Full wwPDB EM Validation Report ⓘ

Dec 4, 2024 – 03:51 am GMT

PDB ID	:	9GUQ
EMDB ID	:	EMD-51616
Title	:	30S PIC (Pre-Initiation complex)
Authors	:	Rahil, H.; Weixlbaumer, A.; Webster, M.W.
Deposited on	:	2024-09-20
Resolution	:	3.10 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:

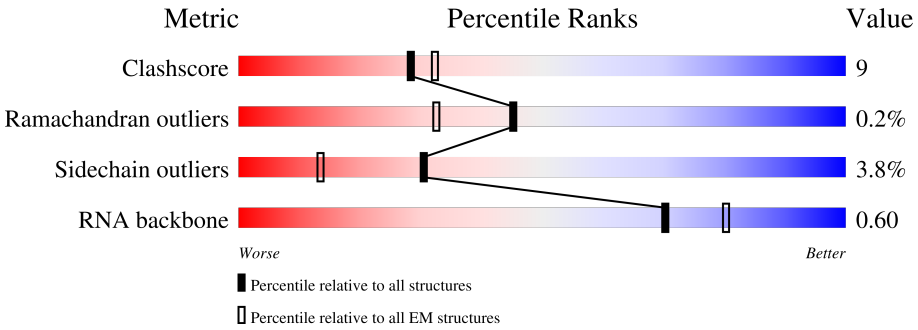
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	52% 42% 6%
2	B	557	19% 24% 6% 69%
3	C	241	72% 21% 6%
4	D	233	76% 14% 9%
5	E	206	81% 18%
6	F	156	84% 16%
7	G	131	51% 27% 21%

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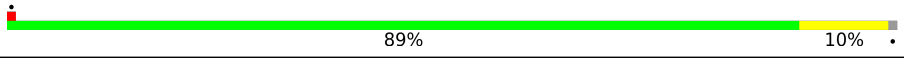
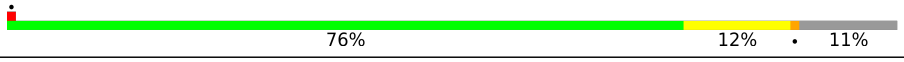
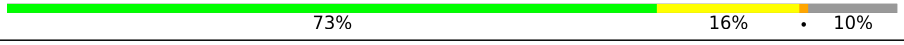
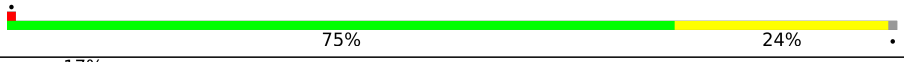
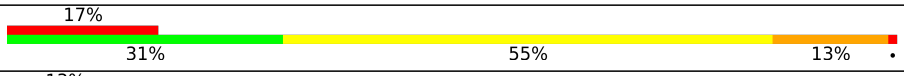
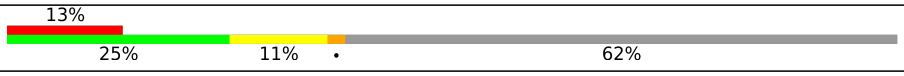
Mol	Chain	Length	Quality of chain
8	H	156	
9	I	130	
10	J	130	
11	K	103	
12	L	129	
13	M	124	
14	N	118	
15	O	101	
16	P	89	
17	Q	82	
18	R	84	
19	S	75	
20	T	92	
21	U	87	
22	V	71	
23	W	77	
24	X	53	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 55411 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		
2	B	172	1094	674	196	224	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, non-modified isoform.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	125	ASP	GLU	conflict	UNP P02358

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	153	Total	C	N	O	S	0	0
			1203	750	231	218	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 tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	20	Total	C	N	O	P	0	0
			427	191	77	139	20		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

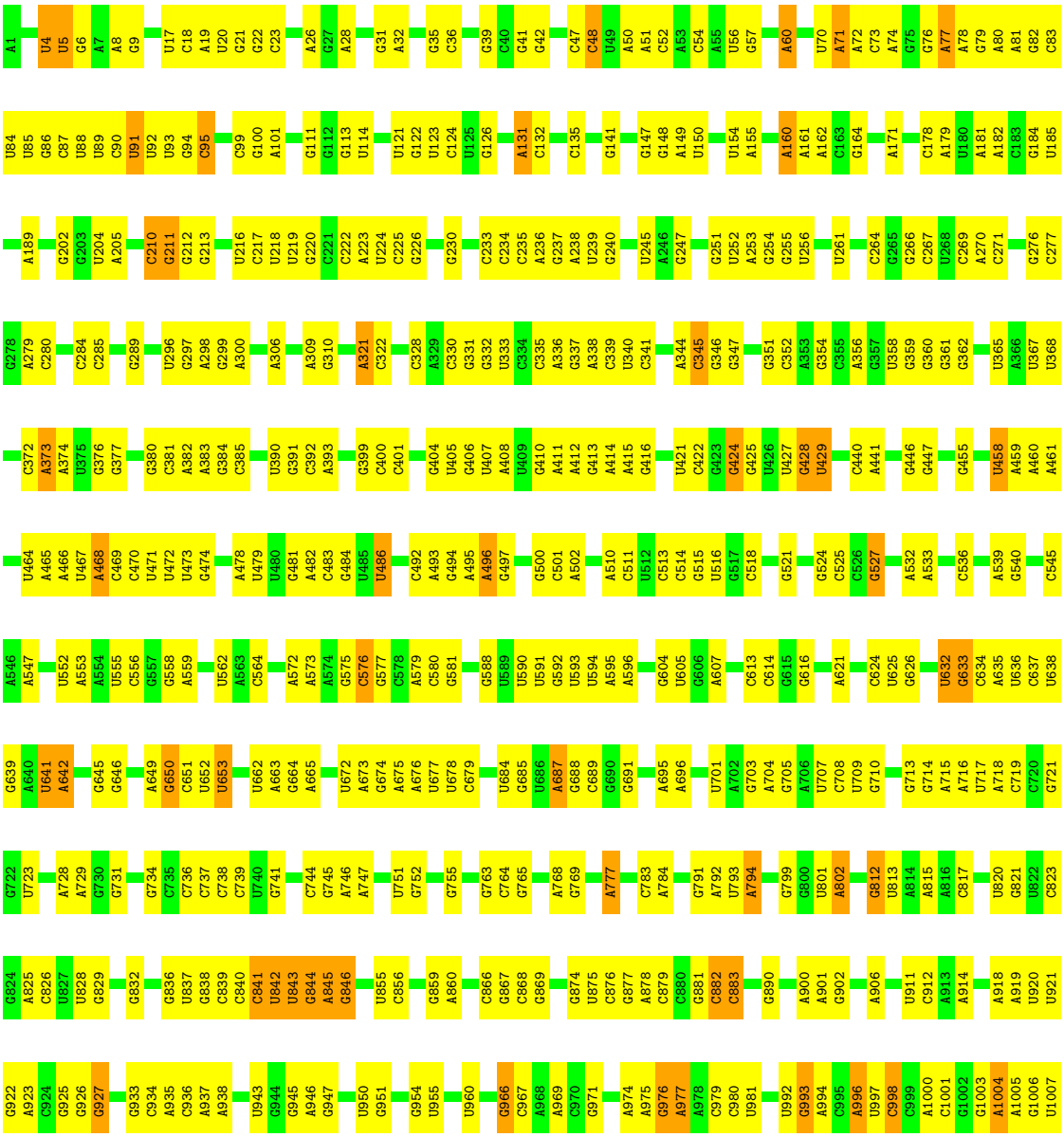
Mol	Chain	Residues	Atoms		AltConf
25	A	127	Total	Mg	0
			127	127	
25	X	1	Total	Mg	0
			1	1	

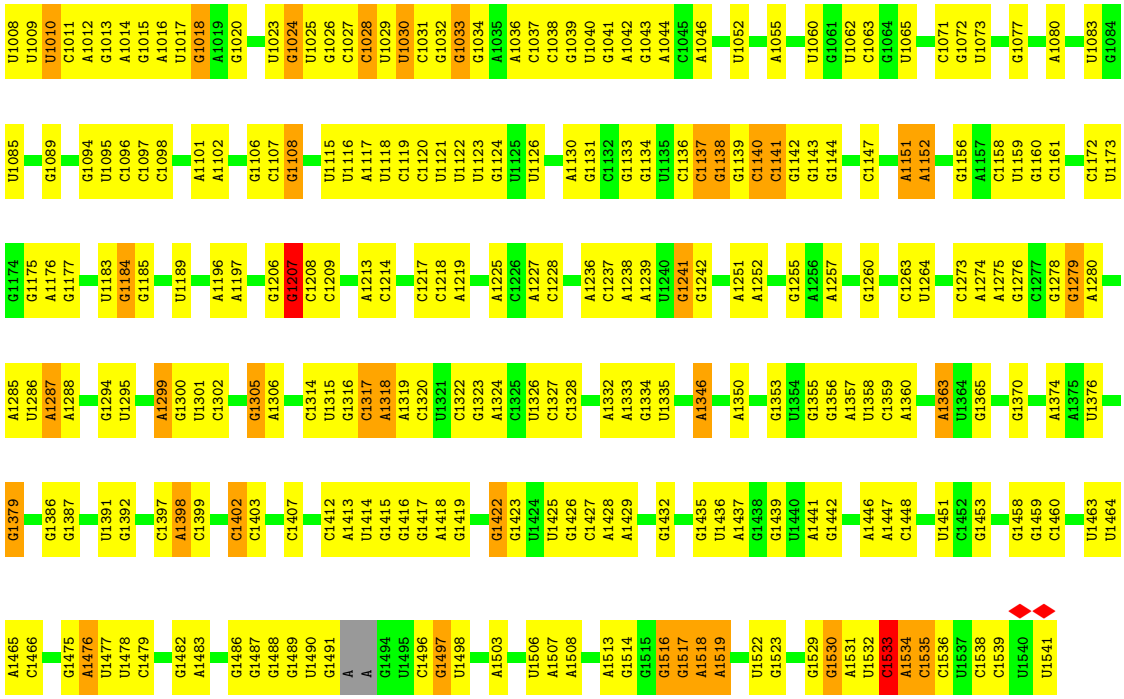
3 Residue-property plots (i)

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

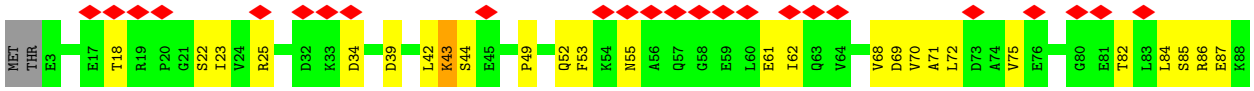
Chain A:

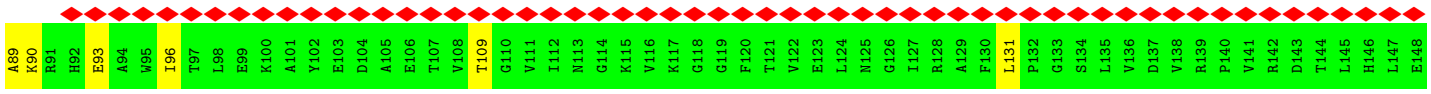


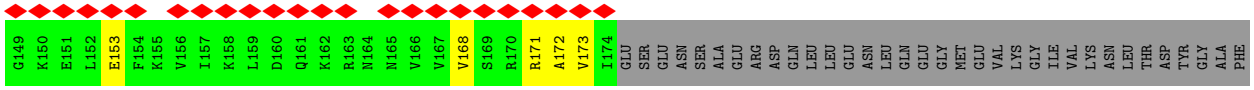


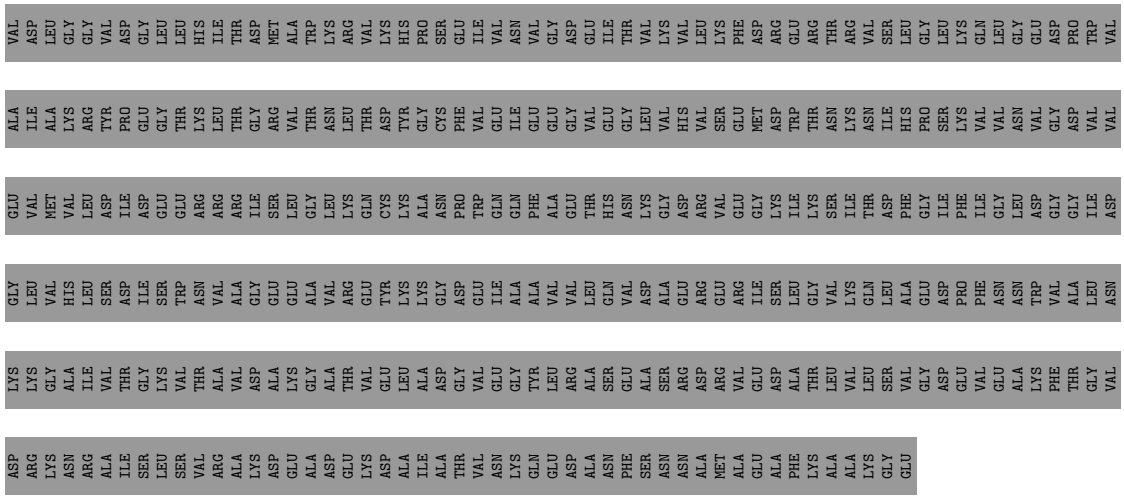
- Molecule 2: 30S ribosomal protein S1

Chain B:



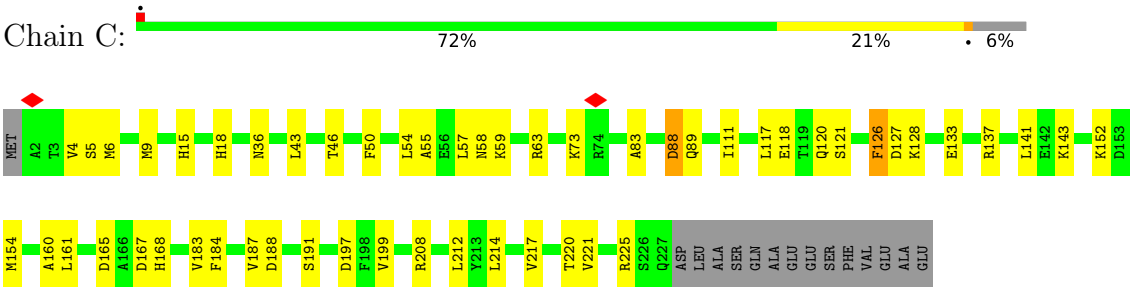






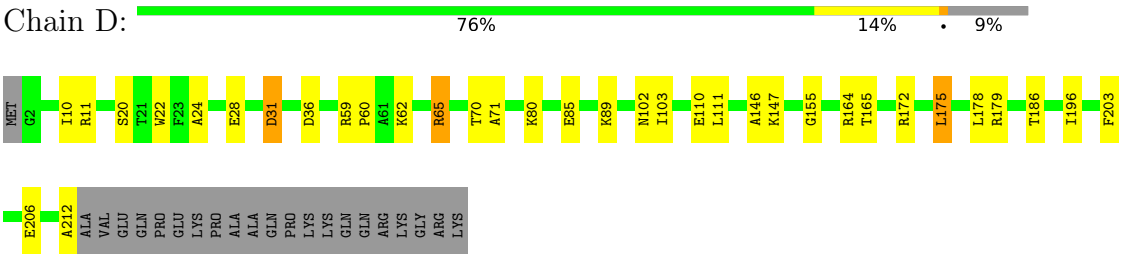
• Molecule 3: 30S ribosomal protein S2

Chain C:



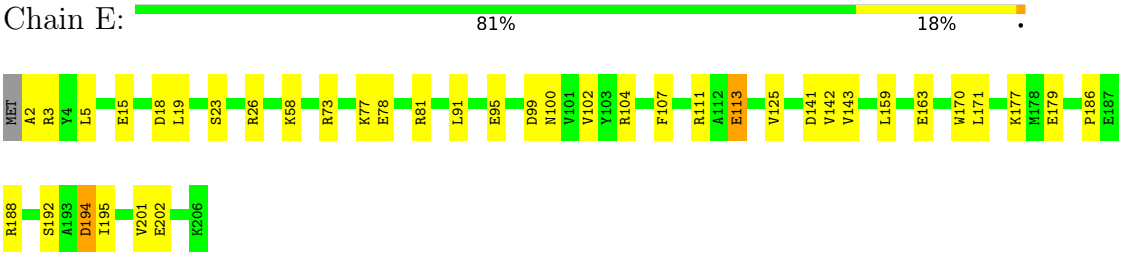
• Molecule 4: Small ribosomal subunit protein uS3

Chain D:



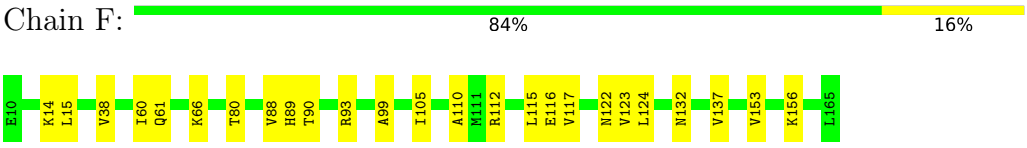
• Molecule 5: Small ribosomal subunit protein uS4

Chain E:



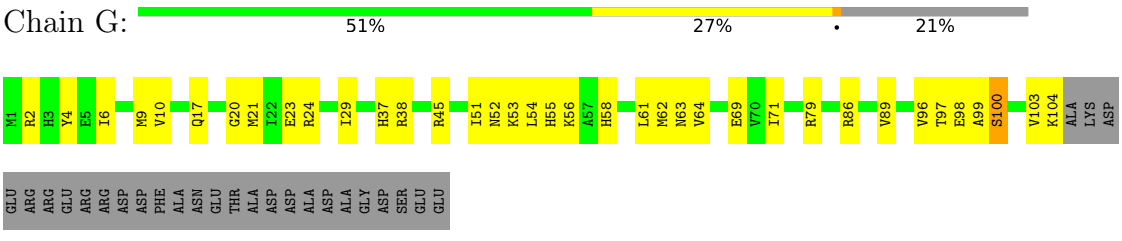
• Molecule 6: 30S ribosomal protein S5

Chain F:



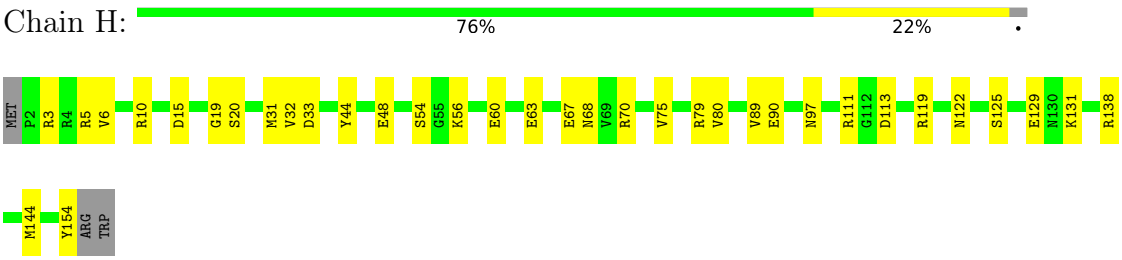
• Molecule 7: Small ribosomal subunit protein bS6, non-modified isoform

Chain G:



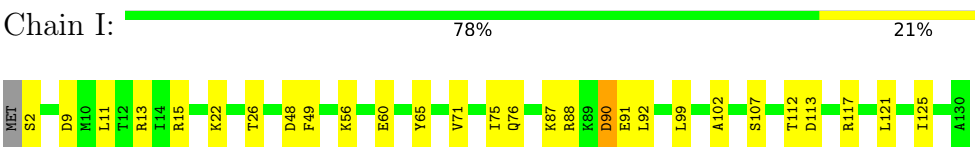
• Molecule 8: 30S ribosomal protein S7

Chain H:



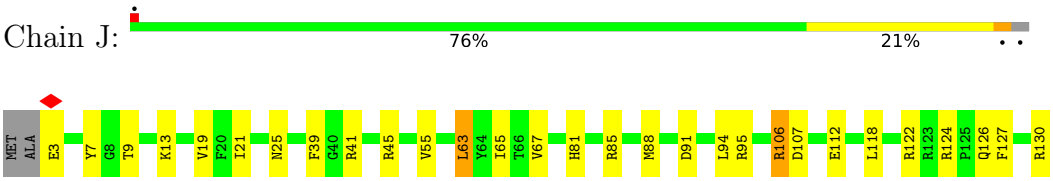
• Molecule 9: 30S ribosomal protein S8

Chain I:



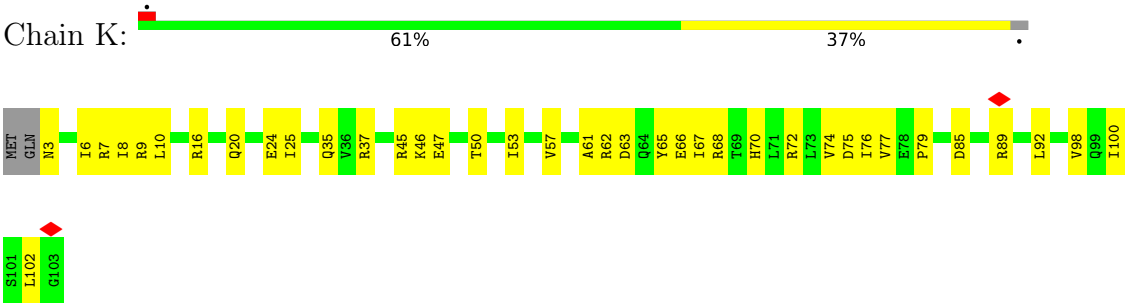
• Molecule 10: 30S ribosomal protein S9

Chain J:



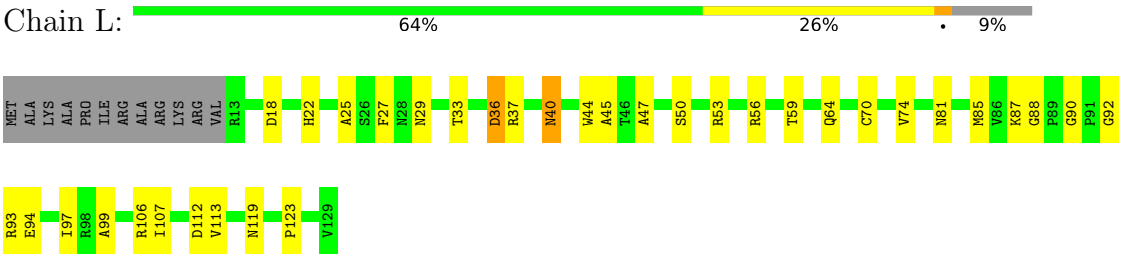
• Molecule 11: 30S ribosomal protein S10

Chain K:



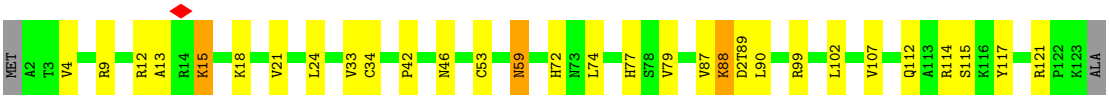
• Molecule 12: 30S ribosomal protein S11

Chain L:



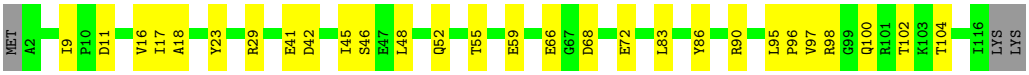
• Molecule 13: 30S ribosomal protein S12

Chain M:



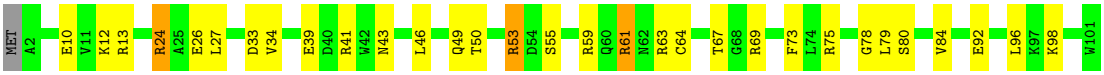
• Molecule 14: 30S ribosomal protein S13

Chain N:



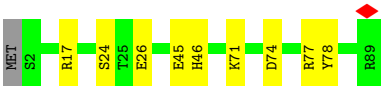
• Molecule 15: 30S ribosomal protein S14

Chain O:



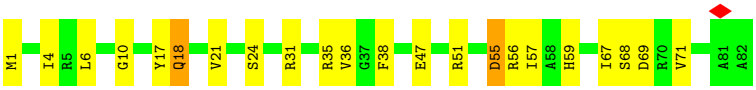
• Molecule 16: Small ribosomal subunit protein uS15

Chain P:



• Molecule 17: 30S ribosomal protein S16

Chain Q:

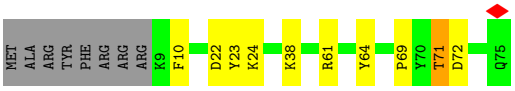


• Molecule 18: 30S ribosomal protein S17

Chain R:

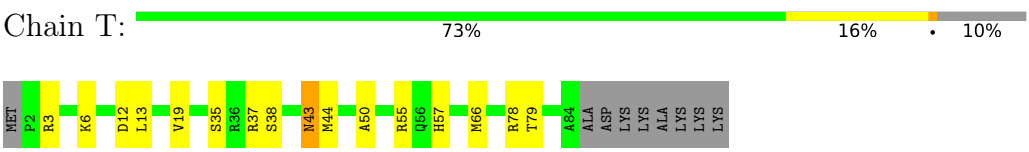
• Molecule 19: 30S ribosomal protein S18

Chain S:



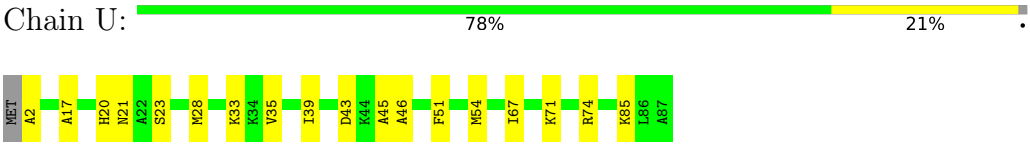
• Molecule 20: 30S ribosomal protein S19

Chain T:



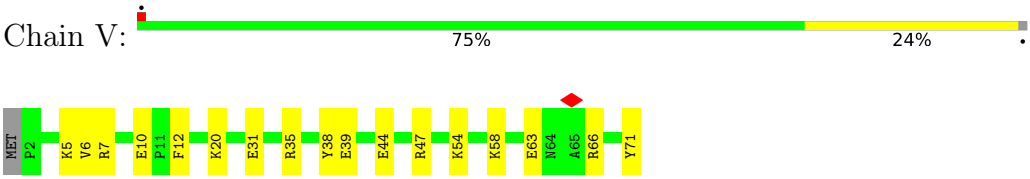
• Molecule 21: 30S ribosomal protein S20

Chain U:



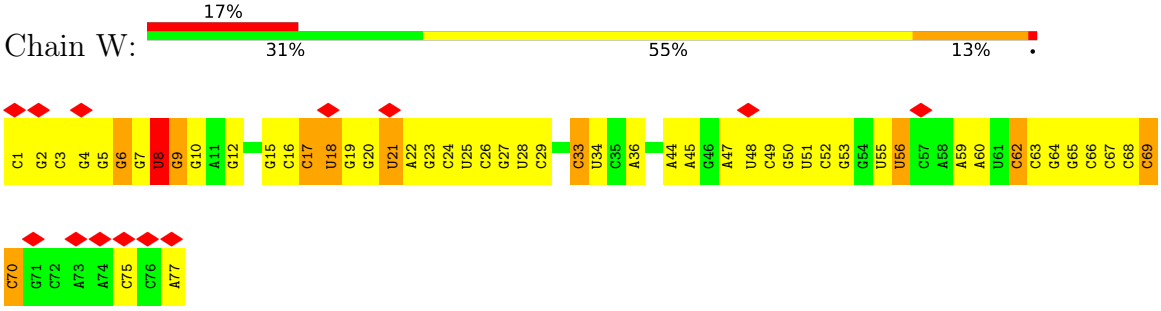
• Molecule 22: 30S ribosomal protein S21

Chain V:



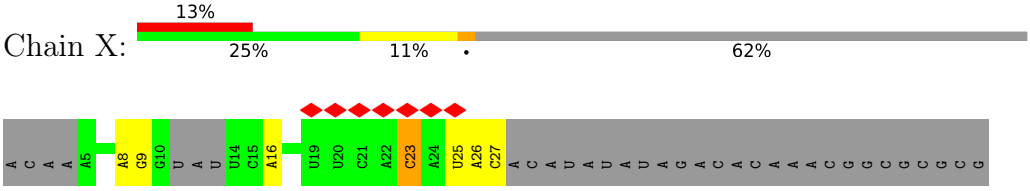
• Molecule 23: tRNA(fmet) P-site

Chain W:



• Molecule 24: 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	20551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	1.745	Depositor
Minimum map value	-0.554	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.253	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 5MC, 4OC, OMC, 5MU, MA6, UR3, MG, 2MG, 4SU, PSU, D2T, G7M

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	0.62	0/36692	0.80	10/57230 (0.0%)
2	B	0.25	0/1102	0.45	0/1504
3	C	0.30	0/1796	0.50	0/2420
4	D	0.34	0/1680	0.53	0/2263
5	E	0.33	0/1665	0.54	0/2227
6	F	0.34	0/1165	0.53	0/1568
7	G	0.34	0/867	0.52	0/1171
8	H	0.29	0/1219	0.53	0/1635
9	I	0.33	0/989	0.50	0/1326
10	J	0.34	0/1043	0.58	0/1387
11	K	0.32	0/818	0.55	0/1105
12	L	0.32	0/893	0.54	0/1205
13	M	0.36	0/954	0.59	0/1279
14	N	0.30	0/900	0.55	0/1204
15	O	0.34	0/817	0.53	0/1088
16	P	0.30	0/722	0.53	0/964
17	Q	0.36	0/659	0.56	0/884
18	R	0.31	0/657	0.53	0/881
19	S	0.34	0/563	0.55	0/754
20	T	0.33	0/680	0.52	0/915
21	U	0.30	0/676	0.47	0/895
22	V	0.29	0/598	0.59	0/792
23	W	0.44	1/1725 (0.1%)	0.89	2/2687 (0.1%)
24	X	0.32	0/476	0.77	0/737
All	All	0.53	1/59356 (0.0%)	0.73	12/88121 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	1	C	OP3-P	-10.54	1.48	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	883	C	N3-C2-O2	-7.89	116.38	121.90
1	A	882	C	N3-C2-O2	-6.82	117.13	121.90
1	A	812	G	O4'-C1'-N9	6.46	113.37	108.20
23	W	69	C	N1-C2-O2	-6.26	115.15	118.90
1	A	1533	C	C2-N1-C1'	6.16	125.58	118.80
1	A	998	C	N3-C2-O2	-5.82	117.83	121.90
1	A	1533	C	N1-C2-O2	5.77	122.36	118.90
23	W	69	C	N3-C2-O2	5.46	125.72	121.90
1	A	998	C	N1-C2-O2	5.29	122.08	118.90
1	A	883	C	C6-N1-C2	-5.12	118.25	120.30
1	A	536	C	C2-N1-C1'	5.08	124.39	118.80
1	A	641	U	P-O3'-C3'	5.02	125.73	119.70

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	A	33023	0	16643	510	0
2	B	1094	0	866	26	0
3	C	1765	0	1792	34	0
4	D	1653	0	1727	19	0
5	E	1643	0	1707	31	0
6	F	1152	0	1196	17	0
7	G	848	0	846	27	0
8	H	1203	0	1254	20	0
9	I	979	0	1031	17	0
10	J	1031	0	1076	17	0
11	K	808	0	845	26	0
12	L	877	0	887	22	0
13	M	951	0	1010	20	0
14	N	891	0	952	19	0
15	O	805	0	844	24	0
16	P	714	0	734	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	649	0	666	16	0
18	R	648	0	691	9	0
19	S	554	0	573	9	0
20	T	663	0	688	15	0
21	U	670	0	719	11	0
22	V	590	0	629	10	0
23	W	1645	0	842	43	0
24	X	427	0	217	4	0
25	A	127	0	0	0	0
25	X	1	0	0	0	0
All	All	55411	0	38435	850	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 (850) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:U:H3	1:A:1475:G:H1	1.05	0.91
1:A:1006:G:H1	1:A:1023:U:H3	1.21	0.88
23:W:8:4SU:H5"	23:W:50:G:H5'	1.55	0.85
1:A:1418:A:N6	1:A:1482:G:O2'	2.08	0.85
1:A:1423:G:H1	1:A:1477:U:H3	1.24	0.85
10:J:130:ARG:NH2	23:W:34:U:OP2	2.11	0.84
11:K:65:TYR:HB3	15:O:96:LEU:HD11	1.60	0.83
1:A:1040:U:H2'	1:A:1041:G:H8	1.44	0.81
1:A:76:G:H1	1:A:93:U:H3	1.25	0.81
1:A:150:U:H3	1:A:171:A:H62	1.31	0.78
3:C:58:ASN:HB3	3:C:220:THR:HG22	1.66	0.78
8:H:111:ARG:HD2	8:H:119:ARG:HG3	1.65	0.78
1:A:405:U:OP2	5:E:3:ARG:NH2	2.16	0.78
2:B:52:GLN:HB3	2:B:86:ARG:HB2	1.66	0.76
1:A:1006:G:N2	1:A:1023:U:O2	2.19	0.75
14:N:23:TYR:HB3	14:N:66:GLU:HB3	1.69	0.75
6:F:99:ALA:HB2	6:F:124:LEU:HG	1.69	0.75
9:I:11:LEU:HD22	9:I:75:ILE:HD11	1.69	0.74
1:A:859:G:H2'	1:A:860:A:H8	1.53	0.73
1:A:744:C:H2'	1:A:745:G:H8	1.54	0.72
8:H:75:VAL:HG21	8:H:144:MET:HG2	1.71	0.72
1:A:677:U:H3	1:A:713:G:H22	1.37	0.72
5:E:100:ASN:OD1	5:E:111:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:63:C:H2'	23:W:64:G:H8	1.54	0.72
1:A:933:G:N7	8:H:3:ARG:NH1	2.37	0.72
15:O:41:ARG:NH2	20:T:6:LYS:O	2.23	0.71
1:A:1118:U:OP1	10:J:106:ARG:NH1	2.23	0.71
12:L:93:ARG:NH2	12:L:112:ASP:OD2	2.23	0.71
1:A:8:A:N6	5:E:202:GLU:O	2.23	0.71
1:A:297:G:N2	1:A:300:A:OP2	2.22	0.71
1:A:261:U:OP2	21:U:74:ARG:NH2	2.24	0.71
1:A:713:G:H2'	1:A:714:G:C8	2.27	0.69
7:G:37:HIS:HB3	7:G:97:THR:HG22	1.74	0.69
2:B:70:VAL:HG22	2:B:86:ARG:HD3	1.75	0.69
17:Q:4:ILE:HG12	17:Q:21:VAL:HG22	1.74	0.69
1:A:1052:U:O2'	1:A:1055:A:OP2	2.12	0.68
2:B:43:LYS:HE2	3:C:18:HIS:HD2	1.59	0.68
3:C:6:MET:HA	3:C:9:MET:HE2	1.76	0.68
1:A:1137:C:O2	1:A:1138:G:N1	2.27	0.68
2:B:93:GLU:HA	2:B:96:ILE:HB	1.76	0.68
9:I:92:LEU:O	9:I:117:ARG:NH2	2.27	0.68
1:A:1535:C:H2'	1:A:1536:C:H6	1.57	0.67
6:F:14:LYS:NZ	6:F:116:GLU:OE1	2.28	0.67
1:A:1530:G:H2'	1:A:1531:A:H8	1.60	0.67
1:A:1037:C:H2'	1:A:1038:C:H6	1.60	0.67
1:A:71:A:H61	1:A:99:C:H1'	1.60	0.67
1:A:1328:C:O2'	14:N:29:ARG:NH2	2.28	0.67
1:A:616:G:O2'	17:Q:47:GLU:OE2	2.12	0.67
9:I:9:ASP:OD2	9:I:13:ARG:NH1	2.27	0.66
17:Q:18:GLN:HE21	17:Q:35:ARG:HE	1.41	0.66
1:A:492:C:H2'	1:A:493:A:C8	2.29	0.66
1:A:501:C:OP1	13:M:114:ARG:NH2	2.28	0.66
14:N:16:VAL:HG13	14:N:17:ILE:HD12	1.78	0.66
12:L:18:ASP:OD2	12:L:37:ARG:NH2	2.29	0.66
3:C:187:VAL:HG23	3:C:191:SER:HB2	1.77	0.65
4:D:111:LEU:HD11	4:D:146:ALA:HB2	1.78	0.65
18:R:5:ILE:HD12	18:R:62:ARG:HG3	1.78	0.65
1:A:1535:C:H2'	1:A:1536:C:C6	2.31	0.65
1:A:460:A:H2'	1:A:461:A:C8	2.31	0.65
1:A:1414:U:H2'	1:A:1415:G:H8	1.60	0.65
1:A:1239:A:H62	1:A:1299:A:H62	1.43	0.65
1:A:981:U:O2'	15:O:61:ARG:NH1	2.30	0.65
17:Q:1:MET:SD	17:Q:24:SER:OG	2.54	0.65
1:A:1147:C:O2'	10:J:7:TYR:OH	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:H2'	1:A:1131:G:H8	1.62	0.64
10:J:88:MET:HE1	10:J:95:ARG:HB2	1.80	0.64
1:A:407:U:O2'	5:E:113:GLU:OE1	2.15	0.64
1:A:1516:2MG:N2	1:A:1519:MA6:OP2	2.30	0.64
1:A:980:C:O2'	15:O:13:ARG:NH1	2.30	0.64
1:A:1363:A:O2'	1:A:1365:G:N7	2.26	0.64
5:E:194:ASP:OD1	5:E:194:ASP:N	2.30	0.64
1:A:1359:C:OP2	15:O:75:ARG:NH1	2.31	0.64
7:G:4:TYR:HD2	7:G:71:ILE:HG13	1.63	0.64
14:N:86:TYR:OH	14:N:90:ARG:NH2	2.30	0.64
1:A:235:C:H2'	1:A:236:A:H8	1.64	0.63
3:C:88:ASP:HB2	3:C:225:ARG:HH12	1.63	0.63
1:A:714:G:H2'	1:A:715:A:C8	2.33	0.63
1:A:859:G:H2'	1:A:860:A:C8	2.33	0.63
1:A:1417:G:O2'	1:A:1483:A:N6	2.32	0.63
1:A:460:A:H2'	1:A:461:A:H8	1.62	0.63
1:A:674:G:N2	1:A:717:U:O2	2.29	0.63
22:V:5:LYS:NZ	22:V:6:VAL:O	2.27	0.63
1:A:1029:U:O2'	1:A:1032:G:O6	2.12	0.63
13:M:88:LYS:O	13:M:90:LEU:N	2.32	0.63
1:A:736:C:OP1	19:S:61:ARG:NH1	2.31	0.63
1:A:738:C:OP1	7:G:2:ARG:NH1	2.32	0.62
1:A:1391:U:H2'	1:A:1392:G:C8	2.34	0.62
3:C:161:LEU:HB2	3:C:183:VAL:HG12	1.81	0.62
4:D:179:ARG:NE	4:D:206:GLU:OE2	2.32	0.62
23:W:4:G:H2'	23:W:5:G:C8	2.35	0.62
1:A:1305:G:H21	1:A:1332:A:H2	1.45	0.62
3:C:160:ALA:HB1	3:C:184:PHE:HE1	1.64	0.62
1:A:76:G:H2'	1:A:77:A:C8	2.35	0.62
1:A:356:A:N3	1:A:368:U:O2'	2.27	0.62
1:A:1037:C:H2'	1:A:1038:C:C6	2.35	0.61
7:G:21:MET:HG2	7:G:24:ARG:HH22	1.63	0.61
1:A:751:U:OP1	16:P:17:ARG:NH2	2.33	0.61
23:W:23:G:H2'	23:W:24:C:C6	2.35	0.61
23:W:64:G:H2'	23:W:65:G:H8	1.64	0.61
13:M:33:VAL:HG22	13:M:79:VAL:HG12	1.82	0.61
14:N:11:ASP:HA	14:N:45:ILE:HB	1.82	0.61
1:A:147:G:H2'	1:A:148:G:C8	2.35	0.61
10:J:81:HIS:CE1	10:J:85:ARG:HH21	2.17	0.61
23:W:51:U:H2'	23:W:52:C:C6	2.36	0.61
1:A:335:C:H2'	1:A:336:A:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:GLU:OE1	2:B:87:GLU:N	2.31	0.61
8:H:113:ASP:OD2	8:H:122:ASN:ND2	2.33	0.61
1:A:310:G:H5"	17:Q:31:ARG:HB2	1.81	0.61
1:A:1439:G:OP1	21:U:33:LYS:NZ	2.34	0.61
7:G:29:ILE:HD13	7:G:64:VAL:HG11	1.83	0.61
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	1.99	0.61
15:O:39:GLU:OE1	15:O:43:ASN:ND2	2.33	0.61
19:S:71:THR:OG1	19:S:72:ASP:N	2.33	0.61
1:A:126:G:OP1	1:A:605:U:O2'	2.19	0.60
1:A:1422:G:N2	1:A:1478:U:O2	2.26	0.60
1:A:459:A:H2'	1:A:460:A:H8	1.64	0.60
1:A:1005:A:OP2	1:A:1024:G:N2	2.32	0.60
1:A:1488:G:H2'	1:A:1489:G:C8	2.36	0.60
2:B:44:SER:OG	2:B:82:THR:N	2.32	0.60
1:A:765:G:H1	1:A:812:G:HO2'	1.50	0.60
2:B:53:PHE:HE1	2:B:68:VAL:HG11	1.66	0.60
6:F:110:ALA:HB1	6:F:137:VAL:HG23	1.84	0.60
23:W:15:G:N2	23:W:49:C:O2	2.28	0.60
1:A:1323:G:H2'	1:A:1324:A:C8	2.36	0.60
1:A:673:A:H2'	1:A:674:G:C8	2.36	0.60
1:A:1422:G:H1	1:A:1478:U:H3	1.49	0.60
21:U:35:VAL:HG21	21:U:54:MET:HG2	1.84	0.60
1:A:79:G:H2'	1:A:80:A:C8	2.36	0.60
1:A:1040:U:H2'	1:A:1041:G:C8	2.32	0.60
1:A:459:A:H2'	1:A:460:A:C8	2.37	0.60
1:A:877:G:C2	1:A:878:A:N7	2.70	0.60
14:N:11:ASP:OD1	14:N:46:SER:N	2.34	0.60
1:A:1322:C:OP1	20:T:78:ARG:NH2	2.34	0.60
5:E:95:GLU:OE2	5:E:104:ARG:NH1	2.35	0.60
7:G:69:GLU:OE1	7:G:69:GLU:N	2.29	0.59
11:K:8:ILE:HG12	11:K:100:ILE:HG12	1.82	0.59
1:A:80:A:H2'	1:A:81:A:C8	2.37	0.59
1:A:405:U:O4	5:E:2:ALA:N	2.35	0.59
1:A:744:C:H2'	1:A:745:G:C8	2.36	0.59
1:A:1152:A:OP1	11:K:70:HIS:ND1	2.35	0.59
2:B:23:ILE:HA	2:B:71:ALA:HA	1.83	0.59
15:O:49:GLN:NE2	20:T:12:ASP:OD1	2.34	0.59
23:W:23:G:H2'	23:W:24:C:H6	1.67	0.59
1:A:562:U:C4	13:M:15:LYS:HG2	2.37	0.59
1:A:1279:G:OP1	11:K:9:ARG:NH2	2.35	0.59
16:P:24:SER:OG	16:P:26:GLU:OE1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:H2'	1:A:1252:A:C8	2.37	0.59
1:A:31:G:O2'	1:A:48:C:N4	2.36	0.59
1:A:979:C:O2	15:O:59:ARG:NH1	2.36	0.59
1:A:1464:U:H2'	1:A:1465:A:H8	1.68	0.59
6:F:105:ILE:O	6:F:112:ARG:NH2	2.35	0.59
15:O:24:ARG:NH1	15:O:55:SER:OG	2.36	0.59
1:A:56:U:H2'	1:A:57:G:H8	1.67	0.59
1:A:333:U:OP1	21:U:2:ALA:N	2.35	0.59
1:A:447:G:N1	1:A:486:U:OP2	2.30	0.59
1:A:997:U:H2'	1:A:998:C:H6	1.68	0.59
11:K:7:ARG:NH1	11:K:75:ASP:OD2	2.35	0.59
1:A:974:A:OP1	15:O:69:ARG:NH2	2.35	0.59
3:C:18:HIS:NE2	3:C:188:ASP:OD2	2.36	0.58
1:A:707:U:H2'	1:A:708:C:H6	1.68	0.58
1:A:875:U:O2'	9:I:15:ARG:NH1	2.35	0.58
5:E:188:ARG:NH2	5:E:195:ILE:O	2.36	0.58
15:O:10:GLU:HG3	15:O:63:ARG:HD2	1.84	0.58
7:G:10:VAL:HG22	7:G:58:HIS:HB3	1.85	0.58
1:A:380:G:N2	1:A:383:A:OP2	2.30	0.58
1:A:890:G:O2'	1:A:906:A:N6	2.35	0.58
1:A:1425:U:O2	1:A:1475:G:N2	2.24	0.58
1:A:837:U:H2'	1:A:838:G:H8	1.69	0.58
1:A:404:G:O6	5:E:2:ALA:N	2.37	0.58
5:E:78:GLU:OE2	5:E:81:ARG:NH2	2.32	0.58
1:A:230:G:OP1	17:Q:31:ARG:NH2	2.36	0.58
1:A:1356:G:H2'	1:A:1357:A:C8	2.39	0.58
23:W:63:C:H2'	23:W:64:G:C8	2.35	0.58
1:A:321:A:H2'	1:A:322:C:H6	1.69	0.58
1:A:1004:A:H2'	1:A:1005:A:O4'	2.04	0.58
12:L:123:PRO:HD2	22:V:38:TYR:HB2	1.85	0.58
1:A:408:A:O3'	5:E:23:SER:OG	2.22	0.57
1:A:1239:A:H62	1:A:1299:A:N6	2.02	0.57
23:W:4:G:H2'	23:W:5:G:H8	1.68	0.57
1:A:1218:C:H2'	1:A:1219:A:C8	2.39	0.57
1:A:56:U:H2'	1:A:57:G:C8	2.39	0.57
1:A:539:A:H2'	1:A:540:G:C8	2.39	0.57
1:A:745:G:H2'	1:A:746:A:C8	2.40	0.57
11:K:53:ILE:HD11	11:K:61:ALA:HB1	1.87	0.57
1:A:321:A:H2'	1:A:322:C:C6	2.39	0.57
1:A:411:A:OP2	5:E:26:ARG:NH2	2.37	0.57
1:A:976:G:OP2	1:A:1358:U:O2'	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:C:H2'	1:A:1072:G:H8	1.70	0.57
7:G:100:SER:O	7:G:104:LYS:NZ	2.37	0.57
1:A:728:A:H2'	1:A:729:A:C8	2.39	0.57
7:G:38:ARG:HB3	7:G:63:ASN:HB3	1.86	0.57
1:A:427:U:OP2	1:A:428:G:O2'	2.20	0.56
1:A:1120:C:H2'	1:A:1121:U:H6	1.70	0.56
11:K:35:GLN:HG3	11:K:77:VAL:HG23	1.87	0.56
1:A:689:C:OP1	12:L:29:ASN:ND2	2.37	0.56
1:A:1538:C:H2'	1:A:1539:C:C6	2.41	0.56
7:G:4:TYR:CD2	7:G:71:ILE:HG13	2.39	0.56
1:A:235:C:H2'	1:A:236:A:C8	2.40	0.56
2:B:22:SER:O	2:B:72:LEU:N	2.35	0.56
6:F:156:LYS:HD2	9:I:71:VAL:HA	1.87	0.56
4:D:31:ASP:OD1	4:D:31:ASP:N	2.36	0.56
10:J:130:ARG:HH22	23:W:33:OMC:P	2.29	0.56
1:A:1488:G:H2'	1:A:1489:G:H8	1.71	0.56
2:B:171:ARG:O	2:B:173:VAL:N	2.39	0.56
9:I:90:ASP:OD1	9:I:90:ASP:N	2.39	0.56
10:J:21:ILE:HD13	10:J:63:LEU:HB3	1.88	0.56
1:A:390:U:H2'	1:A:391:G:H8	1.70	0.56
1:A:1427:C:H2'	1:A:1428:A:H8	1.71	0.56
1:A:1038:C:H2'	1:A:1039:G:C8	2.41	0.55
2:B:43:LYS:HE2	3:C:18:HIS:CD2	2.41	0.55
21:U:28:MET:HE1	21:U:67:ILE:HD12	1.88	0.55
1:A:384:G:H2'	1:A:385:C:C6	2.41	0.55
13:M:102:LEU:HD12	13:M:102:LEU:H	1.70	0.55
1:A:17:U:H2'	1:A:18:C:C6	2.41	0.55
1:A:78:A:H2'	1:A:79:G:C8	2.42	0.55
21:U:17:ALA:O	21:U:21:ASN:ND2	2.23	0.55
1:A:81:A:H2'	1:A:82:G:C8	2.40	0.55
15:O:92:GLU:OE1	15:O:92:GLU:N	2.39	0.55
1:A:996:A:H2'	1:A:997:U:C6	2.41	0.55
14:N:52:GLN:O	14:N:55:THR:OG1	2.17	0.55
1:A:1010:U:H2'	1:A:1011:C:H6	1.71	0.55
1:A:1010:U:H2'	1:A:1011:C:C6	2.42	0.55
2:B:87:GLU:HA	2:B:90:LYS:HG2	1.87	0.55
23:W:66:C:H2'	23:W:67:C:C6	2.42	0.55
1:A:216:U:H2'	1:A:217:C:C6	2.41	0.55
1:A:868:C:H2'	1:A:869:G:O4'	2.07	0.55
10:J:7:TYR:HH	10:J:9:THR:HG1	1.55	0.55
1:A:360:G:H2'	1:A:361:G:C8	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:A:H5”	20:T:3:ARG:HH12	1.72	0.54
1:A:1534:A:H3’	1:A:1535:C:C6	2.42	0.54
2:B:25:ARG:HA	2:B:69:ASP:HA	1.89	0.54
1:A:79:G:H2’	1:A:80:A:H8	1.70	0.54
1:A:524:G:H2’	1:A:525:C:C6	2.43	0.54
1:A:946:A:O2’	1:A:1333:A:N3	2.37	0.54
11:K:20:GLN:O	11:K:24:GLU:HG2	2.06	0.54
23:W:8:4SU:H6	23:W:8:4SU:O5’	2.07	0.54
1:A:820:U:H4’	1:A:821:G:OP2	2.07	0.54
11:K:8:ILE:HB	11:K:74:VAL:HG23	1.89	0.54
1:A:1314:C:H2’	1:A:1315:U:C6	2.43	0.54
7:G:21:MET:HG2	7:G:24:ARG:NH2	2.22	0.54
1:A:254:G:N2	18:R:18:GLU:OE2	2.41	0.54
1:A:728:A:H2’	1:A:729:A:H8	1.72	0.54
1:A:1522:U:H2’	1:A:1523:G:H8	1.73	0.54
3:C:59:LYS:HG2	3:C:63:ARG:HH21	1.72	0.54
1:A:719:C:H1’	19:S:38:LYS:HB2	1.90	0.54
1:A:1314:C:H2’	1:A:1315:U:H6	1.73	0.54
1:A:1507:A:H2’	1:A:1508:A:C8	2.43	0.54
20:T:35:SER:OG	20:T:38:SER:OG	2.21	0.54
16:P:74:ASP:OD2	16:P:77:ARG:NH1	2.41	0.54
1:A:946:A:H2’	1:A:947:G:C8	2.43	0.54
1:A:1219:A:H5”	15:O:53:ARG:HH12	1.73	0.54
12:L:81:ASN:HA	12:L:106:ARG:HB2	1.90	0.54
3:C:55:ALA:HA	3:C:58:ASN:HD21	1.73	0.54
3:C:88:ASP:HB2	3:C:225:ARG:NH1	2.23	0.53
3:C:126:PHE:HD1	3:C:127:ASP:H	1.56	0.53
10:J:118:LEU:HD22	10:J:124:ARG:HG2	1.90	0.53
15:O:64:CYS:HB2	15:O:80:SER:HB3	1.90	0.53
1:A:35:G:H2’	1:A:36:C:C6	2.43	0.53
1:A:458:U:H3	1:A:474:G:H1	1.55	0.53
1:A:1412:C:H2’	1:A:1413:A:C8	2.43	0.53
1:A:1451:U:O2’	1:A:1453:G:N7	2.41	0.53
7:G:38:ARG:NH1	7:G:98:GLU:O	2.42	0.53
15:O:49:GLN:HE22	20:T:12:ASP:HA	1.72	0.53
1:A:1447:A:OP1	1:A:1448:C:N4	2.38	0.53
1:A:299:G:H2’	1:A:300:A:C8	2.44	0.53
1:A:1316:G:N1	1:A:1319:A:OP2	2.38	0.53
1:A:1317:C:N3	20:T:37:ARG:NH1	2.44	0.53
1:A:1533:C:H4’	1:A:1534:A:O5’	2.08	0.53
23:W:68:C:H2’	23:W:69:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:G:N2	1:A:365:U:OP2	2.41	0.53
1:A:1486:G:H2'	1:A:1487:G:C8	2.43	0.53
17:Q:56:ARG:HH12	17:Q:59:HIS:CD2	2.26	0.53
1:A:390:U:H2'	1:A:391:G:C8	2.44	0.53
1:A:707:U:H2'	1:A:708:C:C6	2.44	0.53
1:A:1513:A:H2'	1:A:1514:G:C8	2.43	0.53
1:A:501:C:H2'	1:A:502:A:H8	1.74	0.53
1:A:674:G:H2'	1:A:675:A:C8	2.43	0.53
1:A:825:A:H2'	1:A:826:C:H6	1.73	0.53
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.08	0.53
5:E:104:ARG:HH21	5:E:111:ARG:HH22	1.57	0.52
22:V:39:GLU:OE2	22:V:47:ARG:NH2	2.43	0.52
23:W:2:G:H2'	23:W:3:C:C6	2.43	0.52
1:A:653:U:O5'	9:I:56:LYS:NZ	2.41	0.52
1:A:1287:A:H2'	1:A:1288:A:C8	2.45	0.52
1:A:1478:U:H2'	1:A:1479:C:C6	2.44	0.52
1:A:765:G:N2	1:A:813:U:OP2	2.33	0.52
10:J:39:PHE:O	10:J:45:ARG:NH1	2.42	0.52
1:A:739:C:OP2	7:G:2:ARG:NH2	2.43	0.52
13:M:72:HIS:HB3	13:M:99:ARG:HH22	1.73	0.52
1:A:1033:G:H2'	1:A:1034:G:H8	1.74	0.52
4:D:24:ALA:HB1	4:D:28:GLU:HG2	1.92	0.52
1:A:1003:G:N2	1:A:1005:A:O5'	2.43	0.52
20:T:50:ALA:HB1	20:T:57:HIS:HB3	1.91	0.52
1:A:407:U:H2'	1:A:408:A:H8	1.73	0.52
1:A:844:G:H3'	1:A:844:G:N3	2.25	0.52
1:A:876:C:H2'	1:A:877:G:H8	1.75	0.52
1:A:1391:U:H2'	1:A:1392:G:H8	1.74	0.52
2:B:55:ASN:ND2	2:B:61:GLU:OE1	2.43	0.52
1:A:922:G:H2'	1:A:923:A:C8	2.45	0.52
1:A:1041:G:H2'	1:A:1042:A:C8	2.45	0.52
1:A:736:C:H2'	1:A:737:C:H6	1.74	0.51
1:A:1413:A:H2	1:A:1487:G:H22	1.57	0.51
13:M:21:VAL:HG11	13:M:24:LEU:HD22	1.92	0.51
1:A:1379:G:OP2	8:H:5:ARG:NH1	2.44	0.51
6:F:115:LEU:HD13	6:F:123:VAL:HG11	1.91	0.51
8:H:54:SER:OG	8:H:56:LYS:NZ	2.41	0.51
1:A:28:A:O2'	1:A:296:U:OP1	2.28	0.51
1:A:555:U:H2'	1:A:556:C:C6	2.46	0.51
1:A:1143:G:H2'	1:A:1144:G:H8	1.74	0.51
1:A:687:A:N7	1:A:701:U:N3	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:C:H2'	1:A:1120:C:H6	1.76	0.51
1:A:1120:C:H2'	1:A:1121:U:C6	2.46	0.51
2:B:18:THR:O	3:C:36:ASN:ND2	2.43	0.51
10:J:55:VAL:HG21	10:J:94:LEU:HD13	1.93	0.51
23:W:2:G:H2'	23:W:3:C:H6	1.76	0.51
1:A:1436:U:H2'	1:A:1437:A:H8	1.75	0.51
4:D:36:ASP:OD1	4:D:59:ARG:NH1	2.39	0.51
12:L:25:ALA:HB1	12:L:90:GLY:HA3	1.93	0.51
1:A:339:C:H2'	1:A:340:U:H6	1.76	0.50
1:A:996:A:H2'	1:A:997:U:H6	1.76	0.50
1:A:1323:G:H2'	1:A:1324:A:H8	1.76	0.50
1:A:1513:A:H2'	1:A:1514:G:H8	1.76	0.50
13:M:59:ASN:N	13:M:59:ASN:OD1	2.44	0.50
23:W:4:G:C2	23:W:5:G:C5	2.99	0.50
1:A:938:A:N3	1:A:1376:U:O2'	2.39	0.50
1:A:1386:G:H2'	1:A:1387:G:H8	1.76	0.50
1:A:337:G:H2'	1:A:338:A:C8	2.45	0.50
1:A:401:C:O2'	1:A:621:A:N3	2.39	0.50
7:G:99:ALA:HB1	7:G:103:VAL:HG21	1.93	0.50
1:A:746:A:H2'	1:A:747:A:C8	2.47	0.50
1:A:1397:C:O4'	24:X:23:C:N4	2.45	0.50
1:A:1538:C:H2'	1:A:1539:C:H6	1.77	0.50
1:A:1077:G:N2	1:A:1080:A:OP2	2.35	0.50
1:A:945:G:C2	1:A:946:A:C8	3.00	0.50
1:A:1183:U:O2'	1:A:1185:G:OP2	2.30	0.50
1:A:1397:C:O2	24:X:23:C:N4	2.42	0.50
10:J:130:ARG:NH1	23:W:33:OMC:OP2	2.28	0.50
11:K:3:ASN:HB3	11:K:79:PRO:HD2	1.93	0.50
11:K:67:ILE:HG12	15:O:96:LEU:HD13	1.92	0.50
23:W:64:G:H2'	23:W:65:G:C8	2.45	0.50
1:A:545:C:OP1	5:E:58:LYS:NZ	2.45	0.50
1:A:1011:C:H2'	1:A:1012:A:H8	1.76	0.50
6:F:89:HIS:CD2	6:F:90:THR:HG23	2.47	0.50
8:H:67:GLU:HA	8:H:70:ARG:HH21	1.76	0.50
12:L:64:GLN:HG3	12:L:99:ALA:HB2	1.94	0.50
1:A:552:U:C2	1:A:553:A:C8	3.00	0.50
1:A:1417:G:N2	1:A:1482:G:H2'	2.26	0.50
1:A:1477:U:H2'	1:A:1478:U:C6	2.47	0.50
7:G:45:ARG:O	7:G:56:LYS:HA	2.12	0.50
15:O:46:LEU:O	15:O:50:THR:HG23	2.12	0.50
23:W:62:C:H2'	23:W:63:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:G:H2'	1:A:1007:U:H6	1.77	0.49
7:G:51:ILE:HG22	7:G:52:ASN:ND2	2.26	0.49
23:W:24:C:H2'	23:W:25:U:H6	1.77	0.49
9:I:26:THR:HG22	9:I:60:GLU:HG2	1.94	0.49
1:A:270:A:H2'	1:A:271:C:C6	2.46	0.49
5:E:188:ARG:NH1	5:E:192:SER:O	2.42	0.49
1:A:801:U:H2'	1:A:802:A:H8	1.77	0.49
7:G:9:MET:HG2	7:G:86:ARG:HB2	1.94	0.49
20:T:19:VAL:HG11	20:T:44:MET:HG2	1.93	0.49
1:A:500:G:H2'	1:A:501:C:C6	2.47	0.49
1:A:845:A:H8	19:S:10:PHE:CD1	2.29	0.49
20:T:12:ASP:OD2	20:T:35:SER:OG	2.21	0.49
1:A:335:C:H2'	1:A:336:A:C8	2.47	0.49
1:A:253:A:H2'	1:A:254:G:C8	2.47	0.49
1:A:1476:A:H2'	1:A:1477:U:C6	2.48	0.49
9:I:102:ALA:N	9:I:113:ASP:OD2	2.46	0.49
21:U:43:ASP:OD1	21:U:46:ALA:N	2.33	0.49
1:A:17:U:H2'	1:A:18:C:H6	1.77	0.49
1:A:223:A:H2'	1:A:224:U:C6	2.48	0.49
1:A:309:A:H2'	1:A:310:G:H8	1.77	0.49
17:Q:55:ASP:N	17:Q:55:ASP:OD1	2.44	0.49
1:A:407:U:H2'	1:A:408:A:C8	2.48	0.49
1:A:440:C:C2	1:A:441:A:C8	3.01	0.49
1:A:1490:U:H2'	1:A:1491:G:C8	2.47	0.49
4:D:20:SER:OG	4:D:22:TRP:NE1	2.46	0.49
11:K:46:LYS:HG2	11:K:68:ARG:HG3	1.95	0.49
12:L:88:GLY:O	12:L:93:ARG:NH1	2.46	0.49
23:W:68:C:H2'	23:W:69:C:H6	1.78	0.49
1:A:1126:U:OP1	11:K:7:ARG:NH2	2.45	0.48
1:A:1425:U:H2'	1:A:1426:G:H8	1.78	0.48
2:B:42:LEU:HD13	2:B:75:VAL:HG13	1.93	0.48
8:H:97:ASN:N	8:H:97:ASN:OD1	2.45	0.48
3:C:183:VAL:HG23	3:C:197:ASP:H	1.77	0.48
23:W:62:C:H2'	23:W:63:C:H6	1.77	0.48
1:A:202:G:O2'	1:A:468:A:H8	1.94	0.48
1:A:946:A:H2'	1:A:947:G:H8	1.78	0.48
1:A:1427:C:H2'	1:A:1428:A:C8	2.48	0.48
1:A:1489:G:H2'	1:A:1490:U:C6	2.48	0.48
3:C:88:ASP:O	3:C:89:GLN:NE2	2.45	0.48
7:G:20:GLY:O	7:G:23:GLU:HG2	2.14	0.48
12:L:33:THR:HG22	12:L:44:TRP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:A:H61	1:A:558:G:H1'	1.79	0.48
1:A:219:U:H2'	1:A:220:G:H8	1.78	0.48
1:A:384:G:H2'	1:A:385:C:H6	1.76	0.48
1:A:791:G:O6	1:A:792:A:N6	2.44	0.48
1:A:1458:G:H2'	1:A:1459:G:H8	1.78	0.48
3:C:54:LEU:HG	3:C:220:THR:HG21	1.95	0.48
16:P:45:GLU:HG3	16:P:46:HIS:HD1	1.77	0.48
1:A:338:A:H2'	1:A:339:C:H6	1.78	0.48
1:A:842:U:H4'	1:A:846:G:C6	2.49	0.48
1:A:1038:C:H2'	1:A:1039:G:H8	1.77	0.48
1:A:1273:C:H2'	1:A:1274:A:O4'	2.12	0.48
1:A:1436:U:H2'	1:A:1437:A:C8	2.48	0.48
10:J:7:TYR:OH	10:J:9:THR:OG1	2.25	0.48
1:A:337:G:H2'	1:A:338:A:H8	1.78	0.48
1:A:472:U:H2'	1:A:473:U:C6	2.49	0.48
1:A:638:U:C2	1:A:639:G:C8	3.02	0.48
1:A:707:U:H4'	12:L:22:HIS:ND1	2.28	0.48
1:A:843:U:OP1	1:A:844:G:N1	2.46	0.48
10:J:19:VAL:HG22	10:J:65:ILE:HG23	1.94	0.48
11:K:66:GLU:OE2	11:K:68:ARG:NH2	2.36	0.48
3:C:117:LEU:HD21	3:C:137:ARG:HG3	1.96	0.48
1:A:645:G:C2	1:A:646:G:C8	3.02	0.47
1:A:1350:A:O2'	8:H:33:ASP:OD1	2.32	0.47
1:A:22:G:H2'	1:A:23:C:H6	1.78	0.47
1:A:1033:G:C4	1:A:1034:G:C8	3.02	0.47
5:E:102:VAL:HG22	5:E:107:PHE:HB2	1.95	0.47
23:W:49:C:O2'	23:W:60:A:H1'	2.14	0.47
1:A:184:G:H2'	1:A:185:U:C6	2.49	0.47
1:A:270:A:H2'	1:A:271:C:H6	1.80	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.50	0.47
2:B:52:GLN:HE22	2:B:85:SER:HA	1.79	0.47
3:C:57:LEU:HD13	3:C:217:VAL:HG13	1.96	0.47
4:D:70:THR:OG1	4:D:71:ALA:N	2.47	0.47
19:S:22:ASP:O	19:S:24:LYS:N	2.47	0.47
1:A:76:G:H2'	1:A:77:A:H8	1.77	0.47
3:C:73:LYS:HD2	3:C:165:ASP:HB2	1.96	0.47
12:L:22:HIS:HD2	12:L:85:MET:HB2	1.79	0.47
13:M:87:VAL:HG23	13:M:90:LEU:HB3	1.95	0.47
1:A:625:U:H2'	1:A:626:G:H8	1.79	0.47
1:A:1130:A:H2'	1:A:1131:G:C8	2.46	0.47
1:A:1206:G:H2'	1:A:1207:2MG:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:42:PRO:HB2	13:M:46:ASN:HB2	1.95	0.47
1:A:882:C:O2'	1:A:883:C:H5'	2.15	0.47
3:C:111:ILE:HD12	3:C:152:LYS:HA	1.95	0.47
4:D:147:LYS:HB2	4:D:203:PHE:CD2	2.49	0.47
1:A:575:G:H4'	1:A:576:C:H5"	1.96	0.47
1:A:936:C:C2	1:A:937:A:C8	3.02	0.47
1:A:993:G:O2'	1:A:994:A:N7	2.47	0.47
1:A:1017:U:HO2'	1:A:1018:G:H8	1.58	0.47
1:A:1487:G:C2	1:A:1488:G:C8	3.02	0.47
4:D:155:GLY:O	4:D:196:ILE:HG12	2.13	0.47
4:D:175:LEU:HD12	4:D:175:LEU:HA	1.72	0.47
5:E:95:GLU:HG2	5:E:186:PRO:HG3	1.97	0.47
13:M:72:HIS:HB2	13:M:74:LEU:HD13	1.95	0.47
15:O:49:GLN:NE2	20:T:13:LEU:H	2.12	0.47
20:T:55:ARG:HH22	20:T:79:THR:HG21	1.79	0.47
23:W:6:G:N1	23:W:69:C:N3	2.62	0.47
23:W:27:G:H22	23:W:45:A:H2	1.62	0.47
1:A:22:G:H2'	1:A:23:C:C6	2.50	0.47
1:A:636:U:H2'	1:A:637:C:H6	1.80	0.47
1:A:878:A:C2	1:A:879:C:C2	3.03	0.47
1:A:1137:C:H1'	1:A:1138:G:N2	2.29	0.47
1:A:1255:G:OP2	11:K:45:ARG:NH2	2.47	0.47
1:A:736:C:H2'	1:A:737:C:C6	2.50	0.47
1:A:950:U:H2'	1:A:951:G:C8	2.50	0.47
6:F:89:HIS:CD2	6:F:90:THR:H	2.33	0.47
1:A:358:U:H2'	1:A:359:G:H8	1.80	0.47
1:A:501:C:H2'	1:A:502:A:C8	2.49	0.47
1:A:900:A:H2'	1:A:901:A:C8	2.50	0.47
1:A:1039:G:H2'	1:A:1040:U:C6	2.50	0.47
1:A:1062:U:H2'	1:A:1063:C:C6	2.49	0.47
1:A:1117:A:N6	1:A:1156:G:H22	2.12	0.47
1:A:1175:G:H2'	1:A:1176:A:H8	1.79	0.47
7:G:63:ASN:ND2	7:G:96:VAL:O	2.48	0.47
14:N:41:GLU:N	14:N:41:GLU:OE1	2.47	0.47
1:A:35:G:H2'	1:A:36:C:H6	1.80	0.46
1:A:1530:G:H2'	1:A:1531:A:C8	2.46	0.46
2:B:71:ALA:H	2:B:89:ALA:HB2	1.79	0.46
4:D:164:ARG:NE	24:X:25:U:O2	2.48	0.46
9:I:87:LYS:HG3	9:I:125:ILE:HD11	1.98	0.46
21:U:43:ASP:OD1	21:U:45:ALA:N	2.48	0.46
22:V:7:ARG:N	22:V:10:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:6:G:C2	23:W:69:C:C2	3.03	0.46
1:A:411:A:P	5:E:26:ARG:HH22	2.38	0.46
1:A:708:C:H2'	1:A:709:U:H6	1.79	0.46
1:A:710:G:OP1	7:G:53:LYS:NZ	2.42	0.46
1:A:1008:U:H2'	1:A:1009:U:H6	1.80	0.46
1:A:1118:U:H2'	1:A:1119:C:H6	1.79	0.46
14:N:98:ARG:HB2	14:N:100:GLN:HE22	1.81	0.46
1:A:562:U:H1'	13:M:12:ARG:HB3	1.98	0.46
1:A:1176:A:H2'	1:A:1177:G:C8	2.50	0.46
1:A:1417:G:H2'	1:A:1482:G:N2	2.31	0.46
1:A:1463:U:H2'	1:A:1464:U:C6	2.50	0.46
5:E:159:LEU:O	5:E:163:GLU:HG2	2.14	0.46
6:F:38:VAL:HG12	6:F:117:VAL:HG11	1.98	0.46
1:A:93:U:H2'	1:A:95:C:H5	1.81	0.46
1:A:455:G:C2	1:A:478:A:C2	3.03	0.46
1:A:1098:C:O2'	22:V:71:TYR:OXT	2.31	0.46
1:A:1121:U:C2	1:A:1122:U:C5	3.03	0.46
1:A:1121:U:H2'	1:A:1122:U:H6	1.80	0.46
3:C:15:HIS:HB3	3:C:43:LEU:HD11	1.98	0.46
11:K:6:ILE:HG13	11:K:76:ILE:HB	1.98	0.46
1:A:253:A:H2'	1:A:254:G:H8	1.80	0.46
1:A:284:C:H2'	1:A:285:C:C6	2.51	0.46
1:A:624:C:H4'	17:Q:10:GLY:HA2	1.98	0.46
1:A:1096:C:H2'	1:A:1097:C:H6	1.80	0.46
5:E:170:TRP:CE2	5:E:186:PRO:HB3	2.51	0.46
12:L:97:ILE:HG22	22:V:12:PHE:HZ	1.81	0.46
14:N:42:ASP:OD1	14:N:42:ASP:N	2.49	0.46
14:N:55:THR:O	14:N:59:GLU:HG2	2.15	0.46
1:A:122:G:H2'	1:A:123:U:H6	1.81	0.46
1:A:338:A:H2'	1:A:339:C:C6	2.50	0.46
7:G:51:ILE:O	7:G:54:LEU:HB3	2.16	0.46
12:L:119:ASN:OD1	22:V:35:ARG:NH2	2.44	0.46
15:O:79:LEU:HB2	15:O:84:VAL:HG23	1.98	0.46
1:A:222:C:H2'	1:A:223:A:H8	1.81	0.46
1:A:284:C:H2'	1:A:285:C:H6	1.80	0.46
1:A:539:A:H2'	1:A:540:G:H8	1.81	0.46
1:A:676:A:H2'	1:A:677:U:H6	1.80	0.46
3:C:4:VAL:HG11	3:C:212:LEU:HD11	1.98	0.46
1:A:684:U:H2'	1:A:685:G:O4'	2.16	0.46
1:A:1478:U:H2'	1:A:1479:C:H6	1.81	0.46
23:W:24:C:H2'	23:W:25:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:G:H2'	1:A:185:U:H6	1.80	0.45
1:A:704:A:C4	1:A:705:G:C8	3.04	0.45
1:A:1107:C:C4	1:A:1108:G:C8	3.04	0.45
14:N:68:ASP:O	14:N:72:GLU:HG2	2.15	0.45
23:W:33:OMC:H1'	23:W:33:OMC:HM23	1.66	0.45
1:A:21:G:H2'	1:A:22:G:C8	2.51	0.45
1:A:1016:A:HO2'	1:A:1217:C:HO2'	1.63	0.45
1:A:1120:C:C2	1:A:1121:U:C5	3.04	0.45
1:A:1414:U:H2'	1:A:1415:G:C8	2.46	0.45
1:A:1497:G:H1'	1:A:1518:MA6:H2	1.97	0.45
14:N:68:ASP:N	14:N:68:ASP:OD1	2.50	0.45
1:A:339:C:H2'	1:A:340:U:C6	2.51	0.45
4:D:10:ILE:HG23	4:D:11:ARG:HG3	1.98	0.45
8:H:56:LYS:HB3	8:H:60:GLU:CD	2.37	0.45
8:H:129:GLU:HG3	8:H:131:LYS:HD3	1.99	0.45
11:K:85:ASP:O	11:K:89:ARG:HG2	2.17	0.45
12:L:92:GLY:C	12:L:94:GLU:H	2.20	0.45
1:A:204:U:H2'	1:A:205:A:O4'	2.15	0.45
1:A:236:A:H2'	1:A:237:G:C8	2.52	0.45
1:A:468:A:H3'	1:A:469:C:H6	1.81	0.45
1:A:839:C:H2'	1:A:840:C:C6	2.52	0.45
1:A:866:C:C4	1:A:867:G:H1'	2.52	0.45
3:C:120:GLN:HB3	3:C:126:PHE:HE2	1.82	0.45
10:J:112:GLU:OE2	10:J:122:ARG:NH2	2.43	0.45
1:A:19:A:H2'	1:A:20:U:C6	2.51	0.45
1:A:500:G:H2'	1:A:501:C:H6	1.81	0.45
1:A:677:U:O2	1:A:777:A:O2'	2.34	0.45
1:A:1305:G:HO2'	1:A:1306:A:H8	1.60	0.45
5:E:170:TRP:CD2	5:E:186:PRO:HB3	2.52	0.45
22:V:31:GLU:OE2	22:V:35:ARG:NE	2.34	0.45
1:A:154:U:H2'	1:A:155:A:H8	1.81	0.45
1:A:204:U:C2	1:A:205:A:C8	3.05	0.45
1:A:632:U:H5'	1:A:633:G:C8	2.51	0.45
1:A:651:C:H2'	1:A:652:U:C6	2.51	0.45
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.84	0.45
12:L:47:ALA:O	12:L:50:SER:OG	2.34	0.45
12:L:107:ILE:HG13	22:V:12:PHE:CE1	2.52	0.45
14:N:90:ARG:HD2	14:N:95:LEU:HB2	1.98	0.45
1:A:575:G:C4	1:A:881:G:N2	2.85	0.45
1:A:634:C:H2'	1:A:635:A:H8	1.81	0.45
17:Q:67:ILE:HG23	17:Q:71:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:69:PRO:HB2	19:S:71:THR:O	2.17	0.45
1:A:901:A:C5	1:A:902:G:H1'	2.51	0.45
1:A:1083:U:O2'	1:A:1102:A:OP2	2.31	0.45
1:A:1151:A:HO2'	1:A:1152:A:H8	1.59	0.45
3:C:126:PHE:C	3:C:128:LYS:H	2.20	0.45
1:A:344:A:OP2	1:A:345:C:N4	2.39	0.44
1:A:678:U:H2'	1:A:679:C:H6	1.82	0.44
1:A:1121:U:H2'	1:A:1122:U:C6	2.53	0.44
7:G:86:ARG:NH1	19:S:64:TYR:O	2.50	0.44
1:A:26:A:N6	1:A:558:G:H1'	2.32	0.44
1:A:1029:U:H5"	1:A:1030:U:OP1	2.17	0.44
1:A:1036:A:H2'	1:A:1037:C:C6	2.52	0.44
1:A:1355:G:H2'	1:A:1356:G:H8	1.82	0.44
1:A:1465:A:H2'	1:A:1466:C:C6	2.52	0.44
8:H:89:VAL:HG12	8:H:90:GLU:O	2.17	0.44
23:W:56:PSU:N3	23:W:59:A:OP2	2.29	0.44
17:Q:38:PHE:HE2	17:Q:51:ARG:HE	1.64	0.44
1:A:494:G:O2'	1:A:496:A:H1'	2.17	0.44
3:C:83:ALA:HB2	3:C:214:LEU:HB3	1.99	0.44
1:A:113:G:H2'	1:A:114:U:C6	2.53	0.44
1:A:950:U:H2'	1:A:951:G:H8	1.81	0.44
1:A:977:A:O2'	1:A:979:C:OP2	2.35	0.44
2:B:131:LEU:HA	2:B:168:VAL:O	2.18	0.44
1:A:217:C:H2'	1:A:218:U:H6	1.83	0.44
1:A:468:A:H5"	1:A:469:C:H5	1.82	0.44
1:A:1005:A:C6	1:A:1006:G:H1'	2.52	0.44
1:A:1015:G:O2'	1:A:1218:C:O2'	2.34	0.44
1:A:1477:U:H2'	1:A:1478:U:H6	1.82	0.44
5:E:15:GLU:HG3	5:E:19:LEU:HD11	2.00	0.44
12:L:36:ASP:OD1	12:L:37:ARG:N	2.51	0.44
23:W:28:U:H2'	23:W:29:C:H6	1.82	0.44
1:A:792:A:H1'	1:A:794:A:N7	2.33	0.44
1:A:874:G:C6	1:A:875:U:C4	3.06	0.44
1:A:1152:A:P	11:K:72:ARG:HH22	2.41	0.44
1:A:1189:U:OP1	15:O:98:LYS:NZ	2.51	0.44
8:H:15:ASP:OD1	8:H:20:SER:N	2.33	0.44
23:W:16:C:O2'	23:W:62:C:OP1	2.36	0.44
1:A:410:G:H2'	1:A:429:U:C4	2.52	0.44
16:P:71:LYS:HB2	16:P:78:TYR:CD1	2.53	0.44
1:A:513:C:H2'	1:A:514:C:C6	2.53	0.44
1:A:634:C:H2'	1:A:635:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:47:A:H2'	23:W:48:U:H5"	2.00	0.44
1:A:18:C:OP1	6:F:132:ASN:ND2	2.46	0.43
1:A:90:C:H2'	1:A:91:U:C6	2.53	0.43
1:A:1376:U:O4	8:H:10:ARG:NH2	2.29	0.43
1:A:1533:C:H1'	1:A:1534:A:OP2	2.17	0.43
5:E:202:GLU:OE1	6:F:112:ARG:NH1	2.42	0.43
7:G:6:ILE:HG12	7:G:89:VAL:HG13	2.00	0.43
11:K:25:ILE:HD11	11:K:92:LEU:HD21	2.00	0.43
14:N:46:SER:C	14:N:48:LEU:H	2.22	0.43
1:A:160:A:H2'	1:A:161:A:C8	2.53	0.43
1:A:769:G:H4'	1:A:1513:A:H4'	2.00	0.43
1:A:1118:U:H2'	1:A:1119:C:C6	2.53	0.43
1:A:1275:A:H2'	1:A:1276:G:O4'	2.17	0.43
1:A:1326:U:H2'	1:A:1327:C:C6	2.53	0.43
1:A:1422:G:C2	1:A:1479:C:C2	3.07	0.43
6:F:156:LYS:HG2	9:I:71:VAL:HG13	2.00	0.43
1:A:237:G:H5"	18:R:27:ARG:NH2	2.33	0.43
1:A:255:G:H2'	1:A:256:U:C6	2.53	0.43
1:A:373:A:C2	1:A:374:A:C8	3.07	0.43
1:A:399:G:H2'	1:A:400:C:C6	2.53	0.43
1:A:405:U:C5	5:E:5:LEU:HD11	2.54	0.43
1:A:745:G:H2'	1:A:746:A:H8	1.80	0.43
1:A:1060:U:H5"	11:K:53:ILE:HD12	2.00	0.43
12:L:56:ARG:O	12:L:59:THR:OG1	2.36	0.43
1:A:470:C:H2'	1:A:471:U:C6	2.53	0.43
1:A:613:C:H2'	1:A:614:C:C6	2.54	0.43
1:A:1115:U:H2'	1:A:1116:U:C6	2.53	0.43
1:A:1123:U:O2'	1:A:1124:G:H5'	2.19	0.43
1:A:1496:C:O2'	1:A:1517:G:N1	2.52	0.43
6:F:88:VAL:HG22	6:F:93:ARG:HG2	2.00	0.43
6:F:153:VAL:HG11	9:I:99:LEU:HG	2.00	0.43
1:A:35:G:N3	13:M:115:SER:OG	2.52	0.43
1:A:80:A:C6	1:A:81:A:N6	2.86	0.43
1:A:691:G:O6	12:L:53:ARG:NH2	2.52	0.43
1:A:707:U:C2	1:A:708:C:C5	3.07	0.43
1:A:1134:G:N1	1:A:1141:C:N3	2.67	0.43
5:E:141:ASP:OD1	5:E:142:VAL:N	2.51	0.43
6:F:60:ILE:HG13	6:F:61:GLN:N	2.33	0.43
1:A:60:A:OP1	1:A:331:G:N1	2.38	0.43
1:A:264:C:O2'	18:R:66:PRO:O	2.36	0.43
1:A:825:A:H2'	1:A:826:C:C6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:A:H2'	1:A:1001:C:C6	2.54	0.43
1:A:1263:C:H2'	1:A:1264:U:H6	1.84	0.43
1:A:1458:G:H2'	1:A:1459:G:C8	2.54	0.43
3:C:217:VAL:O	3:C:221:VAL:HG22	2.18	0.43
5:E:18:ASP:OD1	5:E:19:LEU:N	2.52	0.43
13:M:34:CYS:SG	13:M:53:CYS:HB2	2.58	0.43
23:W:9:G:O2'	23:W:10:G:N7	2.45	0.43
1:A:411:A:H4'	1:A:412:A:H5'	2.00	0.43
1:A:1013:G:N2	1:A:1016:A:OP2	2.37	0.43
8:H:31:MET:HG2	8:H:32:VAL:N	2.34	0.43
8:H:63:GLU:O	8:H:67:GLU:HG3	2.19	0.43
1:A:1000:A:C6	1:A:1041:G:C6	3.07	0.43
2:B:49:PRO:HD2	2:B:52:GLN:NE2	2.33	0.43
7:G:103:VAL:HG22	7:G:104:LYS:HZ2	1.83	0.43
1:A:376:G:H2'	1:A:377:G:H8	1.84	0.43
1:A:855:U:H2'	1:A:856:C:H6	1.84	0.43
4:D:60:PRO:HG3	4:D:65:ARG:HH21	1.84	0.43
15:O:26:GLU:HG3	15:O:27:LEU:N	2.32	0.43
1:A:161:A:H2'	1:A:162:A:C8	2.54	0.43
1:A:514:C:C2	1:A:515:G:C8	3.07	0.43
1:A:823:C:HO2'	9:I:2:SER:N	2.17	0.43
1:A:943:U:H1'	10:J:126:GLN:HE22	1.84	0.43
1:A:1096:C:H2'	1:A:1097:C:C6	2.54	0.43
2:B:86:ARG:HH11	2:B:89:ALA:HB3	1.84	0.43
7:G:103:VAL:HG22	7:G:104:LYS:NZ	2.34	0.43
13:M:107:VAL:HG12	13:M:117:TYR:HB3	2.00	0.43
1:A:100:G:C4	1:A:101:A:C8	3.07	0.42
1:A:552:U:N3	1:A:553:A:N7	2.67	0.42
1:A:763:G:H2'	1:A:764:C:H6	1.84	0.42
1:A:920:U:C2	1:A:921:U:C5	3.07	0.42
1:A:954:G:H2'	1:A:955:U:C6	2.53	0.42
1:A:1315:U:O2	1:A:1360:A:H2	2.01	0.42
1:A:1346:A:N1	1:A:1374:A:H5"	2.34	0.42
1:A:1428:A:H2'	1:A:1429:A:C8	2.54	0.42
2:B:53:PHE:CD2	2:B:62:ILE:HD13	2.54	0.42
23:W:66:C:C2	23:W:67:C:C5	3.07	0.42
1:A:652:U:O4	1:A:752:G:O2'	2.23	0.42
1:A:1014:A:C2	1:A:1219:A:H1'	2.53	0.42
2:B:39:ASP:OD2	3:C:208:ARG:NE	2.47	0.42
7:G:61:LEU:HD23	7:G:62:MET:N	2.34	0.42
18:R:68:SER:OG	18:R:69:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:G:C2	1:A:213:G:C8	3.07	0.42
1:A:482:A:H2'	1:A:483:C:O4'	2.19	0.42
1:A:649:A:H2'	1:A:650:G:O4'	2.20	0.42
1:A:662:U:H2'	1:A:663:A:C8	2.54	0.42
3:C:88:ASP:OD1	3:C:88:ASP:N	2.53	0.42
1:A:154:U:H2'	1:A:155:A:C8	2.54	0.42
1:A:500:G:H5"	13:M:121:ARG:NH1	2.33	0.42
1:A:562:U:N3	13:M:13:ALA:O	2.53	0.42
1:A:881:G:OP2	13:M:9:ARG:NH2	2.52	0.42
1:A:1435:G:H2'	1:A:1436:U:C6	2.53	0.42
1:A:1465:A:H2'	1:A:1466:C:H6	1.84	0.42
1:A:1519:MA6:O5'	1:A:1519:MA6:H8	2.19	0.42
2:B:72:LEU:HD23	2:B:84:LEU:HD21	2.01	0.42
4:D:102:ASN:O	4:D:103:ILE:HG13	2.20	0.42
11:K:45:ARG:NE	11:K:47:GLU:OE2	2.52	0.42
17:Q:6:LEU:HB3	17:Q:17:TYR:HB3	2.02	0.42
1:A:923:A:O2'	1:A:1399:C:OP2	2.29	0.42
1:A:1008:U:H2'	1:A:1009:U:C6	2.54	0.42
21:U:67:ILE:HD11	21:U:71:LYS:HE2	2.01	0.42
1:A:276:G:H2'	1:A:277:C:H6	1.85	0.42
1:A:424:G:H2'	1:A:425:G:H8	1.83	0.42
1:A:514:C:H2'	1:A:515:G:H8	1.83	0.42
1:A:783:C:H2'	1:A:784:A:H8	1.85	0.42
1:A:925:G:C2	1:A:927:G:C8	3.07	0.42
14:N:95:LEU:HB3	14:N:96:PRO:HD2	2.01	0.42
15:O:12:LYS:HB2	15:O:12:LYS:HE3	1.83	0.42
19:S:22:ASP:C	19:S:24:LYS:H	2.23	0.42
22:V:54:LYS:HZ2	22:V:58:LYS:HE3	1.84	0.42
1:A:111:G:O6	1:A:330:C:N4	2.46	0.42
1:A:1106:G:H5"	4:D:172:ARG:HB3	2.02	0.42
1:A:1124:G:H3'	11:K:37:ARG:HH21	1.85	0.42
1:A:1140:C:O2'	1:A:1141:C:H6	2.03	0.42
1:A:1241:G:H2'	1:A:1242:G:H8	1.85	0.42
1:A:1355:G:H2'	1:A:1356:G:C8	2.54	0.42
1:A:1402:4OC:H6	1:A:1402:4OC:O5'	2.20	0.42
2:B:109:THR:HA	2:B:153:GLU:HA	2.01	0.42
5:E:125:VAL:HG12	5:E:143:VAL:HG22	2.01	0.42
14:N:9:ILE:HG23	14:N:18:ALA:HB1	2.00	0.42
14:N:83:LEU:HD11	20:T:66:MET:HG2	2.02	0.42
23:W:17:C:H5"	23:W:18:U:H6	1.85	0.42
24:X:8:A:H2'	24:X:9:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:A:OP2	1:A:111:G:N2	2.53	0.42
1:A:135:C:N3	17:Q:1:MET:HB2	2.35	0.42
1:A:1236:A:H2'	1:A:1237:C:C6	2.54	0.42
23:W:24:C:C2	23:W:25:U:C5	3.07	0.42
1:A:695:A:H2'	1:A:696:A:C8	2.54	0.42
1:A:708:C:H2'	1:A:709:U:C6	2.55	0.42
1:A:131:A:H2'	1:A:132:C:C6	2.55	0.42
1:A:392:C:C2	1:A:393:A:C8	3.08	0.42
1:A:464:U:O2'	1:A:466:A:N7	2.41	0.42
1:A:911:U:H2'	1:A:912:C:C6	2.55	0.42
1:A:1218:C:H2'	1:A:1219:A:H8	1.81	0.42
3:C:143:LYS:HE3	3:C:143:LYS:HB2	1.78	0.42
8:H:15:ASP:OD1	8:H:19:GLY:N	2.53	0.42
21:U:20:HIS:O	21:U:23:SER:OG	2.30	0.42
1:A:210:C:H4'	1:A:211:G:H5"	2.01	0.41
1:A:1027:C:C2	1:A:1028:C:C5	3.08	0.41
4:D:62:LYS:HA	4:D:62:LYS:HD3	1.86	0.41
5:E:177:LYS:HD2	5:E:177:LYS:HA	1.94	0.41
6:F:66:LYS:HE2	6:F:66:LYS:HB2	1.88	0.41
8:H:125:SER:O	8:H:129:GLU:HG2	2.20	0.41
18:R:59:VAL:HG13	18:R:75:LEU:HD13	2.01	0.41
1:A:178:C:C2	1:A:179:A:C8	3.08	0.41
1:A:381:C:H2'	1:A:382:A:O4'	2.20	0.41
1:A:415:A:C4	1:A:416:G:C8	3.08	0.41
1:A:593:U:H2'	1:A:594:U:C6	2.55	0.41
1:A:1038:C:C2	1:A:1039:G:C8	3.08	0.41
1:A:1041:G:C2	1:A:1042:A:C5	3.08	0.41
1:A:1397:C:O2'	1:A:1398:A:OP1	2.34	0.41
1:A:593:U:H2'	1:A:594:U:H6	1.86	0.41
1:A:672:U:H2'	1:A:673:A:C8	2.55	0.41
1:A:687:A:C2	1:A:704:A:C5	3.08	0.41
1:A:1130:A:H61	1:A:1144:G:H1'	1.85	0.41
1:A:1415:G:C4	1:A:1416:G:C8	3.08	0.41
18:R:76:VAL:HG12	18:R:77:ARG:HG2	2.03	0.41
21:U:51:PHE:O	21:U:54:MET:HG3	2.20	0.41
1:A:189:A:H8	1:A:189:A:OP2	2.03	0.41
1:A:580:C:H2'	1:A:581:G:O4'	2.21	0.41
1:A:841:C:H5'	1:A:842:U:OP2	2.20	0.41
1:A:1006:G:H2'	1:A:1007:U:C6	2.56	0.41
1:A:1496:C:H2'	1:A:1497:G:O4'	2.19	0.41
3:C:127:ASP:OD1	3:C:127:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:ASN:HD22	20:T:43:ASN:H	1.68	0.41
23:W:69:C:H2'	23:W:70:C:C6	2.56	0.41
1:A:664:G:H22	1:A:741:G:H1	1.69	0.41
1:A:1299:A:O2'	1:A:1301:U:O4'	2.33	0.41
1:A:1459:G:H2'	1:A:1460:C:C6	2.55	0.41
8:H:44:TYR:O	8:H:48:GLU:HG2	2.20	0.41
12:L:40:ASN:OD1	12:L:40:ASN:N	2.50	0.41
17:Q:69:ASP:OD1	17:Q:69:ASP:N	2.53	0.41
1:A:20:U:H2'	1:A:21:G:O4'	2.21	0.41
1:A:202:G:O2'	1:A:468:A:H2'	2.20	0.41
1:A:1011:C:H2'	1:A:1012:A:C8	2.54	0.41
1:A:1333:A:H2'	1:A:1334:G:O4'	2.21	0.41
1:A:1447:A:P	1:A:1448:C:H41	2.42	0.41
5:E:91:LEU:HD23	5:E:91:LEU:HA	1.82	0.41
18:R:19:LYS:HD3	18:R:48:ASP:O	2.21	0.41
1:A:88:U:C4	1:A:89:U:C4	3.08	0.41
1:A:839:C:H2'	1:A:840:C:H6	1.86	0.41
1:A:1071:C:H2'	1:A:1072:G:C8	2.53	0.41
1:A:1072:G:H2'	1:A:1073:U:C6	2.55	0.41
1:A:1172:C:H2'	1:A:1173:U:C6	2.55	0.41
1:A:1208:C:H2'	1:A:1209:C:H6	1.86	0.41
2:B:72:LEU:HD23	2:B:72:LEU:HA	1.94	0.41
15:O:33:ASP:OD1	15:O:34:VAL:N	2.54	0.41
1:A:73:C:C2	1:A:74:A:C8	3.09	0.41
1:A:252:U:C2	1:A:253:A:N7	2.89	0.41
1:A:340:U:H2'	1:A:341:C:H6	1.86	0.41
4:D:80:LYS:HD2	4:D:80:LYS:HA	1.85	0.41
4:D:85:GLU:O	4:D:89:LYS:HG3	2.20	0.41
7:G:17:GLN:N	7:G:17:GLN:OE1	2.54	0.41
17:Q:36:VAL:HG21	17:Q:57:ILE:HD11	2.02	0.41
1:A:233:C:H2'	1:A:234:C:H6	1.86	0.41
1:A:236:A:H2'	1:A:237:G:H8	1.86	0.41
1:A:405:U:C6	5:E:5:LEU:HD11	2.56	0.41
1:A:855:U:H2'	1:A:856:C:C6	2.56	0.41
1:A:1151:A:O2'	1:A:1152:A:H8	2.04	0.41
3:C:154:MET:HB2	3:C:154:MET:HE3	1.94	0.41
6:F:80:THR:HG23	6:F:122:ASN:O	2.21	0.41
8:H:68:ASN:O	8:H:138:ARG:NH1	2.54	0.41
11:K:50:THR:HG22	11:K:62:ARG:HE	1.86	0.41
12:L:87:LYS:HB3	12:L:113:VAL:HG13	2.02	0.41
1:A:41:G:H2'	1:A:42:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:U:H2'	1:A:626:G:C8	2.54	0.41
1:A:878:A:H2'	1:A:879:C:C6	2.56	0.41
1:A:1027:C:H2'	1:A:1028:C:C6	2.56	0.41
1:A:1294:G:H2'	1:A:1295:U:C6	2.56	0.41
11:K:10:LEU:HD23	11:K:98:VAL:HG22	2.03	0.41
13:M:4:VAL:HG13	18:R:34:TYR:HB3	2.03	0.41
1:A:269:C:H2'	1:A:270:A:H8	1.85	0.40
4:D:212:ALA:HB2	11:K:16:ARG:NE	2.36	0.40
9:I:22:LYS:O	9:I:65:TYR:OH	2.32	0.40
11:K:6:ILE:HG22	11:K:102:LEU:HG	2.03	0.40
12:L:45:ALA:HB3	12:L:70:CYS:HB2	2.03	0.40
13:M:90:LEU:HD12	13:M:90:LEU:HA	1.92	0.40
15:O:73:PHE:CZ	15:O:78:GLY:HA2	2.55	0.40
1:A:4:U:O2'	1:A:5:U:OP2	2.32	0.40
1:A:123:U:H2'	1:A:124:C:C6	2.56	0.40
1:A:224:U:H2'	1:A:225:C:C6	2.56	0.40
1:A:590:U:H2'	1:A:591:U:H6	1.86	0.40
1:A:594:U:H2'	1:A:595:A:O4'	2.21	0.40
1:A:845:A:C2	1:A:846:G:H5'	2.55	0.40
1:A:1184:G:C2	1:A:1185:G:C8	3.10	0.40
9:I:48:ASP:OD1	9:I:49:PHE:N	2.55	0.40
19:S:10:PHE:O	19:S:10:PHE:CG	2.73	0.40
1:A:6:G:H4'	1:A:298:A:H4'	2.02	0.40
1:A:217:C:H2'	1:A:218:U:C6	2.57	0.40
1:A:575:G:C4	1:A:881:G:C2	3.09	0.40
1:A:604:G:H2'	1:A:605:U:O4'	2.21	0.40
1:A:642:A:N7	9:I:107:SER:HA	2.36	0.40
1:A:715:A:H2'	1:A:716:A:C8	2.56	0.40
1:A:763:G:H2'	1:A:764:C:C6	2.56	0.40
1:A:768:A:H4'	1:A:1523:G:N2	2.36	0.40
5:E:73:ARG:HH11	5:E:77:LYS:HE3	1.86	0.40
9:I:88:ARG:HB2	9:I:91:GLU:OE1	2.21	0.40
17:Q:68:SER:HB3	17:Q:71:VAL:HG22	2.03	0.40
23:W:17:C:H5"	23:W:18:U:C6	2.56	0.40
1:A:337:G:C2	1:A:338:A:C5	3.08	0.40
1:A:936:C:C4	1:A:937:A:N7	2.90	0.40
1:A:1160:G:C2	1:A:1161:C:C6	3.10	0.40
14:N:90:ARG:HG2	14:N:97:VAL:HA	2.04	0.40
23:W:26:C:C2	23:W:27:G:C8	3.09	0.40
1:A:238:A:H2'	1:A:239:U:O4'	2.21	0.40
1:A:471:U:H2'	1:A:472:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:C:H2'	1:A:514:C:H6	1.86	0.40
1:A:737:C:H2'	1:A:738:C:C6	2.56	0.40
1:A:1318:A:OP1	20:T:3:ARG:NH2	2.39	0.40
1:A:1418:A:N6	1:A:1482:G:HO2'	2.13	0.40
3:C:118:GLU:HB2	3:C:141:LEU:HD11	2.02	0.40
10:J:130:ARG:HD3	23:W:36:A:OP2	2.21	0.40
23:W:28:U:H2'	23:W:29:C:C6	2.57	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	170/557 (30%)	161 (95%)	8 (5%)	1 (1%)	22 53
3	C	224/241 (93%)	208 (93%)	16 (7%)	0	100 100
4	D	209/233 (90%)	201 (96%)	8 (4%)	0	100 100
5	E	203/206 (98%)	198 (98%)	5 (2%)	0	100 100
6	F	154/156 (99%)	140 (91%)	14 (9%)	0	100 100
7	G	102/131 (78%)	97 (95%)	5 (5%)	0	100 100
8	H	151/156 (97%)	140 (93%)	11 (7%)	0	100 100
9	I	127/130 (98%)	122 (96%)	5 (4%)	0	100 100
10	J	126/130 (97%)	114 (90%)	12 (10%)	0	100 100
11	K	99/103 (96%)	95 (96%)	3 (3%)	1 (1%)	13 42
12	L	115/129 (89%)	106 (92%)	9 (8%)	0	100 100
13	M	119/124 (96%)	107 (90%)	11 (9%)	1 (1%)	16 48
14	N	113/118 (96%)	108 (96%)	5 (4%)	0	100 100
15	O	98/101 (97%)	95 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	P	86/89 (97%)	85 (99%)	1 (1%)	0	100 100
17	Q	80/82 (98%)	80 (100%)	0	0	100 100
18	R	78/84 (93%)	73 (94%)	5 (6%)	0	100 100
19	S	65/75 (87%)	59 (91%)	5 (8%)	1 (2%)	8 33
20	T	81/92 (88%)	81 (100%)	0	0	100 100
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	2552/3095 (82%)	2421 (95%)	127 (5%)	4 (0%)	45 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	ALA
19	S	23	TYR
13	M	88	LYS
11	K	57	VAL

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	74/461 (16%)	72 (97%)	2 (3%)	40 67
3	C	187/199 (94%)	177 (95%)	10 (5%)	19 48
4	D	172/190 (90%)	165 (96%)	7 (4%)	26 57
5	E	172/173 (99%)	166 (96%)	6 (4%)	31 61
6	F	119/119 (100%)	118 (99%)	1 (1%)	79 89
7	G	91/112 (81%)	88 (97%)	3 (3%)	33 62
8	H	126/129 (98%)	122 (97%)	4 (3%)	34 63
9	I	104/105 (99%)	100 (96%)	4 (4%)	28 59
10	J	106/107 (99%)	96 (91%)	10 (9%)	7 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	88/90 (98%)	87 (99%)	1 (1%)	70 84
12	L	90/99 (91%)	86 (96%)	4 (4%)	24 54
13	M	102/103 (99%)	97 (95%)	5 (5%)	21 51
14	N	93/96 (97%)	91 (98%)	2 (2%)	47 71
15	O	83/84 (99%)	79 (95%)	4 (5%)	21 51
16	P	76/77 (99%)	76 (100%)	0	100 100
17	Q	65/65 (100%)	63 (97%)	2 (3%)	35 63
18	R	74/78 (95%)	68 (92%)	6 (8%)	9 33
19	S	58/65 (89%)	57 (98%)	1 (2%)	56 78
20	T	72/79 (91%)	71 (99%)	1 (1%)	62 81
21	U	65/66 (98%)	63 (97%)	2 (3%)	35 63
22	V	60/61 (98%)	56 (93%)	4 (7%)	13 40
All	All	2077/2558 (81%)	1998 (96%)	79 (4%)	30 59

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	34	ASP
2	B	43	LYS
3	C	5	SER
3	C	46	THR
3	C	50	PHE
3	C	88	ASP
3	C	121	SER
3	C	126	PHE
3	C	133	GLU
3	C	167	ASP
3	C	168	HIS
3	C	199	VAL
4	D	31	ASP
4	D	65	ARG
4	D	110	GLU
4	D	165	THR
4	D	175	LEU
4	D	178	LEU
4	D	186	THR
5	E	99	ASP
5	E	113	GLU

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Mol	Chain	Res	Type
5	E	171	LEU
5	E	179	GLU
5	E	194	ASP
5	E	201	VAL
6	F	15	LEU
7	G	55	HIS
7	G	79	ARG
7	G	100	SER
8	H	6	VAL
8	H	79	ARG
8	H	80	VAL
8	H	154	TYR
9	I	76	GLN
9	I	90	ASP
9	I	112	THR
9	I	121	LEU
10	J	3	GLU
10	J	13	LYS
10	J	25	ASN
10	J	41	ARG
10	J	63	LEU
10	J	67	VAL
10	J	91	ASP
10	J	106	ARG
10	J	107	ASP
10	J	127	PHE
11	K	63	ASP
12	L	27	PHE
12	L	36	ASP
12	L	40	ASN
12	L	74	VAL
13	M	15	LYS
13	M	18	LYS
13	M	59	ASN
13	M	77	HIS
13	M	112	GLN
14	N	102	THR
14	N	104	THR
15	O	24	ARG
15	O	53	ARG
15	O	61	ARG
15	O	67	THR

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Mol	Chain	Res	Type
17	Q	18	GLN
17	Q	55	ASP
18	R	18	GLU
18	R	28	PHE
18	R	29	VAL
18	R	33	ILE
18	R	49	GLU
18	R	75	LEU
19	S	71	THR
20	T	43	ASN
21	U	39	ILE
21	U	85	LYS
22	V	20	LYS
22	V	44	GLU
22	V	63	GLU
22	V	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	39	HIS
3	C	58	ASN
3	C	94	HIS
3	C	109	GLN
4	D	41	GLN
5	E	40	GLN
6	F	73	ASN
6	F	89	HIS
6	F	135	ASN
7	G	52	ASN
8	H	68	ASN
8	H	86	GLN
10	J	81	HIS
10	J	126	GLN
11	K	4	GLN
12	L	15	GLN
15	O	49	GLN
17	Q	18	GLN
17	Q	59	HIS
20	T	43	ASN
21	U	13	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1534/1541 (99%)	228 (14%)	2 (0%)
23	W	76/77 (98%)	16 (21%)	1 (1%)
24	X	18/53 (33%)	4 (22%)	0
All	All	1628/1671 (97%)	248 (15%)	3 (0%)

All (248) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	C
1	A	54	C
1	A	60	A
1	A	70	U
1	A	71	A
1	A	72	A
1	A	77	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	91	U
1	A	92	U
1	A	94	G
1	A	95	C
1	A	121	U
1	A	131	A
1	A	141	G
1	A	149	A
1	A	160	A
1	A	164	G
1	A	181	A
1	A	182	A

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Mol	Chain	Res	Type
1	A	210	C
1	A	211	G
1	A	226	G
1	A	240	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	306	A
1	A	321	A
1	A	328	C
1	A	332	G
1	A	345	C
1	A	346	G
1	A	347	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	406	G
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	428	G
1	A	429	U
1	A	446	G
1	A	458	U
1	A	465	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

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Mol	Chain	Res	Type
1	A	495	A
1	A	496	A
1	A	497	G
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	527	G7M
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	588	G
1	A	592	G
1	A	596	A
1	A	607	A
1	A	632	U
1	A	633	G
1	A	642	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	687	A
1	A	688	G
1	A	703	G
1	A	718	A
1	A	721	G
1	A	723	U
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	799	G
1	A	802	A

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Mol	Chain	Res	Type
1	A	815	A
1	A	817	C
1	A	828	U
1	A	829	G
1	A	832	G
1	A	836	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	845	A
1	A	846	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
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	996	A
1	A	1004	A
1	A	1010	U
1	A	1018	G
1	A	1020	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1043	G
1	A	1044	A
1	A	1046	A
1	A	1065	U

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Mol	Chain	Res	Type
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1133	G
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1151	A
1	A	1152	A
1	A	1158	C
1	A	1159	U
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	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1257	A
1	A	1260	G
1	A	1278	G
1	A	1279	G
1	A	1280	A
1	A	1285	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

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Mol	Chain	Res	Type
1	A	1318	A
1	A	1320	C
1	A	1335	U
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1398	A
1	A	1419	G
1	A	1422	G
1	A	1432	G
1	A	1441	A
1	A	1442	G
1	A	1446	A
1	A	1476	A
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1532	U
1	A	1533	C
1	A	1534	A
1	A	1535	C
1	A	1541	U
23	W	6	G
23	W	7	G
23	W	8	4SU
23	W	9	G
23	W	12	G
23	W	17	C
23	W	18	U
23	W	19	G
23	W	21	H2U
23	W	22	A
23	W	44	A
23	W	53	G
23	W	62	C
23	W	70	C
23	W	75	C

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Mol	Chain	Res	Type
23	W	77	A
24	X	16	A
24	X	23	C
24	X	26	A
24	X	27	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	641	U
1	A	1533	C
23	W	20	G

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

17 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	$\#\|Z\| > 2$
13	D2T	M	89	13	7,9,10	1.05	0	6,11,13	2.20	2 (33%)
23	H2U	W	21	23	18,21,22	2.76	5 (27%)	21,30,33	2.00	5 (23%)
1	PSU	A	516	25,1	18,21,22	1.07	2 (11%)	22,30,33	1.79	5 (22%)
1	MA6	A	1519	1	18,26,27	1.35	3 (16%)	19,38,41	4.07	2 (10%)
1	2MG	A	966	1	18,26,27	2.29	7 (38%)	16,38,41	1.48	4 (25%)
1	2MG	A	1516	1	18,26,27	2.30	7 (38%)	16,38,41	1.49	4 (25%)
23	4SU	W	8	23	18,21,22	3.94	8 (44%)	26,30,33	2.35	6 (23%)
1	MA6	A	1518	1	18,26,27	1.34	3 (16%)	19,38,41	3.92	2 (10%)
23	OMC	W	33	23	19,22,23	2.76	8 (42%)	26,31,34	0.65	0
1	5MC	A	967	1	18,22,23	3.95	7 (38%)	26,32,35	1.06	2 (7%)
23	5MU	W	55	23	19,22,23	1.42	6 (31%)	28,32,35	2.02	6 (21%)
23	PSU	W	56	23	18,21,22	0.97	1 (5%)	22,30,33	1.80	5 (22%)
1	2MG	A	1207	1	18,26,27	2.33	7 (38%)	16,38,41	1.42	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	UR3	A	1498	25,1	19,22,23	2.62	7 (36%)	26,32,35	1.25	1 (3%)
1	4OC	A	1402	1	20,23,24	3.40	9 (45%)	26,32,35	0.88	1 (3%)
1	G7M	A	527	1	20,26,27	2.32	8 (40%)	17,39,42	1.41	2 (11%)
1	5MC	A	1407	1	18,22,23	3.96	7 (38%)	26,32,35	0.95	1 (3%)

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
13	D2T	M	89	13	-	1/7/12/14	-
23	H2U	W	21	23	-	7/7/38/39	0/2/2/2
1	PSU	A	516	25,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	2MG	A	966	1	-	1/5/27/28	0/3/3/3
1	2MG	A	1516	1	-	2/5/27/28	0/3/3/3
23	4SU	W	8	23	-	2/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
23	OMC	W	33	23	-	1/9/27/28	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
23	5MU	W	55	23	-	0/7/25/26	0/2/2/2
23	PSU	W	56	23	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	UR3	A	1498	25,1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	G7M	A	527	1	-	3/3/25/26	0/3/3/3
1	5MC	A	1407	1	-	2/7/25/26	0/2/2/2

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C6-C5	9.89	1.50	1.34
1	A	1407	5MC	C6-C5	9.86	1.50	1.34
23	W	8	4SU	C4-N3	8.74	1.47	1.37
23	W	21	H2U	C2-N1	8.15	1.47	1.35
23	W	8	4SU	C2-N1	7.41	1.50	1.38
1	A	967	5MC	C4-N3	7.23	1.46	1.34
1	A	1407	5MC	C4-N3	7.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C4-N3	7.00	1.45	1.32
1	A	1407	5MC	C2-N3	6.75	1.50	1.36
1	A	967	5MC	C2-N3	6.72	1.50	1.36
1	A	1498	UR3	C2-N1	6.50	1.47	1.38
1	A	1402	4OC	C6-C5	6.44	1.50	1.35
23	W	21	H2U	C2-N3	6.18	1.49	1.38
23	W	8	4SU	C6-C5	6.12	1.49	1.35
1	A	1498	UR3	C6-C5	6.02	1.49	1.35
1	A	1402	4OC	C2-N3	5.91	1.48	1.36
23	W	8	4SU	C2-N3	5.91	1.48	1.38
23	W	8	4SU	C5-C4	5.87	1.50	1.42
23	W	33	OMC	C6-C5	5.68	1.48	1.35
23	W	33	OMC	C2-N3	5.53	1.47	1.36
1	A	1407	5MC	C4-N4	5.37	1.48	1.34
1	A	967	5MC	C4-N4	5.33	1.48	1.34
1	A	1407	5MC	C6-N1	5.28	1.47	1.38
1	A	967	5MC	C6-N1	5.11	1.46	1.38
23	W	8	4SU	C4-S4	-5.00	1.58	1.68
23	W	33	OMC	C4-N3	4.95	1.44	1.34
1	A	527	G7M	C6-N1	4.94	1.45	1.37
1	A	1402	4OC	C4-N4	4.91	1.46	1.35
1	A	1207	2MG	C2-N2	4.83	1.44	1.33
1	A	1498	UR3	C2-N3	4.80	1.48	1.39
1	A	1402	4OC	O2-C2	-4.75	1.14	1.23
1	A	967	5MC	C2-N1	4.64	1.50	1.40
1	A	1407	5MC	C2-N1	4.63	1.50	1.40
23	W	33	OMC	C4-N4	4.62	1.44	1.33
1	A	966	2MG	C2-N2	4.57	1.43	1.33
1	A	1516	2MG	C2-N2	4.56	1.43	1.33
1	A	527	G7M	C2-N3	4.40	1.43	1.33
1	A	1402	4OC	C5-C4	4.28	1.49	1.40
1	A	1207	2MG	C4-N3	4.18	1.47	1.37
23	W	21	H2U	C4-N3	4.08	1.44	1.37
1	A	966	2MG	C4-N3	4.03	1.47	1.37
1	A	527	G7M	C2-N2	4.02	1.43	1.34
1	A	1402	4OC	C2-N1	3.99	1.48	1.40
1	A	1516	2MG	C4-N3	3.99	1.47	1.37
1	A	966	2MG	C2-N1	3.90	1.43	1.36
23	W	33	OMC	C2-N1	3.88	1.48	1.40
1	A	1516	2MG	C6-N1	3.87	1.43	1.37
1	A	1516	2MG	C2-N1	3.85	1.42	1.36
1	A	1207	2MG	C2-N1	3.83	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	2MG	C6-N1	3.83	1.43	1.37
1	A	1207	2MG	C6-N1	3.78	1.43	1.37
1	A	527	G7M	C4-N3	3.63	1.46	1.37
1	A	1402	4OC	CM4-N4	3.51	1.51	1.45
1	A	1207	2MG	O6-C6	-3.37	1.16	1.23
1	A	1516	2MG	O6-C6	-3.33	1.16	1.23
1	A	966	2MG	O6-C6	-3.31	1.16	1.23
1	A	1518	MA6	C2-N3	3.21	1.37	1.32
1	A	1402	4OC	C6-N1	3.16	1.45	1.38
1	A	1519	MA6	C2-N3	3.13	1.37	1.32
23	W	8	4SU	C6-N1	3.09	1.45	1.38
1	A	516	PSU	C6-C5	3.02	1.38	1.35
23	W	33	OMC	C6-N1	3.00	1.45	1.38
23	W	56	PSU	C6-C5	2.94	1.38	1.35
1	A	1519	MA6	C10-N6	2.91	1.52	1.45
1	A	1516	2MG	C5-C6	2.88	1.53	1.47
1	A	1518	MA6	C10-N6	2.85	1.52	1.45
1	A	1519	MA6	C5-C4	-2.84	1.33	1.40
23	W	55	5MU	C6-C5	2.83	1.39	1.34
1	A	1498	UR3	C6-N1	2.77	1.44	1.38
1	A	527	G7M	C2-N1	2.76	1.44	1.37
1	A	966	2MG	C5-C6	2.75	1.53	1.47
1	A	1518	MA6	C5-C4	-2.71	1.33	1.40
23	W	55	5MU	C4-N3	-2.69	1.33	1.38
1	A	1207	2MG	C5-C6	2.67	1.52	1.47
1	A	527	G7M	O6-C6	-2.57	1.18	1.23
1	A	966	2MG	C5-C4	-2.57	1.36	1.43
1	A	1207	2MG	C5-C4	-2.55	1.36	1.43
1	A	1516	2MG	C5-C4	-2.52	1.36	1.43
1	A	967	5MC	O2-C2	-2.51	1.19	1.23
23	W	55	5MU	C2-N1	2.42	1.42	1.38
23	W	33	OMC	C5-C4	2.38	1.48	1.42
1	A	1498	UR3	O4-C4	-2.38	1.18	1.23
1	A	527	G7M	C5-C4	-2.37	1.34	1.39
1	A	527	G7M	C5-C6	2.37	1.51	1.45
1	A	1407	5MC	O2-C2	-2.36	1.19	1.23
1	A	1498	UR3	O2-C2	-2.22	1.18	1.22
23	W	8	4SU	O2-C2	-2.20	1.19	1.23
23	W	33	OMC	O2-C2	-2.17	1.19	1.23
23	W	55	5MU	C4-C5	2.17	1.48	1.44
23	W	21	H2U	O2-C2	-2.10	1.19	1.23
23	W	21	H2U	O4-C4	-2.10	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	55	5MU	C6-N1	-2.08	1.34	1.38
1	A	516	PSU	O4'-C1'	-2.05	1.41	1.43
1	A	1498	UR3	C5-C4	2.02	1.49	1.43
23	W	55	5MU	C2-N3	-2.02	1.34	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1519	MA6	N1-C6-N6	-16.68	99.50	117.06
1	A	1518	MA6	N1-C6-N6	-16.12	100.09	117.06
23	W	8	4SU	C4-N3-C2	-7.43	120.12	127.34
23	W	21	H2U	C4-N3-C2	-6.38	120.50	125.79
23	W	8	4SU	C5-C4-N3	5.85	120.12	114.69
1	A	1519	MA6	N3-C2-N1	-5.40	120.24	128.68
1	A	1518	MA6	N3-C2-N1	-5.19	120.56	128.68
23	W	55	5MU	C4-N3-C2	-4.95	120.94	127.35
23	W	55	5MU	N3-C2-N1	4.86	121.34	114.89
1	A	1498	UR3	C4-N3-C2	-4.71	120.13	124.56
23	W	56	PSU	N1-C2-N3	4.61	120.36	115.13
1	A	516	PSU	C4-N3-C2	-4.43	119.95	126.34
23	W	56	PSU	C4-N3-C2	-4.43	119.96	126.34
23	W	55	5MU	C5-C4-N3	4.39	119.06	115.31
1	A	516	PSU	N1-C2-N3	4.23	119.92	115.13
13	M	89	D2T	CB1-SB-CB	4.08	109.82	102.44
23	W	8	4SU	C5-C4-S4	-4.05	119.25	124.47
23	W	8	4SU	N3-C2-N1	3.99	120.19	114.89
23	W	55	5MU	O4-C4-C5	-3.86	120.43	124.90
1	A	527	G7M	C2-N1-C6	-3.82	118.07	125.10
23	W	21	H2U	N3-C2-N1	3.80	120.67	116.65
1	A	967	5MC	C5-C6-N1	-3.59	119.64	123.34
1	A	1207	2MG	C5-C6-N1	3.59	120.29	113.95
1	A	1516	2MG	C5-C6-N1	3.58	120.27	113.95
23	W	55	5MU	C5-C6-N1	-3.53	119.71	123.34
1	A	966	2MG	C5-C6-N1	3.50	120.13	113.95
1	A	1407	5MC	C5-C6-N1	-2.95	120.30	123.34
1	A	516	PSU	O2-C2-N1	-2.94	119.55	122.79
23	W	21	H2U	C5-C6-N1	2.92	121.22	111.61
23	W	56	PSU	O2-C2-N1	-2.76	119.75	122.79
23	W	8	4SU	O2-C2-N1	-2.62	119.30	122.79
13	M	89	D2T	OD2-CG-CB	2.62	118.81	113.15
1	A	966	2MG	C8-N7-C5	2.60	107.94	102.99
23	W	21	H2U	C5-C4-N3	2.59	119.55	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1516	2MG	C8-N7-C5	2.51	107.78	102.99
1	A	1207	2MG	C8-N7-C5	2.50	107.76	102.99
1	A	516	PSU	O4'-C1'-C2'	2.46	108.61	105.14
23	W	21	H2U	O2-C2-N1	-2.45	120.03	123.11
1	A	966	2MG	CM2-N2-C2	-2.39	118.57	123.86
1	A	1516	2MG	CM2-N2-C2	-2.39	118.58	123.86
1	A	1207	2MG	O6-C6-C5	-2.38	119.72	124.37
23	W	56	PSU	C6-N1-C2	-2.37	120.26	122.68
1	A	966	2MG	O6-C6-C5	-2.33	119.83	124.37
1	A	1516	2MG	O6-C6-C5	-2.30	119.89	124.37
1	A	516	PSU	C6-N1-C2	-2.26	120.37	122.68
23	W	8	4SU	C1'-N1-C2	2.25	121.64	117.57
1	A	1402	4OC	C6-C5-C4	2.18	119.63	116.96
1	A	527	G7M	O6-C6-N1	2.06	123.09	120.65
23	W	56	PSU	C6-C5-C4	2.06	119.64	118.20
1	A	967	5MC	CM5-C5-C6	-2.04	120.12	122.85
23	W	55	5MU	C1'-N1-C2	2.03	121.24	117.57

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
23	W	21	H2U	O4'-C1'-N1-C6
23	W	33	OMC	C1'-C2'-O2'-CM2
1	A	1519	MA6	C3'-C4'-C5'-O5'
23	W	8	4SU	O4'-C4'-C5'-O5'
23	W	8	4SU	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	1516	2MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	1402	4OC	O4'-C4'-C5'-O5'
23	W	21	H2U	C4'-C5'-O5'-P
23	W	21	H2U	O4'-C4'-C5'-O5'
13	M	89	D2T	CG-CB-SB-CB1
23	W	21	H2U	C3'-C4'-C5'-O5'
23	W	21	H2U	C2'-C1'-N1-C2
1	A	527	G7M	C4'-C5'-O5'-P
1	A	966	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
23	W	21	H2U	C2'-C1'-N1-C6
23	W	21	H2U	O4'-C1'-N1-C2
1	A	1407	5MC	C3'-C4'-C5'-O5'
1	A	1516	2MG	C3'-C4'-C5'-O5'
1	A	1407	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	2	0
1	A	1516	2MG	1	0
23	W	8	4SU	2	0
1	A	1518	MA6	2	0
23	W	33	OMC	3	0
23	W	56	PSU	1	0
1	A	1207	2MG	1	0
1	A	1402	4OC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 128 ligands modelled in this entry, 128 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.

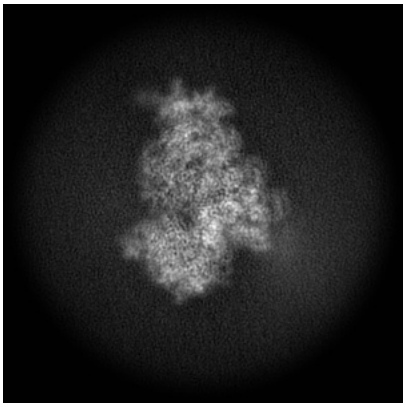
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51616. These allow visual inspection of the internal detail of the map and identification of artifacts.

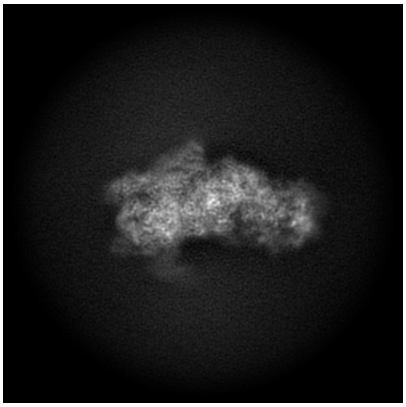
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

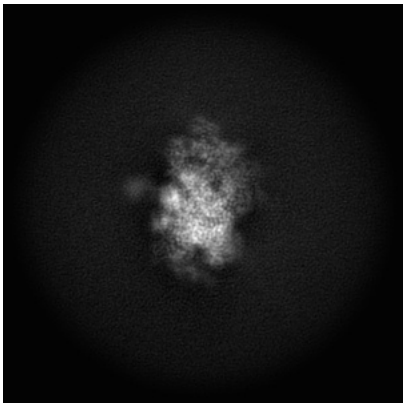
6.1.1 Primary map



X



Y

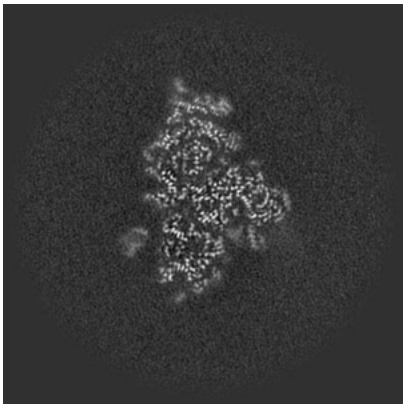


Z

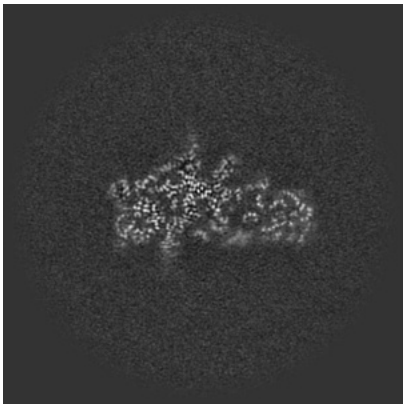
The images above show the map projected in three orthogonal directions.

6.2 Central slices

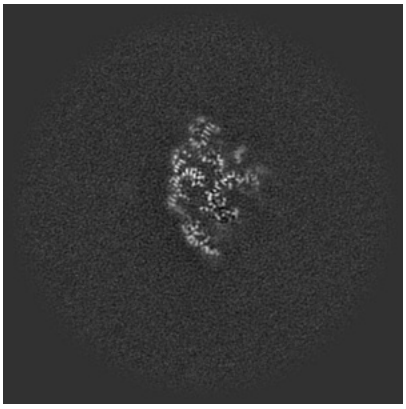
6.2.1 Primary map



X Index: 250



Y Index: 250

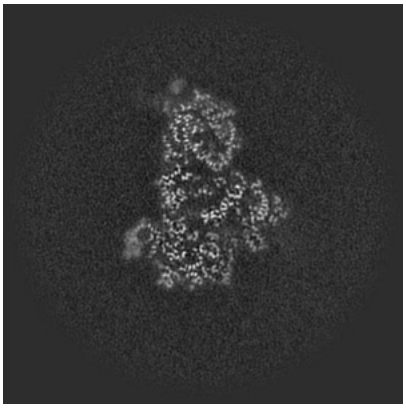


Z Index: 250

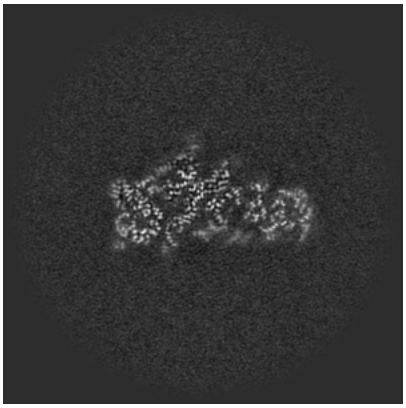
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 238



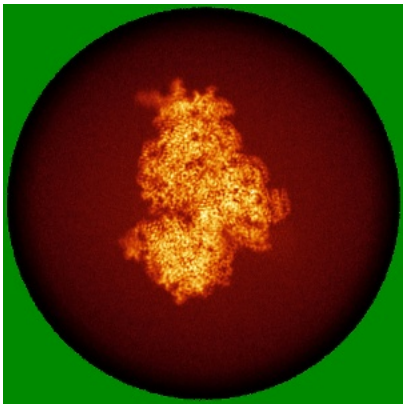
Y Index: 248

Z Index: 257

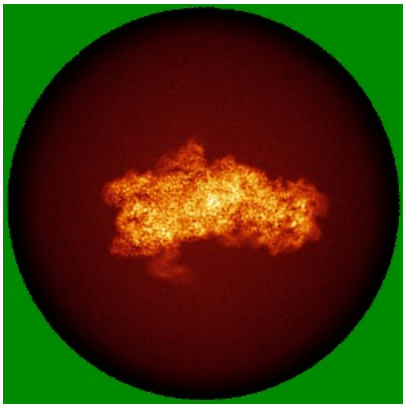
The images above show the largest variance slices of the map in three orthogonal directions.

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

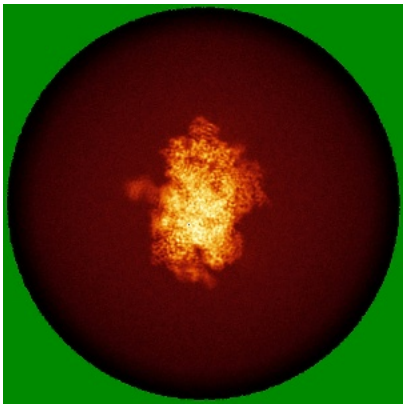
6.4.1 Primary map



X



Y

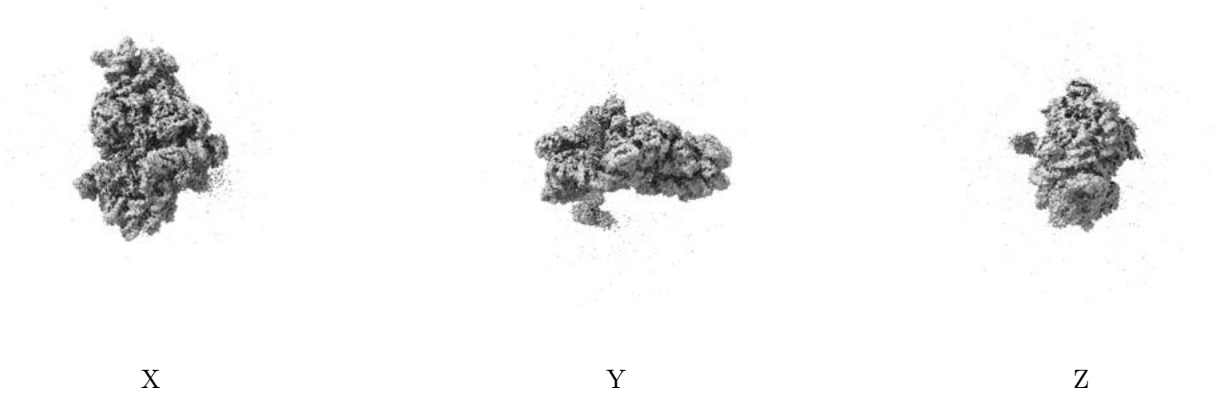


Z

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

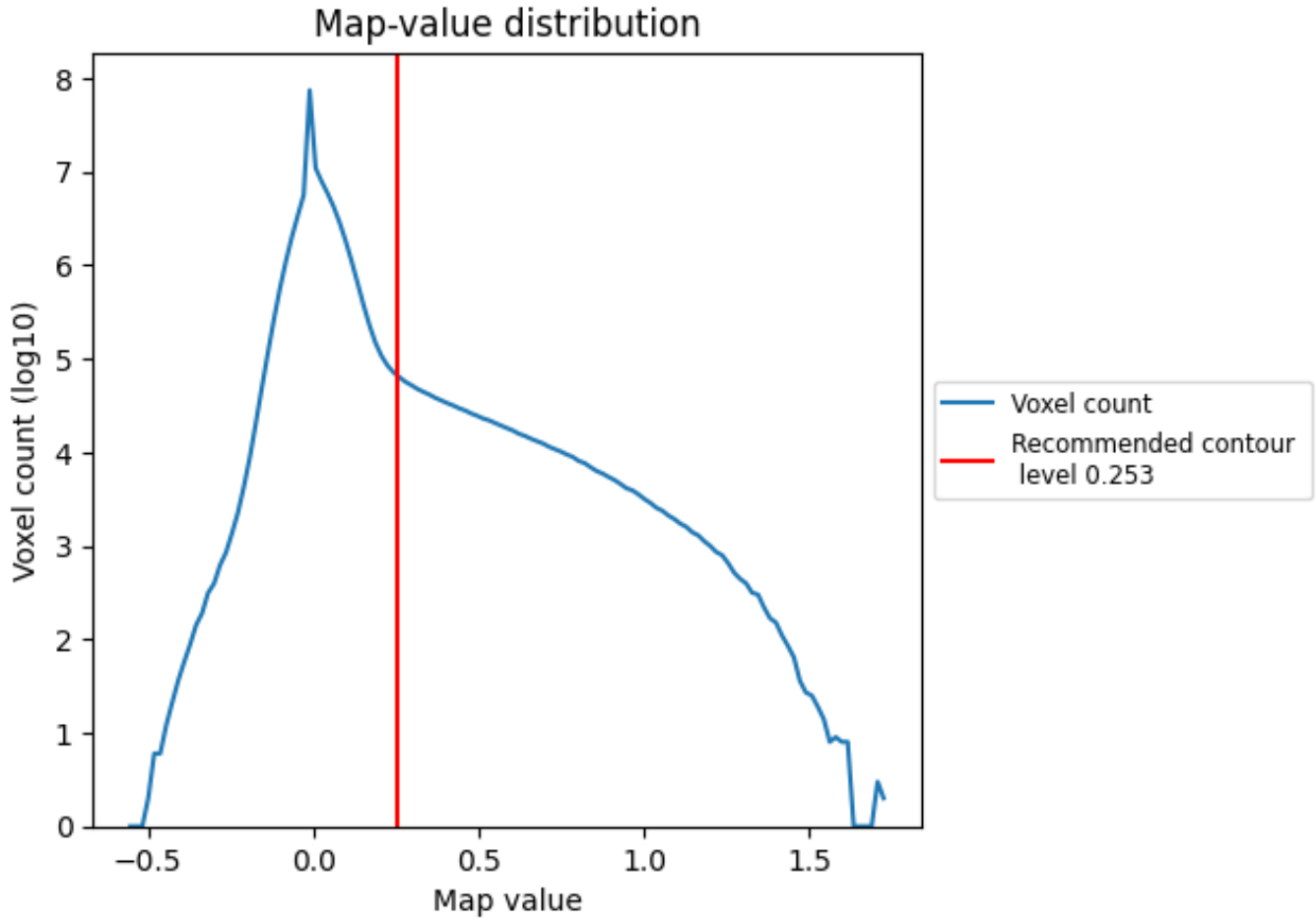
6.6 Mask visualisation (i)

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

7 Map analysis

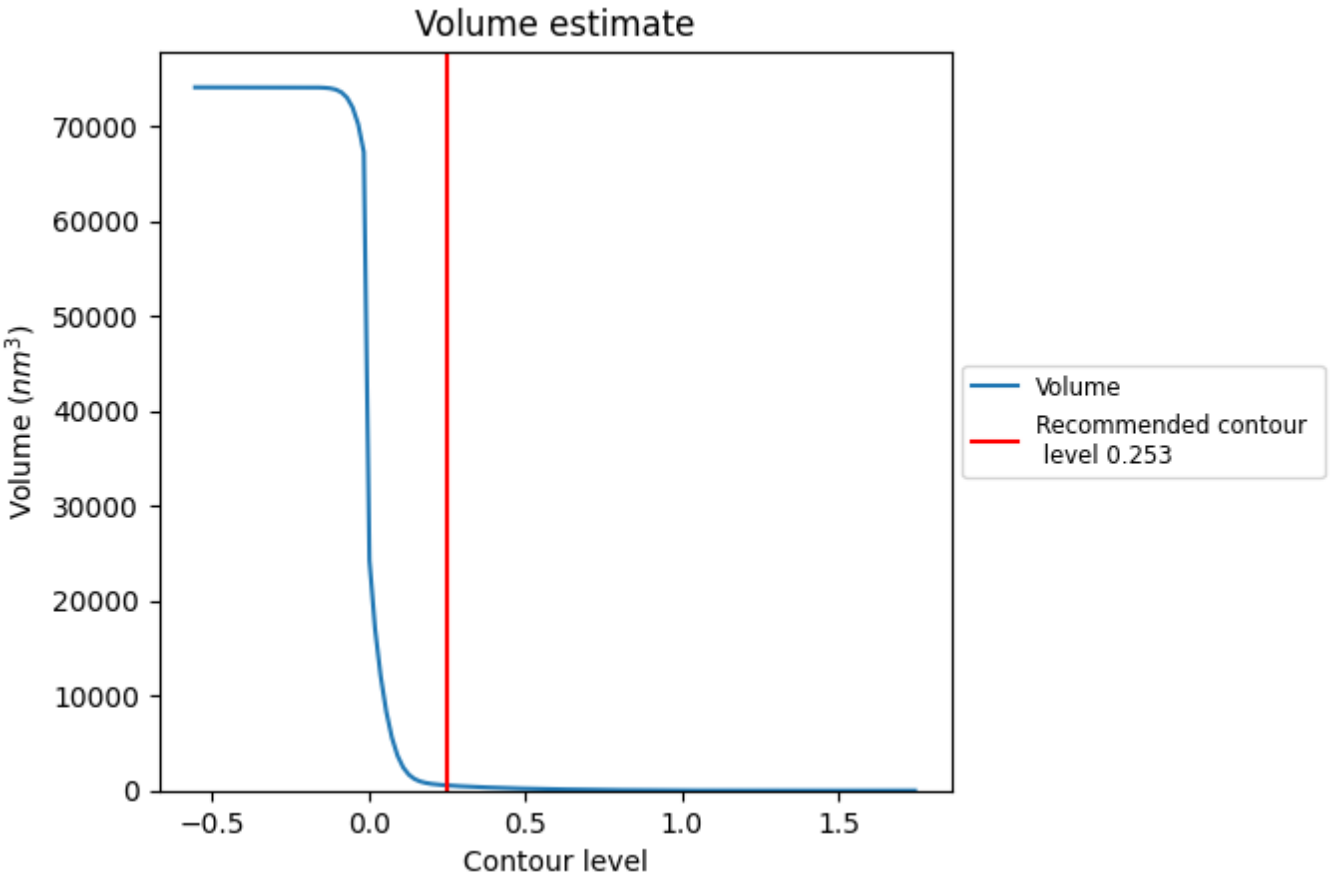
This section contains the results of statistical analysis of the map.

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.

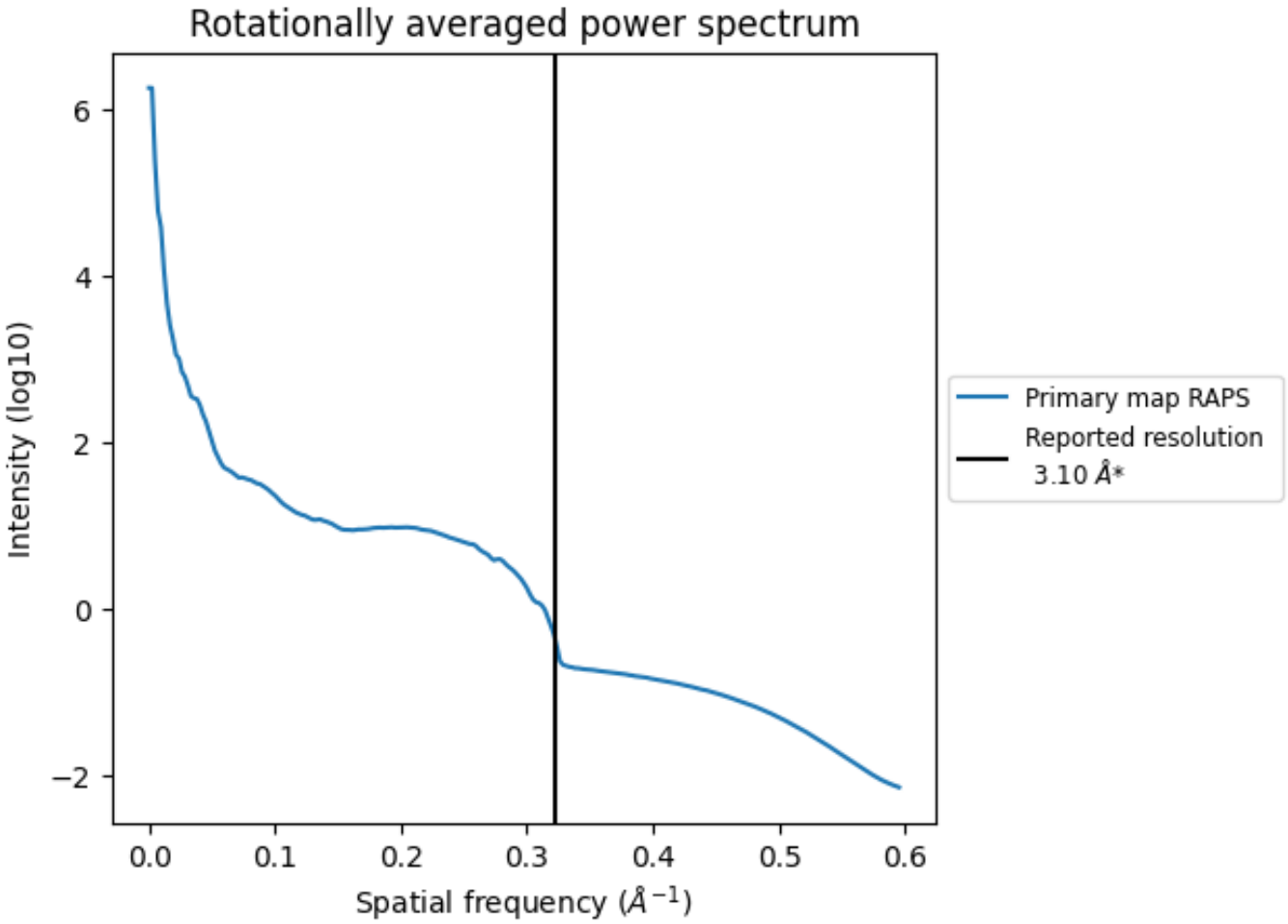
7.2 Volume estimate



The volume at the recommended contour level is 541 nm^3; this corresponds to an approximate mass of 489 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 0.323 $Å^{-1}$

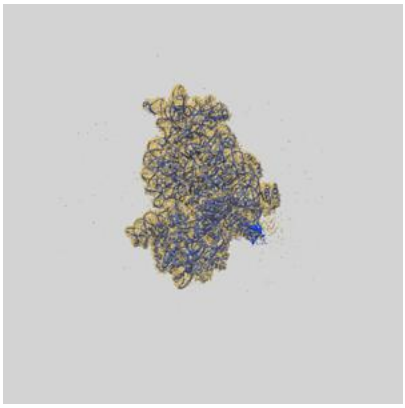
8 Fourier-Shell correlation

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

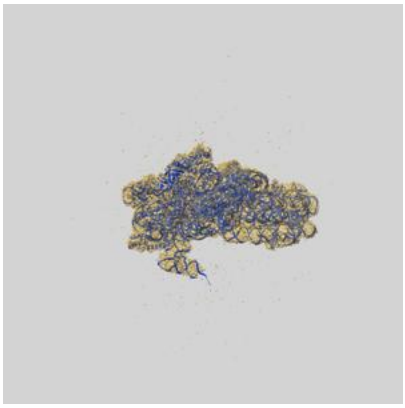
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51616 and PDB model 9GUQ. Per-residue inclusion information can be found in section 3 on page 8.

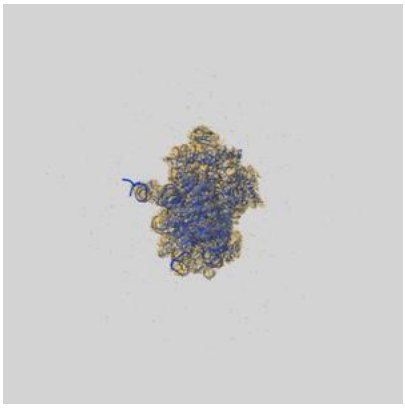
9.1 Map-model overlay



X



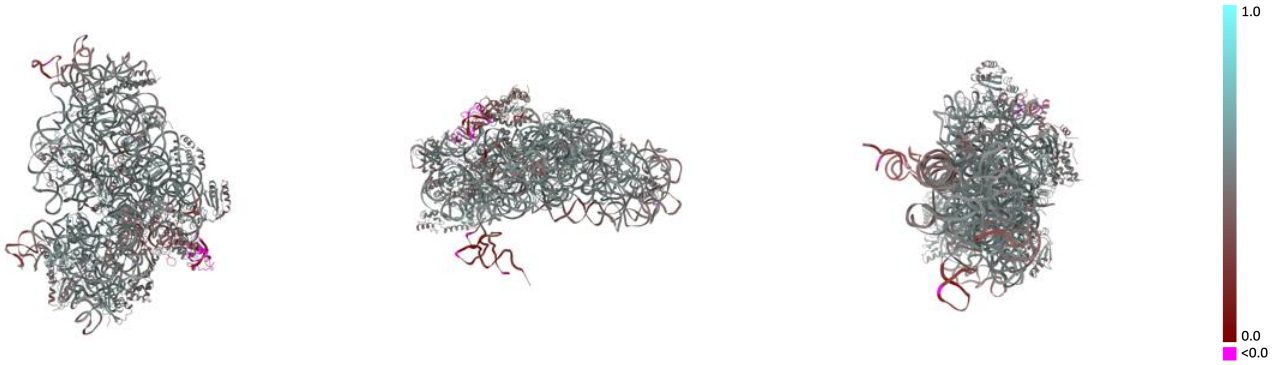
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.253 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.

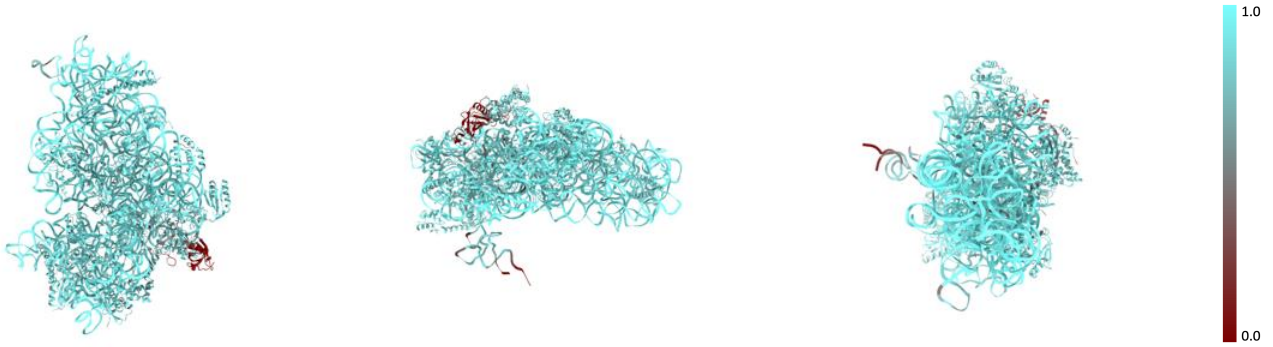
9.2 Q-score mapped to coordinate model



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.

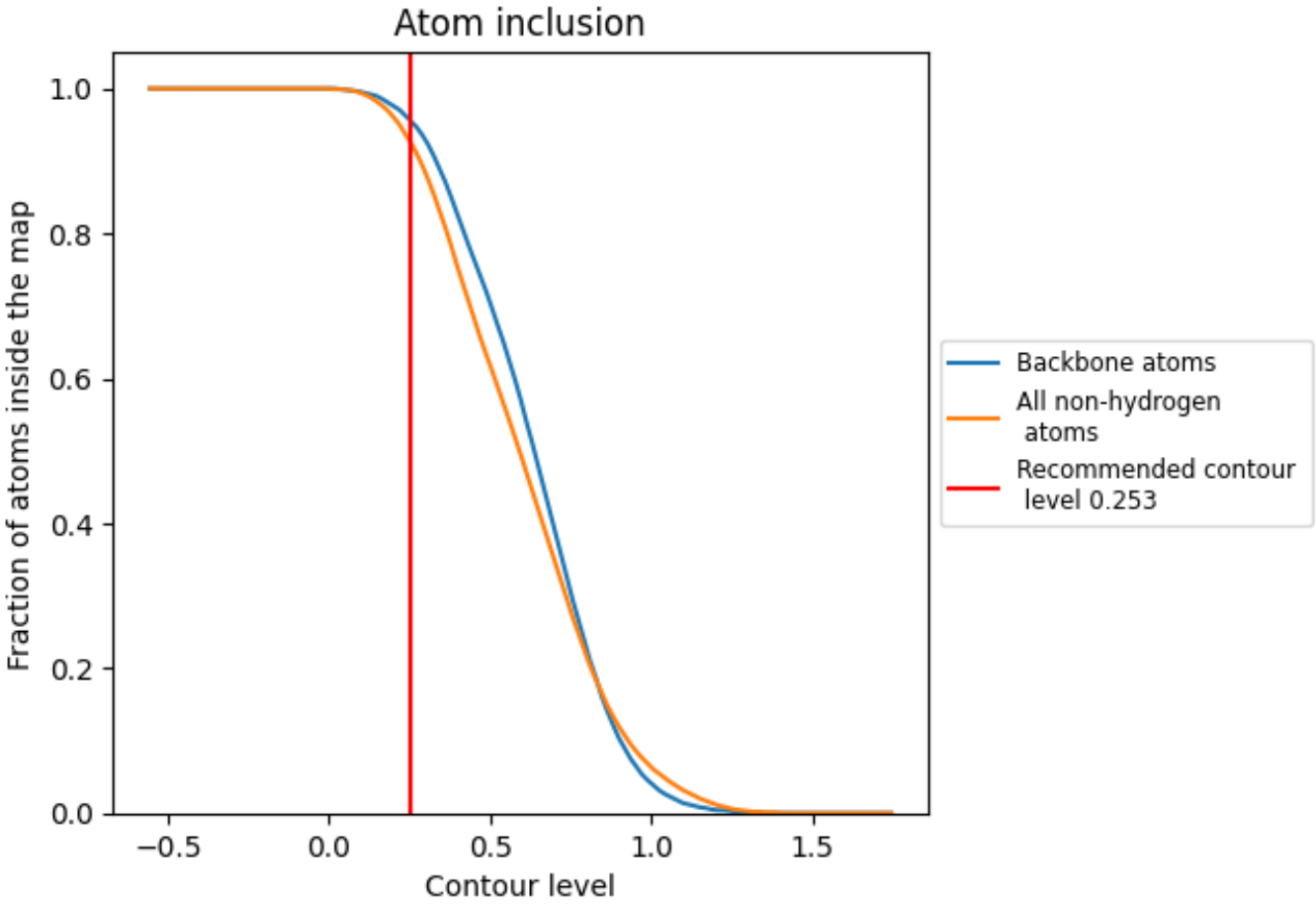
9.3 Atom inclusion mapped to coordinate model



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 (0.253).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.4870
A	0.9840	0.5000
B	0.3630	0.2480
C	0.8600	0.4740
D	0.8890	0.5220
E	0.8880	0.5010
F	0.8880	0.5240
G	0.8830	0.4770
H	0.8550	0.4700
I	0.8930	0.5350
J	0.9010	0.5150
K	0.8570	0.4880
L	0.8860	0.5000
M	0.9030	0.5300
N	0.8910	0.4820
O	0.9160	0.5300
P	0.8990	0.4980
Q	0.9110	0.5150
R	0.8700	0.4990
S	0.8710	0.5010
T	0.9230	0.5100
U	0.8990	0.4790
V	0.7700	0.4510
W	0.7240	0.2640
X	0.5940	0.3110