



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:38 PM UTC

PDB ID : 9DUK / pdb_00009duk
EMDB ID : EMD-47168
Title : Structure of mutant 30S subunit with extended helix 26, version 3
Authors : Boyko, K.; Cate, J.
Deposited on : 2024-10-03
Resolution : 2.56 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

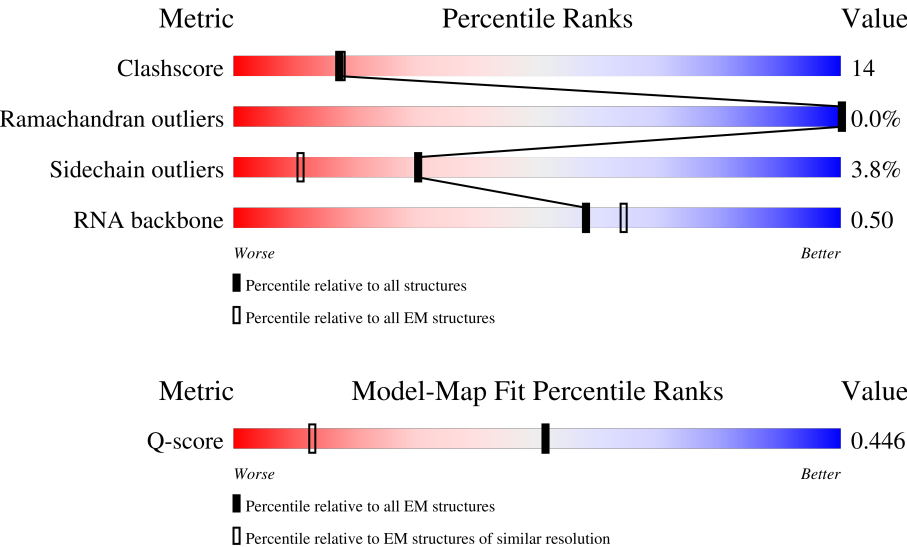
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.56 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7558 (2.06 - 3.06)

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

Mol	Chain	Length	Quality of chain
1	B	234	96% 70% 25% . .
2	C	233	88% 54% 33% . 12%
3	D	206	51% 60% 36% .

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Mol	Chain	Length	Quality of chain
4	E	167	
5	F	135	
6	G	179	
7	H	130	
8	I	130	
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	U	71	
21	A	1533	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51578 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 protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	116	Total	C	N	O	S	0	0
			869	536	172	158	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

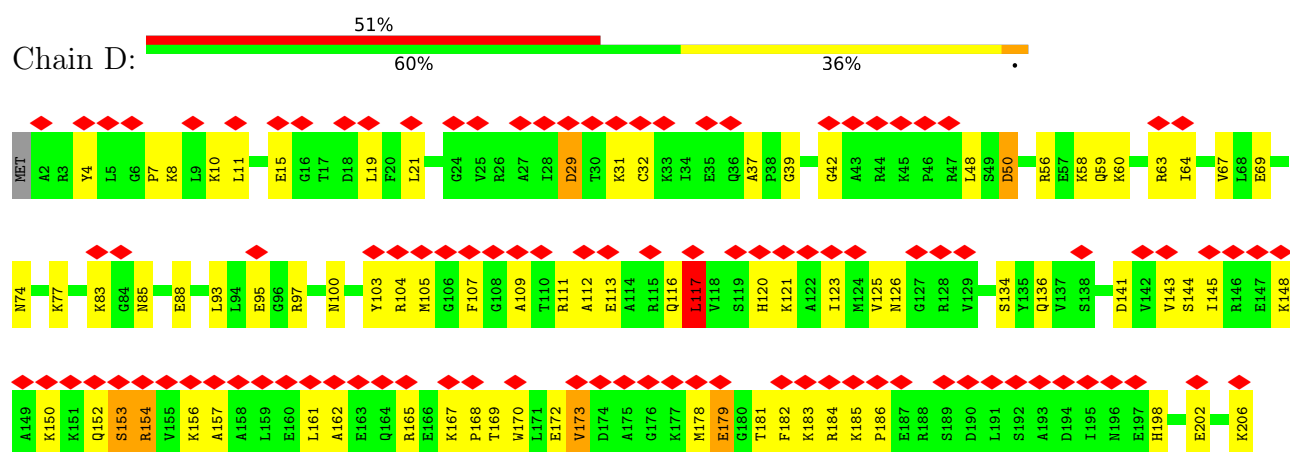
Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 20 is a protein called 30S ribosomal protein S21.

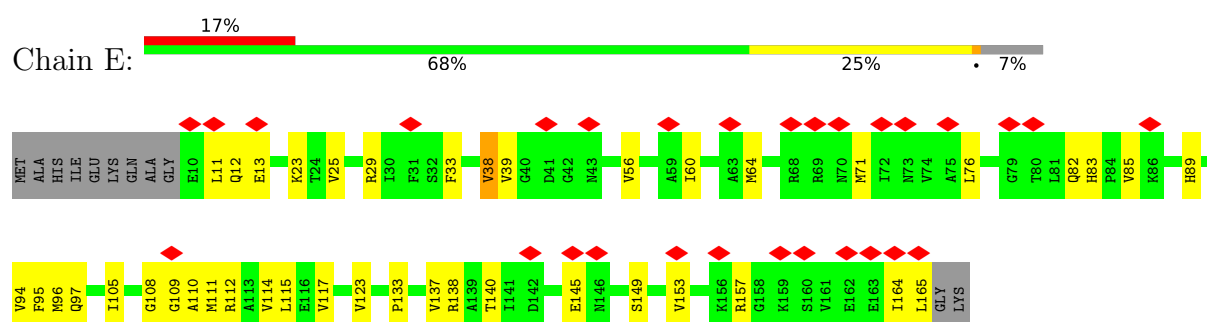
Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 21 is a RNA chain called 16S rRNA.

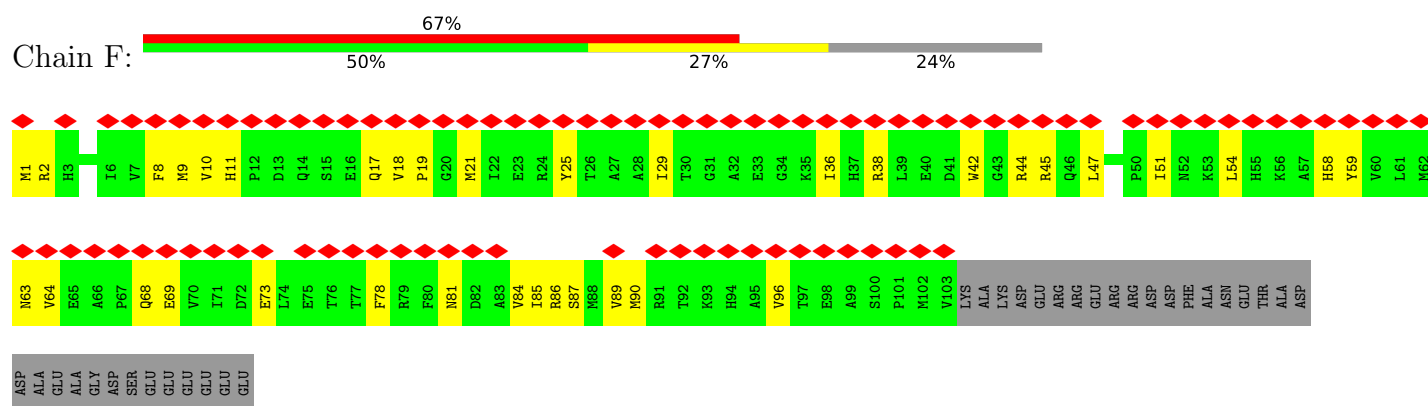
Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	1518	Total	C	N	O	P	0	0
			32586	14539	5981	10548	1518		



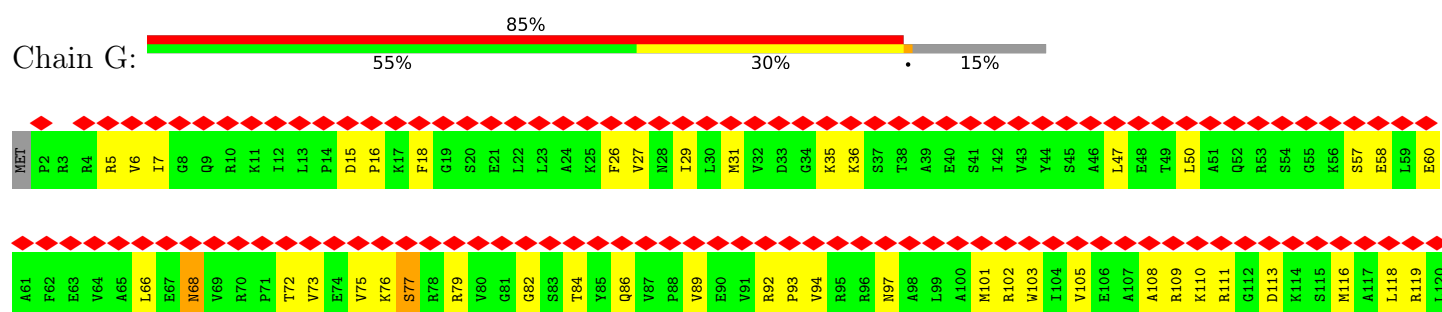
• Molecule 4: 30S ribosomal protein S5

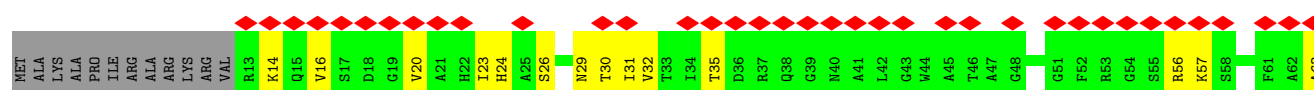


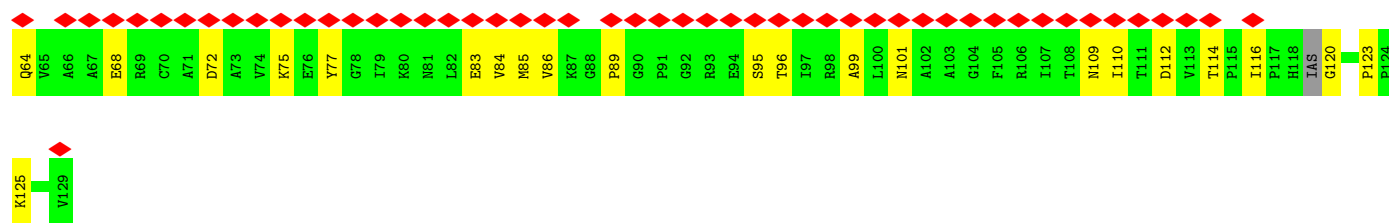
• Molecule 5: 30S ribosomal protein S6



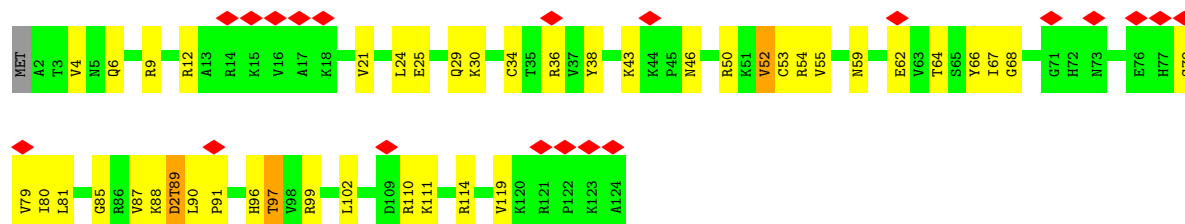
• Molecule 6: 30S ribosomal protein S7







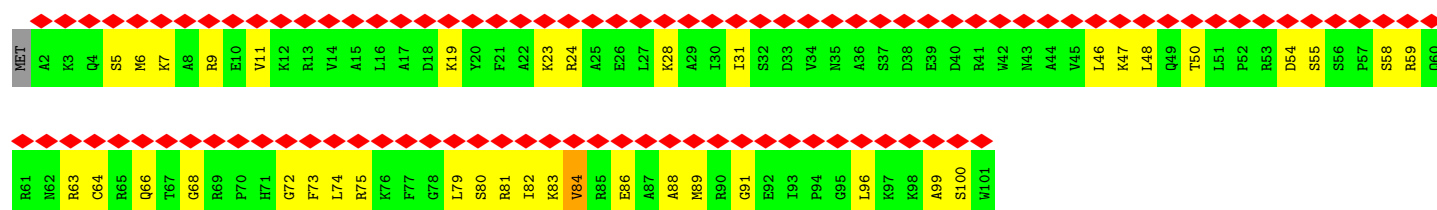
- Molecule 11: Small ribosomal subunit protein uS12



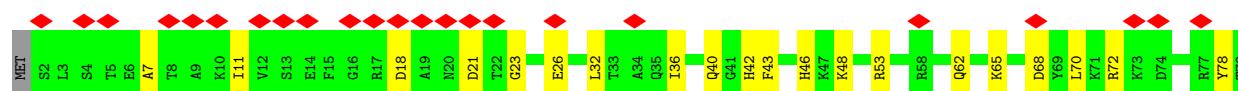
- Molecule 12: 30S ribosomal protein S13

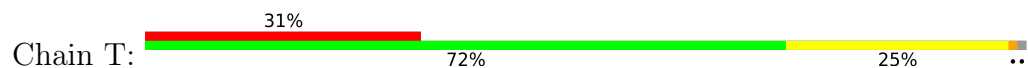


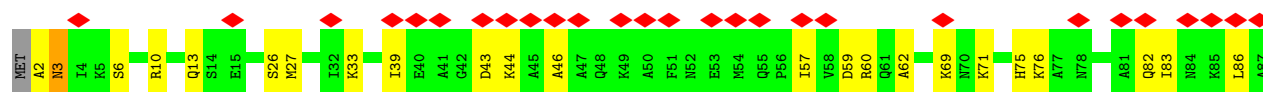
- Molecule 13: Small ribosomal subunit protein uS14



- Molecule 14: Small ribosomal subunit protein uS15



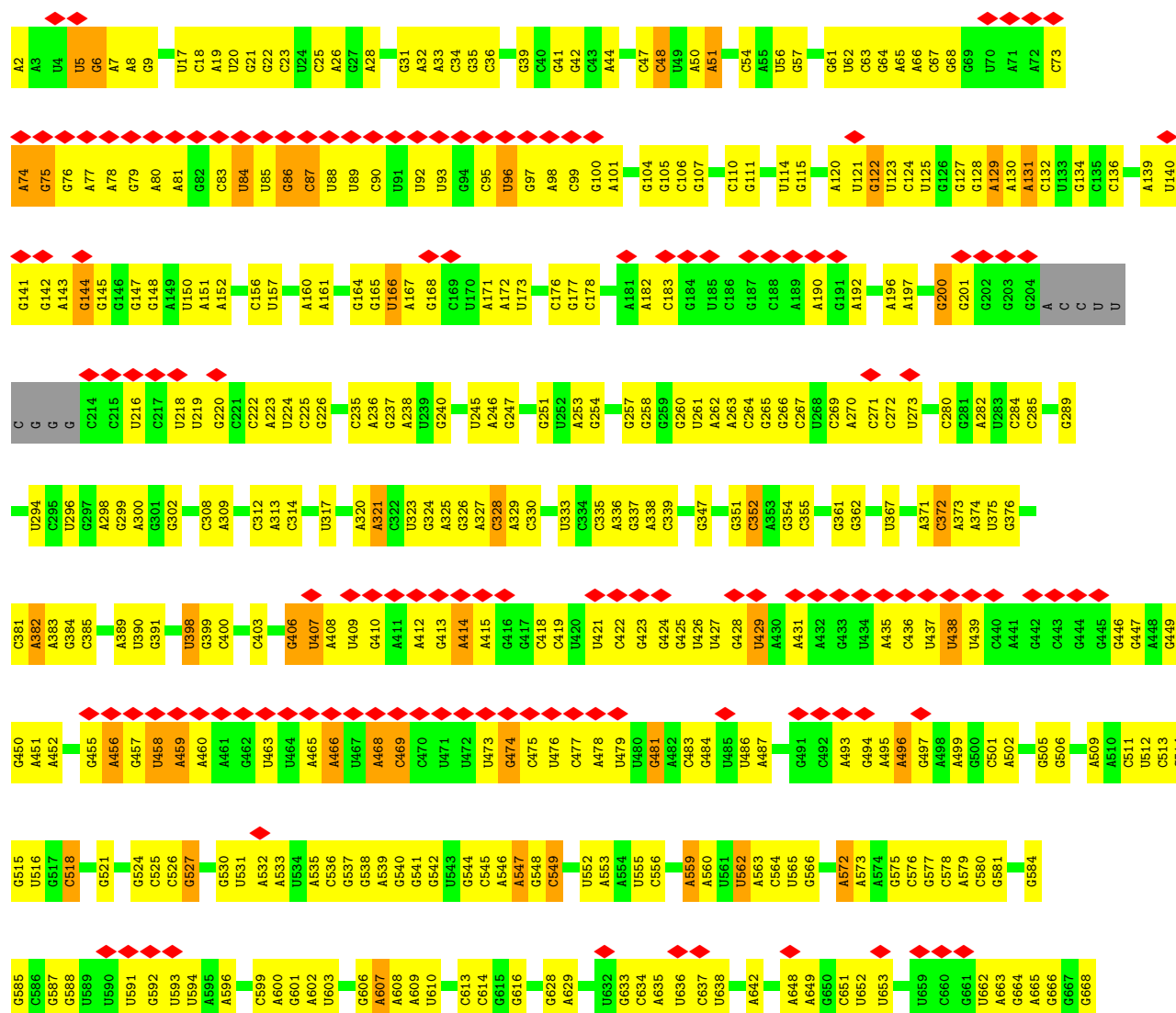
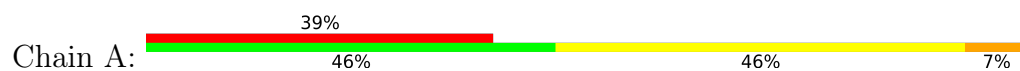




- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S rRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.594	Depositor
Minimum map value	-1.801	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.256	Depositor
Map size ($\text{\AA}$)	369.6, 369.6, 369.6	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	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: 4OC, UR3, MA6, G7M, D2T, 5MC, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.20	0/1784	0.40	0/2403
2	C	0.18	0/1651	0.39	0/2225
3	D	0.70	1/1665 (0.1%)	0.55	2/2227 (0.1%)
4	E	0.16	0/1165	0.33	0/1568
5	F	0.21	0/858	0.39	0/1160
6	G	0.13	0/1219	0.36	0/1635
7	H	0.15	0/989	0.31	0/1326
8	I	0.16	0/1034	0.38	0/1375
9	J	0.85	2/796 (0.3%)	0.86	4/1077 (0.4%)
10	K	0.17	0/884	0.36	0/1191
11	L	0.22	0/960	0.44	0/1286
12	M	0.15	0/900	0.37	0/1204
13	N	0.14	0/817	0.41	0/1088
14	O	0.15	0/722	0.36	0/964
15	P	0.17	0/653	0.40	0/877
16	Q	0.15	0/650	0.38	0/871
17	R	0.19	0/553	0.38	0/742
18	S	0.13	0/685	0.34	0/922
19	T	0.18	0/676	0.37	0/895
20	U	0.13	0/597	0.30	0/792
21	A	0.52	1/36287 (0.0%)	0.63	3/56598 (0.0%)
All	All	0.46	4/55545 (0.0%)	0.57	9/82426 (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
2	C	0	1
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7	PRO	N-CD	-27.06	1.09	1.47
9	J	55	PRO	N-CD	20.88	1.76	1.47
9	J	55	PRO	CG-CD	-10.58	1.14	1.50
21	A	1406	U	C2'-O2'	5.16	1.50	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	55	PRO	N-CD-CG	-21.59	70.82	103.20
3	D	7	PRO	N-CD-CG	11.90	121.06	103.20
9	J	55	PRO	CA-CB-CG	-9.86	85.76	104.50
9	J	55	PRO	CA-N-CD	-7.34	101.73	112.00
21	A	1406	U	C1'-O4'-C4'	-6.29	103.61	109.90
21	A	1406	U	C4'-C3'-O3'	-6.07	103.89	113.00
9	J	55	PRO	N-CA-CB	-5.46	98.02	103.48
3	D	117	LEU	N-CA-C	-5.02	106.85	113.12
21	A	1406	U	C4'-C3'-C2'	-5.01	97.58	102.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	59	ARG	Sidechain
3	D	154	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1753	0	1780	45	0
2	C	1624	0	1696	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1643	0	1707	74	0
4	E	1152	0	1196	32	0
5	F	839	0	833	24	0
6	G	1203	0	1254	40	0
7	H	979	0	1031	33	0
8	I	1022	0	1070	73	0
9	J	786	0	828	26	0
10	K	869	0	880	28	0
11	L	957	0	1017	33	0
12	M	891	0	952	45	0
13	N	805	0	844	50	0
14	O	714	0	734	16	0
15	P	643	0	661	22	0
16	Q	641	0	682	24	0
17	R	544	0	565	19	0
18	S	668	0	693	37	0
19	T	670	0	719	19	0
20	U	589	0	629	21	0
21	A	32586	0	16416	591	0
All	All	51578	0	36187	1164	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 14.

All (1164) 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)
9:J:55:PRO:CD	9:J:55:PRO:N	1.77	1.23
3:D:150:LYS:HG2	3:D:178:MET:HE3	1.41	1.02
3:D:105:MET:HE2	3:D:107:PHE:CZ	1.94	1.01
8:I:42:GLU:HG2	8:I:45:ARG:NH2	1.80	0.96
9:J:53:ILE:HD12	21:A:1060:U:H5''	1.47	0.96
8:I:88:MET:HE1	8:I:104:VAL:HG13	1.49	0.91
2:C:130:PHE:O	2:C:134:MET:HG2	1.73	0.89
18:S:44:MET:HG2	18:S:47:LEU:HD12	1.55	0.88
3:D:170:TRP:HA	3:D:184:ARG:HH12	1.40	0.86
1:B:27:MET:HE1	1:B:193:PRO:CG	2.06	0.86
21:A:1086:U:H3	21:A:1099:G:H22	1.25	0.84
6:G:97:ASN:O	6:G:101:MET:HE2	1.77	0.83
1:B:27:MET:HE1	1:B:193:PRO:HG3	1.61	0.83
21:A:447:G:H21	21:A:487:A:H62	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:946:A:H2'	21:A:947:G:H8	1.44	0.80
8:I:45:ARG:HG2	8:I:46:MET:HE3	1.62	0.80
21:A:1306:A:H62	21:A:1331:G:N2	1.78	0.80
13:N:5:SER:C	13:N:9:ARG:HE	1.90	0.80
3:D:153:SER:HA	3:D:156:LYS:HG3	1.64	0.80
19:T:44:LYS:HD2	19:T:86:LEU:HB3	1.61	0.80
18:S:44:MET:CG	18:S:47:LEU:HD12	2.11	0.79
11:L:29:GLN:HB3	11:L:81:LEU:HD22	1.64	0.79
8:I:45:ARG:HG2	8:I:46:MET:CE	2.13	0.78
21:A:946:A:H2'	21:A:947:G:C8	2.18	0.78
21:A:673:A:H2'	21:A:674:G:C8	2.19	0.78
8:I:42:GLU:HG2	8:I:45:ARG:HH21	1.45	0.78
21:A:1242:G:H1	21:A:1295:U:H3	1.32	0.76
8:I:21:ILE:HD11	8:I:61:LEU:HD13	1.66	0.75
21:A:723:U:H2'	21:A:855:U:H4'	1.69	0.75
16:Q:60:GLU:HG3	16:Q:76:VAL:HB	1.69	0.74
21:A:950:U:H3	21:A:1231:G:H1	1.34	0.74
7:H:10:MET:HA	7:H:27:MET:HE1	1.69	0.74
8:I:18:ARG:HH12	21:A:1130:A:H5'	1.51	0.74
21:A:1218:C:H2'	21:A:1219:A:C8	2.22	0.74
21:A:984:C:N3	21:A:1222:G:N2	2.35	0.73
16:Q:25:ILE:HB	16:Q:42:THR:HG23	1.71	0.72
3:D:105:MET:HE3	3:D:173:VAL:HG13	1.69	0.72
3:D:50:ASP:OD1	3:D:50:ASP:N	2.22	0.72
3:D:56:ARG:NH2	21:A:544:G:OP1	2.23	0.71
3:D:105:MET:SD	3:D:107:PHE:CE2	2.83	0.71
4:E:157:ARG:HH21	7:H:43:GLU:HG3	1.55	0.71
1:B:70:VAL:HB	1:B:163:VAL:HG13	1.72	0.71
3:D:60:LYS:O	3:D:64:ILE:HG22	1.91	0.71
8:I:42:GLU:HA	8:I:45:ARG:HH21	1.54	0.71
2:C:65:ARG:HG2	2:C:102:ASN:HD21	1.54	0.71
21:A:988:G:H1'	21:A:1015:G:H22	1.55	0.71
11:L:50:ARG:HG3	11:L:90:LEU:HD21	1.72	0.70
3:D:150:LYS:HG2	3:D:178:MET:CE	2.17	0.70
7:H:105:SER:HB2	7:H:126:ILE:HD11	1.71	0.70
21:A:1407:5MC:O2'	21:A:1408:A:H5'	1.91	0.70
2:C:142:MET:SD	2:C:149:ILE:HG22	2.32	0.70
21:A:1323:G:N2	21:A:1361:G:O2'	2.24	0.70
2:C:57:ILE:HG13	2:C:64:ILE:HD11	1.73	0.70
12:M:34:LEU:HD13	12:M:41:GLU:HG2	1.74	0.69
15:P:47:GLU:OE1	15:P:48:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:GLU:OE2	9:J:94:ALA:HB3	1.92	0.69
21:A:1407:5MC:H2'	21:A:1408:A:H8	1.58	0.69
8:I:5:GLN:HG2	8:I:22:LYS:HE2	1.74	0.69
11:L:114:ARG:HB3	11:L:119:VAL:HB	1.72	0.69
12:M:24:GLY:O	12:M:29:ARG:NH1	2.25	0.69
13:N:5:SER:O	13:N:9:ARG:NE	2.25	0.69
18:S:44:MET:HE3	18:S:62:VAL:HG21	1.74	0.69
21:A:1306:A:H62	21:A:1331:G:H21	1.39	0.69
6:G:47:LEU:HD13	6:G:58:GLU:HG3	1.75	0.69
21:A:1096:C:H2'	21:A:1097:C:H6	1.57	0.69
6:G:57:SER:HB2	6:G:60:GLU:HB2	1.74	0.68
7:H:64:LYS:HE2	7:H:71:VAL:HG21	1.75	0.68
3:D:170:TRP:HA	3:D:184:ARG:NH1	2.08	0.68
21:A:79:G:H22	21:A:90:C:H42	1.41	0.68
8:I:88:MET:HE1	8:I:104:VAL:CG1	2.24	0.68
18:S:11:ILE:HG13	18:S:38:SER:HB3	1.76	0.68
11:L:55:VAL:HG21	11:L:80:ILE:HD11	1.76	0.68
21:A:324:G:N1	21:A:327:A:OP2	2.27	0.68
2:C:156:ARG:HH21	21:A:1055:A:H1'	1.59	0.68
13:N:5:SER:CB	13:N:9:ARG:HH21	2.06	0.67
10:K:109:ASN:ND2	20:U:4:ILE:O	2.23	0.67
6:G:140:ASP:HA	6:G:143:ARG:HG2	1.76	0.67
3:D:58:LYS:NZ	21:A:545:C:OP1	2.27	0.67
11:L:25:GLU:OE1	11:L:59:ASN:ND2	2.22	0.67
3:D:105:MET:CE	3:D:107:PHE:CZ	2.75	0.67
12:M:78:LYS:HA	12:M:81:MET:CE	2.23	0.67
9:J:9:ARG:HH12	9:J:71:LEU:HD21	1.60	0.67
2:C:183:ASP:HB3	2:C:202:ILE:HB	1.76	0.66
10:K:114:THR:HG21	20:U:28:VAL:HG13	1.76	0.66
21:A:147:G:H2'	21:A:148:G:C8	2.29	0.66
21:A:713:G:H2'	21:A:714:G:C8	2.29	0.66
21:A:677:U:H3	21:A:713:G:H22	1.43	0.66
21:A:1441:A:H62	21:A:1461:G:H21	1.43	0.66
13:N:6:MET:HA	13:N:9:ARG:CD	2.26	0.66
21:A:1032:G:H2'	21:A:1033:G:H4'	1.76	0.66
3:D:31:LYS:O	21:A:413:G:N1	2.27	0.66
7:H:32:LEU:O	7:H:36:ILE:HG12	1.95	0.66
21:A:1071:C:H2'	21:A:1072:G:H8	1.60	0.66
21:A:1315:U:H2'	21:A:1316:G:C8	2.31	0.66
4:E:11:LEU:HD21	4:E:71:MET:HE1	1.76	0.65
13:N:73:PHE:HE2	13:N:75:ARG:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:6:MET:HA	13:N:9:ARG:HD2	1.78	0.65
9:J:27:GLU:OE2	9:J:31:ARG:NH2	2.30	0.65
21:A:728:A:H2'	21:A:729:A:C8	2.32	0.65
21:A:1265:C:H2'	21:A:1266:G:C8	2.30	0.65
21:A:269:C:H2'	21:A:270:A:H8	1.61	0.65
21:A:1017:U:H2'	21:A:1018:G:C8	2.31	0.65
1:B:183:VAL:HG12	1:B:196:VAL:HG13	1.79	0.64
3:D:112:ALA:HB1	21:A:407:U:H5''	1.78	0.64
16:Q:21:ILE:HD11	16:Q:75:LEU:HD21	1.78	0.64
17:R:11:CYS:HB3	17:R:48:ARG:HH11	1.63	0.64
21:A:481:G:O2'	21:A:483:C:N4	2.29	0.64
21:A:999:C:H2'	21:A:1000:A:H8	1.62	0.64
1:B:148:LEU:HD23	1:B:151:ILE:HD11	1.79	0.64
8:I:18:ARG:HH11	8:I:20:PHE:HE2	1.44	0.64
18:S:29:LYS:HG2	18:S:30:PRO:HD2	1.80	0.64
18:S:77:THR:O	21:A:958:A:N6	2.31	0.64
21:A:999:C:H2'	21:A:1000:A:C8	2.33	0.64
21:A:1027:C:H2'	21:A:1028:C:C6	2.33	0.64
21:A:1305:G:N1	21:A:1331:G:N3	2.46	0.64
8:I:42:GLU:CG	8:I:45:ARG:HH21	2.10	0.63
11:L:43:LYS:HG3	11:L:91:PRO:HD3	1.79	0.63
8:I:123:ARG:HB2	21:A:1349:A:H5''	1.80	0.63
15:P:57:ILE:HG21	15:P:75:ILE:HD11	1.80	0.63
21:A:1253:G:H2'	21:A:1254:A:C8	2.33	0.63
21:A:473:U:H2'	21:A:474:G:H8	1.64	0.63
6:G:113:ASP:OD2	6:G:122:ASN:ND2	2.31	0.63
8:I:47:VAL:HG13	8:I:80:ARG:HD3	1.79	0.63
13:N:6:MET:HE2	13:N:63:ARG:HH22	1.63	0.63
16:Q:47:HIS:HB3	16:Q:74:THR:HG22	1.81	0.63
21:A:473:U:H2'	21:A:474:G:C8	2.33	0.63
4:E:12:GLN:HG2	4:E:117:VAL:HG12	1.81	0.63
12:M:13:LYS:NZ	21:A:1302:C:OP2	2.31	0.63
13:N:5:SER:HB2	13:N:9:ARG:HH21	1.64	0.63
18:S:18:LYS:HA	18:S:21:LYS:HE3	1.81	0.62
8:I:74:GLY:N	21:A:1372:U:OP1	2.29	0.62
12:M:54:ASP:OD1	12:M:57:ARG:NH1	2.33	0.62
13:N:64:CYS:HB2	13:N:80:SER:H	1.64	0.62
18:S:63:THR:H	18:S:66:MET:HE1	1.65	0.62
3:D:165:ARG:O	3:D:167:LYS:NZ	2.31	0.62
3:D:116:GLN:NE2	21:A:406:G:N3	2.48	0.62
3:D:104:ARG:HB3	3:D:168:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:14:LYS:H	10:K:14:LYS:HD2	1.65	0.62
21:A:664:G:H22	21:A:741:G:H1	1.45	0.62
4:E:94:VAL:HB	4:E:111:MET:HE3	1.80	0.62
4:E:115:LEU:HD13	4:E:123:VAL:HG11	1.81	0.62
12:M:90:ARG:NH1	21:A:1226:C:OP2	2.31	0.62
18:S:51:VAL:O	18:S:58:VAL:N	2.33	0.62
21:A:1175:G:H2'	21:A:1176:A:H8	1.64	0.62
21:A:390:U:H2'	21:A:391:G:C8	2.34	0.62
21:A:1391:U:H2'	21:A:1392:G:C8	2.35	0.61
8:I:85:ARG:HA	8:I:88:MET:HG2	1.82	0.61
21:A:84:U:O2'	21:A:86:G:N2	2.32	0.61
21:A:413:G:H4'	21:A:414:A:H5''	1.82	0.61
21:A:746:A:H2'	21:A:747:A:C8	2.35	0.61
7:H:84:ARG:NH2	21:A:587:G:OP1	2.33	0.61
21:A:539:A:H2'	21:A:540:G:C8	2.36	0.61
21:A:1382:C:H2'	21:A:1383:C:H6	1.65	0.61
9:J:42:LEU:HD11	9:J:73:LEU:HB2	1.81	0.61
13:N:75:ARG:NH2	21:A:1360:A:OP2	2.34	0.61
15:P:4:ILE:HG12	15:P:21:VAL:HG22	1.81	0.61
21:A:978:A:H61	21:A:1316:G:H1'	1.66	0.61
21:A:1250:A:H2'	21:A:1251:A:C8	2.35	0.61
21:A:1017:U:H2'	21:A:1018:G:H8	1.64	0.61
8:I:7:TYR:HE1	8:I:18:ARG:HB2	1.66	0.60
18:S:50:ALA:HB1	18:S:57:HIS:HB3	1.83	0.60
15:P:5:ARG:HB2	21:A:376:G:H5''	1.82	0.60
8:I:122:ARG:NH1	21:A:1345:U:OP1	2.34	0.60
13:N:6:MET:HE1	21:A:981:U:H5'	1.84	0.60
21:A:1295:U:O2'	21:A:1302:C:N4	2.34	0.60
21:A:745:G:H2'	21:A:746:A:H8	1.66	0.60
1:B:118:GLU:OE2	1:B:152:LYS:NZ	2.31	0.60
2:C:108:LYS:HE3	2:C:144:LEU:HD23	1.83	0.60
11:L:54:ARG:HH22	11:L:62:GLU:HG3	1.66	0.60
21:A:56:U:H2'	21:A:57:G:C8	2.36	0.60
21:A:269:C:H2'	21:A:270:A:C8	2.36	0.60
21:A:1007:U:H2'	21:A:1008:U:H6	1.67	0.60
21:A:323:U:H2'	21:A:324:G:O4'	2.02	0.60
21:A:1412:C:H2'	21:A:1413:A:C8	2.37	0.60
8:I:18:ARG:NE	8:I:66:THR:OG1	2.29	0.60
7:H:108:LYS:HD3	7:H:121:LEU:HD11	1.83	0.59
19:T:10:ARG:NH2	21:A:107:G:N7	2.50	0.59
21:A:514:C:H2'	21:A:515:G:H8	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:HIS:HB2	13:N:89:MET:HE2	1.83	0.59
2:C:53:SER:HB3	2:C:115:LEU:HG	1.84	0.59
3:D:202:GLU:O	21:A:8:A:N6	2.35	0.59
18:S:37:ARG:NH1	21:A:1317:C:N3	2.49	0.59
21:A:75:G:H2'	21:A:76:G:H8	1.66	0.59
3:D:100:ASN:O	3:D:104:ARG:HG2	2.02	0.59
3:D:198:HIS:O	3:D:202:GLU:HG2	2.01	0.59
6:G:16:PRO:HB3	8:I:46:MET:HG3	1.85	0.59
6:G:75:VAL:HB	6:G:86:GLN:HB3	1.84	0.59
7:H:13:ARG:HD2	7:H:27:MET:HE3	1.84	0.59
7:H:77:ARG:NH1	7:H:79:SER:O	2.35	0.59
1:B:134:ALA:O	1:B:138:THR:OG1	2.20	0.59
21:A:1251:A:N3	21:A:1369:C:O2'	2.33	0.59
20:U:12:PHE:CZ	20:U:16:LEU:HD22	2.37	0.59
10:K:120:GLY:N	21:A:716:A:N3	2.50	0.59
17:R:11:CYS:HB2	17:R:47:THR:HA	1.83	0.59
1:B:114:LEU:HD22	1:B:144:LEU:HB3	1.84	0.59
12:M:79:ARG:O	12:M:83:LEU:HB2	2.03	0.59
21:A:200:G:H2'	21:A:201:G:H8	1.68	0.59
21:A:737:C:H2'	21:A:738:C:C6	2.38	0.59
8:I:42:GLU:CG	8:I:45:ARG:NH2	2.61	0.59
21:A:17:U:H2'	21:A:18:C:C6	2.37	0.59
21:A:769:G:H4'	21:A:1513:A:H4'	1.84	0.59
21:A:1405:G:H2'	21:A:1406:U:H6	1.68	0.59
1:B:31:ILE:HG21	1:B:39:HIS:CD2	2.38	0.59
1:B:27:MET:HE1	1:B:193:PRO:CD	2.32	0.58
2:C:73:PRO:HG3	2:C:105:GLU:HG2	1.84	0.58
19:T:43:ASP:OD1	19:T:46:ALA:N	2.35	0.58
1:B:30:PHE:O	1:B:42:ASN:N	2.35	0.58
21:A:1317:C:H3'	21:A:1318:A:H8	1.67	0.58
6:G:140:ASP:O	6:G:144:MET:HG3	2.03	0.58
21:A:1237:C:H4'	21:A:1300:G:H22	1.68	0.58
2:C:19:ASN:O	2:C:40:ARG:NH2	2.36	0.58
4:E:38:VAL:HG11	4:E:114:VAL:HG22	1.85	0.58
7:H:22:LYS:O	7:H:65:TYR:OH	2.21	0.58
21:A:148:G:O2'	21:A:1446:A:N3	2.32	0.58
21:A:1060:U:H2'	21:A:1061:G:H8	1.69	0.58
2:C:69:HIS:HA	2:C:104:ALA:HB3	1.84	0.58
3:D:67:VAL:HG22	3:D:97:ARG:HH11	1.69	0.58
3:D:105:MET:HE2	3:D:107:PHE:CE2	2.36	0.58
6:G:31:MET:HE1	6:G:35:LYS:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:130:ASN:HA	6:G:135:VAL:HG21	1.85	0.58
8:I:92:GLU:H	8:I:92:GLU:CD	2.11	0.58
15:P:28:ARG:HD2	21:A:375:U:O2'	2.02	0.58
21:A:674:G:H2'	21:A:675:A:H8	1.67	0.58
21:A:811:C:O2'	21:A:901:A:N1	2.35	0.58
15:P:12:LYS:HG2	15:P:13:LYS:HG2	1.84	0.58
21:A:501:C:H2'	21:A:502:A:H8	1.68	0.58
21:A:552:U:H2'	21:A:553:A:H8	1.68	0.58
21:A:608:A:H2'	21:A:609:A:O4'	2.04	0.58
21:A:745:G:H2'	21:A:746:A:C8	2.39	0.58
2:C:143:ARG:HG3	2:C:144:LEU:HD12	1.86	0.58
8:I:106:ARG:HH12	21:A:1117:A:H5''	1.68	0.58
21:A:337:G:H2'	21:A:338:A:C8	2.38	0.58
21:A:524:G:H2'	21:A:525:C:C6	2.39	0.58
21:A:1060:U:H2'	21:A:1061:G:C8	2.38	0.58
21:A:1266:G:N2	21:A:1269:A:OP2	2.31	0.58
6:G:26:PHE:HD1	6:G:101:MET:HG3	1.67	0.58
14:O:68:ASP:O	14:O:72:ARG:HG2	2.03	0.58
21:A:976:G:H8	21:A:1358:U:H2'	1.69	0.58
2:C:188:GLU:N	2:C:188:GLU:OE2	2.37	0.58
5:F:29:ILE:HD12	5:F:64:VAL:HG11	1.86	0.58
10:K:16:VAL:HG12	10:K:77:TYR:HB3	1.86	0.58
21:A:131:A:H2'	21:A:132:C:C6	2.38	0.57
4:E:164:ILE:HG22	4:E:165:LEU:HD12	1.86	0.57
5:F:90:MET:HE1	17:R:23:TYR:CE1	2.40	0.57
4:E:13:GLU:HG2	4:E:39:VAL:HG12	1.85	0.57
4:E:94:VAL:HB	4:E:111:MET:CE	2.34	0.57
13:N:24:ARG:NH1	13:N:55:SER:OG	2.33	0.57
13:N:79:LEU:HB2	13:N:84:VAL:HG23	1.86	0.57
20:U:46:LYS:HD3	21:A:1528:U:C4	2.40	0.57
21:A:600:A:H2'	21:A:601:G:C8	2.40	0.57
18:S:18:LYS:HD3	18:S:31:LEU:HD23	1.86	0.57
2:C:161:GLU:O	21:A:1055:A:O2'	2.23	0.57
7:H:88:ARG:NH1	21:A:600:A:OP2	2.38	0.57
21:A:555:U:H2'	21:A:556:C:C6	2.40	0.56
1:B:31:ILE:HG21	1:B:39:HIS:HD2	1.70	0.56
1:B:80:VAL:HG22	1:B:214:LEU:HD11	1.86	0.56
3:D:105:MET:CE	3:D:107:PHE:CE2	2.88	0.56
5:F:9:MET:HE2	5:F:86:ARG:HB3	1.86	0.56
21:A:21:G:H2'	21:A:22:G:C8	2.39	0.56
21:A:501:C:H2'	21:A:502:A:C8	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:990:C:H2'	21:A:991:U:C6	2.40	0.56
21:A:1007:U:H2'	21:A:1008:U:C6	2.41	0.56
16:Q:66:PRO:O	21:A:264:C:O2'	2.23	0.56
18:S:63:THR:HG23	18:S:65:GLU:H	1.70	0.56
6:G:29:ILE:HG21	6:G:101:MET:HB3	1.86	0.56
7:H:36:ILE:HD13	7:H:110:VAL:HG11	1.88	0.56
8:I:19:VAL:HG22	8:I:65:ILE:HG23	1.88	0.56
8:I:42:GLU:O	8:I:46:MET:HG2	2.06	0.56
12:M:78:LYS:HA	12:M:81:MET:HE3	1.86	0.56
14:O:46:HIS:ND1	21:A:668:G:O2'	2.37	0.56
18:S:63:THR:HG22	18:S:66:MET:HE1	1.86	0.56
3:D:104:ARG:NH2	3:D:111:ARG:HH22	2.04	0.56
13:N:28:LYS:NZ	21:A:1316:G:OP1	2.32	0.56
21:A:455:G:H2'	21:A:456:A:H8	1.71	0.56
21:A:1356:G:H2'	21:A:1357:A:C8	2.41	0.56
11:L:54:ARG:HH22	11:L:62:GLU:CG	2.17	0.56
12:M:107:ARG:N	21:A:948:C:OP1	2.39	0.56
16:Q:7:THR:HG22	16:Q:62:ARG:HB3	1.87	0.56
1:B:31:ILE:HD13	1:B:39:HIS:HB3	1.86	0.56
6:G:15:ASP:OD1	6:G:18:PHE:N	2.34	0.56
11:L:110:ARG:HB3	11:L:119:VAL:HG21	1.88	0.56
21:A:262:A:H2'	21:A:263:A:H8	1.70	0.56
2:C:4:LYS:HE3	21:A:1191:A:H5''	1.87	0.56
21:A:600:A:H2'	21:A:601:G:H8	1.71	0.56
5:F:25:TYR:CE2	5:F:78:PHE:HE1	2.24	0.55
19:T:2:ALA:N	21:A:333:U:OP1	2.39	0.55
11:L:36:ARG:HG2	11:L:38:TYR:CD1	2.41	0.55
3:D:121:LYS:HE2	21:A:439:U:H5''	1.89	0.55
8:I:119:ARG:HH21	21:A:1233:G:H4'	1.71	0.55
21:A:384:G:H2'	21:A:385:C:C6	2.41	0.55
21:A:993:G:O2'	21:A:994:A:N7	2.38	0.55
2:C:70:THR:HG21	2:C:76:VAL:HG21	1.88	0.55
3:D:85:ASN:HB3	3:D:88:GLU:HB2	1.87	0.55
12:M:71:ARG:O	12:M:75:MET:HG3	2.07	0.55
4:E:29:ARG:NH2	21:A:1397:C:OP2	2.39	0.55
18:S:77:THR:HB	21:A:1221:G:H4'	1.89	0.55
1:B:107:VAL:HA	1:B:110:SER:HB3	1.88	0.55
4:E:96:MET:HE1	4:E:140:THR:HG23	1.89	0.55
6:G:111:ARG:NH1	6:G:126:ASP:OD2	2.39	0.55
6:G:35:LYS:NZ	21:A:1290:G:OP1	2.40	0.55
8:I:85:ARG:HA	8:I:88:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:36:SER:HA	17:R:72:ASP:HB3	1.89	0.55
2:C:131:ARG:O	2:C:135:LYS:HG2	2.07	0.54
2:C:183:ASP:HB2	2:C:204:LYS:HE3	1.87	0.54
21:A:518:C:O2'	21:A:530:G:N2	2.40	0.54
21:A:1422:G:H1	21:A:1478:U:H3	1.53	0.54
7:H:7:ILE:HD11	7:H:32:LEU:HD23	1.88	0.54
21:A:92:U:H2'	21:A:93:U:C6	2.43	0.54
21:A:1346:A:N1	21:A:1374:A:H5''	2.22	0.54
6:G:92:ARG:HG2	6:G:93:PRO:HD2	1.90	0.54
21:A:41:G:H2'	21:A:42:G:H8	1.72	0.54
21:A:714:G:H2'	21:A:715:A:C8	2.42	0.54
21:A:1005:A:H8	21:A:1024:G:H21	1.53	0.54
8:I:96:SER:HA	8:I:99:ARG:HB2	1.90	0.54
4:E:96:MET:CE	4:E:140:THR:HG23	2.38	0.54
21:A:562:U:H5'	21:A:563:A:C5	2.43	0.54
21:A:715:A:H2'	21:A:716:A:C8	2.42	0.54
2:C:9:GLY:HA3	13:N:89:MET:HE3	1.90	0.54
5:F:2:ARG:NH2	21:A:739:C:OP2	2.40	0.54
5:F:17:GLN:N	5:F:17:GLN:OE1	2.41	0.54
5:F:18:VAL:HA	5:F:21:MET:HG2	1.90	0.54
8:I:6:TYR:HB2	8:I:21:ILE:CG2	2.38	0.54
1:B:166:ALA:HB2	1:B:185:ALA:HB1	1.89	0.54
2:C:86:LYS:O	2:C:90:VAL:HG23	2.08	0.54
2:C:189:ALA:HB3	2:C:196:ILE:HB	1.90	0.54
8:I:126:GLN:NE2	21:A:1232:U:OP1	2.37	0.54
13:N:47:LYS:O	13:N:50:THR:OG1	2.24	0.54
19:T:27:MET:HE1	19:T:57:ILE:HG23	1.89	0.54
21:A:41:G:H2'	21:A:42:G:C8	2.43	0.54
21:A:634:C:H2'	21:A:635:A:H8	1.72	0.54
21:A:904:U:H2'	21:A:905:U:C6	2.42	0.54
21:A:1027:C:H42	21:A:1035:A:H61	1.55	0.54
21:A:505:G:H2'	21:A:506:G:C8	2.43	0.54
2:C:42:TYR:CE1	2:C:46:GLU:HG2	2.43	0.53
9:J:32:THR:HG22	9:J:82:LYS:HG2	1.90	0.53
10:K:20:VAL:HG22	10:K:83:GLU:HB2	1.90	0.53
18:S:4:SER:HA	21:A:1313:U:OP2	2.08	0.53
21:A:337:G:H2'	21:A:338:A:H8	1.73	0.53
2:C:20:SER:OG	2:C:40:ARG:NH2	2.26	0.53
3:D:144:SER:HA	3:D:179:GLU:HB2	1.89	0.53
21:A:1120:C:H2'	21:A:1121:U:C6	2.43	0.53
21:A:262:A:H2'	21:A:263:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:476:U:H2'	21:A:477:C:C6	2.43	0.53
1:B:154:MET:HE3	1:B:158:PRO:HD3	1.89	0.53
5:F:69:GLU:O	5:F:73:GLU:OE1	2.25	0.53
8:I:6:TYR:HB2	8:I:21:ILE:HG23	1.89	0.53
18:S:66:MET:HB2	18:S:74:PHE:CZ	2.44	0.53
21:A:957:U:H2'	21:A:959:A:OP2	2.08	0.53
2:C:7:PRO:O	2:C:11:ARG:NH1	2.37	0.53
2:C:63:SER:HB2	2:C:98:PRO:O	2.09	0.53
21:A:455:G:H2'	21:A:456:A:C8	2.44	0.53
21:A:447:G:N2	21:A:487:A:H62	2.00	0.53
12:M:101:ARG:HD2	21:A:950:U:OP2	2.08	0.53
18:S:51:VAL:N	18:S:58:VAL:O	2.37	0.53
21:A:73:C:O2'	21:A:74:A:H8	1.92	0.53
21:A:75:G:H2'	21:A:76:G:C8	2.44	0.53
21:A:859:G:H2'	21:A:860:A:C8	2.44	0.53
15:P:70:ARG:HH22	21:A:451:A:H5'	1.74	0.53
21:A:56:U:H2'	21:A:57:G:H8	1.74	0.53
17:R:26:ILE:HD11	17:R:67:LEU:HB3	1.91	0.52
16:Q:22:VAL:HG22	16:Q:45:HIS:CD2	2.44	0.52
21:A:79:G:H1	21:A:90:C:H42	1.57	0.52
21:A:80:A:H2'	21:A:81:A:H8	1.74	0.52
21:A:372:C:O2	21:A:389:A:N6	2.42	0.52
21:A:559:A:H4'	21:A:560:A:H3'	1.91	0.52
21:A:1314:C:H2'	21:A:1315:U:C6	2.44	0.52
2:C:71:ALA:HB2	2:C:109:PRO:HB3	1.91	0.52
3:D:10:LYS:HE3	21:A:542:G:OP1	2.10	0.52
8:I:6:TYR:O	8:I:21:ILE:HG22	2.09	0.52
21:A:77:A:H2'	21:A:78:A:C8	2.44	0.52
21:A:222:C:H2'	21:A:223:A:H8	1.74	0.52
21:A:1391:U:H2'	21:A:1392:G:H8	1.74	0.52
21:A:1224:U:O2	21:A:1322:C:H5'	2.10	0.52
10:K:101:ASN:ND2	20:U:12:PHE:CD2	2.77	0.52
14:O:18:ASP:OD1	14:O:21:ASP:HB2	2.09	0.52
15:P:64:GLY:O	21:A:136:C:O2'	2.20	0.52
16:Q:53:CYS:SG	16:Q:75:LEU:HD11	2.49	0.52
21:A:2:A:H1'	21:A:613:C:O2'	2.09	0.52
3:D:29:ASP:OD1	3:D:29:ASP:N	2.41	0.52
9:J:55:PRO:HG2	9:J:56:HIS:N	2.25	0.52
13:N:6:MET:HE2	13:N:63:ARG:NH2	2.24	0.52
18:S:70:LYS:N	18:S:73:GLU:OE2	2.43	0.52
21:A:160:A:H2'	21:A:161:A:O4'	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:976:G:C8	21:A:1358:U:H2'	2.44	0.52
8:I:128:SER:OG	8:I:130:ARG:OXT	2.25	0.52
21:A:864:A:H2'	21:A:865:A:C8	2.45	0.52
1:B:97:LEU:HD22	21:A:1103:C:H5''	1.91	0.52
15:P:70:ARG:NH2	21:A:451:A:H5'	2.25	0.52
21:A:1308:U:H2'	21:A:1309:G:C8	2.45	0.52
7:H:29:SER:HB3	7:H:57:PRO:HB2	1.91	0.52
21:A:410:G:H2'	21:A:429:U:C4	2.44	0.52
21:A:1095:U:H2'	21:A:1096:C:C6	2.45	0.52
21:A:1315:U:O2'	21:A:1360:A:O2'	2.26	0.52
12:M:33:ILE:HG22	12:M:56:LEU:HD22	1.92	0.52
17:R:61:ARG:NH2	21:A:736:C:OP1	2.43	0.52
19:T:3:ASN:OD1	19:T:3:ASN:N	2.42	0.52
21:A:494:G:H2'	21:A:496:A:H1'	1.92	0.52
21:A:1253:G:H2'	21:A:1254:A:H8	1.73	0.51
7:H:16:ASN:ND2	21:A:826:C:O2	2.43	0.51
21:A:299:G:H2'	21:A:300:A:C8	2.45	0.51
21:A:1023:U:N3	21:A:1024:G:O6	2.43	0.51
21:A:1138:G:H3'	21:A:1138:G:N3	2.25	0.51
1:B:94:HIS:HB2	1:B:146:ASN:O	2.10	0.51
1:B:107:VAL:O	1:B:111:ILE:HG23	2.10	0.51
4:E:60:ILE:O	4:E:64:MET:HG2	2.09	0.51
11:L:85:GLY:O	11:L:96:HIS:ND1	2.38	0.51
4:E:76:LEU:O	4:E:82:GLN:NE2	2.43	0.51
10:K:23:ILE:HG22	10:K:32:VAL:HG13	1.92	0.51
11:L:4:VAL:HG23	16:Q:34:TYR:HB3	1.92	0.51
18:S:64:ASP:O	18:S:67:VAL:HG22	2.11	0.51
21:A:335:C:H2'	21:A:336:A:H8	1.74	0.51
2:C:72:ARG:HB3	2:C:75:ILE:HG23	1.93	0.51
3:D:59:GLN:O	3:D:63:ARG:HG3	2.11	0.51
3:D:117:LEU:HB3	3:D:123:ILE:HD11	1.93	0.51
8:I:85:ARG:HA	8:I:88:MET:CG	2.39	0.51
12:M:9:ILE:HB	12:M:18:ALA:HB1	1.92	0.51
17:R:23:TYR:HE2	17:R:65:LEU:HD12	1.75	0.51
21:A:98:A:H2'	21:A:99:C:C6	2.46	0.51
21:A:165:G:H2'	21:A:166:U:H6	1.75	0.51
21:A:634:C:H2'	21:A:635:A:C8	2.46	0.51
21:A:1291:U:H2'	21:A:1292:G:H8	1.75	0.51
8:I:124:ARG:HG2	8:I:125:PRO:HD2	1.93	0.51
15:P:77:GLU:HA	15:P:81:ALA:HB2	1.92	0.51
21:A:944:G:N1	21:A:1338:G:OP2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:LYS:HE2	21:A:429:U:H6	1.74	0.51
6:G:36:LYS:NZ	21:A:1374:A:OP1	2.42	0.51
6:G:102:ARG:NH1	21:A:939:G:OP1	2.43	0.51
8:I:27:LYS:HE3	8:I:62:ASP:HB3	1.93	0.51
8:I:42:GLU:CA	8:I:45:ARG:HH21	2.23	0.51
21:A:253:A:H2'	21:A:254:G:C8	2.46	0.51
21:A:512:U:H2'	21:A:513:C:C6	2.45	0.51
21:A:1223:C:OP2	21:A:1224:U:H2'	2.11	0.51
4:E:133:PRO:O	4:E:137:VAL:HG13	2.11	0.51
11:L:111:LYS:HB2	21:A:538:G:H5''	1.91	0.51
21:A:165:G:H2'	21:A:166:U:C6	2.46	0.51
21:A:746:A:H2'	21:A:747:A:H8	1.73	0.51
3:D:126:ASN:ND2	3:D:141:ASP:OD1	2.44	0.51
9:J:87:LEU:HB2	9:J:88:MET:HE2	1.93	0.51
10:K:72:ASP:O	10:K:75:LYS:HG3	2.11	0.51
11:L:110:ARG:NH2	21:A:537:G:OP1	2.44	0.51
21:A:1120:C:H2'	21:A:1121:U:H6	1.75	0.51
21:A:1171:A:H2'	21:A:1172:C:C6	2.45	0.51
21:A:1159:U:O4'	21:A:1182:G:N2	2.43	0.50
21:A:1175:G:H2'	21:A:1176:A:C8	2.45	0.50
21:A:1404:C:H2'	21:A:1405:G:C8	2.46	0.50
3:D:104:ARG:HH21	3:D:111:ARG:HH22	1.57	0.50
10:K:24:HIS:HB3	10:K:31:ILE:HB	1.92	0.50
10:K:64:GLN:O	10:K:68:GLU:HG2	2.11	0.50
18:S:78:ARG:HH21	21:A:1223:C:P	2.35	0.50
21:A:1142:G:C2	21:A:1143:G:H1'	2.46	0.50
2:C:19:ASN:N	13:N:91:GLY:O	2.43	0.50
3:D:117:LEU:O	3:D:123:ILE:HG12	2.11	0.50
15:P:4:ILE:HG22	15:P:71:VAL:HG11	1.93	0.50
21:A:1116:U:O2	21:A:1184:G:O6	2.28	0.50
3:D:95:GLU:HB3	3:D:186:PRO:HG2	1.92	0.50
16:Q:45:HIS:HB3	16:Q:71:LYS:HG3	1.92	0.50
21:A:1313:U:H2'	21:A:1314:C:C6	2.45	0.50
8:I:46:MET:HA	8:I:46:MET:HE2	1.93	0.50
9:J:7:ARG:HB3	9:J:101:SER:HB3	1.93	0.50
21:A:224:U:H2'	21:A:225:C:C6	2.47	0.50
21:A:399:G:H2'	21:A:400:C:C6	2.46	0.50
21:A:635:A:H2'	21:A:636:U:H6	1.76	0.50
8:I:116:VAL:HG11	9:J:62:ARG:HB2	1.92	0.50
12:M:22:ILE:HG23	12:M:66:GLU:HG2	1.94	0.50
12:M:107:ARG:NH2	12:M:111:GLY:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:47:HIS:O	16:Q:75:LEU:HD23	2.10	0.50
21:A:22:G:O2'	21:A:913:A:N1	2.38	0.50
21:A:527:G7M:O2'	21:A:535:A:N1	2.43	0.50
21:A:579:A:H2'	21:A:580:C:C6	2.46	0.50
21:A:1410:A:H2'	21:A:1411:C:C6	2.47	0.50
3:D:152:GLN:CD	21:A:437:U:H4'	2.36	0.50
21:A:376:G:C4	21:A:389:A:C2	3.00	0.50
21:A:1223:C:P	21:A:1224:U:H2'	2.52	0.50
21:A:313:A:H2'	21:A:314:C:C6	2.47	0.50
21:A:736:C:H2'	21:A:737:C:C6	2.47	0.50
7:H:7:ILE:O	7:H:11:LEU:HG	2.12	0.49
8:I:31:ASN:HB2	8:I:38:TYR:CE1	2.47	0.49
14:O:32:LEU:HD11	14:O:62:GLN:OE1	2.12	0.49
18:S:51:VAL:HG21	18:S:71:LEU:HB3	1.94	0.49
21:A:501:C:H1'	21:A:549:C:H1'	1.94	0.49
21:A:1181:G:H1'	21:A:1182:G:C8	2.46	0.49
21:A:1282:C:H2'	21:A:1283:U:C6	2.46	0.49
3:D:202:GLU:OE2	4:E:105:ILE:N	2.33	0.49
4:E:85:VAL:HG22	4:E:96:MET:HB2	1.93	0.49
5:F:47:LEU:HD22	17:R:66:SER:HB3	1.93	0.49
6:G:26:PHE:O	6:G:29:ILE:HG22	2.12	0.49
10:K:116:ILE:O	21:A:675:A:O2'	2.29	0.49
12:M:56:LEU:O	12:M:60:VAL:N	2.46	0.49
12:M:59:GLU:HA	12:M:62:LYS:HG3	1.94	0.49
20:U:40:LYS:NZ	21:A:1526:G:N7	2.60	0.49
21:A:176:C:H2'	21:A:177:G:N3	2.28	0.49
21:A:335:C:H2'	21:A:336:A:C8	2.48	0.49
21:A:628:G:H2'	21:A:629:A:C8	2.47	0.49
21:A:1086:U:H3	21:A:1099:G:N2	2.03	0.49
21:A:1435:G:H2'	21:A:1436:U:C6	2.47	0.49
3:D:39:GLY:HA3	21:A:542:G:H5'	1.94	0.49
12:M:40:ALA:HB3	12:M:43:VAL:HG23	1.94	0.49
21:A:246:A:C2	21:A:282:A:C5	3.01	0.49
8:I:28:ILE:HG12	8:I:63:LEU:HD12	1.95	0.49
13:N:88:ALA:HB2	13:N:96:LEU:HD23	1.95	0.49
21:A:1169:A:H2'	21:A:1170:A:C8	2.47	0.49
3:D:32:CYS:HB3	21:A:429:U:OP2	2.13	0.49
16:Q:10:GLY:HA3	16:Q:25:ILE:HD13	1.94	0.49
18:S:77:THR:HG21	21:A:1321:U:O2	2.12	0.49
21:A:1022:A:H2'	21:A:1023:U:O4'	2.12	0.49
4:E:109:GLY:HA2	4:E:112:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:62:GLU:O	11:L:62:GLU:HG2	2.13	0.49
19:T:71:LYS:NZ	21:A:261:U:OP2	2.33	0.49
21:A:123:U:H2'	21:A:124:C:C6	2.47	0.49
21:A:635:A:H2'	21:A:636:U:C6	2.47	0.49
3:D:31:LYS:HE2	21:A:429:U:H2'	1.93	0.49
21:A:201:G:O2'	21:A:469:C:O2'	2.26	0.49
21:A:312:C:H2'	21:A:313:A:C8	2.48	0.49
21:A:737:C:H2'	21:A:738:C:H6	1.78	0.49
21:A:219:U:H2'	21:A:220:G:H8	1.77	0.49
21:A:591:U:H2'	21:A:592:G:C8	2.48	0.49
21:A:1287:A:H2'	21:A:1288:A:C8	2.48	0.49
2:C:47:LEU:HD13	2:C:52:VAL:HG21	1.94	0.49
21:A:418:C:H2'	21:A:419:C:C6	2.48	0.49
1:B:95:ARG:NH1	1:B:95:ARG:HA	2.27	0.48
1:B:113:ARG:NE	1:B:140:GLU:OE2	2.32	0.48
1:B:187:VAL:HG23	1:B:191:SER:HB3	1.95	0.48
2:C:110:GLU:HB2	2:C:144:LEU:HD22	1.95	0.48
12:M:77:ILE:O	12:M:81:MET:HG3	2.13	0.48
21:A:1295:U:H2'	21:A:1296:C:C6	2.48	0.48
2:C:35:SER:O	2:C:39:VAL:HG22	2.13	0.48
10:K:20:VAL:N	10:K:35:THR:O	2.46	0.48
21:A:719:C:OP2	21:A:720:C:N4	2.44	0.48
21:A:1463:U:H2'	21:A:1464:U:C6	2.48	0.48
2:C:6:HIS:HB2	13:N:89:MET:CE	2.43	0.48
11:L:12:ARG:NH1	21:A:563:A:N3	2.61	0.48
13:N:63:ARG:HB3	13:N:68:GLY:HA2	1.95	0.48
16:Q:58:VAL:HB	16:Q:80:GLU:HB2	1.94	0.48
21:A:150:U:H2'	21:A:151:A:H8	1.79	0.48
21:A:867:G:O2'	21:A:873:A:N1	2.42	0.48
2:C:83:ASP:O	2:C:87:LEU:HG	2.13	0.48
10:K:112:ASP:H	20:U:2:PRO:HB2	1.78	0.48
20:U:22:SER:HA	20:U:25:LYS:HG2	1.96	0.48
21:A:382:A:H2'	21:A:383:A:C8	2.48	0.48
2:C:20:SER:HB3	2:C:22:TRP:NE1	2.29	0.48
2:C:20:SER:HG	2:C:40:ARG:HH22	1.58	0.48
5:F:51:ILE:O	5:F:54:LEU:HG	2.13	0.48
21:A:427:U:O2'	21:A:541:G:OP1	2.23	0.48
21:A:911:U:H2'	21:A:912:C:C6	2.48	0.48
21:A:1033:G:H3'	21:A:1034:G:C8	2.48	0.48
21:A:1119:C:H2'	21:A:1120:C:H6	1.78	0.48
3:D:83:LYS:HB3	3:D:83:LYS:HE2	1.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:125:VAL:HG22	3:D:143:VAL:HA	1.96	0.48
9:J:52:LEU:O	13:N:81:ARG:NH1	2.46	0.48
10:K:56:ARG:HG2	10:K:56:ARG:HH11	1.78	0.48
12:M:77:ILE:HG22	12:M:81:MET:HE2	1.95	0.48
21:A:1151:A:O2'	21:A:1152:A:H5''	2.12	0.48
2:C:22:TRP:HD1	2:C:57:ILE:HG22	1.78	0.48
12:M:78:LYS:HA	12:M:81:MET:HE2	1.92	0.48
12:M:96:PRO:HA	12:M:109:ARG:HG3	1.95	0.48
14:O:70:LEU:HD23	14:O:78:TYR:HA	1.95	0.48
21:A:54:C:H2'	21:A:352:C:H41	1.78	0.48
21:A:64:G:H4'	21:A:65:A:H5''	1.96	0.48
21:A:389:A:H3'	21:A:390:U:H6	1.78	0.48
21:A:859:G:H2'	21:A:860:A:H8	1.78	0.48
21:A:1049:U:H4'	21:A:1050:G:H5''	1.96	0.48
21:A:1306:A:H2'	21:A:1307:U:C6	2.48	0.48
3:D:172:GLU:HB2	3:D:183:LYS:NZ	2.29	0.48
11:L:88:LYS:HE3	21:A:526:C:OP2	2.14	0.48
12:M:93:ARG:HB3	12:M:95:LEU:HG	1.95	0.48
16:Q:53:CYS:SG	16:Q:59:VAL:HG11	2.54	0.48
18:S:44:MET:HG3	18:S:47:LEU:HD12	1.93	0.48
21:A:128:G:H2'	21:A:129:A:C8	2.49	0.48
21:A:144:G:H2'	21:A:145:G:C8	2.48	0.48
21:A:167:A:H2'	21:A:168:G:H8	1.79	0.48
21:A:1002:G:C2	21:A:1003:G:H1'	2.49	0.48
21:A:1009:U:H2'	21:A:1010:U:C6	2.49	0.48
21:A:1152:A:H2'	21:A:1153:G:C8	2.49	0.48
1:B:35:ARG:CZ	1:B:36:ASN:HB2	2.44	0.48
12:M:102:THR:O	21:A:1226:C:O2'	2.30	0.48
21:A:28:A:O2'	21:A:296:U:OP1	2.26	0.48
5:F:2:ARG:HH22	21:A:739:C:P	2.37	0.48
5:F:36:ILE:HD13	5:F:64:VAL:HG22	1.95	0.48
11:L:21:VAL:HG21	21:A:553:A:H5''	1.96	0.48
17:R:9:LYS:HA	17:R:46:GLY:HA3	1.95	0.48
19:T:39:ILE:HD11	19:T:83:ILE:HG13	1.96	0.48
21:A:1162:C:H2'	21:A:1163:A:H8	1.79	0.48
9:J:52:LEU:HB2	13:N:81:ARG:HD2	1.96	0.47
21:A:31:G:O2'	21:A:48:C:N4	2.47	0.47
21:A:51:A:N7	21:A:114:U:O2'	2.47	0.47
21:A:493:A:H2'	21:A:494:G:C8	2.48	0.47
21:A:1477:U:H2'	21:A:1478:U:C6	2.49	0.47
2:C:112:ASP:O	2:C:116:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:34:CYS:HB2	11:L:78:SER:H	1.79	0.47
13:N:9:ARG:NH2	21:A:1217:C:OP1	2.46	0.47
21:A:1315:U:HO2'	21:A:1360:A:HO2'	1.61	0.47
4:E:89:HIS:CE1	4:E:138:ARG:HD3	2.50	0.47
21:A:868:C:H2'	21:A:869:G:O4'	2.15	0.47
4:E:157:ARG:HH21	7:H:43:GLU:CG	2.25	0.47
5:F:45:ARG:HB2	5:F:59:TYR:HD2	1.78	0.47
21:A:1218:C:H2'	21:A:1219:A:H8	1.76	0.47
21:A:1273:C:H2'	21:A:1274:A:O4'	2.15	0.47
8:I:55:VAL:HG23	8:I:57:MET:HB2	1.96	0.47
12:M:81:MET:HA	12:M:88:GLY:HA3	1.97	0.47
21:A:35:G:H2'	21:A:36:C:C6	2.49	0.47
21:A:1412:C:H2'	21:A:1413:A:H8	1.78	0.47
21:A:1124:G:N2	21:A:1125:U:O4	2.33	0.47
21:A:1236:A:H4'	21:A:1304:G:H4'	1.96	0.47
21:A:1313:U:H2'	21:A:1314:C:H6	1.79	0.47
1:B:27:MET:HG3	1:B:30:PHE:HD2	1.80	0.47
3:D:148:LYS:NZ	21:A:438:U:OP1	2.43	0.47
8:I:21:ILE:CG2	8:I:86:ALA:HB1	2.44	0.47
13:N:5:SER:O	13:N:9:ARG:CD	2.62	0.47
21:A:200:G:H2'	21:A:201:G:C8	2.48	0.47
21:A:294:U:OP1	21:A:610:U:O2'	2.25	0.47
21:A:691:G:O2'	21:A:797:C:H4'	2.13	0.47
21:A:955:U:H2'	21:A:956:U:O4'	2.15	0.47
21:A:1140:C:H2'	21:A:1141:C:H6	1.80	0.47
21:A:1157:A:H4'	21:A:1158:C:O4'	2.15	0.47
1:B:68:LEU:HD23	1:B:161:LEU:HD11	1.95	0.47
15:P:76:LYS:NZ	21:A:473:U:OP1	2.48	0.47
21:A:475:C:H2'	21:A:476:U:C6	2.50	0.47
21:A:1096:C:H2'	21:A:1097:C:C6	2.45	0.47
21:A:1125:U:O2'	21:A:1126:U:H2'	2.15	0.47
2:C:42:TYR:CE1	2:C:90:VAL:HG11	2.50	0.47
3:D:157:ALA:O	3:D:161:LEU:HG	2.15	0.47
6:G:110:LYS:HB3	6:G:110:LYS:HE2	1.67	0.47
11:L:66:TYR:O	11:L:97:THR:HG23	2.15	0.47
14:O:78:TYR:O	14:O:82:ILE:HG23	2.14	0.47
21:A:77:A:H2'	21:A:78:A:H8	1.78	0.47
21:A:79:G:N2	21:A:90:C:H42	2.12	0.47
21:A:114:U:H2'	21:A:115:G:C8	2.50	0.47
21:A:458:U:H2'	21:A:459:A:C8	2.50	0.47
21:A:602:A:H2'	21:A:603:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1300:G:N2	21:A:1301:U:O4	2.36	0.47
4:E:94:VAL:CB	4:E:111:MET:HE3	2.45	0.47
6:G:84:THR:HB	6:G:86:GLN:HE21	1.80	0.47
9:J:6:ILE:HB	9:J:76:ILE:HB	1.97	0.47
11:L:46:ASN:ND2	11:L:89:D2T:SB	2.88	0.47
12:M:89:LEU:O	12:M:93:ARG:HD2	2.14	0.47
13:N:48:LEU:HD21	21:A:1317:C:H4'	1.97	0.47
16:Q:14:SER:HA	16:Q:55:ILE:HD11	1.97	0.47
18:S:54:GLY:HA2	21:A:1220:G:N3	2.30	0.47
21:A:607:A:H2'	21:A:608:A:C8	2.51	0.47
21:A:613:C:H2'	21:A:614:C:C6	2.49	0.47
21:A:637:C:H2'	21:A:638:U:C6	2.50	0.47
13:N:46:LEU:HD22	18:S:13:LEU:HD13	1.96	0.46
19:T:59:ASP:OD1	19:T:76:LYS:NZ	2.47	0.46
19:T:60:ARG:NH2	21:A:178:C:OP2	2.47	0.46
21:A:1149:C:H2'	21:A:1150:A:C8	2.50	0.46
8:I:7:TYR:CE1	8:I:18:ARG:HB2	2.49	0.46
14:O:23:GLY:HA3	21:A:750:C:O2	2.14	0.46
16:Q:46:VAL:HG11	16:Q:75:LEU:HD22	1.96	0.46
20:U:17:ARG:HA	20:U:20:LYS:HG2	1.97	0.46
21:A:257:G:H2'	21:A:258:G:H8	1.79	0.46
5:F:10:VAL:HB	5:F:58:HIS:HB3	1.97	0.46
13:N:58:SER:OG	21:A:1316:G:H4'	2.15	0.46
21:A:1354:U:H2'	21:A:1355:G:C8	2.50	0.46
3:D:74:ASN:O	3:D:77:LYS:HG3	2.15	0.46
6:G:27:VAL:O	6:G:31:MET:N	2.47	0.46
8:I:33:ARG:HD3	8:I:38:TYR:HA	1.98	0.46
11:L:12:ARG:HD3	21:A:562:U:H1'	1.98	0.46
17:R:65:LEU:O	17:R:67:LEU:HG	2.16	0.46
21:A:993:G:H2'	21:A:995:C:H41	1.80	0.46
21:A:1032:G:C6	21:A:1033:G:H1'	2.51	0.46
21:A:1308:U:H2'	21:A:1309:G:H8	1.80	0.46
21:A:1407:5MC:C2	21:A:1408:A:C8	3.03	0.46
7:H:96:MET:HG2	7:H:99:LEU:HB2	1.98	0.46
8:I:50:GLN:HB3	8:I:103:PHE:CZ	2.51	0.46
9:J:11:LYS:HB2	9:J:97:ASP:HB3	1.97	0.46
21:A:33:A:H2'	21:A:34:C:C6	2.51	0.46
21:A:321:A:N7	21:A:328:C:O2'	2.48	0.46
21:A:943:U:H2'	21:A:944:G:O4'	2.16	0.46
21:A:1064:G:H21	21:A:1190:G:H1'	1.81	0.46
8:I:130:ARG:HH11	8:I:130:ARG:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:107:ARG:H	21:A:948:C:P	2.39	0.46
21:A:427:U:H2'	21:A:428:G:C8	2.50	0.46
21:A:447:G:H21	21:A:487:A:N6	2.04	0.46
21:A:821:G:H2'	21:A:822:U:C6	2.50	0.46
21:A:1239:A:H61	21:A:1296:C:H2'	1.80	0.46
21:A:1316:G:H22	21:A:1318:A:H3'	1.80	0.46
2:C:78:GLY:HA3	2:C:83:ASP:HB2	1.97	0.46
3:D:153:SER:HA	3:D:156:LYS:HZ2	1.80	0.46
9:J:50:THR:HG22	9:J:62:ARG:HG2	1.97	0.46
14:O:65:LYS:NZ	21:A:581:G:OP1	2.48	0.46
8:I:88:MET:CE	8:I:104:VAL:HG13	2.35	0.46
16:Q:59:VAL:HG12	16:Q:78:VAL:HG22	1.98	0.46
21:A:601:G:H2'	21:A:602:A:H8	1.81	0.46
21:A:1354:U:H2'	21:A:1355:G:H8	1.81	0.46
3:D:69:GLU:HB3	21:A:546:A:P	2.56	0.46
8:I:18:ARG:HH22	8:I:64:TYR:HE1	1.61	0.46
8:I:114:LYS:HA	8:I:121:ALA:HA	1.97	0.46
16:Q:71:LYS:HD3	21:A:254:G:H5''	1.97	0.46
21:A:1050:G:H2'	21:A:1051:C:C6	2.51	0.46
7:H:41:LYS:HB2	7:H:46:ILE:HD11	1.98	0.46
8:I:10:GLY:HA3	8:I:82:GLY:N	2.31	0.46
9:J:24:GLU:HG3	9:J:90:LEU:HD21	1.96	0.46
11:L:66:TYR:CG	11:L:87:VAL:HG21	2.50	0.46
13:N:64:CYS:HA	13:N:79:LEU:HA	1.97	0.46
21:A:591:U:H2'	21:A:592:G:H8	1.81	0.46
21:A:674:G:H2'	21:A:675:A:C8	2.49	0.46
1:B:68:LEU:HD22	1:B:158:PRO:HG3	1.97	0.45
1:B:126:PHE:CD1	1:B:126:PHE:N	2.85	0.45
2:C:189:ALA:O	2:C:196:ILE:N	2.38	0.45
3:D:162:ALA:HA	3:D:165:ARG:HD3	1.98	0.45
5:F:81:ASN:OD1	5:F:84:VAL:N	2.37	0.45
21:A:263:A:H2'	21:A:264:C:C6	2.51	0.45
21:A:1321:U:H3'	21:A:1322:C:H2'	1.97	0.45
21:A:1355:G:H2'	21:A:1356:G:H8	1.81	0.45
3:D:19:LEU:HD22	3:D:64:ILE:HB	1.98	0.45
4:E:95:PHE:CE2	4:E:97:GLN:HG3	2.50	0.45
13:N:6:MET:HA	13:N:9:ARG:NE	2.31	0.45
14:O:26:GLU:OE2	14:O:81:LEU:HD22	2.16	0.45
16:Q:49:GLU:C	16:Q:51:ASN:H	2.23	0.45
19:T:62:ALA:HB1	19:T:69:LYS:HA	1.98	0.45
21:A:110:C:H2'	21:A:111:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:264:C:H2'	21:A:265:G:O4'	2.16	0.45
21:A:1064:G:H1'	21:A:1190:G:H21	1.81	0.45
21:A:1250:A:N3	21:A:1370:G:O2'	2.43	0.45
2:C:139:GLN:O	2:C:143:ARG:HG2	2.16	0.45
7:H:79:SER:HB2	7:H:85:ILE:H	1.81	0.45
11:L:68:GLY:O	11:L:99:ARG:NH1	2.46	0.45
21:A:190:A:O5'	21:A:190:A:H8	1.98	0.45
21:A:236:A:H2'	21:A:237:G:C8	2.52	0.45
21:A:270:A:H2'	21:A:271:C:C6	2.51	0.45
21:A:376:G:C2	21:A:389:A:C2	3.05	0.45
21:A:821:G:H2'	21:A:822:U:H6	1.82	0.45
21:A:1209:C:H2'	21:A:1210:C:C5	2.51	0.45
21:A:1235:U:O2'	21:A:1305:G:H5'	2.16	0.45
3:D:58:LYS:HB3	3:D:58:LYS:HE3	1.68	0.45
6:G:5:ARG:O	6:G:5:ARG:HG3	2.17	0.45
12:M:55:THR:O	12:M:59:GLU:HG2	2.16	0.45
12:M:67:GLY:HA2	12:M:70:ARG:HD2	1.99	0.45
21:A:5:U:H4'	21:A:6:G:O5'	2.17	0.45
21:A:167:A:H2'	21:A:168:G:C8	2.51	0.45
21:A:381:C:H2'	21:A:382:A:O4'	2.17	0.45
5:F:69:GLU:O	5:F:73:GLU:CD	2.60	0.45
8:I:39:PHE:HE2	8:I:48:VAL:HG21	1.82	0.45
15:P:1:MET:O	15:P:24:SER:OG	2.33	0.45
18:S:18:LYS:HA	18:S:21:LYS:HG2	1.97	0.45
21:A:832:G:H1	21:A:854:U:H3	1.63	0.45
21:A:1100:C:N4	21:A:1103:C:OP1	2.49	0.45
21:A:1305:G:N2	21:A:1332:A:C8	2.84	0.45
3:D:109:ALA:H	3:D:113:GLU:CD	2.24	0.45
4:E:56:VAL:O	4:E:60:ILE:HG13	2.17	0.45
6:G:116:MET:HB2	21:A:1240:U:OP1	2.16	0.45
15:P:42:ILE:HG13	21:A:449:G:O2'	2.17	0.45
19:T:27:MET:SD	19:T:27:MET:C	3.00	0.45
21:A:253:A:H2'	21:A:254:G:H8	1.80	0.45
21:A:562:U:H5'	21:A:563:A:C4	2.52	0.45
21:A:751:U:H2'	21:A:752:G:O4'	2.17	0.45
21:A:978:A:C2	21:A:1316:G:N2	2.85	0.45
21:A:1023:U:H2'	21:A:1024:G:C8	2.52	0.45
1:B:95:ARG:HE	21:A:1100:C:P	2.40	0.45
4:E:108:GLY:O	4:E:112:ARG:HG3	2.16	0.45
7:H:107:SER:HA	21:A:642:A:C8	2.52	0.45
8:I:114:LYS:NZ	21:A:1367:C:OP2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:89:PRO:HA	20:U:29:LEU:HD11	1.98	0.45
10:K:123:PRO:HB2	20:U:38:TYR:N	2.32	0.45
14:O:36:ILE:O	14:O:40:GLN:HG2	2.17	0.45
17:R:73:ARG:HH21	21:A:676:A:H5'	1.82	0.45
19:T:13:GLN:NE2	21:A:104:G:OP2	2.50	0.45
21:A:130:A:N3	21:A:263:A:O2'	2.38	0.45
21:A:662:U:H2'	21:A:663:A:C8	2.52	0.45
21:A:1114:C:H2'	21:A:1115:U:O4'	2.15	0.45
7:H:79:SER:OG	7:H:124:GLU:OE2	2.27	0.45
8:I:100:LYS:HB3	8:I:100:LYS:HE3	1.61	0.45
13:N:81:ARG:H	13:N:81:ARG:HG3	1.59	0.45
21:A:96:U:H2'	21:A:97:G:C8	2.52	0.45
21:A:651:C:H2'	21:A:652:U:C6	2.52	0.45
21:A:715:A:H2'	21:A:716:A:H8	1.80	0.45
21:A:1147:C:H2'	21:A:1148:U:H6	1.82	0.45
21:A:1221:G:OP1	21:A:1321:U:N3	2.44	0.45
21:A:1518:MA6:H5''	21:A:1518:MA6:H8	1.99	0.45
1:B:26:LYS:C	1:B:27:MET:SD	3.00	0.45
2:C:116:VAL:HG11	2:C:200:VAL:HG11	1.99	0.45
4:E:149:SER:O	4:E:153:VAL:HG23	2.17	0.45
6:G:76:LYS:HE3	6:G:89:VAL:HG11	1.99	0.45
8:I:42:GLU:OE1	8:I:46:MET:SD	2.75	0.45
21:A:593:U:H2'	21:A:594:U:C6	2.52	0.45
21:A:881:G:H2'	21:A:882:C:O4'	2.17	0.45
21:A:1053:G:H4'	21:A:1054:C:H5''	1.97	0.45
1:B:6:MET:H	1:B:6:MET:HG2	1.54	0.45
1:B:27:MET:HE1	1:B:193:PRO:CB	2.45	0.45
21:A:679:C:H2'	21:A:680:C:C6	2.52	0.45
21:A:1071:C:H2'	21:A:1072:G:C8	2.47	0.45
21:A:1304:G:H1'	21:A:1333:A:H61	1.82	0.45
21:A:1407:5MC:H2'	21:A:1408:A:C8	2.44	0.45
21:A:1500:A:H5''	21:A:1508:A:H5''	1.98	0.45
3:D:103:TYR:CD2	3:D:104:ARG:HD3	2.51	0.44
8:I:114:LYS:NZ	8:I:118:LEU:O	2.42	0.44
12:M:51:GLY:O	12:M:55:THR:HG23	2.17	0.44
21:A:22:G:H2'	21:A:23:C:C6	2.52	0.44
21:A:235:C:H2'	21:A:236:A:C8	2.52	0.44
21:A:514:C:H2'	21:A:515:G:C8	2.48	0.44
21:A:957:U:H1'	21:A:960:U:C4	2.52	0.44
21:A:1464:U:H2'	21:A:1465:A:H8	1.81	0.44
1:B:161:LEU:HD23	1:B:181:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:11:LEU:O	3:D:15:GLU:HB2	2.18	0.44
8:I:113:ARG:NH2	21:A:1368:A:OP1	2.49	0.44
15:P:45:GLU:O	15:P:46:LYS:HB2	2.17	0.44
18:S:44:MET:SD	18:S:49:ILE:HD12	2.58	0.44
1:B:203:ASN:O	1:B:213:TYR:HE2	2.00	0.44
3:D:144:SER:OG	3:D:145:ILE:N	2.50	0.44
4:E:108:GLY:O	4:E:112:ARG:N	2.40	0.44
6:G:77:SER:HB3	6:G:86:GLN:HE22	1.82	0.44
8:I:47:VAL:O	8:I:80:ARG:HG3	2.17	0.44
12:M:87:ARG:HD2	21:A:1309:G:OP1	2.17	0.44
15:P:18:GLN:OE1	15:P:35:ARG:NE	2.33	0.44
16:Q:12:VAL:HG12	16:Q:55:ILE:HA	2.00	0.44
21:A:22:G:H2'	21:A:23:C:H6	1.82	0.44
21:A:900:A:H2'	21:A:901:A:C8	2.53	0.44
6:G:137:LYS:HE3	6:G:141:VAL:HG23	1.99	0.44
7:H:46:ILE:HA	7:H:64:LYS:HG2	1.99	0.44
18:S:15:LEU:HD13	18:S:38:SER:HB2	2.00	0.44
21:A:324:G:N2	21:A:326:G:H3'	2.32	0.44
21:A:1152:A:H2'	21:A:1153:G:H8	1.83	0.44
21:A:1162:C:H2'	21:A:1163:A:C8	2.52	0.44
3:D:8:LYS:HB3	3:D:21:LEU:HB3	1.99	0.44
6:G:79:ARG:NH1	6:G:82:GLY:H	2.16	0.44
9:J:56:HIS:CD2	21:A:973:G:H1'	2.53	0.44
21:A:1115:U:H2'	21:A:1116:U:C6	2.52	0.44
6:G:68:ASN:OD1	6:G:68:ASN:N	2.50	0.44
8:I:57:MET:SD	8:I:60:LYS:HE3	2.58	0.44
16:Q:6:ARG:HH11	21:A:127:G:H4'	1.82	0.44
16:Q:20:SER:HB3	16:Q:71:LYS:HD2	2.00	0.44
18:S:19:VAL:O	18:S:23:VAL:HG23	2.18	0.44
21:A:67:C:H2'	21:A:68:G:C8	2.52	0.44
21:A:373:A:O2'	21:A:451:A:N7	2.51	0.44
21:A:686:U:O4	21:A:703:G:O2'	2.28	0.44
1:B:68:LEU:HB3	1:B:161:LEU:HD13	2.00	0.44
2:C:107:ARG:HB2	2:C:107:ARG:HH11	1.82	0.44
3:D:206:LYS:HB2	21:A:8:A:C6	2.53	0.44
4:E:83:HIS:CG	7:H:96:MET:HG3	2.52	0.44
11:L:50:ARG:HB3	11:L:90:LEU:HD11	1.99	0.44
12:M:114:LYS:HE2	12:M:114:LYS:HB2	1.89	0.44
21:A:695:A:H2'	21:A:696:A:C8	2.53	0.44
21:A:1237:C:H4'	21:A:1300:G:N2	2.31	0.44
21:A:1323:G:C6	21:A:1324:A:C6	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:TRP:CH2	2:C:32:ASN:HB3	2.53	0.44
3:D:4:TYR:CD2	3:D:11:LEU:HD11	2.53	0.44
10:K:63:ALA:HB1	10:K:96:THR:OG1	2.18	0.44
12:M:114:LYS:H	21:A:1228:C:H5'	1.83	0.44
14:O:7:ALA:O	14:O:11:ILE:HD12	2.18	0.44
19:T:82:GLN:O	19:T:86:LEU:HD13	2.18	0.44
21:A:371:A:O2'	21:A:373:A:N7	2.41	0.44
21:A:967:5MC:H2'	21:A:968:A:C8	2.53	0.44
21:A:1242:G:N2	21:A:1295:U:O2	2.46	0.44
6:G:50:LEU:HD11	6:G:121:ALA:HA	2.00	0.44
12:M:113:ARG:HD3	21:A:1229:A:OP2	2.18	0.44
13:N:7:LYS:H	13:N:7:LYS:HG2	1.66	0.44
21:A:539:A:H2'	21:A:540:G:H8	1.83	0.44
21:A:676:A:H2'	21:A:677:U:H6	1.83	0.44
21:A:1316:G:N2	21:A:1318:A:H3'	2.33	0.44
1:B:188:ASP:OD1	1:B:203:ASN:HA	2.18	0.43
8:I:18:ARG:NH1	8:I:20:PHE:CE2	2.86	0.43
8:I:57:MET:HG3	8:I:61:LEU:CD1	2.48	0.43
10:K:110:ILE:HG13	20:U:19:PHE:CG	2.53	0.43
10:K:125:LYS:HD3	21:A:780:A:H5''	1.99	0.43
12:M:27:LYS:HA	12:M:27:LYS:HD2	1.65	0.43
12:M:115:PRO:HA	21:A:1228:C:H4'	2.00	0.43
14:O:89:ARG:HH11	14:O:89:ARG:HG3	1.82	0.43
21:A:131:A:O2'	21:A:262:A:N3	2.41	0.43
21:A:134:G:H1'	21:A:325:A:C5	2.53	0.43
21:A:218:U:H2'	21:A:219:U:O4'	2.17	0.43
21:A:1047:G:N2	21:A:1213:A:H2	2.16	0.43
1:B:27:MET:CE	1:B:193:PRO:HG3	2.40	0.43
3:D:116:GLN:HB3	3:D:154:ARG:HH12	1.83	0.43
18:S:10:PHE:CE2	21:A:1318:A:H4'	2.53	0.43
21:A:22:G:H4'	21:A:885:G:C8	2.53	0.43
21:A:171:A:H2'	21:A:172:A:C8	2.53	0.43
21:A:1070:U:H2'	21:A:1071:C:C6	2.53	0.43
21:A:1288:A:H2'	21:A:1289:A:C8	2.53	0.43
21:A:1498:UR3:O5'	21:A:1498:UR3:H6	2.18	0.43
3:D:37:ALA:O	3:D:42:GLY:HA3	2.19	0.43
10:K:89:PRO:HB3	20:U:29:LEU:HG	2.00	0.43
13:N:28:LYS:HD3	21:A:1317:C:OP2	2.18	0.43
18:S:23:VAL:HG22	18:S:47:LEU:HD11	2.00	0.43
21:A:540:G:H2'	21:A:541:G:O4'	2.18	0.43
21:A:1518:MA6:H3'	21:A:1519:MA6:H8	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:190:HIS:HD1	2:C:195:VAL:HG22	1.84	0.43
6:G:108:ALA:O	6:G:119:ARG:HD2	2.18	0.43
7:H:15:ARG:NH2	7:H:75:ILE:O	2.36	0.43
8:I:106:ARG:NH1	21:A:1117:A:H5''	2.32	0.43
9:J:7:ARG:HA	9:J:75:ASP:OD1	2.19	0.43
13:N:31:ILE:HD11	13:N:48:LEU:HD22	1.99	0.43
15:P:47:GLU:OE2	21:A:616:G:O2'	2.36	0.43
21:A:722:G:H5'	21:A:723:U:OP1	2.18	0.43
21:A:1107:C:C4	21:A:1108:G:C8	3.07	0.43
1:B:7:ARG:O	1:B:10:LEU:HG	2.19	0.43
2:C:67:THR:HA	2:C:102:ASN:HB2	2.00	0.43
6:G:109:ARG:HA	6:G:116:MET:HE1	2.01	0.43
20:U:44:GLU:HA	20:U:47:ARG:HG2	2.00	0.43
21:A:61:G:H2'	21:A:62:U:C6	2.54	0.43
21:A:302:G:O2'	21:A:556:C:H5''	2.18	0.43
21:A:1355:G:H2'	21:A:1356:G:C8	2.54	0.43
21:A:1469:C:H3'	21:A:1470:U:H6	1.83	0.43
8:I:21:ILE:CD1	8:I:61:LEU:HD13	2.41	0.43
8:I:69:GLY:HA2	21:A:1250:A:O3'	2.19	0.43
9:J:50:THR:HG23	9:J:64:GLN:HG2	2.00	0.43
13:N:23:LYS:HA	13:N:23:LYS:HD3	1.82	0.43
17:R:40:VAL:HG11	17:R:45:THR:HG23	2.01	0.43
21:A:537:G:H2'	21:A:538:G:C8	2.54	0.43
21:A:575:G:O2'	21:A:821:G:H5'	2.18	0.43
21:A:584:G:H2'	21:A:585:G:H8	1.84	0.43
21:A:648:A:H2'	21:A:649:A:C8	2.54	0.43
21:A:1005:A:O3'	21:A:1037:C:O2'	2.33	0.43
21:A:1413:A:H2'	21:A:1414:U:O4'	2.19	0.43
2:C:159:GLY:HA2	2:C:193:TYR:CE2	2.54	0.43
4:E:157:ARG:NH1	7:H:99:LEU:O	2.51	0.43
5:F:11:HIS:HE1	5:F:54:LEU:HD21	1.84	0.43
11:L:24:LEU:HD23	11:L:30:LYS:HG2	2.00	0.43
14:O:43:PHE:HB3	14:O:53:ARG:HH22	1.83	0.43
21:A:124:C:H2'	21:A:125:U:C6	2.53	0.43
21:A:284:C:H2'	21:A:285:C:H6	1.83	0.43
21:A:1124:G:O2'	21:A:1145:A:N6	2.52	0.43
2:C:42:TYR:CZ	2:C:90:VAL:HG11	2.53	0.43
10:K:84:VAL:HB	10:K:110:ILE:HD13	2.01	0.43
21:A:62:U:OP1	21:A:385:C:O2'	2.37	0.43
21:A:156:C:H2'	21:A:157:U:O4'	2.19	0.43
21:A:593:U:H2'	21:A:594:U:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:67:VAL:HG11	8:I:79:ILE:HD11	2.01	0.43
10:K:112:ASP:HB3	20:U:2:PRO:HG2	1.99	0.43
11:L:54:ARG:NH2	11:L:62:GLU:CG	2.81	0.43
17:R:38:LYS:HG2	21:A:718:A:C2	2.54	0.43
21:A:537:G:H2'	21:A:538:G:H8	1.84	0.43
21:A:945:G:N2	21:A:1334:G:O2'	2.52	0.43
21:A:1148:U:H2'	21:A:1149:C:O4'	2.18	0.43
2:C:108:LYS:CE	2:C:144:LEU:HD23	2.48	0.43
15:P:7:ALA:HA	15:P:28:ARG:HG2	1.99	0.43
17:R:59:ILE:O	17:R:63:ARG:HG3	2.18	0.43
19:T:33:LYS:NZ	21:A:1438:G:H5''	2.33	0.43
21:A:62:U:H2'	21:A:63:C:C6	2.54	0.43
21:A:120:A:O2'	21:A:122:G:N7	2.37	0.43
21:A:757:U:H2'	21:A:758:C:O4'	2.19	0.43
21:A:920:U:H2'	21:A:921:U:C6	2.54	0.43
21:A:984:C:H2'	21:A:985:C:H6	1.84	0.43
21:A:1180:A:O2'	21:A:1184:G:H1'	2.19	0.43
21:A:1222:G:H2'	21:A:1223:C:O4'	2.19	0.43
3:D:134:SER:HB2	21:A:403:C:OP1	2.19	0.42
12:M:23:TYR:O	12:M:65:VAL:HB	2.18	0.42
14:O:80:GLN:O	14:O:84:ARG:HG3	2.19	0.42
21:A:25:C:H2'	21:A:26:A:C8	2.53	0.42
21:A:139:A:H2'	21:A:140:U:C6	2.54	0.42
21:A:1125:U:O2'	21:A:1126:U:O5'	2.34	0.42
21:A:1172:C:H2'	21:A:1173:U:C6	2.53	0.42
1:B:25:PRO:HB3	21:A:828:U:H2'	2.00	0.42
2:C:36:ASP:HB3	2:C:40:ARG:NH1	2.34	0.42
2:C:108:LYS:HE3	2:C:144:LEU:CD2	2.49	0.42
13:N:83:LYS:HD3	13:N:83:LYS:HA	1.80	0.42
17:R:62:ALA:HB3	17:R:68:LEU:HD12	2.00	0.42
21:A:1065:U:H5''	21:A:1190:G:N2	2.34	0.42
21:A:1118:U:H1'	21:A:1179:A:C5	2.54	0.42
5:F:42:TRP:CE3	5:F:59:TYR:HB3	2.54	0.42
8:I:12:ARG:HD2	8:I:107:ASP:HB3	2.02	0.42
15:P:56:ARG:HD2	15:P:56:ARG:HA	1.61	0.42
21:A:151:A:C5	21:A:152:A:C8	3.07	0.42
21:A:425:G:C6	21:A:426:U:C4	3.07	0.42
2:C:6:HIS:HB3	13:N:89:MET:HE3	2.01	0.42
7:H:35:ALA:O	7:H:39:VAL:HG23	2.19	0.42
12:M:29:ARG:NH1	12:M:63:PHE:HB3	2.34	0.42
17:R:26:ILE:HG23	17:R:30:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:71:THR:OG1	17:R:72:ASP:N	2.52	0.42
21:A:86:G:O2'	21:A:87:C:O5'	2.35	0.42
21:A:712:A:H2'	21:A:713:G:O4'	2.20	0.42
21:A:838:G:H2'	21:A:839:C:C6	2.54	0.42
21:A:935:A:H2'	21:A:936:C:O4'	2.20	0.42
21:A:1209:C:H2'	21:A:1210:C:C6	2.55	0.42
21:A:1497:G:O2'	21:A:1518:MA6:H92	2.19	0.42
1:B:126:PHE:N	1:B:126:PHE:HD1	2.17	0.42
2:C:22:TRP:CG	2:C:59:ARG:HE	2.37	0.42
2:C:184:TYR:HA	2:C:200:VAL:O	2.19	0.42
6:G:111:ARG:NH2	6:G:122:ASN:HB3	2.34	0.42
9:J:66:GLU:HB2	13:N:99:ALA:HB2	2.00	0.42
13:N:66:GLN:HB2	13:N:83:LYS:HG3	2.02	0.42
21:A:100:G:C4	21:A:101:A:C8	3.07	0.42
21:A:196:A:N3	21:A:222:C:H1'	2.34	0.42
21:A:308:C:H2'	21:A:309:A:C8	2.55	0.42
21:A:980:C:H3'	21:A:981:U:C6	2.55	0.42
3:D:120:HIS:HA	21:A:439:U:O4'	2.19	0.42
3:D:167:LYS:HD2	3:D:167:LYS:H	1.84	0.42
4:E:110:ALA:HB1	4:E:137:VAL:HG12	2.01	0.42
6:G:5:ARG:NH2	6:G:7:ILE:HG13	2.34	0.42
12:M:26:GLY:N	21:A:1329:A:H5''	2.35	0.42
21:A:628:G:H2'	21:A:629:A:H8	1.84	0.42
21:A:922:G:H2'	21:A:923:A:C8	2.54	0.42
21:A:1042:A:N3	21:A:1042:A:H2'	2.35	0.42
21:A:1392:G:H4'	21:A:1531:A:O5'	2.20	0.42
5:F:1:MET:HE3	5:F:1:MET:HB2	1.80	0.42
7:H:64:LYS:HG3	7:H:71:VAL:HG21	2.00	0.42
8:I:7:TYR:CE2	21:A:1147:C:H4'	2.55	0.42
12:M:116:ILE:HD11	21:A:1228:C:H1'	2.00	0.42
13:N:5:SER:C	13:N:9:ARG:NE	2.68	0.42
13:N:72:GLY:HA2	21:A:975:A:O2'	2.19	0.42
13:N:74:LEU:HD23	13:N:74:LEU:HA	1.88	0.42
19:T:75:HIS:HE1	21:A:260:G:OP1	2.03	0.42
20:U:35:ARG:NH2	21:A:718:A:O2'	2.53	0.42
21:A:547:A:H4'	21:A:548:G:O5'	2.20	0.42
5:F:90:MET:HE1	17:R:23:TYR:HE1	1.81	0.42
6:G:113:ASP:CG	6:G:118:LEU:HD22	2.45	0.42
7:H:113:ASP:HB2	7:H:117:ARG:HH21	1.85	0.42
8:I:11:ARG:HH21	21:A:1149:C:P	2.43	0.42
21:A:66:A:H8	21:A:66:A:P	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:768:A:N3	21:A:1512:U:O2'	2.48	0.42
21:A:1117:A:N6	21:A:1156:G:H1	2.18	0.42
21:A:1293:C:C2	21:A:1294:G:C8	3.08	0.42
21:A:1526:G:H2'	21:A:1527:U:C6	2.55	0.42
5:F:42:TRP:HE3	5:F:59:TYR:HB3	1.85	0.42
6:G:103:TRP:CH2	6:G:141:VAL:HG21	2.55	0.42
7:H:88:ARG:HB3	21:A:600:A:OP1	2.20	0.42
12:M:97:VAL:HB	21:A:1308:U:H5''	2.02	0.42
21:A:697:U:O2	21:A:798:U:H1'	2.20	0.42
2:C:157:LEU:HD12	2:C:166:GLU:OE1	2.20	0.42
3:D:104:ARG:HG3	3:D:170:TRP:HE1	1.85	0.42
4:E:23:LYS:HB2	4:E:23:LYS:HE2	1.84	0.42
4:E:25:VAL:HA	21:A:922:G:H4'	2.02	0.42
11:L:50:ARG:CB	11:L:90:LEU:HD11	2.50	0.42
18:S:36:ARG:HD3	21:A:1220:G:O3'	2.20	0.42
18:S:63:THR:H	18:S:66:MET:CE	2.33	0.42
21:A:79:G:H22	21:A:90:C:N4	2.12	0.42
21:A:398:U:H2'	21:A:399:G:C8	2.54	0.42
21:A:565:U:OP2	21:A:566:G:O2'	2.33	0.42
21:A:802:A:H3'	21:A:803:G:H8	1.85	0.42
21:A:855:U:OP2	21:A:871:U:N3	2.40	0.42
21:A:1008:U:H3'	21:A:1009:U:H5''	2.02	0.42
21:A:1198:G:H2'	21:A:1199:U:C6	2.55	0.42
21:A:1319:A:C8	21:A:1323:G:C6	3.08	0.42
2:C:11:ARG:HA	2:C:14:ILE:HD12	2.02	0.41
2:C:16:LYS:HA	2:C:16:LYS:HD3	1.76	0.41
2:C:67:THR:HG23	2:C:102:ASN:HB2	2.02	0.41
2:C:75:ILE:HG13	2:C:76:VAL:N	2.31	0.41
6:G:66:LEU:HD23	6:G:66:LEU:HA	1.91	0.41
7:H:46:ILE:HD12	7:H:46:ILE:C	2.45	0.41
21:A:451:A:H4'	21:A:452:A:O4'	2.20	0.41
21:A:1307:U:H2'	21:A:1308:U:C6	2.54	0.41
21:A:1324:A:H2'	21:A:1325:C:C6	2.55	0.41
21:A:1486:G:H2'	21:A:1487:G:O4'	2.20	0.41
21:A:1524:C:H2'	21:A:1525:G:C8	2.55	0.41
3:D:67:VAL:HG22	3:D:97:ARG:NH1	2.34	0.41
21:A:223:A:H2'	21:A:224:U:C6	2.55	0.41
21:A:776:G:N1	21:A:802:A:OP1	2.46	0.41
21:A:1151:A:O2'	21:A:1152:A:H8	2.03	0.41
2:C:150:LYS:HG2	2:C:201:TRP:CE3	2.55	0.41
3:D:107:PHE:CZ	3:D:178:MET:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:38:ARG:HB3	5:F:63:ASN:OD1	2.20	0.41
8:I:21:ILE:HD12	8:I:63:LEU:CD2	2.50	0.41
8:I:130:ARG:OXT	21:A:970:C:N4	2.53	0.41
10:K:23:ILE:HG12	10:K:85:MET:O	2.20	0.41
11:L:52:VAL:HG12	11:L:66:TYR:CD1	2.56	0.41
13:N:79:LEU:HD22	13:N:83:LYS:HB3	2.02	0.41
13:N:82:ILE:O	13:N:86:GLU:HG3	2.21	0.41
16:Q:40:ARG:HE	16:Q:40:ARG:HA	1.86	0.41
18:S:11:ILE:HD11	18:S:15:LEU:HD22	2.00	0.41
21:A:865:A:H2'	21:A:866:C:C6	2.56	0.41
21:A:1063:C:OP2	21:A:1064:G:O2'	2.21	0.41
5:F:8:PHE:HA	5:F:87:SER:HA	2.03	0.41
12:M:7:ILE:HG22	12:M:8:ASN:O	2.21	0.41
21:A:599:C:H2'	21:A:600:A:H8	1.86	0.41
21:A:606:G:P	21:A:607:A:H5'	2.60	0.41
21:A:1246:A:C6	21:A:1292:G:C6	3.08	0.41
1:B:206:ALA:O	1:B:210:VAL:HG23	2.21	0.41
2:C:149:ILE:HD13	2:C:202:ILE:HG12	2.01	0.41
11:L:52:VAL:HG11	11:L:90:LEU:HD13	2.03	0.41
12:M:27:LYS:O	12:M:31:LYS:HG3	2.20	0.41
21:A:19:A:O2'	21:A:572:A:N1	2.48	0.41
21:A:222:C:H2'	21:A:223:A:C8	2.54	0.41
21:A:272:C:H2'	21:A:273:U:C6	2.56	0.41
21:A:466:A:H2'	21:A:468:A:C8	2.56	0.41
6:G:97:ASN:C	6:G:101:MET:HE2	2.45	0.41
12:M:14:HIS:HA	12:M:44:LYS:HA	2.03	0.41
15:P:3:THR:HG23	15:P:5:ARG:HD3	2.02	0.41
15:P:57:ILE:O	15:P:61:VAL:HG23	2.20	0.41
21:A:446:G:H2'	21:A:447:G:O4'	2.21	0.41
21:A:1013:G:N2	21:A:1015:G:H3'	2.36	0.41
2:C:72:ARG:O	2:C:76:VAL:HG23	2.20	0.41
3:D:74:ASN:O	3:D:77:LYS:HE3	2.20	0.41
3:D:105:MET:SD	3:D:107:PHE:HE2	2.37	0.41
8:I:30:ILE:HA	8:I:65:ILE:O	2.20	0.41
11:L:53:CYS:SG	11:L:67:ILE:HD11	2.61	0.41
13:N:19:LYS:NZ	21:A:1007:U:OP1	2.41	0.41
15:P:41:PRO:HB2	21:A:450:G:H4'	2.03	0.41
21:A:838:G:H2'	21:A:839:C:H6	1.84	0.41
21:A:967:5MC:H2'	21:A:968:A:H8	1.85	0.41
3:D:107:PHE:CD2	3:D:145:ILE:HD11	2.56	0.41
5:F:18:VAL:N	5:F:19:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:104:VAL:HG22	7:H:125:ILE:HD13	2.01	0.41
10:K:64:GLN:HG3	10:K:99:ALA:HB2	2.03	0.41
10:K:83:GLU:HB3	10:K:109:ASN:HB2	2.02	0.41
11:L:30:LYS:HD2	11:L:30:LYS:HA	1.80	0.41
18:S:18:LYS:NZ	18:S:32:ARG:O	2.44	0.41
20:U:17:ARG:O	20:U:20:LYS:HG2	2.21	0.41
21:A:128:G:O2'	21:A:129:A:H5'	2.20	0.41
21:A:578:C:O2'	21:A:728:A:N3	2.45	0.41
21:A:580:C:H2'	21:A:581:G:O4'	2.20	0.41
21:A:912:C:O2'	21:A:913:A:H5'	2.21	0.41
21:A:1098:C:H2'	21:A:1099:G:C8	2.55	0.41
1:B:61:ALA:HB3	1:B:224:GLY:HA3	2.03	0.41
1:B:140:GLU:HA	1:B:143:LYS:HG2	2.03	0.41
2:C:142:MET:HE3	2:C:142:MET:HA	2.03	0.41
4:E:33:PHE:CD1	4:E:56:VAL:HG22	2.56	0.41
10:K:29:ASN:OD1	10:K:30:THR:N	2.52	0.41
13:N:7:LYS:O	13:N:11:VAL:HG23	2.20	0.41
14:O:78:TYR:OH	14:O:89:ARG:O	2.37	0.41
18:S:62:VAL:HA	18:S:66:MET:SD	2.61	0.41
20:U:17:ARG:HA	20:U:20:LYS:HZ3	1.86	0.41
20:U:46:LYS:HE2	20:U:46:LYS:HB3	1.90	0.41
20:U:47:ARG:HG3	20:U:48:ALA:N	2.35	0.41
21:A:79:G:O6	21:A:80:A:N6	2.53	0.41
21:A:105:G:H2'	21:A:106:C:C6	2.56	0.41
21:A:505:G:H2'	21:A:506:G:H8	1.83	0.41
21:A:978:A:C8	21:A:979:C:H5	2.39	0.41
21:A:1185:G:H2'	21:A:1186:G:C8	2.56	0.41
21:A:1219:A:H2'	21:A:1220:G:H8	1.85	0.41
21:A:1372:U:H2'	21:A:1373:G:O4'	2.20	0.41
21:A:1406:U:C5	21:A:1407:5MC:CM5	3.04	0.41
2:C:42:TYR:O	2:C:46:GLU:HG3	2.21	0.41
2:C:178:LEU:HD23	2:C:178:LEU:HA	1.95	0.41
12:M:23:TYR:HB2	12:M:70:ARG:NH2	2.36	0.41
21:A:408:A:H2'	21:A:409:U:O4'	2.20	0.41
21:A:601:G:H2'	21:A:602:A:C8	2.56	0.41
21:A:730:G:C5	21:A:731:G:H1'	2.56	0.41
21:A:1424:U:H2'	21:A:1425:U:O4'	2.21	0.41
9:J:55:PRO:HD2	21:A:1059:C:O2	2.21	0.40
19:T:33:LYS:HD3	21:A:1439:G:OP1	2.21	0.40
20:U:8:GLU:OE1	20:U:8:GLU:N	2.47	0.40
21:A:7:A:H5'	21:A:298:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:20:U:H2'	21:A:21:G:O4'	2.21	0.40
21:A:237:G:H2'	21:A:238:A:H8	1.86	0.40
21:A:460:A:N6	21:A:473:U:O4	2.54	0.40
21:A:1077:G:N2	21:A:1080:A:OP2	2.51	0.40
21:A:1233:G:H2'	21:A:1234:C:C6	2.55	0.40
21:A:1513:A:H2'	21:A:1514:G:C8	2.56	0.40
1:B:118:GLU:CD	1:B:152:LYS:HZ1	2.26	0.40
3:D:182:PHE:HZ	3:D:185:LYS:HA	1.87	0.40
6:G:31:MET:HE1	6:G:35:LYS:H	1.85	0.40
7:H:111:MET:HE2	7:H:111:MET:HB3	1.91	0.40
9:J:12:ALA:HB3	9:J:18:ILE:HB	2.02	0.40
11:L:6:GLN:HG2	11:L:9:ARG:NH2	2.37	0.40
13:N:6:MET:CE	21:A:981:U:H5'	2.50	0.40
21:A:320:A:H2'	21:A:321:A:O4'	2.21	0.40
21:A:860:A:H2'	21:A:861:G:O4'	2.21	0.40
21:A:939:G:H2'	21:A:940:C:C6	2.55	0.40
21:A:984:C:H2'	21:A:985:C:C6	2.56	0.40
21:A:1140:C:H2'	21:A:1141:C:C6	2.56	0.40
2:C:162:ILE:HD12	2:C:162:ILE:C	2.46	0.40
10:K:57:LYS:NZ	21:A:691:G:O6	2.30	0.40
13:N:54:ASP:CG	13:N:59:ARG:HH21	2.29	0.40
14:O:42:HIS:ND1	21:A:739:C:O2'	2.42	0.40
17:R:61:ARG:HE	17:R:61:ARG:HB2	1.70	0.40
19:T:43:ASP:OD1	19:T:44:LYS:N	2.54	0.40
21:A:1141:C:H2'	21:A:1142:G:C8	2.57	0.40
21:A:1203:C:H2'	21:A:1204:A:C8	2.56	0.40
1:B:30:PHE:CD1	1:B:201:PRO:HG3	2.57	0.40
2:C:58:GLU:OE2	9:J:94:ALA:CB	2.67	0.40
8:I:34:SER:O	8:I:38:TYR:N	2.48	0.40
9:J:6:ILE:HG23	9:J:102:LEU:HG	2.03	0.40
9:J:40:ILE:HB	9:J:73:LEU:HB3	2.03	0.40
16:Q:6:ARG:HE	16:Q:6:ARG:HB3	1.60	0.40
19:T:39:ILE:HD13	19:T:82:GLN:HB2	2.02	0.40
21:A:201:G:H1	21:A:216:U:H3	1.70	0.40
21:A:1027:C:H2'	21:A:1028:C:H6	1.82	0.40
21:A:1350:A:H2'	21:A:1351:U:C6	2.55	0.40
2:C:6:HIS:CB	13:N:89:MET:CE	2.99	0.40
3:D:93:LEU:HA	3:D:136:GLN:HE22	1.85	0.40
3:D:100:ASN:HD22	3:D:111:ARG:HH21	1.69	0.40
6:G:130:ASN:HA	6:G:135:VAL:HG11	2.03	0.40
8:I:10:GLY:HA2	8:I:81:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:235:C:H2'	21:A:236:A:H8	1.85	0.40
21:A:361:G:H2'	21:A:362:G:O4'	2.21	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	
1	B	222/234 (95%)	206 (93%)	16 (7%)	0	100	100
2	C	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
3	D	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
4	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
5	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
6	G	151/179 (84%)	137 (91%)	14 (9%)	0	100	100
7	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
8	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
9	J	96/103 (93%)	94 (98%)	1 (1%)	1 (1%)	12	17
10	K	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
11	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
12	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
13	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
14	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
16	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
17	R	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
18	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	84/87 (97%)	84 (100%)	0	0	100	100
20	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
All	All	2366/2569 (92%)	2245 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	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	
1	B	186/193 (96%)	177 (95%)	9 (5%)	23	34
2	C	170/190 (90%)	166 (98%)	4 (2%)	43	59
3	D	172/173 (99%)	163 (95%)	9 (5%)	21	31
4	E	119/126 (94%)	117 (98%)	2 (2%)	53	68
5	F	90/116 (78%)	85 (94%)	5 (6%)	19	28
6	G	126/147 (86%)	119 (94%)	7 (6%)	19	28
7	H	104/105 (99%)	100 (96%)	4 (4%)	29	42
8	I	105/107 (98%)	101 (96%)	4 (4%)	29	42
9	J	86/90 (96%)	79 (92%)	7 (8%)	11	16
10	K	89/98 (91%)	86 (97%)	3 (3%)	32	47
11	L	102/103 (99%)	97 (95%)	5 (5%)	22	33
12	M	93/96 (97%)	91 (98%)	2 (2%)	45	61
13	N	83/84 (99%)	81 (98%)	2 (2%)	43	59
14	O	76/77 (99%)	75 (99%)	1 (1%)	61	74
15	P	65/65 (100%)	65 (100%)	0	100	100
16	Q	73/78 (94%)	69 (94%)	4 (6%)	19	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	57/65 (88%)	55 (96%)	2 (4%)	32	46
18	S	72/79 (91%)	71 (99%)	1 (1%)	59	73
19	T	65/66 (98%)	62 (95%)	3 (5%)	24	35
20	U	60/61 (98%)	59 (98%)	1 (2%)	53	68
All	All	1993/2119 (94%)	1918 (96%)	75 (4%)	30	42

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	TRP
1	B	41	ILE
1	B	70	VAL
1	B	102	THR
1	B	107	VAL
1	B	129	LEU
1	B	130	THR
1	B	138	THR
1	B	194	ASP
2	C	15	VAL
2	C	75	ILE
2	C	131	ARG
2	C	192	THR
3	D	29	ASP
3	D	48	LEU
3	D	50	ASP
3	D	117	LEU
3	D	153	SER
3	D	169	THR
3	D	173	VAL
3	D	179	GLU
3	D	181	THR
4	E	38	VAL
4	E	145	GLU
5	F	44	ARG
5	F	68	GLN
5	F	85	ILE
5	F	89	VAL
5	F	96	VAL
6	G	6	VAL
6	G	68	ASN
6	G	72	THR

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Mol	Chain	Res	Type
6	G	73	VAL
6	G	77	SER
6	G	94	VAL
6	G	105	VAL
7	H	31	LYS
7	H	60	GLU
7	H	79	SER
7	H	117	ARG
8	I	29	VAL
8	I	30	ILE
8	I	67	VAL
8	I	96	SER
9	J	10	LEU
9	J	18	ILE
9	J	27	GLU
9	J	28	THR
9	J	32	THR
9	J	85	ASP
9	J	100	ILE
10	K	26	SER
10	K	86	VAL
10	K	95	SER
11	L	52	VAL
11	L	64	THR
11	L	79	VAL
11	L	97	THR
11	L	102	LEU
12	M	75	MET
12	M	83	LEU
13	N	84	VAL
13	N	100	SER
14	O	48	LYS
16	Q	13	VAL
16	Q	21	ILE
16	Q	29	VAL
16	Q	42	THR
17	R	18	VAL
17	R	66	SER
18	S	74	PHE
19	T	3	ASN
19	T	6	SER
19	T	26	SER

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Mol	Chain	Res	Type
20	U	3	VAL

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

Mol	Chain	Res	Type
1	B	109	GLN
2	C	102	ASN
2	C	139	GLN
3	D	136	GLN
5	F	11	HIS
5	F	94	HIS
6	G	86	GLN
8	I	75	GLN
9	J	20	GLN
10	K	15	GLN
10	K	24	HIS
10	K	81	ASN
12	M	12	HIS
12	M	52	GLN
13	N	43	ASN
14	O	50	HIS
14	O	80	GLN
15	P	40	ASN
16	Q	50	ASN
18	S	43	ASN
19	T	61	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1514/1533 (98%)	258 (17%)	7 (0%)

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	5	U
21	A	6	G
21	A	9	G
21	A	32	A
21	A	39	G

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Mol	Chain	Res	Type
21	A	44	A
21	A	47	C
21	A	48	C
21	A	50	A
21	A	51	A
21	A	74	A
21	A	75	G
21	A	83	C
21	A	84	U
21	A	85	U
21	A	86	G
21	A	87	C
21	A	88	U
21	A	89	U
21	A	95	C
21	A	96	U
21	A	121	U
21	A	122	G
21	A	129	A
21	A	131	A
21	A	141	G
21	A	142	G
21	A	143	A
21	A	144	G
21	A	164	G
21	A	166	U
21	A	173	U
21	A	182	A
21	A	183	C
21	A	192	A
21	A	197	A
21	A	200	G
21	A	226	G
21	A	240	G
21	A	245	U
21	A	247	G
21	A	251	G
21	A	266	G
21	A	267	C
21	A	280	C
21	A	289	G
21	A	317	U

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Mol	Chain	Res	Type
21	A	321	A
21	A	328	C
21	A	329	A
21	A	330	C
21	A	339	C
21	A	347	G
21	A	351	G
21	A	352	C
21	A	354	G
21	A	355	C
21	A	367	U
21	A	372	C
21	A	374	A
21	A	382	A
21	A	398	U
21	A	406	G
21	A	407	U
21	A	412	A
21	A	414	A
21	A	415	A
21	A	421	U
21	A	422	C
21	A	423	G
21	A	424	G
21	A	429	U
21	A	431	A
21	A	435	A
21	A	436	C
21	A	456	A
21	A	457	G
21	A	458	U
21	A	459	A
21	A	463	U
21	A	465	A
21	A	466	A
21	A	468	A
21	A	469	C
21	A	474	G
21	A	478	A
21	A	479	U
21	A	481	G
21	A	484	G

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Mol	Chain	Res	Type
21	A	486	U
21	A	495	A
21	A	496	A
21	A	497	G
21	A	499	A
21	A	509	A
21	A	511	C
21	A	518	C
21	A	521	G
21	A	531	U
21	A	532	A
21	A	533	A
21	A	536	C
21	A	547	A
21	A	549	C
21	A	559	A
21	A	562	U
21	A	564	C
21	A	572	A
21	A	573	A
21	A	576	C
21	A	577	G
21	A	588	G
21	A	596	A
21	A	607	A
21	A	633	G
21	A	653	U
21	A	665	A
21	A	666	G
21	A	687	A
21	A	702	A
21	A	703	G
21	A	721	G
21	A	723	U
21	A	724	G
21	A	734	G
21	A	746	A
21	A	747	A
21	A	748	G
21	A	755	G
21	A	774	G
21	A	777	A

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Mol	Chain	Res	Type
21	A	793	U
21	A	794	A
21	A	815	A
21	A	817	C
21	A	821	G
21	A	870	U
21	A	889	A
21	A	890	G
21	A	914	A
21	A	926	G
21	A	934	C
21	A	935	A
21	A	936	C
21	A	960	U
21	A	966	G
21	A	967	5MC
21	A	968	A
21	A	969	A
21	A	975	A
21	A	976	G
21	A	977	A
21	A	982	U
21	A	992	U
21	A	994	A
21	A	996	A
21	A	1003	G
21	A	1004	A
21	A	1005	A
21	A	1009	U
21	A	1019	A
21	A	1021	A
21	A	1024	G
21	A	1027	C
21	A	1028	C
21	A	1030	U
21	A	1031	C
21	A	1032	G
21	A	1033	G
21	A	1034	G
21	A	1036	A
21	A	1037	C
21	A	1039	G

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Mol	Chain	Res	Type
21	A	1043	G
21	A	1044	A
21	A	1064	G
21	A	1065	U
21	A	1070	U
21	A	1084	G
21	A	1085	U
21	A	1094	G
21	A	1095	U
21	A	1101	A
21	A	1108	G
21	A	1117	A
21	A	1130	A
21	A	1137	C
21	A	1138	G
21	A	1139	G
21	A	1140	C
21	A	1159	U
21	A	1193	G
21	A	1196	A
21	A	1197	A
21	A	1212	U
21	A	1213	A
21	A	1214	C
21	A	1224	U
21	A	1225	A
21	A	1226	C
21	A	1227	A
21	A	1228	C
21	A	1238	A
21	A	1240	U
21	A	1258	G
21	A	1275	A
21	A	1280	A
21	A	1286	U
21	A	1287	A
21	A	1297	G
21	A	1300	G
21	A	1305	G
21	A	1306	A
21	A	1315	U
21	A	1317	C

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Mol	Chain	Res	Type
21	A	1319	A
21	A	1320	C
21	A	1331	G
21	A	1332	A
21	A	1336	C
21	A	1346	A
21	A	1348	U
21	A	1353	G
21	A	1357	A
21	A	1360	A
21	A	1361	G
21	A	1368	A
21	A	1370	G
21	A	1371	G
21	A	1379	G
21	A	1397	C
21	A	1407	5MC
21	A	1419	G
21	A	1428	A
21	A	1432	G
21	A	1441	A
21	A	1442	G
21	A	1446	A
21	A	1450	U
21	A	1451	U
21	A	1452	C
21	A	1487	G
21	A	1492	A
21	A	1494	G
21	A	1497	G
21	A	1499	A
21	A	1503	A
21	A	1506	U
21	A	1507	A
21	A	1517	G
21	A	1518	MA6
21	A	1519	MA6
21	A	1520	C
21	A	1529	G
21	A	1530	G
21	A	1531	A
21	A	1532	U

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Mol	Chain	Res	Type
21	A	1534	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	5	U
21	A	438	U
21	A	966	G
21	A	1026	G
21	A	1035	A
21	A	1319	A
21	A	1530	G

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

9 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
21	5MC	A	967	21	19,22,23	0.83	1 (5%)	26,32,35	0.67	0
21	G7M	A	527	21	23,26,27	1.56	3 (13%)	34,39,42	1.73	5 (14%)
21	4OC	A	1402	21	20,23,24	0.39	0	25,32,35	0.45	0
21	MA6	A	1518	21	23,26,27	0.29	0	33,38,41	0.64	1 (3%)
21	PSU	A	516	21	18,21,22	1.10	1 (5%)	21,30,33	1.99	6 (28%)
21	MA6	A	1519	21	23,26,27	0.29	0	33,38,41	0.71	1 (3%)
21	5MC	A	1407	21	19,22,23	0.91	2 (10%)	26,32,35	0.78	1 (3%)
21	UR3	A	1498	21	19,22,23	0.30	0	26,32,35	0.72	0
11	D2T	L	89	11	8,9,10	1.26	2 (25%)	6,11,13	1.67	3 (50%)

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
21	5MC	A	967	21	-	2/7/25/26	0/2/2/2
21	G7M	A	527	21	-	1/7/25/26	0/3/3/3
21	4OC	A	1402	21	-	0/9/29/30	0/2/2/2
21	MA6	A	1518	21	-	4/11/29/30	0/3/3/3
21	PSU	A	516	21	-	0/7/25/26	0/2/2/2
21	MA6	A	1519	21	-	2/11/29/30	0/3/3/3
21	5MC	A	1407	21	-	0/7/25/26	0/2/2/2
21	UR3	A	1498	21	-	0/7/25/26	0/2/2/2
11	D2T	L	89	11	-	4/7/12/14	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	527	G7M	C5-N7	-5.09	1.33	1.39
21	A	516	PSU	C6-C5	3.43	1.39	1.35
21	A	967	5MC	C5-C4	-3.31	1.41	1.44
21	A	527	G7M	C5-C4	3.06	1.45	1.38
21	A	1407	5MC	C5-C4	-2.99	1.41	1.44
21	A	527	G7M	C6-N1	-2.69	1.33	1.38
11	L	89	D2T	CB-CA	-2.28	1.54	1.54
21	A	1407	5MC	O5'-C5'	2.27	1.50	1.44
11	L	89	D2T	OD2-CG	-2.08	1.24	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	527	G7M	N9-C4-N3	5.44	136.82	125.95
21	A	527	G7M	C5-C4-N3	-5.37	118.00	128.15
21	A	516	PSU	N1-C2-N3	4.90	120.34	115.17
21	A	516	PSU	C4-N3-C2	-4.88	119.65	126.37
21	A	527	G7M	C2-N3-C4	4.68	120.36	112.30
21	A	516	PSU	O2-C2-N1	-3.07	119.63	122.79
21	A	1519	MA6	C2-N1-C6	2.78	118.63	111.83
21	A	1518	MA6	C2-N1-C6	2.77	118.59	111.83
11	L	89	D2T	O-C-CA	-2.52	118.29	124.77
21	A	516	PSU	C6-N1-C2	-2.41	120.46	122.69
11	L	89	D2T	OD1-CG-CB	-2.38	117.47	122.44
21	A	516	PSU	C6-C5-C4	2.36	119.77	118.17
21	A	527	G7M	O6-C6-C5	-2.35	122.78	128.01
21	A	1407	5MC	C5-C6-N1	-2.26	120.86	123.31
21	A	527	G7M	C5-C6-N1	2.11	116.20	111.84
21	A	516	PSU	O4'-C1'-C2'	2.09	108.05	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	89	D2T	OD2-CG-CB	2.04	117.55	113.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	89	D2T	CA-CB-CG-OD1
11	L	89	D2T	CA-CB-CG-OD2
21	A	1518	MA6	C5-C6-N6-C9
21	A	967	5MC	O4'-C1'-N1-C2
21	A	1518	MA6	N1-C6-N6-C9
21	A	967	5MC	O4'-C1'-N1-C6
21	A	1519	MA6	C5-C6-N6-C10
21	A	1518	MA6	C3'-C4'-C5'-O5'
21	A	527	G7M	C3'-C4'-C5'-O5'
11	L	89	D2T	CG-CB-SB-CB1
21	A	1518	MA6	C5-C6-N6-C10
21	A	1519	MA6	C4'-C5'-O5'-P
11	L	89	D2T	SB-CB-CG-OD2

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	967	5MC	2	0
21	A	527	G7M	1	0
21	A	1518	MA6	3	0
21	A	1519	MA6	1	0
21	A	1407	5MC	5	0
21	A	1498	UR3	1	0
11	L	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

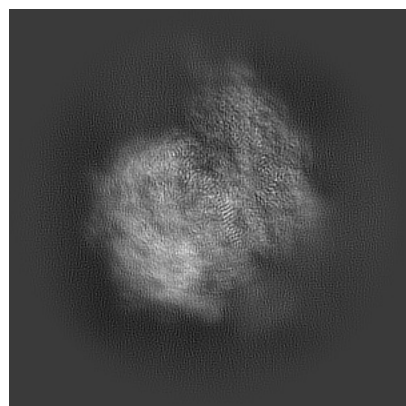
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47168. These allow visual inspection of the internal detail of the map and identification of artifacts.

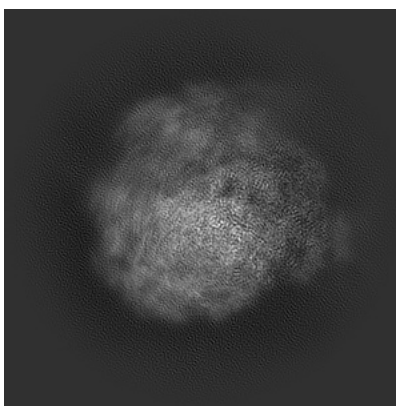
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

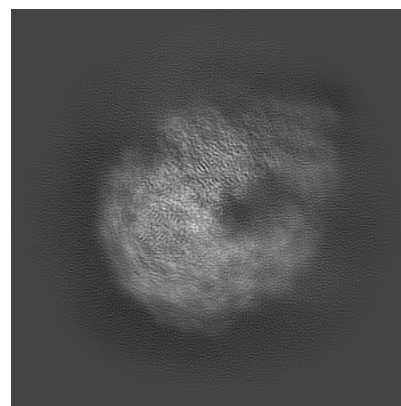
6.1.1 Primary map



X

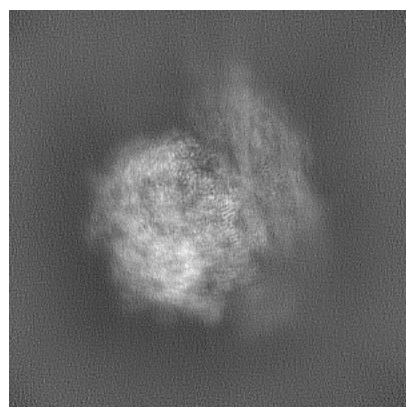


Y

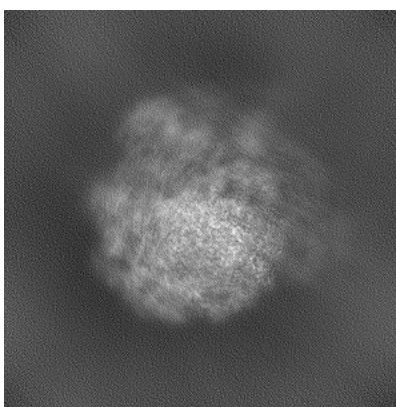


Z

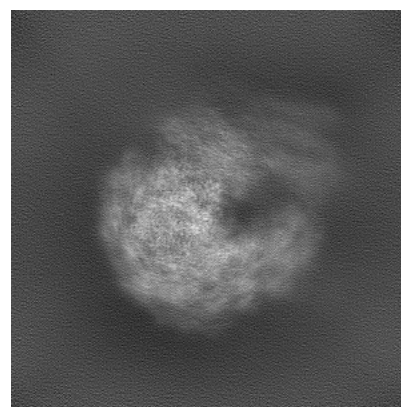
6.1.2 Raw map



X



Y

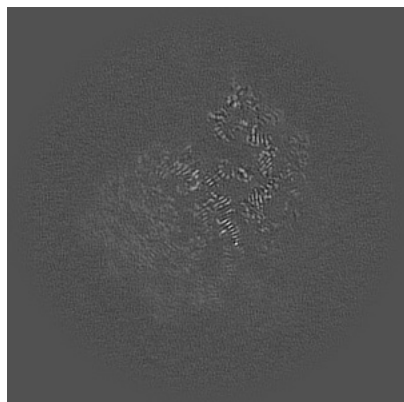


Z

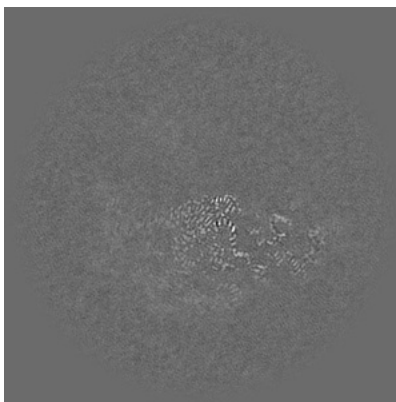
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

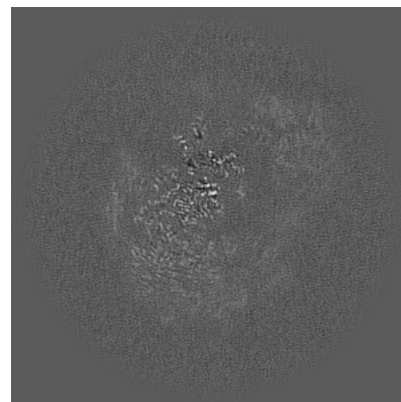
6.2.1 Primary map



X Index: 224

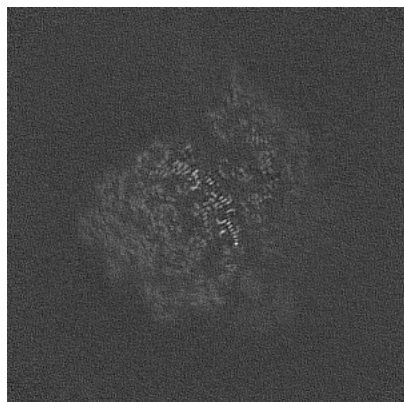


Y Index: 224

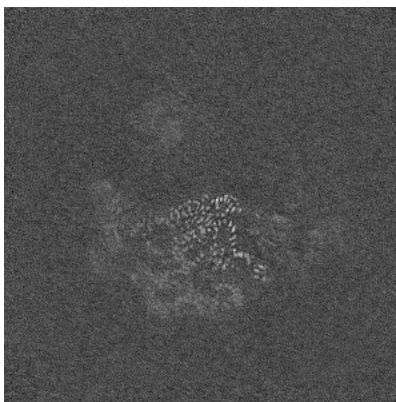


Z Index: 224

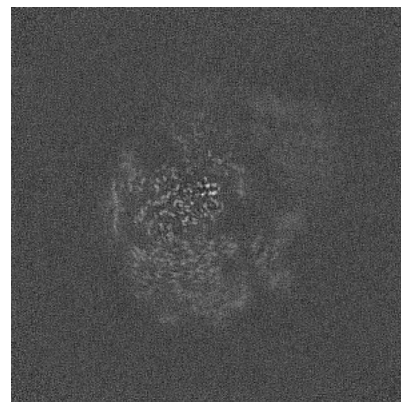
6.2.2 Raw map



X Index: 224



Y Index: 224

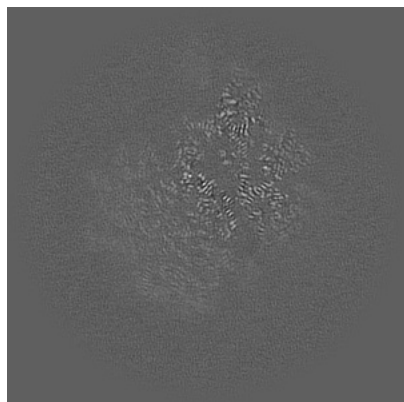


Z Index: 224

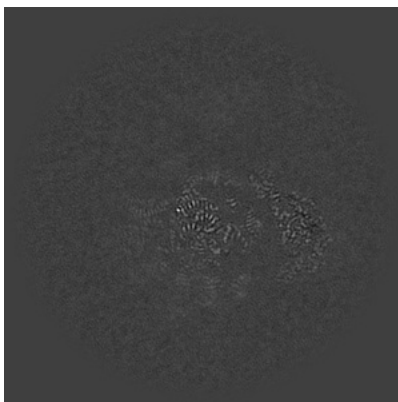
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

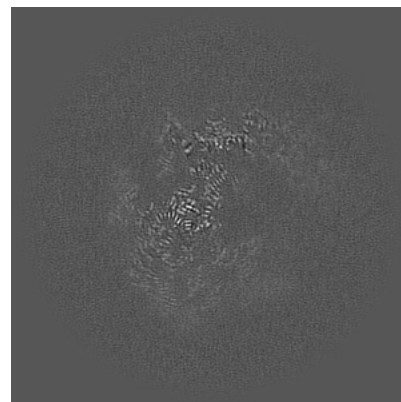
6.3.1 Primary map



X Index: 208

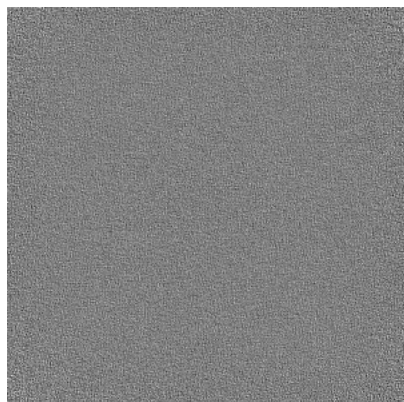


Y Index: 244

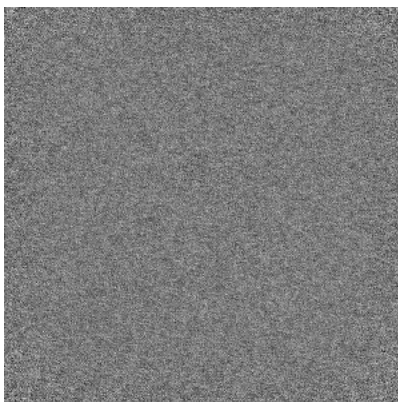


Z Index: 256

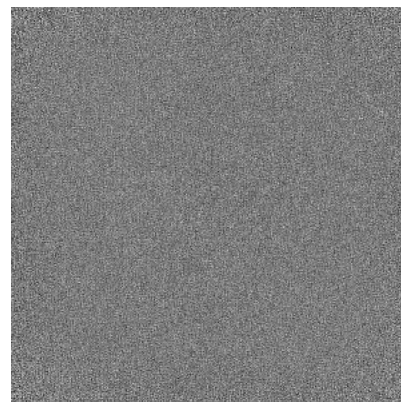
6.3.2 Raw map



X Index: 0



Y Index: 0

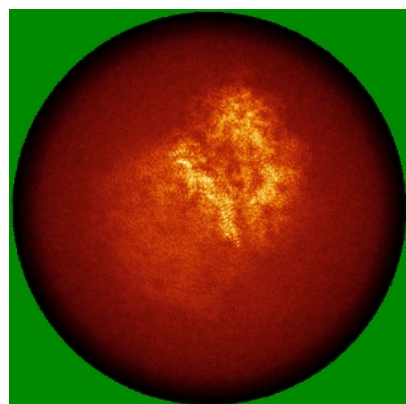


Z Index: 0

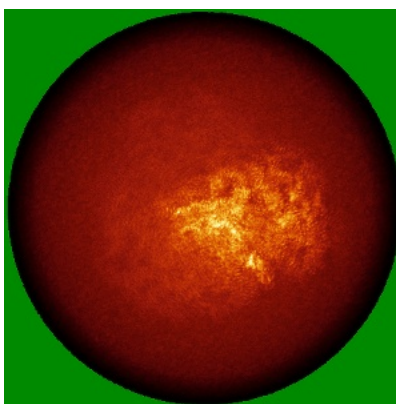
The images above show the largest variance slices of the map in three orthogonal directions.

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

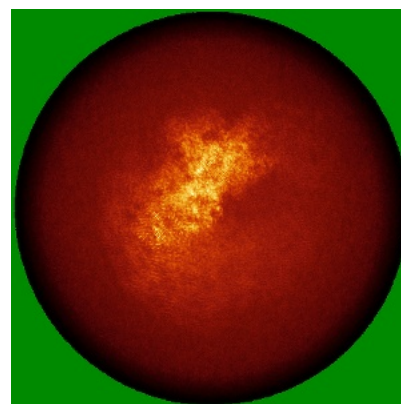
6.4.1 Primary map



X

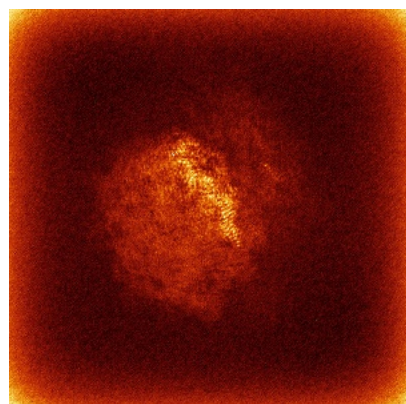


Y

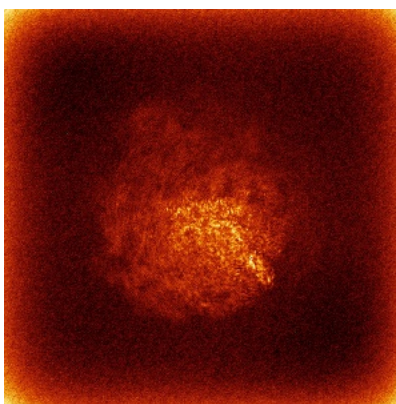


Z

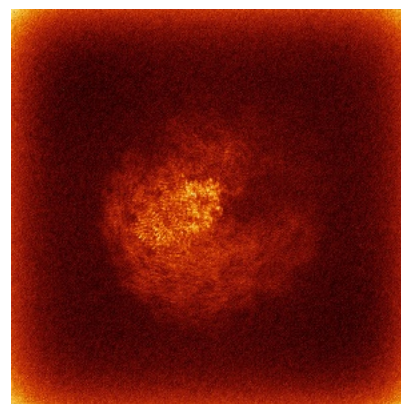
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

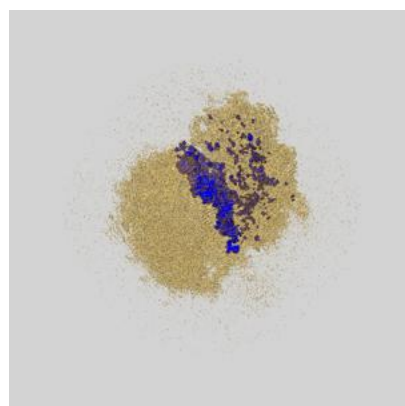
6.6 Mask visualisation [i](#)

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

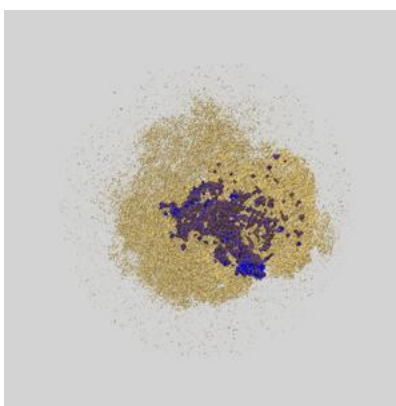
A mask typically either:

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

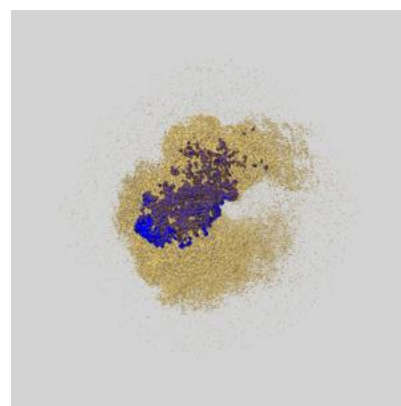
6.6.1 emd_47168_msk_1.map [i](#)



X



Y

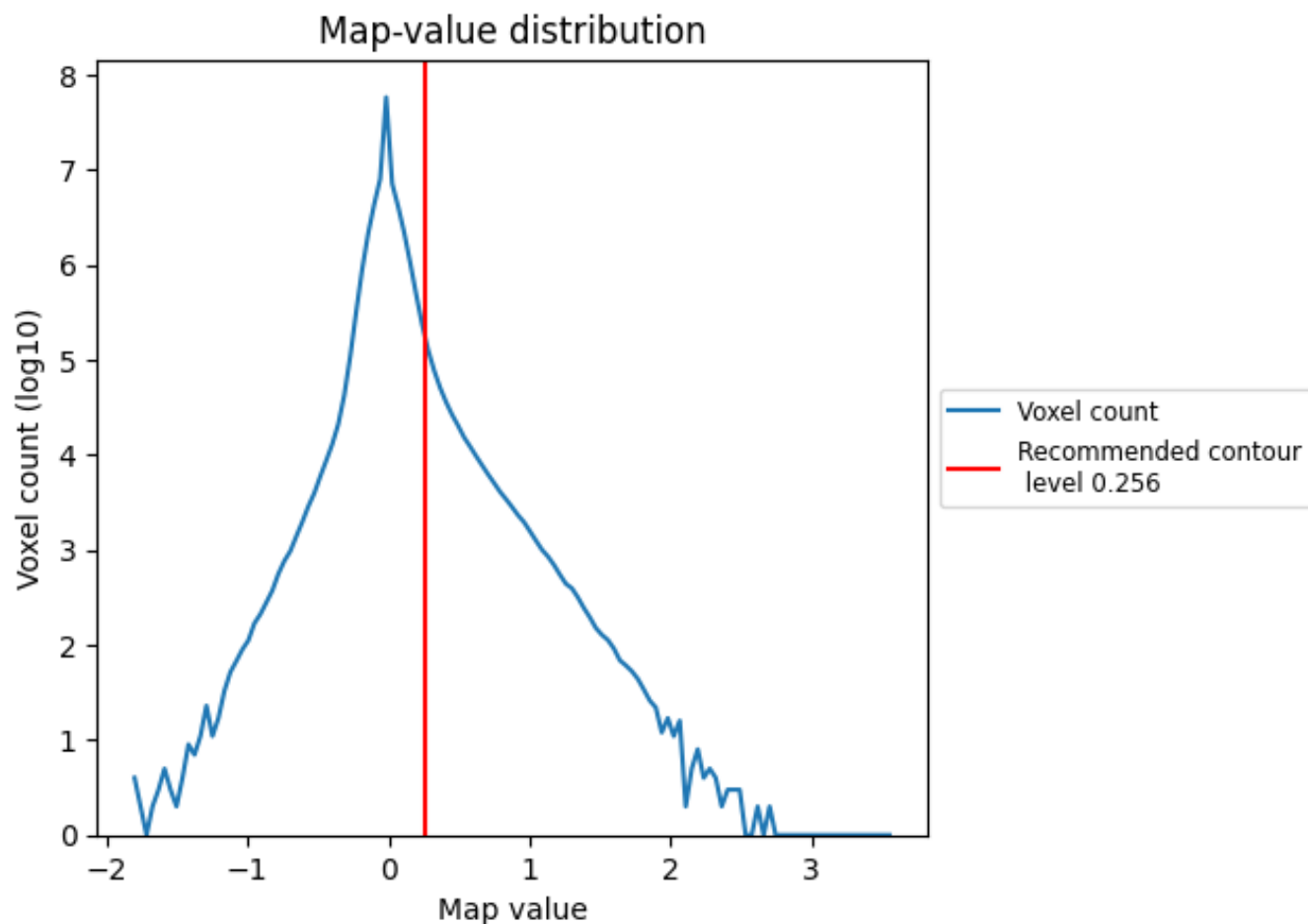


Z

7 Map analysis [i](#)

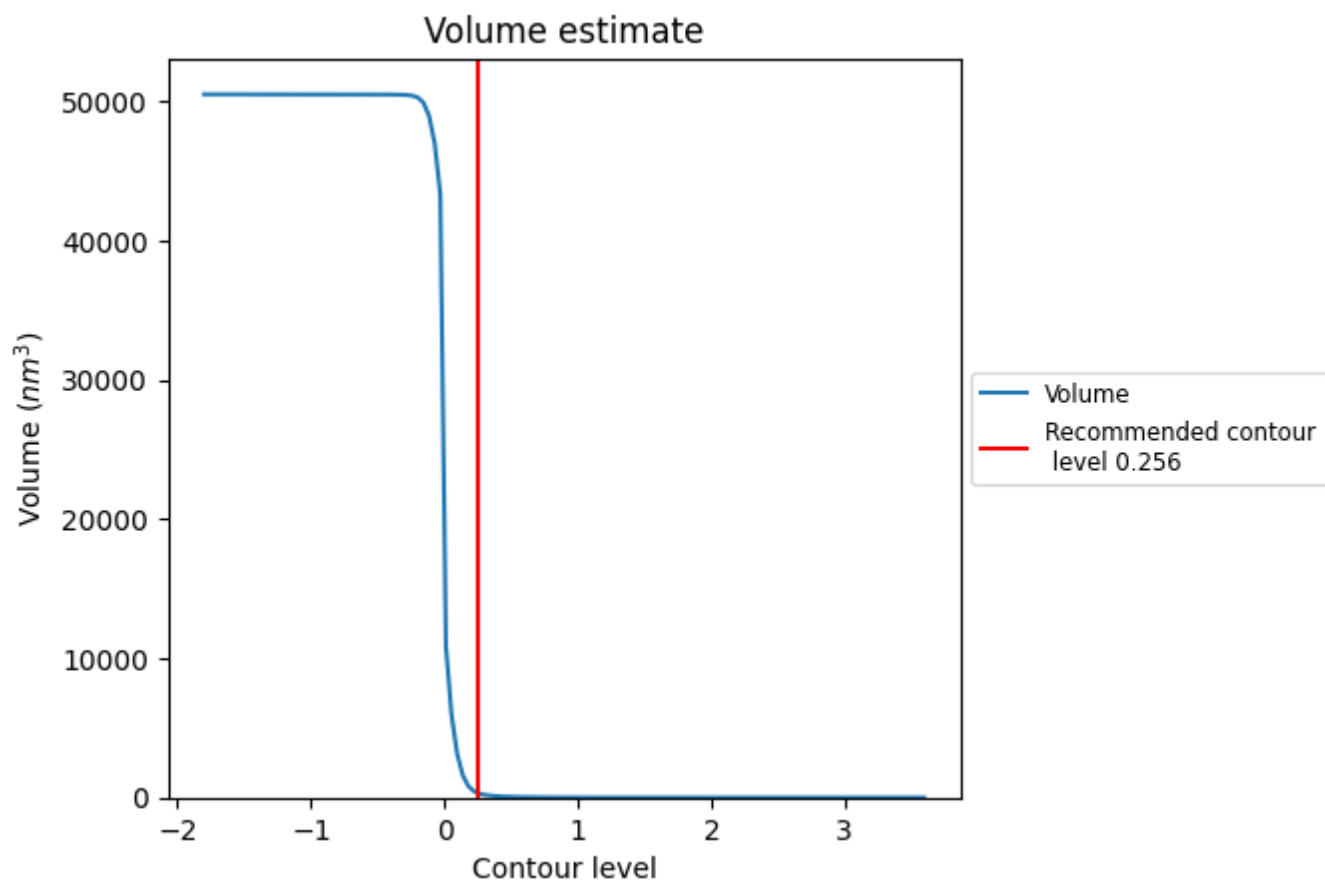
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

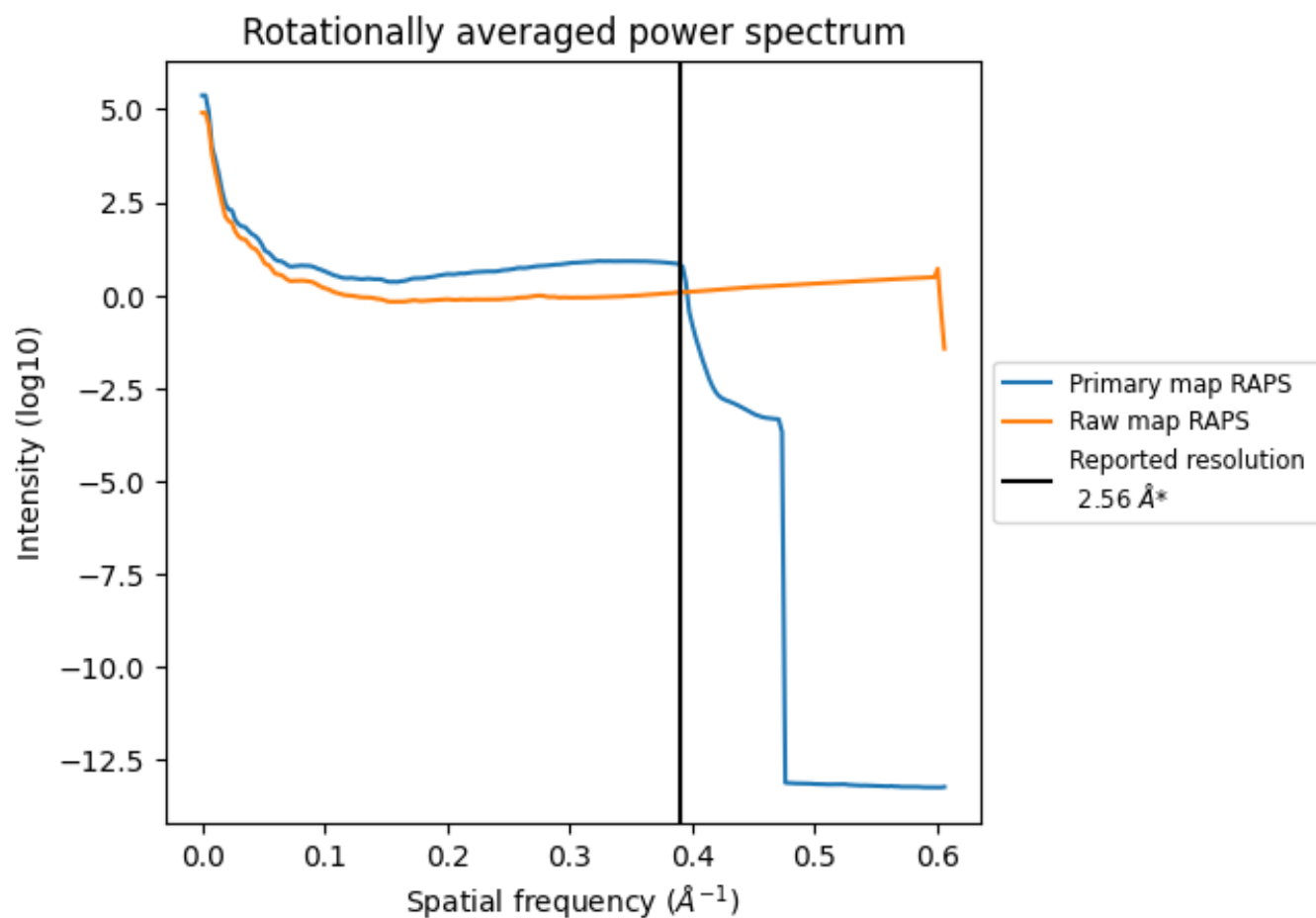
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 310 nm³; this corresponds to an approximate mass of 280 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

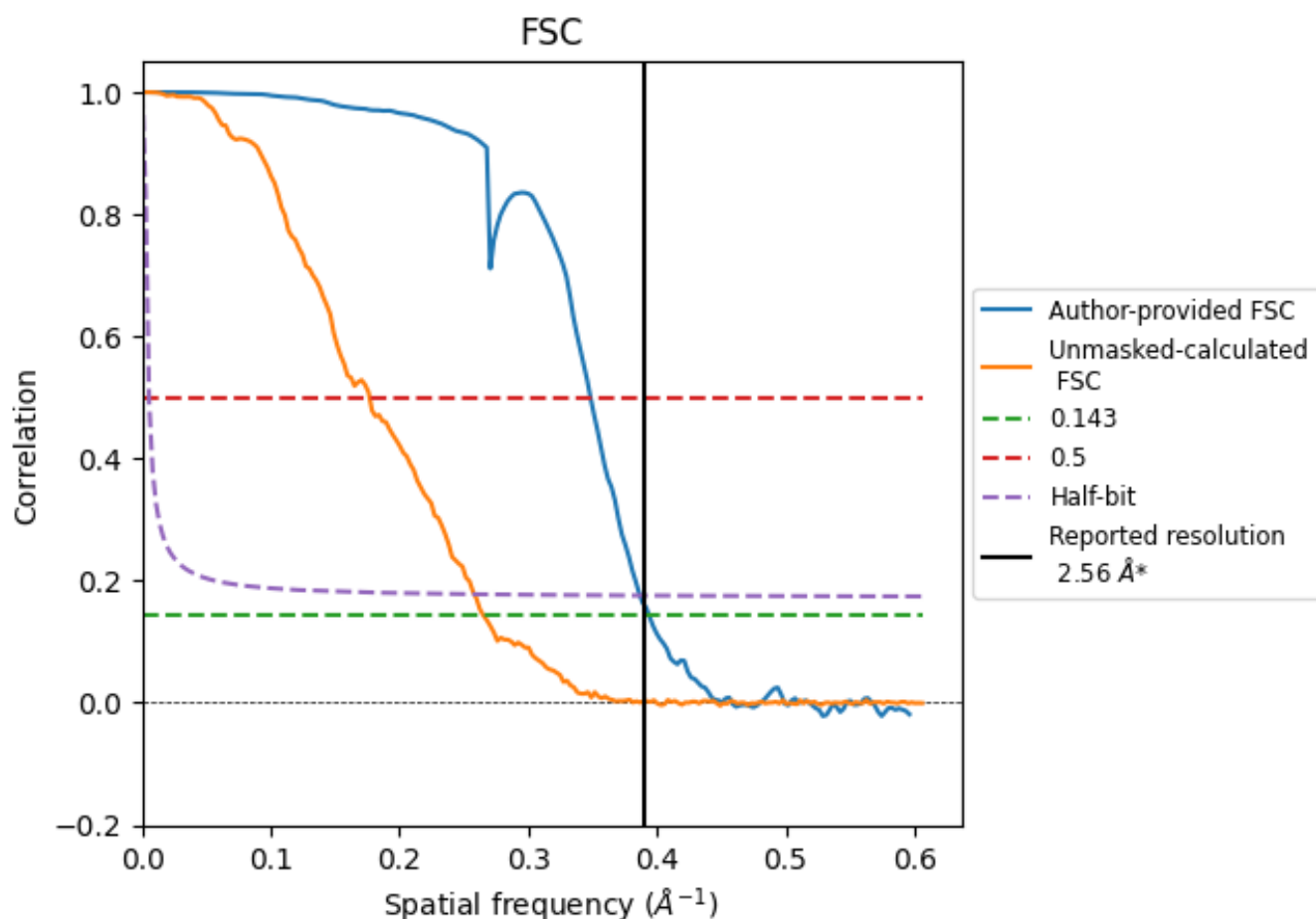


*Reported resolution corresponds to spatial frequency of 0.391 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.391 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

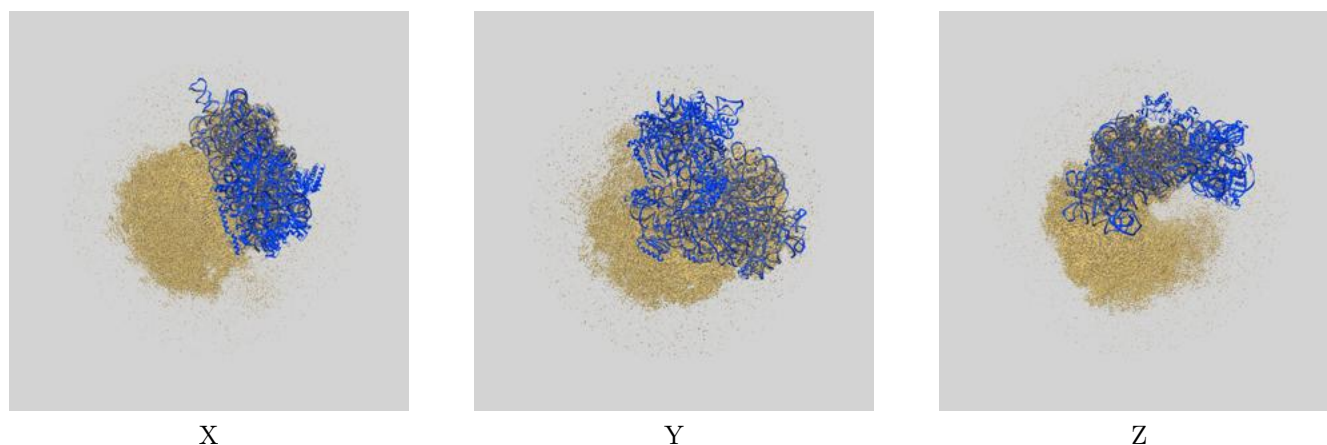
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.54	2.87	2.58
Unmasked-calculated*	3.77	5.66	3.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 2.56 by more than 10 %

9 Map-model fit [i](#)

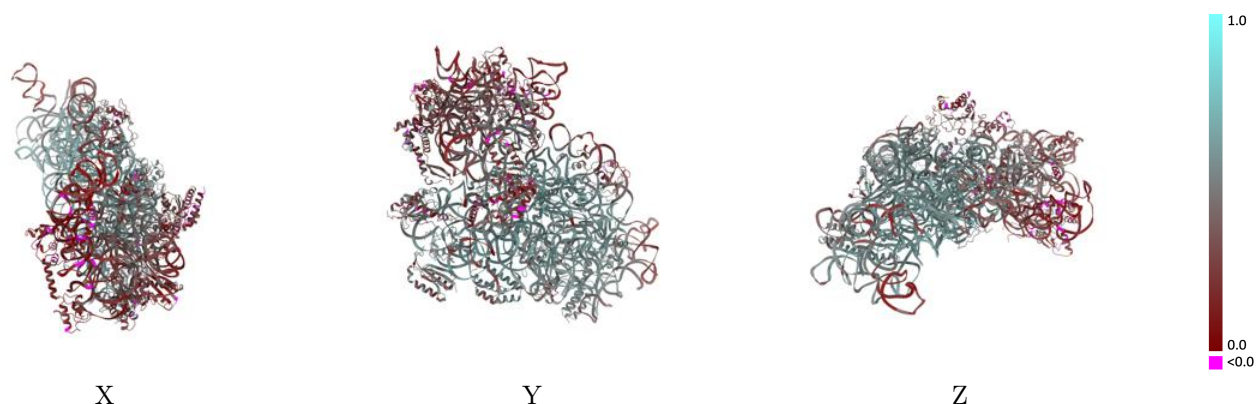
This section contains information regarding the fit between EMDB map EMD-47168 and PDB model 9DUK. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



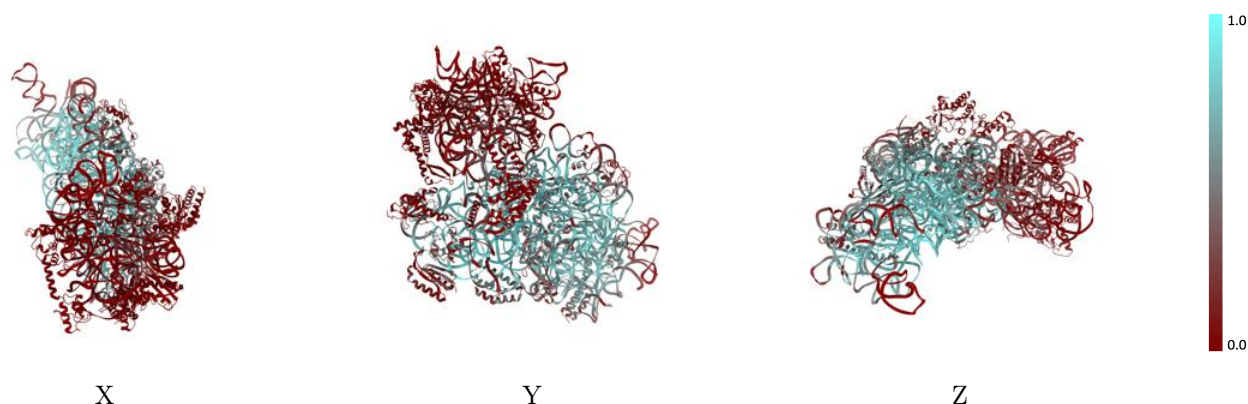
The images above show the 3D surface view of the map at the recommended contour level 0.256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



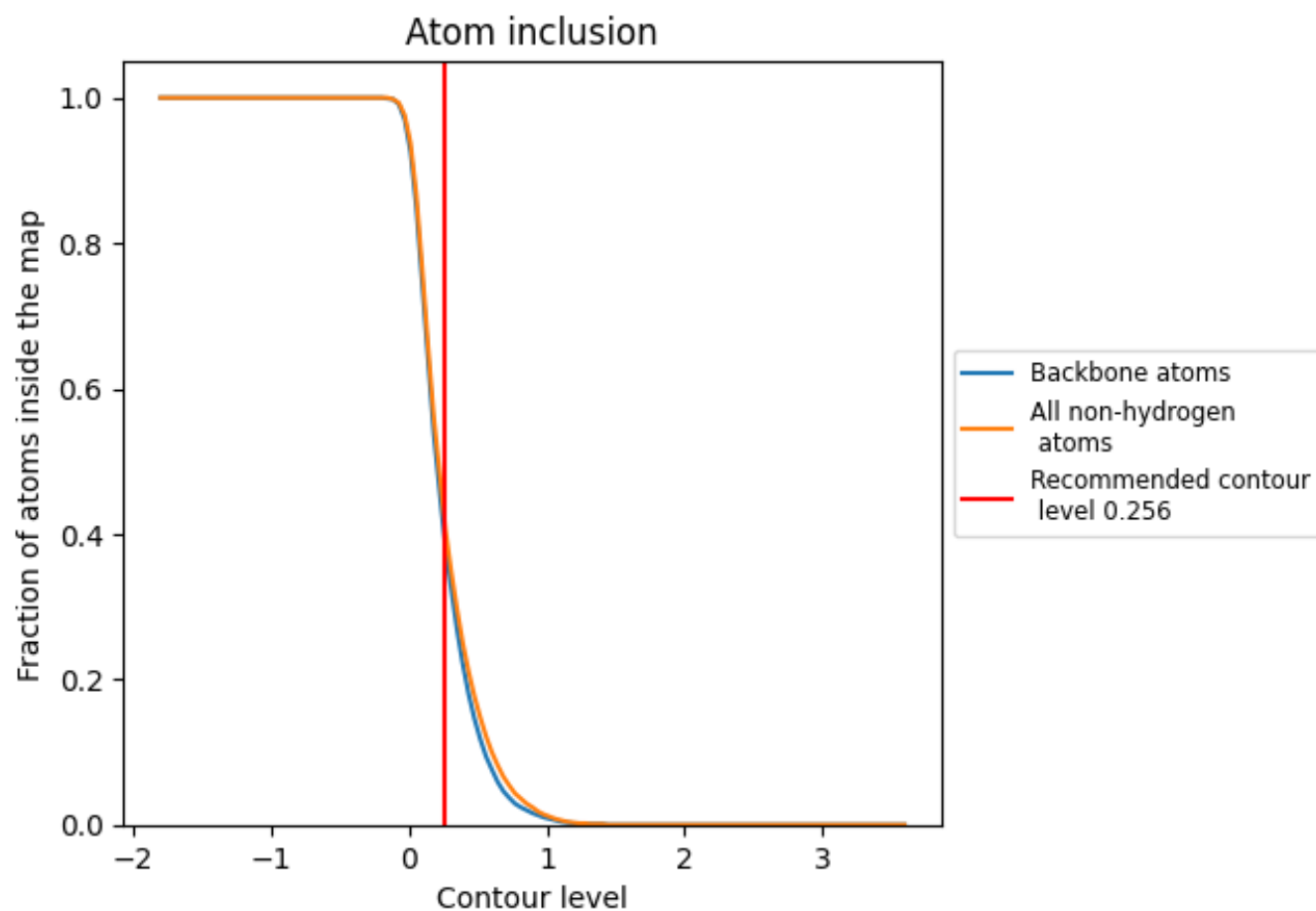
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.256).

9.4 Atom inclusion ⓘ



At the recommended contour level, 40% of all backbone atoms, 42% 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 (0.256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4200	 0.4460
A	 0.5170	 0.4680
B	 0.0030	 0.2580
C	 0.0610	 0.3890
D	 0.4120	 0.4480
E	 0.5980	 0.5930
F	 0.1980	 0.4540
G	 0.0140	 0.3150
H	 0.5010	 0.5580
I	 0.0310	 0.3120
J	 0.0340	 0.3450
K	 0.2620	 0.4840
L	 0.6480	 0.5750
M	 0.0050	 0.2180
N	 0.0280	 0.2670
O	 0.5460	 0.5580
P	 0.6420	 0.5730
Q	 0.4370	 0.5200
R	 0.3160	 0.4900
S	 0.0020	 0.1870
T	 0.5650	 0.5600
U	 0.0070	 0.1950

