Full wwPDB EM Validation Report

Feb 8, 2025 – 02:07 PM EST

PDB ID	:	9DUL
EMDB ID	:	EMD-47169
Title	:	Structure of mutant 30S subunit with extended helix 26, version 4
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:

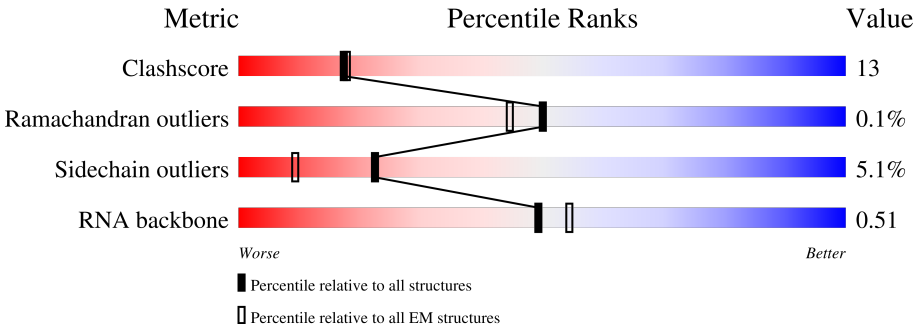
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (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)
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	1533	35% 46% 44% 9%
2	B	234	87% 56% 38%
3	C	233	63% 59% 27% 12%
4	D	206	83% 60% 33% 5%
5	E	167	5% 81% 13% 7%
6	F	135	19% 47% 27% 24%
7	G	179	82% 51% 33% 15%

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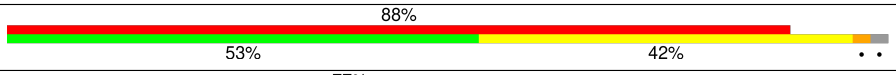
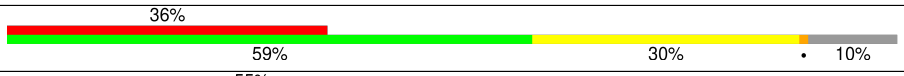
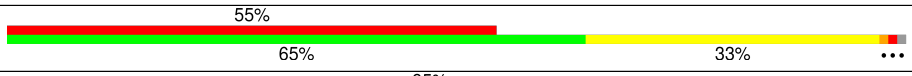
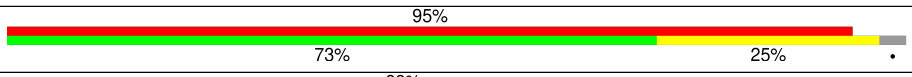
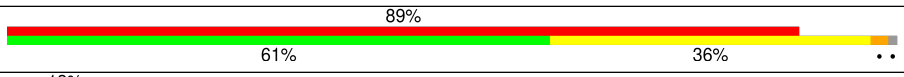
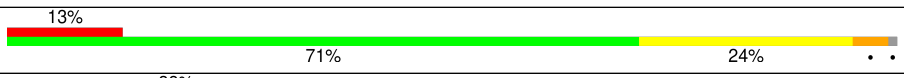
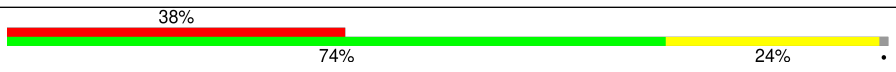
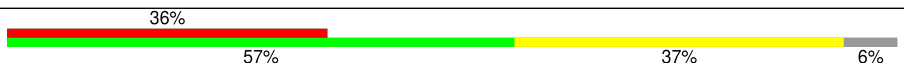
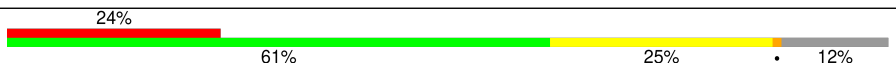
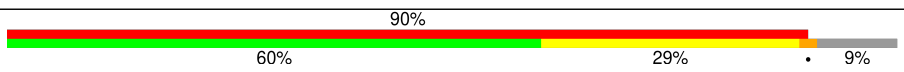
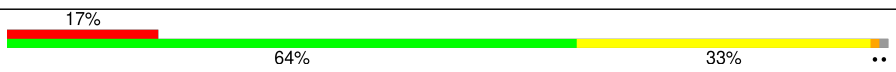
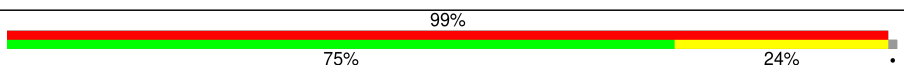
Mol	Chain	Length	Quality of chain
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51552 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1517	32560	14528	5974	10541	1517	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	966	C	G	conflict	GB 2852408577

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

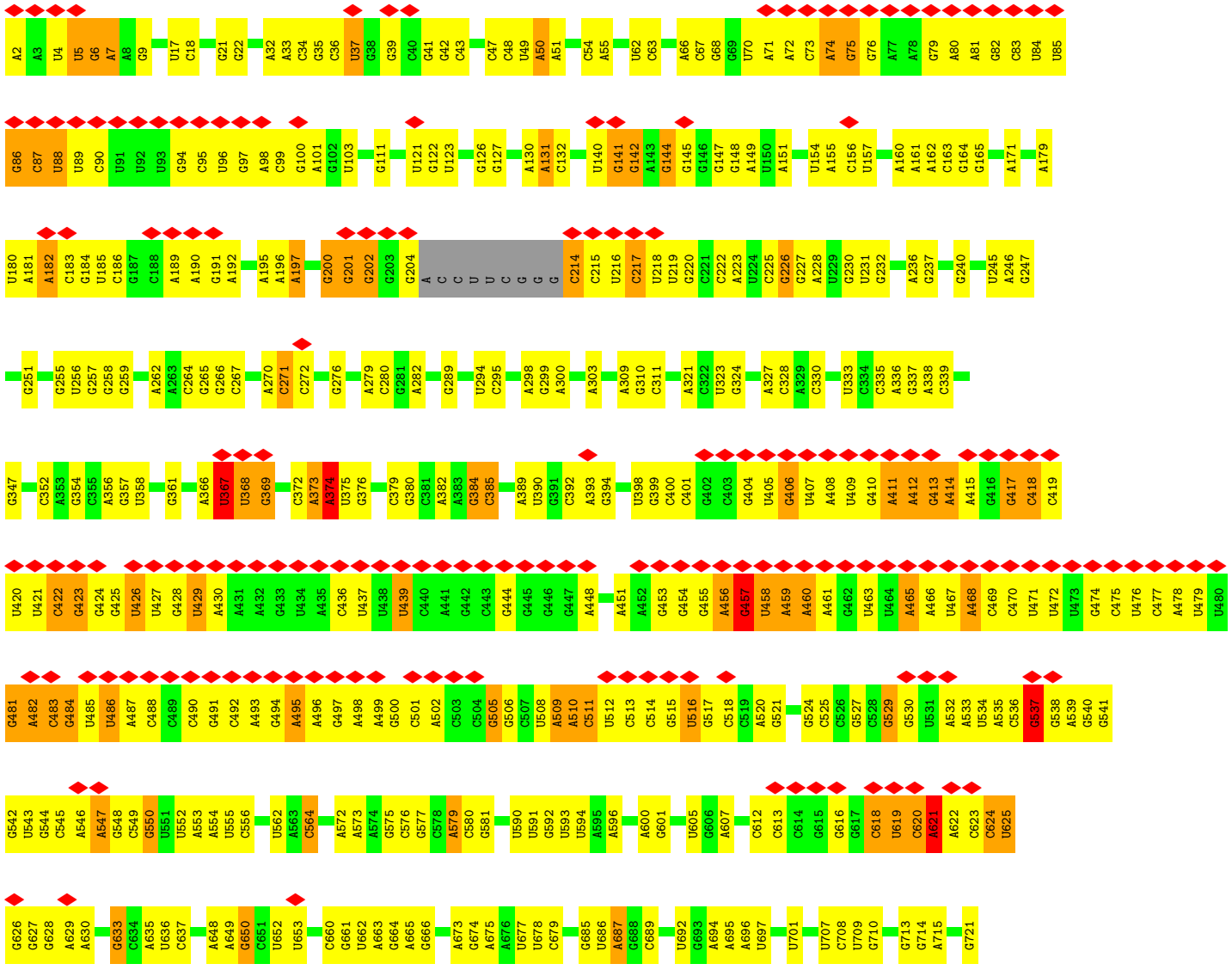
Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total 589	C 366	N 125	O 97	S 1	0	0

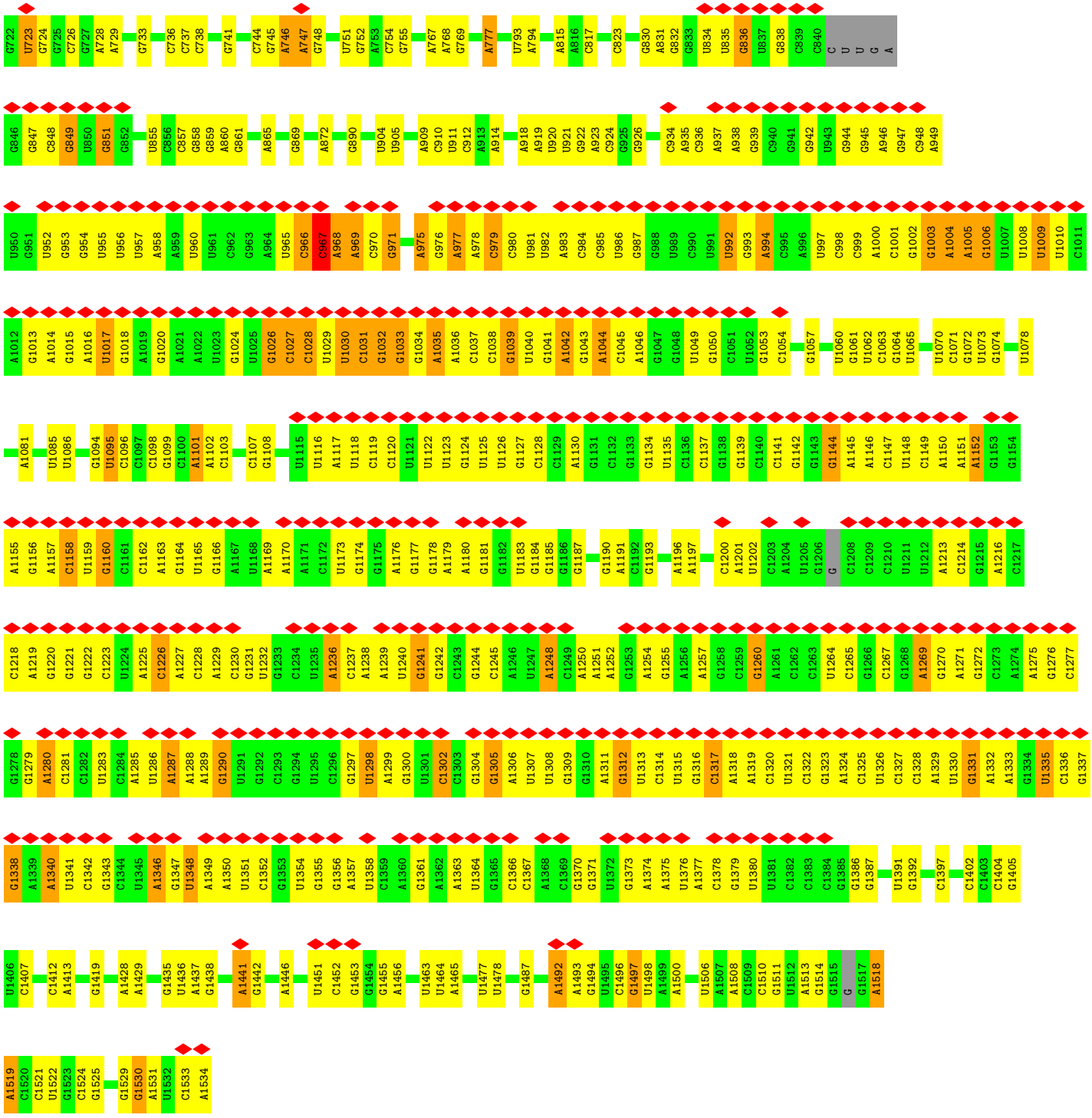
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S rRNA

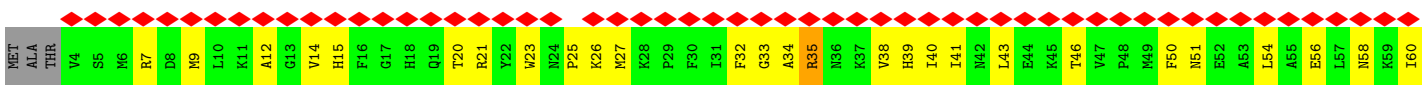
Chain A:

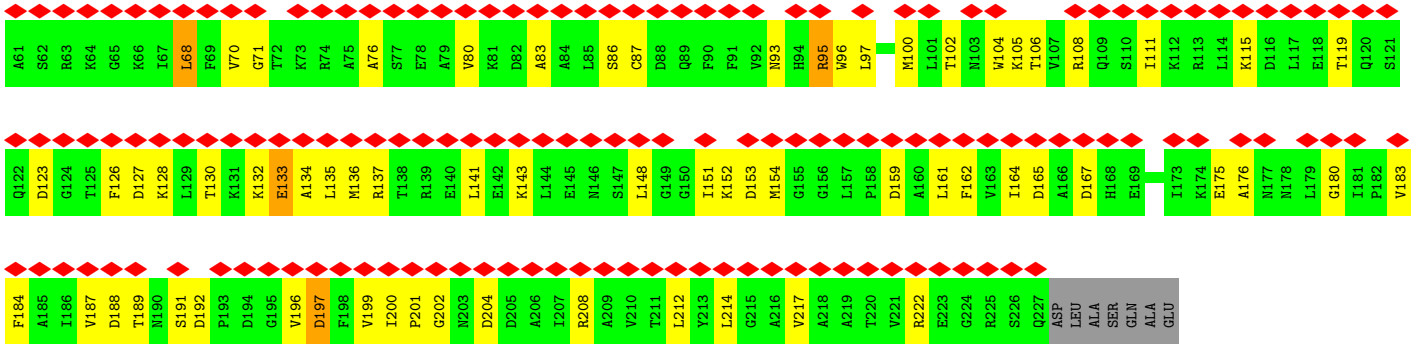




• Molecule 2: Small ribosomal subunit protein uS2

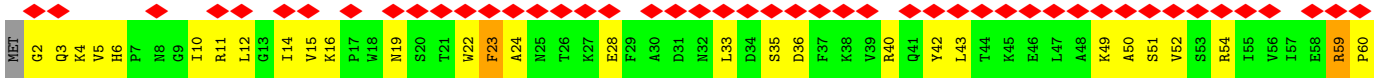
Chain B:





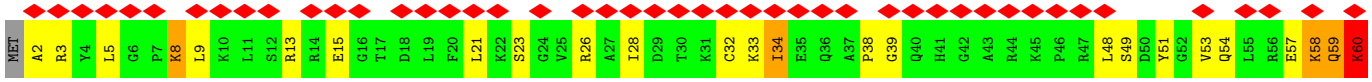
• Molecule 3: Small ribosomal subunit protein uS3

Chain C:



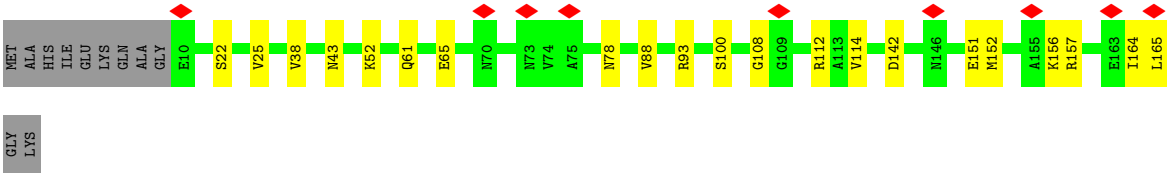
• Molecule 4: Small ribosomal subunit protein uS4

Chain D:



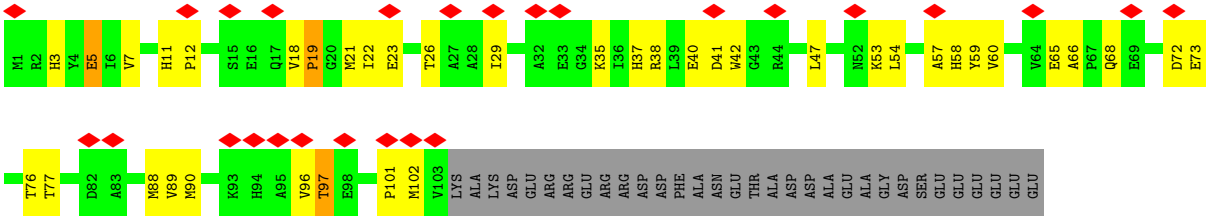
• Molecule 5: Small ribosomal subunit protein uS5

Chain E:



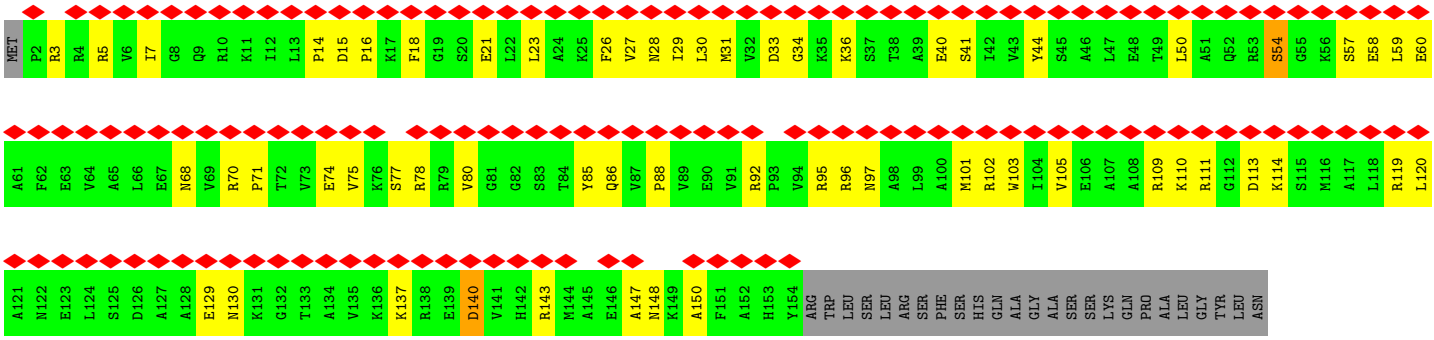
• Molecule 6: Small ribosomal subunit protein bS6

Chain F:



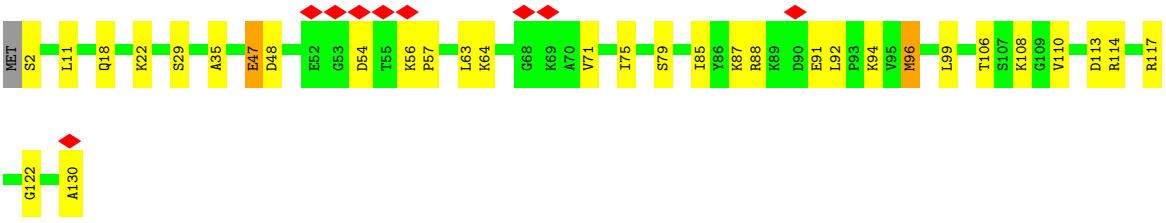
• Molecule 7: Small ribosomal subunit protein uS7

Chain G:



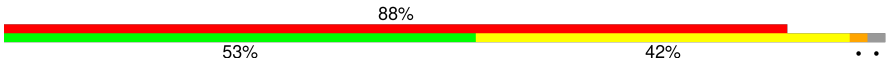
• Molecule 8: Small ribosomal subunit protein uS8

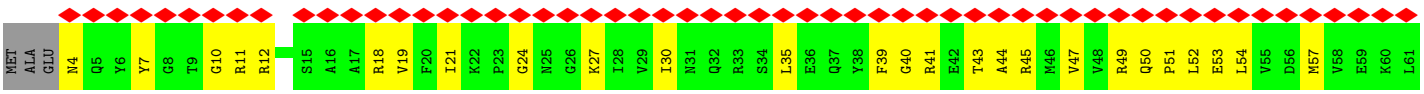
Chain H:

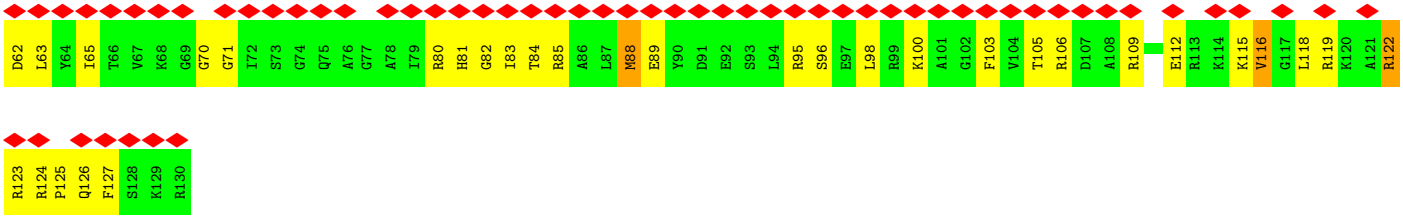


• Molecule 9: Small ribosomal subunit protein uS9

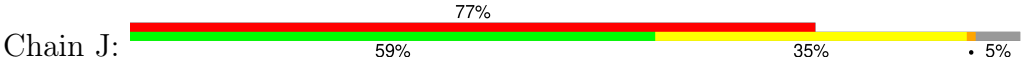
Chain I:

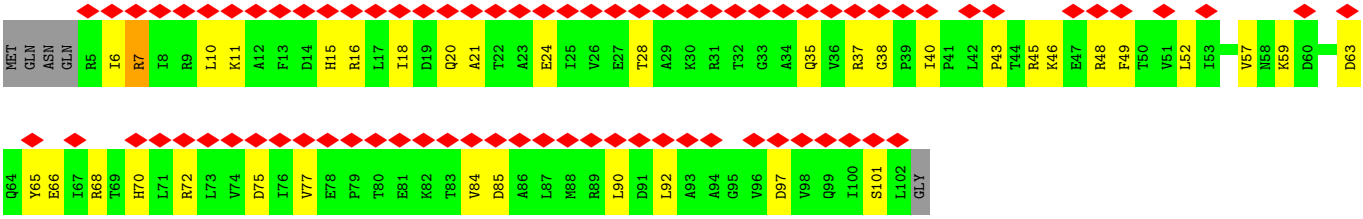




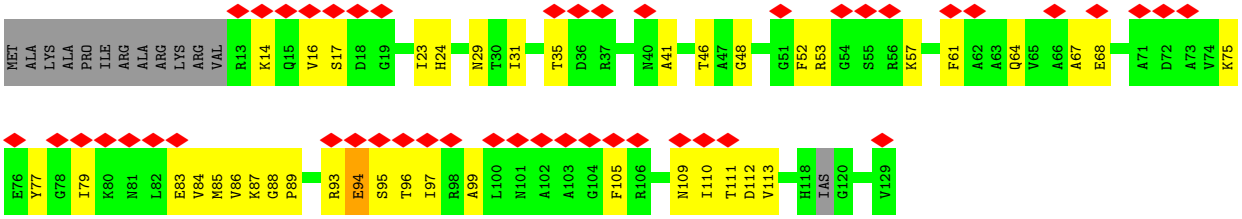


• Molecule 10: Small ribosomal subunit protein uS10

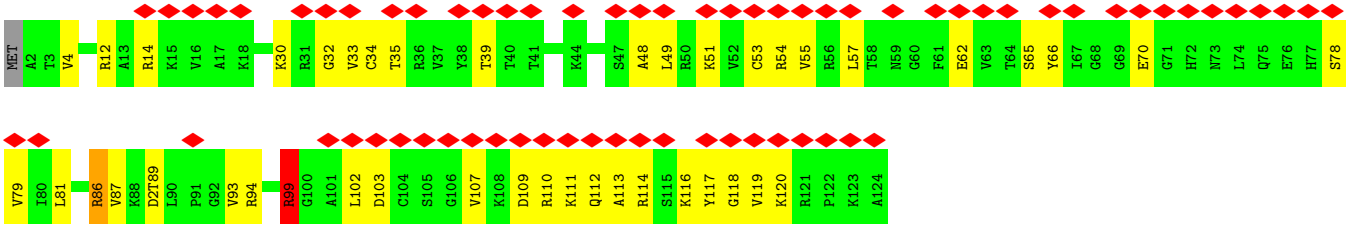




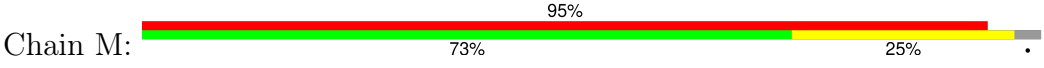
• Molecule 11: Small ribosomal subunit protein uS11

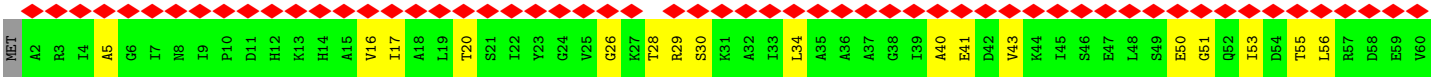


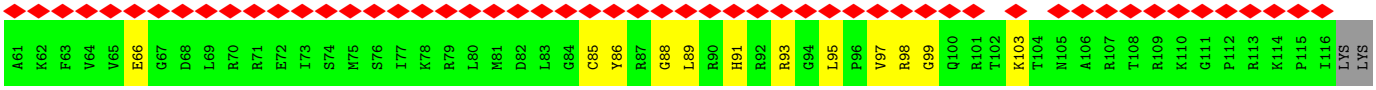
• Molecule 12: Small ribosomal subunit protein uS12



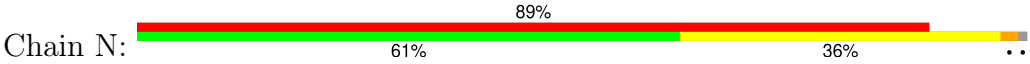
• Molecule 13: Small ribosomal subunit protein uS13

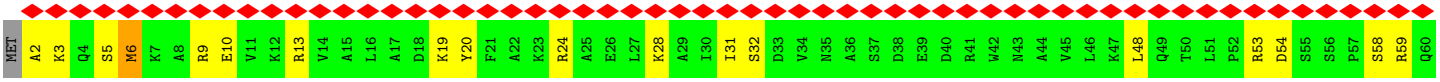


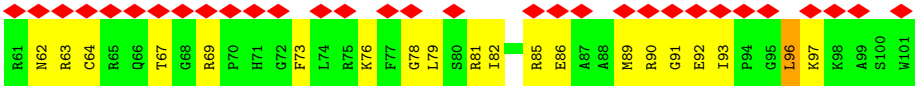




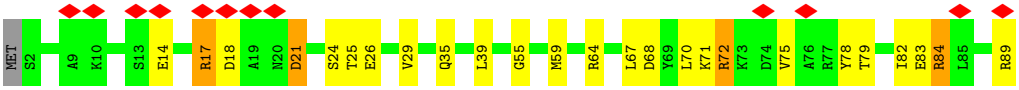
• Molecule 14: Small ribosomal subunit protein uS14



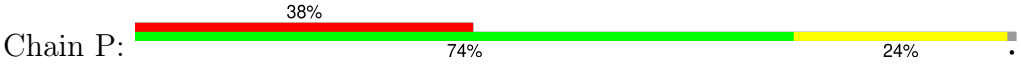


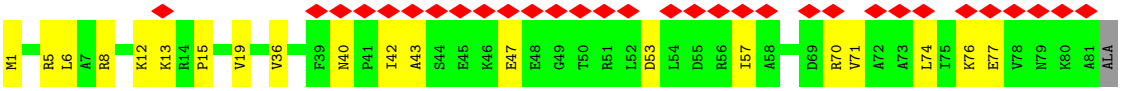


• Molecule 15: Small ribosomal subunit protein uS15

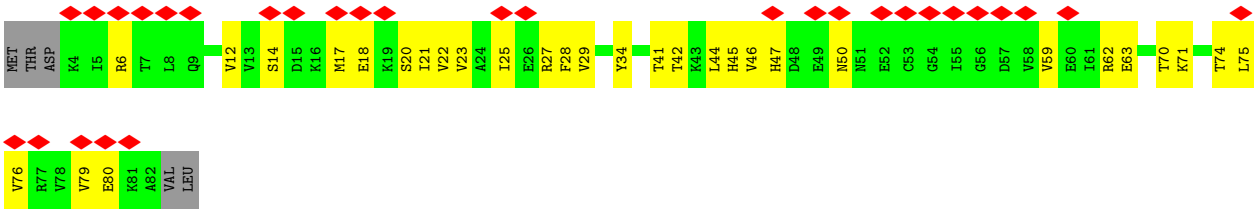


• Molecule 16: Small ribosomal subunit protein bS16

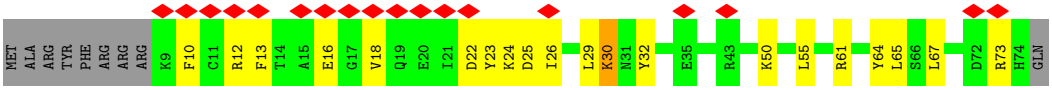




• Molecule 17: Small ribosomal subunit protein uS17

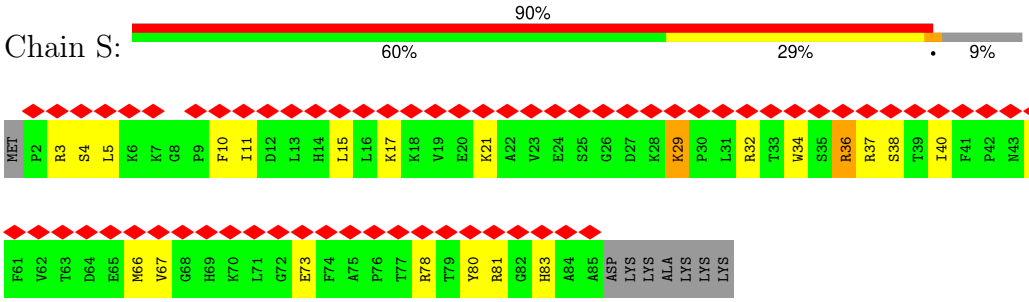


• Molecule 18: Small ribosomal subunit protein bS18



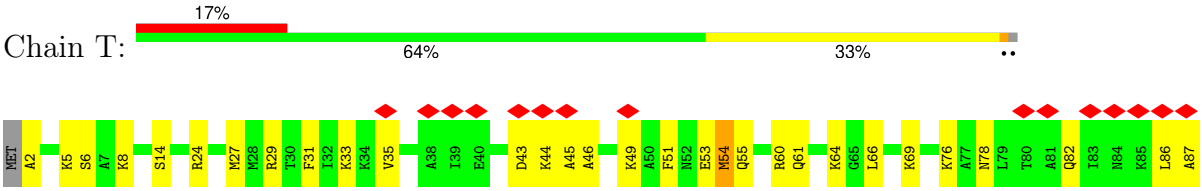
• Molecule 19: Small ribosomal subunit protein uS19

Chain S:



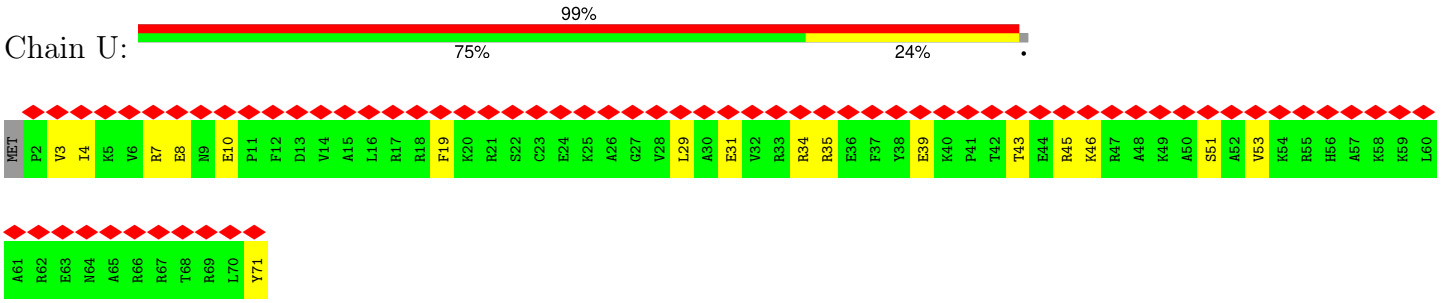
• Molecule 20: Small ribosomal subunit protein bS20

Chain T:



• Molecule 21: Small ribosomal subunit protein bS21

Chain U:



4 Experimental information (i)

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 ($e^-/Å^2$)	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	4.905	Depositor
Minimum map value	-1.524	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.334	Depositor
Map size (Å)	369.376, 369.376, 369.376	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.45	0/36256	0.93	33/56546 (0.1%)
2	B	0.29	0/1784	0.58	0/2403
3	C	0.30	0/1651	0.59	0/2225
4	D	0.33	0/1665	0.70	2/2227 (0.1%)
5	E	0.31	0/1165	0.57	0/1568
6	F	0.33	0/858	0.66	2/1160 (0.2%)
7	G	0.28	0/1219	0.56	0/1635
8	H	0.33	0/989	0.57	0/1326
9	I	0.36	0/1034	0.68	1/1375 (0.1%)
10	J	0.29	0/796	0.63	0/1077
11	K	0.34	0/884	0.72	2/1191 (0.2%)
12	L	0.33	0/960	0.71	1/1286 (0.1%)
13	M	0.26	0/900	0.61	0/1204
14	N	0.28	0/817	0.60	0/1088
15	O	0.29	0/722	0.58	0/964
16	P	0.32	0/653	0.63	0/877
17	Q	0.31	0/650	0.60	0/871
18	R	0.31	0/553	0.59	0/742
19	S	0.36	0/685	0.62	0/922
20	T	0.31	0/676	0.58	0/895
21	U	0.33	0/597	0.64	0/792
All	All	0.41	0/55514	0.84	41/82374 (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
3	C	0	1
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
19	S	0	1
21	U	0	1
All	All	0	5

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	60	LYS	CB-CA-C	8.03	126.46	110.40
11	K	89	PRO	N-CD-CG	-7.91	91.34	103.20
1	A	472	U	C5-C6-N1	7.12	126.26	122.70
1	A	537	G	N3-C4-N9	6.89	130.14	126.00
1	A	367	U	C5-C6-N1	6.75	126.08	122.70
1	A	373	A	OP1-P-O3'	6.57	119.65	105.20
1	A	214	C	C2-N1-C1'	6.51	125.96	118.80
1	A	965	U	OP1-P-O3'	6.44	119.36	105.20
1	A	620	C	P-O3'-C3'	6.39	127.37	119.70
1	A	979	C	N1-C2-O2	6.39	122.73	118.90
1	A	620	C	O3'-P-O5'	6.34	116.05	104.00
6	F	19	PRO	N-CD-CG	-6.25	93.83	103.20
4	D	59	GLN	CB-CA-C	-6.25	97.91	110.40
1	A	979	C	N3-C2-O2	-6.12	117.62	121.90
1	A	993	G	N3-C4-N9	6.10	129.66	126.00
6	F	19	PRO	CA-N-CD	-6.09	102.98	111.50
9	I	57	MET	CA-CB-CG	6.08	123.64	113.30
11	K	89	PRO	CA-N-CD	-5.86	103.29	111.50
1	A	537	G	C6-C5-N7	-5.73	126.96	130.40
1	A	439	U	N3-C2-O2	-5.68	118.23	122.20
1	A	472	U	C5-C4-O4	-5.66	122.50	125.90
1	A	612	C	C6-N1-C2	-5.63	118.05	120.30
1	A	537	G	N9-C4-C5	-5.62	103.15	105.40
1	A	872	A	O4'-C1'-N9	5.53	112.62	108.20
1	A	439	U	N1-C2-O2	5.46	126.62	122.80
1	A	439	U	C2-N1-C1'	5.44	124.22	117.70
1	A	457	G	OP2-P-O3'	5.40	117.08	105.20
1	A	1236	A	OP2-P-O3'	5.36	117.00	105.20
1	A	1158	C	C2-N1-C1'	5.35	124.69	118.80
12	L	99	ARG	CB-CA-C	5.30	121.00	110.40
1	A	374	A	OP1-P-OP2	-5.21	111.79	119.60
1	A	217	C	N1-C2-O2	5.19	122.01	118.90
1	A	537	G	C8-N9-C1'	-5.18	120.26	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	621	A	OP1-P-OP2	-5.15	111.87	119.60
1	A	625	U	O4'-C1'-N1	5.15	112.32	108.20
1	A	967	5MC	OP2-P-O3'	5.15	116.53	105.20
1	A	537	G	N1-C6-O6	5.12	122.97	119.90
1	A	575	G	N3-C4-N9	-5.06	122.96	126.00
1	A	1032	G	OP2-P-O3'	5.06	116.33	105.20
1	A	259	G	OP1-P-OP2	-5.05	112.03	119.60
1	A	1035	A	P-O3'-C3'	5.02	125.73	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	59	ARG	Sidechain
4	D	105	MET	Peptide
12	L	99	ARG	Sidechain
19	S	36	ARG	Sidechain
21	U	45	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	A	32560	0	16406	661	0
2	B	1753	0	1780	69	0
3	C	1624	0	1696	48	0
4	D	1643	0	1707	67	0
5	E	1152	0	1196	9	0
6	F	839	0	833	26	0
7	G	1203	0	1254	44	0
8	H	979	0	1031	18	0
9	I	1022	0	1070	47	0
10	J	786	0	828	23	0
11	K	869	0	880	38	0
12	L	957	0	1017	39	0
13	M	891	0	952	26	0
14	N	805	0	844	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	714	0	734	14	0
16	P	643	0	661	17	0
17	Q	641	0	682	26	0
18	R	544	0	565	20	0
19	S	668	0	693	34	0
20	T	670	0	719	22	0
21	U	589	0	629	11	0
All	All	51552	0	36177	1144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1144) 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:73:C:HO2'	1:A:74:A:H8	0.99	0.94
1:A:55:A:H62	1:A:357:G:H21	1.13	0.93
1:A:1009:U:H3	1:A:1020:G:H1	0.93	0.90
1:A:486:U:H2'	1:A:487:A:H8	1.38	0.86
1:A:673:A:H2'	1:A:674:G:C8	2.13	0.83
1:A:406:G:H5'	4:D:5:LEU:HD22	1.61	0.81
20:T:24:ARG:HD2	20:T:61:GLN:HE22	1.46	0.80
1:A:490:C:H5"	4:D:146:ARG:HH22	1.45	0.79
19:S:11:ILE:HG13	19:S:38:SER:HB3	1.63	0.79
1:A:664:G:H22	1:A:741:G:H1	1.26	0.79
1:A:55:A:H62	1:A:357:G:N2	1.80	0.78
1:A:406:G:N3	4:D:116:GLN:NE2	2.33	0.77
1:A:509:A:H2	1:A:544:G:H4'	1.49	0.77
2:B:126:PHE:HB3	2:B:134:ALA:HB1	1.67	0.76
3:C:66:VAL:HG21	3:C:91:VAL:HG21	1.69	0.75
1:A:1157:A:H61	1:A:1178:G:H1'	1.50	0.75
12:L:33:VAL:HG22	12:L:79:VAL:HG22	1.68	0.75
1:A:35:G:H2'	1:A:36:C:C6	2.22	0.75
1:A:1160:G:H1	1:A:1176:A:N6	1.85	0.74
1:A:1127:G:H1	1:A:1145:A:H61	1.34	0.74
1:A:376:G:H5"	16:P:5:ARG:HB2	1.69	0.74
1:A:1321:U:O2'	19:S:78:ARG:NH1	2.20	0.74
4:D:126:ASN:ND2	4:D:141:ASP:OD1	2.20	0.74
1:A:456:A:H3'	1:A:457:G:H8	1.53	0.74
11:K:64:GLN:HG3	11:K:99:ALA:HB2	1.70	0.74
5:E:164:ILE:HG22	5:E:165:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:G:N2	1:A:469:C:O2	2.21	0.73
1:A:621:A:H2'	1:A:622:A:H8	1.52	0.73
1:A:1325:C:H2'	1:A:1326:U:H6	1.52	0.73
18:R:13:PHE:HD1	18:R:18:VAL:HG21	1.53	0.73
1:A:1193:G:O6	3:C:2:GLY:N	2.22	0.73
1:A:1367:C:H5"	9:I:116:VAL:HG12	1.72	0.72
12:L:39:THR:HG22	12:L:51:LYS:HE3	1.70	0.72
1:A:618:C:N4	1:A:621:A:OP2	2.21	0.72
1:A:215:C:H1'	1:A:465:A:H62	1.55	0.72
4:D:9:LEU:HD13	4:D:32:CYS:HB3	1.72	0.72
2:B:86:SER:O	2:B:222:ARG:NH1	2.21	0.71
1:A:2:A:N3	1:A:613:C:O2'	2.23	0.71
1:A:1335:U:H5"	1:A:1336:C:H5'	1.71	0.71
4:D:183:LYS:O	4:D:184:ARG:NH1	2.23	0.71
1:A:486:U:H2'	1:A:487:A:C8	2.24	0.71
1:A:1160:G:H1	1:A:1176:A:H61	1.39	0.71
1:A:509:A:C2	1:A:544:G:H4'	2.26	0.71
1:A:481:G:H21	1:A:482:A:H61	1.37	0.70
1:A:980:C:O2'	14:N:13:ARG:NH1	2.24	0.70
1:A:1218:C:H2'	1:A:1219:A:C8	2.27	0.70
1:A:1218:C:H2'	1:A:1219:A:H8	1.57	0.70
2:B:151:ILE:HB	2:B:154:MET:HE2	1.74	0.70
17:Q:20:SER:HB3	17:Q:71:LYS:HE3	1.72	0.69
1:A:374:A:O3'	16:P:70:ARG:NH1	2.26	0.69
11:K:83:GLU:HG2	11:K:109:ASN:HB2	1.74	0.69
1:A:677:U:H3	1:A:713:G:H22	1.38	0.69
1:A:81:A:N6	1:A:88:U:O4	2.24	0.69
2:B:32:PHE:HB3	2:B:40:ILE:HG23	1.75	0.69
12:L:53:CYS:O	12:L:65:SER:N	2.21	0.68
15:O:14:GLU:HG3	15:O:84:ARG:HH21	1.55	0.68
1:A:1354:U:H2'	1:A:1355:G:H8	1.58	0.68
1:A:545:C:O2'	1:A:549:C:H5"	1.94	0.68
2:B:15:HIS:ND1	2:B:40:ILE:HD11	2.09	0.68
1:A:1305:G:H22	1:A:1331:G:H1'	1.57	0.68
1:A:1313:U:H2'	1:A:1314:C:C6	2.28	0.68
9:I:84:THR:HG23	9:I:98:LEU:HD22	1.76	0.68
10:J:48:ARG:HG2	10:J:66:GLU:HG3	1.75	0.67
1:A:147:G:H2'	1:A:148:G:C8	2.30	0.67
1:A:1191:A:H5"	3:C:4:LYS:HE3	1.77	0.67
19:S:40:ILE:HG23	19:S:44:MET:HG3	1.74	0.67
19:S:10:PHE:HE2	19:S:37:ARG:HG3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:A:N3	1:A:368:U:O2'	2.28	0.67
9:I:88:MET:HG2	9:I:95:ARG:HB2	1.77	0.67
1:A:633:G:OP2	8:H:88:ARG:NH2	2.27	0.67
11:K:46:THR:HG22	11:K:48:GLY:H	1.59	0.66
13:M:16:VAL:HB	13:M:41:GLU:HB3	1.77	0.66
1:A:1327:C:H2'	1:A:1328:C:C6	2.30	0.66
3:C:131:ARG:O	3:C:135:LYS:HG3	1.95	0.66
2:B:167:ASP:OD2	2:B:191:SER:HA	1.95	0.66
14:N:28:LYS:HA	14:N:31:ILE:HD12	1.78	0.66
20:T:55:GLN:HG2	20:T:76:LYS:HD2	1.78	0.66
4:D:15:GLU:HG3	4:D:60:LYS:HB2	1.78	0.66
1:A:37:U:OP2	12:L:120:LYS:NZ	2.29	0.66
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.66
1:A:466:A:H2'	1:A:468:A:C8	2.32	0.65
1:A:623:C:H2'	1:A:624:C:C6	2.31	0.65
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.78	0.65
1:A:823:C:HO2'	8:H:2:SER:N	1.94	0.65
1:A:255:G:H4'	17:Q:18:GLU:HG2	1.77	0.65
1:A:1320:C:H41	19:S:37:ARG:HB3	1.61	0.65
1:A:1328:C:H5"	13:M:28:THR:HB	1.77	0.65
6:F:37:HIS:HB3	6:F:97:THR:HG22	1.78	0.65
1:A:1101:A:OP2	2:B:95:ARG:NH1	2.30	0.65
14:N:9:ARG:HB3	14:N:13:ARG:HH21	1.61	0.65
1:A:1530:G:H2'	1:A:1531:A:H8	1.60	0.65
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.79	0.65
12:L:110:ARG:NE	12:L:112:GLN:O	2.29	0.65
4:D:105:MET:HB3	4:D:171:LEU:HD13	1.79	0.65
3:C:50:ALA:HB1	3:C:76:VAL:HG22	1.79	0.64
3:C:43:LEU:HD13	3:C:68:ILE:HD11	1.79	0.64
1:A:536:C:H2'	1:A:537:G:H8	1.62	0.64
9:I:30:ILE:HG12	9:I:65:ILE:HB	1.79	0.64
20:T:29:ARG:O	20:T:33:LYS:HD2	1.97	0.64
1:A:515:G:H2'	1:A:516:PSU:H6	1.63	0.64
1:A:216:U:H2'	1:A:217:C:C6	2.33	0.63
1:A:405:U:O4	4:D:3:ARG:N	2.31	0.63
1:A:1309:G:OP1	13:M:91:HIS:NE2	2.28	0.63
1:A:1373:G:H4'	7:G:31:MET:HE2	1.79	0.63
1:A:500:G:H2'	1:A:501:C:C6	2.33	0.63
1:A:620:C:H2'	1:A:621:A:C8	2.33	0.63
9:I:11:ARG:HD2	9:I:106:ARG:HH21	1.63	0.63
1:A:17:U:H2'	1:A:18:C:C6	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ASN:OD1	7:G:130:ASN:ND2	2.32	0.63
12:L:110:ARG:HB3	12:L:119:VAL:HG11	1.81	0.63
1:A:1222:G:OP2	1:A:1322:C:N4	2.30	0.63
12:L:114:ARG:HB3	12:L:119:VAL:O	1.99	0.63
1:A:453:G:OP1	16:P:76:LYS:NZ	2.32	0.63
6:F:29:ILE:HG23	6:F:66:ALA:HB2	1.81	0.63
1:A:1524:C:H2'	1:A:1525:G:C8	2.34	0.62
1:A:505:G:OP2	1:A:535:A:H5'	1.98	0.62
1:A:1072:G:H21	2:B:106:THR:HG21	1.62	0.62
1:A:1241:G:H2'	1:A:1242:G:H8	1.63	0.62
14:N:64:CYS:HB3	14:N:69:ARG:H	1.63	0.62
2:B:15:HIS:HB3	2:B:43:LEU:HD11	1.81	0.62
6:F:38:ARG:NH2	6:F:96:VAL:HG12	2.14	0.62
11:K:23:ILE:HG12	11:K:96:THR:HG21	1.82	0.62
1:A:1156:G:O2'	1:A:1180:A:N6	2.27	0.62
1:A:1313:U:H2'	1:A:1314:C:H6	1.63	0.62
1:A:1530:G:H2'	1:A:1531:A:C8	2.35	0.62
1:A:542:G:H5'	4:D:39:GLY:HA3	1.81	0.62
4:D:57:GLU:HG2	4:D:199:LEU:HB2	1.82	0.62
1:A:366:A:O2'	1:A:394:G:N2	2.33	0.61
1:A:1086:U:H3	1:A:1099:G:H22	1.47	0.61
9:I:96:SER:O	9:I:100:LYS:HG2	2.00	0.61
1:A:405:U:H3	1:A:499:A:H62	1.48	0.61
1:A:490:C:H2'	1:A:491:G:H8	1.66	0.61
1:A:744:C:H2'	1:A:745:G:H8	1.64	0.61
1:A:1147:C:H1'	9:I:18:ARG:HH21	1.66	0.61
2:B:102:THR:OG1	2:B:175:GLU:HG2	2.00	0.61
7:G:75:VAL:HB	7:G:86:GLN:HB3	1.82	0.61
1:A:1297:G:N2	1:A:1298:U:O4	2.27	0.61
10:J:38:GLY:HA2	10:J:40:ILE:HG13	1.80	0.61
1:A:1354:U:H2'	1:A:1355:G:C8	2.36	0.61
16:P:36:VAL:HB	16:P:53:ASP:HB3	1.83	0.61
1:A:67:C:H2'	1:A:68:G:C8	2.36	0.61
1:A:1001:C:H2'	1:A:1002:G:H8	1.66	0.61
1:A:1232:U:H5"	9:I:126:GLN:HB3	1.82	0.61
13:M:34:LEU:HD13	13:M:41:GLU:HA	1.83	0.61
1:A:55:A:N6	1:A:357:G:H21	1.91	0.60
1:A:1391:U:H2'	1:A:1392:G:C8	2.35	0.60
2:B:23:TRP:CZ3	2:B:25:PRO:HA	2.37	0.60
4:D:95:GLU:OE1	4:D:100:ASN:ND2	2.34	0.60
1:A:1513:A:H2'	1:A:1514:G:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:C:H2'	1:A:35:G:C8	2.37	0.60
1:A:502:A:H4'	12:L:116:LYS:HE3	1.84	0.60
13:M:85:CYS:SG	13:M:88:GLY:N	2.69	0.60
1:A:945:G:C2	1:A:946:A:C8	2.90	0.60
10:J:46:LYS:HD3	10:J:68:ARG:HG2	1.82	0.60
14:N:9:ARG:HB3	14:N:13:ARG:NH2	2.16	0.60
1:A:1312:G:H5'	19:S:5:LEU:HG	1.83	0.60
1:A:422:C:O2	1:A:423:G:N1	2.34	0.59
1:A:481:G:H21	1:A:482:A:N6	2.00	0.59
9:I:21:ILE:HG12	9:I:63:LEU:HD22	1.83	0.59
1:A:692:U:O2'	1:A:694:A:N7	2.28	0.59
1:A:1169:A:H2'	1:A:1170:A:C8	2.37	0.59
2:B:12:ALA:HB1	2:B:208:ARG:HB3	1.83	0.59
3:C:52:VAL:HG22	3:C:70:THR:HB	1.85	0.59
1:A:227:G:H2'	1:A:228:A:O4'	2.03	0.59
9:I:47:VAL:HG13	9:I:80:ARG:HD3	1.84	0.59
1:A:131:A:H2'	1:A:132:C:C6	2.36	0.59
1:A:579:A:H2'	1:A:580:C:C6	2.36	0.59
1:A:946:A:O2'	1:A:1333:A:N3	2.29	0.59
1:A:270:A:H2'	1:A:271:C:C6	2.38	0.59
1:A:236:A:H2'	1:A:237:G:C8	2.38	0.59
1:A:80:A:H2'	1:A:81:A:H8	1.67	0.59
1:A:333:U:OP1	20:T:2:ALA:N	2.36	0.59
1:A:536:C:C2	1:A:537:G:N7	2.71	0.59
1:A:1241:G:H2'	1:A:1242:G:C8	2.38	0.59
1:A:618:C:N4	1:A:621:A:N7	2.51	0.59
13:M:40:ALA:HB3	13:M:43:VAL:HG23	1.84	0.59
9:I:7:TYR:HE1	9:I:18:ARG:HB3	1.68	0.58
4:D:28:ILE:HG23	4:D:34:ILE:HG21	1.83	0.58
6:F:90:MET:SD	18:R:61:ARG:NE	2.73	0.58
1:A:622:A:C8	1:A:623:C:C5	2.91	0.58
1:A:1127:G:H1	1:A:1145:A:N6	2.01	0.58
11:K:14:LYS:HE3	11:K:77:TYR:HE2	1.68	0.58
11:K:110:ILE:HG23	21:U:4:ILE:HB	1.85	0.58
12:L:34:CYS:HA	12:L:55:VAL:HG22	1.84	0.58
1:A:621:A:H2'	1:A:622:A:C8	2.37	0.58
1:A:635:A:O2'	17:Q:6:ARG:NH1	2.37	0.58
1:A:1220:G:OP1	14:N:53:ARG:NH1	2.36	0.58
1:A:835:U:H3	1:A:851:G:H1	1.52	0.58
12:L:114:ARG:O	12:L:118:GLY:N	2.37	0.58
1:A:524:G:H2'	1:A:525:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:C:O2'	1:A:621:A:H5'	2.03	0.58
1:A:1412:C:H2'	1:A:1413:A:C8	2.38	0.58
2:B:104:TRP:CZ2	2:B:108:ARG:HG3	2.38	0.58
8:H:47:GLU:OE1	8:H:48:ASP:HB2	2.04	0.58
1:A:157:U:H1'	1:A:165:G:N2	2.18	0.58
1:A:537:G:OP1	12:L:110:ARG:NH2	2.37	0.58
1:A:1009:U:O2	1:A:1020:G:N2	2.26	0.58
1:A:493:A:H2'	1:A:494:G:C5	2.39	0.57
1:A:1141:C:H2'	1:A:1142:G:C8	2.39	0.57
1:A:538:G:H2'	1:A:539:A:C8	2.39	0.57
1:A:674:G:H2'	1:A:675:A:H8	1.69	0.57
5:E:157:ARG:NH1	8:H:99:LEU:O	2.37	0.57
18:R:23:TYR:HA	18:R:29:LEU:HD11	1.85	0.57
1:A:375:U:H5"	16:P:70:ARG:HG2	1.87	0.57
1:A:548:G:H2'	1:A:549:C:C6	2.39	0.57
1:A:1173:U:H2'	1:A:1174:G:C8	2.38	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.40	0.57
1:A:979:C:O2	14:N:59:ARG:NH1	2.36	0.57
1:A:1254:A:H2'	1:A:1255:G:C8	2.39	0.57
9:I:40:GLY:HA2	9:I:45:ARG:HH21	1.69	0.57
1:A:1223:C:OP2	19:S:78:ARG:NH2	2.35	0.57
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.86	0.57
1:A:977:A:O2'	1:A:1223:C:N4	2.38	0.57
1:A:1122:U:H2'	1:A:1123:U:C6	2.39	0.57
12:L:30:LYS:O	12:L:81:LEU:HD12	2.04	0.57
1:A:831:A:H5'	2:B:21:ARG:HE	1.70	0.57
1:A:1116:U:H2'	1:A:1117:A:C8	2.40	0.57
2:B:26:LYS:NZ	2:B:192:ASP:OD1	2.38	0.57
1:A:400:C:H2'	1:A:401:C:O4'	2.05	0.57
1:A:501:C:P	12:L:114:ARG:HH22	2.28	0.57
1:A:955:U:O2'	19:S:83:HIS:ND1	2.37	0.57
1:A:1008:U:H3'	1:A:1009:U:H5"	1.86	0.57
10:J:24:GLU:HB2	10:J:90:LEU:HD21	1.85	0.57
1:A:191:G:H2'	1:A:192:A:H8	1.70	0.56
1:A:303:A:OP1	12:L:14:ARG:NH1	2.39	0.56
1:A:714:G:H2'	1:A:715:A:C8	2.40	0.56
4:D:48:LEU:HD22	4:D:49:SER:H	1.69	0.56
1:A:182:A:N1	1:A:223:A:O2'	2.39	0.56
1:A:407:U:N3	1:A:408:A:N7	2.53	0.56
1:A:508:U:H1'	1:A:509:A:N7	2.19	0.56
1:A:539:A:H2'	1:A:540:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:U:H2'	1:A:591:U:C6	2.40	0.56
1:A:986:U:H1'	19:S:55:ARG:HA	1.87	0.56
3:C:43:LEU:HD11	3:C:66:VAL:HG11	1.87	0.56
4:D:177:LYS:HG3	4:D:179:GLU:HG2	1.87	0.56
7:G:27:VAL:O	7:G:31:MET:N	2.39	0.56
15:O:18:ASP:OD1	15:O:21:ASP:HB2	2.05	0.56
17:Q:62:ARG:HD3	17:Q:76:VAL:HG22	1.87	0.56
1:A:1015:G:H2'	1:A:1016:A:C8	2.41	0.56
4:D:58:LYS:HE3	4:D:203:LEU:HD23	1.86	0.56
6:F:38:ARG:HD3	6:F:40:GLU:OE1	2.06	0.56
1:A:41:G:H2'	1:A:42:G:H8	1.71	0.56
1:A:73:C:O2'	1:A:74:A:O5'	2.24	0.56
1:A:427:U:OP1	4:D:13:ARG:NH1	2.34	0.56
1:A:662:U:H2'	1:A:663:A:C8	2.41	0.56
1:A:1003:G:N2	1:A:1004:A:O2'	2.38	0.56
1:A:979:C:OP1	1:A:1223:C:N4	2.39	0.56
1:A:1464:U:H2'	1:A:1465:A:H8	1.71	0.56
7:G:50:LEU:O	7:G:54:SER:HB3	2.05	0.56
1:A:202:G:O2'	1:A:468:A:N3	2.31	0.56
1:A:404:G:H4'	1:A:439:U:O2	2.06	0.56
1:A:414:A:H62	1:A:430:A:H2	1.50	0.56
1:A:555:U:H2'	1:A:556:C:C6	2.41	0.56
1:A:636:U:H2'	1:A:637:C:C6	2.41	0.56
1:A:723:U:H2'	1:A:855:U:H4'	1.87	0.56
1:A:1239:A:O2'	7:G:114:LYS:O	2.20	0.56
2:B:15:HIS:O	2:B:40:ILE:HD12	2.05	0.56
1:A:552:U:H2'	1:A:553:A:H8	1.71	0.56
1:A:613:C:C2	1:A:628:G:N2	2.74	0.56
1:A:1157:A:N7	1:A:1180:A:N6	2.54	0.56
5:E:38:VAL:HG11	5:E:114:VAL:HG22	1.87	0.56
9:I:85:ARG:NH2	9:I:89:GLU:HG3	2.21	0.56
12:L:102:LEU:HD22	12:L:102:LEU:H	1.71	0.56
17:Q:25:ILE:HB	17:Q:42:THR:HG22	1.87	0.56
1:A:200:G:H2'	1:A:201:G:C8	2.41	0.56
1:A:482:A:H8	1:A:482:A:OP1	1.89	0.56
11:K:84:VAL:HB	11:K:110:ILE:HA	1.88	0.56
12:L:110:ARG:HH21	12:L:113:ALA:HB3	1.71	0.56
16:P:19:VAL:HG13	16:P:36:VAL:HG23	1.88	0.56
1:A:50:A:N6	1:A:361:G:H4'	2.21	0.55
1:A:1254:A:H2'	1:A:1255:G:H8	1.71	0.55
4:D:116:GLN:OE1	4:D:154:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:58:GLU:N	7:G:58:GLU:OE1	2.39	0.55
8:H:79:SER:HB2	8:H:85:ILE:HB	1.87	0.55
1:A:490:C:OP1	4:D:146:ARG:NH1	2.34	0.55
4:D:118:VAL:HG22	4:D:123:ILE:HG13	1.88	0.55
1:A:255:G:H2'	1:A:256:U:C6	2.41	0.55
1:A:746:A:H2'	1:A:747:A:C8	2.42	0.55
7:G:29:ILE:HD13	7:G:101:MET:HB2	1.89	0.55
16:P:5:ARG:HA	16:P:71:VAL:HG21	1.87	0.55
1:A:616:G:O2'	16:P:47:GLU:HG3	2.07	0.55
1:A:618:C:H5'	1:A:619:U:H5"	1.87	0.55
1:A:1122:U:H2'	1:A:1123:U:H6	1.72	0.55
1:A:1327:C:H2'	1:A:1328:C:H6	1.70	0.55
10:J:6:ILE:HD11	10:J:84:VAL:HG22	1.88	0.55
11:K:111:THR:HG23	21:U:3:VAL:HG12	1.89	0.55
14:N:2:ALA:N	14:N:67:THR:O	2.40	0.55
14:N:73:PHE:CZ	14:N:78:GLY:HA2	2.41	0.55
1:A:160:A:H2'	1:A:161:A:O4'	2.06	0.55
1:A:723:U:C4	21:U:53:VAL:HG22	2.41	0.55
1:A:1318:A:H5"	19:S:3:ARG:NH1	2.22	0.55
6:F:38:ARG:NH2	6:F:96:VAL:O	2.40	0.55
1:A:436:C:H2'	1:A:437:U:O4'	2.07	0.55
6:F:42:TRP:HB2	6:F:59:TYR:O	2.07	0.55
12:L:48:ALA:O	12:L:49:LEU:HD23	2.06	0.55
1:A:538:G:H2'	1:A:539:A:H8	1.72	0.55
1:A:673:A:H2'	1:A:674:G:H8	1.66	0.55
2:B:20:THR:O	2:B:23:TRP:HD1	1.90	0.55
1:A:276:G:H5'	17:Q:17:MET:HE3	1.88	0.55
1:A:918:A:H2'	1:A:919:A:C8	2.42	0.55
1:A:1157:A:N6	1:A:1178:G:H1'	2.19	0.55
4:D:124:MET:N	4:D:144:SER:O	2.33	0.55
10:J:18:ILE:HD11	10:J:72:ARG:HG2	1.89	0.55
12:L:110:ARG:NH2	12:L:113:ALA:HB3	2.22	0.55
13:M:51:GLY:O	13:M:55:THR:HG23	2.07	0.55
20:T:35:VAL:HG21	20:T:54:MET:HE3	1.89	0.55
1:A:1141:C:H2'	1:A:1142:G:H8	1.71	0.55
1:A:1304:G:O6	1:A:1331:G:O2'	2.25	0.55
1:A:492:C:H2'	1:A:493:A:C8	2.42	0.54
1:A:1002:G:C2	1:A:1003:G:H1'	2.42	0.54
2:B:51:ASN:HA	2:B:54:LEU:HD12	1.89	0.54
3:C:70:THR:HG21	3:C:76:VAL:HG21	1.89	0.54
7:G:57:SER:HB3	7:G:60:GLU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:13:ARG:HD2	14:N:59:ARG:HB3	1.89	0.54
1:A:280:C:N3	17:Q:41:THR:HG23	2.22	0.54
1:A:1269:A:H2'	1:A:1270:G:O4'	2.08	0.54
1:A:1325:C:H2'	1:A:1326:U:C6	2.39	0.54
9:I:118:LEU:HD23	9:I:124:ARG:HA	1.89	0.54
10:J:49:PHE:HZ	14:N:76:LYS:HD3	1.71	0.54
16:P:40:ASN:HB3	16:P:43:ALA:HB2	1.90	0.54
1:A:546:A:H4'	1:A:549:C:H5'	1.89	0.54
1:A:546:A:H5"	4:D:70:ARG:NH2	2.22	0.54
1:A:948:C:H2'	1:A:949:A:H8	1.72	0.54
12:L:99:ARG:HB3	12:L:117:TYR:O	2.07	0.54
1:A:999:C:H2'	1:A:1000:A:C8	2.42	0.54
1:A:1351:U:H2'	1:A:1352:C:C6	2.43	0.54
2:B:20:THR:HA	2:B:39:HIS:CD2	2.43	0.54
11:K:79:ILE:HB	11:K:105:PHE:HE1	1.72	0.54
1:A:685:G:H2'	1:A:686:U:C6	2.42	0.54
2:B:12:ALA:HA	2:B:208:ARG:NH2	2.23	0.54
1:A:323:U:H2'	1:A:324:G:O4'	2.08	0.54
1:A:457:G:H3'	1:A:458:U:H5"	1.88	0.54
1:A:512:U:H2'	1:A:513:C:C6	2.42	0.54
1:A:1098:C:O2'	21:U:71:TYR:O	2.26	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.22	0.54
1:A:410:G:H2'	1:A:429:U:C5	2.43	0.54
3:C:28:GLU:O	3:C:28:GLU:HG3	2.07	0.54
5:E:151:GLU:H	5:E:151:GLU:CD	2.10	0.54
1:A:549:C:H2'	1:A:550:G:O4'	2.07	0.54
1:A:1043:G:O2'	1:A:1044:A:O5'	2.26	0.54
1:A:1225:A:H2'	1:A:1226:C:C6	2.43	0.54
1:A:1342:C:H2'	1:A:1343:G:C8	2.42	0.54
4:D:23:SER:HB3	4:D:161:LEU:HD13	1.88	0.54
1:A:405:U:H4'	1:A:498:A:C6	2.42	0.54
1:A:428:G:OP1	1:A:430:A:H1'	2.07	0.54
1:A:542:G:H2'	1:A:543:U:C6	2.42	0.54
1:A:834:U:H2'	1:A:835:U:C6	2.43	0.54
10:J:20:GLN:O	10:J:24:GLU:HG2	2.07	0.54
1:A:401:C:O2'	1:A:621:A:N3	2.32	0.53
1:A:493:A:H2'	1:A:494:G:C4	2.42	0.53
9:I:45:ARG:HB3	9:I:49:ARG:NH2	2.22	0.53
18:R:22:ASP:OD1	18:R:24:LYS:HE2	2.07	0.53
21:U:31:GLU:OE2	21:U:34:ARG:NH2	2.41	0.53
9:I:124:ARG:HB3	9:I:124:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:VAL:N	12:L:103:ASP:OD2	2.22	0.53
15:O:68:ASP:O	15:O:72:ARG:HG2	2.09	0.53
1:A:536:C:H2'	1:A:537:G:C8	2.41	0.53
1:A:1264:U:H2'	1:A:1265:C:C6	2.43	0.53
3:C:35:SER:OG	3:C:59:ARG:NH2	2.42	0.53
4:D:54:GLN:HG2	4:D:199:LEU:O	2.08	0.53
1:A:425:G:H2'	1:A:426:U:C6	2.44	0.53
2:B:96:TRP:NE1	2:B:175:GLU:OE2	2.33	0.53
8:H:113:ASP:OD1	8:H:114:ARG:N	2.41	0.53
1:A:922:G:H4'	5:E:25:VAL:HA	1.91	0.53
1:A:1166:G:N1	1:A:1169:A:OP2	2.42	0.53
14:N:90:ARG:NE	14:N:92:GLU:OE1	2.41	0.53
20:T:44:LYS:HE3	20:T:87:ALA:HB2	1.89	0.53
15:O:75:VAL:O	15:O:79:THR:HG23	2.09	0.53
1:A:75:G:H2'	1:A:76:G:H8	1.73	0.53
1:A:544:G:H2'	1:A:545:C:C6	2.44	0.53
1:A:1014:A:N3	1:A:1219:A:H1'	2.24	0.53
1:A:80:A:H2'	1:A:81:A:C8	2.44	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.91	0.53
1:A:191:G:H2'	1:A:192:A:C8	2.43	0.53
1:A:1317:C:O2	19:S:37:ARG:NH2	2.40	0.53
3:C:87:LEU:O	3:C:91:VAL:HG12	2.10	0.53
11:K:17:SER:HA	11:K:79:ILE:HA	1.91	0.53
15:O:71:LYS:HD2	15:O:78:TYR:CE2	2.43	0.53
20:T:24:ARG:HD2	20:T:61:GLN:NE2	2.20	0.53
1:A:417:G:N2	1:A:541:G:H5'	2.24	0.52
2:B:43:LEU:HA	2:B:46:THR:HB	1.90	0.52
6:F:19:PRO:O	6:F:23:GLU:HG2	2.08	0.52
1:A:437:U:H1'	4:D:154:ARG:HH12	1.75	0.52
1:A:1049:U:OP1	14:N:3:LYS:HG2	2.09	0.52
1:A:1221:G:H5'	19:S:36:ARG:HD3	1.92	0.52
5:E:61:GLN:O	5:E:65:GLU:HG3	2.10	0.52
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.91	0.52
17:Q:14:SER:HB3	17:Q:22:VAL:HB	1.90	0.52
1:A:511:C:H2'	1:A:534:U:H1'	1.90	0.52
4:D:174:ASP:O	4:D:178:MET:HA	2.10	0.52
1:A:1149:C:H2'	1:A:1150:A:C8	2.45	0.52
1:A:1386:G:H2'	1:A:1387:G:H8	1.74	0.52
1:A:1178:G:N2	1:A:1181:G:OP2	2.42	0.52
16:P:12:LYS:HG2	16:P:13:LYS:HG2	1.92	0.52
17:Q:59:VAL:HB	17:Q:75:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:78:ASN:O	20:T:82:GLN:HG3	2.09	0.52
1:A:1346:A:OP1	9:I:122:ARG:NH1	2.43	0.52
2:B:56:GLU:O	2:B:60:ILE:HG13	2.09	0.52
4:D:172:GLU:HG3	4:D:183:LYS:HD2	1.90	0.52
11:K:16:VAL:HG23	11:K:79:ILE:HG12	1.91	0.52
13:M:86:TYR:HA	13:M:89:LEU:HD12	1.92	0.52
1:A:357:G:OP1	1:A:367:U:H6	1.92	0.52
1:A:838:G:C5	1:A:849:G:C6	2.97	0.52
1:A:1013:G:N2	1:A:1016:A:OP2	2.43	0.52
1:A:161:A:H2'	1:A:162:A:C8	2.45	0.52
17:Q:79:VAL:HG12	17:Q:80:GLU:HG3	1.92	0.52
1:A:200:G:H2'	1:A:201:G:H8	1.74	0.52
1:A:983:A:OP1	14:N:9:ARG:NH1	2.43	0.52
6:F:72:ASP:O	6:F:76:THR:HG23	2.10	0.52
1:A:830:G:H2'	1:A:831:A:C8	2.45	0.52
2:B:133:GLU:O	2:B:137:ARG:HG3	2.09	0.52
4:D:125:VAL:O	4:D:128:ARG:HD2	2.09	0.52
1:A:728:A:H2'	1:A:729:A:C8	2.45	0.51
1:A:1375:A:H2'	1:A:1376:U:O4'	2.10	0.51
1:A:1464:U:H2'	1:A:1465:A:C8	2.45	0.51
2:B:104:TRP:CH2	2:B:108:ARG:HG3	2.45	0.51
19:S:32:ARG:HG2	19:S:34:TRP:CH2	2.45	0.51
1:A:41:G:H2'	1:A:42:G:C8	2.45	0.51
1:A:1163:A:H2'	1:A:1164:G:C8	2.45	0.51
1:A:1342:C:H5"	9:I:127:PHE:HD2	1.75	0.51
11:K:24:HIS:HB3	11:K:31:ILE:HB	1.93	0.51
1:A:512:U:H2'	1:A:513:C:H6	1.74	0.51
1:A:952:U:H2'	1:A:953:G:H8	1.74	0.51
1:A:1306:A:H2'	1:A:1307:U:O4'	2.10	0.51
1:A:505:G:H2'	1:A:506:G:C8	2.45	0.51
1:A:1276:G:H2'	1:A:1277:C:C6	2.45	0.51
7:G:57:SER:OG	7:G:58:GLU:N	2.42	0.51
1:A:707:U:H2'	1:A:708:C:C6	2.44	0.51
1:A:744:C:H2'	1:A:745:G:C8	2.44	0.51
1:A:1125:U:O2'	1:A:1126:U:O5'	2.28	0.51
1:A:1163:A:H2'	1:A:1164:G:H8	1.75	0.51
1:A:1255:G:OP2	10:J:45:ARG:NH2	2.43	0.51
3:C:5:VAL:HG11	3:C:10:ILE:HD12	1.92	0.51
4:D:118:VAL:HG11	4:D:133:ALA:HA	1.93	0.51
1:A:103:U:H1'	1:A:171:A:N1	2.26	0.51
1:A:835:U:OP1	18:R:50:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:A:N3	1:A:1326:U:H1'	2.25	0.51
5:E:108:GLY:O	5:E:112:ARG:N	2.40	0.51
8:H:18:GLN:HG2	8:H:63:LEU:HD13	1.93	0.51
9:I:88:MET:CG	9:I:95:ARG:HB2	2.40	0.51
7:G:31:MET:HE1	7:G:36:LYS:HB2	1.91	0.51
1:A:1002:G:N3	1:A:1003:G:H1'	2.26	0.51
1:A:1323:G:C6	1:A:1324:A:C6	2.99	0.51
7:G:80:VAL:HG21	7:G:85:TYR:CD2	2.45	0.51
1:A:86:G:H1'	1:A:87:C:O4'	2.11	0.51
1:A:1031:C:O3'	1:A:1032:G:N2	2.44	0.51
1:A:1350:A:P	9:I:123:ARG:HG3	2.51	0.51
2:B:119:THR:O	2:B:123:ASP:HB2	2.10	0.51
6:F:7:VAL:HG11	18:R:65:LEU:HD13	1.93	0.51
1:A:1124:G:OP1	10:J:37:ARG:NH1	2.44	0.51
7:G:70:ARG:NH1	7:G:97:ASN:OD1	2.35	0.51
1:A:36:C:H2'	1:A:37:U:O4'	2.11	0.50
20:T:51:PHE:HA	20:T:54:MET:HG2	1.93	0.50
1:A:34:C:H2'	1:A:35:G:H8	1.74	0.50
1:A:35:G:H2'	1:A:36:C:H6	1.75	0.50
1:A:389:A:H3'	1:A:390:U:H6	1.76	0.50
1:A:1223:C:P	19:S:78:ARG:HH21	2.34	0.50
14:N:82:ILE:O	14:N:86:GLU:HG3	2.11	0.50
16:P:6:LEU:HD23	16:P:19:VAL:HG23	1.92	0.50
1:A:516:PSU:C2	1:A:517:G:C6	3.00	0.50
1:A:517:G:N2	1:A:530:G:OP1	2.45	0.50
7:G:14:PRO:HA	7:G:21:GLU:HA	1.93	0.50
13:M:5:ALA:O	13:M:66:GLU:HG3	2.12	0.50
20:T:24:ARG:NH1	20:T:61:GLN:OE1	2.44	0.50
1:A:197:A:N1	1:A:220:G:O2'	2.34	0.50
1:A:1187:G:H5'	9:I:115:LYS:HE3	1.93	0.50
1:A:1320:C:H2'	1:A:1321:U:C6	2.47	0.50
1:A:1323:G:H2'	1:A:1324:A:C8	2.46	0.50
3:C:23:PHE:HD1	3:C:24:ALA:N	2.10	0.50
7:G:86:GLN:HB2	7:G:148:ASN:OD1	2.12	0.50
19:S:36:ARG:NH1	19:S:52:HIS:O	2.43	0.50
20:T:24:ARG:HH12	20:T:66:LEU:HB2	1.77	0.50
1:A:547:A:OP1	4:D:70:ARG:NH1	2.44	0.50
1:A:999:C:H2'	1:A:1000:A:H8	1.75	0.50
1:A:1510:C:H2'	1:A:1511:G:C8	2.47	0.50
11:K:85:MET:HE3	11:K:113:VAL:HG11	1.93	0.50
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:ASP:OD1	20:T:45:ALA:N	2.44	0.50
1:A:190:A:H2'	1:A:191:G:O4'	2.12	0.50
1:A:413:G:H1'	1:A:428:G:H21	1.77	0.50
1:A:510:A:N3	1:A:543:U:O2'	2.37	0.50
1:A:580:C:H2'	1:A:581:G:O4'	2.12	0.50
1:A:1063:C:OP2	1:A:1064:G:O2'	2.27	0.50
1:A:1162:C:H2'	1:A:1163:A:C8	2.47	0.50
1:A:1280:A:O2'	1:A:1281:C:H5'	2.12	0.50
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.93	0.50
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.94	0.50
1:A:148:G:N3	1:A:1446:A:H2	2.10	0.50
1:A:979:C:O2	1:A:979:C:H2'	2.12	0.50
1:A:1032:G:H3'	1:A:1033:G:H4'	1.94	0.50
1:A:1236:A:H2'	1:A:1237:C:C6	2.47	0.50
1:A:1455:G:H2'	1:A:1456:A:O4'	2.12	0.50
2:B:33:GLY:H	2:B:40:ILE:HG22	1.76	0.50
1:A:1298:U:H4'	1:A:1299:A:O4'	2.12	0.49
1:A:154:U:H2'	1:A:155:A:C8	2.47	0.49
1:A:992:U:O4	1:A:1043:G:O2'	2.23	0.49
2:B:12:ALA:HA	2:B:208:ARG:HH21	1.77	0.49
2:B:76:ALA:O	2:B:80:VAL:HG12	2.12	0.49
1:A:544:G:OP1	4:D:59:GLN:NE2	2.45	0.49
1:A:1329:A:H5"	13:M:26:GLY:N	2.27	0.49
1:A:1343:G:H4'	9:I:124:ARG:HB2	1.94	0.49
2:B:115:LYS:O	2:B:119:THR:HG23	2.13	0.49
12:L:66:TYR:HB2	12:L:93:VAL:CG1	2.42	0.49
1:A:619:U:O2	4:D:132:ILE:HG12	2.13	0.49
1:A:1060:U:H2'	1:A:1061:G:H8	1.78	0.49
1:A:1302:C:H5'	13:M:17:ILE:HG21	1.93	0.49
1:A:1380:U:O2'	7:G:3:ARG:NH1	2.44	0.49
16:P:74:LEU:HA	16:P:77:GLU:HG2	1.95	0.49
1:A:618:C:C2	1:A:622:A:N6	2.81	0.49
1:A:999:C:N3	1:A:1042:A:N6	2.61	0.49
1:A:1376:U:H2'	1:A:1377:A:H8	1.77	0.49
13:M:93:ARG:HH22	19:S:80:TYR:HD2	1.60	0.49
4:D:65:TYR:CE2	4:D:94:LEU:HB3	2.48	0.49
9:I:10:GLY:HA3	9:I:81:HIS:HB3	1.95	0.49
1:A:1287:A:H2'	1:A:1288:A:C8	2.48	0.49
6:F:42:TRP:CE2	6:F:102:MET:HG3	2.47	0.49
17:Q:62:ARG:N	17:Q:74:THR:O	2.28	0.49
19:S:40:ILE:HG23	19:S:44:MET:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:U:H2'	1:A:97:G:H8	1.78	0.49
19:S:17:LYS:O	19:S:21:LYS:HG3	2.13	0.49
1:A:958:A:C2	19:S:55:ARG:HB3	2.48	0.49
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.46	0.49
11:K:53:ARG:NH1	11:K:57:LYS:HE3	2.28	0.49
1:A:512:U:H5	1:A:534:U:H4'	1.78	0.49
1:A:746:A:H5'	1:A:836:G:H21	1.78	0.49
1:A:375:U:OP1	16:P:70:ARG:HB2	2.13	0.48
1:A:411:A:H4'	1:A:412:A:OP1	2.13	0.48
1:A:1328:C:OP1	13:M:28:THR:OG1	2.20	0.48
18:R:12:ARG:NH1	18:R:16:GLU:OE2	2.46	0.48
19:S:52:HIS:HB2	19:S:57:HIS:CE1	2.48	0.48
1:A:830:G:H2'	1:A:831:A:H8	1.76	0.48
1:A:1271:A:H2'	1:A:1272:G:H8	1.77	0.48
11:K:16:VAL:HG22	11:K:77:TYR:HB3	1.94	0.48
11:K:93:ARG:CZ	21:U:29:LEU:HD21	2.43	0.48
1:A:1147:C:H2'	1:A:1148:U:H6	1.78	0.48
2:B:111:ILE:HD12	2:B:152:LYS:HA	1.95	0.48
3:C:42:TYR:CZ	3:C:90:VAL:HG11	2.48	0.48
20:T:82:GLN:O	20:T:86:LEU:N	2.46	0.48
1:A:922:G:H2'	1:A:923:A:C8	2.48	0.48
1:A:1057:G:O2'	3:C:188:GLU:OE1	2.27	0.48
1:A:1314:C:H2'	1:A:1315:U:H6	1.78	0.48
2:B:97:LEU:HD12	2:B:97:LEU:H	1.79	0.48
4:D:190:ASP:OD1	4:D:190:ASP:N	2.46	0.48
1:A:126:G:OP1	1:A:605:U:O2'	2.20	0.48
1:A:154:U:H2'	1:A:155:A:H8	1.78	0.48
1:A:544:G:H5"	4:D:59:GLN:NE2	2.28	0.48
1:A:859:G:H2'	1:A:860:A:C8	2.48	0.48
1:A:1005:A:H3'	1:A:1006:G:H8	1.79	0.48
2:B:162:PHE:HA	2:B:184:PHE:O	2.13	0.48
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.46	0.48
4:D:54:GLN:HB3	4:D:203:LEU:HD13	1.95	0.48
11:K:46:THR:HG22	11:K:48:GLY:N	2.26	0.48
1:A:338:A:H2'	1:A:339:C:O4'	2.13	0.48
1:A:1147:C:H4'	9:I:7:TYR:CE2	2.47	0.48
1:A:1309:G:C6	1:A:1329:A:C6	3.02	0.48
1:A:1349:A:H5"	9:I:123:ARG:HB2	1.96	0.48
2:B:164:ILE:HG23	2:B:204:ASP:HB2	1.95	0.48
9:I:24:GLY:HA3	9:I:62:ASP:CG	2.34	0.48
11:K:75:LYS:HD2	11:K:75:LYS:HA	1.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:112:ASP:HB2	21:U:19:PHE:CZ	2.48	0.48
20:T:46:ALA:HA	20:T:49:LYS:HG2	1.95	0.48
1:A:324:G:N1	1:A:327:A:OP2	2.47	0.48
1:A:624:C:H2'	1:A:625:U:C6	2.48	0.48
1:A:1071:C:H2'	1:A:1072:G:H8	1.76	0.48
1:A:1340:A:H2'	1:A:1341:U:O4'	2.14	0.48
4:D:100:ASN:OD1	4:D:111:ARG:NH2	2.38	0.48
4:D:150:LYS:HE2	4:D:178:MET:CE	2.44	0.48
11:K:113:VAL:HG12	18:R:73:ARG:HD3	1.95	0.48
1:A:1321:U:OP2	1:A:1322:C:O2'	2.23	0.48
3:C:19:ASN:O	3:C:40:ARG:NH2	2.47	0.48
6:F:11:HIS:ND1	6:F:12:PRO:HD2	2.28	0.48
9:I:27:LYS:HB2	9:I:27:LYS:HE2	1.72	0.48
9:I:39:PHE:HB3	9:I:44:ALA:HB3	1.96	0.48
1:A:407:U:C2	1:A:408:A:N7	2.82	0.48
1:A:515:G:H2'	1:A:516:PSU:C6	2.47	0.48
1:A:613:C:OP1	4:D:81:ARG:HD2	2.14	0.48
7:G:147:ALA:C	7:G:148:ASN:HD22	2.17	0.48
9:I:35:LEU:HD13	9:I:49:ARG:NH1	2.28	0.48
1:A:652:U:O4	1:A:752:G:O2'	2.25	0.48
1:A:1027:C:H2'	1:A:1028:C:C6	2.48	0.48
1:A:1176:A:H3'	1:A:1177:G:C8	2.49	0.48
1:A:1518:MA6:H103	1:A:1519:MA6:H102	1.96	0.48
3:C:150:LYS:HD2	3:C:201:TRP:CE3	2.49	0.48
1:A:148:G:O2'	1:A:1446:A:N3	2.35	0.47
1:A:148:G:H2'	1:A:149:A:O4'	2.14	0.47
1:A:562:U:H1'	12:L:12:ARG:HB3	1.96	0.47
1:A:923:A:H2'	1:A:924:C:C6	2.49	0.47
1:A:1152:A:P	10:J:72:ARG:HH22	2.37	0.47
4:D:105:MET:HB2	4:D:173:VAL:HG22	1.95	0.47
7:G:26:PHE:HD1	7:G:101:MET:HB3	1.78	0.47
8:H:35:ALA:HB1	8:H:110:VAL:HB	1.96	0.47
12:L:99:ARG:HH11	12:L:107:VAL:HG22	1.79	0.47
19:S:32:ARG:HA	19:S:50:ALA:HB3	1.97	0.47
1:A:517:G:H21	1:A:530:G:P	2.37	0.47
1:A:666:G:H5'	1:A:726:C:H1'	1.94	0.47
1:A:1225:A:H2'	1:A:1226:C:C5	2.49	0.47
2:B:130:THR:O	2:B:132:LYS:N	2.47	0.47
1:A:33:A:H2'	1:A:34:C:C6	2.49	0.47
1:A:225:C:H2'	1:A:226:G:O4'	2.13	0.47
1:A:978:A:C8	1:A:979:C:H5	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:ARG:HG2	10:J:101:SER:O	2.14	0.47
11:K:67:ALA:HB2	11:K:96:THR:HG23	1.95	0.47
11:K:87:LYS:CG	11:K:113:VAL:HG23	2.44	0.47
1:A:156:C:H2'	1:A:157:U:O4'	2.14	0.47
1:A:232:G:H1'	1:A:262:A:N1	2.29	0.47
1:A:399:G:H2'	1:A:400:C:C6	2.49	0.47
1:A:1125:U:C2	1:A:1127:G:C8	3.02	0.47
1:A:1317:C:H4'	14:N:48:LEU:HD21	1.97	0.47
7:G:36:LYS:O	7:G:40:GLU:HB2	2.14	0.47
1:A:405:U:O4	4:D:2:ALA:N	2.48	0.47
1:A:713:G:H2'	1:A:714:G:C8	2.50	0.47
1:A:1260:G:H4'	1:A:1283:U:O2'	2.13	0.47
1:A:1404:C:H2'	1:A:1405:G:C8	2.50	0.47
7:G:74:GLU:HG2	7:G:75:VAL:H	1.79	0.47
7:G:129:GLU:O	7:G:129:GLU:HG2	2.13	0.47
14:N:54:ASP:OD1	14:N:59:ARG:NH2	2.47	0.47
1:A:257:G:H2'	1:A:258:G:H8	1.80	0.47
1:A:707:U:H2'	1:A:708:C:H6	1.80	0.47
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.47
1:A:1329:A:H5"	13:M:26:GLY:H	1.80	0.47
3:C:64:ILE:HG22	3:C:97:VAL:HG23	1.97	0.47
18:R:13:PHE:O	18:R:18:VAL:HB	2.14	0.47
1:A:406:G:C8	1:A:495:A:C2	3.03	0.47
1:A:613:C:C2	1:A:628:G:C2	3.02	0.47
1:A:939:G:OP1	7:G:95:ARG:NH2	2.37	0.47
1:A:997:U:H2'	1:A:998:C:O4'	2.15	0.47
1:A:1081:A:N7	5:E:52:LYS:HE2	2.29	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.49	0.47
1:A:1155:A:H2'	1:A:1156:G:O4'	2.15	0.47
4:D:69:GLU:OE2	4:D:204:TYR:OH	2.30	0.47
9:I:10:GLY:HA3	9:I:82:GLY:N	2.30	0.47
10:J:21:ALA:HB1	10:J:92:LEU:HD22	1.96	0.47
12:L:32:GLY:O	12:L:79:VAL:HA	2.14	0.47
18:R:26:ILE:HD11	18:R:67:LEU:HB3	1.97	0.47
1:A:618:C:N4	1:A:621:A:C8	2.83	0.47
1:A:1001:C:H2'	1:A:1002:G:C8	2.47	0.47
2:B:197:ASP:OD1	2:B:197:ASP:N	2.47	0.47
4:D:51:TYR:CE1	4:D:203:LEU:HD11	2.49	0.47
7:G:150:ALA:HA	11:K:61:PHE:HB3	1.97	0.47
9:I:115:LYS:HB2	9:I:118:LEU:HD12	1.96	0.47
10:J:35:GLN:HG2	10:J:77:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:C:H2'	1:A:420:U:O4'	2.15	0.47
1:A:1307:U:H2'	1:A:1308:U:O4'	2.14	0.47
3:C:33:LEU:HD11	14:N:93:ILE:HG23	1.96	0.47
1:A:622:A:H3'	1:A:623:C:H6	1.80	0.47
1:A:736:C:H2'	1:A:737:C:C6	2.49	0.47
1:A:968:A:C8	1:A:1062:U:H4'	2.49	0.47
1:A:1306:A:H62	1:A:1331:G:H21	1.62	0.47
15:O:55:GLY:O	15:O:59:MET:HG3	2.15	0.47
1:A:418:C:H2'	1:A:419:C:C6	2.50	0.46
1:A:1347:G:O2'	1:A:1373:G:O6	2.20	0.46
1:A:1371:G:H5"	9:I:70:GLY:HA2	1.98	0.46
1:A:195:A:H2'	1:A:196:A:C8	2.50	0.46
1:A:454:G:C2	1:A:455:G:C8	3.03	0.46
1:A:653:U:OP1	8:H:56:LYS:NZ	2.21	0.46
1:A:674:G:H2'	1:A:675:A:C8	2.48	0.46
1:A:745:G:H5"	1:A:851:G:O2'	2.16	0.46
6:F:47:LEU:HD21	6:F:57:ALA:HB3	1.96	0.46
6:F:73:GLU:O	6:F:77:THR:HG23	2.14	0.46
7:G:26:PHE:HZ	7:G:120:LEU:HD11	1.80	0.46
10:J:24:GLU:O	10:J:28:THR:HG22	2.15	0.46
1:A:1017:U:H2'	1:A:1018:G:C8	2.50	0.46
1:A:1271:A:H2'	1:A:1272:G:C8	2.50	0.46
1:A:407:U:O4	1:A:408:A:N6	2.49	0.46
1:A:475:C:H2'	1:A:476:U:C6	2.50	0.46
1:A:685:G:O2'	1:A:686:U:O4'	2.29	0.46
7:G:92:ARG:O	7:G:96:ARG:N	2.43	0.46
12:L:99:ARG:NH1	12:L:107:VAL:HG22	2.30	0.46
1:A:246:A:C2	1:A:282:A:C5	3.03	0.46
1:A:276:G:H5'	17:Q:17:MET:CE	2.45	0.46
1:A:944:G:O2'	1:A:1338:G:O6	2.23	0.46
1:A:1332:A:H2'	1:A:1333:A:C8	2.51	0.46
4:D:156:LYS:HD3	4:D:156:LYS:N	2.30	0.46
17:Q:20:SER:HB3	17:Q:71:LYS:CE	2.43	0.46
17:Q:27:ARG:HH11	17:Q:29:VAL:HG11	1.81	0.46
1:A:955:U:HO2'	19:S:83:HIS:CE1	2.33	0.46
2:B:80:VAL:HA	2:B:214:LEU:HD21	1.97	0.46
2:B:176:ALA:O	2:B:180:GLY:N	2.48	0.46
10:J:63:ASP:HB3	10:J:65:TYR:CZ	2.51	0.46
1:A:1119:C:H2'	1:A:1120:C:H6	1.80	0.46
3:C:52:VAL:HG13	3:C:68:ILE:HG23	1.97	0.46
11:K:88:GLY:O	11:K:93:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:55:VAL:O	12:L:62:GLU:HA	2.16	0.46
20:T:54:MET:HG3	20:T:55:GLN:N	2.30	0.46
1:A:379:C:H2'	1:A:380:G:O4'	2.16	0.46
1:A:709:U:H2'	1:A:710:G:H8	1.81	0.46
1:A:942:G:H1	1:A:1341:U:H3	1.64	0.46
1:A:955:U:H2'	1:A:956:U:C6	2.49	0.46
1:A:1264:U:H2'	1:A:1265:C:H6	1.80	0.46
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.98	0.46
9:I:54:LEU:HD13	9:I:103:PHE:HE2	1.81	0.46
21:U:31:GLU:OE2	21:U:35:ARG:NE	2.39	0.46
1:A:1030:U:H5"	1:A:1032:G:O6	2.15	0.46
2:B:128:LYS:H	2:B:128:LYS:HD2	1.81	0.46
2:B:162:PHE:CE1	2:B:217:VAL:HG11	2.51	0.46
13:M:93:ARG:HH12	19:S:80:TYR:HD2	1.64	0.46
1:A:660:C:H2'	1:A:661:G:O4'	2.15	0.46
1:A:1180:A:OP1	9:I:105:THR:OG1	2.33	0.46
1:A:1226:C:H3'	13:M:95:LEU:HD11	1.98	0.46
3:C:49:LYS:HB3	3:C:49:LYS:HE2	1.68	0.46
1:A:140:U:H2'	1:A:141:G:O4'	2.16	0.45
1:A:237:G:H5"	17:Q:27:ARG:NH2	2.31	0.45
1:A:521:G:OP1	12:L:70:GLU:HA	2.15	0.45
1:A:737:C:H5'	6:F:89:VAL:O	2.16	0.45
1:A:1147:C:H2'	1:A:1148:U:C6	2.51	0.45
1:A:236:A:H2'	1:A:237:G:H8	1.79	0.45
1:A:483:C:H2'	1:A:484:G:C8	2.51	0.45
1:A:1162:C:H2'	1:A:1163:A:H8	1.79	0.45
1:A:357:G:H5'	1:A:367:U:H2'	1.98	0.45
1:A:426:U:OP1	4:D:33:LYS:HD3	2.17	0.45
1:A:1314:C:OP2	19:S:4:SER:OG	2.20	0.45
3:C:131:ARG:NH1	3:C:166:GLU:HG2	2.32	0.45
7:G:113:ASP:HB3	7:G:119:ARG:HG3	1.98	0.45
13:M:97:VAL:HG23	13:M:98:ARG:HG3	1.98	0.45
14:N:90:ARG:HE	14:N:92:GLU:CD	2.20	0.45
1:A:1160:G:N2	1:A:1176:A:N1	2.61	0.45
2:B:100:MET:HE1	2:B:148:LEU:HD22	1.97	0.45
3:C:86:LYS:O	3:C:90:VAL:HG23	2.16	0.45
4:D:65:TYR:HB3	4:D:67:VAL:HG23	1.97	0.45
12:L:35:THR:OG1	12:L:54:ARG:O	2.22	0.45
1:A:111:G:O6	1:A:330:C:N4	2.48	0.45
1:A:374:A:H4'	1:A:451:A:OP2	2.16	0.45
1:A:554:A:H2'	1:A:555:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:A:C5	1:A:622:A:N7	2.85	0.45
7:G:18:PHE:CD1	7:G:59:LEU:HG	2.51	0.45
10:J:10:LEU:HA	10:J:97:ASP:O	2.16	0.45
13:M:50:GLU:OE1	13:M:53:ILE:HD11	2.17	0.45
1:A:429:U:O4'	1:A:430:A:H8	1.99	0.45
1:A:505:G:H2'	1:A:506:G:H8	1.82	0.45
1:A:593:U:H2'	1:A:594:U:C6	2.51	0.45
1:A:677:U:O2	1:A:777:A:O2'	2.21	0.45
1:A:945:G:C4	1:A:1337:G:H1'	2.51	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.17	0.45
2:B:68:LEU:HD23	2:B:70:VAL:HG22	1.99	0.45
9:I:19:VAL:HG11	9:I:83:ILE:HA	1.98	0.45
11:K:68:GLU:OE2	11:K:68:GLU:HA	2.15	0.45
20:T:82:GLN:O	20:T:86:LEU:HB2	2.17	0.45
1:A:470:C:H2'	1:A:471:U:O4'	2.17	0.45
1:A:1477:U:H2'	1:A:1478:U:C6	2.51	0.45
2:B:26:LYS:HB2	2:B:26:LYS:HE3	1.65	0.45
2:B:208:ARG:O	2:B:212:LEU:HD13	2.17	0.45
3:C:15:VAL:HG11	3:C:179:ARG:O	2.17	0.45
3:C:23:PHE:HE2	10:J:11:LYS:HB3	1.80	0.45
7:G:16:PRO:HD2	7:G:44:TYR:OH	2.17	0.45
7:G:26:PHE:CE2	7:G:120:LEU:HD21	2.52	0.45
7:G:31:MET:HE2	7:G:34:GLY:HA2	1.99	0.45
1:A:184:G:H2'	1:A:185:U:C6	2.51	0.45
1:A:1229:A:H2'	1:A:1230:C:C6	2.52	0.45
1:A:1250:A:H2'	1:A:1251:A:C8	2.51	0.45
1:A:66:A:H8	1:A:66:A:P	2.40	0.45
1:A:481:G:O2'	1:A:483:C:N4	2.48	0.45
1:A:663:A:H5'	1:A:836:G:OP1	2.17	0.45
1:A:751:U:H4'	15:O:24:SER:HA	1.99	0.45
1:A:847:G:H2'	1:A:848:C:C6	2.51	0.45
1:A:1072:G:N2	2:B:106:THR:HG21	2.31	0.45
10:J:15:HIS:HB3	10:J:70:HIS:CE1	2.52	0.45
1:A:392:C:H2'	1:A:393:A:H8	1.82	0.45
1:A:533:A:N6	1:A:536:C:C2	2.85	0.45
1:A:591:U:H2'	1:A:592:G:H8	1.82	0.45
1:A:592:G:C6	1:A:648:A:C6	3.05	0.45
1:A:623:C:C2	1:A:624:C:C5	3.06	0.45
1:A:696:A:H2'	1:A:697:U:H6	1.82	0.45
1:A:954:G:O6	13:M:103:LYS:HE3	2.17	0.45
1:A:985:C:H2'	1:A:986:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:H1'	1:A:1190:G:N2	2.32	0.45
1:A:1319:A:C8	1:A:1323:G:C6	3.04	0.45
1:A:1371:G:O3'	9:I:71:GLY:HA3	2.17	0.45
3:C:10:ILE:HD13	3:C:178:LEU:HD11	1.99	0.45
4:D:100:ASN:HA	4:D:111:ARG:HG2	1.99	0.45
7:G:28:ASN:HA	7:G:31:MET:HB3	1.98	0.45
1:A:455:G:C4	1:A:456:A:C8	3.05	0.44
1:A:1316:G:H4'	14:N:58:SER:OG	2.17	0.44
2:B:32:PHE:HB3	2:B:40:ILE:CG2	2.45	0.44
4:D:72:PHE:CE1	4:D:94:LEU:HD11	2.51	0.44
18:R:32:TYR:CG	18:R:55:LEU:HD21	2.52	0.44
1:A:1355:G:C4	1:A:1356:G:C8	3.05	0.44
1:A:1355:G:H2'	1:A:1356:G:H8	1.82	0.44
2:B:183:VAL:HG23	2:B:196:VAL:HG13	1.98	0.44
2:B:187:VAL:O	2:B:201:PRO:HA	2.16	0.44
3:C:109:PRO:HG2	3:C:110:GLU:OE2	2.17	0.44
3:C:175:LEU:HA	3:C:175:LEU:HD23	1.68	0.44
4:D:85:ASN:HB2	4:D:88:GLU:CG	2.47	0.44
1:A:957:U:H5"	19:S:81:ARG:HH12	1.83	0.44
1:A:1309:G:O6	1:A:1329:A:N6	2.49	0.44
7:G:74:GLU:O	7:G:88:PRO:HA	2.18	0.44
11:K:94:GLU:CD	11:K:94:GLU:H	2.21	0.44
19:S:40:ILE:HG23	19:S:44:MET:SD	2.57	0.44
1:A:736:C:H2'	1:A:737:C:H6	1.83	0.44
1:A:1330:U:O2'	1:A:1331:G:H5'	2.18	0.44
1:A:1441:A:C8	1:A:1442:G:C8	3.05	0.44
2:B:71:GLY:O	2:B:93:ASN:HA	2.17	0.44
4:D:13:ARG:HD2	4:D:32:CYS:HB2	1.98	0.44
12:L:66:TYR:HB2	12:L:93:VAL:HG11	1.99	0.44
1:A:635:A:H2'	1:A:636:U:C6	2.52	0.44
1:A:754:C:H4'	15:O:72:ARG:HH22	1.83	0.44
1:A:952:U:H2'	1:A:953:G:C8	2.51	0.44
1:A:1026:G:O2'	1:A:1027:C:OP1	2.28	0.44
1:A:1347:G:C8	9:I:109:ARG:HB3	2.52	0.44
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.49	0.44
8:H:106:THR:HG22	8:H:122:GLY:O	2.17	0.44
17:Q:62:ARG:HB3	17:Q:76:VAL:CG2	2.48	0.44
1:A:398:U:H2'	1:A:399:G:C8	2.53	0.44
1:A:512:U:C5	1:A:534:U:H4'	2.53	0.44
1:A:515:G:C6	1:A:537:G:O6	2.71	0.44
1:A:532:A:O2'	3:C:161:GLU:OE2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:U:H2'	1:A:752:G:O4'	2.18	0.44
1:A:980:C:H2'	1:A:981:U:O4'	2.17	0.44
2:B:34:ALA:O	2:B:35:ARG:HG3	2.18	0.44
1:A:368:U:O2'	1:A:369:G:OP2	2.36	0.44
1:A:1176:A:H3'	1:A:1177:G:H8	1.82	0.44
1:A:1179:A:H2'	1:A:1180:A:O4'	2.17	0.44
3:C:22:TRP:CD2	3:C:59:ARG:HD2	2.53	0.44
7:G:97:ASN:O	7:G:101:MET:HG3	2.18	0.44
15:O:35:GLN:HE21	15:O:39:LEU:HG	1.81	0.44
17:Q:25:ILE:HD13	17:Q:44:LEU:HD12	2.00	0.44
1:A:142:G:O2'	1:A:196:A:N1	2.40	0.44
1:A:357:G:H5'	1:A:367:U:C2'	2.47	0.44
1:A:1038:C:C4	1:A:1039:G:N7	2.85	0.44
1:A:1130:A:C8	1:A:1146:A:C2	3.06	0.44
4:D:13:ARG:NH2	4:D:38:PRO:HA	2.33	0.44
20:T:60:ARG:O	20:T:64:LYS:HG2	2.18	0.44
21:U:7:ARG:O	21:U:10:GLU:HB3	2.18	0.44
1:A:300:A:O2'	1:A:564:C:N3	2.45	0.44
1:A:909:A:N3	1:A:1413:A:O2'	2.41	0.44
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.48	0.44
1:A:144:G:H2'	1:A:145:G:O4'	2.18	0.43
1:A:687:A:C8	1:A:701:U:C4	3.05	0.43
1:A:737:C:H2'	1:A:738:C:H6	1.83	0.43
2:B:105:LYS:HB3	2:B:105:LYS:HE2	1.66	0.43
11:K:35:THR:HG22	11:K:41:ALA:HA	2.00	0.43
14:N:85:ARG:O	14:N:89:MET:HG2	2.18	0.43
19:S:51:VAL:O	19:S:57:HIS:HA	2.18	0.43
1:A:185:U:H2'	1:A:186:C:C6	2.54	0.43
1:A:404:G:O6	4:D:2:ALA:N	2.51	0.43
1:A:454:G:C6	1:A:455:G:N7	2.86	0.43
1:A:938:A:H1'	1:A:1377:A:H5'	1.99	0.43
2:B:20:THR:HA	2:B:39:HIS:NE2	2.33	0.43
3:C:51:SER:OG	3:C:72:ARG:HG2	2.18	0.43
3:C:100:GLN:HE21	3:C:102:ASN:HD21	1.66	0.43
1:A:505:G:P	1:A:535:A:H5'	2.57	0.43
1:A:649:A:H2'	1:A:650:G:O4'	2.18	0.43
1:A:971:G:P	1:A:1231:G:H21	2.41	0.43
1:A:1270:G:C2	1:A:1271:A:C5	3.06	0.43
1:A:1328:C:C4	1:A:1329:A:N7	2.86	0.43
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.43
3:C:16:LYS:HE2	3:C:181:ASP:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:PHE:O	4:D:75:TYR:HB2	2.18	0.43
20:T:31:PHE:CE1	20:T:53:GLU:HG2	2.53	0.43
1:A:32:A:OP1	1:A:398:U:H1'	2.19	0.43
1:A:79:G:O6	1:A:80:A:N6	2.52	0.43
1:A:618:C:H5'	1:A:619:U:C5'	2.46	0.43
1:A:1346:A:N1	1:A:1374:A:H5"	2.33	0.43
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.18	0.43
1:A:1428:A:H2'	1:A:1429:A:O4'	2.18	0.43
2:B:40:ILE:HD12	2:B:40:ILE:HA	1.83	0.43
4:D:101:VAL:HG21	4:D:182:PHE:HE2	1.83	0.43
7:G:102:ARG:O	7:G:105:VAL:HG12	2.17	0.43
9:I:112:GLU:HG2	9:I:115:LYS:HZ3	1.83	0.43
10:J:52:LEU:HB2	14:N:81:ARG:HD2	2.00	0.43
11:K:14:LYS:HE3	11:K:77:TYR:CE2	2.52	0.43
14:N:93:ILE:HG21	14:N:96:LEU:HD12	2.00	0.43
1:A:838:G:H1'	1:A:849:G:N2	2.34	0.43
1:A:1530:G:C2'	1:A:1531:A:H8	2.29	0.43
2:B:70:VAL:HG21	2:B:161:LEU:HD22	2.00	0.43
7:G:110:LYS:HB3	7:G:110:LYS:HE2	1.68	0.43
1:A:1072:G:H2'	1:A:1073:U:C6	2.53	0.43
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.88	0.43
4:D:198:HIS:O	4:D:202:GLU:HG2	2.19	0.43
7:G:140:ASP:OD1	7:G:143:ARG:NH1	2.51	0.43
1:A:127:G:N2	17:Q:63:GLU:OE2	2.51	0.43
1:A:398:U:H2'	1:A:399:G:H8	1.84	0.43
1:A:482:A:H8	1:A:482:A:P	2.41	0.43
1:A:514:C:C4	1:A:515:G:N7	2.87	0.43
1:A:537:G:H2'	1:A:538:G:O4'	2.19	0.43
1:A:545:C:HO2'	1:A:549:C:H5"	1.81	0.43
1:A:1032:G:H3'	1:A:1032:G:N3	2.33	0.43
1:A:1119:C:H2'	1:A:1120:C:C6	2.54	0.43
1:A:1305:G:N1	1:A:1331:G:C4	2.87	0.43
1:A:1322:C:H5"	13:M:99:GLY:HA3	2.00	0.43
2:B:83:ALA:O	2:B:87:CYS:HB2	2.18	0.43
3:C:54:ARG:HD3	3:C:69:HIS:CG	2.53	0.43
9:I:118:LEU:HA	9:I:125:PRO:HD3	2.00	0.43
16:P:19:VAL:HG13	16:P:36:VAL:CG2	2.48	0.43
1:A:82:G:N3	1:A:82:G:H2'	2.34	0.43
1:A:529:G:H5"	1:A:530:G:OP2	2.19	0.43
1:A:1053:G:N7	1:A:1200:C:H5"	2.33	0.43
1:A:1117:A:H5"	9:I:106:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.53	0.43
1:A:1436:U:H2'	1:A:1437:A:C8	2.54	0.43
2:B:9:MET:SD	2:B:14:VAL:HG11	2.59	0.43
2:B:35:ARG:O	2:B:38:VAL:HG12	2.18	0.43
4:D:105:MET:HE1	4:D:107:PHE:CE2	2.53	0.43
4:D:184:ARG:HG3	4:D:185:LYS:N	2.34	0.43
15:O:78:TYR:O	15:O:82:ILE:HG23	2.18	0.43
1:A:99:C:O2'	1:A:100:G:H8	2.01	0.43
1:A:185:U:H2'	1:A:186:C:H6	1.84	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.43
1:A:1144:G:H8	1:A:1144:G:OP2	2.02	0.43
1:A:1308:U:OP1	13:M:97:VAL:HG22	2.18	0.43
2:B:135:LEU:HD12	2:B:135:LEU:HA	1.82	0.43
13:M:26:GLY:O	13:M:30:SER:HB2	2.19	0.43
15:O:17:ARG:NH1	15:O:26:GLU:OE1	2.52	0.43
17:Q:12:VAL:HA	17:Q:23:VAL:HG22	2.00	0.43
1:A:412:A:C6	1:A:414:A:H1'	2.54	0.43
1:A:865:A:H5'	1:A:1078:U:O4	2.19	0.43
1:A:1329:A:OP1	13:M:29:ARG:HB2	2.19	0.43
1:A:1463:U:H2'	1:A:1464:U:C6	2.53	0.43
1:A:1510:C:H2'	1:A:1511:G:H8	1.84	0.43
3:C:85:GLU:O	3:C:89:LYS:HD2	2.19	0.43
11:K:85:MET:HE3	11:K:85:MET:HB3	1.98	0.43
11:K:113:VAL:HG12	18:R:73:ARG:CD	2.48	0.43
12:L:70:GLU:O	12:L:70:GLU:HG2	2.18	0.43
12:L:86:ARG:HA	12:L:94:ARG:HA	2.00	0.43
19:S:45:ILE:HD11	19:S:67:VAL:HG21	2.01	0.43
1:A:858:G:O6	1:A:869:G:H3'	2.19	0.42
1:A:978:A:C8	1:A:979:C:C5	3.07	0.42
1:A:978:A:C2	1:A:1319:A:C4	3.07	0.42
1:A:1057:G:H5"	3:C:154:SER:OG	2.19	0.42
1:A:1183:U:O2'	1:A:1185:G:OP2	2.37	0.42
1:A:1346:A:H5'	1:A:1348:U:O4'	2.19	0.42
3:C:169:ARG:HE	3:C:169:ARG:HB3	1.61	0.42
6:F:5:GLU:OE2	18:R:24:LYS:NZ	2.47	0.42
8:H:54:ASP:OD1	8:H:54:ASP:N	2.41	0.42
11:K:53:ARG:HA	11:K:53:ARG:HD2	1.86	0.42
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.01	0.42
18:R:30:LYS:HE3	18:R:30:LYS:HB3	1.72	0.42
19:S:32:ARG:HE	19:S:57:HIS:CD2	2.37	0.42
1:A:5:U:H4'	1:A:6:G:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:C:H4'	1:A:967:5MC:OP1	2.19	0.42
1:A:1017:U:H2'	1:A:1018:G:H8	1.84	0.42
1:A:1103:C:H5"	2:B:97:LEU:HD23	2.00	0.42
5:E:88:VAL:HG22	5:E:93:ARG:HG2	2.00	0.42
8:H:87:LYS:HD2	8:H:91:GLU:O	2.19	0.42
9:I:50:GLN:HA	9:I:53:GLU:HG2	2.01	0.42
17:Q:21:ILE:CG1	17:Q:46:VAL:HB	2.50	0.42
1:A:309:A:O2'	1:A:607:A:N1	2.49	0.42
1:A:408:A:C6	1:A:409:U:C4	3.08	0.42
1:A:1248:A:C5	1:A:1290:G:C2	3.06	0.42
4:D:49:SER:O	4:D:53:VAL:N	2.45	0.42
12:L:32:GLY:HA2	12:L:57:LEU:HA	2.01	0.42
1:A:309:A:H2'	1:A:310:G:H8	1.85	0.42
1:A:984:C:H2'	1:A:985:C:C6	2.54	0.42
1:A:1101:A:H4'	1:A:1102:A:O5'	2.19	0.42
1:A:1134:G:H2'	1:A:1135:U:O4'	2.19	0.42
1:A:1496:C:H2'	1:A:1497:G:O4'	2.19	0.42
7:G:15:ASP:CG	7:G:23:LEU:HD23	2.40	0.42
8:H:92:LEU:HD12	8:H:117:ARG:HG3	2.01	0.42
1:A:195:A:H1'	1:A:222:C:O2'	2.19	0.42
1:A:476:U:H2'	1:A:477:C:O4'	2.20	0.42
1:A:1040:U:H2'	1:A:1041:G:C8	2.54	0.42
1:A:1446:A:OP1	1:A:1446:A:H8	2.02	0.42
2:B:196:VAL:HB	2:B:199:VAL:HG12	2.01	0.42
4:D:177:LYS:HA	4:D:177:LYS:HD2	1.85	0.42
11:K:87:LYS:HG2	11:K:113:VAL:HG23	2.01	0.42
12:L:99:ARG:HD2	12:L:99:ARG:HA	1.69	0.42
1:A:294:U:H2'	1:A:295:C:C6	2.54	0.42
1:A:947:G:C6	1:A:948:C:C4	3.07	0.42
1:A:1123:U:O2'	1:A:1124:G:H5'	2.19	0.42
1:A:1127:G:C2	1:A:1128:C:C5	3.07	0.42
1:A:1165:U:H2'	1:A:1166:G:O4'	2.20	0.42
8:H:96:MET:CE	8:H:130:ALA:HB1	2.49	0.42
14:N:20:TYR:HB3	14:N:24:ARG:HG3	2.00	0.42
1:A:257:G:H2'	1:A:258:G:C8	2.55	0.42
1:A:967:5MC:O2'	1:A:968:A:OP2	2.36	0.42
1:A:1521:C:H2'	1:A:1522:U:C6	2.54	0.42
2:B:7:ARG:O	2:B:7:ARG:HD3	2.19	0.42
2:B:50:PHE:CD1	2:B:200:ILE:HG12	2.55	0.42
9:I:118:LEU:CD2	9:I:124:ARG:HG2	2.49	0.42
12:L:110:ARG:HB3	12:L:119:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:A:H5'	10:J:43:PRO:HA	2.01	0.42
3:C:6:HIS:CG	14:N:89:MET:HB3	2.54	0.42
6:F:53:LYS:O	6:F:53:LYS:HG3	2.20	0.42
14:N:62:ASN:HB3	14:N:73:PHE:CE2	2.54	0.42
18:R:10:PHE:HE2	18:R:12:ARG:NH2	2.18	0.42
18:R:10:PHE:O	18:R:10:PHE:CG	2.71	0.42
18:R:13:PHE:CD1	18:R:18:VAL:HG21	2.44	0.42
18:R:23:TYR:HE2	18:R:65:LEU:HD12	1.84	0.42
1:A:62:U:H2'	1:A:63:C:C6	2.55	0.42
1:A:414:A:N6	1:A:430:A:H2	2.14	0.42
17:Q:74:THR:HB	17:Q:75:LEU:H	1.77	0.42
1:A:459:A:H2'	1:A:460:A:H8	1.85	0.42
1:A:1073:U:C2	1:A:1074:G:C8	3.08	0.42
1:A:1118:U:H1'	1:A:1179:A:C4	2.54	0.42
1:A:1311:A:C6	1:A:1312:G:C5	3.08	0.42
1:A:70:U:H1'	1:A:71:A:N7	2.35	0.41
1:A:737:C:H2'	1:A:738:C:C6	2.55	0.41
1:A:1032:G:N2	1:A:1033:G:O4'	2.53	0.41
1:A:1070:U:H2'	1:A:1071:C:C6	2.55	0.41
1:A:1220:G:O3'	19:S:36:ARG:HD3	2.20	0.41
3:C:12:LEU:HD21	14:N:91:GLY:HA3	2.02	0.41
6:F:3:HIS:NE2	6:F:65:GLU:OE1	2.53	0.41
7:G:30:LEU:HD12	7:G:105:VAL:HG23	2.02	0.41
11:K:29:ASN:ND2	11:K:57:LYS:HE2	2.35	0.41
1:A:439:U:O2	1:A:439:U:H2'	2.20	0.41
1:A:904:U:H2'	1:A:905:U:C6	2.55	0.41
1:A:975:A:O4'	1:A:1358:U:H1'	2.20	0.41
4:D:57:GLU:OE1	4:D:199:LEU:HD12	2.20	0.41
6:F:101:PRO:HB3	18:R:25:ASP:OD1	2.20	0.41
17:Q:45:HIS:HB2	17:Q:70:THR:O	2.20	0.41
1:A:189:A:H2'	1:A:190:A:C8	2.56	0.41
1:A:335:C:H2'	1:A:336:A:C8	2.56	0.41
1:A:427:U:O5'	1:A:428:G:H2'	2.21	0.41
1:A:552:U:C2	1:A:553:A:C8	3.09	0.41
1:A:1144:G:O6	1:A:1145:A:N6	2.52	0.41
1:A:1267:C:H6	1:A:1267:C:OP1	2.04	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.41
7:G:70:ARG:HD3	7:G:97:ASN:OD1	2.20	0.41
8:H:108:LYS:HA	8:H:108:LYS:HD3	1.81	0.41
1:A:55:A:H2'	1:A:55:A:N3	2.35	0.41
1:A:123:U:H5"	1:A:311:C:O2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:C:H2'	1:A:265:G:O4'	2.20	0.41
1:A:299:G:H2'	1:A:300:A:C8	2.55	0.41
1:A:936:C:C2	1:A:937:A:C8	3.09	0.41
1:A:969:A:H2'	1:A:970:C:O4'	2.20	0.41
1:A:1251:A:H2'	1:A:1252:A:C8	2.55	0.41
1:A:1500:A:H5"	1:A:1508:A:H5"	2.03	0.41
11:K:84:VAL:O	11:K:111:THR:N	2.36	0.41
17:Q:47:HIS:HB3	17:Q:74:THR:HG22	2.02	0.41
1:A:7:A:H5'	1:A:298:A:O4'	2.19	0.41
1:A:49:U:C2	1:A:361:G:N2	2.89	0.41
1:A:626:G:H2'	1:A:627:G:C8	2.55	0.41
1:A:832:G:C6	1:A:855:U:C4	3.08	0.41
1:A:994:A:N3	1:A:994:A:H2'	2.36	0.41
1:A:1107:C:H5"	3:C:173:VAL:HG23	2.02	0.41
1:A:1201:A:H4'	1:A:1202:U:O5'	2.21	0.41
1:A:1244:G:H2'	1:A:1245:C:C6	2.55	0.41
4:D:8:LYS:HG3	4:D:21:LEU:HD22	2.01	0.41
7:G:5:ARG:NH1	7:G:7:ILE:HD12	2.34	0.41
9:I:41:ARG:HG3	9:I:43:THR:H	1.85	0.41
10:J:65:TYR:HB3	14:N:96:LEU:HD21	2.02	0.41
14:N:6:MET:HA	14:N:6:MET:CE	2.51	0.41
14:N:78:GLY:C	14:N:79:LEU:HD23	2.40	0.41
20:T:61:GLN:OE1	20:T:61:GLN:HA	2.20	0.41
1:A:71:A:C2	1:A:100:G:C8	3.09	0.41
1:A:230:G:H2'	1:A:231:U:O4'	2.20	0.41
1:A:426:U:H6	1:A:426:U:O5'	2.02	0.41
1:A:600:A:H2'	1:A:601:G:C8	2.55	0.41
1:A:1118:U:H2'	1:A:1119:C:C6	2.56	0.41
1:A:1438:G:OP1	20:T:29:ARG:HD3	2.20	0.41
9:I:47:VAL:O	9:I:50:GLN:HB2	2.21	0.41
1:A:89:U:H2'	1:A:90:C:C6	2.55	0.41
1:A:216:U:H2'	1:A:217:C:C5	2.55	0.41
1:A:593:U:H2'	1:A:594:U:H6	1.85	0.41
1:A:678:U:H2'	1:A:679:C:H6	1.85	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.08	0.41
1:A:1271:A:C2	1:A:1272:G:C5	3.09	0.41
3:C:149:ILE:HG13	3:C:201:TRP:O	2.21	0.41
7:G:150:ALA:HB2	11:K:52:PHE:HE2	1.86	0.41
9:I:51:PRO:HB2	9:I:83:ILE:HG22	2.03	0.41
1:A:218:U:H2'	1:A:219:U:O4'	2.21	0.41
1:A:511:C:O2'	1:A:512:U:OP2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:U:OP2	1:A:723:U:H4'	2.21	0.41
4:D:177:LYS:O	4:D:177:LYS:NZ	2.29	0.41
11:K:16:VAL:CG2	11:K:79:ILE:HG12	2.51	0.41
12:L:4:VAL:HG23	17:Q:34:TYR:HB3	2.03	0.41
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.87	0.41
1:A:21:G:H2'	1:A:22:G:C8	2.55	0.41
1:A:412:A:O2'	1:A:413:G:H4'	2.21	0.41
1:A:546:A:H4'	1:A:548:G:O2'	2.20	0.41
1:A:946:A:C2	1:A:947:G:C5	3.09	0.41
1:A:1216:A:H5"	14:N:5:SER:HB3	2.03	0.41
1:A:1306:A:H62	1:A:1331:G:N2	2.19	0.41
1:A:1315:U:O2'	1:A:1361:G:O4'	2.34	0.41
1:A:1347:G:H22	1:A:1374:A:P	2.44	0.41
1:A:1366:C:OP1	9:I:119:ARG:NH1	2.54	0.41
1:A:1402:4OC:O5'	1:A:1402:4OC:H6	2.21	0.41
1:A:1492:A:H2'	1:A:1493:A:C8	2.56	0.41
2:B:161:LEU:HB2	2:B:183:VAL:HG12	2.02	0.41
2:B:188:ASP:HB2	2:B:204:ASP:OD2	2.20	0.41
4:D:142:VAL:HA	4:D:180:GLY:O	2.21	0.41
6:F:11:HIS:HE1	6:F:54:LEU:HD21	1.86	0.41
6:F:22:ILE:O	6:F:26:THR:HG23	2.21	0.41
13:M:20:THR:HG22	13:M:26:GLY:O	2.21	0.41
16:P:42:ILE:HG22	16:P:42:ILE:O	2.20	0.41
1:A:216:U:H2'	1:A:217:C:H6	1.86	0.41
1:A:255:G:C2	1:A:272:C:C2	3.08	0.41
1:A:505:G:H8	1:A:505:G:OP1	2.05	0.41
2:B:41:ILE:HD13	2:B:202:GLY:H	1.86	0.41
2:B:41:ILE:HD13	2:B:202:GLY:N	2.35	0.41
3:C:206:GLU:HG2	3:C:207:ILE:H	1.85	0.41
14:N:62:ASN:HB3	14:N:73:PHE:CZ	2.56	0.41
19:S:15:LEU:HD13	19:S:38:SER:HB2	2.04	0.41
19:S:29:LYS:H	19:S:29:LYS:HD2	1.86	0.41
1:A:41:G:C2	1:A:42:G:C5	3.09	0.40
1:A:695:A:H2'	1:A:696:A:C8	2.56	0.40
1:A:920:U:H2'	1:A:921:U:C6	2.56	0.40
1:A:986:U:H2'	1:A:987:G:O4'	2.21	0.40
1:A:1053:G:H4'	1:A:1054:C:H5"	2.03	0.40
2:B:152:LYS:HE3	2:B:153:ASP:OD1	2.21	0.40
3:C:91:VAL:HG11	3:C:101:ILE:HD11	2.03	0.40
4:D:54:GLN:CB	4:D:203:LEU:HD13	2.51	0.40
6:F:18:VAL:HA	6:F:21:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:5:LEU:HD23	19:S:5:LEU:HA	1.95	0.40
1:A:86:G:H1'	1:A:87:C:C1'	2.51	0.40
1:A:96:U:H2'	1:A:97:G:C8	2.55	0.40
1:A:149:A:H1'	1:A:1446:A:C2	2.57	0.40
1:A:237:G:H5"	17:Q:27:ARG:HH21	1.85	0.40
1:A:337:G:H2'	1:A:338:A:C8	2.56	0.40
1:A:466:A:H2'	1:A:468:A:N7	2.36	0.40
1:A:678:U:H2'	1:A:679:C:C6	2.56	0.40
1:A:836:G:C6	1:A:851:G:C5	3.10	0.40
1:A:1158:C:C4	1:A:1160:G:C8	3.09	0.40
1:A:1533:C:H4'	1:A:1534:A:C8	2.56	0.40
2:B:27:MET:HG3	2:B:189:THR:HA	2.03	0.40
3:C:149:ILE:HA	3:C:201:TRP:O	2.21	0.40
3:C:181:ASP:HB2	3:C:205:GLY:O	2.21	0.40
7:G:71:PRO:HG3	7:G:103:TRP:CH2	2.56	0.40
12:L:4:VAL:CG2	17:Q:34:TYR:HB3	2.51	0.40
13:M:85:CYS:HB2	19:S:73:GLU:HB3	2.03	0.40
1:A:767:A:H2'	1:A:768:A:O4'	2.20	0.40
1:A:911:U:H2'	1:A:912:C:C6	2.57	0.40
1:A:981:U:H6	1:A:981:U:O5'	2.05	0.40
1:A:1309:G:C6	1:A:1329:A:N1	2.89	0.40
1:A:1355:G:N3	1:A:1356:G:C8	2.89	0.40
6:F:97:THR:O	6:F:97:THR:OG1	2.34	0.40
11:K:86:VAL:HG22	11:K:112:ASP:HA	2.03	0.40
12:L:66:TYR:CG	12:L:87:VAL:HG21	2.56	0.40
15:O:72:ARG:HG2	15:O:72:ARG:H	1.76	0.40
16:P:53:ASP:O	16:P:57:ILE:HG13	2.21	0.40
21:U:8:GLU:C	21:U:10:GLU:H	2.24	0.40
1:A:384:G:H2'	1:A:385:C:C6	2.56	0.40
1:A:407:U:H1'	4:D:116:GLN:OE1	2.22	0.40
1:A:408:A:H2'	1:A:409:U:H6	1.86	0.40
1:A:520:A:OP2	12:L:48:ALA:HB1	2.21	0.40
1:A:909:A:H2'	1:A:910:C:O4'	2.22	0.40
1:A:1279:G:H4'	1:A:1281:C:H5	1.86	0.40
2:B:41:ILE:HG21	2:B:201:PRO:HB2	2.04	0.40
3:C:11:ARG:HA	3:C:14:ILE:HD12	2.02	0.40
6:F:88:MET:HE3	18:R:64:TYR:HD2	1.86	0.40
12:L:33:VAL:HA	12:L:78:SER:O	2.22	0.40
14:N:64:CYS:SG	14:N:67:THR:N	2.91	0.40
20:T:24:ARG:NH1	20:T:66:LEU:HD22	2.36	0.40
21:U:39:GLU:HG3	21:U:43:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:G:C5	1:A:101:A:C8	3.10	0.40
1:A:179:A:H2'	1:A:180:U:O4'	2.22	0.40
1:A:214:C:O2	1:A:214:C:H2'	2.22	0.40
1:A:692:U:H2'	1:A:694:A:OP2	2.22	0.40
1:A:1289:A:H2'	1:A:1290:G:H5'	2.04	0.40
1:A:1518:MA6:H8	1:A:1518:MA6:O5'	2.22	0.40
6:F:68:GLN:H	6:F:68:GLN:HG3	1.55	0.40
7:G:148:ASN:HD22	7:G:148:ASN:N	2.18	0.40
11:K:93:ARG:O	11:K:97:ILE:HG13	2.22	0.40
14:N:19:LYS:HE3	14:N:20:TYR:CE1	2.57	0.40
20:T:2:ALA:O	20:T:8:LYS:NZ	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/234 (95%)	207 (93%)	15 (7%)	0	100	100
3	C	204/233 (88%)	193 (95%)	10 (5%)	1 (0%)	25	34
4	D	203/206 (98%)	191 (94%)	12 (6%)	0	100	100
5	E	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
6	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
7	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
8	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	I	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
10	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	13	17
11	K	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	110 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	N	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
18	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
All	All	2366/2569 (92%)	2240 (95%)	124 (5%)	2 (0%)	50	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
3	C	60	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/193 (96%)	174 (94%)	12 (6%)	14	19
3	C	170/190 (90%)	160 (94%)	10 (6%)	16	22
4	D	172/173 (99%)	157 (91%)	15 (9%)	8	10
5	E	119/126 (94%)	112 (94%)	7 (6%)	16	22
6	F	90/116 (78%)	86 (96%)	4 (4%)	24	34
7	G	126/147 (86%)	118 (94%)	8 (6%)	15	20
8	H	104/105 (99%)	100 (96%)	4 (4%)	28	41
9	I	105/107 (98%)	100 (95%)	5 (5%)	21	30
10	J	86/90 (96%)	81 (94%)	5 (6%)	17	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	89/98 (91%)	87 (98%)	2 (2%)	47 63
12	L	102/103 (99%)	98 (96%)	4 (4%)	27 40
13	M	93/96 (97%)	93 (100%)	0	100 100
14	N	83/84 (99%)	79 (95%)	4 (5%)	21 30
15	O	76/77 (99%)	69 (91%)	7 (9%)	7 9
16	P	65/65 (100%)	64 (98%)	1 (2%)	60 75
17	Q	73/78 (94%)	71 (97%)	2 (3%)	40 54
18	R	57/65 (88%)	56 (98%)	1 (2%)	54 70
19	S	72/79 (91%)	70 (97%)	2 (3%)	38 53
20	T	65/66 (98%)	59 (91%)	6 (9%)	7 9
21	U	60/61 (98%)	58 (97%)	2 (3%)	33 46
All	All	1993/2119 (94%)	1892 (95%)	101 (5%)	22 28

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	35	ARG
2	B	58	ASN
2	B	68	LEU
2	B	95	ARG
2	B	127	ASP
2	B	133	GLU
2	B	136	MET
2	B	141	LEU
2	B	143	LYS
2	B	159	ASP
2	B	165	ASP
2	B	197	ASP
3	C	3	GLN
3	C	23	PHE
3	C	85	GLU
3	C	107	ARG
3	C	143	ARG
3	C	154	SER
3	C	169	ARG
3	C	178	LEU
3	C	181	ASP
3	C	185	ASN

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Mol	Chain	Res	Type
4	D	8	LYS
4	D	26	ARG
4	D	34	ILE
4	D	58	LYS
4	D	60	LYS
4	D	70	ARG
4	D	105	MET
4	D	124	MET
4	D	128	ARG
4	D	156	LYS
4	D	178	MET
4	D	181	THR
4	D	188	ARG
4	D	190	ASP
4	D	206	LYS
5	E	22	SER
5	E	43	ASN
5	E	78	ASN
5	E	100	SER
5	E	142	ASP
5	E	152	MET
5	E	156	LYS
6	F	5	GLU
6	F	35	LYS
6	F	60	VAL
6	F	97	THR
7	G	41	SER
7	G	54	SER
7	G	77	SER
7	G	78	ARG
7	G	109	ARG
7	G	111	ARG
7	G	137	LYS
7	G	140	ASP
8	H	22	LYS
8	H	47	GLU
8	H	94	LYS
8	H	96	MET
9	I	4	ASN
9	I	12	ARG
9	I	88	MET
9	I	116	VAL

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Mol	Chain	Res	Type
9	I	122	ARG
10	J	7	ARG
10	J	16	ARG
10	J	59	LYS
10	J	75	ASP
10	J	85	ASP
11	K	94	GLU
11	K	95	SER
12	L	86	ARG
12	L	99	ARG
12	L	109	ASP
12	L	111	LYS
14	N	6	MET
14	N	32	SER
14	N	96	LEU
14	N	97	LYS
15	O	17	ARG
15	O	21	ASP
15	O	64	ARG
15	O	72	ARG
15	O	83	GLU
15	O	84	ARG
15	O	89	ARG
16	P	1	MET
17	Q	28	PHE
17	Q	50	ASN
18	R	30	LYS
19	S	29	LYS
19	S	66	MET
20	T	5	LYS
20	T	6	SER
20	T	14	SER
20	T	27	MET
20	T	54	MET
20	T	69	LYS
21	U	46	LYS
21	U	51	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	19	ASN

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Mol	Chain	Res	Type
3	C	100	GLN
4	D	59	GLN
7	G	130	ASN
7	G	148	ASN
16	P	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1533 (98%)	252 (16%)	6 (0%)

All (252) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	9	G
1	A	37	U
1	A	39	G
1	A	43	C
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	72	A
1	A	74	A
1	A	75	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	94	G
1	A	95	C
1	A	98	A
1	A	121	U
1	A	122	G

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Mol	Chain	Res	Type
1	A	130	A
1	A	131	A
1	A	141	G
1	A	142	G
1	A	144	G
1	A	151	A
1	A	163	C
1	A	164	G
1	A	181	A
1	A	182	A
1	A	183	C
1	A	197	A
1	A	200	G
1	A	201	G
1	A	202	G
1	A	204	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	271	C
1	A	279	A
1	A	289	G
1	A	321	A
1	A	328	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	358	U
1	A	367	U
1	A	369	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	385	C
1	A	406	G
1	A	411	A

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Mol	Chain	Res	Type
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	417	G
1	A	418	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	426	U
1	A	429	U
1	A	444	G
1	A	448	A
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	460	A
1	A	461	A
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	474	G
1	A	478	A
1	A	479	U
1	A	481	G
1	A	482	A
1	A	483	C
1	A	484	G
1	A	485	U
1	A	486	U
1	A	488	C
1	A	495	A
1	A	496	A
1	A	497	G
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C

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Mol	Chain	Res	Type
1	A	529	G
1	A	537	G
1	A	547	A
1	A	550	G
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	596	A
1	A	618	C
1	A	619	U
1	A	621	A
1	A	624	C
1	A	629	A
1	A	630	A
1	A	633	G
1	A	650	G
1	A	665	A
1	A	687	A
1	A	689	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	733	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	836	G
1	A	849	G
1	A	851	G
1	A	857	C
1	A	890	G
1	A	914	A
1	A	926	G

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Mol	Chain	Res	Type
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	C
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	992	U
1	A	994	A
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1006	G
1	A	1009	U
1	A	1010	U
1	A	1017	U
1	A	1024	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1037	C
1	A	1039	G
1	A	1042	A
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1050	G
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A

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Mol	Chain	Res	Type
1	A	1137	C
1	A	1139	G
1	A	1144	G
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1248	A
1	A	1257	A
1	A	1260	G
1	A	1269	A
1	A	1275	A
1	A	1280	A
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1290	G
1	A	1298	U
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1331	G
1	A	1335	U
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1348	U
1	A	1363	A
1	A	1364	U
1	A	1370	G

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Mol	Chain	Res	Type
1	A	1378	C
1	A	1379	G
1	A	1397	C
1	A	1419	G
1	A	1441	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1506	U
1	A	1529	G
1	A	1530	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	368	U
1	A	411	A
1	A	967	5MC
1	A	1026	G
1	A	1035	A

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

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	$\#\|Z\| > 2$
1	4OC	A	1402	1	20,23,24	0.38	0	25,32,35	0.52	0
1	5MC	A	1407	1	19,22,23	0.70	1 (5%)	26,32,35	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	G7M	A	527	1	20,26,27	1.21	2 (10%)	16,39,42	0.62	0
1	PSU	A	516	1	18,21,22	1.04	2 (11%)	21,30,33	1.85	5 (23%)
1	5MC	A	967	1	19,22,23	0.81	1 (5%)	26,32,35	0.96	1 (3%)
1	MA6	A	1519	1	19,26,27	1.11	1 (5%)	18,38,41	1.99	3 (16%)
1	UR3	A	1498	1	19,22,23	0.30	0	26,32,35	0.87	2 (7%)
1	MA6	A	1518	1	19,26,27	1.02	1 (5%)	18,38,41	1.87	4 (22%)
12	D2T	L	89	12	8,9,10	1.59	2 (25%)	6,11,13	1.46	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
12	D2T	L	89	12	-	4/7/12/14	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	G7M	C5-C4	3.48	1.46	1.39
12	L	89	D2T	CB-CG	3.28	1.57	1.52
1	A	967	5MC	C5-C4	-3.16	1.41	1.44
1	A	516	PSU	C6-C5	3.04	1.38	1.35
1	A	1519	MA6	C6-C5	2.78	1.49	1.44
1	A	1407	5MC	C5-C4	-2.70	1.42	1.44
1	A	527	G7M	C6-N1	-2.61	1.33	1.37
1	A	1518	MA6	C6-C5	2.50	1.48	1.44
1	A	516	PSU	O4'-C1'	-2.11	1.40	1.43
12	L	89	D2T	CB-SB	2.08	1.84	1.82

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1519	MA6	C2-N1-C6	5.66	122.39	116.84
1	A	1518	MA6	C2-N1-C6	5.12	121.86	116.84
1	A	516	PSU	C4-N3-C2	-4.68	119.93	126.37
1	A	516	PSU	N1-C2-N3	4.25	119.65	115.17
1	A	1519	MA6	N3-C2-N1	-4.02	123.22	128.67
1	A	516	PSU	O2-C2-N1	-3.55	119.12	122.79
1	A	1518	MA6	N3-C2-N1	-3.38	124.08	128.67
1	A	1519	MA6	C4-C5-N7	-3.36	105.78	109.34
1	A	1518	MA6	C4-C5-N7	-3.25	105.91	109.34
1	A	1518	MA6	N1-C6-N6	3.17	120.50	116.83
1	A	516	PSU	O4'-C1'-C2'	2.35	108.40	105.15
12	L	89	D2T	OD1-CG-CB	-2.32	117.58	122.44
1	A	1498	UR3	C4-N3-C2	-2.30	122.73	124.58
1	A	967	5MC	C2'-C1'-N1	-2.13	107.32	113.25
1	A	516	PSU	C6-N1-C2	-2.11	120.73	122.69
1	A	1498	UR3	C6-N1-C2	-2.00	120.16	121.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CA-CB-CG-OD1
12	L	89	D2T	CA-CB-CG-OD2
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	967	5MC	C4'-C5'-O5'-P
1	A	967	5MC	C3'-C4'-C5'-O5'
12	L	89	D2T	SB-CB-CG-OD2
12	L	89	D2T	CG-CB-SB-CB1
1	A	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	516	PSU	3	0
1	A	967	5MC	2	0
1	A	1519	MA6	1	0
1	A	1518	MA6	2	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

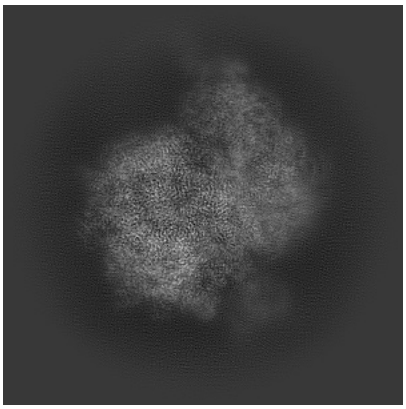
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47169. These allow visual inspection of the internal detail of the map and identification of artifacts.

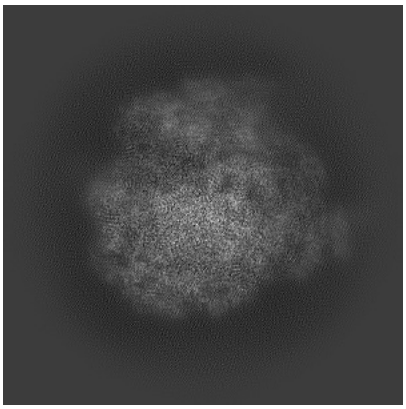
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

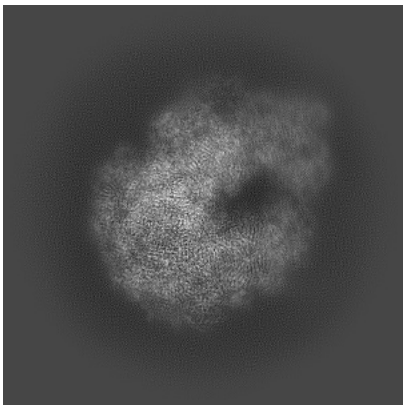
6.1.1 Primary map



X

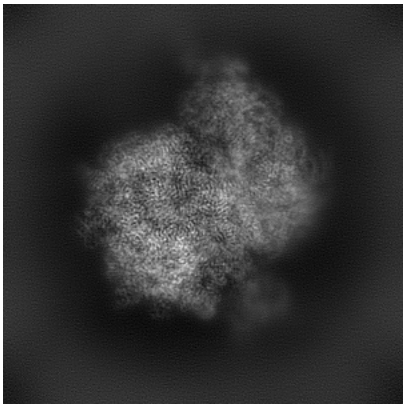


Y

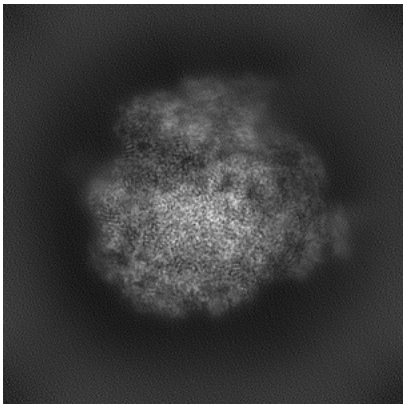


Z

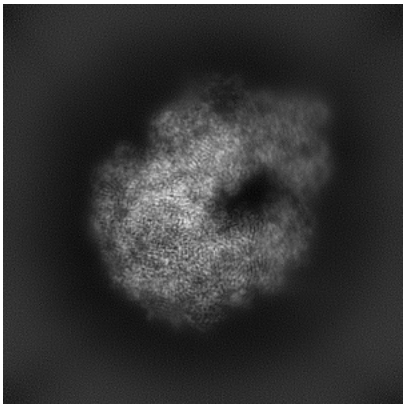
6.1.2 Raw map



X



Y

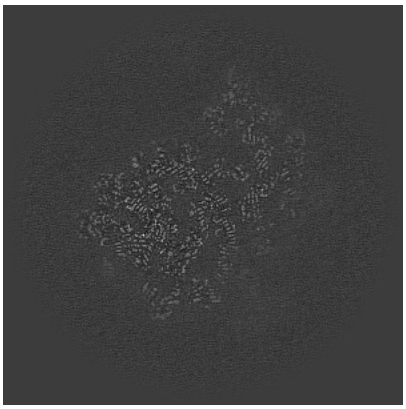


Z

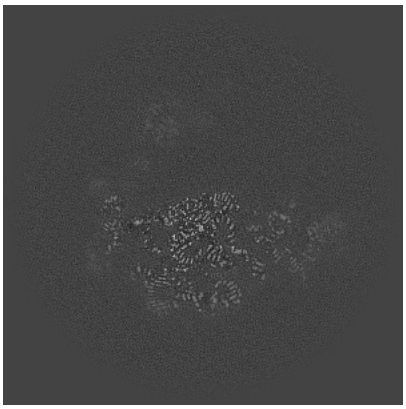
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

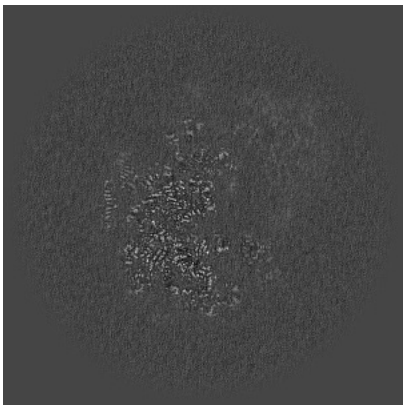
6.2.1 Primary map



X Index: 224

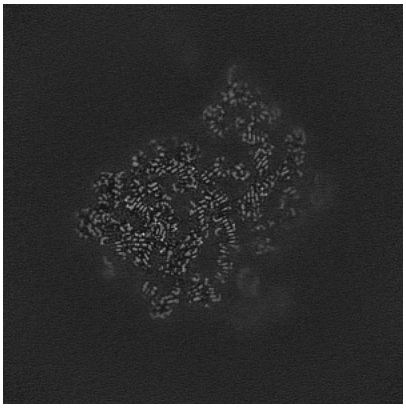


Y Index: 224

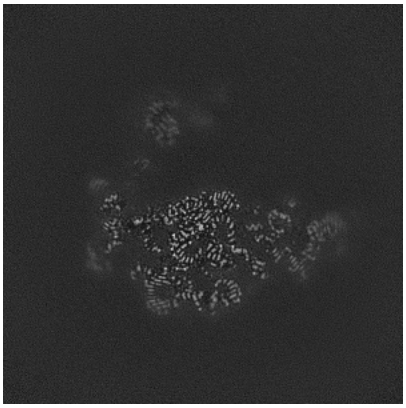


Z Index: 224

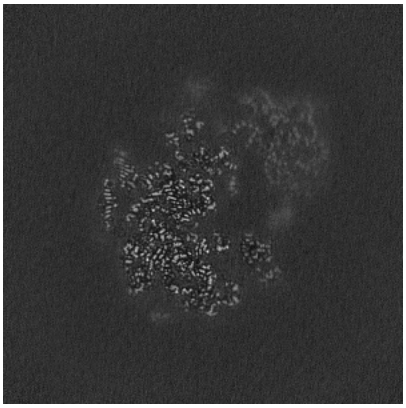
6.2.2 Raw map



X Index: 224



Y Index: 224

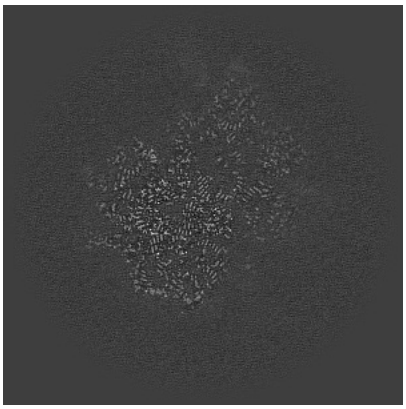


Z Index: 224

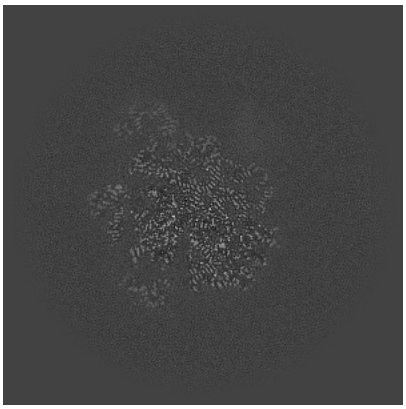
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

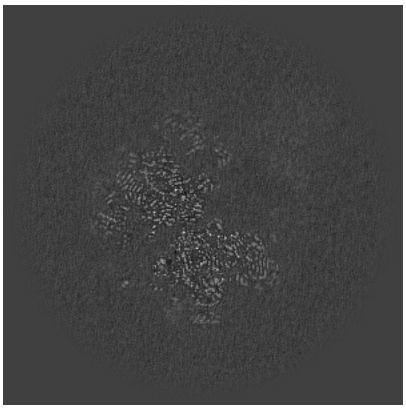
6.3.1 Primary map



X Index: 206

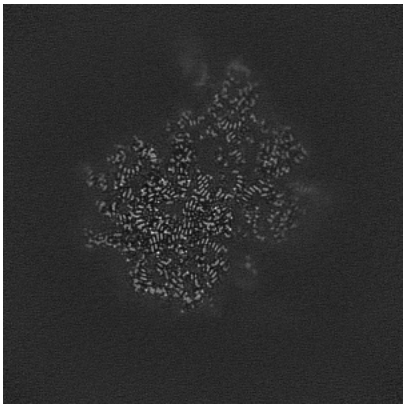


Y Index: 172

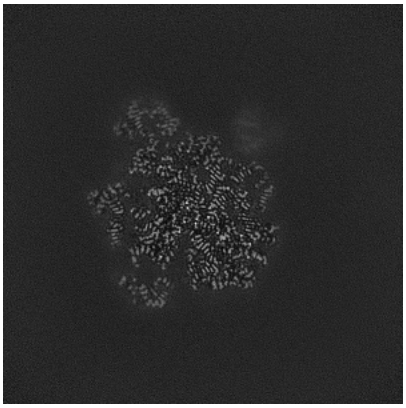


Z Index: 199

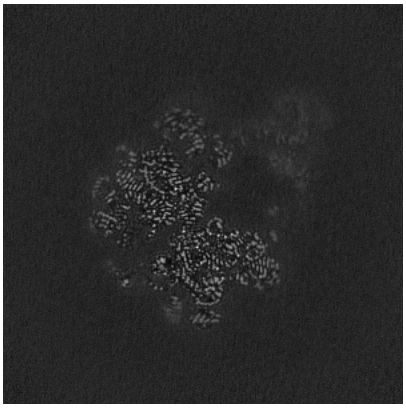
6.3.2 Raw map



X Index: 206



Y Index: 171

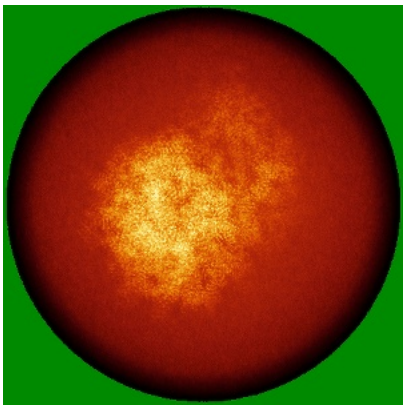


Z Index: 199

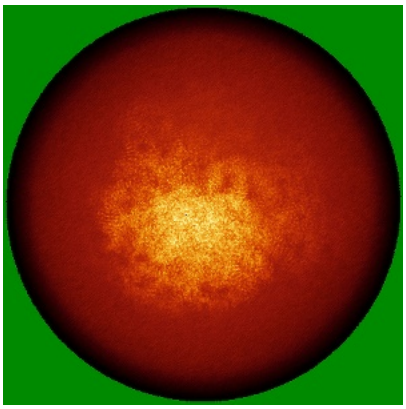
The images above show the largest variance slices of the map in three orthogonal directions.

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

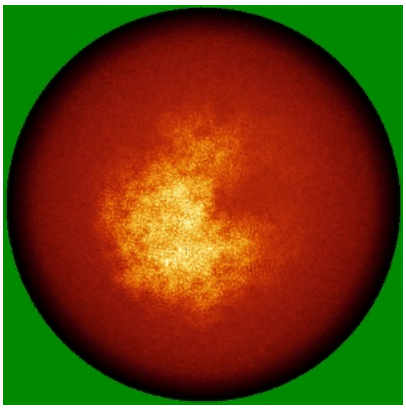
6.4.1 Primary map



X

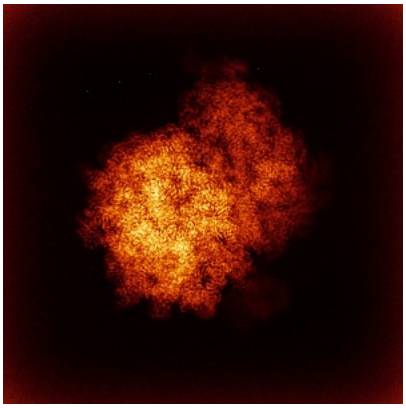


Y

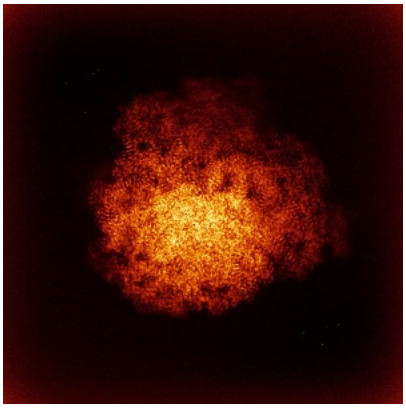


Z

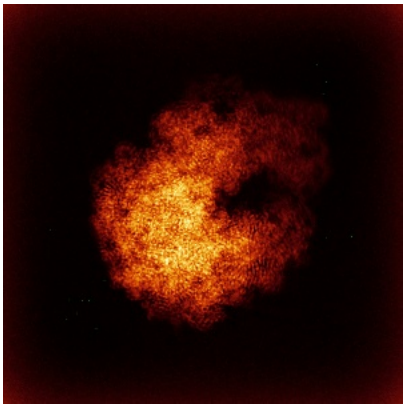
6.4.2 Raw map



X



Y

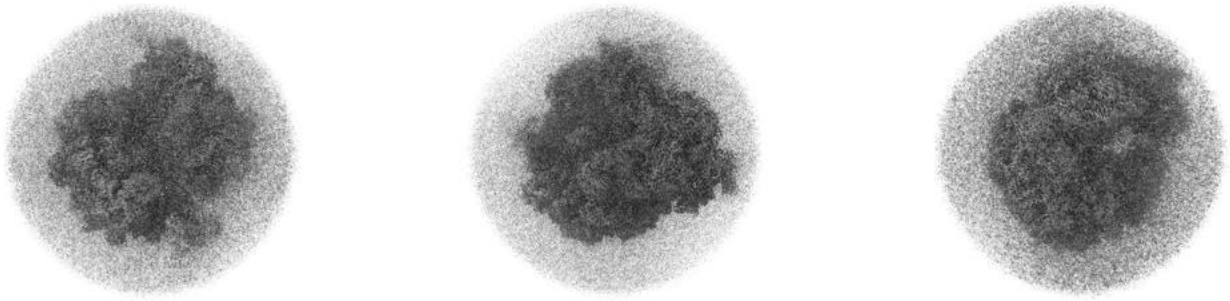


Z

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

6.5 Orthogonal surface views (i)

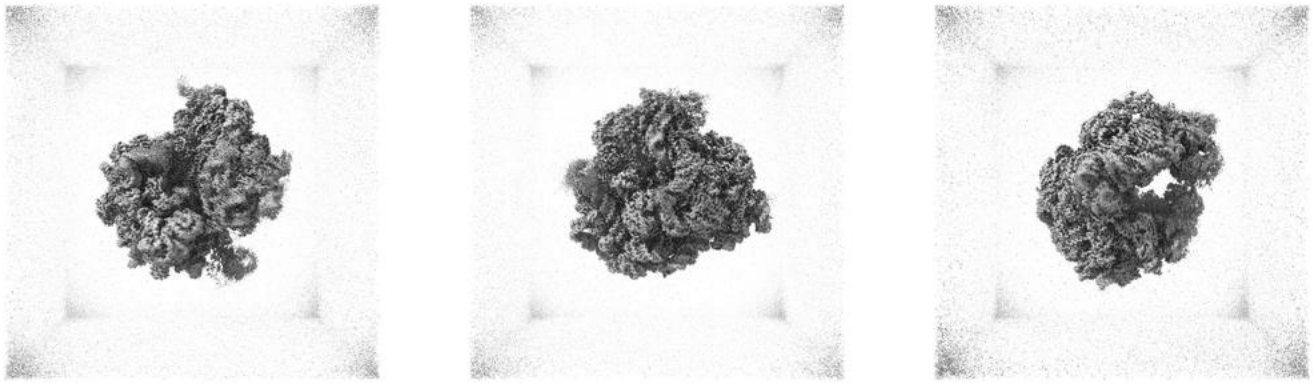
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.334. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

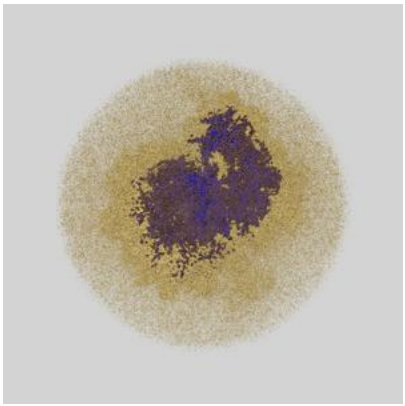
6.6 Mask visualisation (i)

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

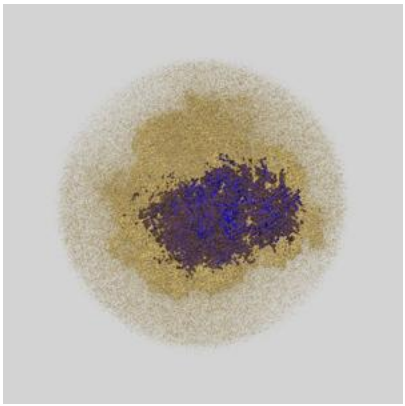
A mask typically either:

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

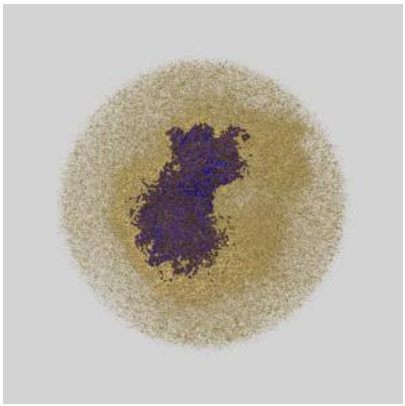
6.6.1 emd_47169_msk_1.map (i)



X



Y

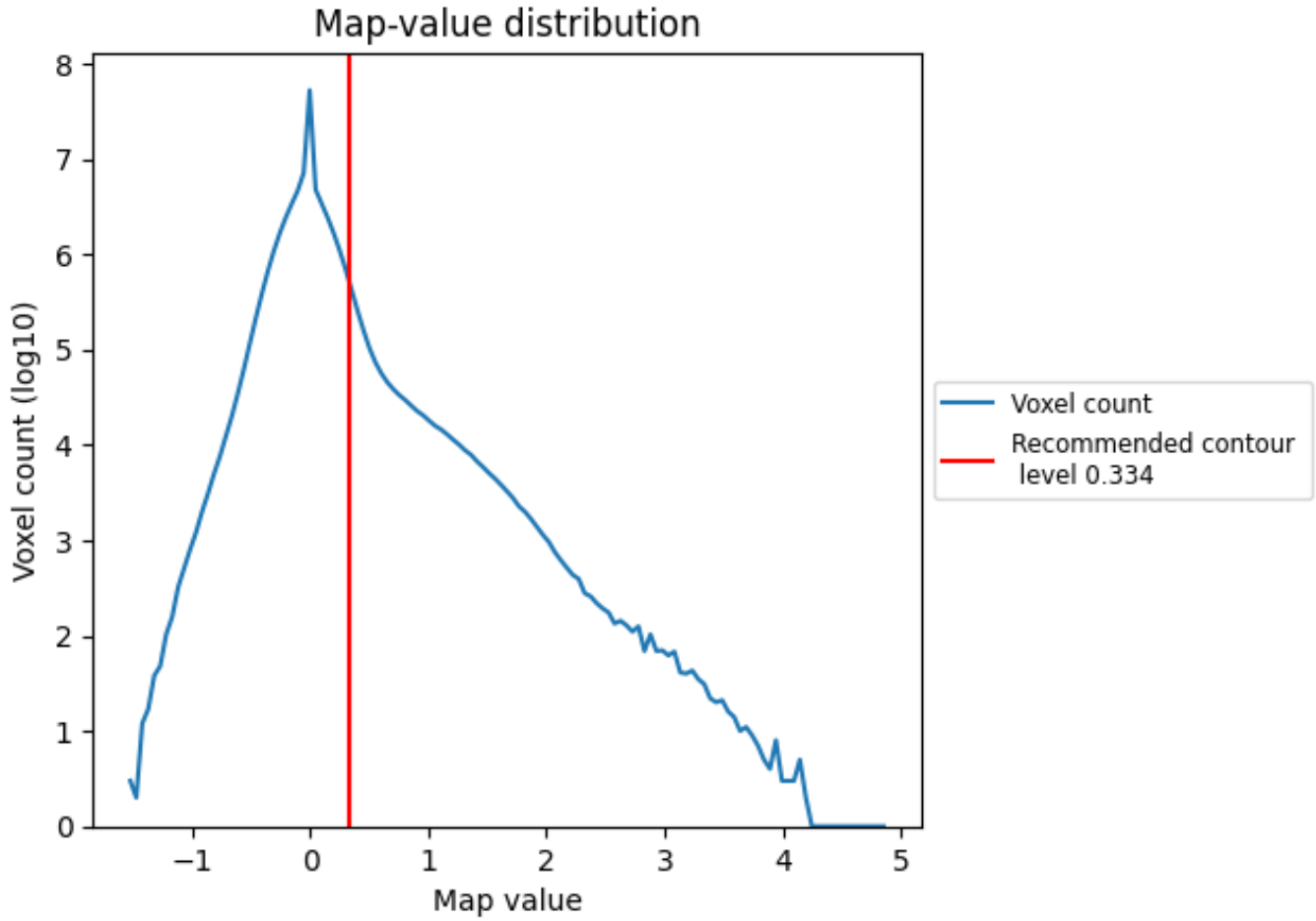


Z

7 Map analysis

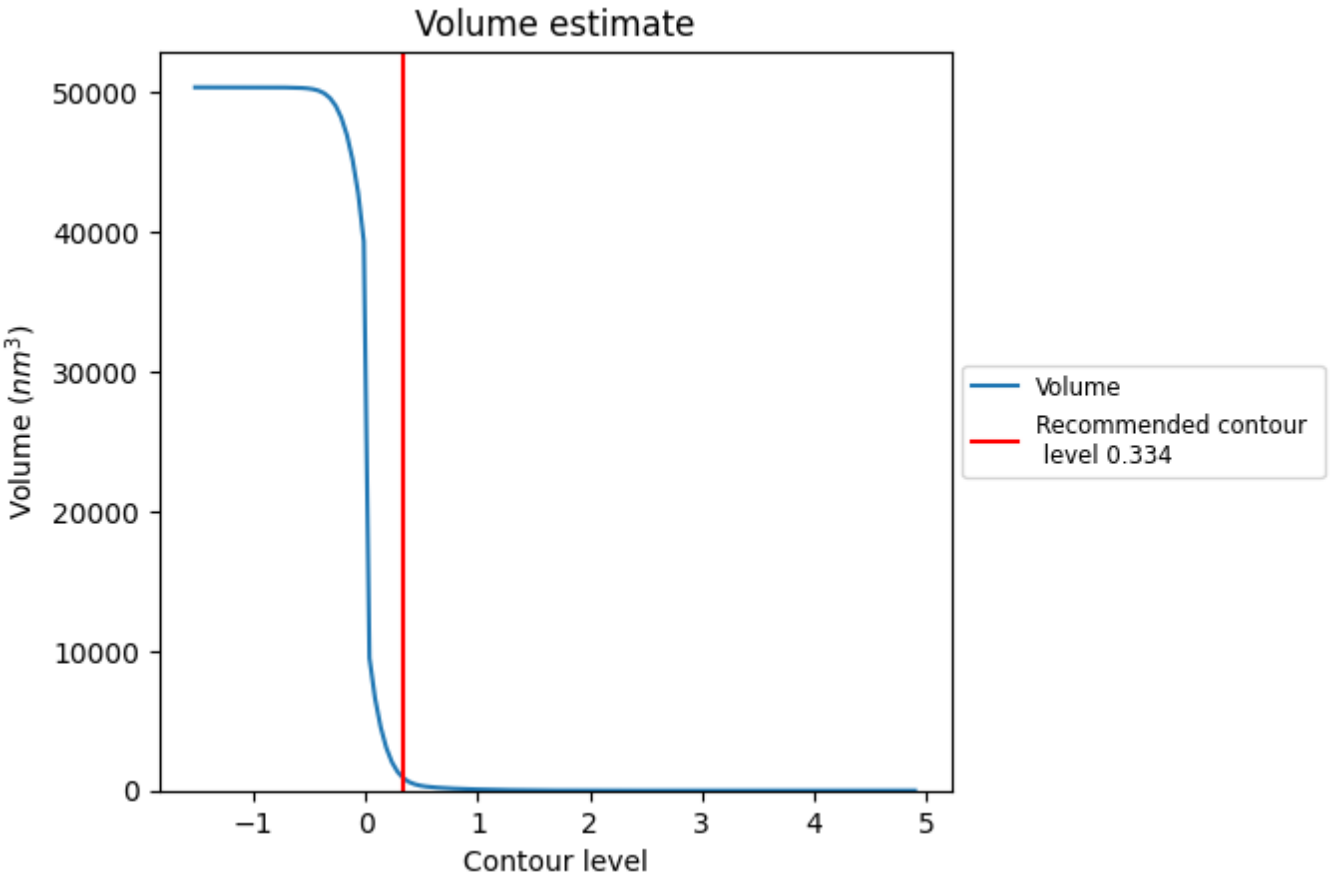
This section contains the results of statistical analysis of the map.

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.

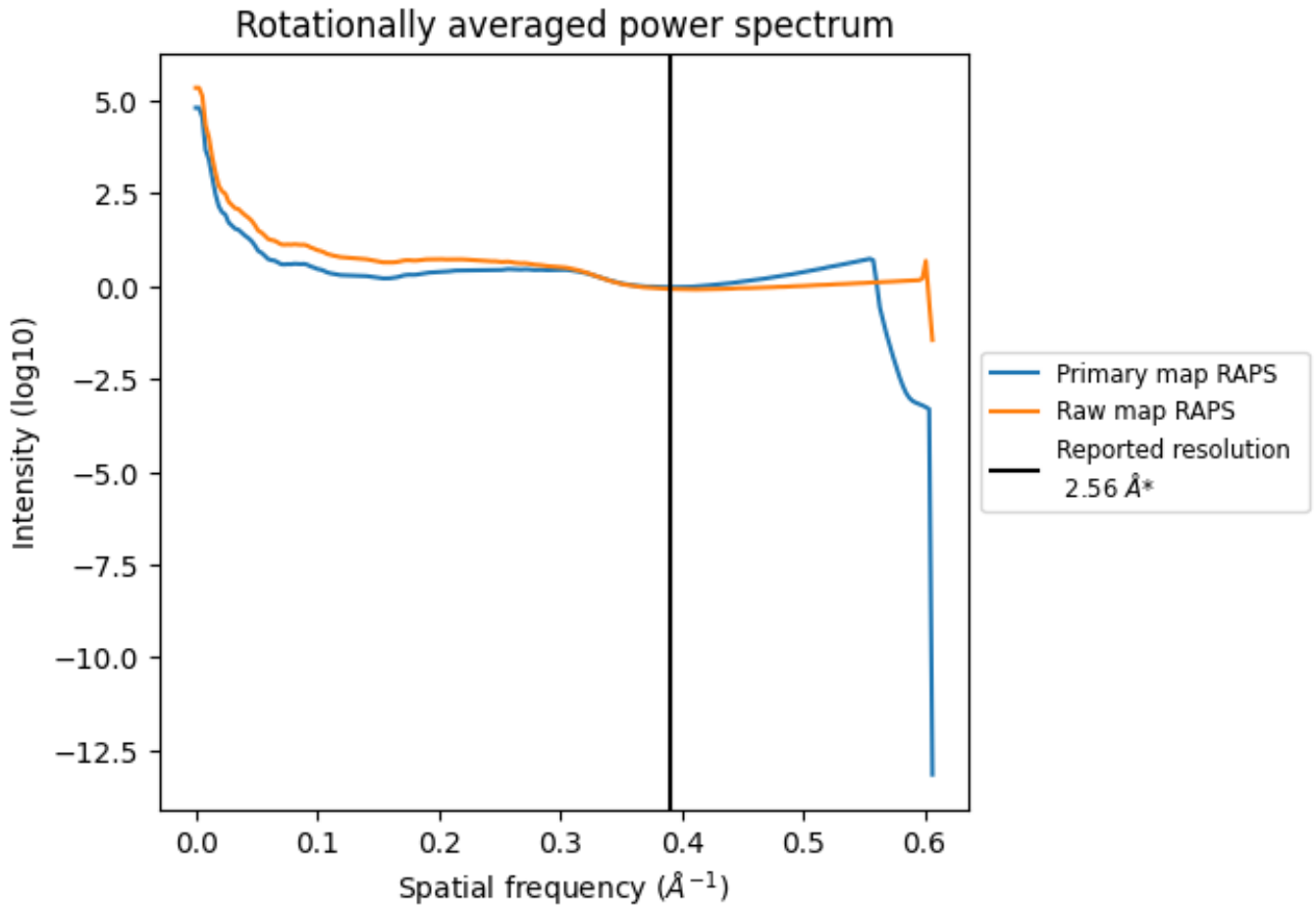
7.2 Volume estimate (i)



The volume at the recommended contour level is 905 nm^3; this corresponds to an approximate mass of 817 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)

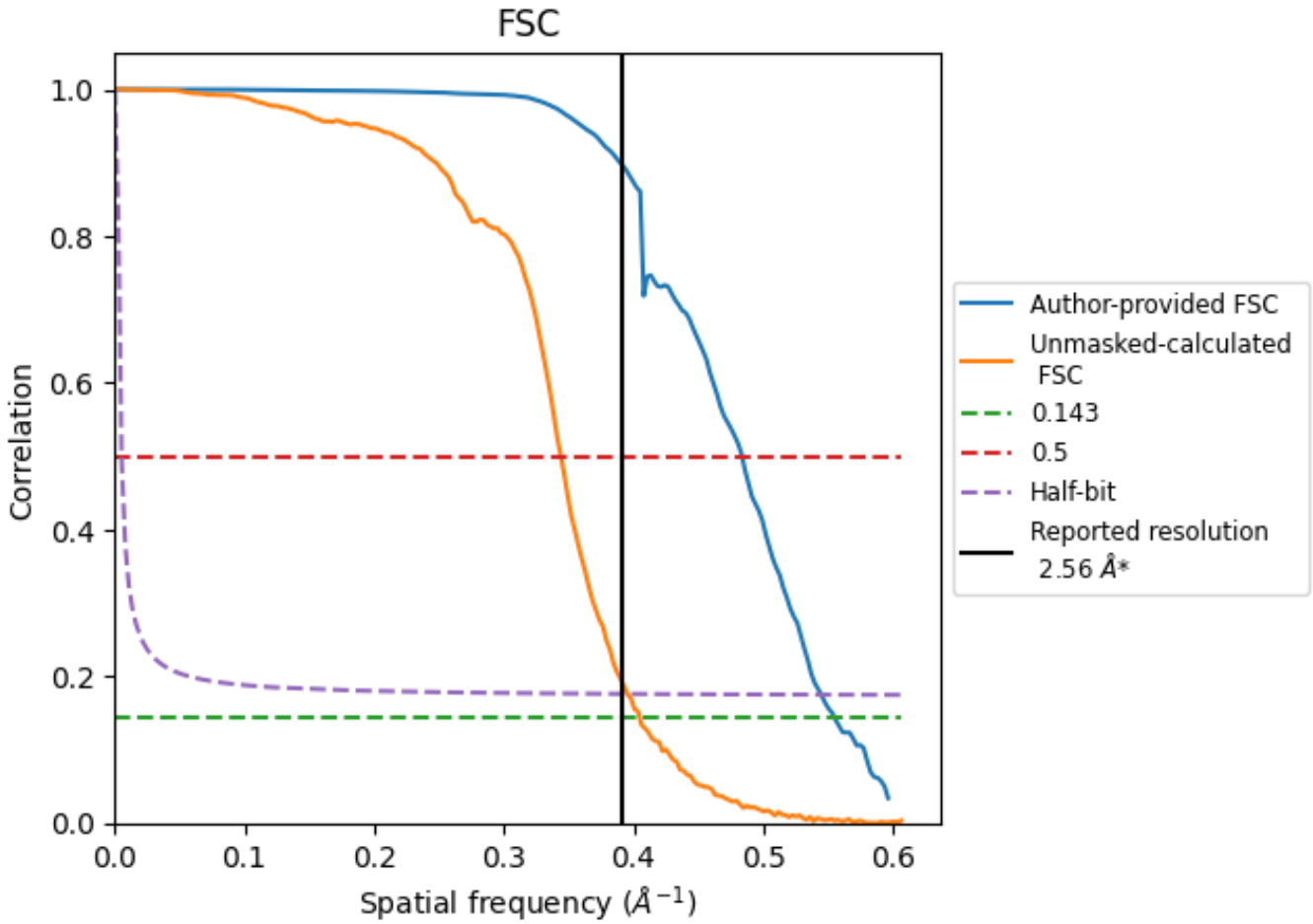


*Reported resolution corresponds to spatial frequency of 0.391 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8.2 Resolution estimates (i)

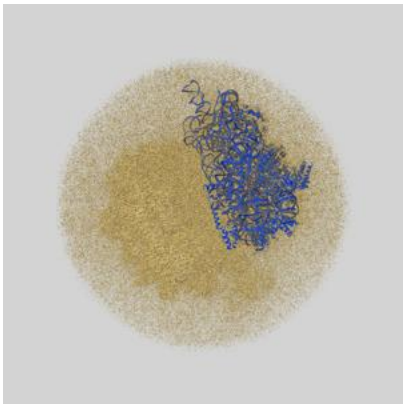
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	1.80	2.07	1.84
Unmasked-calculated*	2.47	2.91	2.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 1.80 differs from the reported value 2.56 by more than 10 %

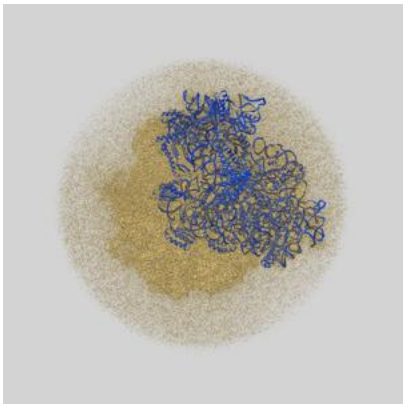
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47169 and PDB model 9DUL. Per-residue inclusion information can be found in section 3 on page 8.

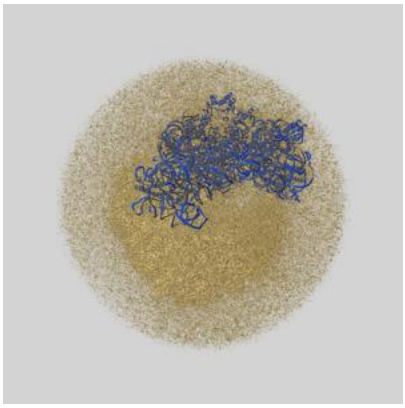
9.1 Map-model overlay



X



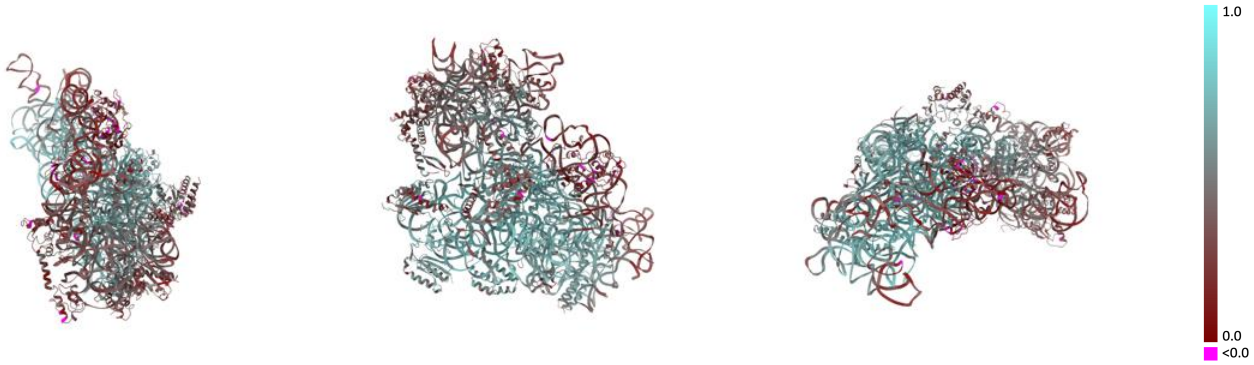
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.334 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

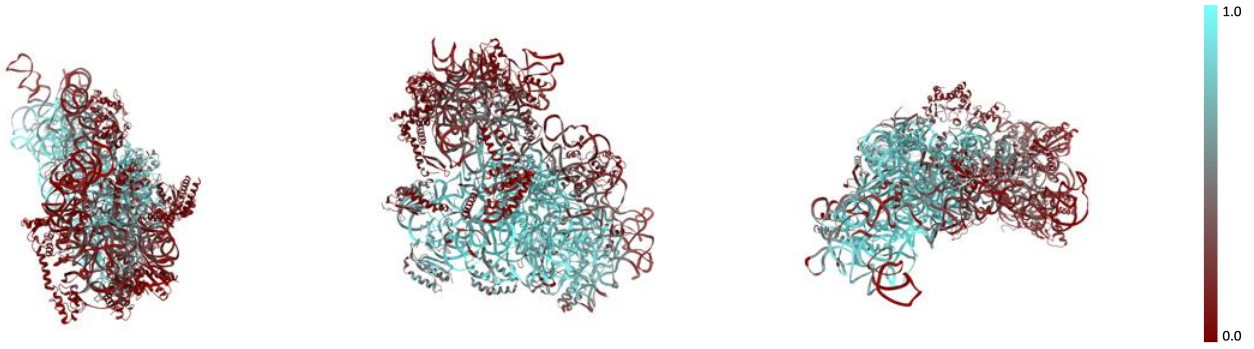
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

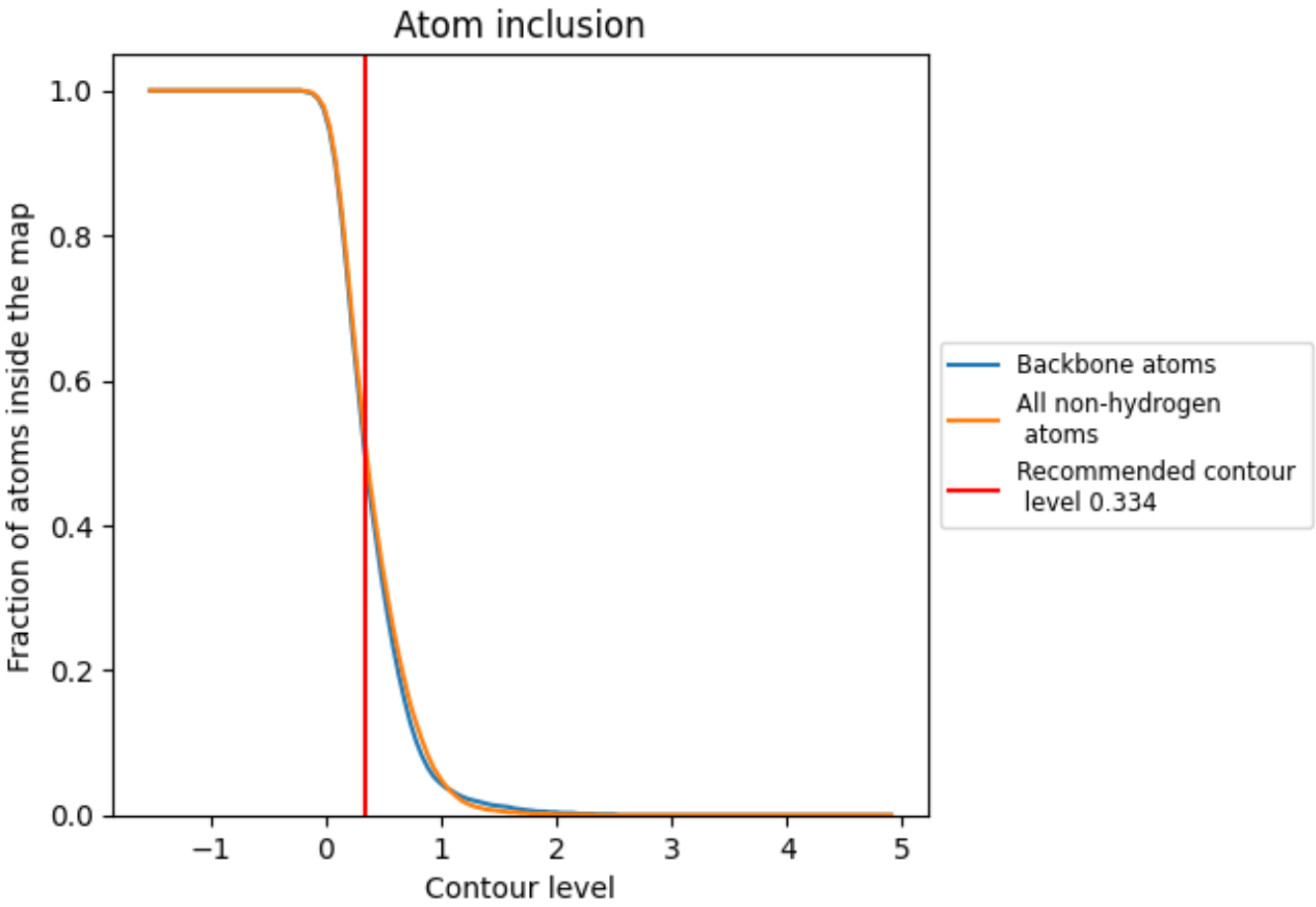
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.334).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 52% 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 (0.334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.5100
A	0.6140	0.5420
B	0.1390	0.3880
C	0.2960	0.4920
D	0.2060	0.2350
E	0.8160	0.6970
F	0.5490	0.5670
G	0.1200	0.3710
H	0.7900	0.6850
I	0.1460	0.3710
J	0.1790	0.3920
K	0.5310	0.5540
L	0.4510	0.3880
M	0.0980	0.3170
N	0.1780	0.3940
O	0.7350	0.6570
P	0.5200	0.4810
Q	0.5420	0.5210
R	0.6120	0.6020
S	0.0640	0.2970
T	0.7160	0.6430
U	0.0300	0.2550