	2.18	0.43
37:2:1555:SPM:H122	37:2:1583:SPM:H21	2.00	0.43
37:2:1568:SPM:H131	27:Z:132:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:120:SER:O	12:K:122:LYS:NZ	2.51	0.43
30:c:96:LEU:HB2	30:c:106:TYR:HE1	1.81	0.43
31:d:29:ARG:HH12	31:d:62:TRP:HA	1.84	0.43
1:2:10:G:O2'	7:F:65:GLN:OE1	2.32	0.43
1:2:219:A:H2'	1:2:220:U:C6	2.54	0.43
1:2:416:C:H2'	1:2:417:G:O4'	2.19	0.43
1:2:924:U:C2	1:2:1188:G:C6	3.06	0.43
1:2:1273:G:OP1	16:O:117:ARG:NH1	2.47	0.43
2:A:41:ILE:HG12	2:A:74:ASN:ND2	2.33	0.43
5:D:127:THR:HG23	5:D:128:HIS:HD2	1.84	0.43
12:K:107:ASP:O	12:K:110:MET:HG3	2.18	0.43
13:L:90:ARG:O	13:L:90:ARG:HG2	2.18	0.43
15:N:135:ASP:C	15:N:135:ASP:OD1	2.62	0.43
27:Z:96:MET:HE3	27:Z:96:MET:HA	2.00	0.43
31:d:35:GLU:N	31:d:35:GLU:OE1	2.51	0.43
34:4:9:G:H1'	34:4:45:G:H2'	2.00	0.43
34:4:50:U:O4	34:4:64:G:O6	2.37	0.43
1:2:1492:C:H2'	1:2:1493:C:H6	1.84	0.43
7:F:9:ASN:HB2	7:F:12:GLU:CD	2.44	0.43
9:H:186:GLU:HB3	25:X:70:ARG:NH2	2.33	0.43
10:I:71:LYS:HB3	10:I:133:TYR:CZ	2.54	0.43
17:P:10:ARG:HG3	17:P:10:ARG:HH11	1.83	0.43
22:U:45:PHE:CE1	22:U:46:LYS:HE2	2.54	0.43
26:Y:27:TYR:OH	28:3:44:GLU:HG3	2.19	0.43
34:4:20:H2U:O2'	34:4:22:G:OP1	2.33	0.43
1:2:366:C:H2'	1:2:367:G:C8	2.54	0.43
1:2:625:G:OP1	37:2:1564:SPM:N5	2.52	0.43
1:2:940:G:H21	1:2:1327:A:H5'	1.84	0.43
1:2:1061:OMG:HM22	1:2:1062:A:H5'	2.01	0.43
1:2:1120:G:N7	20:S:44:LYS:NZ	2.60	0.43
1:2:1366:OMC:HM22	1:2:1367:C:H5'	2.01	0.43
7:F:126:CYS:HB2	7:F:153:PRO:HA	2.00	0.43
7:F:148:ASP:OD1	7:F:148:ASP:N	2.50	0.43
8:G:197:ARG:HG2	8:G:205:ILE:HD11	2.01	0.43
18:Q:32:GLU:HB3	18:Q:76:ARG:NH2	2.34	0.43
24:W:64:ILE:O	24:W:65:MET:HG3	2.19	0.43
34:4:24:U:H2'	34:4:25:C:C6	2.53	0.43
1:2:273:C:H2'	1:2:274:C:H6	1.84	0.43
1:2:995:U:H2'	1:2:996:C:C5	2.54	0.43
6:E:127:ILE:HG13	6:E:128:LYS:H	1.84	0.43
6:E:153:LYS:O	6:E:156:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:180:LYS:HE3	9:H:180:LYS:HB2	1.75	0.43
21:T:94:LYS:HB2	21:T:94:LYS:HE3	1.82	0.43
1:2:367:G:N1	1:2:370:A:OP2	2.49	0.42
1:2:988:G:O2'	1:2:989:C:O5'	2.35	0.42
1:2:1448:G:O2'	1:2:1449:A:H5'	2.19	0.42
9:H:33:LEU:H	31:d:62:TRP:CG	2.36	0.42
10:I:71:LYS:HG3	10:I:72:CYS:N	2.33	0.42
21:T:25:MET:HE1	21:T:33:LEU:HD11	2.00	0.42
21:T:67:ASN:OD1	21:T:67:ASN:N	2.51	0.42
34:4:52:G:H2'	34:4:53:G:C8	2.51	0.42
1:2:260:G:H2'	1:2:261:G:C8	2.53	0.42
1:2:843:C:O2	1:2:844:G:C8	2.72	0.42
1:2:855:A:H2'	1:2:856:C:C6	2.53	0.42
2:A:36:THR:HA	2:A:37:PRO:HD3	1.90	0.42
3:B:211:VAL:HG23	3:B:212:ILE:HG23	2.02	0.42
5:D:97:THR:OG1	5:D:98:GLU:OE1	2.33	0.42
9:H:30:TYR:CE2	9:H:132:PRO:HG2	2.54	0.42
9:H:190:LEU:HA	9:H:193:ARG:HB2	2.02	0.42
31:d:21:ILE:HD11	31:d:60:VAL:HB	2.00	0.42
1:2:267:A:OP2	11:J:54:LYS:NZ	2.42	0.42
1:2:671:A:H2'	1:2:672:OMG:C8	2.54	0.42
1:2:1077:A:H2'	1:2:1078:C:H6	1.83	0.42
1:2:1172:C:H2'	1:2:1173:C:C6	2.54	0.42
12:K:29:ARG:HA	22:U:156:TYR:CE1	2.55	0.42
28:3:70:CYS:SG	28:3:77:TYR:HB3	2.59	0.42
1:2:311:A:O2'	1:2:312:G:H5'	2.19	0.42
1:2:446:G:H21	23:V:42:THR:HG21	1.84	0.42
1:2:519:C:H5'	1:2:525:G:N2	2.34	0.42
1:2:695:U:H2'	1:2:696:G:H8	1.83	0.42
1:2:908:G:O6	37:2:1580:SPM:H121	2.19	0.42
1:2:1095:C:OP1	22:U:129:PRO:HB2	2.20	0.42
1:2:1164:A:H4'	1:2:1165:G:H5''	2.01	0.42
1:2:1350:C:H2'	1:2:1351:U:C6	2.55	0.42
1:2:1447:A:H2'	1:2:1448:G:C8	2.50	0.42
1:2:1466:4AC:O7	1:2:1466:4AC:H5	2.18	0.42
13:L:4:LYS:H	13:L:4:LYS:CE	2.33	0.42
20:S:25:LYS:H	20:S:31:ASN:HD21	1.66	0.42
23:V:92:LYS:HE2	23:V:92:LYS:HB2	1.80	0.42
1:2:73:C:OP2	1:2:209:U:N3	2.39	0.42
1:2:207:U:H2'	1:2:208:A:H8	1.84	0.42
1:2:787:A:H2'	1:2:788:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:828:A:H5'	37:2:1566:SPM:N5	2.35	0.42
1:2:974:A:H2	26:Y:53:LYS:HE3	1.84	0.42
5:D:157:VAL:HG13	5:D:158:THR:HG23	2.01	0.42
13:L:52:ARG:NE	13:L:63:GLU:OE2	2.53	0.42
15:N:139:LYS:HE2	15:N:139:LYS:HB3	1.79	0.42
31:d:24:LEU:HD23	31:d:24:LEU:HA	1.76	0.42
1:2:329:G:N1	1:2:332:A:OP2	2.52	0.42
1:2:497:A:H2'	1:2:498:G:H8	1.84	0.42
1:2:938:U:O4	13:L:51:MET:N	2.52	0.42
1:2:1161:G:H2'	1:2:1162:U:C6	2.54	0.42
2:A:20:TYR:CD2	2:A:41:ILE:HD12	2.54	0.42
3:B:74:ASP:O	3:B:78:ILE:HG13	2.20	0.42
12:K:51:GLU:OE1	12:K:51:GLU:HA	2.19	0.42
15:N:118:ASP:OD1	15:N:118:ASP:C	2.63	0.42
22:U:22:ILE:O	22:U:26:GLU:HG2	2.19	0.42
25:X:77:ARG:HD2	25:X:77:ARG:N	2.34	0.42
28:3:27:LYS:NZ	28:3:89:ALA:HB3	2.33	0.42
29:a:20:TYR:CD2	29:a:25:ASN:ND2	2.86	0.42
1:2:72:G:H2'	1:2:209:U:O2	2.19	0.42
1:2:141:A:H2'	1:2:142:A:O4'	2.18	0.42
1:2:558:C:H2'	1:2:559:A:C8	2.54	0.42
1:2:786:U:H2'	1:2:833:U:O4	2.19	0.42
1:2:926:OMG:HM22	1:2:927:G:H5'	2.00	0.42
1:2:967:G:O6	28:3:37:ASN:HB2	2.19	0.42
1:2:1232:A:H2'	1:2:1233:A:C8	2.54	0.42
1:2:1283:A:O2'	1:2:1287:G:N7	2.40	0.42
1:2:1434:C:H2'	1:2:1435:C:H6	1.84	0.42
3:B:146:LEU:HD12	3:B:168:VAL:O	2.19	0.42
6:E:145:ASP:OD1	6:E:145:ASP:C	2.63	0.42
9:H:18:THR:O	9:H:18:THR:OG1	2.38	0.42
15:N:32:THR:HG22	15:N:37:LEU:HD12	2.01	0.42
15:N:134:LEU:O	15:N:138:TYR:HB2	2.20	0.42
23:V:107:GLN:OE1	23:V:107:GLN:HA	2.19	0.42
26:Y:36:LEU:HB3	26:Y:38:ASN:O	2.19	0.42
31:d:33:THR:HG23	31:d:35:GLU:H	1.85	0.42
34:4:35:A:H2'	34:4:36:U:H6	1.83	0.42
1:2:161:U:H2'	1:2:162:A:C8	2.55	0.42
1:2:649:G:H2'	1:2:650:G:C8	2.55	0.42
5:D:117:ASN:H	5:D:121:GLN:NE2	2.18	0.42
12:K:98:GLU:H	12:K:98:GLU:CD	2.19	0.42
15:N:77:LEU:HD21	15:N:105:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:11:ARG:HH22	20:S:12:ILE:HD13	1.85	0.42
20:S:25:LYS:NZ	20:S:26:ASP:H	2.18	0.42
21:T:54:LEU:HA	21:T:54:LEU:HD23	1.84	0.42
21:T:108:HIS:ND1	21:T:113:TYR:OH	2.52	0.42
27:Z:164:ASP:C	27:Z:164:ASP:OD1	2.63	0.42
30:c:14:LYS:HE2	30:c:14:LYS:HA	2.02	0.42
30:c:96:LEU:HD22	30:c:97:TYR:N	2.35	0.42
1:2:796:A:H2'	1:2:797:U:C6	2.55	0.42
1:2:971:G:H2'	1:2:972:C:O4'	2.19	0.42
1:2:986:U:C4	1:2:987:U:C4	3.08	0.42
1:2:1349:G:H2'	1:2:1350:C:C6	2.55	0.42
2:A:197:ASN:OD1	2:A:197:ASN:N	2.52	0.42
3:B:142:PRO:HG2	3:B:165:ILE:HD13	2.02	0.42
6:E:31:HIS:CG	6:E:80:GLY:HA3	2.55	0.42
6:E:102:ARG:HA	6:E:102:ARG:HD3	1.83	0.42
16:O:17:ASP:OD1	16:O:17:ASP:C	2.63	0.42
28:3:110:LEU:C	28:3:110:LEU:CD1	2.86	0.42
1:2:559:A:H2'	1:2:560:C:C6	2.55	0.42
1:2:663:A:C5	1:2:664:U:C5	3.08	0.42
1:2:736:A:H2'	1:2:737:G:C8	2.55	0.42
1:2:1436:U:O2'	1:2:1437:G:OP1	2.29	0.42
37:2:1577:SPM:H31	37:2:1577:SPM:H61	1.64	0.42
2:A:19:TRP:CE2	2:A:37:PRO:HG3	2.55	0.42
3:B:127:ILE:O	3:B:130:THR:OG1	2.27	0.42
8:G:59:LEU:HB3	8:G:114:THR:HB	2.02	0.42
9:H:173:ASP:OD2	9:H:175:LYS:HG2	2.20	0.42
14:M:120:THR:OG1	14:M:121:ILE:N	2.51	0.42
23:V:8:LYS:HD2	23:V:14:GLU:OE1	2.19	0.42
34:4:36:U:C2	34:4:37:A:C8	3.08	0.42
1:2:138:G:N7	37:2:1575:SPM:H32	2.35	0.41
1:2:591:U:H2'	1:2:592:G:H8	1.86	0.41
1:2:1126:C:H2'	1:2:1127:G:H8	1.85	0.41
37:2:1555:SPM:H71	37:2:1555:SPM:H41	1.86	0.41
37:2:1562:SPM:H92	37:2:1562:SPM:H122	1.76	0.41
2:A:114:ASP:OD1	2:A:114:ASP:N	2.42	0.41
3:B:199:TRP:NE1	3:B:218:LEU:HD23	2.34	0.41
4:C:28:LYS:HD2	4:C:28:LYS:HA	1.82	0.41
9:H:91:LEU:HD12	30:c:97:TYR:CZ	2.54	0.41
11:J:67:ASP:HB2	11:J:125:LEU:HD12	2.01	0.41
11:J:127:LYS:HA	11:J:127:LYS:HE2	2.01	0.41
16:O:142:ILE:HD12	21:T:125:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:44:C:H3'	1:2:45:U:C5'	2.50	0.41
1:2:326:A:O2'	8:G:191:ARG:NH2	2.53	0.41
1:2:534:G:O2'	1:2:780:G:H5'	2.20	0.41
1:2:571:C:H2'	1:2:572:C:H6	1.85	0.41
1:2:941:A:N6	1:2:1187:C:O5'	2.53	0.41
1:2:1478:4AC:O7	1:2:1478:4AC:H5	2.19	0.41
2:A:114:ASP:O	2:A:195:PRO:HG3	2.20	0.41
3:B:21:LYS:HE3	3:B:21:LYS:HB2	1.83	0.41
3:B:24:LEU:H	3:B:24:LEU:HD22	1.85	0.41
12:K:107:ASP:OD1	12:K:107:ASP:C	2.62	0.41
14:M:33:ILE:HD12	14:M:33:ILE:C	2.45	0.41
16:O:57:ASP:O	16:O:61:LYS:HG2	2.21	0.41
22:U:19:ARG:NH1	22:U:141:GLU:OE1	2.49	0.41
26:Y:32:ASN:C	26:Y:33:LYS:HD2	2.45	0.41
28:3:36:THR:HA	28:3:98:SER:HB3	2.02	0.41
1:2:159:C:OP2	39:2:1608:HOH:O	2.22	0.41
1:2:193:A:H2'	1:2:194:A:C8	2.55	0.41
1:2:543:G:H2'	1:2:544:C:C6	2.56	0.41
1:2:634:U:C2	1:2:635:A:C8	3.08	0.41
1:2:1003:A:H2'	1:2:1004:G:O4'	2.19	0.41
2:A:40:ASP:OD1	2:A:42:THR:N	2.53	0.41
2:A:96:LEU:HB3	2:A:125:LEU:HD11	2.01	0.41
9:H:57:ILE:HA	9:H:60:ARG:HG3	2.03	0.41
11:J:114:ARG:O	11:J:118:ASP:HB2	2.20	0.41
18:Q:97:ARG:CZ	18:Q:141:PRO:HB3	2.50	0.41
1:2:56:A:OP1	1:2:336:G:N1	2.40	0.41
1:2:340:C:O2'	1:2:1397:A:N3	2.49	0.41
1:2:794:A:H2'	1:2:795:C:C6	2.56	0.41
1:2:1241:G:H1'	1:2:1246:C:O2	2.20	0.41
5:D:54:GLN:O	5:D:58:LEU:HG	2.21	0.41
7:F:138:VAL:HG11	7:F:201:THR:HG22	2.02	0.41
9:H:63:ASN:OD1	9:H:75:LYS:HE3	2.20	0.41
12:K:124:MET:HE2	13:L:60:LYS:N	2.27	0.41
15:N:44:LEU:HG	15:N:50:ALA:HB2	2.01	0.41
28:3:6:TYR:HB2	28:3:55:GLU:OE2	2.20	0.41
28:3:88:GLU:HA	28:3:92:LEU:O	2.20	0.41
34:4:66:C:H2'	34:4:67:C:C6	2.55	0.41
1:2:29:G:H2'	1:2:30:C:H6	1.84	0.41
1:2:38:G:N7	37:2:1584:SPM:H41	2.35	0.41
1:2:644:G:C1'	14:M:33:ILE:HD11	2.50	0.41
1:2:807:G:H2'	1:2:808:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:976:G:H2'	1:2:977:C:H6	1.86	0.41
1:2:1096:U:C2	1:2:1098:C:C4	3.03	0.41
1:2:1314:A:H2'	1:2:1315:C:C6	2.56	0.41
2:A:130:CYS:SG	2:A:134:GLN:HB2	2.60	0.41
7:F:91:ILE:HG21	7:F:191:VAL:HG12	2.02	0.41
8:G:65:THR:HA	8:G:74:LYS:HA	2.03	0.41
22:U:76:ILE:HD13	22:U:76:ILE:HA	1.82	0.41
24:W:40:CYS:SG	24:W:42:SER:OG	2.77	0.41
25:X:15:GLU:OE2	25:X:45:GLU:HG2	2.20	0.41
29:a:14:LEU:HD23	29:a:14:LEU:HA	1.88	0.41
1:2:91:G:OP1	37:2:1557:SPM:H91	2.20	0.41
1:2:478:C:H2'	1:2:479:A:O4'	2.19	0.41
1:2:855:A:H2'	1:2:856:C:H6	1.84	0.41
1:2:1044:C:C2	1:2:1045:U:C5	3.08	0.41
1:2:1114:U:H4'	13:L:42:PRO:HG3	2.03	0.41
1:2:1418:G:H2'	1:2:1419:G:C8	2.56	0.41
7:F:8:LEU:HB2	7:F:48:ASP:HB3	2.03	0.41
7:F:9:ASN:OD1	7:F:9:ASN:N	2.52	0.41
9:H:89:ILE:HD11	9:H:97:PRO:CA	2.47	0.41
9:H:145:THR:O	9:H:148:LYS:N	2.53	0.41
16:O:78:TRP:CH2	22:U:40:ALA:HB2	2.54	0.41
22:U:143:PHE:HE1	22:U:153:LEU:HB3	1.85	0.41
26:Y:40:LYS:HA	26:Y:40:LYS:HD2	1.83	0.41
26:Y:55:ASN:ND2	26:Y:57:ARG:HG2	2.36	0.41
27:Z:2:PRO:HG2	27:Z:6:ARG:HG2	2.01	0.41
27:Z:118:MET:SD	27:Z:129:ALA:HB3	2.61	0.41
30:c:29:LYS:HA	30:c:35:LYS:HD3	2.01	0.41
1:2:569:G:C4	1:2:570:A:C8	3.09	0.41
1:2:569:G:C2	1:2:570:A:C8	3.09	0.41
1:2:751:A:O2'	1:2:753:A:N7	2.49	0.41
1:2:1173:C:H2'	1:2:1174:G:O4'	2.20	0.41
3:B:29:LYS:HB2	3:B:76:ARG:HD2	2.03	0.41
6:E:103:PHE:O	6:E:104:MET:HG3	2.21	0.41
9:H:68:PRO:HG2	9:H:70:ARG:HG2	2.02	0.41
9:H:85:ALA:O	9:H:89:ILE:HG23	2.21	0.41
12:K:24:TYR:CE1	12:K:65:ASP:HB3	2.55	0.41
15:N:57:LYS:HG2	15:N:73:VAL:HG12	2.03	0.41
18:Q:123:LEU:HD23	18:Q:123:LEU:HA	1.87	0.41
25:X:28:ASP:OD1	25:X:28:ASP:N	2.52	0.41
27:Z:170:ALA:HB1	27:Z:172:LEU:HD23	2.02	0.41
28:3:66:LEU:HA	28:3:69:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:58:U:H2'	1:2:59:C:C6	2.56	0.41
1:2:303:A:H2'	1:2:304:G:O4'	2.21	0.41
1:2:947:A:H5'	1:2:948:C:OP2	2.21	0.41
1:2:1172:C:H2'	1:2:1173:C:H6	1.86	0.41
1:2:1365:G:H2'	1:2:1366:OMC:O4'	2.20	0.41
1:2:1369:G:H2'	1:2:1370:U:C6	2.55	0.41
1:2:1467:4AC:H5	1:2:1467:4AC:O7	2.20	0.41
34:4:66:C:H2'	34:4:67:C:H6	1.84	0.41
1:2:65:C:H2'	1:2:66:U:C6	2.56	0.41
1:2:310:G:H5''	1:2:311:A:OP1	2.21	0.41
1:2:314:C:H2'	1:2:315:C:H6	1.85	0.41
1:2:338:G:O2'	8:G:191:ARG:O	2.33	0.41
1:2:974:A:H1'	26:Y:57:ARG:CZ	2.50	0.41
1:2:1068:A:N7	39:2:1640:HOH:O	2.37	0.41
1:2:1070:C:C2	1:2:1071:C:C5	3.09	0.41
1:2:1125:C:C2	1:2:1126:C:C5	3.08	0.41
1:2:1315:C:OP1	37:2:1579:SPM:H61	2.21	0.41
1:2:1331:U:OP2	37:2:1569:SPM:H132	2.20	0.41
1:2:1444:G:HO2'	1:2:1445:G:H8	1.65	0.41
2:A:114:ASP:OD2	2:A:154:SER:OG	2.38	0.41
2:A:153:LEU:HD23	2:A:153:LEU:HA	1.90	0.41
3:B:134:PRO:HA	3:B:139:TYR:CD2	2.56	0.41
5:D:99:GLN:O	5:D:103:GLU:HG2	2.20	0.41
8:G:23:VAL:HB	8:G:107:PHE:CE1	2.56	0.41
8:G:32:ILE:HG23	8:G:35:GLU:HG3	2.03	0.41
9:H:25:PRO:O	9:H:28:LYS:HG3	2.21	0.41
9:H:119:TYR:CD2	25:X:77:ARG:HD3	2.56	0.41
10:I:50:PHE:HA	10:I:62:THR:O	2.20	0.41
11:J:92:ARG:HA	11:J:92:ARG:NH1	2.36	0.41
12:K:59:ASP:HB2	12:K:63:LYS:NZ	2.35	0.41
16:O:138:THR:HG21	30:c:6:LYS:NZ	2.36	0.41
25:X:22:GLU:CB	25:X:44:LEU:HD21	2.51	0.41
28:3:17:ASP:HA	28:3:20:LEU:HB2	2.02	0.41
28:3:56:ASP:CA	28:3:60:GLU:OE2	2.53	0.41
31:d:34:LEU:HD22	31:d:50:TYR:HB2	2.03	0.41
34:4:27:U:H2'	34:4:28:C:H6	1.85	0.41
1:2:52:OMU:HM22	1:2:53:G:O4'	2.20	0.41
1:2:184:U:C2	1:2:185:C:C5	3.08	0.41
1:2:327:C:H2'	1:2:328:U:C6	2.56	0.41
1:2:579:C:OP1	37:2:1590:SPM:N14	2.54	0.41
1:2:958:C:OP1	29:a:55:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1186:C:OP1	1:2:1188:G:H8	2.04	0.41
1:2:1188:G:OP1	16:O:131:ARG:HB3	2.21	0.41
1:2:1454:G:C2'	1:2:1455:U:H5'	2.50	0.41
3:B:81:ARG:HD3	3:B:81:ARG:HA	1.83	0.41
8:G:43:GLN:OE1	8:G:82:ASP:N	2.54	0.41
9:H:6:LEU:HD21	9:H:8:LEU:CG	2.49	0.41
12:K:7:LEU:HD21	12:K:9:ILE:HD11	2.02	0.41
21:T:84:ILE:HD13	21:T:101:VAL:HG12	2.02	0.41
22:U:12:PRO:HA	22:U:13:PRO:HD3	1.92	0.41
1:2:458:G:H2'	1:2:459:C:H6	1.85	0.40
1:2:709:C:OP2	18:Q:14:ARG:NH2	2.53	0.40
1:2:946:U:H4'	1:2:947:A:O4'	2.21	0.40
1:2:1071:C:H2'	1:2:1072:C:H6	1.86	0.40
1:2:1314:A:H2'	1:2:1315:C:H6	1.85	0.40
37:2:1567:SPM:H32	37:2:1567:SPM:H61	1.94	0.40
8:G:164:ARG:HB3	8:G:196:ILE:HD12	2.04	0.40
9:H:24:ASP:OD1	9:H:27:LEU:HG	2.21	0.40
14:M:66:ALA:HA	14:M:69:LYS:HB2	2.03	0.40
16:O:55:LEU:HG	16:O:59:GLU:HG3	2.03	0.40
20:S:25:LYS:HZ2	20:S:26:ASP:H	1.68	0.40
29:a:39:PRO:HD3	29:a:69:VAL:HG12	2.03	0.40
1:2:264:G:H2'	1:2:265:G:C8	2.56	0.40
1:2:1014:G:H2'	1:2:1015:G:O4'	2.22	0.40
1:2:1070:C:H2'	1:2:1071:C:C6	2.54	0.40
1:2:1096:U:C6	1:2:1098:C:N4	2.89	0.40
6:E:174:SER:OG	6:E:177:SER:OG	2.36	0.40
9:H:125:TYR:O	9:H:192:SER:OG	2.33	0.40
16:O:115:SER:HB3	21:T:113:TYR:CE1	2.57	0.40
22:U:5:MET:HB2	22:U:6:ILE:H	1.75	0.40
1:2:782:A:N6	1:2:841:G:O6	2.54	0.40
1:2:925:U:OP1	37:2:1578:SPM:H41	2.21	0.40
1:2:1293:G:H5''	16:O:33:GLY:N	2.36	0.40
1:2:1350:C:C2	1:2:1351:U:C5	3.10	0.40
2:A:12:ASP:OD1	2:A:13:LYS:N	2.54	0.40
5:D:164:ARG:NH2	5:D:165:PRO:O	2.54	0.40
6:E:177:SER:O	6:E:192:ILE:HA	2.22	0.40
8:G:35:GLU:HG2	8:G:42:PRO:HG3	2.04	0.40
8:G:62:LEU:HB2	8:G:79:PHE:HE1	1.86	0.40
12:K:10:SER:HB3	12:K:89:ALA:HB2	2.03	0.40
21:T:72:THR:OG1	21:T:74:VAL:HG12	2.22	0.40
25:X:76:ALA:O	25:X:78:LYS:NZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:85:LEU:HD23	30:c:106:TYR:HD2	1.85	0.40
30:c:98:SER:OG	30:c:105:ILE:HD11	2.20	0.40
32:e:29:VAL:HG22	32:e:32:VAL:HB	2.04	0.40
1:2:261:G:OP1	19:R:52:LYS:NZ	2.54	0.40
1:2:323:G:OP2	37:2:1562:SPM:N14	2.53	0.40
1:2:504:C:H2'	1:2:505:G:O4'	2.22	0.40
1:2:846:C:O2'	1:2:847:U:H5'	2.22	0.40
1:2:887:C:H2'	1:2:888:G:H8	1.87	0.40
1:2:1196:G:H2'	1:2:1197:U:C6	2.56	0.40
2:A:96:LEU:HB3	2:A:125:LEU:CD1	2.52	0.40
2:A:140:LYS:O	2:A:144:GLU:HG3	2.21	0.40
4:C:55:TYR:CZ	4:C:64:GLY:HA3	2.54	0.40
9:H:173:ASP:CG	9:H:175:LYS:HZ3	2.30	0.40
13:L:93:GLU:OE2	27:Z:37:LEU:HG	2.20	0.40
27:Z:25:GLN:OE1	27:Z:25:GLN:HA	2.22	0.40
28:3:84:LYS:HA	28:3:84:LYS:HD3	1.86	0.40
29:a:23:ILE:N	29:a:23:ILE:HD12	2.36	0.40
1:2:516:A:H2'	1:2:517:C:O4'	2.21	0.40
1:2:574:C:H2'	1:2:575:G:H8	1.86	0.40
1:2:694:C:H2'	1:2:695:U:H6	1.87	0.40
1:2:914:U:H2'	1:2:915:G:H8	1.86	0.40
1:2:965:A:O2'	28:3:34:LYS:HD3	2.22	0.40
8:G:88:PRO:HG2	8:G:91:GLU:HB2	2.02	0.40
9:H:165:GLU:OE2	9:H:177:PHE:N	2.55	0.40
16:O:121:HIS:CE1	16:O:127:VAL:HG11	2.57	0.40
21:T:105:MET:HB3	21:T:113:TYR:CZ	2.57	0.40
26:Y:62:LYS:H	26:Y:62:LYS:HG3	1.70	0.40
29:a:53:ASP:O	29:a:57:LEU:HG	2.21	0.40
34:4:6:G:H2'	34:4:7:G:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	A	184/208 (88%)	180 (98%)	4 (2%)	0	100	100
3	B	213/231 (92%)	210 (99%)	3 (1%)	0	100	100
4	C	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
5	D	164/181 (91%)	161 (98%)	3 (2%)	0	100	100
6	E	236/239 (99%)	228 (97%)	8 (3%)	0	100	100
7	F	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
8	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
9	H	190/193 (98%)	183 (96%)	7 (4%)	0	100	100
10	I	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
11	J	125/133 (94%)	121 (97%)	4 (3%)	0	100	100
12	K	131/137 (96%)	125 (95%)	6 (5%)	0	100	100
13	L	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
14	M	125/132 (95%)	117 (94%)	8 (6%)	0	100	100
15	N	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
16	O	138/165 (84%)	132 (96%)	6 (4%)	0	100	100
17	P	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
18	Q	143/152 (94%)	143 (100%)	0	0	100	100
19	R	111/114 (97%)	110 (99%)	1 (1%)	0	100	100
20	S	64/79 (81%)	63 (98%)	1 (2%)	0	100	100
21	T	126/140 (90%)	126 (100%)	0	0	100	100
22	U	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
23	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
24	W	63/66 (96%)	56 (89%)	6 (10%)	1 (2%)	7	27
25	X	65/83 (78%)	58 (89%)	7 (11%)	0	100	100
26	Y	47/75 (63%)	37 (79%)	10 (21%)	0	100	100
27	Z	194/229 (85%)	190 (98%)	4 (2%)	0	100	100
28	3	115/127 (91%)	102 (89%)	13 (11%)	0	100	100
29	a	69/72 (96%)	69 (100%)	0	0	100	100
30	c	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
31	d	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
32	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
All	All	3875/4194 (92%)	3729 (96%)	145 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	W	23	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	A	168/184 (91%)	163 (97%)	5 (3%)	36	72
3	B	182/198 (92%)	178 (98%)	4 (2%)	45	78
4	C	51/58 (88%)	51 (100%)	0	100	100
5	D	147/158 (93%)	143 (97%)	4 (3%)	39	74
6	E	214/215 (100%)	212 (99%)	2 (1%)	70	89
7	F	180/181 (99%)	179 (99%)	1 (1%)	78	92
8	G	186/187 (100%)	180 (97%)	6 (3%)	34	70
9	H	166/167 (99%)	158 (95%)	8 (5%)	23	56
10	I	113/114 (99%)	112 (99%)	1 (1%)	70	89
11	J	104/110 (94%)	104 (100%)	0	100	100
12	K	109/113 (96%)	105 (96%)	4 (4%)	30	65
13	L	93/94 (99%)	91 (98%)	2 (2%)	45	78
14	M	93/98 (95%)	91 (98%)	2 (2%)	45	78
15	N	122/123 (99%)	120 (98%)	2 (2%)	55	83
16	O	121/142 (85%)	119 (98%)	2 (2%)	53	83
17	P	45/46 (98%)	44 (98%)	1 (2%)	45	78
18	Q	125/129 (97%)	124 (99%)	1 (1%)	73	90
19	R	101/102 (99%)	99 (98%)	2 (2%)	48	80
20	S	63/75 (84%)	61 (97%)	2 (3%)	34	70
21	T	116/126 (92%)	113 (97%)	3 (3%)	40	75
22	U	134/138 (97%)	131 (98%)	3 (2%)	45	78
23	V	92/99 (93%)	89 (97%)	3 (3%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	57/58 (98%)	53 (93%)	4 (7%)	14	40
25	X	58/73 (80%)	53 (91%)	5 (9%)	10	31
26	Y	43/65 (66%)	42 (98%)	1 (2%)	44	78
27	Z	163/195 (84%)	161 (99%)	2 (1%)	63	87
28	3	97/105 (92%)	92 (95%)	5 (5%)	21	53
29	a	61/62 (98%)	59 (97%)	2 (3%)	33	69
30	c	95/96 (99%)	90 (95%)	5 (5%)	20	52
31	d	63/65 (97%)	60 (95%)	3 (5%)	23	56
32	e	40/46 (87%)	39 (98%)	1 (2%)	42	76
All	All	3402/3622 (94%)	3316 (98%)	86 (2%)	42	76

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	72	ILE
2	A	86	HIS
2	A	127	THR
2	A	157	ASP
2	A	194	VAL
3	B	37	VAL
3	B	40	ASP
3	B	99	VAL
3	B	211	VAL
5	D	77	LEU
5	D	92	ASP
5	D	127	THR
5	D	162	LYS
6	E	82	MET
6	E	122	ILE
7	F	207	LEU
8	G	19	ILE
8	G	41	VAL
8	G	46	VAL
8	G	49	LYS
8	G	56	VAL
8	G	97	THR
9	H	5	ASN
9	H	84	LEU
9	H	138	LEU

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Mol	Chain	Res	Type
9	H	151	SER
9	H	188	ILE
9	H	190	LEU
9	H	191	SER
9	H	192	SER
10	I	110	SER
12	K	7	LEU
12	K	8	VAL
12	K	20	THR
12	K	111	LEU
13	L	14	VAL
13	L	28	VAL
14	M	84	TYR
14	M	88	THR
15	N	111	THR
15	N	128	MET
16	O	16	VAL
16	O	134	THR
17	P	9	GLU
18	Q	12	SER
19	R	7	THR
19	R	75	SER
20	S	3	ASN
20	S	22	ASP
21	T	28	ASP
21	T	102	THR
21	T	130	THR
22	U	103	VAL
22	U	106	LEU
22	U	155	VAL
23	V	7	VAL
23	V	24	SER
23	V	64	VAL
24	W	17	LEU
24	W	24	CYS
24	W	28	GLN
24	W	62	VAL
25	X	24	ILE
25	X	28	ASP
25	X	37	THR
25	X	38	GLN
25	X	72	THR

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Mol	Chain	Res	Type
26	Y	47	ILE
27	Z	9	LEU
27	Z	20	GLU
28	3	19	VAL
28	3	36	THR
28	3	39	THR
28	3	86	LEU
28	3	88	GLU
29	a	24	CYS
29	a	72	LEU
30	c	56	LEU
30	c	64	ILE
30	c	74	SER
30	c	77	SER
30	c	96	LEU
31	d	6	ILE
31	d	28	VAL
31	d	34	LEU
32	e	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	117	ASN
5	D	121	GLN
5	D	134	ASN
7	F	208	GLN
8	G	142	GLN
8	G	186	ASN
9	H	71	ASN
9	H	76	HIS
11	J	5	GLN
11	J	52	ASN
13	L	100	GLN
14	M	60	ASN
18	Q	63	GLN
19	R	86	ASN
20	S	31	ASN
23	V	22	GLN
26	Y	51	HIS
27	Z	88	ASN
27	Z	109	HIS

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Mol	Chain	Res	Type
27	Z	123	ASN
27	Z	157	GLN
29	a	25	ASN
31	d	25	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1495/1497 (99%)	240 (16%)	6 (0%)
33	5	12/15 (80%)	8 (66%)	2 (16%)
34	4	76/77 (98%)	13 (17%)	1 (1%)
35	s	9/15 (60%)	9 (100%)	0
All	All	1592/1604 (99%)	270 (16%)	9 (0%)

All (270) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	33	U
1	2	34	C
1	2	43	G
1	2	45	U
1	2	47	A
1	2	60	G
1	2	67	C
1	2	68	C
1	2	70	G
1	2	71	G
1	2	72	G
1	2	73	C
1	2	74	A
1	2	75	A
1	2	76	G
1	2	89	A
1	2	99	A
1	2	101	C
1	2	110	A
1	2	111	A
1	2	112	C
1	2	115	A
1	2	122	G

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Mol	Chain	Res	Type
1	2	138	G
1	2	144	C
1	2	193	A
1	2	195	A
1	2	196	G
1	2	208	A
1	2	209	U
1	2	211	C
1	2	212	C
1	2	213	C
1	2	214	C
1	2	215	G
1	2	225	G
1	2	245	C
1	2	246	OMC
1	2	248	A
1	2	250	C
1	2	252	G
1	2	256	G
1	2	257	U
1	2	267	A
1	2	271	G
1	2	272	C
1	2	278	A
1	2	286	A
1	2	294	G
1	2	311	A
1	2	320	U
1	2	321	U
1	2	333	C
1	2	334	A
1	2	335	A
1	2	336	G
1	2	349	A
1	2	357	C
1	2	358	A
1	2	359	C
1	2	372	G
1	2	377	C
1	2	378	A
1	2	389	G
1	2	395	G

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Mol	Chain	Res	Type
1	2	402	A
1	2	411	G
1	2	417	G
1	2	418	U
1	2	419	A
1	2	420	A
1	2	429	U
1	2	453	A
1	2	454	A
1	2	470	U
1	2	471	C
1	2	477	U
1	2	480	G
1	2	490	U
1	2	491	A
1	2	506	A
1	2	522	A
1	2	523	C
1	2	531	A
1	2	532	A
1	2	535	C
1	2	536	G
1	2	555	A
1	2	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	647	G
1	2	682	U
1	2	707	G
1	2	708	C
1	2	712	A
1	2	714	G
1	2	740	A
1	2	741	A
1	2	752	U
1	2	753	A
1	2	774	A
1	2	776	C
1	2	802	U
1	2	805	G

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Mol	Chain	Res	Type
1	2	806	A
1	2	828	A
1	2	835	A
1	2	853	G
1	2	865	OMG
1	2	877	A
1	2	889	G
1	2	897	C
1	2	924	U
1	2	930	C4J
1	2	931	C
1	2	933	A
1	2	935	G
1	2	939	G
1	2	941	A
1	2	946	U
1	2	957	A
1	2	960	G
1	2	966	U
1	2	967	G
1	2	969	C
1	2	982	G
1	2	983	A
1	2	988	G
1	2	989	C
1	2	990	C
1	2	991	U
1	2	992	G
1	2	995	U
1	2	996	C
1	2	997	G
1	2	1002	G
1	2	1023	C
1	2	1051	G
1	2	1052	U
1	2	1058	A
1	2	1059	A
1	2	1080	A
1	2	1081	G
1	2	1086	U
1	2	1094	U
1	2	1095	C

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Mol	Chain	Res	Type
1	2	1096	U
1	2	1097	C
1	2	1098	C
1	2	1099	G
1	2	1101	G
1	2	1102	C
1	2	1103	C
1	2	1104	G
1	2	1106	G
1	2	1107	A
1	2	1118	G
1	2	1121	A
1	2	1123	U
1	2	1147	G
1	2	1157	G
1	2	1159	A
1	2	1160	G
1	2	1175	A
1	2	1188	G
1	2	1189	C
1	2	1190	A
1	2	1199	A
1	2	1201	A
1	2	1211	A
1	2	1220	U
1	2	1221	U
1	2	1222	C
1	2	1226	C
1	2	1244	A
1	2	1248	C
1	2	1249	U
1	2	1251	A
1	2	1258	G
1	2	1264	G
1	2	1265	U
1	2	1267	G
1	2	1270	A
1	2	1281	A
1	2	1284	C
1	2	1286	C
1	2	1300	A
1	2	1309	U

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Mol	Chain	Res	Type
1	2	1317	G
1	2	1328	A
1	2	1334	G
1	2	1338	A
1	2	1358	A
1	2	1361	C
1	2	1376	C
1	2	1378	C
1	2	1381	G
1	2	1383	G
1	2	1386	G
1	2	1387	G
1	2	1389	G
1	2	1391	G
1	2	1394	G
1	2	1403	C
1	2	1410	U
1	2	1411	U
1	2	1412	G
1	2	1413	G
1	2	1414	G
1	2	1416	G
1	2	1424	G
1	2	1425	A
1	2	1428	U
1	2	1432	C
1	2	1433	U
1	2	1437	G
1	2	1440	A
1	2	1441	G
1	2	1442	G
1	2	1443	G
1	2	1444	G
1	2	1445	G
1	2	1448	G
1	2	1449	A
1	2	1450	A
1	2	1454	G
1	2	1455	U
1	2	1456	A
1	2	1459	A
1	2	1460	A

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Mol	Chain	Res	Type
1	2	1461	G
1	2	1463	U
1	2	1474	G
1	2	1476	A
1	2	1486	G
1	2	1487	G
33	5	3	G
33	5	4	A
33	5	6	U
33	5	7	G
33	5	10	G
33	5	11	A
33	5	12	U
33	5	13	G
34	4	8	4SU
34	4	9	G
34	4	16	C
34	4	17(A)	U
34	4	18	G
34	4	20	H2U
34	4	21	A
34	4	22	G
34	4	46	A
34	4	47	U
34	4	49	G
34	4	74	C
34	4	75	C
35	s	807	G
35	s	808	A
35	s	809	G
35	s	810	G
35	s	811	A
35	s	812	U
35	s	813	G
35	s	814	A
35	s	815	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	256	G
1	2	1102	C

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Mol	Chain	Res	Type
1	2	1188	G
1	2	1436	U
1	2	1443	G
1	2	1455	U
33	5	3	G
33	5	12	U
34	4	74	C

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMG	2	546	1	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
1	OMC	2	313	1	19,22,23	0.82	0	25,31,34	0.97	1 (4%)
1	OMC	2	538	1	19,22,23	0.79	0	25,31,34	0.82	0
1	5MC	2	1368	1	19,22,23	1.45	3 (15%)	26,32,35	1.06	3 (11%)
1	OMC	2	113	1	19,22,23	0.80	0	25,31,34	0.82	0
1	4AC	2	1477	1	21,24,25	0.99	2 (9%)	28,34,37	1.61	6 (21%)
1	OMG	2	865	1	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)
1	4AC	2	1467	1	21,24,25	1.00	2 (9%)	28,34,37	1.40	4 (14%)
1	OMG	2	1018	1	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)
1	OMU	2	52	1	19,22,23	1.27	3 (15%)	25,31,34	1.80	4 (16%)
1	OMG	2	399	1	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)
34	PSU	4	55	34	18,21,22	1.34	2 (11%)	21,30,33	2.04	4 (19%)
1	OMC	2	710	1	19,22,23	0.80	0	25,31,34	0.89	1 (4%)
1	4AC	2	1466	1	21,24,25	0.98	2 (9%)	28,34,37	1.36	4 (14%)
1	4AC	2	1478	1	21,24,25	0.99	2 (9%)	28,34,37	1.41	4 (14%)
1	OMC	2	1060	1	19,22,23	0.80	0	25,31,34	0.76	0
1	OMG	2	337	1	23,26,27	1.21	3 (13%)	32,38,41	2.02	6 (18%)
1	OMG	2	926	1	23,26,27	1.19	3 (13%)	32,38,41	2.04	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	2	494	1	22,25,26	1.47	5 (22%)	30,36,39	2.02	8 (26%)
1	OMU	2	1344	1	19,22,23	1.25	3 (15%)	25,31,34	1.78	6 (24%)
1	OMG	2	1194	1	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
1	OMC	2	246	1	19,22,23	0.82	0	25,31,34	1.01	1 (4%)
1	MA6	2	1475	1	23,26,27	1.50	5 (21%)	33,38,41	2.08	10 (30%)
34	5MU	4	54	34	19,22,23	1.38	6 (31%)	27,32,35	2.08	7 (25%)
1	OMG	2	1061	1	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
1	OMG	2	672	1	23,26,27	1.21	3 (13%)	32,38,41	2.00	6 (18%)
1	C4J	2	930	1	25,29,30	0.64	1 (4%)	28,42,45	0.86	1 (3%)
1	OMU	2	1032	1	19,22,23	1.28	3 (15%)	25,31,34	1.83	4 (16%)
34	4SU	4	8	34	18,21,22	0.20	0	25,30,33	0.33	0
1	6MZ	2	1457	36,1	22,25,26	1.51	5 (22%)	29,36,39	2.17	10 (34%)
1	OMU	2	15	1	19,22,23	1.29	3 (15%)	25,31,34	1.83	4 (16%)
1	OMC	2	481	1	19,22,23	0.81	0	25,31,34	0.94	1 (4%)
34	OMC	4	32	34	19,22,23	0.83	0	25,31,34	1.06	2 (8%)
1	OMC	2	512	1	19,22,23	0.79	0	25,31,34	0.81	0
1	OMG	2	905	1	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
34	H2U	4	20	34	18,21,22	0.27	0	19,30,33	0.40	0
1	OMC	2	1366	1	19,22,23	0.79	0	25,31,34	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	OMC	2	313	1	-	1/9/27/28	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1477	1	-	2/11/29/30	0/2/2/2
1	OMG	2	865	1	-	2/9/27/28	0/3/3/3
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3
34	PSU	4	55	34	-	1/7/25/26	0/2/2/2
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMG	2	926	1	-	0/9/27/28	0/3/3/3
1	A2M	2	494	1	-	0/9/27/28	0/3/3/3
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
1	OMC	2	246	1	-	4/9/27/28	0/2/2/2
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3
34	5MU	4	54	34	-	0/7/25/26	0/2/2/2
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	C4J	2	930	1	-	2/16/34/35	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
34	4SU	4	8	34	-	0/7/25/26	0/2/2/2
1	6MZ	2	1457	36,1	-	0/9/27/28	0/3/3/3
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
34	OMC	4	32	34	-	2/9/27/28	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
34	H2U	4	20	34	-	3/7/38/39	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1368	5MC	C5-C4	5.01	1.47	1.44
1	2	1475	MA6	C5-C4	4.64	1.47	1.39
1	2	1457	6MZ	C5-C4	4.61	1.47	1.39
1	2	494	A2M	C5-C4	4.42	1.47	1.39
34	4	55	PSU	C6-C5	3.38	1.39	1.35
1	2	672	OMG	C5-C4	2.99	1.46	1.38
1	2	1061	OMG	C5-C4	2.98	1.46	1.38
1	2	399	OMG	C5-C4	2.97	1.46	1.38
1	2	15	OMU	C4-N3	-2.96	1.33	1.38
1	2	865	OMG	C5-C4	2.95	1.46	1.38
1	2	546	OMG	C5-C4	2.95	1.46	1.38
1	2	905	OMG	C5-C4	2.93	1.46	1.38
1	2	1194	OMG	C5-C4	2.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1018	OMG	C5-C4	2.92	1.46	1.38
1	2	1032	OMU	C4-N3	-2.91	1.33	1.38
1	2	926	OMG	C5-C4	2.91	1.46	1.38
1	2	337	OMG	C5-C4	2.90	1.46	1.38
1	2	1457	6MZ	C5-C6	2.89	1.48	1.41
1	2	1475	MA6	C5-C6	2.89	1.48	1.41
1	2	52	OMU	C4-N3	-2.87	1.33	1.38
1	2	1344	OMU	C4-N3	-2.79	1.33	1.38
1	2	337	OMG	C6-N1	-2.72	1.33	1.38
1	2	1194	OMG	C6-N1	-2.71	1.33	1.38
1	2	672	OMG	C6-N1	-2.71	1.33	1.38
1	2	1018	OMG	C6-N1	-2.69	1.33	1.38
1	2	905	OMG	C6-N1	-2.68	1.33	1.38
1	2	930	C4J	O4'-C1'	-2.67	1.40	1.43
1	2	1478	4AC	C5-C4	2.65	1.46	1.41
1	2	865	OMG	C6-N1	-2.65	1.33	1.38
1	2	399	OMG	C6-N1	-2.65	1.33	1.38
34	4	55	PSU	C4-N3	-2.64	1.33	1.38
1	2	1061	OMG	C6-N1	-2.63	1.33	1.38
1	2	926	OMG	C6-N1	-2.62	1.33	1.38
34	4	54	5MU	C6-C5	2.61	1.38	1.34
1	2	1467	4AC	C5-C4	2.58	1.46	1.41
1	2	1466	4AC	C5-C4	2.56	1.46	1.41
1	2	1368	5MC	C6-C5	2.53	1.38	1.34
1	2	494	A2M	C5-C6	2.52	1.48	1.41
1	2	1477	4AC	C5-C4	2.52	1.46	1.41
1	2	15	OMU	C2-N3	-2.52	1.33	1.38
34	4	54	5MU	C4-N3	-2.50	1.34	1.38
1	2	546	OMG	C6-N1	-2.46	1.34	1.38
1	2	1032	OMU	C2-N3	-2.45	1.33	1.38
1	2	1467	4AC	C4-N3	-2.45	1.28	1.32
1	2	494	A2M	C5-N7	-2.41	1.34	1.39
34	4	54	5MU	C4-C5	2.41	1.48	1.44
1	2	1368	5MC	C6-N1	-2.37	1.34	1.38
1	2	52	OMU	C2-N3	-2.37	1.33	1.38
1	2	1466	4AC	C4-N3	-2.34	1.28	1.32
1	2	1344	OMU	C2-N3	-2.33	1.33	1.38
1	2	15	OMU	C5-C4	-2.31	1.38	1.43
1	2	1457	6MZ	C5-N7	-2.30	1.34	1.39
1	2	1344	OMU	C5-C4	-2.30	1.38	1.43
1	2	1478	4AC	C4-N3	-2.29	1.29	1.32
34	4	54	5MU	C2-N1	2.27	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1475	MA6	C5-N7	-2.27	1.34	1.39
1	2	672	OMG	C5-N7	-2.26	1.34	1.39
1	2	1018	OMG	C5-N7	-2.25	1.34	1.39
1	2	399	OMG	C5-N7	-2.25	1.34	1.39
1	2	1194	OMG	C5-N7	-2.24	1.34	1.39
1	2	865	OMG	C5-N7	-2.23	1.34	1.39
34	4	54	5MU	C6-N1	-2.22	1.34	1.38
1	2	926	OMG	C5-N7	-2.21	1.34	1.39
1	2	52	OMU	C5-C4	-2.21	1.38	1.43
1	2	337	OMG	C5-N7	-2.20	1.34	1.39
1	2	1477	4AC	C4-N3	-2.20	1.29	1.32
1	2	905	OMG	C5-N7	-2.20	1.34	1.39
1	2	1061	OMG	C5-N7	-2.19	1.34	1.39
1	2	1032	OMU	C5-C4	-2.19	1.39	1.43
1	2	494	A2M	C8-N7	2.14	1.35	1.31
1	2	546	OMG	C5-N7	-2.12	1.34	1.39
1	2	1457	6MZ	C4-N9	-2.12	1.33	1.37
1	2	1457	6MZ	C8-N7	2.09	1.35	1.31
1	2	1475	MA6	C8-N7	2.06	1.35	1.31
1	2	494	A2M	C4-N9	-2.04	1.33	1.37
1	2	1475	MA6	C4-N9	-2.02	1.33	1.37
34	4	54	5MU	C2-N3	-2.00	1.34	1.38

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	672	OMG	C5-C4-N3	-6.38	118.24	128.39
34	4	55	PSU	N1-C2-N3	6.24	121.75	115.17
1	2	926	OMG	C5-C4-N3	-6.23	118.47	128.39
1	2	1018	OMG	C5-C4-N3	-6.18	118.55	128.39
1	2	865	OMG	C5-C4-N3	-6.17	118.57	128.39
1	2	399	OMG	C5-C4-N3	-6.16	118.58	128.39
1	2	1194	OMG	C5-C4-N3	-6.10	118.68	128.39
1	2	905	OMG	C5-C4-N3	-6.10	118.68	128.39
1	2	337	OMG	C5-C4-N3	-6.08	118.72	128.39
1	2	1061	OMG	C5-C4-N3	-6.07	118.73	128.39
1	2	546	OMG	C5-C4-N3	-5.82	119.12	128.39
1	2	1475	MA6	C5-C4-N3	-5.58	119.04	126.72
1	2	494	A2M	C5-C4-N3	-5.58	119.04	126.72
1	2	1457	6MZ	C5-C4-N3	-5.50	119.14	126.72
1	2	926	OMG	C2-N3-C4	5.17	121.21	112.30
1	2	672	OMG	C2-N3-C4	5.08	121.05	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	905	OMG	C2-N3-C4	5.04	120.99	112.30
1	2	399	OMG	C2-N3-C4	5.04	120.98	112.30
1	2	1194	OMG	C2-N3-C4	5.03	120.97	112.30
1	2	1018	OMG	C2-N3-C4	5.02	120.94	112.30
1	2	865	OMG	C2-N3-C4	5.01	120.92	112.30
1	2	337	OMG	C2-N3-C4	5.01	120.92	112.30
1	2	546	OMG	C2-N3-C4	4.96	120.85	112.30
1	2	1061	OMG	C2-N3-C4	4.95	120.83	112.30
34	4	54	5MU	C4-N3-C2	-4.94	120.87	127.34
1	2	15	OMU	C4-N3-C2	-4.92	120.50	126.61
1	2	1032	OMU	C4-N3-C2	-4.84	120.61	126.61
34	4	54	5MU	N3-C2-N1	4.80	121.14	114.89
1	2	52	OMU	C4-N3-C2	-4.75	120.71	126.61
1	2	672	OMG	N9-C4-N3	4.72	135.40	125.95
1	2	1477	4AC	O7-C7-N4	4.66	129.22	121.90
1	2	926	OMG	N9-C4-N3	4.65	135.25	125.95
1	2	1344	OMU	C4-N3-C2	-4.61	120.89	126.61
1	2	1018	OMG	N9-C4-N3	4.61	135.16	125.95
1	2	865	OMG	N9-C4-N3	4.60	135.14	125.95
1	2	399	OMG	N9-C4-N3	4.59	135.13	125.95
1	2	1061	OMG	N9-C4-N3	4.56	135.07	125.95
1	2	1194	OMG	N9-C4-N3	4.54	135.03	125.95
1	2	1467	4AC	O7-C7-N4	4.53	129.03	121.90
1	2	1478	4AC	O7-C7-N4	4.52	129.01	121.90
1	2	494	A2M	N3-C4-N9	4.51	134.83	127.17
1	2	337	OMG	N9-C4-N3	4.47	134.89	125.95
1	2	905	OMG	N9-C4-N3	4.46	134.87	125.95
1	2	1466	4AC	O7-C7-N4	4.45	128.90	121.90
1	2	1457	6MZ	C6-C5-N7	4.40	137.23	132.43
1	2	1475	MA6	C2-N1-C6	4.27	122.25	111.83
1	2	1475	MA6	N3-C4-N9	4.26	134.42	127.17
1	2	15	OMU	C5-C4-N3	4.25	120.76	114.80
34	4	54	5MU	C5-C4-N3	4.22	118.99	115.32
1	2	546	OMG	N9-C4-N3	4.20	134.35	125.95
34	4	55	PSU	C4-N3-C2	-4.20	120.59	126.37
1	2	1032	OMU	N3-C2-N1	4.15	120.30	114.89
1	2	1457	6MZ	C4-C5-N7	-4.14	105.85	110.58
1	2	52	OMU	N3-C2-N1	4.13	120.27	114.89
1	2	1344	OMU	N3-C2-N1	4.10	120.23	114.89
1	2	1457	6MZ	N3-C4-N9	4.06	134.07	127.17
1	2	1475	MA6	C4-C5-N7	-4.01	106.00	110.58
1	2	1032	OMU	C5-C4-N3	3.97	120.36	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	52	OMU	C5-C4-N3	3.96	120.34	114.80
34	4	54	5MU	O4-C4-C5	-3.92	120.43	124.92
1	2	15	OMU	N3-C2-N1	3.92	119.99	114.89
1	2	1344	OMU	C5-C4-N3	3.83	120.16	114.80
1	2	1477	4AC	N4-C4-N3	3.69	119.86	113.87
1	2	1457	6MZ	C2-N3-C4	3.66	120.77	111.83
1	2	1475	MA6	C2-N3-C4	3.65	120.74	111.83
1	2	494	A2M	C2-N3-C4	3.63	120.69	111.83
1	2	1477	4AC	C5-C4-N4	-3.50	117.05	122.94
1	2	546	OMG	C6-C5-N7	3.47	136.60	130.29
34	4	55	PSU	O2-C2-N1	-3.41	119.27	122.79
1	2	930	C4J	C1'-C5-C4	3.39	122.76	117.61
1	2	1457	6MZ	N1-C2-N3	-3.39	123.45	128.58
1	2	337	OMG	C6-C5-N7	3.36	136.40	130.29
1	2	905	OMG	C6-C5-N7	3.36	136.40	130.29
1	2	1467	4AC	CM7-C7-N4	-3.33	109.89	115.27
34	4	54	5MU	C5-C6-N1	-3.30	119.72	123.31
1	2	494	A2M	C4-C5-N7	-3.30	106.80	110.58
1	2	494	A2M	N3-C2-N1	-3.30	123.59	128.58
1	2	1194	OMG	C6-C5-N7	3.29	136.28	130.29
1	2	1475	MA6	N1-C2-N3	-3.27	123.63	128.58
1	2	15	OMU	O4-C4-C5	-3.24	119.58	125.16
1	2	926	OMG	C6-C5-N7	3.24	136.18	130.29
1	2	1061	OMG	C6-C5-N7	3.20	136.12	130.29
1	2	399	OMG	C6-C5-N7	3.17	136.06	130.29
1	2	1018	OMG	C6-C5-N7	3.13	135.98	130.29
1	2	865	OMG	C6-C5-N7	3.13	135.98	130.29
1	2	1344	OMU	O4-C4-C5	-3.11	119.80	125.16
1	2	1478	4AC	N4-C4-N3	3.09	118.88	113.87
1	2	1467	4AC	C5-C4-N4	-3.08	117.75	122.94
1	2	1478	4AC	C5-C4-N4	-3.06	117.78	122.94
1	2	672	OMG	C6-C5-N7	3.05	135.84	130.29
1	2	1032	OMU	O4-C4-C5	-3.04	119.92	125.16
1	2	52	OMU	O4-C4-C5	-3.03	119.94	125.16
1	2	1478	4AC	CM7-C7-N4	-3.00	110.43	115.27
1	2	1466	4AC	C5-C4-N4	-2.98	117.91	122.94
1	2	1466	4AC	N4-C4-N3	2.98	118.71	113.87
1	2	1467	4AC	N4-C4-N3	2.93	118.62	113.87
1	2	1368	5MC	C5-C4-N3	-2.92	118.76	121.75
1	2	1466	4AC	CM7-C7-N4	-2.91	110.56	115.27
1	2	1457	6MZ	C5-N7-C8	2.85	107.93	103.45
1	2	1475	MA6	C5-N7-C8	2.81	107.87	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	494	A2M	C4-N9-C8	2.80	108.67	105.74
1	2	1368	5MC	C5-C6-N1	-2.78	120.29	123.31
1	2	1477	4AC	CM7-C7-N4	-2.78	110.78	115.27
34	4	32	OMC	O2-C2-N3	-2.73	118.02	122.33
1	2	1475	MA6	C4-N9-C8	2.70	108.58	105.74
1	2	246	OMC	O2-C2-N3	-2.65	118.15	122.33
1	2	546	OMG	C4-C5-N7	-2.63	106.50	110.67
1	2	337	OMG	C4-C5-N7	-2.60	106.55	110.67
1	2	905	OMG	C4-C5-N7	-2.59	106.57	110.67
1	2	313	OMC	O2-C2-N3	-2.59	118.25	122.33
1	2	1457	6MZ	C4-N9-C8	2.57	108.44	105.74
1	2	926	OMG	C4-C5-N7	-2.53	106.66	110.67
1	2	1018	OMG	C4-C5-N7	-2.53	106.67	110.67
1	2	1194	OMG	C4-C5-N7	-2.52	106.67	110.67
1	2	672	OMG	C4-C5-N7	-2.52	106.68	110.67
1	2	1061	OMG	C4-C5-N7	-2.51	106.69	110.67
1	2	399	OMG	C4-C5-N7	-2.51	106.70	110.67
1	2	481	OMC	O2-C2-N3	-2.48	118.42	122.33
1	2	865	OMG	C4-C5-N7	-2.47	106.75	110.67
1	2	494	A2M	C5-N7-C8	2.43	107.27	103.45
34	4	54	5MU	O2-C2-N1	-2.31	119.78	122.80
34	4	32	OMC	C1'-N1-C2	2.25	123.41	118.44
1	2	1457	6MZ	C2-N1-C6	2.23	122.63	115.24
1	2	1477	4AC	C1'-N1-C2	2.22	123.35	118.44
1	2	1475	MA6	C6-C5-N7	2.21	136.96	133.43
1	2	926	OMG	O6-C6-C5	-2.20	120.74	126.53
1	2	710	OMC	O2-C2-N3	-2.18	118.90	122.33
1	2	546	OMG	O6-C6-C5	-2.17	120.81	126.53
1	2	1061	OMG	O6-C6-C5	-2.16	120.83	126.53
34	4	54	5MU	C5M-C5-C4	2.16	121.09	118.78
1	2	1194	OMG	O6-C6-C5	-2.16	120.84	126.53
1	2	865	OMG	O6-C6-C5	-2.12	120.94	126.53
1	2	1018	OMG	O6-C6-C5	-2.12	120.94	126.53
1	2	1368	5MC	O2-C2-N3	-2.10	119.01	122.33
1	2	1344	OMU	O2-C2-N1	-2.10	120.06	122.80
1	2	399	OMG	O6-C6-C5	-2.10	120.99	126.53
1	2	1457	6MZ	N9-C8-N7	-2.08	110.99	113.94
1	2	494	A2M	C6-C5-N7	2.07	136.08	132.09
1	2	1475	MA6	N9-C8-N7	-2.06	111.01	113.94
1	2	672	OMG	O6-C6-C5	-2.06	121.11	126.53
1	2	337	OMG	O6-C6-C5	-2.05	121.12	126.53
1	2	905	OMG	O6-C6-C5	-2.04	121.14	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1477	4AC	O2-C2-N3	-2.01	119.16	122.33
34	4	55	PSU	O4'-C1'-C2'	2.01	107.93	105.15
1	2	1344	OMU	C1'-N1-C2	2.00	121.19	117.59

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
1	2	246	OMC	C3'-C4'-C5'-O5'
1	2	246	OMC	O4'-C4'-C5'-O5'
34	4	20	H2U	O4'-C1'-N1-C2
1	2	930	C4J	C3'-C4'-C5'-O5'
34	4	20	H2U	C4'-C5'-O5'-P
1	2	865	OMG	C3'-C4'-C5'-O5'
34	4	32	OMC	C3'-C2'-O2'-CM2
1	2	865	OMG	C4'-C5'-O5'-P
34	4	55	PSU	O4'-C1'-C5-C4
1	2	337	OMG	C4'-C5'-O5'-P
34	4	32	OMC	C2'-C1'-N1-C6
1	2	313	OMC	C2'-C1'-N1-C2
1	2	246	OMC	C3'-C2'-O2'-CM2
1	2	1477	4AC	C4'-C5'-O5'-P
1	2	246	OMC	C2'-C1'-N1-C2
1	2	1477	4AC	C2'-C1'-N1-C2

There are no ring outliers.

26 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	546	OMG	1	0
1	2	538	OMC	2	0
1	2	1368	5MC	1	0
1	2	113	OMC	1	0
1	2	1477	4AC	1	0
1	2	865	OMG	1	0
1	2	1467	4AC	2	0
1	2	1018	OMG	1	0
1	2	52	OMU	1	0
1	2	1466	4AC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1478	4AC	1	0
1	2	1060	OMC	2	0
1	2	337	OMG	1	0
1	2	926	OMG	1	0
1	2	1344	OMU	3	0
1	2	246	OMC	2	0
1	2	1475	MA6	1	0
1	2	1061	OMG	1	0
1	2	672	OMG	2	0
1	2	1032	OMU	1	0
1	2	1457	6MZ	1	0
1	2	481	OMC	1	0
34	4	32	OMC	1	0
1	2	512	OMC	1	0
34	4	20	H2U	1	0
1	2	1366	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 66 are monoatomic - leaving 42 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	$\# Z > 2$
37	SPM	2	1566	-	13,13,13	0.10	0	12,12,12	0.10	0
37	SPM	2	1556	-	13,13,13	0.08	0	12,12,12	0.12	0
37	SPM	2	1589	-	13,13,13	0.09	0	12,12,12	0.11	0
37	SPM	2	1555	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1580	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1563	-	13,13,13	0.07	0	12,12,12	0.10	0
37	SPM	2	1594	-	13,13,13	0.09	0	12,12,12	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	SPM	2	1586	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1570	-	13,13,13	0.08	0	12,12,12	0.09	0
37	SPM	2	1569	-	13,13,13	0.06	0	12,12,12	0.14	0
37	SPM	2	1567	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1592	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1571	-	13,13,13	0.08	0	12,12,12	0.11	0
37	SPM	2	1574	-	13,13,13	0.09	0	12,12,12	0.10	0
37	SPM	2	1577	-	13,13,13	0.10	0	12,12,12	0.10	0
37	SPM	2	1584	1	13,13,13	0.11	0	12,12,12	0.14	0
37	SPM	2	1573	-	13,13,13	0.09	0	12,12,12	0.09	0
37	SPM	2	1585	-	13,13,13	0.11	0	12,12,12	0.11	0
37	SPM	2	1554	-	13,13,13	0.07	0	12,12,12	0.10	0
37	SPM	2	1583	-	13,13,13	0.08	0	12,12,12	0.08	0
37	SPM	2	1560	-	13,13,13	0.07	0	12,12,12	0.10	0
37	SPM	2	1562	-	13,13,13	0.08	0	12,12,12	0.10	0
37	SPM	2	1572	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1578	-	13,13,13	0.10	0	12,12,12	0.06	0
37	SPM	2	1582	-	13,13,13	0.10	0	12,12,12	0.12	0
37	SPM	2	1565	-	13,13,13	0.09	0	12,12,12	0.12	0
37	SPM	2	1587	-	13,13,13	0.09	0	12,12,12	0.09	0
37	SPM	2	1595	-	13,13,13	0.09	0	12,12,12	0.13	0
37	SPM	2	1588	-	13,13,13	0.11	0	12,12,12	0.10	0
37	SPM	2	1581	-	13,13,13	0.10	0	12,12,12	0.06	0
37	SPM	2	1558	-	13,13,13	0.06	0	12,12,12	0.11	0
37	SPM	2	1591	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1579	-	13,13,13	0.07	0	12,12,12	0.11	0
37	SPM	2	1590	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1559	-	13,13,13	0.08	0	12,12,12	0.06	0
37	SPM	2	1557	-	13,13,13	0.09	0	12,12,12	0.07	0
37	SPM	2	1561	-	13,13,13	0.08	0	12,12,12	0.10	0
37	SPM	2	1568	-	13,13,13	0.09	0	12,12,12	0.10	0
37	SPM	2	1593	-	13,13,13	0.11	0	12,12,12	0.09	0
37	SPM	2	1564	-	13,13,13	0.08	0	12,12,12	0.07	0
37	SPM	2	1576	-	13,13,13	0.07	0	12,12,12	0.11	0
37	SPM	2	1575	-	13,13,13	0.09	0	12,12,12	0.08	0

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
37	SPM	2	1566	-	-	1/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SPM	2	1556	-	-	3/11/11/11	-
37	SPM	2	1589	-	-	1/11/11/11	-
37	SPM	2	1555	-	-	3/11/11/11	-
37	SPM	2	1580	-	-	3/11/11/11	-
37	SPM	2	1563	-	-	2/11/11/11	-
37	SPM	2	1594	-	-	5/11/11/11	-
37	SPM	2	1586	-	-	1/11/11/11	-
37	SPM	2	1570	-	-	5/11/11/11	-
37	SPM	2	1569	-	-	1/11/11/11	-
37	SPM	2	1567	-	-	3/11/11/11	-
37	SPM	2	1592	-	-	1/11/11/11	-
37	SPM	2	1571	-	-	2/11/11/11	-
37	SPM	2	1574	-	-	2/11/11/11	-
37	SPM	2	1577	-	-	4/11/11/11	-
37	SPM	2	1584	1	-	2/11/11/11	-
37	SPM	2	1573	-	-	4/11/11/11	-
37	SPM	2	1585	-	-	4/11/11/11	-
37	SPM	2	1554	-	-	2/11/11/11	-
37	SPM	2	1583	-	-	2/11/11/11	-
37	SPM	2	1560	-	-	1/11/11/11	-
37	SPM	2	1562	-	-	2/11/11/11	-
37	SPM	2	1572	-	-	4/11/11/11	-
37	SPM	2	1578	-	-	3/11/11/11	-
37	SPM	2	1582	-	-	2/11/11/11	-
37	SPM	2	1565	-	-	4/11/11/11	-
37	SPM	2	1587	-	-	3/11/11/11	-
37	SPM	2	1595	-	-	5/11/11/11	-
37	SPM	2	1588	-	-	4/11/11/11	-
37	SPM	2	1581	-	-	1/11/11/11	-
37	SPM	2	1558	-	-	2/11/11/11	-
37	SPM	2	1591	-	-	1/11/11/11	-
37	SPM	2	1579	-	-	3/11/11/11	-
37	SPM	2	1590	-	-	3/11/11/11	-
37	SPM	2	1559	-	-	4/11/11/11	-
37	SPM	2	1557	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SPM	2	1561	-	-	3/11/11/11	-
37	SPM	2	1568	-	-	0/11/11/11	-
37	SPM	2	1593	-	-	1/11/11/11	-
37	SPM	2	1564	-	-	3/11/11/11	-
37	SPM	2	1576	-	-	3/11/11/11	-
37	SPM	2	1575	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1562	SPM	C12-C11-N10-C9
37	2	1571	SPM	C7-C6-N5-C4
37	2	1577	SPM	C3-C4-N5-C6
37	2	1577	SPM	C12-C11-N10-C9
37	2	1572	SPM	C7-C6-N5-C4
37	2	1585	SPM	C7-C6-N5-C4
37	2	1587	SPM	C3-C4-N5-C6
37	2	1588	SPM	C3-C4-N5-C6
37	2	1594	SPM	C3-C4-N5-C6
37	2	1554	SPM	C8-C9-N10-C11
37	2	1555	SPM	C12-C11-N10-C9
37	2	1571	SPM	C3-C4-N5-C6
37	2	1572	SPM	C12-C11-N10-C9
37	2	1574	SPM	C7-C6-N5-C4
37	2	1575	SPM	C7-C6-N5-C4
37	2	1579	SPM	C12-C11-N10-C9
37	2	1583	SPM	C3-C4-N5-C6
37	2	1595	SPM	C12-C11-N10-C9
37	2	1556	SPM	C12-C11-N10-C9
37	2	1557	SPM	C3-C4-N5-C6
37	2	1557	SPM	C8-C9-N10-C11
37	2	1560	SPM	C12-C11-N10-C9
37	2	1562	SPM	C8-C9-N10-C11
37	2	1563	SPM	C3-C4-N5-C6
37	2	1576	SPM	C7-C6-N5-C4
37	2	1577	SPM	C7-C6-N5-C4
37	2	1578	SPM	C3-C4-N5-C6

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Mol	Chain	Res	Type	Atoms
37	2	1578	SPM	C8-C9-N10-C11
37	2	1582	SPM	C3-C4-N5-C6
37	2	1588	SPM	C12-C11-N10-C9
37	2	1590	SPM	C7-C6-N5-C4
37	2	1592	SPM	C3-C4-N5-C6
37	2	1595	SPM	N5-C6-C7-C8
37	2	1559	SPM	C12-C11-N10-C9
37	2	1565	SPM	C7-C6-N5-C4
37	2	1574	SPM	C3-C4-N5-C6
37	2	1575	SPM	C8-C9-N10-C11
37	2	1581	SPM	C3-C4-N5-C6
37	2	1583	SPM	C12-C11-N10-C9
37	2	1586	SPM	C7-C6-N5-C4
37	2	1588	SPM	C7-C6-N5-C4
37	2	1555	SPM	C3-C4-N5-C6
37	2	1559	SPM	C3-C4-N5-C6
37	2	1580	SPM	C7-C6-N5-C4
37	2	1590	SPM	C12-C11-N10-C9
37	2	1594	SPM	C7-C6-N5-C4
37	2	1559	SPM	C7-C6-N5-C4
37	2	1573	SPM	C6-C7-C8-C9
37	2	1567	SPM	C8-C9-N10-C11
37	2	1570	SPM	C3-C4-N5-C6
37	2	1573	SPM	C12-C11-N10-C9
37	2	1556	SPM	C8-C9-N10-C11
37	2	1563	SPM	C7-C6-N5-C4
37	2	1564	SPM	C7-C6-N5-C4
37	2	1565	SPM	C3-C4-N5-C6
37	2	1577	SPM	C8-C9-N10-C11
37	2	1582	SPM	C7-C6-N5-C4
37	2	1595	SPM	C3-C4-N5-C6
37	2	1570	SPM	N10-C11-C12-C13
37	2	1556	SPM	C3-C4-N5-C6
37	2	1561	SPM	C7-C6-N5-C4
37	2	1564	SPM	C3-C4-N5-C6
37	2	1570	SPM	C7-C6-N5-C4
37	2	1573	SPM	C3-C4-N5-C6
37	2	1576	SPM	C8-C9-N10-C11
37	2	1573	SPM	C7-C8-C9-N10
37	2	1576	SPM	C6-C7-C8-C9
37	2	1557	SPM	C7-C6-N5-C4
37	2	1565	SPM	C12-C11-N10-C9

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Mol	Chain	Res	Type	Atoms
37	2	1565	SPM	C8-C9-N10-C11
37	2	1585	SPM	C3-C4-N5-C6
37	2	1585	SPM	C8-C9-N10-C11
37	2	1587	SPM	C7-C6-N5-C4
37	2	1587	SPM	C8-C9-N10-C11
37	2	1566	SPM	C8-C9-N10-C11
37	2	1595	SPM	C8-C9-N10-C11
37	2	1567	SPM	C7-C6-N5-C4
37	2	1579	SPM	C3-C4-N5-C6
37	2	1584	SPM	C7-C6-N5-C4
37	2	1591	SPM	C3-C4-N5-C6
37	2	1594	SPM	C12-C11-N10-C9
37	2	1558	SPM	C8-C9-N10-C11
37	2	1561	SPM	C3-C4-N5-C6
37	2	1569	SPM	C3-C4-N5-C6
37	2	1570	SPM	C8-C9-N10-C11
37	2	1579	SPM	C7-C6-N5-C4
37	2	1554	SPM	C12-C11-N10-C9
37	2	1567	SPM	C12-C11-N10-C9
37	2	1561	SPM	C12-C11-N10-C9
37	2	1578	SPM	C12-C11-N10-C9
37	2	1593	SPM	C7-C6-N5-C4
37	2	1589	SPM	C6-C7-C8-C9
37	2	1585	SPM	C6-C7-C8-C9
37	2	1555	SPM	C8-C9-N10-C11
37	2	1564	SPM	C8-C9-N10-C11
37	2	1572	SPM	C3-C4-N5-C6
37	2	1558	SPM	C7-C6-N5-C4
37	2	1570	SPM	C12-C11-N10-C9
37	2	1588	SPM	C8-C9-N10-C11
37	2	1595	SPM	C6-C7-C8-C9
37	2	1559	SPM	C6-C7-C8-C9
37	2	1584	SPM	C6-C7-C8-C9
37	2	1580	SPM	C3-C4-N5-C6
37	2	1594	SPM	C8-C9-N10-C11
37	2	1594	SPM	C6-C7-C8-C9
37	2	1580	SPM	C8-C9-N10-C11
37	2	1590	SPM	C8-C9-N10-C11
37	2	1572	SPM	C6-C7-C8-C9

There are no ring outliers.

33 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1566	SPM	4	0
37	2	1555	SPM	4	0
37	2	1580	SPM	1	0
37	2	1586	SPM	1	0
37	2	1570	SPM	3	0
37	2	1569	SPM	3	0
37	2	1567	SPM	3	0
37	2	1571	SPM	1	0
37	2	1577	SPM	1	0
37	2	1584	SPM	4	0
37	2	1573	SPM	1	0
37	2	1585	SPM	2	0
37	2	1554	SPM	1	0
37	2	1583	SPM	3	0
37	2	1560	SPM	1	0
37	2	1562	SPM	3	0
37	2	1578	SPM	2	0
37	2	1582	SPM	1	0
37	2	1565	SPM	1	0
37	2	1587	SPM	1	0
37	2	1595	SPM	2	0
37	2	1581	SPM	1	0
37	2	1558	SPM	1	0
37	2	1579	SPM	2	0
37	2	1590	SPM	2	0
37	2	1559	SPM	1	0
37	2	1557	SPM	1	0
37	2	1561	SPM	1	0
37	2	1568	SPM	3	0
37	2	1593	SPM	1	0
37	2	1564	SPM	1	0
37	2	1576	SPM	2	0
37	2	1575	SPM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

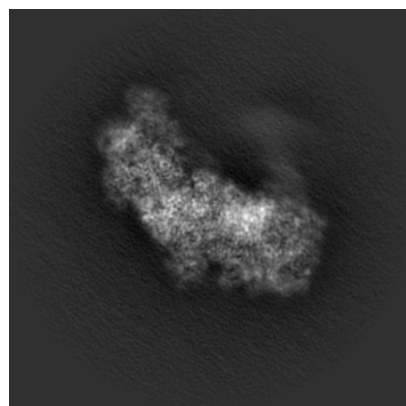
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50709. These allow visual inspection of the internal detail of the map and identification of artifacts.

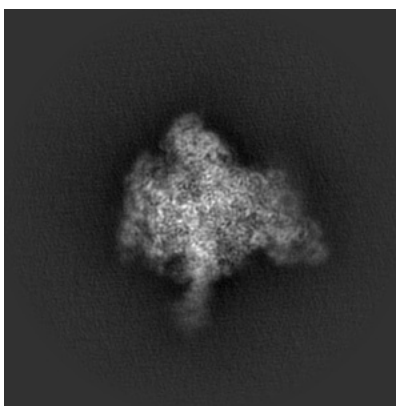
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

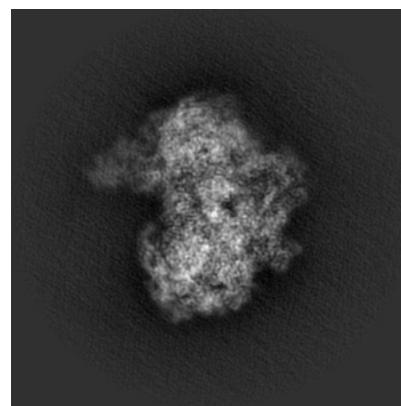
6.1.1 Primary map



X

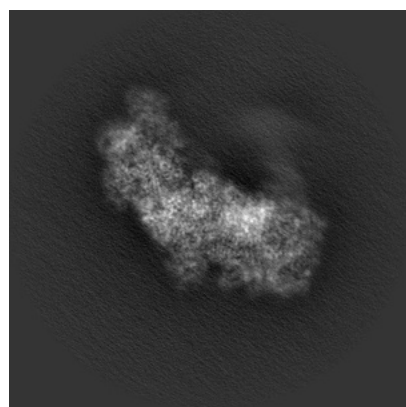


Y

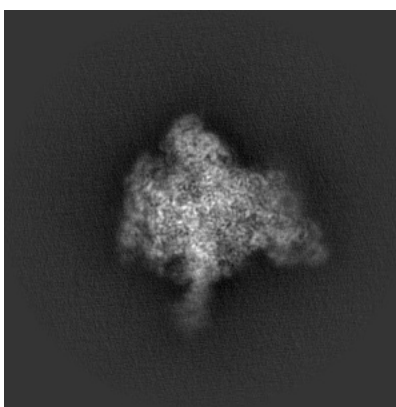


Z

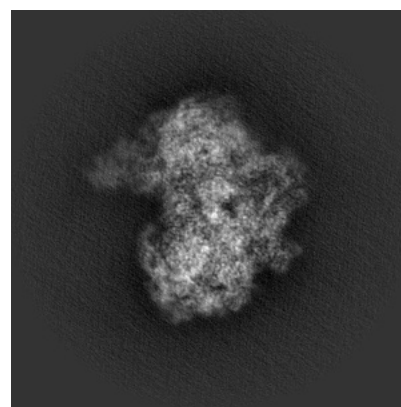
6.1.2 Raw map



X



Y

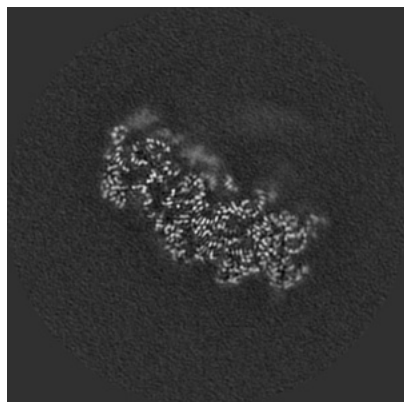


Z

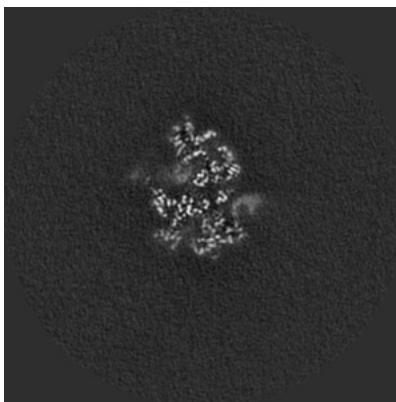
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

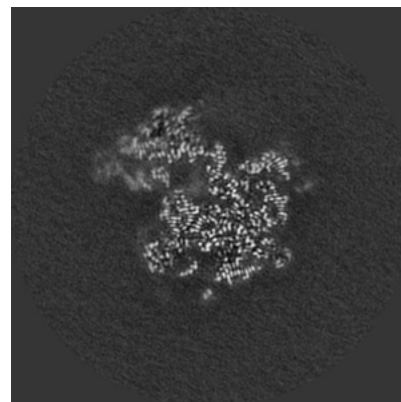
6.2.1 Primary map



X Index: 219

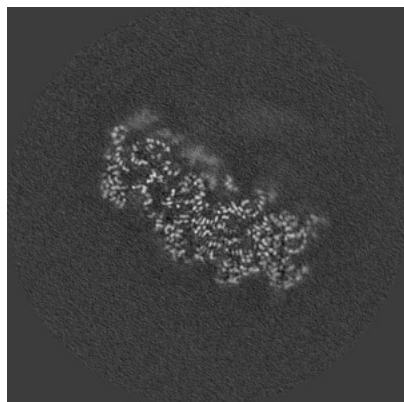


Y Index: 219

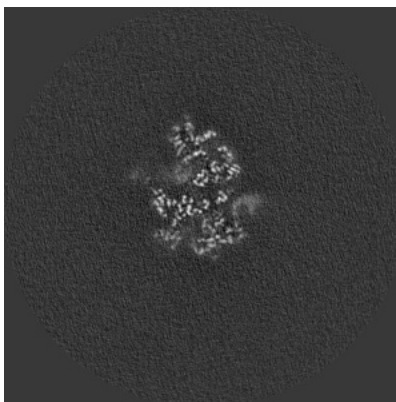


Z Index: 219

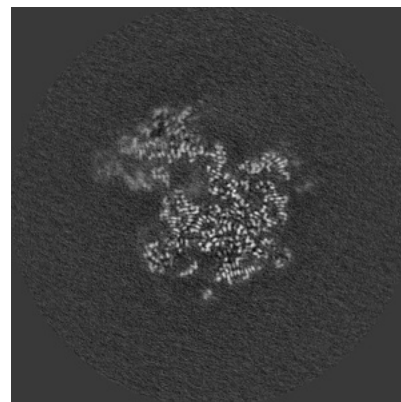
6.2.2 Raw map



X Index: 219



Y Index: 219

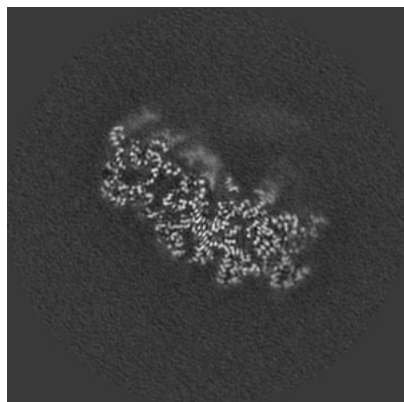


Z Index: 219

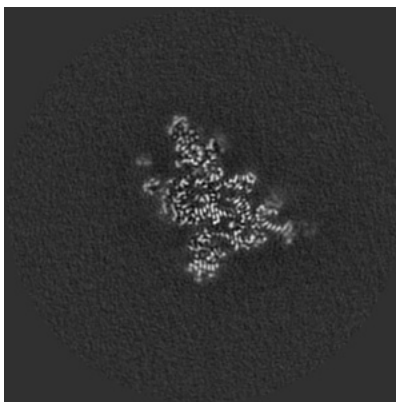
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

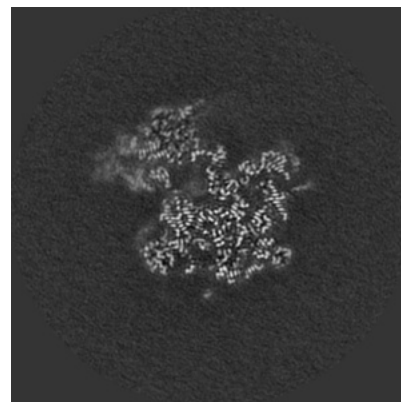
6.3.1 Primary map



X Index: 221

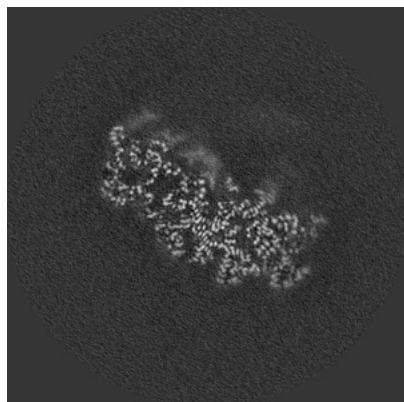


Y Index: 176

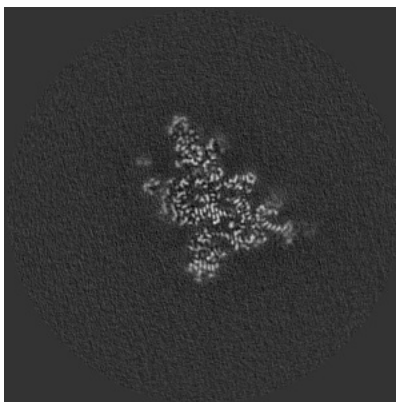


Z Index: 217

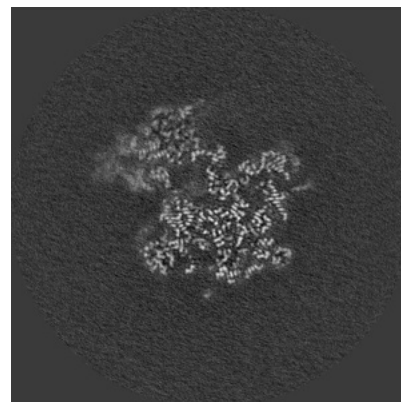
6.3.2 Raw map



X Index: 221



Y Index: 176

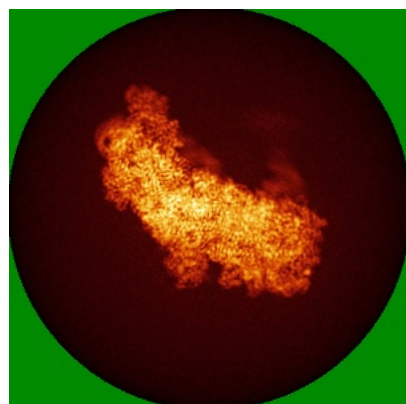


Z Index: 217

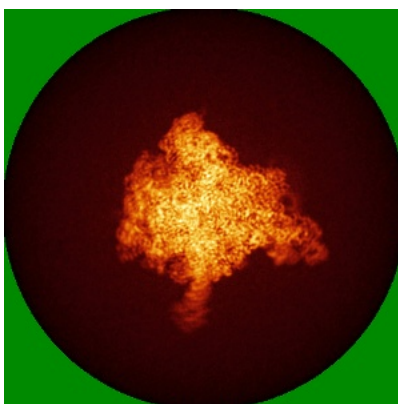
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

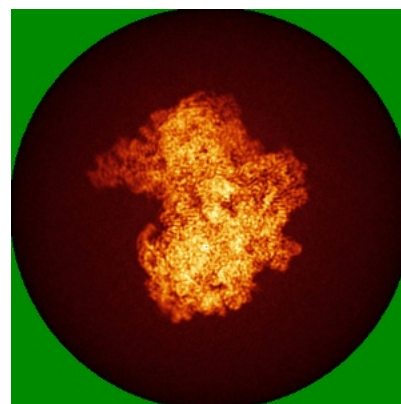
6.4.1 Primary map



X

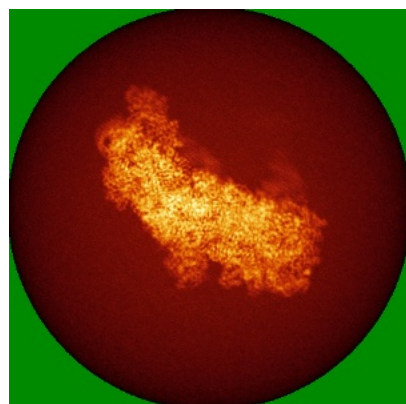


Y

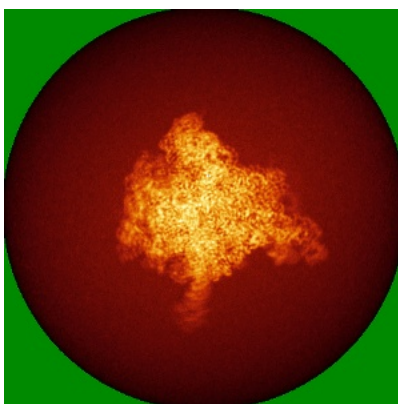


Z

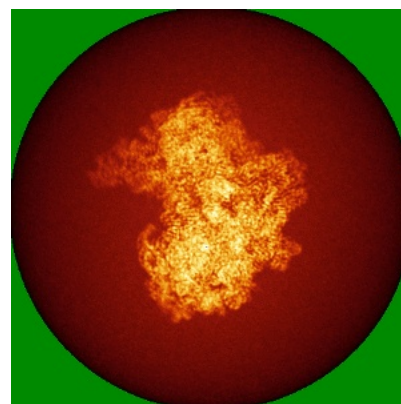
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



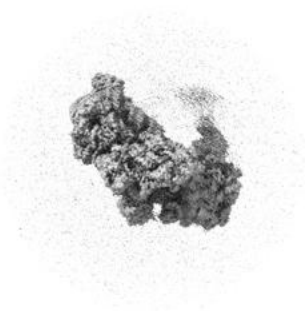
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

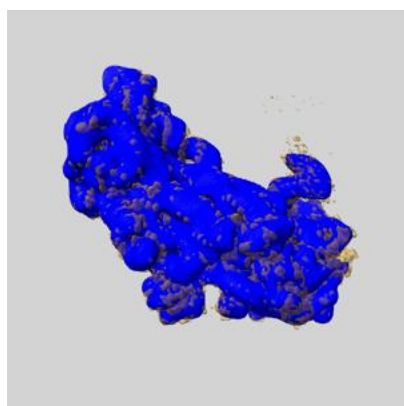
6.6 Mask visualisation [i](#)

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

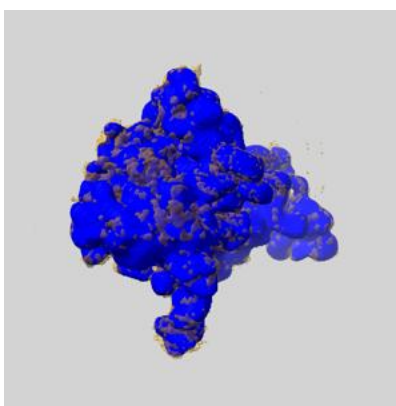
A mask typically either:

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

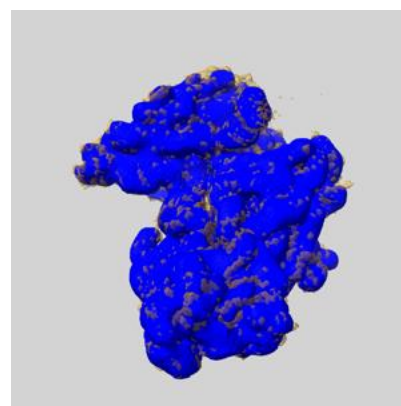
6.6.1 emd_50709_msk_1.map [i](#)



X



Y

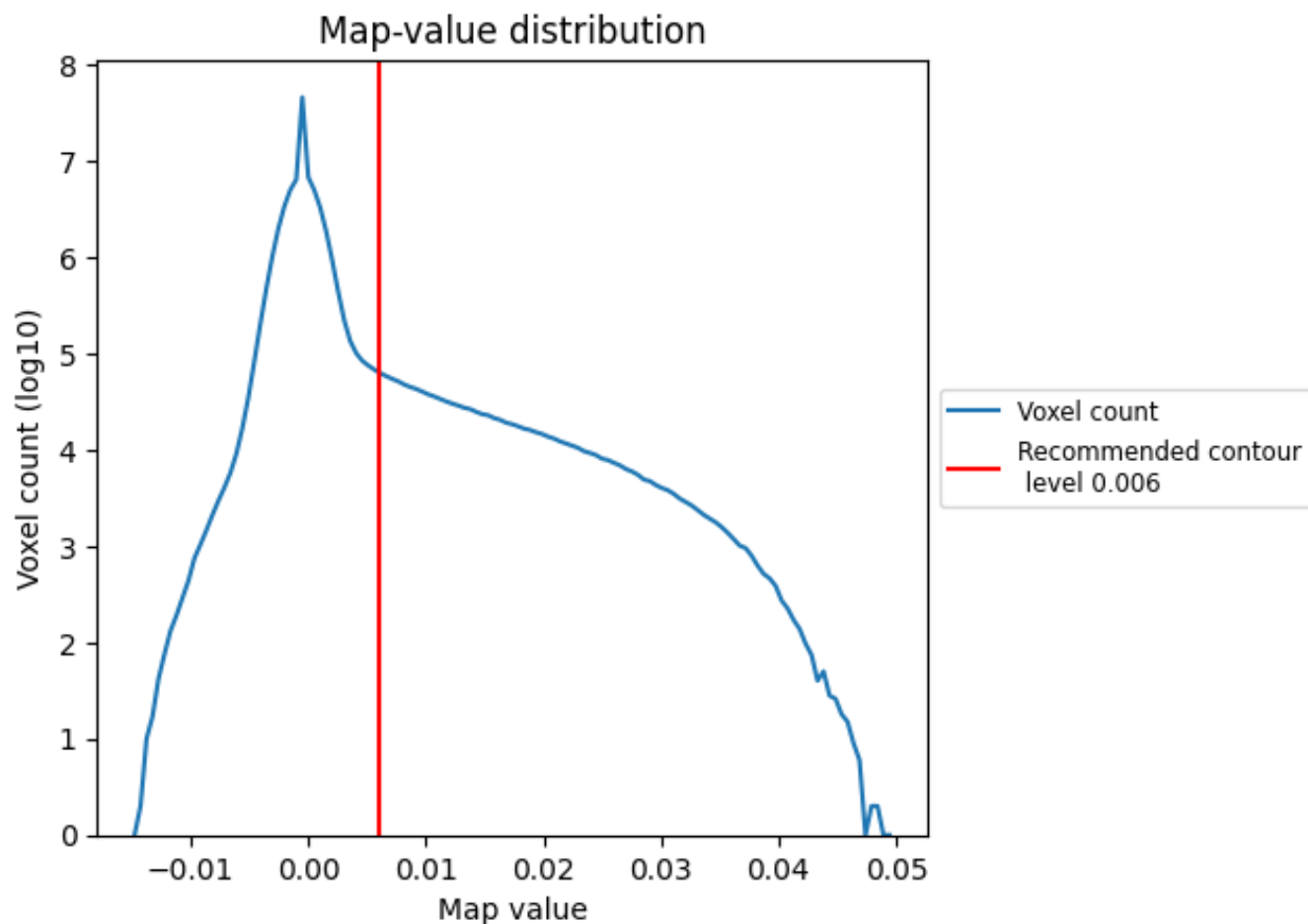


Z

7 Map analysis [i](#)

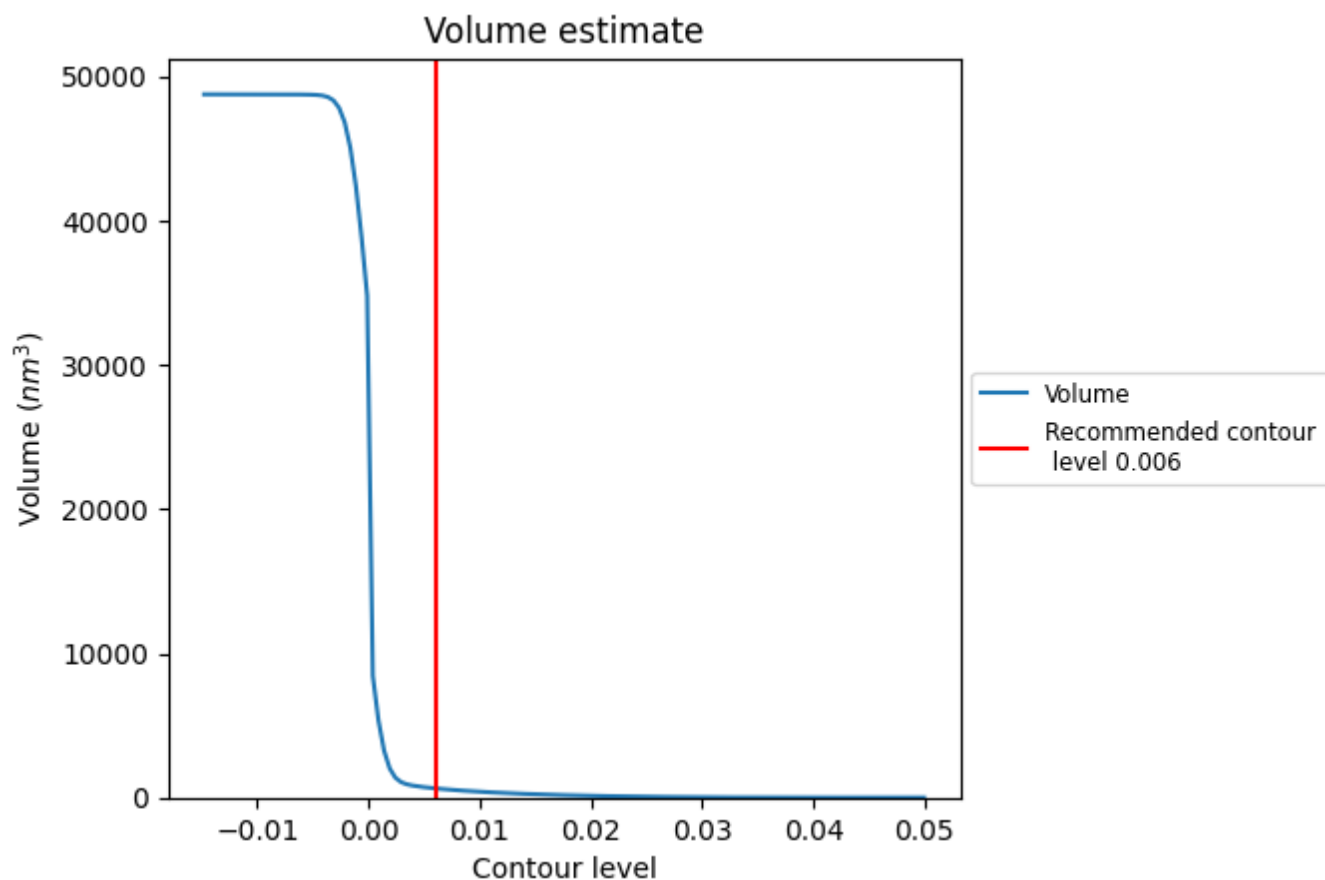
This section contains the results of statistical analysis of the map.

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.

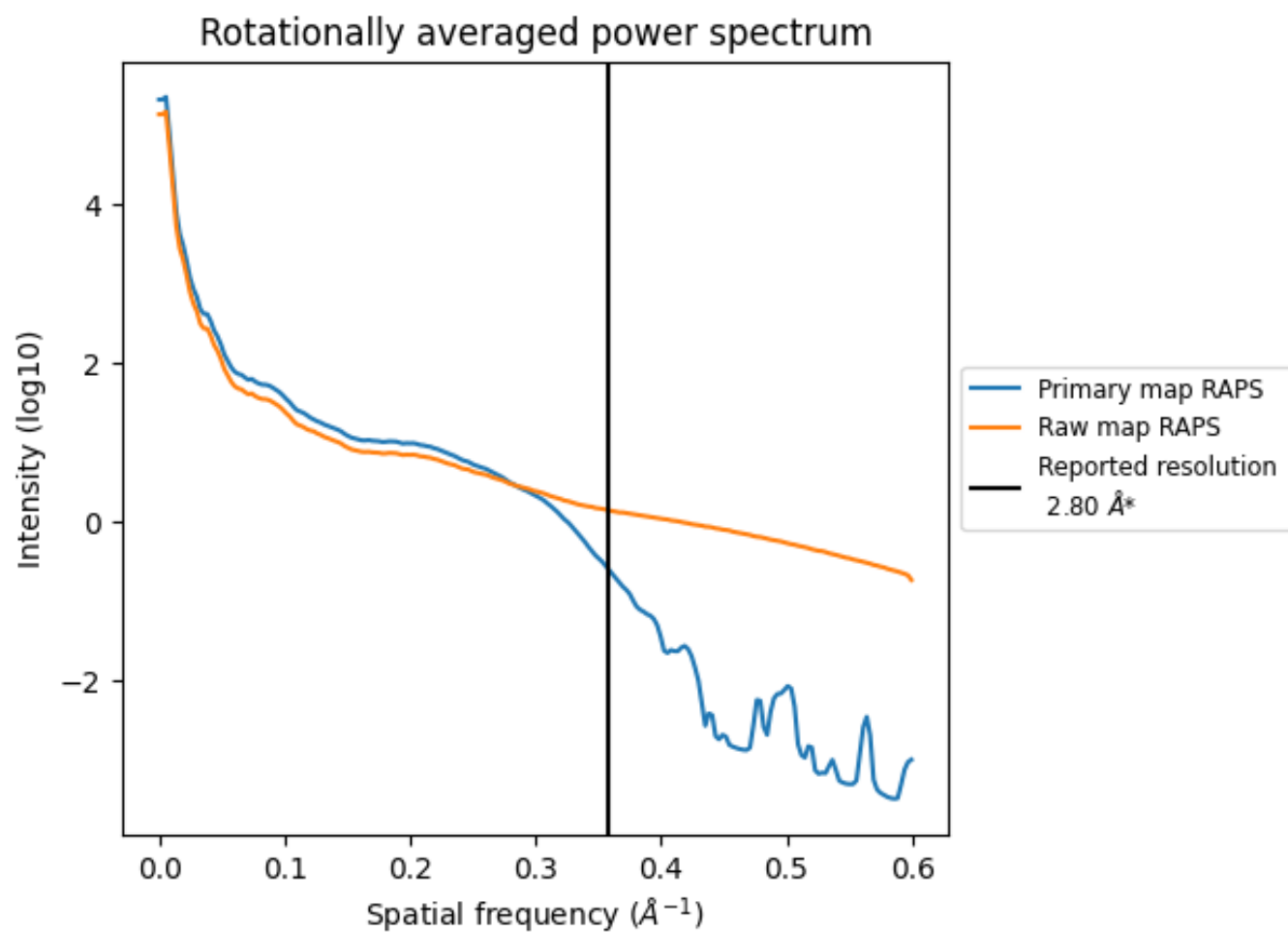
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm^3 ; this corresponds to an approximate mass of 576 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 ⓘ

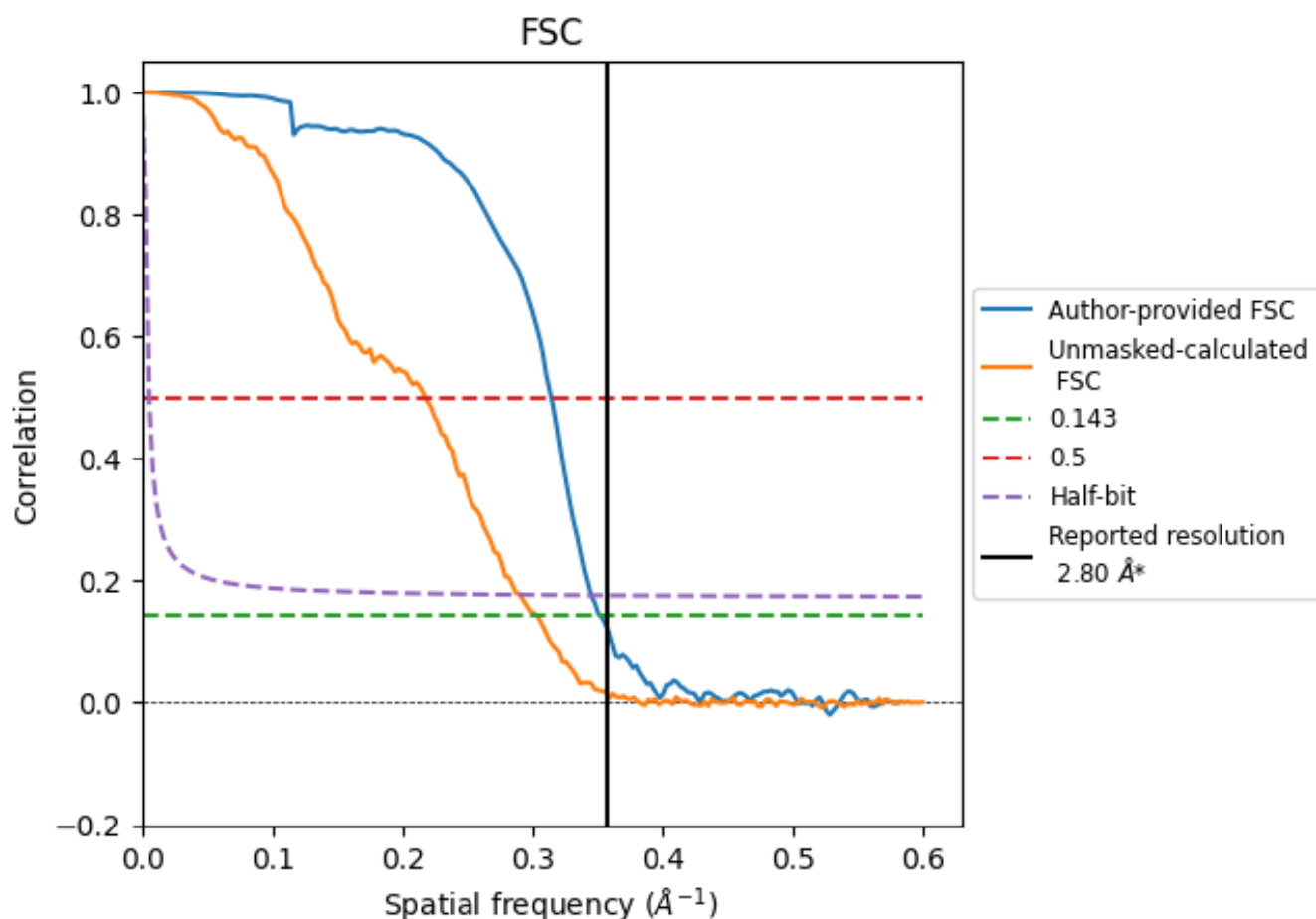


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

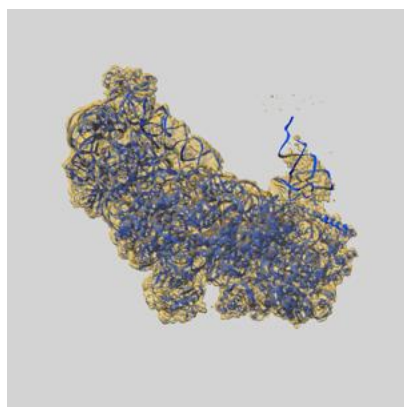
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.18	2.90
Unmasked-calculated*	3.30	4.59	3.44

*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 3.30 differs from the reported value 2.8 by more than 10 %

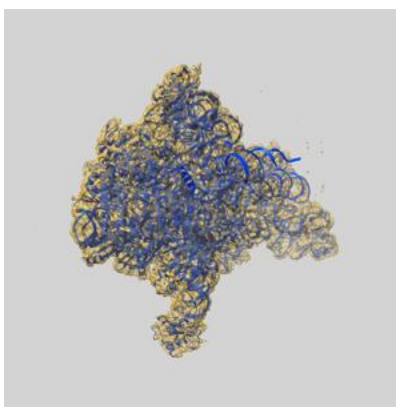
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50709 and PDB model 9FRA. Per-residue inclusion information can be found in section 3 on page 15.

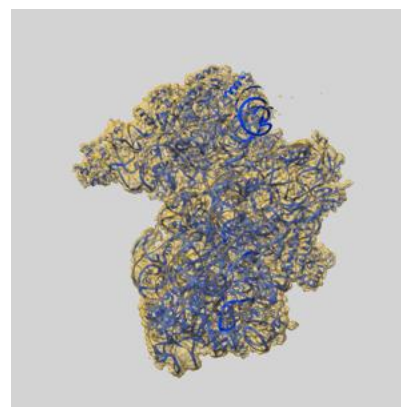
9.1 Map-model overlay [i](#)



X



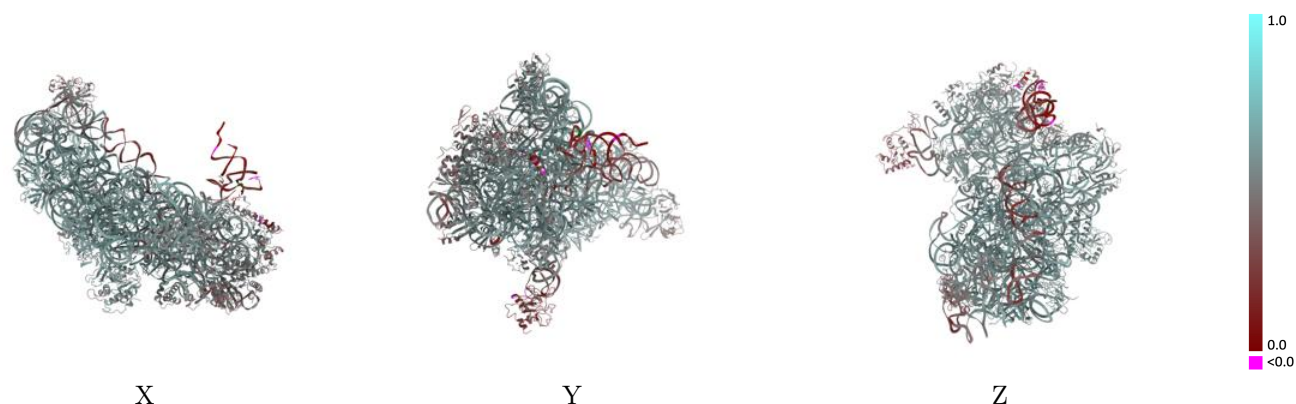
Y



Z

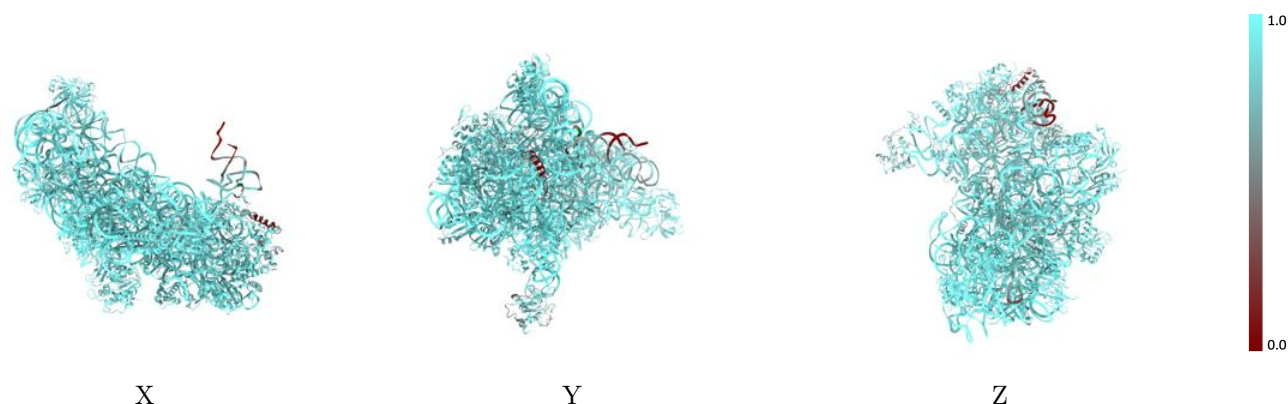
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



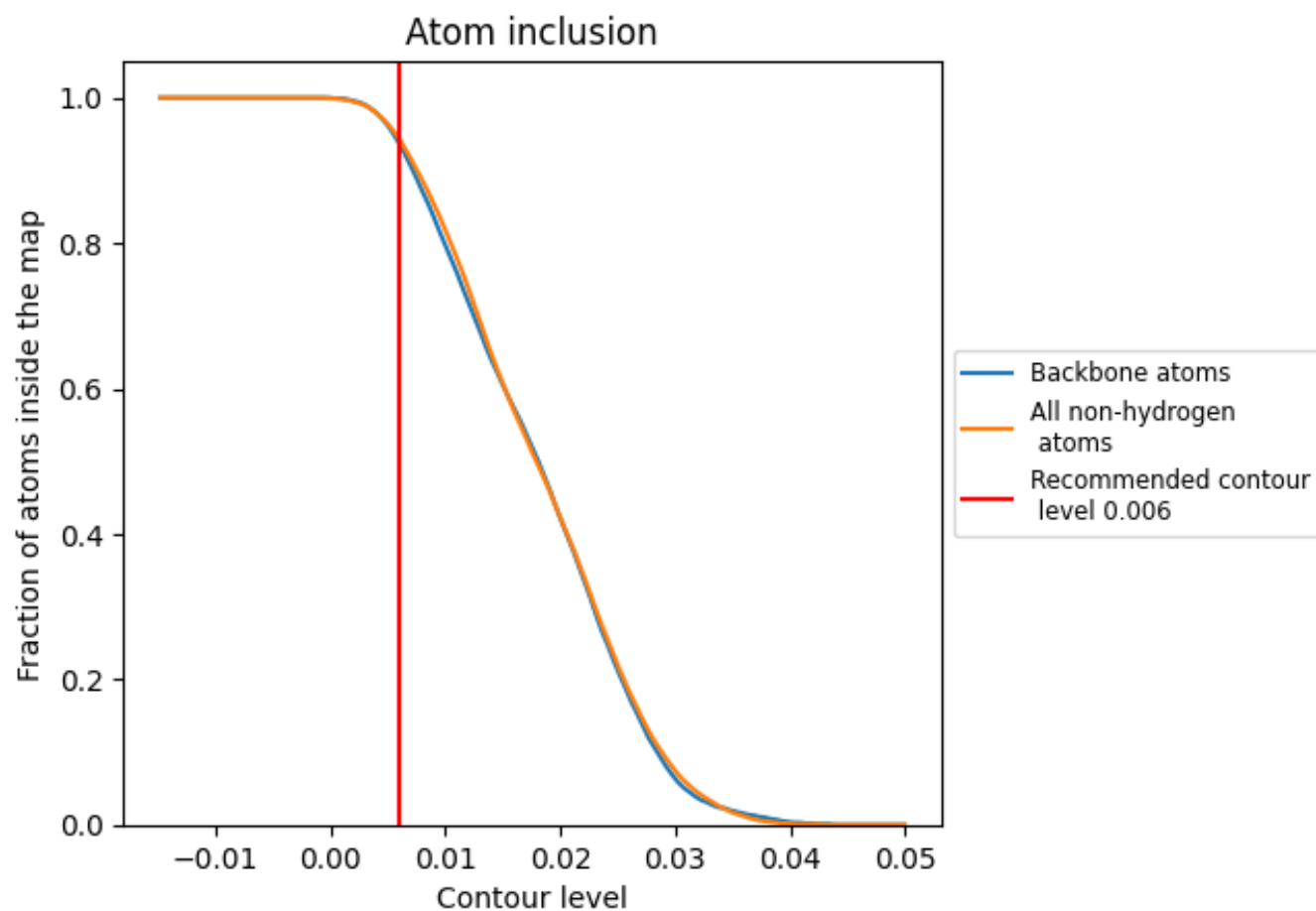
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.006).









































































9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.5330
2	 0.9850	 0.5580
3	 0.6710	 0.2530
4	 0.6830	 0.2520
5	 0.5970	 0.3660
A	 0.9450	 0.5280
B	 0.9240	 0.5430
C	 0.9600	 0.5740
D	 0.9670	 0.5800
E	 0.9700	 0.5840
F	 0.9660	 0.5880
G	 0.9100	 0.4540
H	 0.9020	 0.4940
I	 0.9760	 0.6000
J	 0.9670	 0.5700
K	 0.9510	 0.5230
L	 0.8990	 0.5110
M	 0.9440	 0.5370
N	 0.9630	 0.5820
O	 0.9440	 0.5230
P	 0.9790	 0.5870
Q	 0.9560	 0.5630
R	 0.9730	 0.5950
S	 0.9310	 0.5170
T	 0.9130	 0.5180
U	 0.9430	 0.5230
V	 0.9470	 0.5600
W	 0.9780	 0.5640
X	 0.8970	 0.4650
Y	 0.7120	 0.2570
Z	 0.9380	 0.5450
a	 0.9580	 0.5300
c	 0.5710	 0.3810
d	 0.8480	 0.4180
e	 0.7490	 0.5440
s	 0.7770	 0.2740

