Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 10:10 pm GMT

PDB ID	:	9GUP
EMDB ID	:	EMD-51615
Title	:	30S mRNA delivery complex (open head)
Authors	:	Rahil, H.; Weixlbaumer, A.; Webster, M.W.
Deposited on	:	2024-09-20
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:

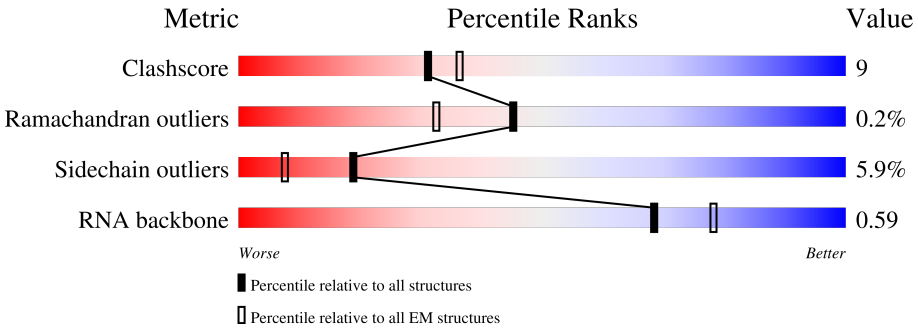
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1541	59% 35% 6%
2	B	557	12% 24% 6% 69%
3	C	241	71% 20% 6%
4	D	233	75% 15% 9%
5	E	206	68% 28%
6	F	156	82% 17%
7	G	131	58% 20% 21%

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Mol	Chain	Length	Quality of chain
8	H	156	8% 70% 24%
9	I	130	85% 14%
10	J	130	73% 23%
11	K	103	6% 74% 21%
12	L	129	74% 16% 9%
13	M	124	77% 19%
14	N	118	74% 21%
15	O	101	82% 15%
16	P	89	88% 10%
17	Q	82	77% 22%
18	R	84	73% 19% 5%
19	S	75	73% 15% 11%
20	T	92	59% 27% 10%
21	U	87	68% 30%
22	V	71	66% 31%
23	X	53	15% 11% 15% 6% 68%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 53689 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1539	33023	14736	6046	10702	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	174	1148	708	201	238	1	0	0

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	226	1765	1116	317	324	8	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	211	1653	1046	310	293	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1643	1026	315	298	4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	156	1152	717	217	212	6	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			808	504	155	148	1		

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 15 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	67	Total	C	N	O	S	0	0
			554	350	104	99	1		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 21 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 22 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	17	Total	C	N	O	P	0	0
			365	163	65	120	17		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

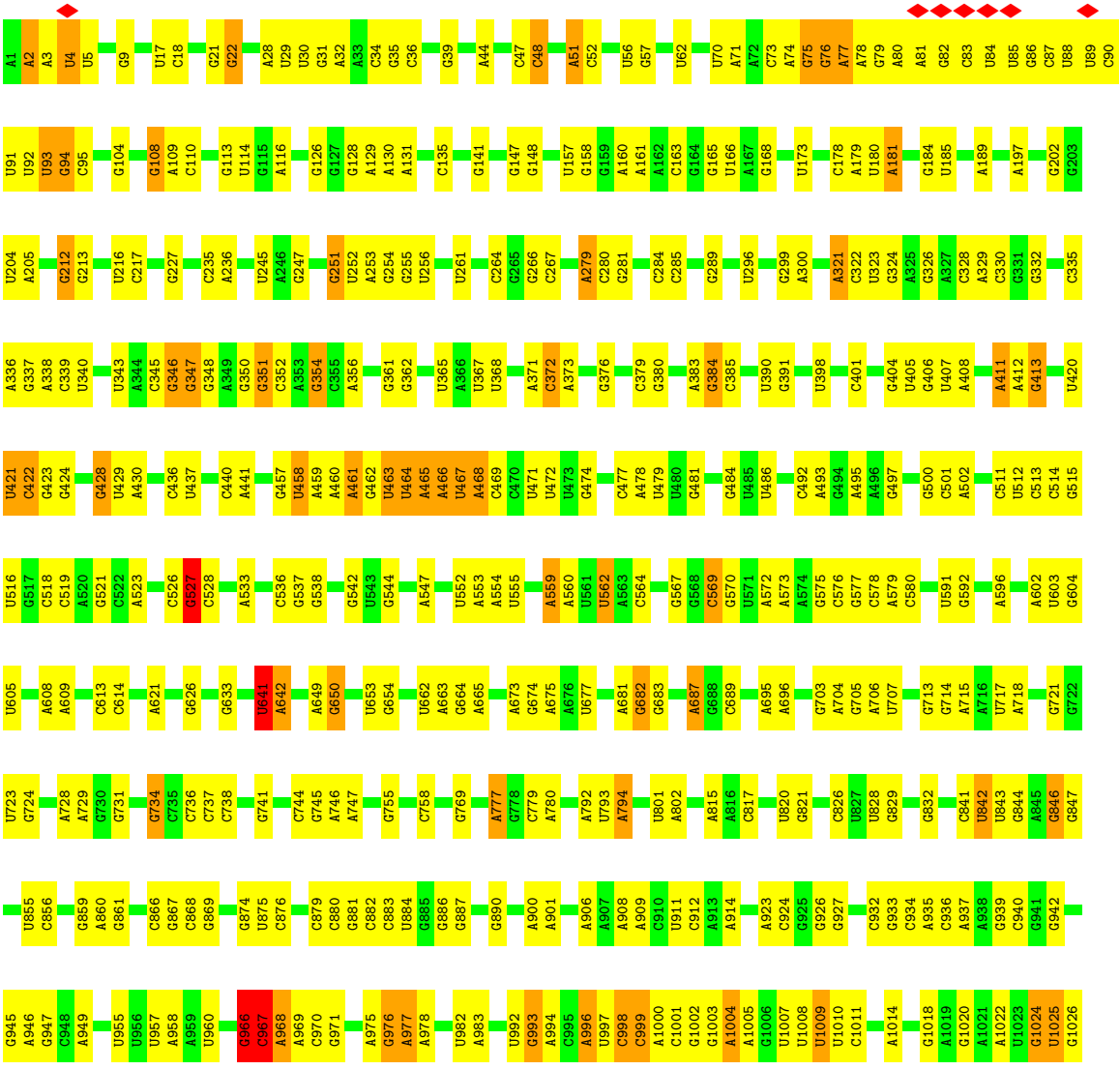
Mol	Chain	Residues	Atoms		AltConf
24	A	86	Total	Mg	0
			86	86	

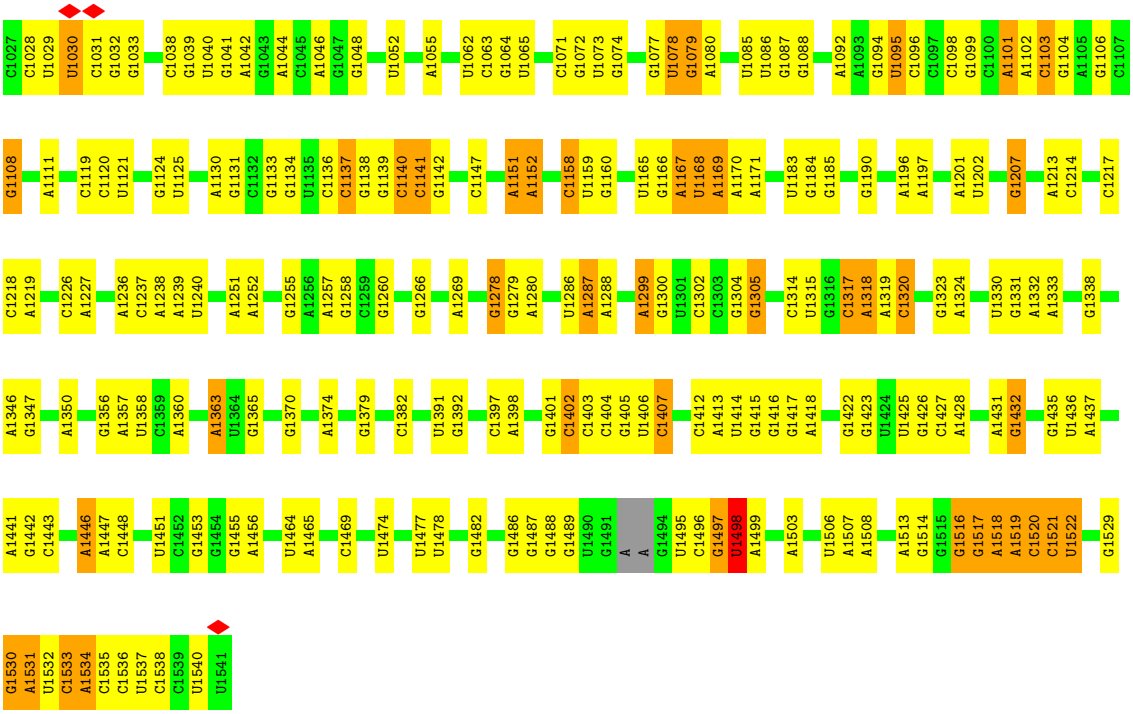
3 Residue-property plots (i)

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: 16S ribosomal RNA

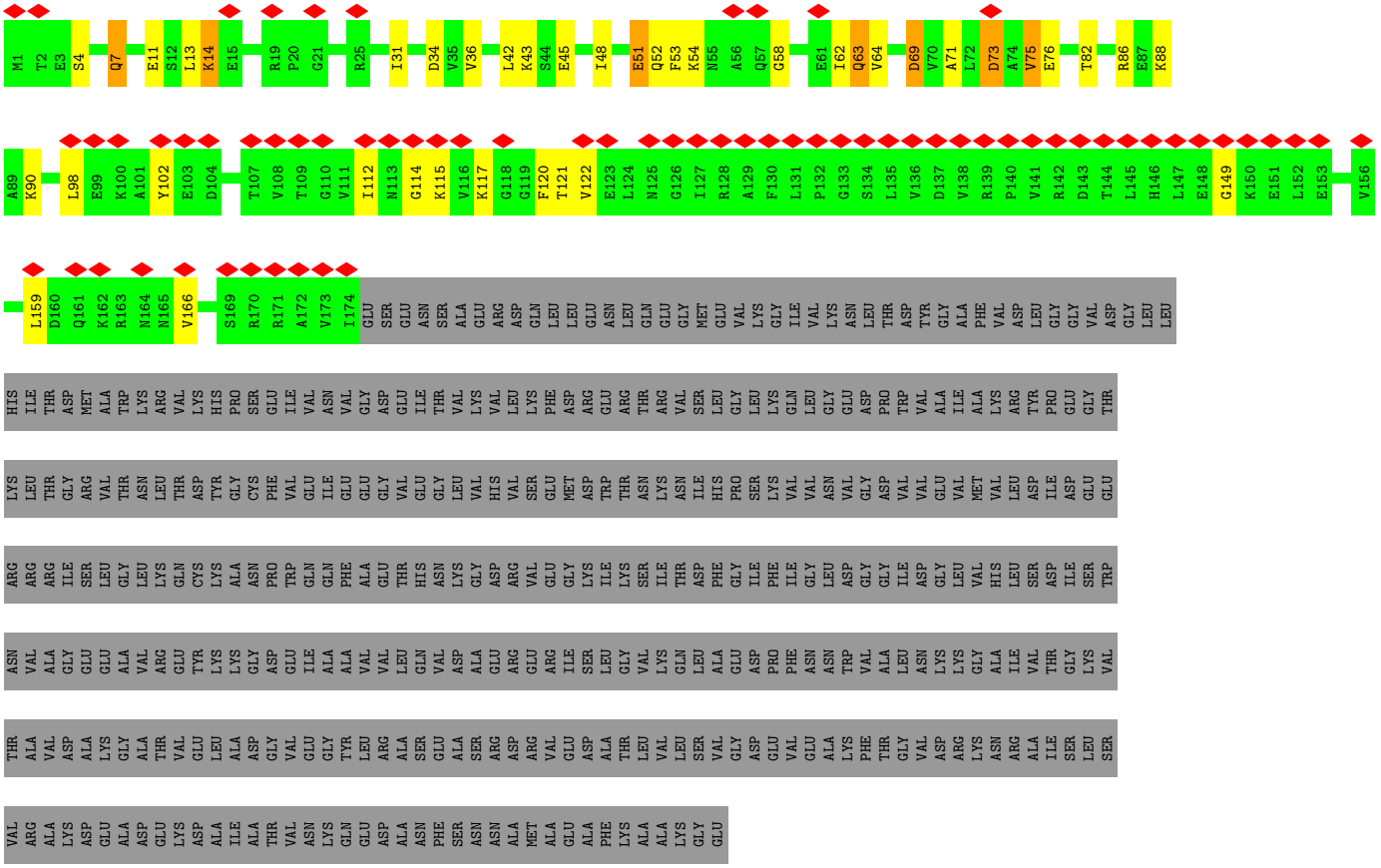
Chain A:





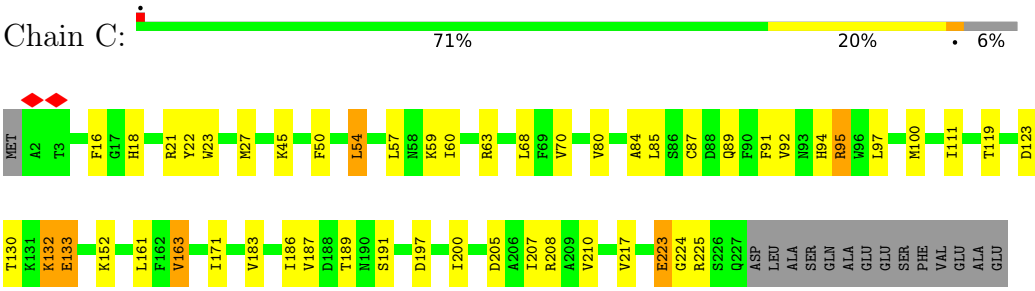
• Molecule 2: 30S ribosomal protein S1

Chain B:



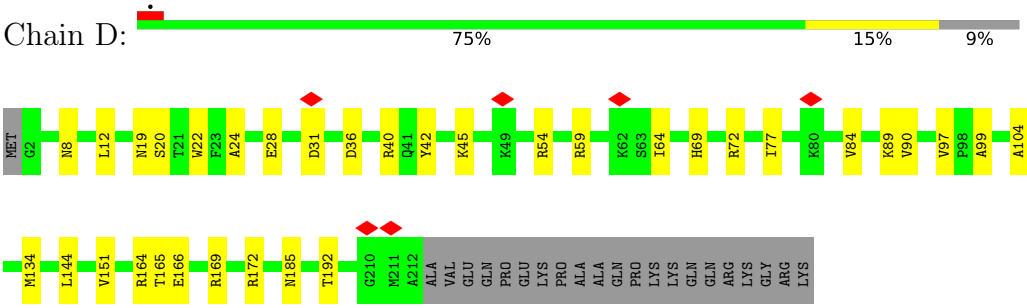
• Molecule 3: 30S ribosomal protein S2

Chain C:



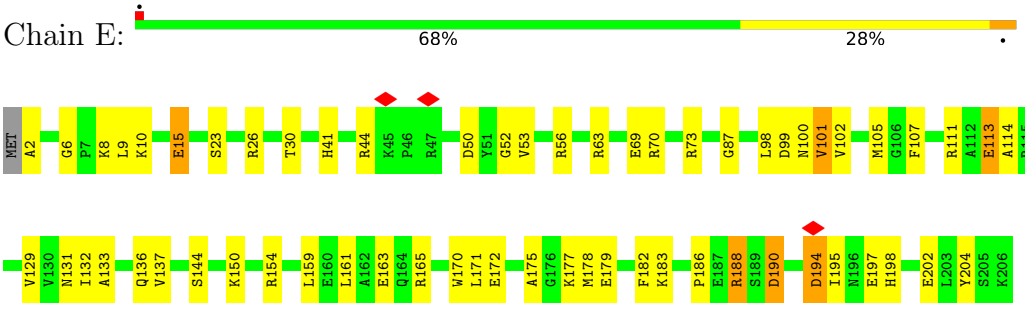
• Molecule 4: Small ribosomal subunit protein uS3

Chain D:



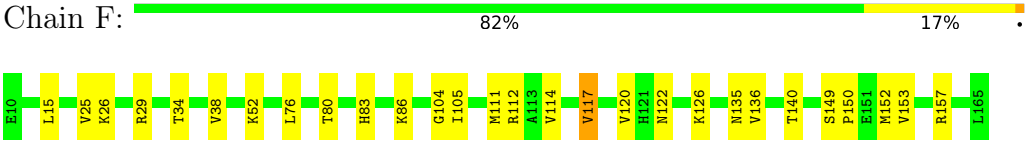
• Molecule 5: Small ribosomal subunit protein uS4

Chain E:



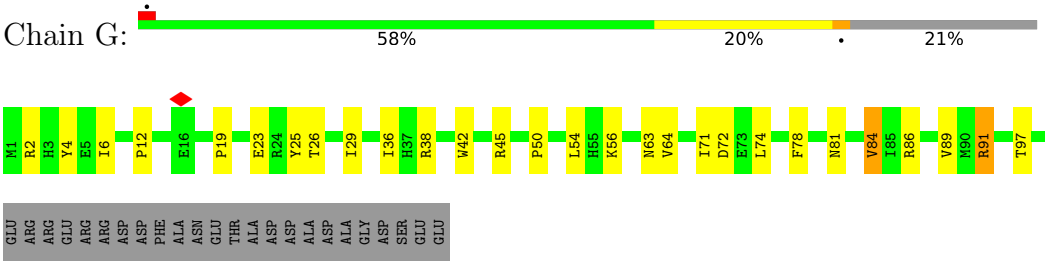
• Molecule 6: 30S ribosomal protein S5

Chain F:



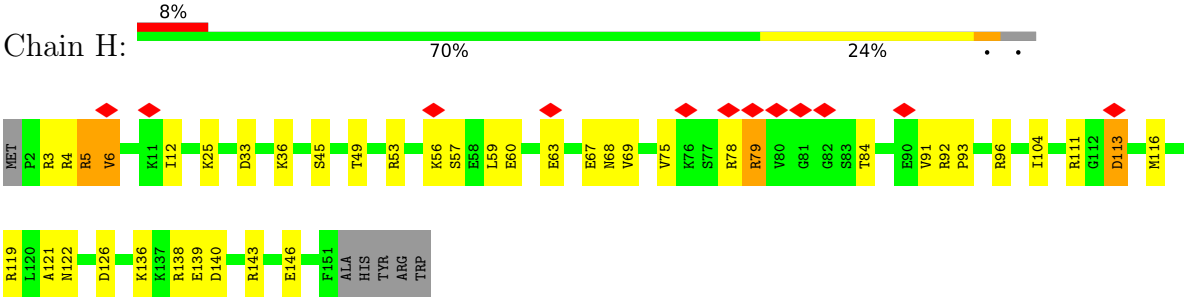
• Molecule 7: Small ribosomal subunit protein bS6

Chain G:



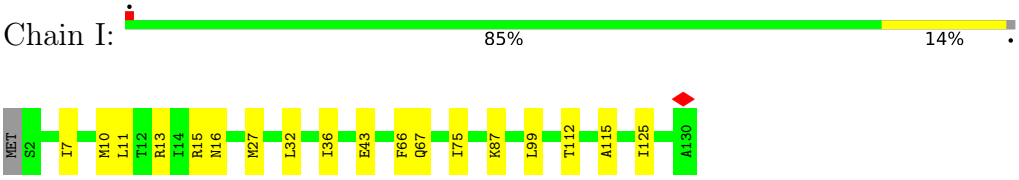
• Molecule 8: 30S ribosomal protein S7

Chain H:



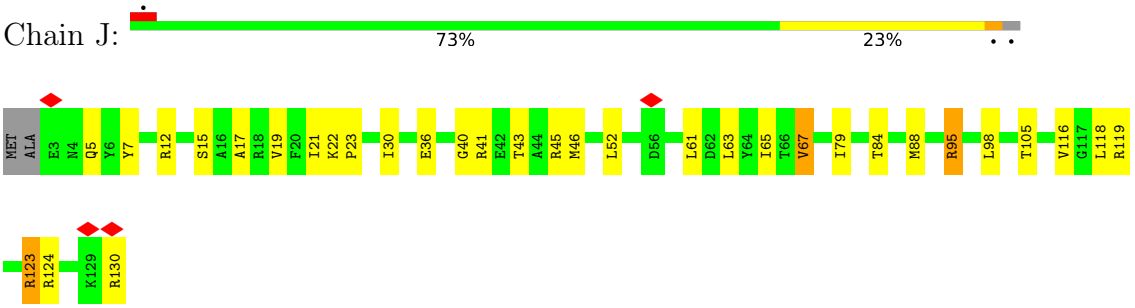
• Molecule 9: 30S ribosomal protein S8

Chain I:



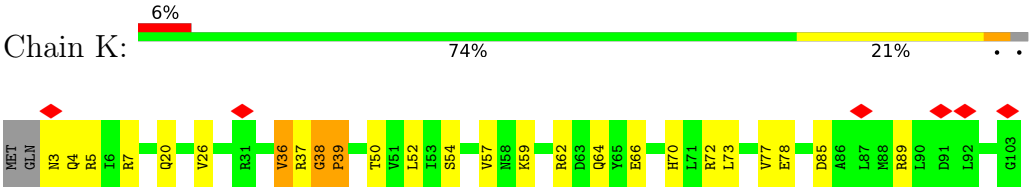
• Molecule 10: 30S ribosomal protein S9

Chain J:



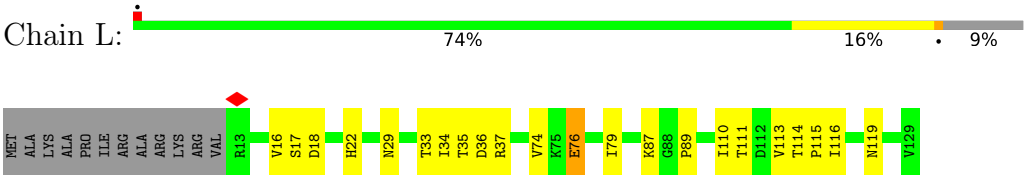
• Molecule 11: 30S ribosomal protein S10

Chain K:



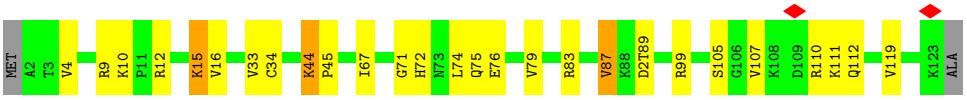
• Molecule 12: 30S ribosomal protein S11

Chain L:



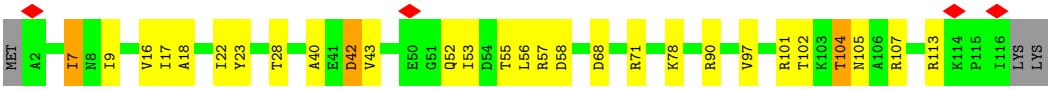
• Molecule 13: 30S ribosomal protein S12

Chain M:



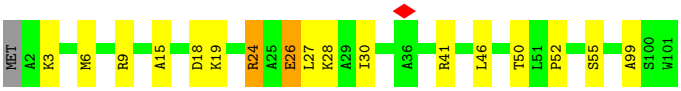
• Molecule 14: 30S ribosomal protein S13

Chain N:



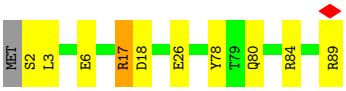
• Molecule 15: 30S ribosomal protein S14

Chain O:



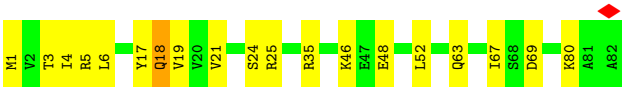
• Molecule 16: Small ribosomal subunit protein uS15

Chain P:



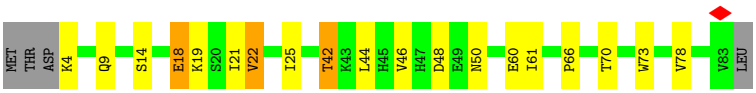
• Molecule 17: 30S ribosomal protein S16

Chain Q:



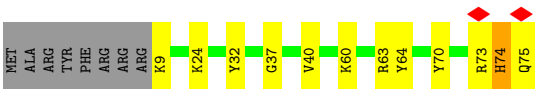
• Molecule 18: 30S ribosomal protein S17

Chain R:



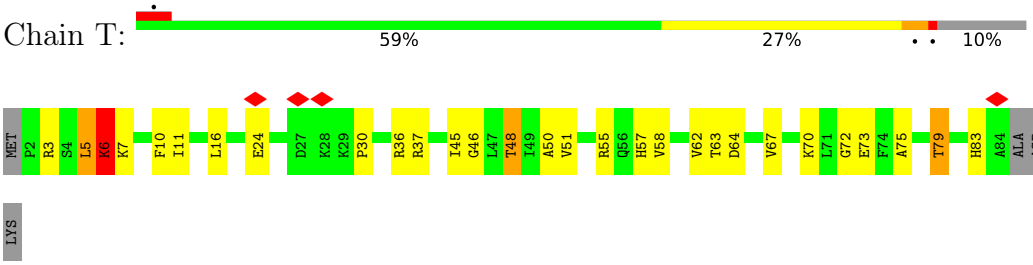
• Molecule 19: 30S ribosomal protein S18

Chain S:



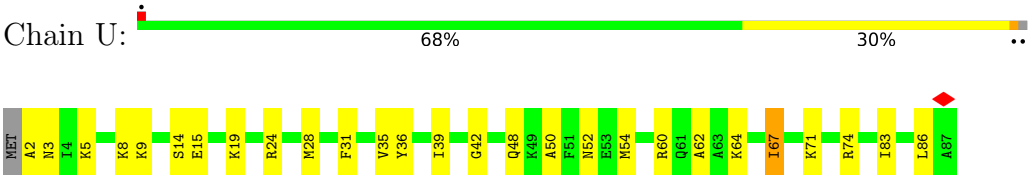
• Molecule 20: 30S ribosomal protein S19

Chain T:



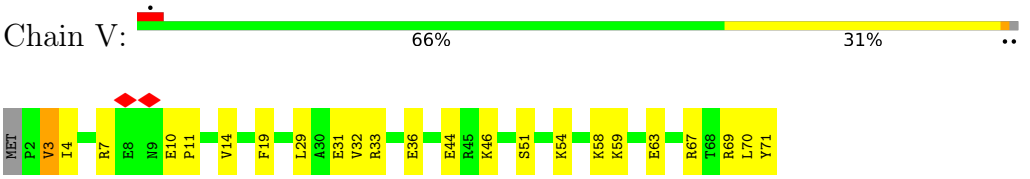
• Molecule 21: 30S ribosomal protein S20

Chain U:



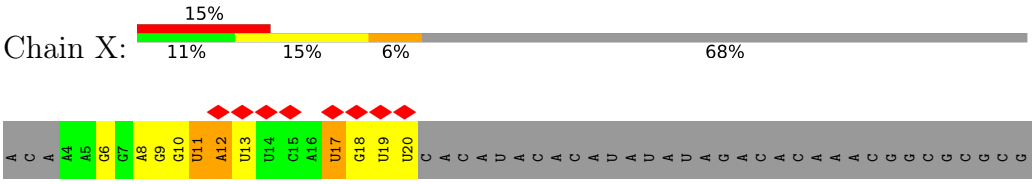
• Molecule 22: 30S ribosomal protein S21

Chain V:



• Molecule 23: mRNA

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52113	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 ($e^-/Å^2$)	49.95	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	7.196	Depositor
Minimum map value	-2.451	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.151	Depositor
Recommended contour level	0.745	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, PSU, D2T, 4OC, G7M, 2MG, UR3, 5MC, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.66	4/36692 (0.0%)	0.78	2/57230 (0.0%)
2	B	0.29	0/1157	0.52	0/1574
3	C	0.33	0/1796	0.53	0/2420
4	D	0.33	0/1680	0.53	0/2263
5	E	0.36	0/1665	0.55	0/2227
6	F	0.33	0/1165	0.53	0/1568
7	G	0.36	0/867	0.53	0/1171
8	H	0.29	0/1190	0.54	0/1595
9	I	0.34	0/989	0.53	0/1326
10	J	0.38	0/1043	0.59	0/1387
11	K	0.35	0/818	0.66	1/1105 (0.1%)
12	L	0.31	0/893	0.56	0/1205
13	M	0.39	0/954	0.65	0/1279
14	N	0.31	0/900	0.57	0/1204
15	O	0.32	0/817	0.55	0/1088
16	P	0.32	0/722	0.54	0/964
17	Q	0.40	0/659	0.58	0/884
18	R	0.34	0/657	0.53	0/881
19	S	0.36	0/563	0.55	0/754
20	T	0.36	0/680	0.61	1/915 (0.1%)
21	U	0.32	0/676	0.47	0/895
22	V	0.31	0/598	0.58	0/792
23	X	0.30	0/408	0.92	0/634
All	All	0.56	4/57589 (0.0%)	0.71	4/85361 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
13	M	0	1
20	T	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1108	G	O3'-P	-6.78	1.53	1.61
1	A	874	G	O3'-P	-6.08	1.53	1.61
1	A	1522	U	O3'-P	-5.66	1.54	1.61
1	A	1531	A	O3'-P	-5.22	1.54	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	641	U	C2'-C3'-O3'	8.41	128.00	109.50
11	K	39	PRO	CB-CA-C	-7.92	92.21	112.00
20	T	6	LYS	CB-CA-C	-7.47	95.46	110.40
1	A	527	G7M	OP1-P-O3'	6.84	120.25	105.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	38	GLY	Peptide
13	M	44	LYS	Peptide
20	T	5	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33023	0	16643	451	0
2	B	1148	0	948	39	0
3	C	1765	0	1792	36	0
4	D	1653	0	1727	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1643	0	1707	42	0
6	F	1152	0	1196	21	0
7	G	848	0	846	14	0
8	H	1176	0	1233	26	0
9	I	979	0	1031	15	0
10	J	1031	0	1076	20	0
11	K	808	0	845	14	0
12	L	877	0	887	20	0
13	M	951	0	1012	15	0
14	N	891	0	952	15	0
15	O	805	0	844	14	0
16	P	714	0	734	7	0
17	Q	649	0	666	11	0
18	R	648	0	691	12	0
19	S	554	0	573	10	0
20	T	663	0	688	23	0
21	U	670	0	719	14	0
22	V	590	0	629	24	0
23	X	365	0	182	11	0
24	A	86	0	0	0	0
All	All	53689	0	37621	771	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 9.

All (771) 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)
2:B:53:PHE:CD2	2:B:62:ILE:HD12	1.61	1.34
2:B:53:PHE:HD2	2:B:62:ILE:CD1	1.41	1.33
2:B:53:PHE:CD2	2:B:62:ILE:CD1	2.18	1.25
2:B:75:VAL:O	2:B:76:GLU:HG3	1.50	1.09
2:B:53:PHE:HD2	2:B:62:ILE:HD12	0.86	1.03
1:A:966:2MG:H5"	1:A:966:2MG:H8	1.20	1.01
1:A:75:G:H4'	1:A:75:G:OP1	1.68	0.91
1:A:966:2MG:H5"	1:A:966:2MG:C8	2.04	0.91
12:L:89:PRO:HB3	22:V:32:VAL:HG21	1.51	0.90
1:A:75:G:C5'	1:A:75:G:H8	1.88	0.86
7:G:26:THR:HG23	7:G:36:ILE:HG13	1.58	0.86
2:B:75:VAL:O	2:B:76:GLU:CG	2.24	0.84
1:A:1533:C:OP2	1:A:1533:C:H2'	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:U:H5”	1:A:422:C:H5	1.44	0.82
1:A:346:G:H3’	1:A:346:G:N3	1.97	0.80
4:D:36:ASP:OD1	4:D:59:ARG:NH1	2.15	0.79
3:C:27:MET:HG2	3:C:189:THR:HA	1.63	0.79
1:A:1520:C:H5”	1:A:1520:C:H6	1.47	0.78
1:A:420:U:H2’	1:A:422:C:C5	2.19	0.78
1:A:1423:G:H1	1:A:1477:U:H3	1.31	0.78
1:A:1382:C:H5’	8:H:79:ARG:HH21	1.50	0.76
20:T:70:LYS:HB2	20:T:73:GLU:HG3	1.67	0.76
1:A:465:A:N3	1:A:465:A:H2’	2.01	0.75
5:E:102:VAL:HG13	5:E:114:ALA:HB1	1.68	0.75
1:A:1350:A:O2’	8:H:33:ASP:OD1	2.05	0.74
1:A:1520:C:H5”	1:A:1520:C:C6	2.23	0.73
5:E:101:VAL:HG21	5:E:137:VAL:HG21	1.70	0.73
1:A:468:A:H3’	1:A:469:C:H6	1.54	0.73
1:A:458:U:H5”	1:A:458:U:H6	1.54	0.73
1:A:664:G:H22	1:A:741:G:H1	1.34	0.73
1:A:407:U:O2’	5:E:113:GLU:OE1	2.06	0.73
1:A:1240:U:OP1	8:H:119:ARG:NH2	2.22	0.73
2:B:75:VAL:C	2:B:76:GLU:HG3	2.08	0.73
2:B:43:LYS:HG3	3:C:16:PHE:HB3	1.70	0.72
1:A:1363:A:O2’	1:A:1365:G:N7	2.20	0.72
2:B:53:PHE:CD2	2:B:62:ILE:HD13	2.22	0.72
1:A:75:G:H8	1:A:75:G:H5’	1.53	0.72
3:C:119:THR:O	3:C:123:ASP:HB2	1.89	0.72
1:A:1374:A:OP1	8:H:36:LYS:NZ	2.19	0.72
1:A:3:A:H5”	1:A:4:U:H5’	1.72	0.72
1:A:77:A:O5’	1:A:77:A:H8	1.72	0.72
2:B:112:ILE:O	2:B:149:GLY:N	2.16	0.72
20:T:36:ARG:NH2	20:T:75:ALA:O	2.23	0.72
2:B:75:VAL:HG22	2:B:76:GLU:HG3	1.72	0.71
1:A:423:G:H5”	1:A:423:G:N3	2.06	0.71
1:A:562:U:H1’	13:M:12:ARG:HB3	1.70	0.71
1:A:421:U:H3’	1:A:422:C:C6	2.26	0.71
1:A:1403:C:O5’	1:A:1403:C:H6	1.73	0.71
8:H:113:ASP:OD2	8:H:122:ASN:ND2	2.23	0.71
1:A:467:U:H3’	1:A:467:U:O2	1.92	0.70
2:B:114:GLY:O	2:B:121:THR:N	2.24	0.70
1:A:75:G:C5’	1:A:75:G:C8	2.73	0.70
21:U:35:VAL:HG21	21:U:54:MET:HG2	1.72	0.70
1:A:826:C:O2	9:I:16:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:U:H3	1:A:474:G:H1	1.40	0.70
13:M:99:ARG:NH1	13:M:105:SER:O	2.26	0.69
1:A:713:G:H2'	1:A:714:G:C8	2.28	0.69
10:J:118:LEU:HD22	10:J:124:ARG:HG2	1.75	0.69
1:A:126:G:OP1	1:A:605:U:O2'	2.09	0.69
1:A:933:G:N7	8:H:3:ARG:NH1	2.40	0.69
1:A:1147:C:O2'	10:J:7:TYR:OH	2.05	0.69
14:N:68:ASP:OD1	14:N:71:ARG:NH1	2.26	0.69
1:A:468:A:H3'	1:A:469:C:C6	2.29	0.68
21:U:15:GLU:OE2	21:U:19:LYS:NZ	2.27	0.67
1:A:1158:C:H5'	3:C:132:LYS:HD3	1.77	0.67
1:A:261:U:OP2	21:U:74:ARG:NH2	2.28	0.67
1:A:421:U:H5"	1:A:422:C:C5	2.27	0.67
2:B:53:PHE:CE2	2:B:62:ILE:CD1	2.78	0.67
1:A:641:U:H1'	1:A:642:A:N7	2.10	0.66
10:J:52:LEU:HD11	10:J:63:LEU:HD11	1.77	0.66
1:A:492:C:H2'	1:A:493:A:C8	2.31	0.66
1:A:526:C:C4	1:A:527:G7M:H1'	2.31	0.66
20:T:46:GLY:N	20:T:62:VAL:O	2.26	0.66
1:A:946:A:H2'	1:A:947:G:C8	2.30	0.66
5:E:100:ASN:OD1	5:E:111:ARG:NH1	2.29	0.65
1:A:255:G:H2'	1:A:256:U:C6	2.30	0.65
3:C:60:ILE:HG12	3:C:63:ARG:HH21	1.62	0.65
1:A:227:G:O2'	17:Q:63:GLN:OE1	2.13	0.65
1:A:75:G:H5'	1:A:75:G:C8	2.31	0.65
1:A:79:G:H2'	1:A:80:A:C8	2.33	0.64
2:B:4:SER:OG	2:B:7:GLN:NE2	2.31	0.64
2:B:73:ASP:OD1	2:B:73:ASP:N	2.30	0.64
22:V:29:LEU:HA	22:V:32:VAL:HG22	1.80	0.64
1:A:347:G:H8	1:A:347:G:OP2	1.81	0.64
1:A:1530:G:H2'	1:A:1531:A:C8	2.32	0.64
6:F:83:HIS:HD2	9:I:99:LEU:HD12	1.62	0.64
10:J:116:VAL:HG13	11:K:62:ARG:HH11	1.61	0.64
1:A:1533:C:OP2	1:A:1533:C:H6	1.80	0.64
1:A:890:G:O2'	1:A:906:A:N6	2.31	0.64
2:B:159:LEU:HA	2:B:166:VAL:HA	1.80	0.63
20:T:50:ALA:HB1	20:T:57:HIS:HB3	1.80	0.63
4:D:20:SER:OG	4:D:22:TRP:NE1	2.31	0.63
13:M:71:GLY:O	13:M:99:ARG:NH2	2.32	0.63
1:A:1536:C:C2	23:X:10:G:N2	2.67	0.62
3:C:97:LEU:HB2	3:C:100:MET:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:2:ARG:HG2	7:G:91:ARG:HH21	1.63	0.62
1:A:1356:G:H2'	1:A:1357:A:C8	2.34	0.62
9:I:11:LEU:HD22	9:I:75:ILE:HD11	1.80	0.62
15:O:6:MET:SD	15:O:9:ARG:NH1	2.72	0.62
8:H:113:ASP:N	8:H:113:ASP:OD1	2.30	0.62
1:A:717:U:O3'	12:L:119:ASN:ND2	2.33	0.62
1:A:673:A:H2'	1:A:674:G:C8	2.34	0.62
1:A:746:A:H2'	1:A:747:A:C8	2.35	0.62
1:A:467:U:O2	1:A:467:U:C3'	2.47	0.62
1:A:626:G:OP1	17:Q:35:ARG:NH2	2.33	0.62
8:H:111:ARG:NH2	8:H:126:ASP:OD2	2.29	0.62
2:B:53:PHE:CE2	2:B:62:ILE:HD13	2.35	0.61
1:A:356:A:N3	1:A:368:U:O2'	2.29	0.61
5:E:194:ASP:OD1	5:E:194:ASP:N	2.21	0.61
1:A:1251:A:H2'	1:A:1252:A:C8	2.35	0.61
1:A:946:A:H2'	1:A:947:G:H8	1.65	0.60
1:A:1239:A:H62	1:A:1299:A:H62	1.48	0.60
12:L:76:GLU:O	12:L:76:GLU:HG2	1.99	0.60
22:V:4:ILE:HG13	22:V:19:PHE:HA	1.83	0.60
11:K:54:SER:OG	11:K:57:VAL:O	2.14	0.60
1:A:859:G:H2'	1:A:860:A:H8	1.66	0.60
1:A:1488:G:H2'	1:A:1489:G:H8	1.67	0.60
17:Q:6:LEU:HB3	17:Q:17:TYR:HB3	1.82	0.60
1:A:993:G:H2'	1:A:993:G:N3	2.16	0.60
1:A:1516:2MG:H2'	1:A:1518:MA6:OP2	2.01	0.60
2:B:69:ASP:OD1	2:B:69:ASP:N	2.35	0.60
1:A:77:A:H2'	1:A:78:A:C8	2.37	0.59
1:A:463:U:H5"	1:A:463:U:C6	2.37	0.59
1:A:999:C:H2'	1:A:1000:A:C8	2.36	0.59
1:A:1005:A:OP2	1:A:1024:G:N2	2.26	0.59
1:A:1537:U:H2'	1:A:1538:C:C6	2.36	0.59
3:C:129:LEU:HD13	3:C:133:GLU:HB2	1.83	0.59
5:E:202:GLU:OE2	6:F:112:ARG:NH1	2.35	0.59
1:A:1062:U:H2'	1:A:1063:C:C6	2.38	0.59
1:A:465:A:H3'	1:A:466:A:C8	2.38	0.59
1:A:1537:U:H2'	1:A:1538:C:H6	1.67	0.59
3:C:27:MET:HG3	3:C:27:MET:O	2.03	0.59
4:D:77:ILE:HA	4:D:84:VAL:HG23	1.84	0.59
6:F:150:PRO:HA	6:F:153:VAL:HG12	1.85	0.59
1:A:401:C:O2'	1:A:621:A:N3	2.32	0.59
1:A:216:U:H1'	1:A:466:A:H61	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:A:O2'	3:C:133:GLU:OE1	2.20	0.58
1:A:1427:C:H2'	1:A:1428:A:H8	1.68	0.58
6:F:114:VAL:HG11	6:F:140:THR:HG21	1.85	0.58
1:A:1518:MA6:H103	1:A:1519:MA6:N6	2.18	0.58
1:A:1130:A:H2'	1:A:1131:G:H8	1.68	0.58
1:A:1397:C:OP2	6:F:29:ARG:NH2	2.37	0.58
6:F:83:HIS:CD2	9:I:99:LEU:HD12	2.38	0.58
1:A:966:2MG:HM23	1:A:967:5MC:H1'	1.85	0.58
8:H:138:ARG:NH1	8:H:139:GLU:OE2	2.37	0.58
1:A:75:G:H2'	1:A:76:G:O4'	2.04	0.58
1:A:859:G:H2'	1:A:860:A:C8	2.39	0.58
1:A:1535:C:H2'	1:A:1536:C:C6	2.38	0.58
1:A:714:G:H2'	1:A:715:A:C8	2.39	0.58
1:A:1519:MA6:N7	1:A:1519:MA6:H93	2.19	0.58
2:B:43:LYS:NZ	3:C:205:ASP:OD2	2.36	0.58
8:H:136:LYS:NZ	8:H:140:ASP:OD1	2.36	0.58
10:J:116:VAL:HG13	11:K:62:ARG:NH1	2.19	0.58
1:A:421:U:H3'	1:A:422:C:H6	1.68	0.57
1:A:477:C:H2'	1:A:478:A:C8	2.39	0.57
2:B:117:LYS:O	23:X:18:G:N2	2.33	0.57
1:A:147:G:H2'	1:A:148:G:C8	2.38	0.57
1:A:1488:G:H2'	1:A:1489:G:C8	2.38	0.57
4:D:19:ASN:OD1	4:D:54:ARG:NH1	2.37	0.57
5:E:159:LEU:O	5:E:163:GLU:HG2	2.03	0.57
1:A:466:A:H8	1:A:466:A:OP2	1.86	0.57
5:E:172:GLU:HB3	5:E:183:LYS:HD3	1.85	0.57
1:A:79:G:H2'	1:A:80:A:H8	1.68	0.57
12:L:111:THR:CG2	22:V:3:VAL:HG12	2.34	0.57
1:A:376:G:H5"	17:Q:5:ARG:HD2	1.87	0.57
4:D:164:ARG:NE	4:D:166:GLU:OE2	2.36	0.57
1:A:1102:A:O2'	1:A:1103:C:H5'	2.05	0.57
1:A:1534:A:C1'	22:V:58:LYS:HG3	2.34	0.57
20:T:5:LEU:C	20:T:7:LYS:H	2.07	0.57
1:A:1217:C:P	15:O:9:ARG:HH21	2.28	0.57
2:B:54:LYS:HB3	2:B:58:GLY:HA2	1.87	0.56
19:S:74:HIS:HD2	19:S:75:GLN:H	1.53	0.56
1:A:1518:MA6:N7	1:A:1518:MA6:H93	2.21	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.40	0.56
12:L:17:SER:HA	12:L:79:ILE:HA	1.87	0.56
22:V:29:LEU:O	22:V:32:VAL:HG22	2.04	0.56
1:A:744:C:H2'	1:A:745:G:H8	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:U:H2'	1:A:1415:G:H8	1.71	0.56
1:A:87:C:H2'	1:A:88:U:C6	2.41	0.56
1:A:408:A:O3'	5:E:23:SER:OG	2.22	0.56
12:L:111:THR:HG22	22:V:3:VAL:HG12	1.87	0.56
1:A:1532:U:C2'	1:A:1533:C:H5'	2.36	0.56
2:B:69:ASP:OD1	2:B:86:ARG:NH1	2.29	0.56
14:N:42:ASP:OD1	14:N:42:ASP:N	2.38	0.56
1:A:93:U:H2'	1:A:94:G:H5"	1.87	0.56
1:A:346:G:N3	1:A:346:G:C3'	2.68	0.56
1:A:255:G:H2'	1:A:256:U:H6	1.71	0.55
1:A:1486:G:H2'	1:A:1487:G:C8	2.42	0.55
12:L:16:VAL:O	12:L:17:SER:OG	2.23	0.55
1:A:1239:A:H62	1:A:1299:A:N6	2.04	0.55
1:A:544:G:OP1	5:E:56:ARG:NH1	2.39	0.55
5:E:98:LEU:O	5:E:102:VAL:HG12	2.07	0.55
3:C:18:HIS:H	3:C:189:THR:HG22	1.71	0.55
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.36	0.55
7:G:4:TYR:CD2	7:G:71:ILE:HG13	2.42	0.55
11:K:66:GLU:HB3	15:O:99:ALA:HB2	1.88	0.55
21:U:28:MET:SD	21:U:67:ILE:HD12	2.47	0.55
11:K:26:VAL:HG23	11:K:36:VAL:HG11	1.87	0.55
1:A:1071:C:H2'	1:A:1072:G:H8	1.72	0.55
1:A:77:A:H8	1:A:77:A:P	2.30	0.54
1:A:1255:G:O2'	1:A:1258:G:N3	2.37	0.54
16:P:26:GLU:OE1	16:P:26:GLU:N	2.38	0.54
1:A:542:G:OP1	5:E:10:LYS:NZ	2.39	0.54
1:A:662:U:H2'	1:A:663:A:C8	2.42	0.54
1:A:1305:G:H21	1:A:1332:A:H2	1.53	0.54
1:A:350:G:H2'	1:A:351:G:C8	2.42	0.54
1:A:413:G:N2	1:A:428:G:H1'	2.23	0.54
15:O:24:ARG:NH1	15:O:55:SER:OG	2.41	0.54
6:F:105:ILE:HD11	6:F:112:ARG:HA	1.88	0.54
22:V:51:SER:HA	22:V:54:LYS:HE3	1.90	0.54
1:A:405:U:O4	5:E:2:ALA:N	2.41	0.54
1:A:422:C:OP2	1:A:422:C:H2'	2.08	0.54
1:A:977:A:H3'	1:A:977:A:N3	2.23	0.54
1:A:996:A:H2'	1:A:997:U:O4'	2.08	0.54
1:A:1320:C:C2	20:T:72:GLY:HA3	2.42	0.54
1:A:1412:C:H2'	1:A:1413:A:C8	2.42	0.54
5:E:99:ASP:OD2	5:E:133:ALA:HB1	2.08	0.54
1:A:204:U:H2'	1:A:205:A:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:C:H2'	1:A:1536:C:H6	1.73	0.54
4:D:134:MET:HB2	4:D:151:VAL:HG21	1.89	0.54
7:G:29:ILE:HD13	7:G:64:VAL:HG11	1.90	0.54
7:G:50:PRO:HD3	19:S:75:GLN:HB2	1.89	0.54
19:S:37:GLY:O	19:S:63:ARG:NH2	2.40	0.54
21:U:42:GLY:HA2	21:U:86:LEU:HD11	1.91	0.54
1:A:474:G:C8	1:A:474:G:H5"	2.42	0.53
1:A:958:A:C5	20:T:55:ARG:NH1	2.76	0.53
1:A:967:5MC:H5"	1:A:968:A:H2'	1.89	0.53
1:A:958:A:C4	20:T:55:ARG:HD3	2.43	0.53
6:F:34:THR:HG22	6:F:52:LYS:HG3	1.89	0.53
23:X:17:U:H3'	23:X:18:G:H8	1.72	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.53
1:A:745:G:H2'	1:A:746:A:C8	2.44	0.53
1:A:1405:G:O2'	1:A:1518:MA6:O2'	2.24	0.53
2:B:69:ASP:O	2:B:86:ARG:NH1	2.42	0.53
1:A:74:A:H2'	1:A:75:G:C4'	2.38	0.53
14:N:90:ARG:HB2	14:N:97:VAL:HG23	1.90	0.53
18:R:25:ILE:HB	18:R:42:THR:HG23	1.90	0.53
1:A:413:G:H21	1:A:428:G:H1'	1.73	0.53
3:C:95:ARG:CZ	3:C:95:ARG:HB3	2.37	0.53
8:H:5:ARG:HG2	8:H:6:VAL:H	1.74	0.53
1:A:380:G:N2	1:A:383:A:OP2	2.38	0.53
1:A:1004:A:OP1	1:A:1025:U:N3	2.39	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.53
3:C:207:ILE:HA	3:C:210:VAL:HG22	1.90	0.53
5:E:26:ARG:HH21	5:E:30:THR:HG22	1.73	0.53
1:A:683:G:H1	1:A:707:U:H3	1.58	0.52
2:B:45:GLU:OE2	3:C:208:ARG:HG3	2.08	0.52
16:P:78:TYR:OH	16:P:89:ARG:O	2.18	0.52
17:Q:5:ARG:HH12	17:Q:24:SER:HA	1.74	0.52
21:U:39:ILE:HD11	21:U:83:ILE:HG13	1.91	0.52
1:A:74:A:H2'	1:A:75:G:O4'	2.09	0.52
1:A:202:G:HO2'	1:A:468:A:H8	1.58	0.52
1:A:1403:C:O5'	1:A:1403:C:C6	2.60	0.52
5:E:15:GLU:OE1	5:E:63:ARG:NH1	2.43	0.52
1:A:1014:A:C2	1:A:1219:A:H1'	2.45	0.52
1:A:1431:A:H2	1:A:1469:C:H41	1.57	0.52
11:K:36:VAL:HG22	11:K:38:GLY:H	1.74	0.52
15:O:52:PRO:O	15:O:55:SER:OG	2.22	0.52
1:A:1347:G:O6	10:J:12:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:LEU:HB3	3:C:133:GLU:CG	2.40	0.52
1:A:75:G:H8	1:A:75:G:H5"	1.69	0.52
10:J:21:ILE:HG12	10:J:63:LEU:HD22	1.91	0.52
1:A:89:U:H2'	1:A:90:C:C6	2.45	0.52
1:A:1052:U:O2'	1:A:1055:A:OP2	2.18	0.52
1:A:1078:U:H1'	6:F:135:ASN:HD21	1.76	0.52
1:A:1078:U:HO2'	1:A:1079:G:P	2.33	0.52
1:A:1391:U:H2'	1:A:1392:G:C8	2.45	0.52
12:L:22:HIS:HB2	12:L:33:THR:HG23	1.92	0.52
1:A:77:A:C8	1:A:77:A:OP2	2.63	0.51
1:A:1498:UR3:H5"	1:A:1519:MA6:H102	1.91	0.51
13:M:110:ARG:HB2	13:M:119:VAL:HG21	1.92	0.51
7:G:19:PRO:O	7:G:23:GLU:HG2	2.10	0.51
1:A:463:U:H2'	1:A:463:U:O2	2.09	0.51
3:C:68:LEU:HD11	3:C:92:VAL:HG23	1.92	0.51
5:E:190:ASP:OD1	5:E:190:ASP:N	2.44	0.51
12:L:110:ILE:HG22	22:V:19:PHE:CE1	2.45	0.51
1:A:81:A:H2'	1:A:82:G:C8	2.46	0.51
1:A:110:C:O2'	17:Q:25:ARG:O	2.28	0.51
7:G:86:ARG:NH1	19:S:64:TYR:O	2.43	0.51
1:A:337:G:H2'	1:A:338:A:C8	2.45	0.51
6:F:76:LEU:HD11	6:F:120:VAL:HG22	1.92	0.51
5:E:198:HIS:CD2	5:E:198:HIS:H	2.27	0.51
11:K:3:ASN:OD1	11:K:4:GLN:N	2.42	0.51
1:A:514:C:H2'	1:A:515:G:H8	1.75	0.51
6:F:38:VAL:HG12	6:F:117:VAL:HG11	1.93	0.51
1:A:501:C:H2'	1:A:502:A:H8	1.76	0.51
1:A:1029:U:O2'	1:A:1032:G:O6	2.23	0.51
1:A:160:A:H2'	1:A:161:A:O4'	2.10	0.51
1:A:758:C:H4'	1:A:880:C:H4'	1.92	0.51
1:A:1151:A:HO2'	1:A:1152:A:H8	1.55	0.50
5:E:175:ALA:O	5:E:178:MET:HG2	2.11	0.50
1:A:216:U:H1'	1:A:466:A:N6	2.25	0.50
2:B:115:LYS:HA	2:B:120:PHE:HA	1.94	0.50
5:E:87:GLY:HA3	5:E:197:GLU:HG3	1.92	0.50
14:N:9:ILE:HG23	14:N:18:ALA:HB1	1.92	0.50
1:A:235:C:H2'	1:A:236:A:C8	2.46	0.50
1:A:347:G:OP2	1:A:347:G:C8	2.63	0.50
1:A:958:A:N7	20:T:55:ARG:NH1	2.59	0.50
2:B:75:VAL:O	2:B:75:VAL:CG2	2.60	0.50
9:I:112:THR:HG23	9:I:115:ALA:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:C:P	14:N:90:ARG:HH22	2.34	0.50
1:A:1314:C:H2'	1:A:1315:U:C6	2.47	0.50
1:A:56:U:H2'	1:A:57:G:H8	1.75	0.50
1:A:923:A:H2'	1:A:924:C:C6	2.46	0.50
1:A:1048:G:H5"	15:O:3:LYS:HD2	1.94	0.50
1:A:1305:G:N2	1:A:1331:G:O2'	2.32	0.50
3:C:94:HIS:O	3:C:95:ARG:C	2.50	0.50
3:C:111:ILE:HD12	3:C:152:LYS:HA	1.94	0.50
1:A:135:C:N3	17:Q:1:MET:HB2	2.27	0.50
1:A:216:U:H2'	1:A:217:C:C6	2.46	0.50
2:B:31:ILE:HG12	2:B:36:VAL:HG13	1.94	0.50
1:A:1071:C:H2'	1:A:1072:G:C8	2.47	0.50
1:A:1391:U:H2'	1:A:1392:G:H8	1.77	0.50
17:Q:4:ILE:HB	17:Q:67:ILE:HD13	1.94	0.50
1:A:1134:G:O6	1:A:1141:C:N4	2.45	0.49
1:A:1098:C:O2'	22:V:71:TYR:OXT	2.23	0.49
1:A:1106:G:O2'	4:D:169:ARG:NH1	2.41	0.49
4:D:110:GLU:HB2	4:D:144:LEU:HD12	1.93	0.49
1:A:945:G:C2	1:A:946:A:C8	3.01	0.49
1:A:1427:C:H2'	1:A:1428:A:C8	2.46	0.49
1:A:1464:U:H2'	1:A:1465:A:H8	1.77	0.49
10:J:65:ILE:HD13	10:J:79:ILE:HG23	1.94	0.49
8:H:57:SER:HB3	8:H:60:GLU:HB2	1.93	0.49
7:G:12:PRO:HB3	7:G:56:LYS:O	2.11	0.49
14:N:104:THR:OG1	14:N:105:ASN:N	2.46	0.49
12:L:114:THR:O	19:S:73:ARG:NH1	2.46	0.49
8:H:63:GLU:O	8:H:67:GLU:HG3	2.13	0.49
8:H:68:ASN:O	8:H:138:ARG:NH2	2.45	0.49
10:J:30:ILE:HG12	10:J:65:ILE:HB	1.95	0.49
1:A:251:G:H4'	1:A:252:U:O5'	2.11	0.49
1:A:518:C:H5'	1:A:519:C:C6	2.47	0.49
1:A:744:C:H2'	1:A:745:G:C8	2.46	0.49
1:A:1119:C:H2'	1:A:1120:C:H6	1.76	0.49
3:C:129:LEU:HB3	3:C:133:GLU:HG2	1.94	0.49
6:F:157:ARG:NH2	9:I:43:GLU:OE1	2.46	0.49
13:M:67:ILE:HD13	13:M:74:LEU:HD22	1.94	0.49
1:A:562:U:C5	13:M:15:LYS:HG2	2.48	0.49
1:A:1534:A:N9	22:V:58:LYS:HG3	2.28	0.49
8:H:69:VAL:HG21	8:H:104:ILE:HD11	1.94	0.49
12:L:18:ASP:HB2	12:L:37:ARG:HH21	1.78	0.49
1:A:235:C:H2'	1:A:236:A:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:A:H2'	1:A:461:A:C8	2.47	0.48
1:A:465:A:H3'	1:A:466:A:H8	1.78	0.48
1:A:826:C:H5'	9:I:13:ARG:CZ	2.43	0.48
1:A:868:C:H2'	1:A:869:G:O4'	2.12	0.48
1:A:949:A:N7	14:N:105:ASN:ND2	2.61	0.48
1:A:1007:U:OP1	15:O:19:LYS:NZ	2.41	0.48
1:A:1498:UR3:OP2	1:A:1498:UR3:H6	2.13	0.48
21:U:67:ILE:HG12	21:U:71:LYS:HD3	1.94	0.48
1:A:745:G:H2'	1:A:746:A:H8	1.78	0.48
1:A:1279:G:C8	1:A:1279:G:H3'	2.48	0.48
1:A:677:U:O2	1:A:777:A:O2'	2.31	0.48
1:A:932:C:H5"	8:H:4:ARG:HD3	1.94	0.48
6:F:80:THR:HG23	6:F:122:ASN:O	2.13	0.48
11:K:52:LEU:HD21	11:K:59:LYS:HA	1.95	0.48
15:O:46:LEU:O	15:O:50:THR:HG23	2.14	0.48
1:A:80:A:C6	1:A:81:A:N6	2.82	0.48
1:A:89:U:H2'	1:A:90:C:H6	1.77	0.48
1:A:1314:C:H2'	1:A:1315:U:H6	1.79	0.48
1:A:1403:C:H2'	1:A:1404:C:C6	2.48	0.48
1:A:1152:A:OP1	11:K:70:HIS:ND1	2.43	0.48
14:N:7:ILE:HD11	14:N:22:ILE:HG12	1.95	0.48
15:O:41:ARG:NH2	20:T:6:LYS:O	2.46	0.48
1:A:523:A:N6	13:M:87:VAL:HG12	2.29	0.48
1:A:923:A:H2'	1:A:924:C:H6	1.77	0.48
1:A:976:G:OP2	1:A:1358:U:O2'	2.31	0.48
1:A:1402:4OC:H6	1:A:1402:4OC:O5'	2.14	0.48
1:A:384:G:H2'	1:A:385:C:C6	2.48	0.48
5:E:6:GLY:O	5:E:8:LYS:NZ	2.42	0.48
1:A:180:U:H2'	1:A:181:A:H5'	1.96	0.48
1:A:734:G:O2'	19:S:60:LYS:HD3	2.14	0.48
1:A:957:U:H4'	20:T:79:THR:HG23	1.94	0.48
22:V:7:ARG:O	22:V:10:GLU:HG2	2.13	0.48
1:A:1426:G:H1	1:A:1474:U:H3	1.60	0.48
1:A:1530:G:H2'	1:A:1531:A:H8	1.77	0.48
1:A:113:G:H1'	1:A:354:G:H5'	1.96	0.48
1:A:1010:U:H2'	1:A:1011:C:H6	1.79	0.48
22:V:29:LEU:O	22:V:32:VAL:CG2	2.61	0.48
1:A:371:A:H2'	1:A:372:C:O4'	2.14	0.47
1:A:1183:U:O2'	1:A:1185:G:OP2	2.31	0.47
1:A:820:U:H4'	1:A:821:G:OP2	2.14	0.47
1:A:883:C:H2'	1:A:884:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:C:C3'	1:A:999:C:C6	2.97	0.47
1:A:1077:G:N1	1:A:1080:A:OP2	2.43	0.47
1:A:1540:U:C2	23:X:6:G:C2	3.02	0.47
1:A:728:A:H2'	1:A:729:A:C8	2.48	0.47
1:A:1124:G:N2	1:A:1125:U:O4	2.38	0.47
1:A:1407:5MC:OP2	1:A:1407:5MC:HM51	2.14	0.47
1:A:1141:C:O2'	1:A:1142:G:H8	1.96	0.47
1:A:1279:G:C8	1:A:1279:G:C3'	2.97	0.47
12:L:89:PRO:HA	22:V:29:LEU:HD22	1.96	0.47
2:B:11:GLU:O	2:B:14:LYS:HG3	2.14	0.47
13:M:33:VAL:HG22	13:M:79:VAL:HG12	1.97	0.47
22:V:29:LEU:HA	22:V:32:VAL:CG2	2.43	0.47
1:A:500:G:H2'	1:A:501:C:C6	2.50	0.47
1:A:1519:MA6:H5"	1:A:1520:C:O4'	2.15	0.47
22:V:29:LEU:CA	22:V:32:VAL:HG22	2.45	0.47
1:A:87:C:H2'	1:A:88:U:H6	1.78	0.47
1:A:254:G:N2	18:R:18:GLU:OE2	2.44	0.47
1:A:335:C:H2'	1:A:336:A:H8	1.79	0.47
1:A:536:C:H2'	1:A:537:G:H8	1.80	0.47
1:A:1102:A:C2'	1:A:1103:C:H5'	2.45	0.47
2:B:52:GLN:O	2:B:90:LYS:NZ	2.37	0.47
11:K:7:ARG:NH1	11:K:73:LEU:HD21	2.29	0.47
4:D:69:HIS:HA	4:D:104:ALA:O	2.14	0.47
21:U:35:VAL:HG22	21:U:50:ALA:HB1	1.96	0.47
1:A:1266:G:N2	1:A:1269:A:OP2	2.36	0.47
1:A:1319:A:P	20:T:3:ARG:HD2	2.54	0.47
7:G:45:ARG:O	7:G:56:LYS:HA	2.14	0.47
1:A:21:G:H2'	1:A:22:G:C8	2.50	0.47
1:A:955:U:O2	20:T:83:HIS:HE1	1.98	0.47
1:A:966:2MG:C8	1:A:966:2MG:C5'	2.90	0.47
1:A:1137:C:H1'	1:A:1138:G:N2	2.30	0.47
1:A:1477:U:H2'	1:A:1478:U:C6	2.50	0.47
12:L:87:LYS:HG3	12:L:115:PRO:HD3	1.96	0.47
1:A:35:G:H2'	1:A:36:C:C6	2.49	0.46
1:A:1008:U:H2'	1:A:1009:U:C6	2.50	0.46
1:A:1319:A:OP2	20:T:3:ARG:HD2	2.15	0.46
8:H:116:MET:HA	8:H:119:ARG:HE	1.80	0.46
9:I:32:LEU:O	9:I:36:ILE:HG13	2.14	0.46
10:J:41:ARG:HD3	10:J:43:THR:HB	1.97	0.46
18:R:19:LYS:NZ	18:R:50:ASN:H	2.12	0.46
20:T:6:LYS:O	20:T:6:LYS:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:U:H2'	1:A:802:A:H8	1.81	0.46
1:A:982:U:H4'	1:A:983:A:O4'	2.14	0.46
1:A:999:C:C6	1:A:999:C:H3'	2.49	0.46
1:A:436:C:H2'	1:A:437:U:C6	2.50	0.46
1:A:1495:U:H2'	1:A:1496:C:C6	2.50	0.46
3:C:21:ARG:HG3	3:C:22:TYR:CE2	2.51	0.46
10:J:88:MET:SD	10:J:95:ARG:NE	2.89	0.46
1:A:536:C:H2'	1:A:537:G:C8	2.50	0.46
1:A:1040:U:H2'	1:A:1041:G:C8	2.51	0.46
3:C:125:THR:HA	3:C:128:LYS:NZ	2.30	0.46
16:P:6:GLU:OE1	16:P:6:GLU:N	2.43	0.46
23:X:11:U:H1'	23:X:12:A:OP2	2.14	0.46
1:A:501:C:H2'	1:A:502:A:C8	2.50	0.46
1:A:1008:U:H2'	1:A:1009:U:H6	1.80	0.46
1:A:1435:G:H2'	1:A:1436:U:C6	2.51	0.46
4:D:114:LYS:HB2	4:D:185:ASN:ND2	2.30	0.46
1:A:62:U:O2'	1:A:379:C:O2	2.34	0.46
1:A:1140:C:HO2'	1:A:1141:C:P	2.39	0.46
5:E:50:ASP:OD1	5:E:50:ASP:N	2.39	0.46
11:K:39:PRO:HA	11:K:73:LEU:O	2.15	0.46
1:A:104:G:N7	21:U:9:LYS:NZ	2.54	0.46
1:A:736:C:H2'	1:A:737:C:H6	1.79	0.46
14:N:16:VAL:HG13	14:N:17:ILE:HD12	1.97	0.46
18:R:44:LEU:HD23	18:R:73:TRP:CD1	2.50	0.46
1:A:390:U:H2'	1:A:391:G:H8	1.81	0.46
1:A:866:C:C4	1:A:867:G:H1'	2.51	0.46
1:A:1004:A:H2'	1:A:1005:A:O4'	2.15	0.46
1:A:1078:U:O2'	1:A:1079:G:OP1	2.25	0.46
2:B:112:ILE:HA	2:B:122:VAL:HA	1.97	0.46
4:D:8:ASN:O	4:D:12:LEU:HG	2.16	0.46
6:F:25:VAL:HG12	6:F:26:LYS:H	1.81	0.46
1:A:706:A:O2'	12:L:33:THR:HG21	2.16	0.46
1:A:1166:G:O2'	1:A:1169:A:N6	2.45	0.46
1:A:1422:G:H1	1:A:1478:U:H3	1.64	0.46
7:G:38:ARG:HB3	7:G:63:ASN:HB3	1.98	0.46
20:T:11:ILE:HD13	20:T:16:LEU:HD13	1.98	0.46
1:A:75:G:C8	1:A:75:G:C4'	3.00	0.45
1:A:299:G:H2'	1:A:300:A:C8	2.51	0.45
1:A:769:G:H4'	1:A:1513:A:H4'	1.98	0.45
1:A:932:C:H2'	1:A:933:G:C8	2.51	0.45
1:A:1436:U:H2'	1:A:1437:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:GLN:HG2	5:E:154:ARG:HH22	1.81	0.45
5:E:188:ARG:NH2	5:E:195:ILE:O	2.49	0.45
1:A:875:U:O2'	9:I:15:ARG:NH1	2.48	0.45
1:A:736:C:H2'	1:A:737:C:C6	2.50	0.45
1:A:1330:U:H4'	14:N:23:TYR:CE2	2.51	0.45
3:C:128:LYS:H	3:C:128:LYS:HD2	1.82	0.45
11:K:50:THR:HG23	11:K:64:GLN:HG2	1.99	0.45
1:A:81:A:H2'	1:A:82:G:H8	1.81	0.45
1:A:440:C:C2	1:A:441:A:C8	3.05	0.45
1:A:1101:A:H5"	3:C:171:ILE:HD11	1.98	0.45
1:A:1455:G:H2'	1:A:1456:A:H8	1.82	0.45
1:A:1532:U:O2'	1:A:1533:C:H5'	2.16	0.45
5:E:50:ASP:O	5:E:53:VAL:HG22	2.17	0.45
5:E:161:LEU:O	5:E:165:ARG:HG3	2.16	0.45
14:N:40:ALA:O	14:N:43:VAL:HG12	2.15	0.45
1:A:404:G:O6	5:E:2:ALA:N	2.49	0.45
1:A:1319:A:C8	1:A:1323:G:C5	3.05	0.45
4:D:64:ILE:HG22	4:D:97:VAL:HG23	1.99	0.45
14:N:107:ARG:NH2	14:N:113:ARG:HA	2.32	0.45
8:H:93:PRO:HA	8:H:96:ARG:HD2	1.99	0.45
23:X:11:U:H4'	23:X:12:A:O5'	2.16	0.45
1:A:73:C:H2'	1:A:74:A:O4'	2.16	0.45
1:A:544:G:OP2	5:E:63:ARG:NH2	2.49	0.45
5:E:102:VAL:HG23	5:E:107:PHE:HB2	1.98	0.45
20:T:63:THR:OG1	20:T:64:ASP:N	2.50	0.45
1:A:591:U:H2'	1:A:592:G:H8	1.81	0.45
1:A:1086:U:H2'	1:A:1087:G:H8	1.82	0.45
6:F:136:VAL:O	6:F:140:THR:HG22	2.17	0.45
8:H:53:ARG:HH22	8:H:121:ALA:HB1	1.80	0.45
16:P:17:ARG:HD2	16:P:17:ARG:O	2.16	0.45
17:Q:18:GLN:HE21	17:Q:35:ARG:NH2	2.15	0.45
1:A:855:U:H2'	1:A:856:C:H6	1.82	0.45
1:A:881:G:P	13:M:9:ARG:HH22	2.39	0.45
1:A:1436:U:H2'	1:A:1437:A:C8	2.51	0.45
16:P:80:GLN:HE22	16:P:84:ARG:NE	2.15	0.45
1:A:34:C:H2'	1:A:35:G:H8	1.82	0.45
1:A:160:A:N6	1:A:347:G:H1'	2.32	0.45
1:A:826:C:H5'	9:I:13:ARG:NH2	2.31	0.45
1:A:1158:C:C4	1:A:1160:G:C8	3.05	0.45
1:A:1317:C:O2	20:T:37:ARG:NH2	2.50	0.45
1:A:1318:A:H5'	20:T:10:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1498:UR3:H4'	1:A:1519:MA6:N1	2.32	0.45
5:E:170:TRP:CD2	5:E:186:PRO:HB3	2.53	0.45
10:J:23:PRO:HA	10:J:61:LEU:HD23	1.98	0.45
21:U:62:ALA:HA	21:U:67:ILE:O	2.17	0.45
1:A:2:A:H8	1:A:2:A:OP2	2.00	0.44
1:A:254:G:OP1	18:R:70:THR:HG22	2.17	0.44
1:A:324:G:N2	1:A:326:G:H3'	2.32	0.44
18:R:14:SER:HB3	18:R:22:VAL:CG1	2.48	0.44
1:A:458:U:H6	1:A:458:U:C5'	2.26	0.44
1:A:689:C:OP1	12:L:29:ASN:ND2	2.46	0.44
1:A:1217:C:OP1	15:O:9:ARG:NE	2.37	0.44
1:A:1320:C:O2	20:T:72:GLY:HA3	2.17	0.44
2:B:53:PHE:HD2	2:B:62:ILE:HD11	1.61	0.44
5:E:41:HIS:HB3	5:E:44:ARG:HE	1.82	0.44
5:E:177:LYS:HD2	5:E:177:LYS:HA	1.74	0.44
12:L:35:THR:OG1	12:L:36:ASP:N	2.51	0.44
1:A:613:C:H2'	1:A:614:C:C6	2.52	0.44
1:A:978:A:C5	1:A:1319:A:C2	3.05	0.44
1:A:1287:A:H2'	1:A:1288:A:C8	2.52	0.44
1:A:1536:C:H2'	1:A:1537:U:C6	2.53	0.44
18:R:9:GLN:HE21	18:R:60:GLU:HG3	1.83	0.44
1:A:569:C:H5"	1:A:570:G:OP1	2.18	0.44
1:A:879:C:H2'	1:A:880:C:C6	2.52	0.44
1:A:886:G:H2'	1:A:887:G:O4'	2.18	0.44
1:A:1519:MA6:H8	1:A:1519:MA6:C5'	2.47	0.44
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.84	0.44
19:S:74:HIS:CD2	19:S:75:GLN:H	2.33	0.44
1:A:474:G:H5"	1:A:474:G:H8	1.82	0.44
1:A:538:G:OP2	13:M:112:GLN:HG3	2.17	0.44
1:A:653:U:HO2'	1:A:654:G:H8	1.65	0.44
1:A:695:A:H2'	1:A:696:A:C8	2.53	0.44
1:A:946:A:O2'	1:A:1333:A:N3	2.40	0.44
3:C:89:GLN:NE2	3:C:225:ARG:HD2	2.32	0.44
3:C:95:ARG:NH2	3:C:97:LEU:HD23	2.33	0.44
23:X:8:A:H2'	23:X:9:G:C8	2.53	0.44
1:A:1072:G:H2'	1:A:1073:U:C6	2.52	0.44
1:A:1356:G:H2'	1:A:1357:A:H8	1.79	0.44
1:A:1413:A:H2	1:A:1487:G:H22	1.64	0.44
3:C:84:ALA:HA	3:C:87:CYS:SG	2.58	0.44
8:H:79:ARG:HA	8:H:84:THR:HA	1.99	0.44
18:R:48:ASP:OD1	18:R:48:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:G:H2'	1:A:362:G:O4'	2.18	0.44
1:A:1279:G:H3'	1:A:1279:G:H8	1.83	0.44
5:E:171:LEU:HD23	5:E:182:PHE:HA	2.00	0.44
10:J:40:GLY:O	10:J:45:ARG:NH1	2.51	0.44
20:T:5:LEU:C	20:T:7:LYS:N	2.71	0.44
1:A:178:C:C2	1:A:179:A:C8	3.06	0.44
1:A:184:G:H2'	1:A:185:U:C6	2.53	0.44
2:B:98:LEU:HD23	2:B:98:LEU:HA	1.84	0.44
10:J:123:ARG:NH1	10:J:124:ARG:O	2.48	0.44
13:M:72:HIS:HA	13:M:99:ARG:HH22	1.83	0.44
21:U:31:PHE:O	21:U:35:VAL:HG23	2.18	0.44
3:C:223:GLU:HG3	3:C:224:GLY:N	2.33	0.43
6:F:15:LEU:HD23	6:F:15:LEU:H	1.82	0.43
9:I:10:MET:HG3	9:I:27:MET:SD	2.58	0.43
10:J:84:THR:HG23	10:J:98:LEU:HD13	1.99	0.43
1:A:1442:G:H2'	1:A:1443:C:C6	2.53	0.43
2:B:13:LEU:HD23	2:B:13:LEU:HA	1.87	0.43
12:L:116:ILE:HD12	22:V:31:GLU:HG2	2.00	0.43
15:O:26:GLU:HG3	15:O:27:LEU:N	2.33	0.43
1:A:264:C:O2'	18:R:66:PRO:O	2.36	0.43
1:A:413:G:H1'	1:A:428:G:H21	1.83	0.43
1:A:467:U:O2	1:A:467:U:H5"	2.17	0.43
1:A:999:C:H6	1:A:999:C:C5'	2.30	0.43
1:A:1534:A:H2'	1:A:1535:C:O4'	2.17	0.43
16:P:18:ASP:OD1	16:P:18:ASP:N	2.49	0.43
1:A:681:A:H2'	1:A:682:G:O4'	2.18	0.43
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.43
1:A:1038:C:H2'	1:A:1039:G:H8	1.83	0.43
22:V:32:VAL:O	22:V:36:GLU:HG3	2.18	0.43
1:A:180:U:C2'	1:A:181:A:H5'	2.48	0.43
1:A:335:C:H2'	1:A:336:A:C8	2.54	0.43
1:A:552:U:C2	1:A:553:A:C8	3.07	0.43
1:A:936:C:C2	1:A:937:A:C8	3.06	0.43
1:A:996:A:N7	1:A:1046:A:O2'	2.50	0.43
1:A:1001:C:H2'	1:A:1002:G:H8	1.83	0.43
3:C:59:LYS:HE3	3:C:59:LYS:HB2	1.92	0.43
9:I:66:PHE:CD2	9:I:67:GLN:HG3	2.53	0.43
1:A:579:A:H2'	1:A:580:C:C6	2.54	0.43
2:B:63:GLN:HG2	2:B:64:VAL:H	1.84	0.43
1:A:462:G:H3'	1:A:463:U:H6	1.84	0.43
1:A:471:U:H2'	1:A:472:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:U:OP1	5:E:44:ARG:NH2	2.52	0.43
1:A:1496:C:H2'	1:A:1497:G:O4'	2.19	0.43
21:U:2:ALA:HB3	21:U:8:LYS:HG2	2.01	0.43
1:A:687:A:C2	1:A:704:A:C5	3.07	0.43
6:F:86:LYS:HE3	6:F:86:LYS:HB3	1.89	0.43
10:J:17:ALA:HB2	10:J:67:VAL:HG13	2.01	0.43
1:A:390:U:H2'	1:A:391:G:C8	2.53	0.43
1:A:1040:U:H2'	1:A:1041:G:H8	1.83	0.43
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.43
1:A:1278:G:H4'	1:A:1279:G:O5'	2.18	0.43
11:K:85:ASP:O	11:K:89:ARG:HG2	2.19	0.43
1:A:842:U:H4'	1:A:846:G:C6	2.54	0.43
1:A:1074:G:O2'	1:A:1101:A:N1	2.40	0.43
1:A:1401:G:H2'	1:A:1402:4OC:O4'	2.19	0.43
1:A:1521:C:H2'	1:A:1522:U:C6	2.53	0.43
13:M:44:LYS:HE3	13:M:44:LYS:HB2	1.71	0.43
1:A:253:A:H2'	1:A:254:G:C8	2.54	0.42
1:A:538:G:H5"	13:M:111:LYS:HB2	2.01	0.42
1:A:608:A:H2'	1:A:609:A:O4'	2.19	0.42
1:A:1120:C:H2'	1:A:1121:U:H6	1.84	0.42
1:A:1319:A:C8	1:A:1323:G:C6	3.07	0.42
20:T:30:PRO:HA	20:T:48:THR:HG23	2.02	0.42
23:X:19:U:H2'	23:X:20:U:O4'	2.18	0.42
1:A:1236:A:H2'	1:A:1237:C:C6	2.54	0.42
1:A:1416:G:H2'	1:A:1417:G:O4'	2.18	0.42
1:A:1137:C:O2	1:A:1138:G:N2	2.52	0.42
5:E:70:ARG:CD	5:E:73:ARG:HH21	2.32	0.42
7:G:42:TRP:HZ2	19:S:24:LYS:HD2	1.84	0.42
1:A:91:U:C2'	1:A:92:U:H5'	2.48	0.42
1:A:279:A:H5"	1:A:281:G:O4'	2.18	0.42
1:A:362:G:N2	1:A:365:U:OP2	2.46	0.42
1:A:1010:U:H2'	1:A:1011:C:C6	2.53	0.42
5:E:102:VAL:HA	5:E:105:MET:HG2	2.01	0.42
15:O:15:ALA:HA	15:O:18:ASP:OD2	2.19	0.42
1:A:204:U:C2	1:A:205:A:C8	3.08	0.42
1:A:384:G:H2'	1:A:385:C:H6	1.84	0.42
1:A:1029:U:H4'	1:A:1030:U:H5	1.85	0.42
3:C:57:LEU:HD13	3:C:217:VAL:HG13	2.01	0.42
18:R:21:ILE:HG13	18:R:46:VAL:HB	2.00	0.42
1:A:321:A:H2'	1:A:322:C:C6	2.55	0.42
1:A:1403:C:H2'	1:A:1404:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:A:N6	1:A:1482:G:O2'	2.50	0.42
7:G:81:ASN:HB3	7:G:84:VAL:HG23	2.02	0.42
15:O:26:GLU:O	15:O:30:ILE:HG22	2.19	0.42
18:R:46:VAL:HG21	18:R:61:ILE:HG21	2.02	0.42
1:A:337:G:H2'	1:A:338:A:H8	1.85	0.42
1:A:1201:A:H4'	1:A:1202:U:H5"	2.02	0.42
1:A:1425:U:H2'	1:A:1426:G:H8	1.84	0.42
1:A:1536:C:C2	23:X:10:G:C2	3.08	0.42
2:B:69:ASP:H	2:B:86:ARG:NH1	2.18	0.42
5:E:177:LYS:HB3	5:E:179:GLU:HG2	2.01	0.42
6:F:153:VAL:HG11	9:I:99:LEU:HD22	2.02	0.42
10:J:46:MET:HE2	10:J:46:MET:HB3	1.85	0.42
12:L:16:VAL:HG23	12:L:17:SER:H	1.85	0.42
14:N:52:GLN:O	14:N:55:THR:OG1	2.33	0.42
1:A:1507:A:H2'	1:A:1508:A:C8	2.54	0.42
2:B:51:GLU:HA	2:B:54:LYS:HD2	2.00	0.42
3:C:84:ALA:CB	3:C:91:PHE:HB3	2.49	0.42
4:D:20:SER:HB2	4:D:40:ARG:HH22	1.85	0.42
1:A:846:G:H2'	1:A:847:G:C8	2.54	0.42
1:A:970:C:N4	10:J:130:ARG:OXT	2.53	0.42
1:A:1236:A:H4'	1:A:1304:G:H4'	2.01	0.42
1:A:1323:G:H2'	1:A:1324:A:H8	1.81	0.42
1:A:1406:U:H2'	1:A:1407:5MC:O4'	2.20	0.42
21:U:24:ARG:HA	21:U:24:ARG:HD3	1.80	0.42
22:V:32:VAL:HG23	22:V:33:ARG:N	2.35	0.42
1:A:704:A:C4	1:A:705:G:C8	3.08	0.42
1:A:932:C:OP2	8:H:3:ARG:HD3	2.20	0.42
1:A:996:A:C2	1:A:997:U:H1'	2.55	0.42
1:A:1446:A:O2'	1:A:1447:A:H5'	2.20	0.42
2:B:75:VAL:O	2:B:75:VAL:HG22	2.19	0.42
1:A:846:G:H2'	1:A:847:G:H8	1.85	0.41
1:A:908:A:H2'	1:A:909:A:H8	1.84	0.41
1:A:1130:A:H2'	1:A:1131:G:C8	2.51	0.41
1:A:1455:G:H2'	1:A:1456:A:C8	2.55	0.41
1:A:28:A:O2'	1:A:296:U:OP1	2.30	0.41
1:A:108:G:H5"	1:A:109:A:H5"	2.02	0.41
1:A:284:C:H2'	1:A:285:C:H6	1.86	0.41
1:A:1317:C:OP2	15:O:28:LYS:HD3	2.21	0.41
1:A:1431:A:O2'	1:A:1432:G:H5'	2.20	0.41
19:S:70:TYR:HB2	19:S:74:HIS:CE1	2.55	0.41
1:A:554:A:H2'	1:A:555:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:A:H4'	1:A:560:A:H3'	2.03	0.41
1:A:674:G:H2'	1:A:675:A:C8	2.55	0.41
1:A:737:C:H2'	1:A:738:C:C6	2.55	0.41
1:A:998:C:H2'	1:A:999:C:H5'	2.01	0.41
4:D:24:ALA:HB1	4:D:28:GLU:HG2	2.01	0.41
5:E:9:LEU:HD23	5:E:9:LEU:HA	1.88	0.41
7:G:25:TYR:CE2	7:G:78:PHE:HE1	2.38	0.41
9:I:87:LYS:HG3	9:I:125:ILE:HD11	2.03	0.41
1:A:1497:G:H1'	1:A:1518:MA6:H2	2.03	0.41
6:F:149:SER:OG	6:F:152:MET:HG2	2.20	0.41
10:J:19:VAL:HG13	10:J:65:ILE:HG12	2.02	0.41
17:Q:19:VAL:HG21	17:Q:52:LEU:HD11	2.02	0.41
1:A:779:C:H2'	1:A:780:A:O4'	2.21	0.41
8:H:140:ASP:HA	8:H:143:ARG:NH1	2.34	0.41
14:N:78:LYS:HD2	14:N:78:LYS:HA	1.92	0.41
19:S:32:TYR:O	19:S:40:VAL:HG12	2.21	0.41
1:A:513:C:H2'	1:A:514:C:C6	2.56	0.41
1:A:1165:U:H2'	1:A:1166:G:O4'	2.20	0.41
2:B:71:ALA:HB3	2:B:88:LYS:HB2	2.03	0.41
3:C:68:LEU:HB3	3:C:161:LEU:HD22	2.01	0.41
3:C:187:VAL:HG22	3:C:191:SER:HB2	2.01	0.41
13:M:110:ARG:HA	13:M:110:ARG:HD2	1.79	0.41
23:X:10:G:H2'	23:X:11:U:C6	2.55	0.41
1:A:602:A:H2'	1:A:603:U:C6	2.56	0.41
1:A:603:U:H2'	1:A:604:G:H8	1.86	0.41
1:A:860:A:H2'	1:A:861:G:O4'	2.21	0.41
1:A:1442:G:H2'	1:A:1443:C:H6	1.85	0.41
4:D:45:LYS:HB3	4:D:45:LYS:HE3	1.87	0.41
9:I:7:ILE:O	9:I:11:LEU:HG	2.21	0.41
16:P:2:SER:OG	16:P:3:LEU:N	2.54	0.41
18:R:22:VAL:HA	18:R:44:LEU:O	2.20	0.41
1:A:1086:U:O5'	1:A:1086:U:O2	2.39	0.41
1:A:212:G:C2	1:A:213:G:C8	3.09	0.41
1:A:212:G:C4	1:A:213:G:C8	3.08	0.41
1:A:407:U:H2'	1:A:408:A:C8	2.56	0.41
1:A:463:U:H3'	1:A:464:U:H6	1.85	0.41
1:A:603:U:H2'	1:A:604:G:C8	2.56	0.41
1:A:1025:U:H4'	1:A:1026:G:H5'	2.02	0.41
1:A:1167:A:H4'	1:A:1168:U:OP2	2.19	0.41
1:A:1404:C:H2'	1:A:1405:G:C8	2.56	0.41
2:B:42:LEU:HB2	2:B:82:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:VAL:HG11	5:E:133:ALA:HA	2.03	0.41
8:H:25:LYS:HE2	8:H:25:LYS:HB2	1.91	0.41
13:M:76:GLU:OE1	13:M:76:GLU:N	2.54	0.41
1:A:31:G:O2'	1:A:48:C:N4	2.54	0.41
1:A:128:G:H2'	1:A:129:A:C8	2.56	0.41
1:A:411:A:H4'	1:A:412:A:H5'	2.02	0.41
1:A:458:U:H2'	1:A:459:A:C8	2.55	0.41
1:A:792:A:H1'	1:A:794:A:N7	2.36	0.41
1:A:1041:G:H2'	1:A:1042:A:C8	2.56	0.41
1:A:1417:G:H2'	1:A:1482:G:N2	2.35	0.41
3:C:70:VAL:O	3:C:163:VAL:HA	2.20	0.41
3:C:85:LEU:HD23	3:C:85:LEU:HA	1.83	0.41
3:C:186:ILE:HD13	3:C:200:ILE:HB	2.03	0.41
5:E:52:GLY:O	5:E:56:ARG:HG2	2.21	0.41
8:H:45:SER:O	8:H:49:THR:HG22	2.21	0.41
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.40
1:A:468:A:H5"	1:A:469:C:H5	1.86	0.40
1:A:526:C:C5	1:A:527:G7M:H1'	2.55	0.40
1:A:900:A:H2'	1:A:901:A:C8	2.56	0.40
1:A:1003:G:N2	1:A:1005:A:O5'	2.53	0.40
1:A:1064:G:H1'	1:A:1190:G:N2	2.35	0.40
1:A:1513:A:H2'	1:A:1514:G:C8	2.56	0.40
5:E:69:GLU:OE2	5:E:204:TYR:OH	2.29	0.40
1:A:421:U:H3'	1:A:422:C:C5	2.56	0.40
4:D:42:TYR:OH	4:D:90:VAL:HG11	2.20	0.40
6:F:104:GLY:O	6:F:122:ASN:HA	2.21	0.40
6:F:111:MET:HA	6:F:114:VAL:HG12	2.02	0.40
7:G:6:ILE:HG12	7:G:89:VAL:HG12	2.04	0.40
17:Q:80:LYS:HB3	17:Q:80:LYS:HE2	1.89	0.40
1:A:29:U:O2'	1:A:30:U:H5'	2.21	0.40
1:A:51:A:N7	1:A:114:U:O2'	2.54	0.40
1:A:466:A:H2'	1:A:468:A:C2	2.56	0.40
1:A:1000:A:O5'	1:A:1000:A:H8	2.04	0.40
1:A:1152:A:P	11:K:72:ARG:HH22	2.45	0.40
1:A:1517:G:H2'	1:A:1518:MA6:C8	2.52	0.40
8:H:113:ASP:HB2	8:H:119:ARG:HG3	2.03	0.40
10:J:36:GLU:HA	10:J:45:ARG:HD3	2.04	0.40
14:N:53:ILE:O	14:N:57:ARG:HG3	2.21	0.40
1:A:339:C:H2'	1:A:340:U:H6	1.86	0.40
1:A:422:C:H4'	1:A:423:G:C5'	2.51	0.40
1:A:1315:U:O2	1:A:1360:A:H2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1464:U:H2'	1:A:1465:A:C8	2.56	0.40
4:D:64:ILE:O	4:D:99:ALA:HA	2.21	0.40
5:E:150:LYS:NZ	5:E:178:MET:HB2	2.36	0.40
8:H:92:ARG:O	8:H:96:ARG:HG3	2.21	0.40
12:L:34:ILE:HD12	12:L:74:VAL:HG11	2.04	0.40
12:L:87:LYS:HB2	12:L:113:VAL:HG13	2.04	0.40
20:T:45:ILE:HD11	20:T:67:VAL:CG2	2.51	0.40
21:U:48:GLN:HE21	21:U:52:ASN:HD21	1.69	0.40
22:V:11:PRO:HG2	22:V:14:VAL:HG23	2.03	0.40
22:V:29:LEU:C	22:V:32:VAL:HG22	2.41	0.40
22:V:69:ARG:NE	22:V:71:TYR:O	2.52	0.40
23:X:17:U:H3'	23:X:18:G:C8	2.52	0.40
1:A:323:U:H2'	1:A:324:G:O4'	2.22	0.40
1:A:649:A:H2'	1:A:650:G:O4'	2.21	0.40
1:A:939:G:H2'	1:A:940:C:C6	2.57	0.40
1:A:978:A:C4	1:A:1319:A:C2	3.09	0.40
1:A:1088:G:H5'	22:V:70:LEU:HD23	2.04	0.40
1:A:1218:C:H2'	1:A:1219:A:C8	2.56	0.40
1:A:1447:A:OP1	1:A:1448:C:N4	2.40	0.40
1:A:1530:G:O6	22:V:46:LYS:NZ	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	172/557 (31%)	158 (92%)	14 (8%)	0	100	100
3	C	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
4	D	209/233 (90%)	204 (98%)	5 (2%)	0	100	100
5	E	203/206 (98%)	199 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	154/156 (99%)	152 (99%)	2 (1%)	0	100 100
7	G	102/131 (78%)	100 (98%)	2 (2%)	0	100 100
8	H	148/156 (95%)	140 (95%)	6 (4%)	2 (1%)	9 30
9	I	127/130 (98%)	122 (96%)	5 (4%)	0	100 100
10	J	126/130 (97%)	118 (94%)	8 (6%)	0	100 100
11	K	99/103 (96%)	96 (97%)	3 (3%)	0	100 100
12	L	115/129 (89%)	109 (95%)	6 (5%)	0	100 100
13	M	119/124 (96%)	113 (95%)	5 (4%)	1 (1%)	16 44
14	N	113/118 (96%)	110 (97%)	3 (3%)	0	100 100
15	O	98/101 (97%)	97 (99%)	1 (1%)	0	100 100
16	P	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
17	Q	80/82 (98%)	78 (98%)	2 (2%)	0	100 100
18	R	78/84 (93%)	75 (96%)	3 (4%)	0	100 100
19	S	65/75 (87%)	63 (97%)	2 (3%)	0	100 100
20	T	81/92 (88%)	80 (99%)	0	1 (1%)	11 34
21	U	84/87 (97%)	84 (100%)	0	0	100 100
22	V	68/71 (96%)	67 (98%)	1 (2%)	0	100 100
All	All	2551/3095 (82%)	2463 (97%)	84 (3%)	4 (0%)	45 73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	5	ARG
8	H	6	VAL
20	T	6	LYS
13	M	45	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	B	86/461 (19%)	76 (88%)	10 (12%)	4 15
3	C	187/199 (94%)	174 (93%)	13 (7%)	12 36
4	D	172/190 (90%)	166 (96%)	6 (4%)	31 65
5	E	172/173 (99%)	159 (92%)	13 (8%)	11 32
6	F	119/119 (100%)	117 (98%)	2 (2%)	56 84
7	G	91/112 (81%)	85 (93%)	6 (7%)	14 39
8	H	124/129 (96%)	115 (93%)	9 (7%)	11 34
9	I	104/105 (99%)	104 (100%)	0	100 100
10	J	106/107 (99%)	98 (92%)	8 (8%)	11 33
11	K	88/90 (98%)	82 (93%)	6 (7%)	13 38
12	L	90/99 (91%)	89 (99%)	1 (1%)	70 90
13	M	102/103 (99%)	93 (91%)	9 (9%)	8 26
14	N	93/96 (97%)	85 (91%)	8 (9%)	8 27
15	O	83/84 (99%)	81 (98%)	2 (2%)	44 77
16	P	76/77 (99%)	75 (99%)	1 (1%)	65 88
17	Q	65/65 (100%)	59 (91%)	6 (9%)	7 24
18	R	74/78 (95%)	69 (93%)	5 (7%)	13 38
19	S	58/65 (89%)	56 (97%)	2 (3%)	32 66
20	T	72/79 (91%)	67 (93%)	5 (7%)	13 37
21	U	65/66 (98%)	58 (89%)	7 (11%)	5 17
22	V	60/61 (98%)	55 (92%)	5 (8%)	9 28
All	All	2087/2558 (82%)	1963 (94%)	124 (6%)	19 44

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	B	14	LYS
2	B	34	ASP
2	B	48	ILE
2	B	51	GLU
2	B	63	GLN
2	B	69	ASP
2	B	73	ASP
2	B	75	VAL
2	B	102	TYR

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Mol	Chain	Res	Type
3	C	23	TRP
3	C	45	LYS
3	C	50	PHE
3	C	54	LEU
3	C	80	VAL
3	C	95	ARG
3	C	130	THR
3	C	132	LYS
3	C	133	GLU
3	C	163	VAL
3	C	183	VAL
3	C	197	ASP
3	C	223	GLU
4	D	31	ASP
4	D	72	ARG
4	D	89	LYS
4	D	165	THR
4	D	172	ARG
4	D	192	THR
5	E	15	GLU
5	E	101	VAL
5	E	113	GLU
5	E	116	GLN
5	E	125	VAL
5	E	129	VAL
5	E	131	ASN
5	E	132	ILE
5	E	136	GLN
5	E	144	SER
5	E	188	ARG
5	E	190	ASP
5	E	194	ASP
6	F	117	VAL
6	F	126	LYS
7	G	54	LEU
7	G	72	ASP
7	G	74	LEU
7	G	84	VAL
7	G	91	ARG
7	G	97	THR
8	H	12	ILE
8	H	56	LYS

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Mol	Chain	Res	Type
8	H	59	LEU
8	H	75	VAL
8	H	78	ARG
8	H	79	ARG
8	H	91	VAL
8	H	113	ASP
8	H	146	GLU
10	J	5	GLN
10	J	15	SER
10	J	22	LYS
10	J	67	VAL
10	J	95	ARG
10	J	105	THR
10	J	119	ARG
10	J	123	ARG
11	K	5	ARG
11	K	20	GLN
11	K	36	VAL
11	K	37	ARG
11	K	77	VAL
11	K	78	GLU
12	L	76	GLU
13	M	4	VAL
13	M	10	LYS
13	M	15	LYS
13	M	16	VAL
13	M	34	CYS
13	M	75	GLN
13	M	83	ARG
13	M	87	VAL
13	M	107	VAL
14	N	7	ILE
14	N	28	THR
14	N	42	ASP
14	N	56	LEU
14	N	58	ASP
14	N	101	ARG
14	N	102	THR
14	N	104	THR
15	O	24	ARG
15	O	26	GLU
16	P	17	ARG

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Mol	Chain	Res	Type
17	Q	3	THR
17	Q	18	GLN
17	Q	21	VAL
17	Q	46	LYS
17	Q	48	GLU
17	Q	69	ASP
18	R	4	LYS
18	R	18	GLU
18	R	22	VAL
18	R	42	THR
18	R	78	VAL
19	S	9	LYS
19	S	74	HIS
20	T	24	GLU
20	T	48	THR
20	T	51	VAL
20	T	58	VAL
20	T	79	THR
21	U	3	ASN
21	U	5	LYS
21	U	14	SER
21	U	36	TYR
21	U	60	ARG
21	U	64	LYS
21	U	67	ILE
22	V	3	VAL
22	V	44	GLU
22	V	59	LYS
22	V	63	GLU
22	V	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	B	63	GLN
3	C	19	GLN
4	D	123	GLN
5	E	59	GLN
5	E	136	GLN
5	E	198	HIS
6	F	135	ASN

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Mol	Chain	Res	Type
7	G	46	GLN
7	G	58	HIS
7	G	63	ASN
8	H	9	GLN
10	J	4	ASN
10	J	37	GLN
10	J	75	GLN
12	L	15	GLN
15	O	35	ASN
15	O	66	GLN
16	P	35	GLN
16	P	80	GLN
17	Q	18	GLN
18	R	9	GLN
19	S	74	HIS
20	T	69	HIS
21	U	13	GLN
21	U	48	GLN
21	U	52	ASN
21	U	70	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1534/1541 (99%)	239 (15%)	10 (0%)
23	X	16/53 (30%)	3 (18%)	1 (6%)
All	All	1550/1594 (97%)	242 (15%)	11 (0%)

All (242) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	U
1	A	5	U
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C

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Mol	Chain	Res	Type
1	A	51	A
1	A	52	C
1	A	70	U
1	A	71	A
1	A	75	G
1	A	76	G
1	A	77	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	93	U
1	A	94	G
1	A	95	C
1	A	108	G
1	A	116	A
1	A	130	A
1	A	131	A
1	A	141	G
1	A	157	U
1	A	158	G
1	A	163	C
1	A	165	G
1	A	166	U
1	A	168	G
1	A	173	U
1	A	181	A
1	A	189	A
1	A	197	A
1	A	212	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C

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Mol	Chain	Res	Type
1	A	332	G
1	A	343	U
1	A	345	C
1	A	346	G
1	A	347	G
1	A	348	G
1	A	351	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	398	U
1	A	406	G
1	A	411	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	457	G
1	A	458	U
1	A	461	A
1	A	463	U
1	A	464	U
1	A	465	A
1	A	466	A
1	A	467	U
1	A	468	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	497	G
1	A	511	C
1	A	521	G
1	A	527	G7M
1	A	528	C
1	A	533	A

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Mol	Chain	Res	Type
1	A	547	A
1	A	559	A
1	A	562	U
1	A	564	C
1	A	567	G
1	A	569	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C
1	A	577	G
1	A	578	C
1	A	596	A
1	A	633	G
1	A	642	A
1	A	650	G
1	A	665	A
1	A	682	G
1	A	687	A
1	A	703	G
1	A	718	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	828	U
1	A	829	G
1	A	832	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	846	G
1	A	876	C
1	A	882	C

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Mol	Chain	Res	Type
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	942	G
1	A	960	U
1	A	966	2MG
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	994	A
1	A	996	A
1	A	998	C
1	A	999	C
1	A	1004	A
1	A	1009	U
1	A	1018	G
1	A	1020	G
1	A	1022	A
1	A	1024	G
1	A	1025	U
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1044	A
1	A	1065	U
1	A	1079	G
1	A	1085	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1099	G
1	A	1101	A
1	A	1103	C

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Mol	Chain	Res	Type
1	A	1104	G
1	A	1108	G
1	A	1133	G
1	A	1136	C
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1151	A
1	A	1152	A
1	A	1158	C
1	A	1159	U
1	A	1167	A
1	A	1168	U
1	A	1169	A
1	A	1170	A
1	A	1171	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1207	2MG
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1257	A
1	A	1260	G
1	A	1278	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1318	A
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1363	A
1	A	1370	G

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Mol	Chain	Res	Type
1	A	1379	G
1	A	1398	A
1	A	1432	G
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1453	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1520	C
1	A	1521	C
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
23	X	12	A
23	X	13	U
23	X	17	U

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	422	C
1	A	428	G
1	A	429	U
1	A	463	U
1	A	467	U
1	A	575	G
1	A	641	U
1	A	966	2MG
1	A	1078	U
1	A	1167	A
23	X	11	U

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

12 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	2MG	A	1207	1	18,26,27	1.35	2 (11%)	16,38,41	1.58	4 (25%)
1	UR3	A	1498	1	19,22,23	1.11	2 (10%)	26,32,35	1.85	6 (23%)
1	MA6	A	1519	1	18,26,27	1.05	1 (5%)	19,38,41	1.80	6 (31%)
1	MA6	A	1518	1	18,26,27	1.11	1 (5%)	19,38,41	2.00	6 (31%)
1	G7M	A	527	1	20,26,27	1.11	2 (10%)	17,39,42	1.19	1 (5%)
1	2MG	A	1516	1	18,26,27	1.06	2 (11%)	16,38,41	1.34	3 (18%)
13	D2T	M	89	13	7,9,10	1.04	0	6,11,13	2.29	2 (33%)
1	2MG	A	966	1	18,26,27	1.08	2 (11%)	16,38,41	1.58	5 (31%)
1	5MC	A	1407	1	18,22,23	1.07	1 (5%)	26,32,35	1.69	5 (19%)
1	5MC	A	967	1	18,22,23	1.18	2 (11%)	26,32,35	1.56	5 (19%)
1	PSU	A	516	24,1	18,21,22	0.86	1 (5%)	22,30,33	0.66	0
1	4OC	A	1402	1	20,23,24	0.79	0	26,32,35	1.47	2 (7%)

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	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	6/7/29/30	0/3/3/3
1	MA6	A	1518	1	-	1/7/29/30	0/3/3/3
1	G7M	A	527	1	-	3/3/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
13	D2T	M	89	13	-	1/7/12/14	-
1	2MG	A	966	1	-	5/5/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	PSU	A	516	24,1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C6-N1	-3.85	1.32	1.37
1	A	527	G7M	C8-N9	3.49	1.39	1.33
1	A	516	PSU	C6-C5	3.34	1.39	1.35
1	A	1407	5MC	C6-N1	-3.26	1.32	1.38
1	A	967	5MC	C6-N1	-2.81	1.33	1.38
1	A	966	2MG	C6-N1	-2.78	1.33	1.37
1	A	1516	2MG	C6-N1	-2.52	1.34	1.37
1	A	1207	2MG	C2-N1	-2.44	1.32	1.36
1	A	1519	MA6	C5-C4	2.40	1.47	1.40
1	A	967	5MC	C6-C5	2.38	1.38	1.34
1	A	1518	MA6	C5-C4	2.34	1.47	1.40
1	A	527	G7M	C8-N7	2.30	1.37	1.33
1	A	966	2MG	C2'-C1'	-2.29	1.50	1.53
1	A	1498	UR3	C5-C4	-2.22	1.38	1.43
1	A	1498	UR3	C6-N1	-2.09	1.32	1.38
1	A	1516	2MG	O4'-C1'	2.05	1.43	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1498	UR3	C4-N3-C2	-5.93	118.98	124.56
1	A	1518	MA6	N1-C6-N6	5.87	123.23	117.06
1	A	1402	4OC	C2'-C1'-N1	-5.82	102.92	114.22
1	A	967	5MC	C5-C6-N1	-4.43	118.78	123.34
1	A	1407	5MC	C5-C6-N1	-4.42	118.79	123.34
13	M	89	D2T	CB1-SB-CB	3.92	109.54	102.44
1	A	1498	UR3	O4'-C1'-C2'	-3.53	98.94	106.64
1	A	1407	5MC	CM5-C5-C6	-3.34	118.39	122.85
1	A	1407	5MC	C2'-C1'-N1	-3.28	103.92	113.22
1	A	1519	MA6	C10-N6-C6	-3.22	109.76	119.51
1	A	1518	MA6	N3-C2-N1	-3.19	123.69	128.68
1	A	527	G7M	C3'-C2'-C1'	-3.17	96.21	100.98
1	A	1519	MA6	N1-C6-N6	3.16	120.38	117.06
1	A	1519	MA6	C9-N6-C6	-3.14	110.01	119.51
1	A	1519	MA6	N3-C2-N1	-3.11	123.83	128.68
13	M	89	D2T	OD2-CG-CB	2.97	119.56	113.15
1	A	967	5MC	C2'-C1'-N1	-2.96	104.82	113.22
1	A	1498	UR3	C3U-N3-C2	2.90	122.39	117.31
1	A	1207	2MG	C5-C6-N1	2.82	118.94	113.95
1	A	1518	MA6	C9-N6-C6	-2.78	111.10	119.51
1	A	966	2MG	C3'-C2'-C1'	2.77	105.15	100.98
1	A	1519	MA6	C4-C5-N7	-2.77	106.52	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	2MG	C5-C6-N1	2.76	118.82	113.95
1	A	1207	2MG	CM2-N2-C2	-2.73	117.84	123.86
1	A	1518	MA6	C3'-C2'-C1'	2.72	105.07	100.98
1	A	1207	2MG	C3'-C2'-C1'	2.71	105.06	100.98
1	A	1407	5MC	C1'-N1-C6	-2.67	116.68	121.12
1	A	1407	5MC	O2-C2-N3	-2.64	118.03	122.33
1	A	1498	UR3	C1'-N1-C2	2.49	121.19	116.99
1	A	1516	2MG	C5-C6-N1	2.48	118.33	113.95
1	A	967	5MC	C5-C4-N3	-2.46	119.02	121.67
1	A	1516	2MG	C8-N7-C5	2.43	107.61	102.99
1	A	966	2MG	O6-C6-C5	-2.41	119.67	124.37
1	A	966	2MG	C8-N7-C5	2.41	107.57	102.99
1	A	967	5MC	O4'-C1'-N1	2.31	113.63	108.36
1	A	1402	4OC	C6-C5-C4	2.29	119.77	116.96
1	A	1498	UR3	C2'-C3'-C4'	-2.27	98.23	102.64
1	A	1518	MA6	C4-C5-N7	-2.27	107.03	109.40
1	A	1498	UR3	O3'-C3'-C4'	-2.26	104.51	111.05
1	A	1207	2MG	C8-N7-C5	2.24	107.27	102.99
1	A	967	5MC	O2-C2-N3	-2.22	118.72	122.33
1	A	1518	MA6	C10-N6-C6	-2.19	112.88	119.51
1	A	966	2MG	CM2-N2-C2	-2.14	119.14	123.86
1	A	1516	2MG	C3'-C2'-C1'	2.06	104.08	100.98
1	A	1519	MA6	C10-N6-C9	-2.06	109.49	116.12

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	966	2MG	N1-C2-N2-CM2
1	A	966	2MG	N3-C2-N2-CM2
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	966	2MG	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C10
1	A	1519	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	527	G7M	C4'-C5'-O5'-P
1	A	966	2MG	C4'-C5'-O5'-P
13	M	89	D2T	CG-CB-SB-CB1

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	4	0
1	A	1519	MA6	6	0
1	A	1518	MA6	6	0
1	A	527	G7M	2	0
1	A	1516	2MG	1	0
1	A	966	2MG	4	0
1	A	1407	5MC	2	0
1	A	967	5MC	2	0
1	A	1402	4OC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 86 ligands modelled in this entry, 86 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

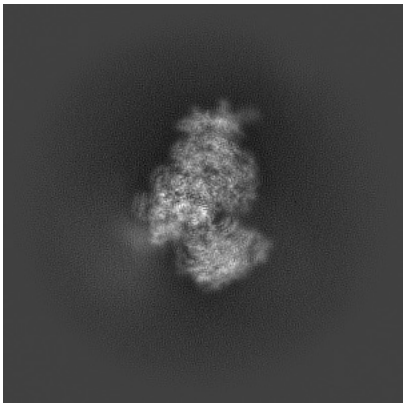
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51615. These allow visual inspection of the internal detail of the map and identification of artifacts.

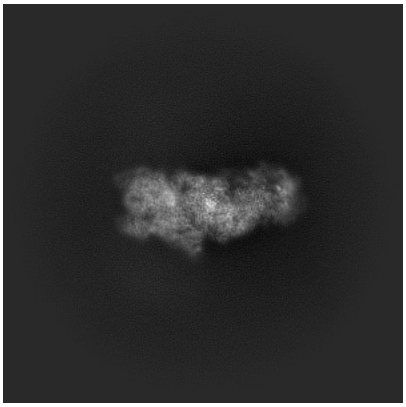
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

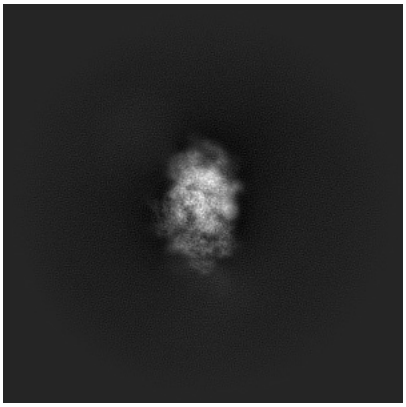
6.1.1 Primary map



X



Y

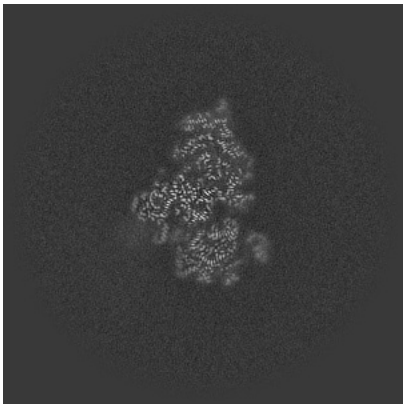


Z

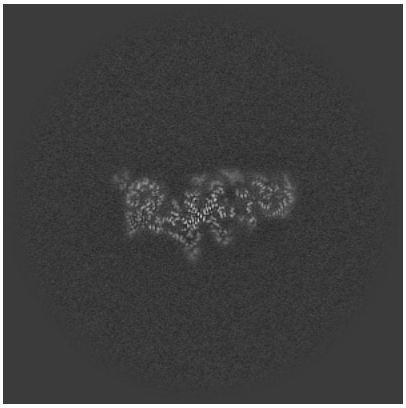
The images above show the map projected in three orthogonal directions.

6.2 Central slices

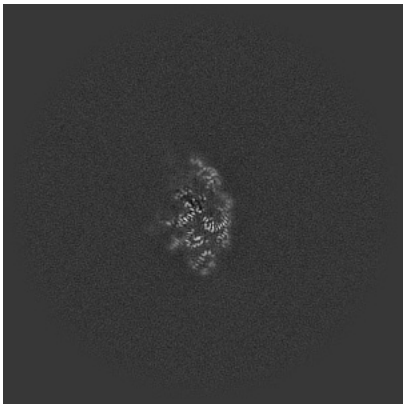
6.2.1 Primary map



X Index: 300



Y Index: 300

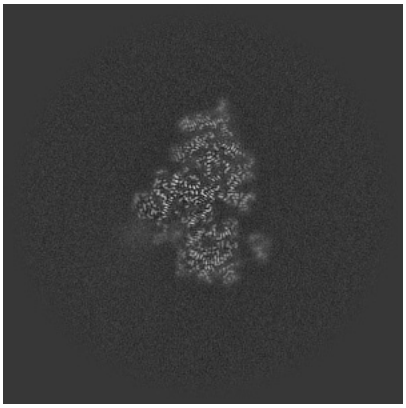


Z Index: 300

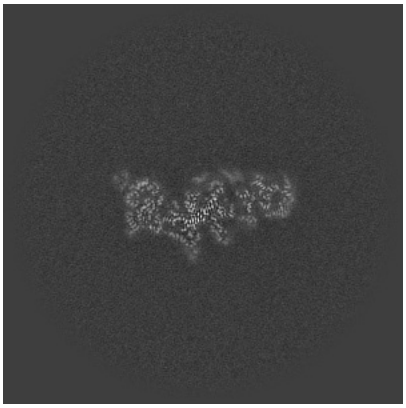
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

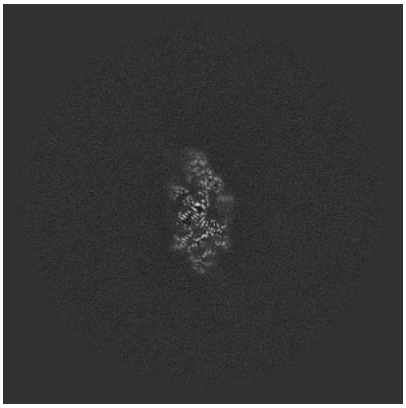
6.3.1 Primary map



X Index: 297



Y Index: 301

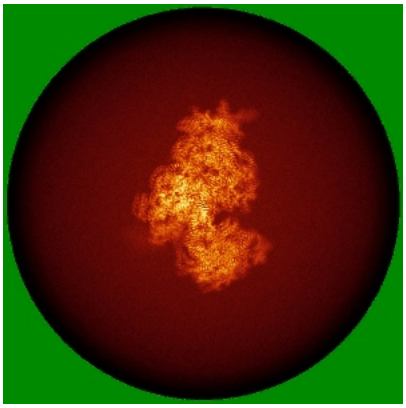


Z Index: 306

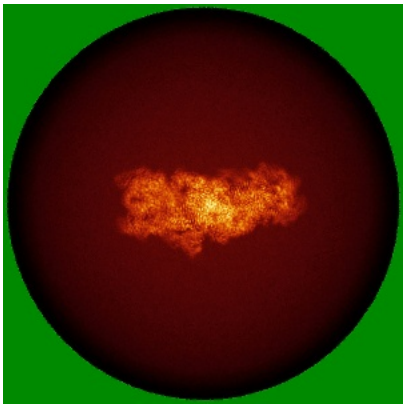
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

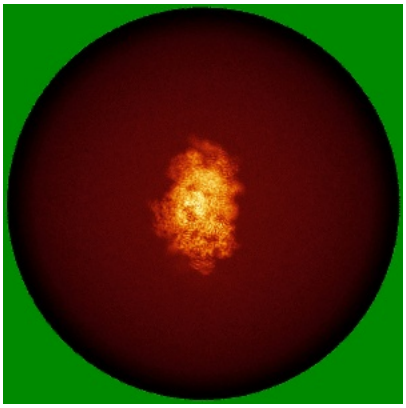
6.4.1 Primary map



X



Y



Z

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 0.745. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

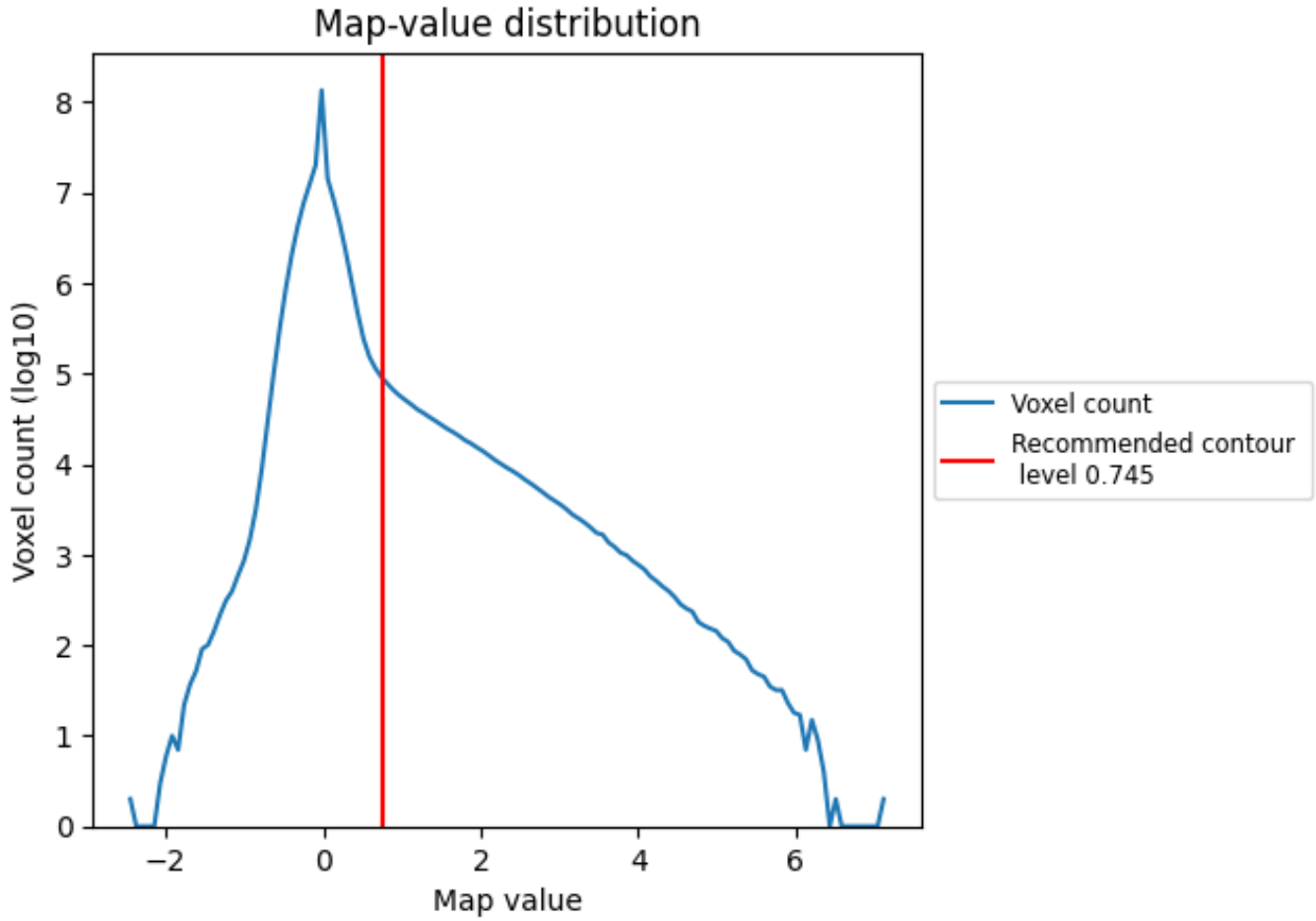
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

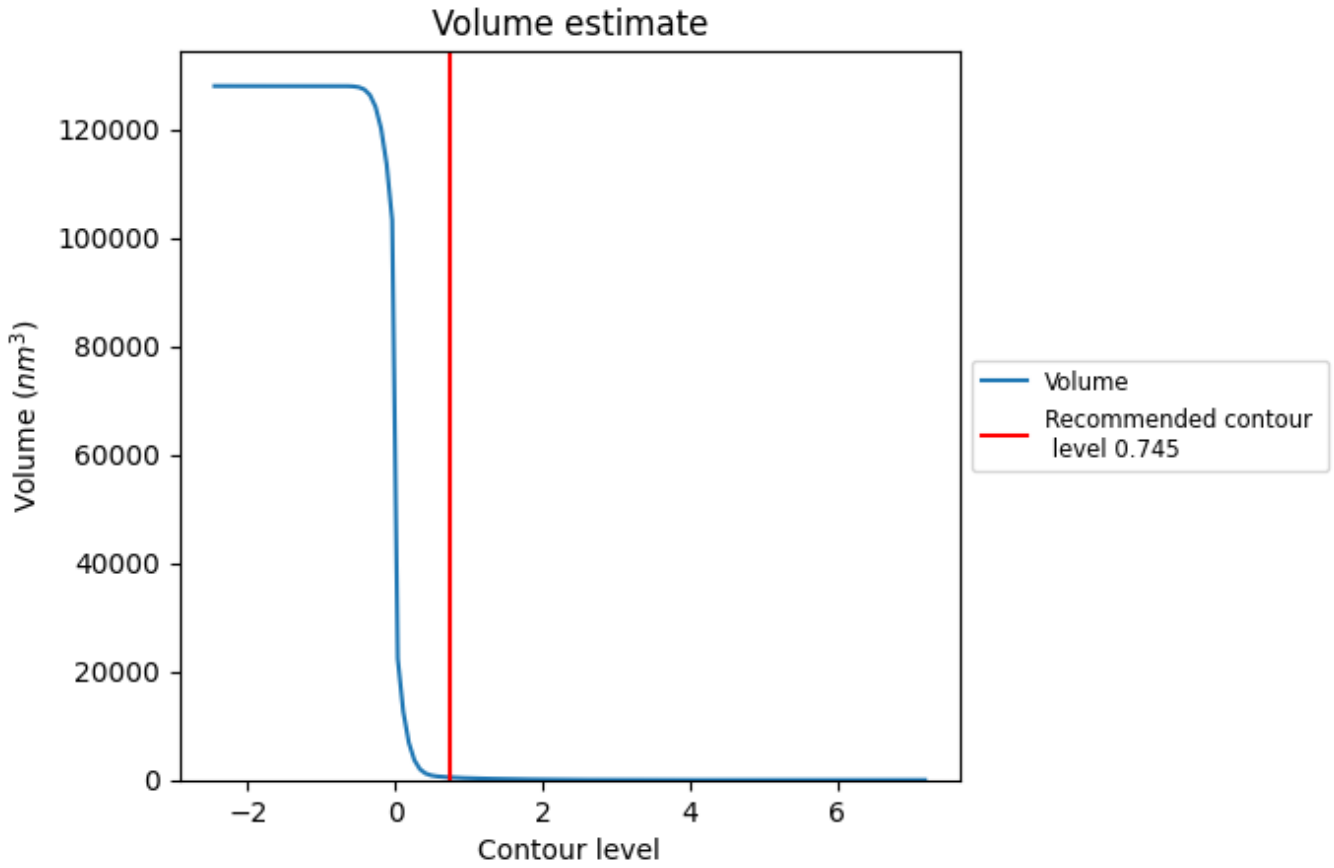
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

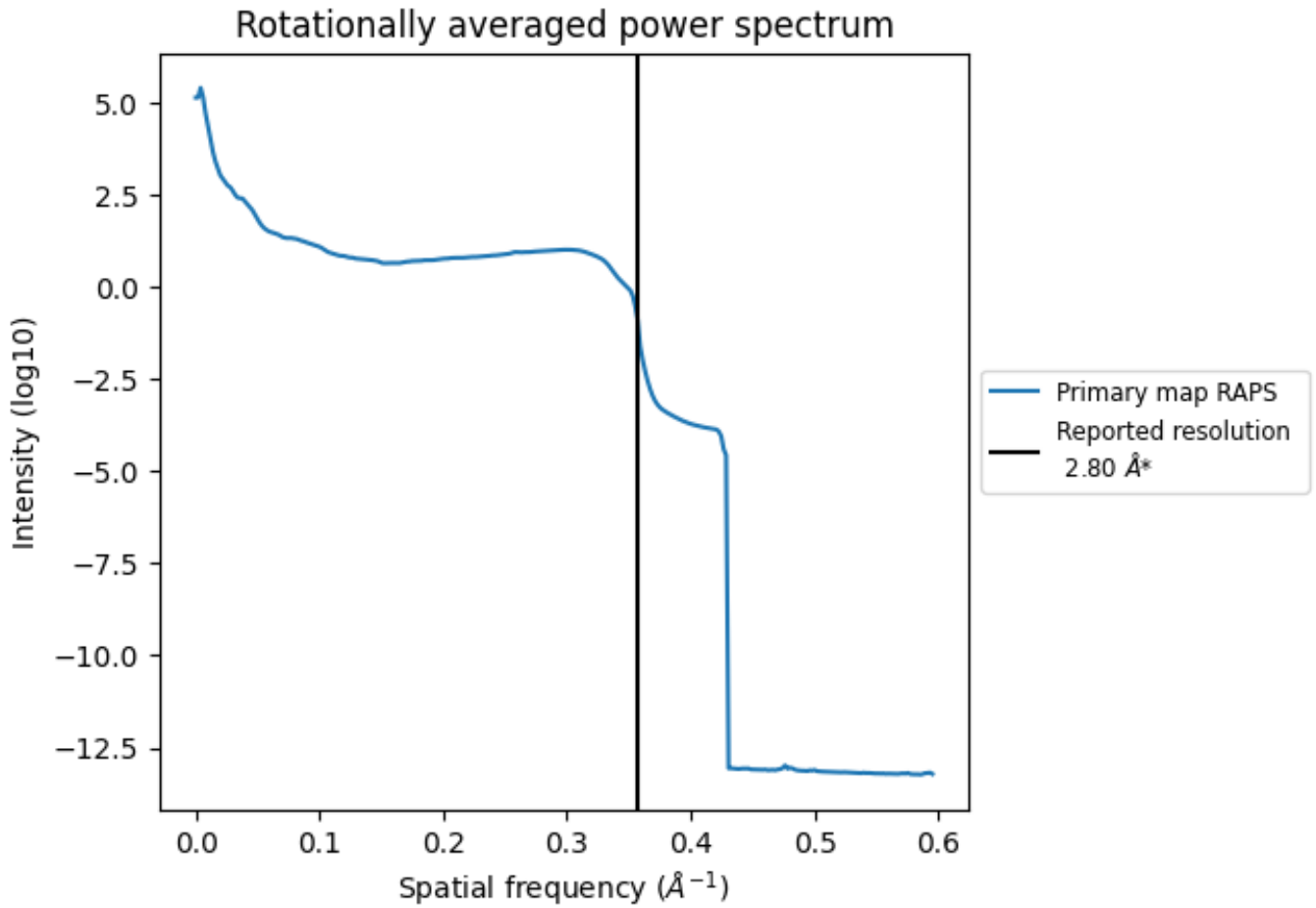
7.2 Volume estimate



The volume at the recommended contour level is 478 nm^3; this corresponds to an approximate mass of 432 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

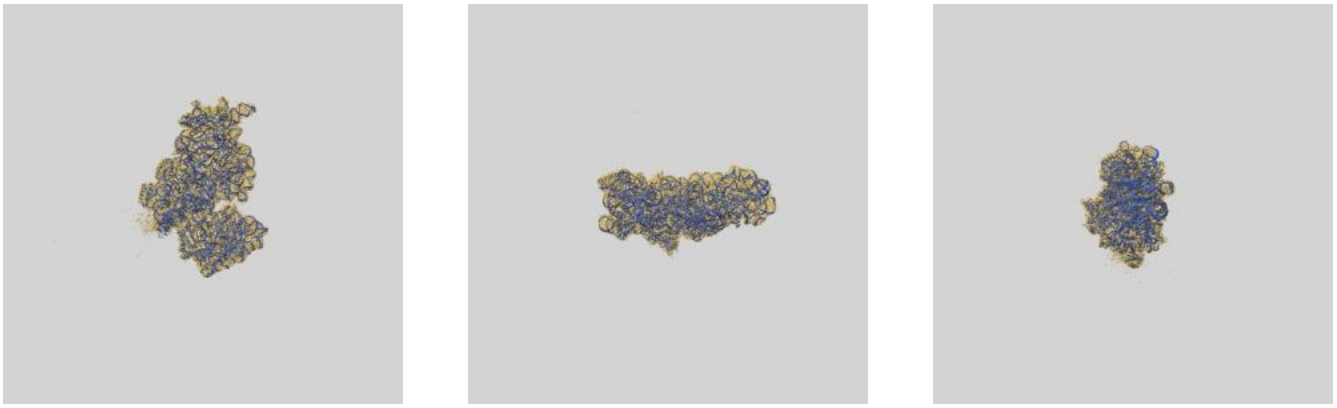
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51615 and PDB model 9GUP. Per-residue inclusion information can be found in section 3 on page 8.

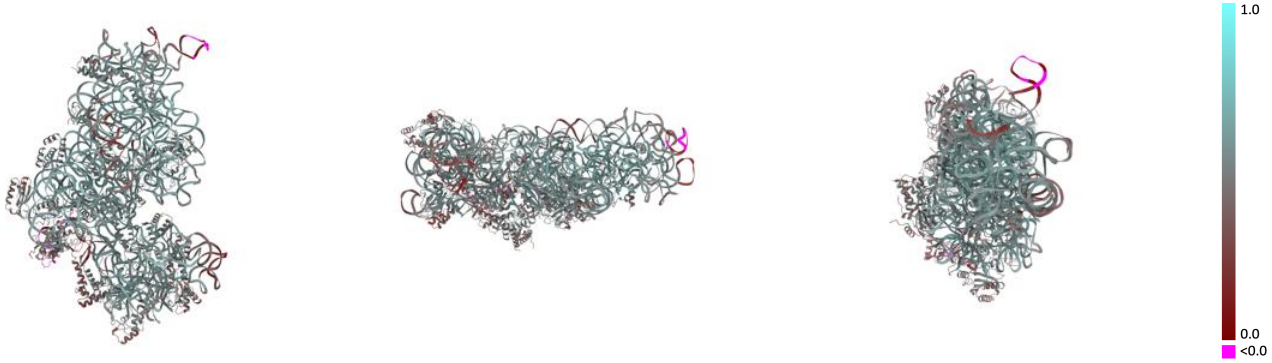
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.745 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.

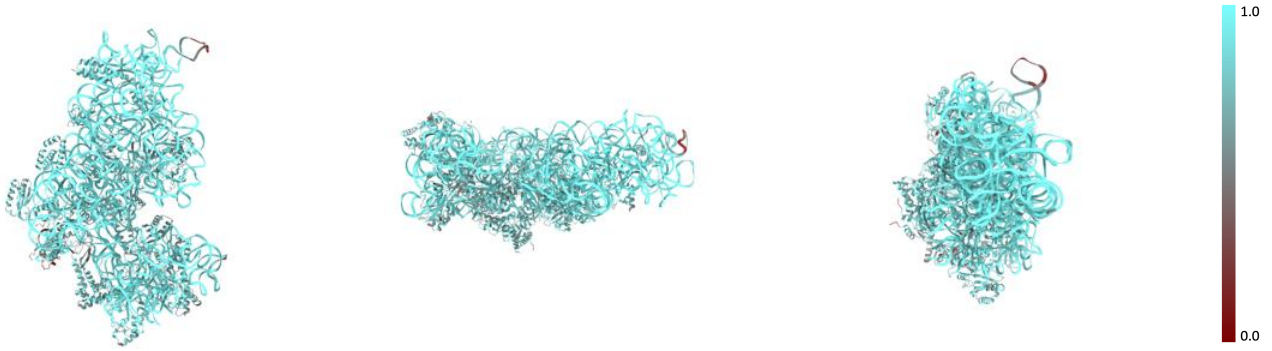
9.2 Q-score mapped to coordinate model



X Y Z

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

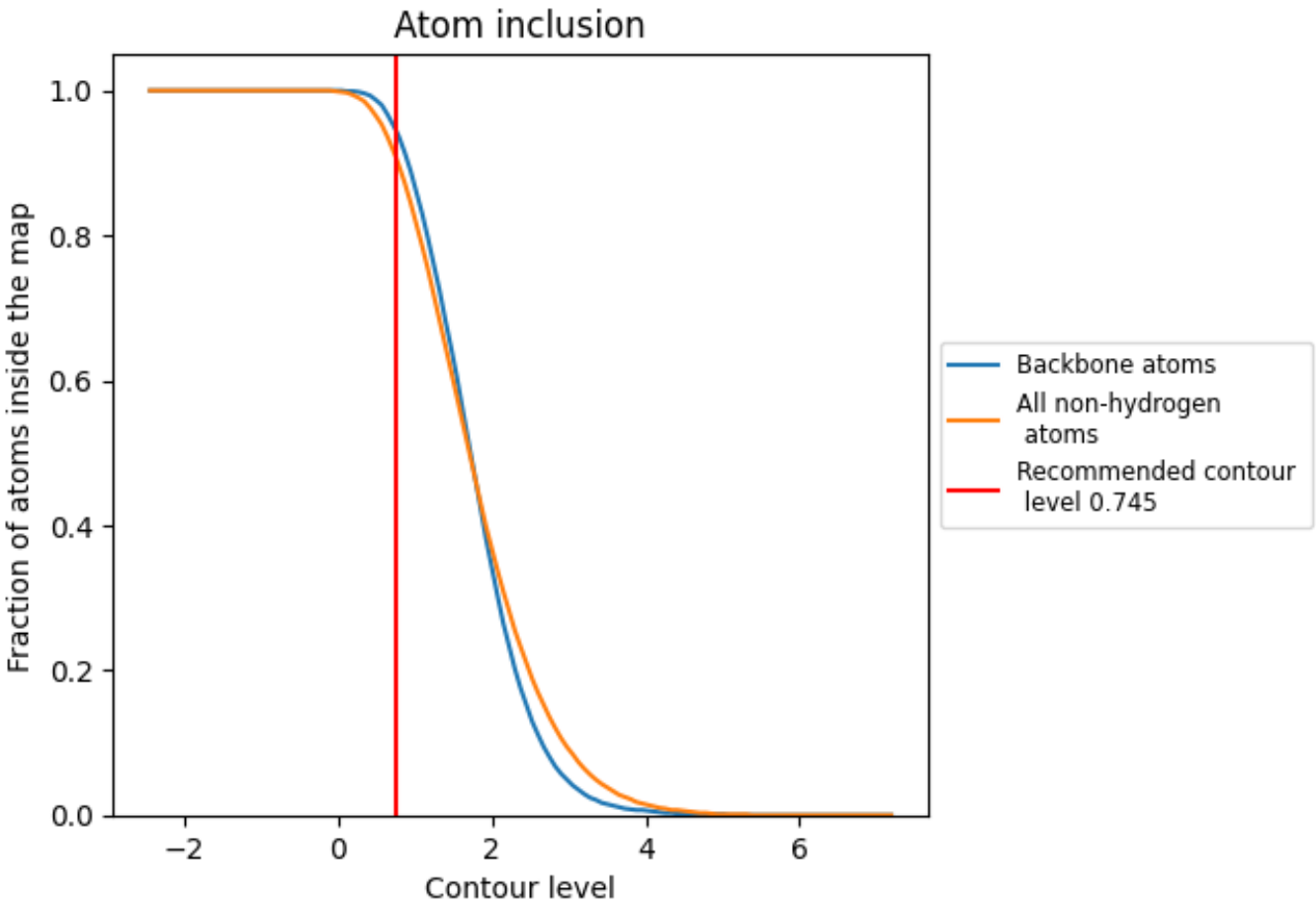
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.745).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.745) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9090	0.5160
A	0.9700	0.5500
B	0.5660	0.2830
C	0.8360	0.4720
D	0.7600	0.4610
E	0.8550	0.4930
F	0.8810	0.5280
G	0.8170	0.4480
H	0.7270	0.3700
I	0.8800	0.5270
J	0.8400	0.4910
K	0.7610	0.4300
L	0.8500	0.4660
M	0.8810	0.5290
N	0.8160	0.4630
O	0.8100	0.4750
P	0.8880	0.5010
Q	0.8820	0.5410
R	0.8560	0.5120
S	0.8520	0.4920
T	0.8550	0.4750
U	0.8750	0.5180
V	0.7660	0.4210
X	0.4470	0.1050