Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 05:02 pm BST

PDB ID	:	8R6F
EMDB ID	:	EMD-18951
Title	:	CryoEM structure of wheat 40S ribosomal subunit, body domain
Authors	:	Kravchenko, O.V.; Baymukhametov, T.N.; Afonina, Z.A.; Vasilenko, K.S.
Deposited on	:	2023-11-22
Resolution	:	2.34 Å(reported)
Based on initial model	:	7qix

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:

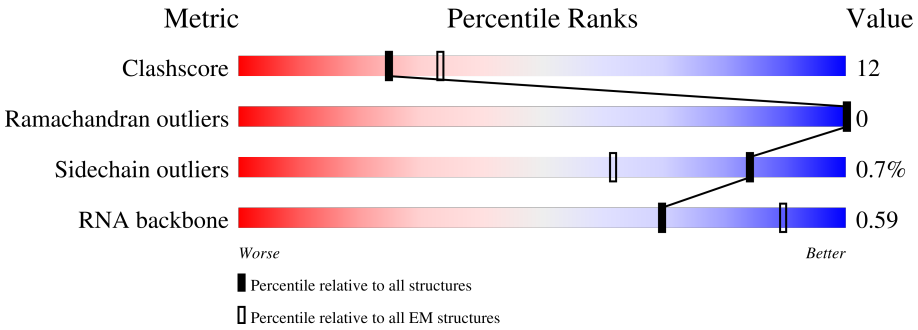
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.34 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	Y	137	66% 25% 9%
2	X	142	81% 17%
3	E	265	81% 17%
4	O	151	64% 23% 14%
5	W	130	75% 24%
6	b	86	6% 97%
7	e	62	77% 23%

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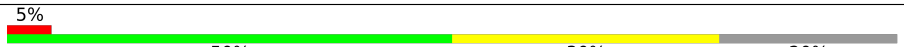
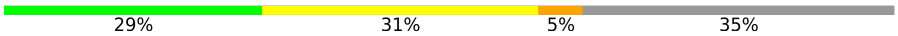
Mol	Chain	Length	Quality of chain
8	k	308	
9	B	263	
10	V	81	
11	a	139	
12	J	195	
13	C	275	
14	G	250	
15	H	192	
16	h	143	
17	L	159	
18	N	151	
19	n	25	
20	I	224	
21	A	1810	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 49016 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	124	Total	C	N	O	S	0	0
			1014	648	196	168	2		

- Molecule 2 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	140	Total	C	N	O	S	0	0
			1088	690	212	183	3		

- Molecule 3 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	260	Total	C	N	O	S	0	0
			2077	1322	387	361	7		

- Molecule 4 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	130	Total	C	N	O	S	0	0
			984	603	195	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	conflict	UNP A0A3B6SS17

- Molecule 5 is a protein called Small ribosomal subunit protein uS8c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	129	Total	C	N	O	S	0	0
			1032	659	188	180	5		

- Molecule 6 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	83	Total	C	N	O	S	0	0
			645	405	117	116	7		

- Molecule 7 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	e	48	Total	C	N	O	0	0
			383	232	87	64		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	199	Total	C	N	O	S	0	0
			1586	1004	285	286	11		

- Molecule 9 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	210	Total	C	N	O	S	0	0
			1716	1094	310	303	9		

- Molecule 10 is a protein called Genome assembly, chromosome: II.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	81	Total	C	N	O	S	0	0
			630	389	116	122	3		

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	98	Total	C	N	O	S	0	0
			794	487	172	128	7		

- Molecule 12 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	181	Total	C	N	O	S	0	0
			1494	947	298	245	4		

- Molecule 13 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	214	Total	C	N	O	S	0	0
			1660	1070	294	287	9		

- Molecule 14 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total	C	N	O	S	0	0
			1856	1157	366	325	8		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	184	Total	C	N	O	S	0	0
			1508	962	278	266	2		

- Molecule 16 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	27	Total	C	N	O	S	0	0
			208	129	34	42	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	146	Total	C	N	O	S	0	0
			1167	745	224	193	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	141	Total	C	N	O	S	0	0
			1138	731	215	190	2		

- Molecule 19 is a protein called Large ribosomal subunit protein eL41z/eL41y/eL41x/eL41w /eL41v.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	n	23	Total	C	N	O	S	0	0
			222	136	59	24	3		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	186	Total	C	N	O	S	0	0
			1510	936	302	268	4		

- Molecule 21 is a RNA chain called RNA (1177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	1177	Total	C	N	O	P	0	0
			25190	11273	4545	8196	1176		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	a	1	Total	Zn	0
			1	1	

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	G	1	Total	Mg	0
			1	1	
23	A	31	Total	Mg	0
			31	31	

- Molecule 24 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
24	A	14	Total	K	0
			14	14	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	Y	6	Total	O	0
			6	6	
25	X	14	Total	O	0
			14	14	
25	E	24	Total	O	0
			24	24	
25	O	3	Total	O	0
			3	3	

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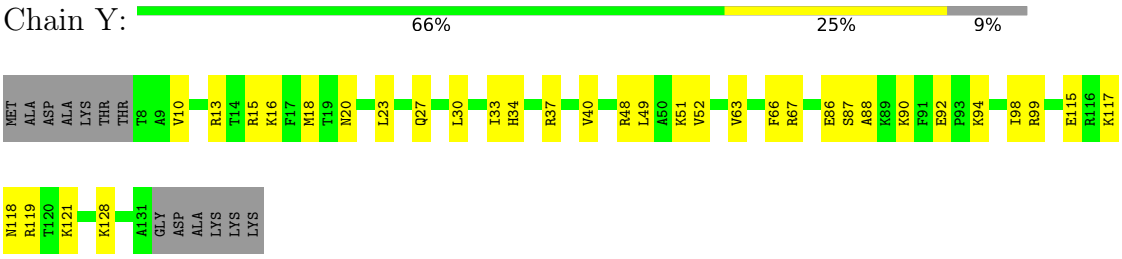
Mol	Chain	Residues	Atoms	AltConf
25	W	6	Total O 6 6	0
25	e	3	Total O 3 3	0
25	B	2	Total O 2 2	0
25	a	8	Total O 8 8	0
25	J	14	Total O 14 14	0
25	C	10	Total O 10 10	0
25	G	7	Total O 7 7	0
25	L	24	Total O 24 24	0
25	N	3	Total O 3 3	0
25	I	18	Total O 18 18	0
25	A	925	Total O 925 925	0

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.

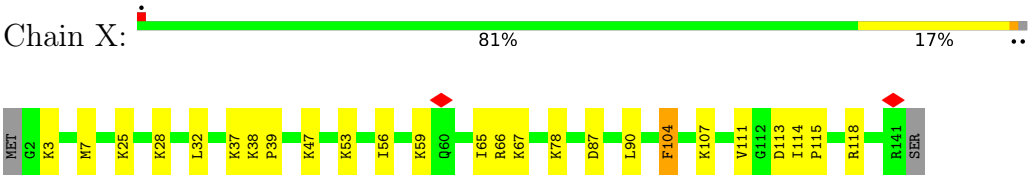
• Molecule 1: 40S ribosomal protein S24

Chain Y:



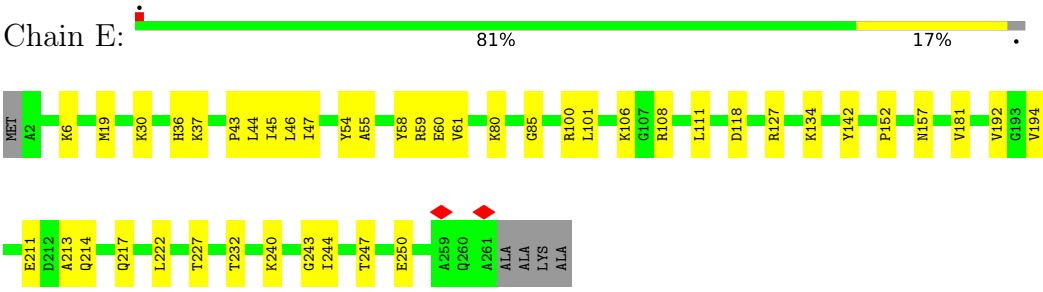
• Molecule 2: 40S ribosomal protein S23

Chain X:



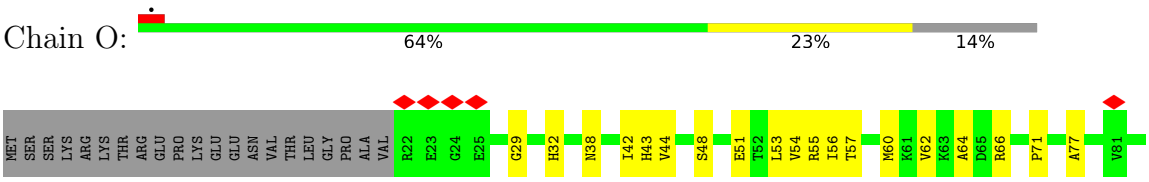
• Molecule 3: 40S ribosomal protein S4

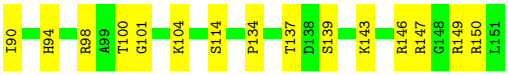
Chain E:



• Molecule 4: 30S ribosomal protein S11, chloroplastic

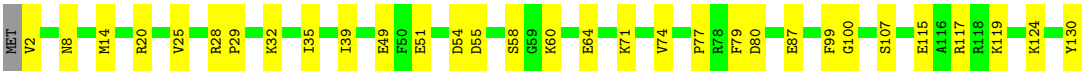
Chain O:





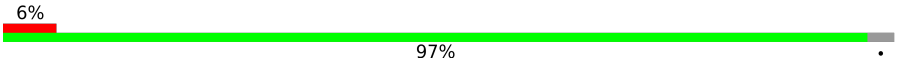
• Molecule 5: Small ribosomal subunit protein uS8c

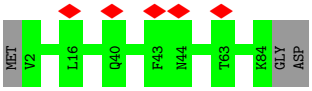
Chain W:



• Molecule 6: 40S ribosomal protein S27

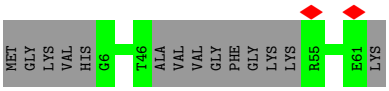
Chain b:





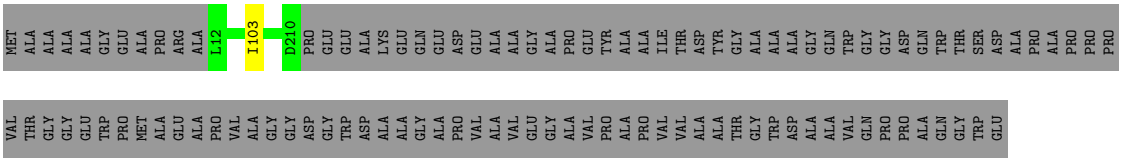
• Molecule 7: 40S ribosomal protein S30

Chain e:



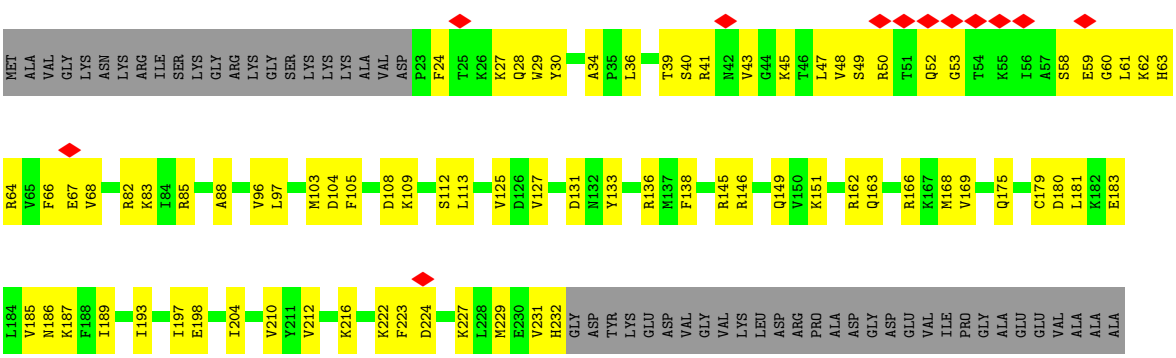
• Molecule 8: Small ribosomal subunit protein uS2

Chain k:



• Molecule 9: Small ribosomal subunit protein eS1

Chain B:

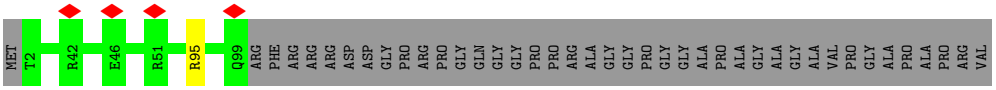


• Molecule 10: Genome assembly, chromosome: II

Chain V:

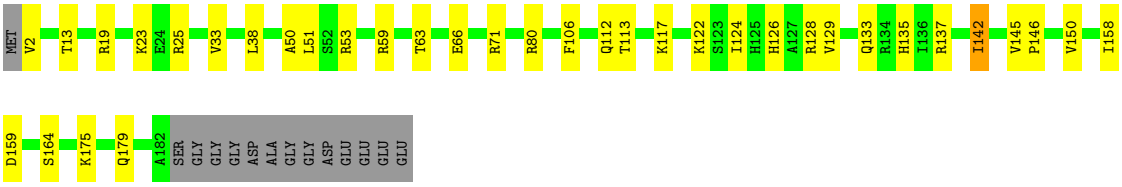
• Molecule 11: 40S ribosomal protein S26

Chain a:



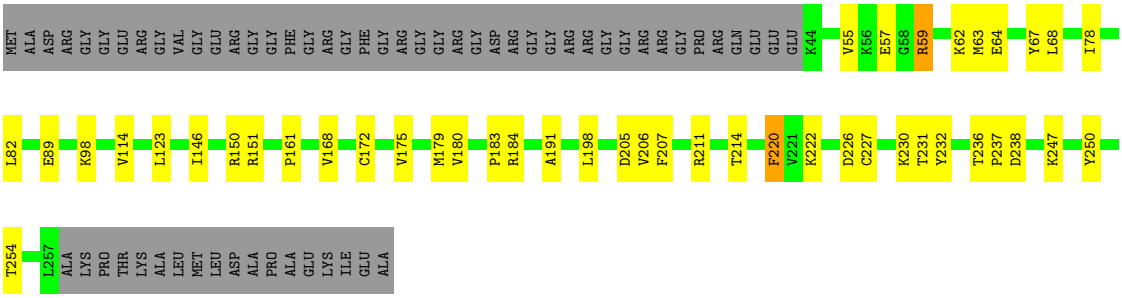
• Molecule 12: 30S ribosomal protein S4, chloroplastic

Chain J:



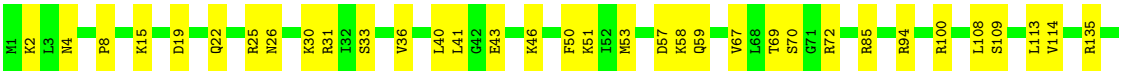
• Molecule 13: S5 DRBM domain-containing protein

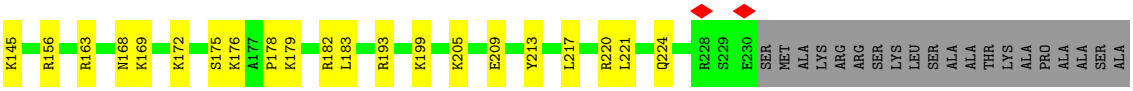
Chain C:



• Molecule 14: 40S ribosomal protein S6

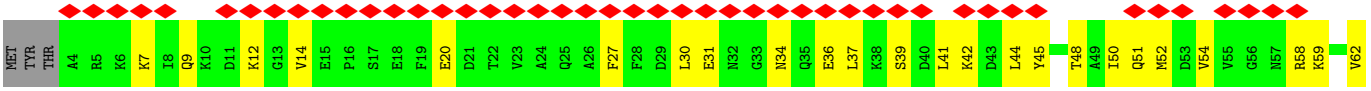
Chain G:

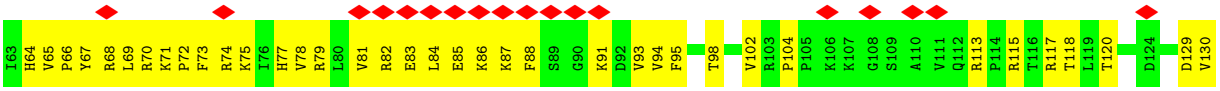


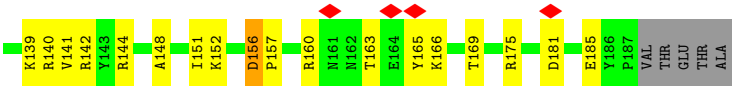


• Molecule 15: 40S ribosomal protein S7

Chain H:

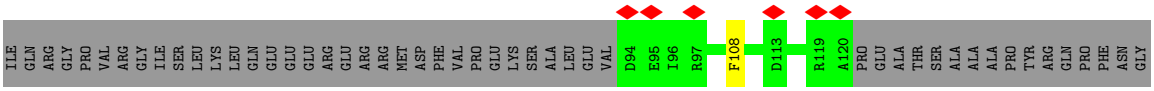


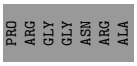




• Molecule 16: 40S ribosomal protein S17

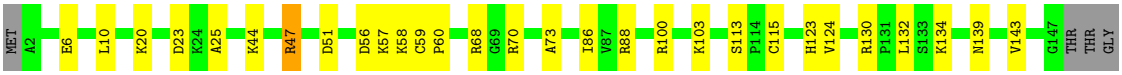
Chain h:





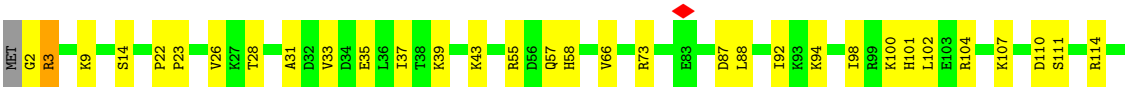
• Molecule 17: Small ribosomal subunit protein uS17 N-terminal domain-containing protein

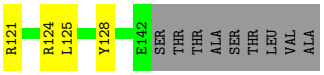
Chain L:



• Molecule 18: Small ribosomal subunit protein uS15 N-terminal domain-containing protein

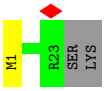
Chain N:





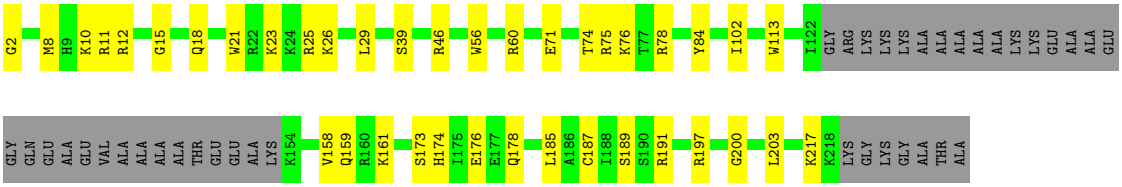
• Molecule 19: Large ribosomal subunit protein eL41z/eL41y/eL41x/eL41w/eL41v

Chain n:



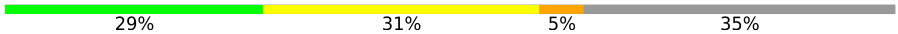
• Molecule 20: 40S ribosomal protein S8

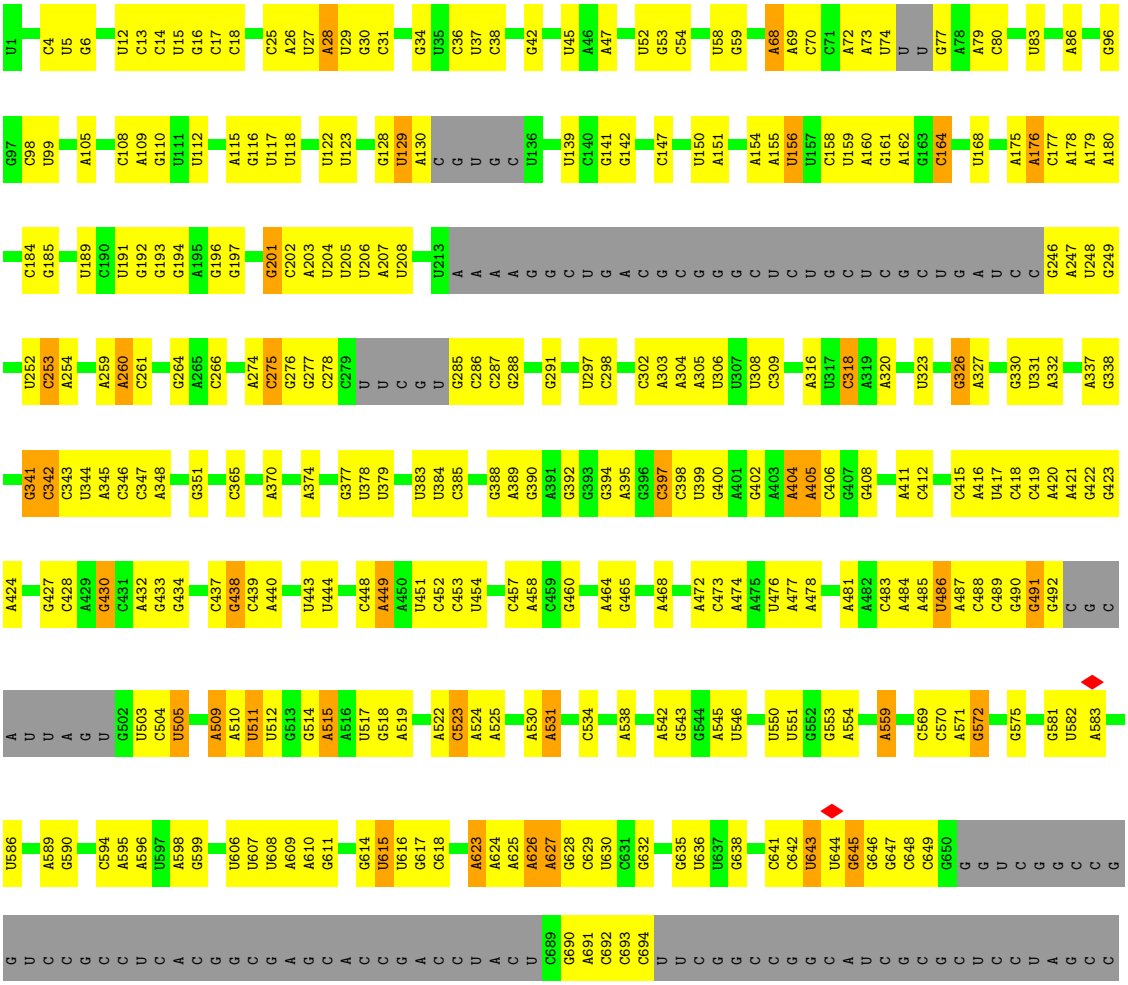
Chain I:

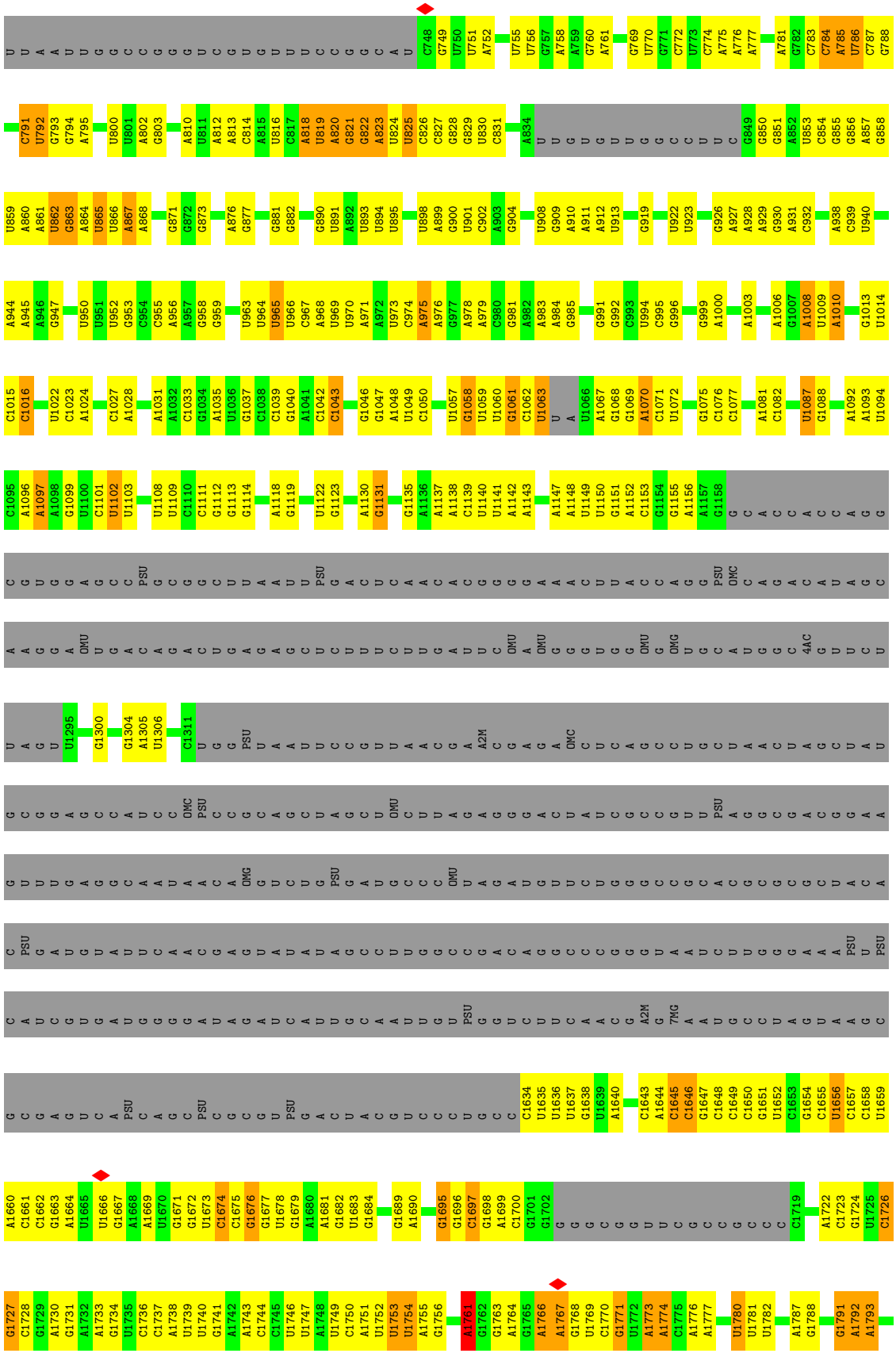


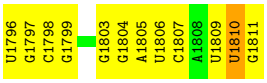
• Molecule 21: RNA (1177-MER)

Chain A:








U1796
G1797
C1798
G1799
G1803
G1804
A1805
U1806
C1807
A1808
U1809
U1810
G1811

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	84	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	9.900	Depositor
Minimum map value	-6.521	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: 6MZ, AME, OMU, K, OMC, MG, 4AC, A2M, OMG, UY1, MA6, IAS, PSU, ZN

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	Y	0.32	0/1029	0.58	0/1366
2	X	0.31	0/1107	0.57	0/1474
3	E	0.28	0/2118	0.56	0/2846
4	O	0.33	0/988	0.60	0/1322
5	W	0.37	0/1050	0.63	0/1405
6	b	0.27	0/656	0.52	0/883
7	e	0.31	0/387	0.63	0/510
8	k	0.32	0/1620	0.56	0/2193
9	B	0.32	0/1745	0.60	0/2344
10	V	0.39	0/628	0.59	0/847
11	a	0.34	0/809	0.57	0/1083
12	J	0.28	0/1522	0.58	0/2037
13	C	0.33	0/1696	0.58	0/2292
14	G	0.29	0/1876	0.60	0/2492
15	H	0.33	0/1535	0.62	0/2065
16	h	0.43	0/209	0.63	0/279
17	L	0.31	0/1193	0.58	0/1599
18	N	0.27	0/1162	0.53	0/1560
19	n	0.39	0/223	0.76	0/283
20	I	0.30	0/1532	0.62	0/2046
21	A	0.30	0/26873	0.78	0/41868
All	All	0.31	0/49958	0.70	0/72794

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1014	0	1099	29	0
2	X	1088	0	1153	20	0
3	E	2077	0	2166	34	0
4	O	984	0	1011	33	0
5	W	1032	0	1068	23	0
6	b	645	0	664	0	0
7	e	383	0	406	0	0
8	k	1586	0	1590	0	0
9	B	1716	0	1790	67	0
10	V	630	0	614	16	0
11	a	794	0	812	0	0
12	J	1494	0	1563	30	0
13	C	1660	0	1743	34	0
14	G	1856	0	1995	47	0
15	H	1508	0	1573	72	0
16	h	208	0	205	0	0
17	L	1167	0	1228	22	0
18	N	1138	0	1228	30	0
19	n	222	0	271	0	0
20	I	1510	0	1555	31	0
21	A	25190	0	12722	475	0
22	a	1	0	0	0	0
23	A	31	0	0	0	0
23	G	1	0	0	0	0
24	A	14	0	0	0	0
25	A	925	0	0	21	0
25	B	2	0	0	0	0
25	C	10	0	0	0	0
25	E	24	0	0	0	0
25	G	7	0	0	0	0
25	I	18	0	0	1	0
25	J	14	0	0	0	0
25	L	24	0	0	2	0
25	N	3	0	0	0	0
25	O	3	0	0	0	0
25	W	6	0	0	0	0
25	X	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	6	0	0	1	0
25	a	8	0	0	0	0
25	e	3	0	0	0	0
All	All	49016	0	36456	843	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 12.

All (843) 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)
21:A:1672:G:H1	21:A:1749:U:H3	1.13	0.94
15:H:88:PHE:HB2	15:H:91:LYS:HD2	1.58	0.85
9:B:34:ALA:O	9:B:41:ARG:HD2	1.76	0.84
9:B:67:GLU:OE1	9:B:85:ARG:HG3	1.78	0.83
20:I:2:GLY:N	21:A:1740:U:HO2'	1.78	0.82
2:X:87:ASP:HB2	21:A:572:G:H4'	1.60	0.82
9:B:27:LYS:HD3	9:B:47:LEU:HD13	1.61	0.82
15:H:66:PRO:HD2	15:H:69:LEU:HD21	1.62	0.82
15:H:31:GLU:HA	15:H:41:LEU:HD13	1.62	0.81
15:H:117:ARG:HH12	21:A:863:G:H5"	1.47	0.80
14:G:43:GLU:OE2	14:G:46:LYS:HE3	1.81	0.79
9:B:162:ARG:HB3	9:B:166:ARG:HH21	1.45	0.79
18:N:87:ASP:CG	18:N:125:LEU:HD21	2.04	0.77
21:A:823:A:H2'	21:A:824:U:C6	2.20	0.76
21:A:784:C:H4'	21:A:785:A:H5'	1.68	0.75
9:B:179:CYS:SG	9:B:187:LYS:NZ	2.60	0.74
12:J:135:HIS:ND1	12:J:164:SER:OG	2.20	0.74
15:H:30:LEU:HB3	15:H:87:LYS:HE3	1.69	0.74
15:H:37:LEU:HD11	15:H:83:GLU:HG3	1.67	0.74
9:B:180:ASP:OD1	9:B:181:LEU:N	2.22	0.73
21:A:691:A:H2'	21:A:692:C:C6	2.24	0.72
4:O:150:ARG:NH1	21:A:1796:U:OP1	2.22	0.72
21:A:876:A:H2'	21:A:877:G:C8	2.24	0.72
9:B:224:ASP:OD2	9:B:227:LYS:HG3	1.89	0.72
21:A:692:C:H2'	21:A:693:C:C6	2.24	0.72
10:V:54:LEU:HD21	10:V:68:LEU:HD13	1.71	0.72
10:V:61:GLN:NE2	21:A:1087:U:O4'	2.23	0.72
10:V:73:GLN:O	10:V:76:ARG:HG2	1.90	0.71
21:A:818:A:H2'	21:A:864:A:C2	2.26	0.71
12:J:175:LYS:NZ	21:A:515:A:OP1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:150:ARG:HB3	13:C:231:THR:HG22	1.71	0.70
21:A:690:G:H2'	21:A:691:A:C8	2.27	0.70
2:X:65:ILE:O	2:X:67:LYS:NZ	2.25	0.69
14:G:4:ASN:ND2	21:A:150:U:O2	2.24	0.69
21:A:873:G:H1	21:A:965:U:H3	1.38	0.69
21:A:444:U:H5'	25:A:2311:HOH:O	1.91	0.69
15:H:72:PRO:HA	15:H:75:LYS:HD2	1.74	0.68
21:A:893:U:H2'	21:A:894:U:C6	2.28	0.68
21:A:141:G:H2'	21:A:142:G:C8	2.29	0.68
18:N:121:ARG:NH1	21:A:873:G:OP1	2.24	0.68
13:C:57:GLU:O	13:C:59:ARG:NH2	2.27	0.68
15:H:65:VAL:HG12	15:H:67:TYR:H	1.60	0.67
9:B:97:LEU:HB3	9:B:232:HIS:CD2	2.29	0.67
14:G:53:MET:HG3	14:G:114:VAL:HG23	1.77	0.67
14:G:25:ARG:NE	14:G:25:ARG:O	2.28	0.67
3:E:58:TYR:OH	3:E:80:LYS:HE3	1.94	0.67
20:I:78:ARG:HH11	20:I:78:ARG:HB2	1.60	0.67
5:W:14:MET:HG2	5:W:25:VAL:HG11	1.77	0.67
21:A:1046:G:H2'	21:A:1047:G:C8	2.29	0.67
21:A:691:A:H2'	21:A:692:C:H6	1.58	0.66
21:A:856:G:H2'	21:A:857:A:C8	2.31	0.66
21:A:890:G:H2'	21:A:891:U:C6	2.31	0.66
1:Y:48:ARG:O	1:Y:52:VAL:HG23	1.95	0.66
20:I:197:ARG:NH1	21:A:261:C:O2	2.29	0.65
9:B:168:MET:HG2	9:B:197:ILE:HG21	1.77	0.65
12:J:2:VAL:N	21:A:465:G:OP1	2.30	0.65
9:B:67:GLU:OE1	9:B:85:ARG:CG	2.44	0.65
18:N:14:SER:HB2	21:A:964:U:H5"	1.79	0.65
13:C:59:ARG:HE	13:C:59:ARG:N	1.93	0.65
9:B:27:LYS:HD3	9:B:47:LEU:CD1	2.26	0.65
20:I:78:ARG:HB2	20:I:78:ARG:NH1	2.11	0.64
21:A:1648:OMC:H5	21:A:1774:6MZ:H6	1.44	0.64
10:V:52:PHE:HZ	10:V:75:LYS:HG3	1.62	0.64
1:Y:88:ALA:O	1:Y:92:GLU:HB2	1.96	0.64
14:G:8:PRO:HD3	14:G:114:VAL:HG13	1.78	0.64
15:H:58:ARG:NH2	15:H:165:TYR:O	2.26	0.64
18:N:110:ASP:O	18:N:114:ARG:HG2	1.98	0.64
21:A:784:C:H4'	21:A:785:A:C5'	2.28	0.64
21:A:1151:G:H2'	21:A:1152:A:C8	2.33	0.63
21:A:690:G:H2'	21:A:691:A:H8	1.61	0.63
12:J:137:ARG:HA	12:J:142:ILE:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:193:ARG:NH2	21:A:288:G:N7	2.40	0.63
2:X:59:LYS:HD2	2:X:113:ASP:HA	1.79	0.63
4:O:147:ARG:HH22	21:A:1796:U:P	2.22	0.63
15:H:70:ARG:O	15:H:74:ARG:HG2	1.98	0.63
21:A:517:U:H2'	21:A:518:G:C8	2.33	0.63
21:A:820:A:H2	21:A:821:G:H1'	1.64	0.63
9:B:175:GLN:N	9:B:175:GLN:OE1	2.32	0.63
14:G:172:LYS:HD2	21:A:73:A:H62	1.64	0.63
15:H:69:LEU:H	15:H:69:LEU:HD23	1.63	0.63
20:I:2:GLY:N	21:A:1740:U:O2'	2.31	0.63
21:A:5:U:H2'	21:A:6:G:H8	1.64	0.63
21:A:944:A:H2'	21:A:945:A:C8	2.33	0.63
15:H:84:LEU:HB3	15:H:88:PHE:CZ	2.33	0.63
3:E:214:GLN:HG3	3:E:244:ILE:HD12	1.82	0.62
21:A:856:G:H2'	21:A:857:A:H8	1.61	0.62
15:H:83:GLU:HA	15:H:86:LYS:HD2	1.80	0.62
21:A:117:U:H2'	21:A:118:U:C6	2.34	0.62
21:A:109:A:H2'	21:A:110:G:C8	2.33	0.62
14:G:213:TYR:O	14:G:217:LEU:HD13	2.00	0.62
21:A:1743:A:N7	25:A:2008:HOH:O	2.31	0.62
17:L:70:ARG:NH1	21:A:803:G:O2'	2.30	0.62
21:A:411:A:H2'	21:A:412:C:C6	2.35	0.62
21:A:1697:C:H2'	21:A:1698:G:C8	2.35	0.61
21:A:824:U:H3	21:A:858:G:H1	1.47	0.61
21:A:893:U:H2'	21:A:894:U:H6	1.64	0.61
12:J:129:VAL:O	12:J:133:GLN:HG2	2.00	0.61
21:A:627:A:N6	21:A:975:A:OP1	2.27	0.61
21:A:929:A:H2'	21:A:930:G:C8	2.35	0.61
5:W:71:LYS:NZ	21:A:1101:C:OP2	2.30	0.61
20:I:76:LYS:HD3	21:A:261:C:H5"	1.80	0.61
9:B:62:LYS:HG2	9:B:63:HIS:CD2	2.36	0.61
18:N:9:LYS:NZ	21:A:1040:G:OP2	2.34	0.61
20:I:174:HIS:O	20:I:178:GLN:HG2	2.01	0.61
21:A:17:C:O2'	21:A:1142:A:N1	2.33	0.61
4:O:143:LYS:HG3	21:A:996:G:P	2.41	0.61
15:H:88:PHE:HE1	15:H:93:VAL:HB	1.66	0.61
21:A:1650:C:H2'	21:A:1651:G:C8	2.36	0.61
12:J:59:ARG:HD3	13:C:183:PRO:HG2	1.83	0.60
13:C:114:VAL:HG23	13:C:146:ILE:HD11	1.84	0.60
21:A:829:G:H1	21:A:853:U:H3	1.49	0.60
1:Y:90:LYS:HB3	1:Y:90:LYS:HZ2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:61:LEU:HA	9:B:64:ARG:HD2	1.83	0.60
21:A:595:A:H2'	21:A:596:A:C8	2.36	0.60
21:A:626:A:HO2'	21:A:1037:G:H5'	1.65	0.59
12:J:23:LYS:HE2	21:A:559:A:H4'	1.83	0.59
14:G:213:TYR:CZ	14:G:217:LEU:HD11	2.36	0.59
15:H:74:ARG:HH22	15:H:129:ASP:HA	1.67	0.59
21:A:785:A:H5"	21:A:786:U:C5	2.37	0.59
21:A:785:A:H5"	21:A:786:U:C6	2.38	0.59
3:E:152:PRO:HD2	14:G:220:ARG:HH12	1.68	0.59
18:N:101:HIS:HA	18:N:104:ARG:HE	1.67	0.59
12:J:175:LYS:O	12:J:179:GLN:HG3	2.02	0.59
14:G:31:ARG:NH2	21:A:1690:A:O3'	2.36	0.59
18:N:87:ASP:OD1	18:N:88:LEU:N	2.35	0.59
14:G:19:ASP:OD1	14:G:19:ASP:N	2.35	0.59
9:B:131:ASP:OD1	9:B:131:ASP:N	2.35	0.59
3:E:181:VAL:HG12	3:E:227:THR:HA	1.84	0.59
20:I:185:LEU:HB3	20:I:203:LEU:HD12	1.83	0.59
21:A:477:A:H1'	25:A:2631:HOH:O	2.02	0.59
5:W:87:GLU:OE1	5:W:117:ARG:NH2	2.35	0.58
21:A:96:G:N7	25:A:2012:HOH:O	2.31	0.58
3:E:55:ALA:HB1	3:E:60:GLU:HB3	1.83	0.58
15:H:59:LYS:O	15:H:91:LYS:HA	2.03	0.58
15:H:27:PHE:CZ	15:H:84:LEU:HD21	2.38	0.58
21:A:5:U:H2'	21:A:6:G:C8	2.38	0.58
4:O:53:LEU:HA	9:B:24:PHE:CE2	2.38	0.58
21:A:1063:U:H3	21:A:1067:A:H61	1.50	0.58
2:X:104:PHE:HB2	2:X:118:ARG:C	2.24	0.58
13:C:67:TYR:OH	13:C:146:ILE:HG22	2.03	0.58
14:G:182:ARG:NH2	21:A:141:G:O6	2.34	0.58
21:A:485:A:H2'	21:A:486:U:C6	2.39	0.58
15:H:115:ARG:HA	15:H:118:THR:HG23	1.86	0.58
18:N:87:ASP:OD2	18:N:125:LEU:HD21	2.04	0.58
21:A:1740:U:H2'	21:A:1741:G:O4'	2.04	0.58
21:A:1696:G:H2'	21:A:1697:C:C6	2.38	0.57
12:J:50:ALA:HA	12:J:53:ARG:NH1	2.19	0.57
18:N:55:ARG:HD3	21:A:965:U:H5'	1.85	0.57
21:A:454:U:H5	25:A:2416:HOH:O	1.87	0.57
21:A:823:A:H2'	21:A:824:U:H6	1.69	0.57
21:A:1743:A:H2'	21:A:1744:C:H6	1.69	0.57
4:O:137:THR:HG23	21:A:891:U:H1'	1.84	0.57
15:H:163:THR:HA	15:H:166:LYS:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:693:C:H2'	21:A:694:C:C6	2.40	0.57
1:Y:48:ARG:HA	1:Y:51:LYS:HE2	1.86	0.57
21:A:1147:A:N7	25:A:2018:HOH:O	2.32	0.57
15:H:71:LYS:HB2	15:H:72:PRO:HD3	1.86	0.57
13:C:55:VAL:HG21	13:C:78:ILE:HG23	1.86	0.57
14:G:85:ARG:HD2	21:A:159:U:H3'	1.87	0.57
5:W:35:ILE:O	5:W:39:ILE:HD12	2.05	0.57
15:H:44:LEU:HG	15:H:73:PHE:CZ	2.40	0.57
5:W:107:SER:HA	21:A:810:A:C8	2.39	0.56
21:A:74:U:O2'	21:A:77:G:N2	2.38	0.56
21:A:464:A:H3'	21:A:465:G:H8	1.70	0.56
21:A:543:G:OP2	21:A:543:G:N2	2.31	0.56
21:A:812:A:H2'	21:A:813:A:H8	1.70	0.56
21:A:1696:G:H2'	21:A:1697:C:H6	1.69	0.56
21:A:451:U:H2'	21:A:452:C:O4'	2.05	0.56
17:L:88:ARG:HD2	25:L:201:HOH:O	2.05	0.56
3:E:106:LYS:NZ	21:A:794:G:OP1	2.34	0.56
15:H:81:VAL:O	15:H:85:GLU:HB2	2.05	0.56
21:A:1659:U:H2'	21:A:1660:A:C8	2.41	0.56
15:H:88:PHE:CE1	15:H:93:VAL:HB	2.40	0.56
18:N:28:THR:HG22	18:N:33:VAL:HG23	1.88	0.56
21:A:323:U:H4'	21:A:327:A:C8	2.41	0.56
15:H:7:LYS:HE2	15:H:7:LYS:HA	1.87	0.56
21:A:430:G:N7	25:A:2024:HOH:O	2.33	0.56
4:O:60:MET:HG3	21:A:904:G:H4'	1.88	0.56
21:A:862:U:H2'	21:A:863:G:H8	1.70	0.56
21:A:1723:C:H2'	21:A:1724:G:H8	1.71	0.56
4:O:29:GLY:O	4:O:94:HIS:N	2.36	0.56
4:O:101:GLY:HA3	4:O:134:PRO:HG2	1.87	0.56
14:G:221:LEU:HD12	14:G:224:GLN:OE1	2.05	0.55
14:G:50:PHE:HB3	14:G:113:LEU:HD22	1.88	0.55
14:G:179:LYS:HG3	21:A:80:C:H1'	1.88	0.55
21:A:1787:A:H2'	21:A:1788:G:C8	2.41	0.55
14:G:168:ASN:OD1	14:G:169:LYS:N	2.39	0.55
15:H:84:LEU:HD22	15:H:95:PHE:HZ	1.71	0.55
3:E:134:LYS:NZ	21:A:202:C:OP1	2.31	0.55
17:L:6:GLU:CG	17:L:10:LEU:HD11	2.36	0.55
21:A:646:G:N2	21:A:694:C:C2	2.74	0.55
9:B:34:ALA:O	9:B:41:ARG:CD	2.52	0.55
9:B:183:GLU:HA	9:B:186:ASN:HB2	1.87	0.55
1:Y:15:ARG:HD2	21:A:783:C:N4	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:818:A:H2'	21:A:864:A:N1	2.22	0.55
21:A:865:U:H2'	21:A:866:U:C6	2.42	0.55
9:B:60:GLY:O	9:B:64:ARG:NE	2.40	0.55
15:H:141:VAL:HG22	15:H:151:ILE:HG12	1.89	0.55
21:A:16:G:H2'	21:A:17:C:C6	2.42	0.55
21:A:758:A:H2	21:A:803:G:H22	1.55	0.55
10:V:9:VAL:HG13	13:C:161:PRO:HG3	1.90	0.54
14:G:156:ARG:HH21	14:G:183:LEU:HD21	1.72	0.54
21:A:820:A:P	21:A:863:G:H22	2.30	0.54
21:A:411:A:H2'	21:A:412:C:H6	1.72	0.54
4:O:32:HIS:HB2	4:O:43:HIS:HB3	1.89	0.54
21:A:12:U:H2'	21:A:13:C:C6	2.43	0.54
21:A:452:C:H2'	21:A:453:C:C6	2.43	0.54
21:A:1092:A:H2'	21:A:1093:A:C8	2.43	0.54
21:A:1069:G:C2'	21:A:1070:A:H5'	2.38	0.54
21:A:1669:A:C2	21:A:1753:U:C2	2.95	0.54
12:J:112:GLN:HE21	12:J:124:ILE:HG13	1.71	0.54
12:J:146:PRO:HD2	21:A:478:A:H5"	1.90	0.54
21:A:385:C:O2'	21:A:761:A:N1	2.36	0.54
21:A:554:A:N3	25:A:2020:HOH:O	2.32	0.54
4:O:100:THR:HG21	4:O:104:LYS:HD2	1.89	0.54
21:A:1739:U:H2'	21:A:1740:U:C6	2.43	0.54
21:A:1787:A:H2'	21:A:1788:G:H8	1.73	0.54
15:H:84:LEU:HD22	15:H:95:PHE:CZ	2.42	0.54
15:H:104:PRO:HD3	21:A:643:U:C2	2.43	0.54
21:A:38:OMC:O2	21:A:474:A:N1	2.41	0.54
21:A:860:A:N1	21:A:862:U:H1'	2.23	0.54
9:B:28:GLN:NE2	9:B:50:ARG:HG3	2.23	0.53
21:A:629:C:H2'	21:A:630:U:C6	2.43	0.53
21:A:15:U:H2'	21:A:16:G:O4'	2.08	0.53
21:A:1119:G:O2'	21:A:1135:G:O6	2.24	0.53
13:C:175:VAL:HG11	13:C:220:PHE:HA	1.91	0.53
14:G:193:ARG:HD2	21:A:287:C:OP2	2.08	0.53
15:H:12:LYS:O	15:H:14:VAL:N	2.40	0.53
17:L:113:SER:OG	17:L:115:CYS:SG	2.59	0.53
21:A:276:G:H2'	21:A:277:G:H8	1.72	0.53
4:O:38:ASN:ND2	21:A:908:U:OP2	2.36	0.53
15:H:152:LYS:HD3	15:H:185:GLU:HG3	1.90	0.53
21:A:108:C:H2'	21:A:109:A:H8	1.74	0.53
9:B:52:GLN:HG2	9:B:53:GLY:H	1.74	0.53
9:B:108:ASP:O	9:B:112:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:50:ALA:HA	12:J:53:ARG:HH12	1.73	0.53
20:I:187:CYS:HB2	20:I:203:LEU:HD21	1.91	0.53
12:J:66:GLU:HG2	12:J:71:ARG:CZ	2.39	0.53
15:H:88:PHE:HD1	15:H:91:LYS:HB2	1.74	0.53
21:A:122:U:H2'	21:A:123:OMU:H6	1.90	0.53
21:A:862:U:H2'	21:A:863:G:C8	2.43	0.53
3:E:211:GLU:HG3	3:E:217:GLN:HG3	1.90	0.53
14:G:2:LYS:HD3	14:G:15:LYS:HD2	1.89	0.53
5:W:2:VAL:N	21:A:1039:C:HO2'	2.06	0.53
10:V:59:ARG:HA	10:V:64:ALA:HB2	1.91	0.53
1:Y:23:LEU:HD11	3:E:60:GLU:HG2	1.91	0.53
1:Y:118:ASN:HA	1:Y:121:LYS:HE3	1.90	0.53
21:A:1069:G:H2'	21:A:1070:A:H5'	1.91	0.53
3:E:47:ILE:HG23	3:E:111:LEU:HD11	1.91	0.52
4:O:53:LEU:HD11	9:B:47:LEU:HD21	1.90	0.52
15:H:120:THR:HG23	21:A:643:U:OP2	2.09	0.52
18:N:31:ALA:O	18:N:35:GLU:HG3	2.10	0.52
9:B:104:ASP:OD1	9:B:105:PHE:N	2.41	0.52
15:H:54:VAL:HG21	15:H:169:THR:HG22	1.91	0.52
15:H:166:LYS:H	15:H:166:LYS:HD2	1.74	0.52
21:A:274:A:H2'	21:A:275:C:O4'	2.09	0.52
21:A:1767:A:HO2'	21:A:1768:G:H8	1.56	0.52
2:X:53:LYS:HE3	2:X:90:LEU:HG	1.91	0.52
4:O:42:ILE:HB	4:O:56:ILE:HG22	1.92	0.52
4:O:66:ARG:HB3	21:A:910:A:H5"	1.91	0.52
18:N:28:THR:CG2	18:N:33:VAL:HG23	2.39	0.52
21:A:344:U:H2'	21:A:345:A:C8	2.45	0.52
21:A:785:A:H2'	21:A:785:A:N3	2.24	0.52
21:A:985:G:H4'	21:A:1787:A:H4'	1.92	0.52
10:V:52:PHE:CZ	10:V:75:LYS:HG3	2.43	0.52
13:C:226:ASP:OD2	13:C:230:LYS:HE3	2.10	0.52
12:J:150:VAL:HG11	12:J:158:ILE:HD11	1.91	0.52
10:V:74:GLN:O	10:V:78:GLU:HG3	2.10	0.52
18:N:22:PRO:HG3	18:N:66:VAL:HA	1.91	0.52
18:N:107:LYS:NZ	21:A:1024:A:OP2	2.43	0.52
21:A:1122:PSU:H2'	21:A:1123:G:C8	2.44	0.52
21:A:1769:U:H2'	21:A:1770:C:C6	2.44	0.52
1:Y:20:ASN:ND2	3:E:54:TYR:O	2.42	0.52
13:C:180:VAL:HB	13:C:207:PHE:HB2	1.92	0.52
21:A:178:A:H2'	21:A:179:A:C8	2.45	0.52
21:A:820:A:H3'	21:A:821:G:H4'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:958:G:H2'	21:A:959:G:H8	1.74	0.52
15:H:41:LEU:O	15:H:41:LEU:HD23	2.10	0.51
15:H:88:PHE:CD1	15:H:91:LYS:HB2	2.46	0.51
18:N:39:LYS:C	18:N:43:LYS:HZ2	2.14	0.51
21:A:1149:U:H2'	21:A:1150:U:C6	2.44	0.51
2:X:28:LYS:O	2:X:32:LEU:HB2	2.09	0.51
2:X:66:ARG:HG3	2:X:114:ILE:HG12	1.91	0.51
21:A:30:G:H2'	21:A:31:C:C6	2.45	0.51
21:A:207:A:H2'	21:A:208:PSU:H6	1.74	0.51
4:O:56:ILE:HG23	4:O:77:ALA:HB1	1.93	0.51
17:L:73:ALA:HB1	17:L:123:HIS:HE1	1.76	0.51
21:A:813:A:H2'	21:A:814:C:H6	1.75	0.51
13:C:151:ARG:HB3	13:C:161:PRO:HB2	1.92	0.51
21:A:1122:PSU:H2'	21:A:1123:G:H8	1.76	0.51
21:A:1743:A:H2'	21:A:1744:C:C6	2.46	0.51
4:O:53:LEU:HD23	4:O:90:ILE:HD11	1.90	0.51
12:J:113:THR:O	12:J:117:LYS:HG2	2.10	0.51
21:A:820:A:C2	21:A:821:G:H1'	2.46	0.51
21:A:1763:G:H2'	21:A:1764:A:C8	2.46	0.51
3:E:37:LYS:NZ	21:A:302:C:OP2	2.43	0.51
17:L:103:LYS:HD2	21:A:636:PSU:OP1	2.11	0.51
21:A:1637:PSU:H2'	21:A:1638:G:C8	2.46	0.51
9:B:66:PHE:HE2	9:B:88:ALA:HB2	1.76	0.51
10:V:32:VAL:HG22	10:V:59:ARG:HD2	1.92	0.51
13:C:179:MET:HG3	13:C:227:CYS:SG	2.51	0.51
21:A:1015:C:H2'	21:A:1016:C:O4'	2.11	0.51
1:Y:20:ASN:ND2	1:Y:23:LEU:HD12	2.26	0.51
4:O:139:SER:N	21:A:932:C:HO2'	2.08	0.51
12:J:137:ARG:NH2	12:J:159:ASP:OD2	2.44	0.51
20:I:12:ARG:HG3	20:I:18:GLN:HG2	1.92	0.51
14:G:172:LYS:NZ	21:A:72:A:N7	2.59	0.50
15:H:117:ARG:NH1	21:A:863:G:H5"	2.22	0.50
21:A:484:A:H2'	21:A:485:A:C8	2.46	0.50
21:A:569:C:O2'	21:A:581:G:N2	2.42	0.50
3:E:100:ARG:NH2	3:E:118:ASP:O	2.44	0.50
9:B:185:VAL:O	9:B:189:ILE:HG12	2.11	0.50
21:A:399:U:H2'	21:A:400:G:O4'	2.11	0.50
21:A:452:C:H2'	21:A:453:C:H6	1.76	0.50
21:A:1750:C:H2'	21:A:1751:A:C8	2.45	0.50
3:E:6:LYS:O	3:E:30:LYS:NZ	2.25	0.50
4:O:38:ASN:OD1	21:A:908:U:H5	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:62:VAL:HG12	4:O:64:ALA:H	1.76	0.50
9:B:198:GLU:HB3	21:A:1061:G:N7	2.26	0.50
21:A:484:A:H2'	21:A:485:A:H8	1.77	0.50
21:A:900:G:H1	21:A:922:U:H3	1.57	0.50
21:A:1699:A:H2'	21:A:1700:C:H6	1.76	0.50
21:A:1736:C:H2'	21:A:1737:C:C6	2.45	0.50
21:A:1796:U:H2'	21:A:1797:G:H8	1.76	0.50
3:E:43:PRO:HD2	3:E:46:LEU:HD22	1.93	0.50
3:E:202:LYS:HE3	25:A:2134:HOH:O	2.12	0.50
9:B:43:VAL:HG13	9:B:68:VAL:HG11	1.94	0.50
15:H:31:GLU:HG2	15:H:41:LEU:HD21	1.93	0.50
17:L:47:ARG:HH21	17:L:51:ASP:CG	2.15	0.50
20:I:173:SER:HA	20:I:176:GLU:HB3	1.94	0.50
17:L:58:LYS:HG2	17:L:132:LEU:HD22	1.93	0.50
21:A:52:U:H2'	21:A:53:G:C8	2.47	0.50
21:A:154:A:H2'	21:A:155:A:O4'	2.11	0.50
21:A:791:C:OP1	21:A:792:U:H4'	2.12	0.50
21:A:488:C:H2'	21:A:489:C:C6	2.46	0.50
21:A:1152:A:H2	25:A:2618:HOH:O	1.94	0.50
21:A:206:U:H2'	21:A:207:A:H8	1.77	0.50
21:A:626:A:O2'	21:A:1037:G:H5'	2.11	0.50
9:B:168:MET:HG2	9:B:197:ILE:CG2	2.40	0.49
13:C:55:VAL:HG11	13:C:78:ILE:HA	1.94	0.49
21:A:524:A:H2'	21:A:525:A:C8	2.46	0.49
21:A:606:PSU:H2'	21:A:607:PSU:H6	1.77	0.49
21:A:1723:C:H2'	21:A:1724:G:C8	2.47	0.49
17:L:134:LYS:HB2	21:A:341:G:H3'	1.94	0.49
18:N:110:ASP:OD2	21:A:882:G:N2	2.37	0.49
20:I:71:GLU:HB3	20:I:113:TRP:CH2	2.47	0.49
21:A:1753:U:H2'	21:A:1754:U:C6	2.48	0.49
15:H:34:ASN:H	15:H:37:LEU:HB2	1.77	0.49
20:I:39:SER:HB3	20:I:60:ARG:HG2	1.93	0.49
2:X:67:LYS:HB3	2:X:90:LEU:HD22	1.94	0.49
15:H:27:PHE:HA	15:H:30:LEU:HG	1.95	0.49
18:N:94:LYS:O	18:N:98:ILE:HG13	2.12	0.49
21:A:589:A:H2'	21:A:590:G:C8	2.48	0.49
21:A:862:U:O2'	21:A:863:G:H5'	2.11	0.49
21:A:867:A:H8	21:A:867:A:OP2	1.96	0.49
3:E:59:ARG:NH2	21:A:449:A:OP2	2.42	0.49
5:W:32:LYS:HG2	21:A:641:C:OP1	2.12	0.49
15:H:9:GLN:OE1	15:H:45:TYR:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:6:GLU:HG2	17:L:10:LEU:HD11	1.93	0.49
20:I:10:LYS:NZ	21:A:326:G:O2'	2.45	0.49
21:A:308:PSU:H2'	21:A:309:C:C6	2.48	0.49
21:A:437:C:H2'	21:A:438:G:O4'	2.13	0.49
21:A:1793:MA6:H8	21:A:1793:MA6:H5"	1.93	0.49
2:X:39:PRO:HA	2:X:78:LYS:HD2	1.93	0.49
9:B:29:TRP:HE3	9:B:45:LYS:O	1.95	0.49
15:H:82:ARG:O	15:H:86:LYS:HG3	2.12	0.49
21:A:611:G:N2	21:A:618:C:H5"	2.27	0.49
1:Y:18:MET:HG2	1:Y:27:GLN:HG3	1.95	0.49
21:A:304:A:H2'	21:A:305:A:C8	2.47	0.49
21:A:486:U:O4	21:A:487:A:N6	2.46	0.49
21:A:1152:A:H2'	21:A:1153:C:C6	2.48	0.49
1:Y:20:ASN:HD21	1:Y:23:LEU:HD12	1.78	0.49
13:C:198:LEU:HD13	13:C:206:VAL:HG11	1.95	0.49
15:H:144:ARG:HE	15:H:148:ALA:HB3	1.77	0.49
21:A:206:U:H2'	21:A:207:A:C8	2.47	0.49
21:A:530:A:H2'	21:A:531:A:O4'	2.13	0.49
18:N:33:VAL:O	18:N:37:ILE:HG13	2.12	0.49
21:A:611:G:H5'	21:A:617:G:N2	2.28	0.49
1:Y:13:ARG:HH21	1:Y:33:ILE:HD13	1.78	0.48
3:E:59:ARG:HH12	21:A:449:A:H5"	1.78	0.48
3:E:240:LYS:HB2	21:A:791:C:C5	2.48	0.48
14:G:70:SER:O	14:G:100:ARG:NH1	2.45	0.48
15:H:48:THR:O	15:H:64:HIS:ND1	2.31	0.48
21:A:397:C:H2'	21:A:398:C:C6	2.47	0.48
21:A:1696:G:O2'	21:A:1697:C:H5'	2.12	0.48
14:G:67:VAL:HG12	14:G:69:THR:HG22	1.95	0.48
1:Y:90:LYS:HB3	1:Y:90:LYS:NZ	2.25	0.48
4:O:55:ARG:NH1	21:A:901:U:O2	2.46	0.48
12:J:175:LYS:HB2	21:A:515:A:H5'	1.95	0.48
20:I:197:ARG:NH2	21:A:204:U:O2	2.44	0.48
21:A:606:PSU:H2'	21:A:607:PSU:C6	2.48	0.48
21:A:966:U:H2'	21:A:967:C:H6	1.79	0.48
5:W:20:ARG:HG3	5:W:20:ARG:HH11	1.77	0.48
18:N:73:ARG:NH1	21:A:864:A:C4	2.80	0.48
21:A:184:C:H2'	21:A:185:G:O4'	2.13	0.48
21:A:207:A:H2'	21:A:208:PSU:C6	2.48	0.48
21:A:859:U:H2'	21:A:860:A:C8	2.48	0.48
21:A:939:C:C4	21:A:1082:C:H4'	2.49	0.48
21:A:1112:G:O2'	21:A:1113:G:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:51:GLN:OE1	15:H:59:LYS:HB3	2.13	0.48
21:A:863:G:O2'	21:A:864:A:H5'	2.13	0.48
12:J:80:ARG:HH22	21:A:770:U:P	2.37	0.48
13:C:191:ALA:HB2	21:A:4:C:H4'	1.96	0.48
15:H:78:VAL:O	15:H:82:ARG:HG3	2.14	0.48
21:A:958:G:H2'	21:A:959:G:C8	2.48	0.48
21:A:1798:C:H2'	21:A:1799:G:C8	2.47	0.48
9:B:193:ILE:O	9:B:197:ILE:HG13	2.13	0.48
17:L:6:GLU:HG3	17:L:10:LEU:HD11	1.95	0.48
21:A:550:U:H2'	21:A:551:U:C6	2.49	0.48
21:A:927:A:H2'	21:A:928:A:C8	2.49	0.48
4:O:150:ARG:HD2	21:A:1780:U:O2	2.14	0.48
15:H:64:HIS:HB3	15:H:98:THR:CG2	2.44	0.48
21:A:1746:U:H2'	21:A:1747:U:C6	2.48	0.48
21:A:755:U:H2'	21:A:756:U:C6	2.48	0.48
21:A:1096:A:H4'	21:A:1097:A:O4'	2.14	0.48
21:A:1730:A:H2'	21:A:1731:G:O4'	2.13	0.48
1:Y:128:LYS:HE2	21:A:86:A:H5"	1.95	0.47
14:G:156:ARG:NH2	14:G:183:LEU:HD21	2.29	0.47
17:L:44:LYS:HD2	17:L:44:LYS:N	2.29	0.47
21:A:860:A:C2	21:A:862:U:H1'	2.49	0.47
17:L:20:LYS:NZ	20:I:71:GLU:OE2	2.48	0.47
13:C:211:ARG:HD2	21:A:1102:U:O4	2.14	0.47
21:A:819:U:H1'	21:A:821:G:C5	2.48	0.47
21:A:1674:C:H2'	21:A:1675:C:C6	2.50	0.47
14:G:22:GLN:OE1	14:G:22:GLN:HA	2.13	0.47
21:A:141:G:H2'	21:A:142:G:H8	1.78	0.47
21:A:488:C:H2'	21:A:489:C:H6	1.80	0.47
21:A:615:OMU:HM23	21:A:615:OMU:H1'	1.57	0.47
21:A:1763:G:H2'	21:A:1764:A:H8	1.78	0.47
9:B:222:LYS:NZ	9:B:223:PHE:O	2.46	0.47
21:A:1770:C:H2'	21:A:1771:G:O4'	2.15	0.47
9:B:47:LEU:HD12	9:B:47:LEU:C	2.35	0.47
21:A:253:C:H2'	21:A:254:A:H8	1.79	0.47
21:A:417:U:H2'	21:A:418:OMC:C6	2.49	0.47
21:A:608:U:H2'	21:A:609:A:O4'	2.15	0.47
21:A:825:U:H2'	21:A:826:C:C6	2.50	0.47
3:E:157:ASN:OD1	3:E:222:LEU:HD21	2.14	0.47
10:V:57:PHE:O	10:V:61:GLN:HG2	2.15	0.47
12:J:19:ARG:O	12:J:25:ARG:NH1	2.46	0.47
15:H:79:ARG:HD3	15:H:82:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:86:ILE:HD11	21:A:351:G:H5"	1.96	0.47
21:A:346:C:H3'	25:A:2206:HOH:O	2.14	0.47
21:A:900:G:H2'	21:A:901:U:C6	2.50	0.47
21:A:926:G:H2'	21:A:927:A:H8	1.80	0.47
21:A:1810:U:H4'	21:A:1811:G:C8	2.50	0.47
9:B:149:GLN:HG3	21:A:1071:C:H4'	1.97	0.47
1:Y:34:HIS:HB2	1:Y:37:ARG:HB2	1.96	0.47
14:G:221:LEU:HD12	14:G:221:LEU:HA	1.79	0.47
21:A:1648:OMC:O2	21:A:1648:OMC:O5'	2.33	0.47
18:N:57:GLN:O	18:N:58:HIS:ND1	2.48	0.47
18:N:88:LEU:O	18:N:92:ILE:HG13	2.15	0.47
21:A:751:U:H2'	21:A:752:A:H8	1.80	0.47
21:A:1042:C:H2'	21:A:1043:C:C6	2.50	0.47
9:B:109:LYS:HE3	9:B:113:LEU:HD21	1.97	0.46
14:G:176:LYS:NZ	21:A:68:A:OP1	2.44	0.46
17:L:60:PRO:HG3	17:L:139:ASN:HB3	1.97	0.46
20:I:189:SER:OG	20:I:200:GLY:HA2	2.15	0.46
21:A:259:A:H2'	21:A:260:A:O4'	2.15	0.46
3:E:19:MET:SD	3:E:108:ARG:HD2	2.56	0.46
20:I:8:MET:HE1	20:I:21:TRP:CD1	2.50	0.46
21:A:36:C:H2'	21:A:37:U:C6	2.51	0.46
21:A:276:G:H2'	21:A:277:G:C8	2.49	0.46
4:O:146:ARG:HG2	21:A:1798:C:OP2	2.15	0.46
18:N:3:ARG:HD3	18:N:3:ARG:HA	1.68	0.46
21:A:108:C:H2'	21:A:109:A:C8	2.50	0.46
15:H:166:LYS:HD2	15:H:166:LYS:N	2.31	0.46
20:I:25:ARG:HA	21:A:404:A:H5"	1.97	0.46
21:A:331:U:H2'	21:A:332:A:C8	2.50	0.46
21:A:347:C:H2'	21:A:348:A:H8	1.80	0.46
13:C:250:TYR:O	13:C:254:THR:HG23	2.15	0.46
21:A:205:U:H2'	21:A:206:U:C6	2.51	0.46
21:A:1057:U:N3	21:A:1058:G:O6	2.49	0.46
5:W:49:GLU:OE2	15:H:144:ARG:HA	2.16	0.46
9:B:67:GLU:OE2	9:B:83:LYS:HB3	2.16	0.46
13:C:62:LYS:HB2	13:C:64:GLU:OE1	2.15	0.46
13:C:175:VAL:HG13	13:C:214:THR:HG22	1.98	0.46
21:A:1059:U:C4	21:A:1060:U:C4	3.04	0.46
21:A:1648:OMC:O2	21:A:1648:OMC:O4'	2.34	0.46
21:A:1648:OMC:H2'	21:A:1649:C:O4'	2.15	0.46
21:A:1695:G:C2	21:A:1696:G:C8	3.04	0.46
4:O:51:GLU:HG2	9:B:64:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:184:ARG:HA	13:C:205:ASP:OD2	2.16	0.46
21:A:813:A:H2'	21:A:814:C:C6	2.51	0.46
21:A:983:A:H2'	21:A:984:A:O4'	2.16	0.46
1:Y:10:VAL:HG11	1:Y:40:VAL:HG21	1.98	0.46
12:J:122:LYS:HD2	21:A:483:C:H4'	1.97	0.46
14:G:156:ARG:HE	14:G:156:ARG:HB3	1.21	0.46
21:A:337:A:H2'	21:A:338:G:C8	2.50	0.46
21:A:969:U:H4'	21:A:970:U:O4'	2.16	0.46
2:X:37:LYS:HE2	2:X:37:LYS:HA	1.98	0.46
5:W:29:PRO:HB3	5:W:58:SER:HB3	1.97	0.46
9:B:58:SER:OG	9:B:59:GLU:OE1	2.33	0.46
9:B:125:VAL:HG13	9:B:127:VAL:HG13	1.98	0.46
18:N:2:GLY:N	21:A:871:G:OP1	2.48	0.46
21:A:27:U:H2'	21:A:28:A2M:H8	1.97	0.46
21:A:518:G:O2'	21:A:519:A:H8	1.98	0.46
21:A:1674:C:H2'	21:A:1675:C:H6	1.81	0.46
21:A:1746:U:H2'	21:A:1747:U:H6	1.81	0.46
21:A:1751:A:C6	21:A:1752:U:C4	3.03	0.46
21:A:1761:A2M:H8	21:A:1761:A2M:H5"	1.97	0.46
20:I:102:ILE:HD12	20:I:203:LEU:HD11	1.97	0.45
21:A:98:C:H2'	21:A:99:U:C6	2.51	0.45
21:A:405:A:H5"	25:A:2047:HOH:O	2.16	0.45
21:A:760:G:N2	21:A:800:U:OP1	2.49	0.45
21:A:1773:A:H2'	21:A:1774:6MZ:H8	1.98	0.45
20:I:8:MET:CE	20:I:21:TRP:CD1	2.99	0.45
21:A:1681:A:H2'	21:A:1682:G:C8	2.51	0.45
1:Y:16:LYS:HE3	21:A:781:A:H62	1.80	0.45
1:Y:115:GLU:O	1:Y:119:ARG:HG3	2.16	0.45
2:X:56:ILE:CD1	2:X:115:PRO:HD2	2.46	0.45
9:B:146:ARG:HH21	21:A:1070:A:H1'	1.81	0.45
9:B:224:ASP:OD2	9:B:227:LYS:HE3	2.16	0.45
9:B:224:ASP:HB3	9:B:227:LYS:HD2	1.98	0.45
15:H:94:VAL:HG11	15:H:130:VAL:HG23	1.99	0.45
21:A:952:U:H2'	21:A:953:G:H8	1.81	0.45
5:W:80:ASP:OD1	5:W:124:LYS:NZ	2.49	0.45
5:W:99:PHE:CD1	13:C:237:PRO:HG2	2.51	0.45
12:J:51:LEU:HD13	12:J:106:PHE:CE1	2.51	0.45
21:A:966:U:H2'	21:A:967:C:C6	2.52	0.45
21:A:1022:U:C2	21:A:1023:C:C5	3.04	0.45
1:Y:86:GLU:CD	1:Y:86:GLU:H	2.19	0.45
4:O:44:VAL:HB	4:O:54:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:850:G:H2'	21:A:851:G:H8	1.82	0.45
21:A:1022:U:H2'	21:A:1023:C:H6	1.82	0.45
14:G:33:SER:O	14:G:51:LYS:NZ	2.47	0.45
14:G:57:ASP:HB3	14:G:100:ARG:HD2	1.98	0.45
21:A:178:A:H2'	21:A:179:A:H8	1.82	0.45
21:A:1058:G:C4	21:A:1059:U:C5	3.05	0.45
3:E:213:ALA:HB3	3:E:244:ILE:HD11	1.97	0.45
4:O:98:ARG:NH2	4:O:100:THR:O	2.49	0.45
14:G:145:LYS:HE2	14:G:145:LYS:HB2	1.82	0.45
15:H:50:ILE:HG22	15:H:62:VAL:HG22	1.99	0.45
20:I:158:VAL:O	20:I:161:LYS:HG2	2.17	0.45
21:A:522:A:C2'	21:A:523:C:H5"	2.47	0.45
21:A:824:U:H2'	21:A:825:U:C6	2.52	0.45
5:W:77:PRO:HD2	5:W:79:PHE:CE2	2.52	0.45
10:V:49:PHE:HZ	13:C:247:LYS:HE2	1.82	0.45
21:A:453:C:H2'	21:A:454:U:C6	2.52	0.45
4:O:149:ARG:NH2	21:A:909:G:OP1	2.50	0.45
9:B:138:PHE:HE2	9:B:216:LYS:HD3	1.81	0.45
21:A:17:C:H2'	21:A:18:C:C6	2.51	0.45
21:A:927:A:H2'	21:A:928:A:H8	1.81	0.45
21:A:1645:C:H4'	21:A:1646:C:H3'	1.99	0.45
5:W:51:GLU:OE1	15:H:142:ARG:HA	2.16	0.45
9:B:162:ARG:HB3	9:B:166:ARG:NH2	2.24	0.45
15:H:175:ARG:CZ	15:H:181:ASP:HA	2.47	0.45
21:A:29:U:H2'	21:A:30:G:H8	1.82	0.45
21:A:594:C:H2'	21:A:595:A:C8	2.52	0.45
21:A:1659:U:H2'	21:A:1660:A:H8	1.82	0.45
9:B:125:VAL:CG2	9:B:169:VAL:HG13	2.47	0.44
14:G:57:ASP:HA	14:G:108:LEU:HA	1.98	0.44
15:H:102:VAL:HG22	15:H:117:ARG:HB3	1.99	0.44
21:A:483:C:H2'	21:A:484:A:H8	1.82	0.44
21:A:1049:U:H2'	21:A:1050:C:C6	2.52	0.44
5:W:115:GLU:O	5:W:119:LYS:HG3	2.17	0.44
13:C:168:VAL:HG13	13:C:227:CYS:SG	2.57	0.44
18:N:128:TYR:CE1	21:A:969:U:H5"	2.53	0.44
21:A:1014:OMU:HM22	21:A:1015:C:O4'	2.17	0.44
21:A:1140:U:H2'	21:A:1141:U:C6	2.52	0.44
21:A:1656:U:H2'	21:A:1657:C:C6	2.52	0.44
21:A:1678:U:H2'	21:A:1679:G:O4'	2.17	0.44
2:X:3:LYS:NZ	21:A:616:U:OP2	2.40	0.44
4:O:48:SER:HB3	9:B:66:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:163:ARG:HH21	14:G:175:SER:HB3	1.81	0.44
20:I:159:GLN:HA	20:I:159:GLN:OE1	2.17	0.44
21:A:130:A:N6	21:A:175:A:O2'	2.50	0.44
21:A:160:A:N6	25:A:2202:HOH:O	2.50	0.44
21:A:416:A:H2'	21:A:417:U:C6	2.52	0.44
4:O:56:ILE:HD12	4:O:60:MET:CE	2.47	0.44
12:J:63:THR:O	12:J:63:THR:HG22	2.18	0.44
13:C:172:CYS:SG	13:C:222:LYS:HE3	2.57	0.44
17:L:130:ARG:NH2	25:L:203:HOH:O	2.49	0.44
21:A:926:G:H2'	21:A:927:A:C8	2.52	0.44
21:A:963:U:H5	25:A:2555:HOH:O	2.01	0.44
21:A:1727:G:H2'	21:A:1728:C:C6	2.53	0.44
2:X:7:MET:HE1	5:W:77:PRO:HB2	2.00	0.44
3:E:192:VAL:HB	3:E:243:GLY:HA3	2.00	0.44
5:W:8:ASN:HB2	5:W:74:VAL:HG21	1.99	0.44
21:A:202:C:C2	21:A:203:A:C8	3.05	0.44
21:A:625:A:HO2'	21:A:1111:C:HO2'	1.62	0.44
21:A:1661:C:H2'	21:A:1662:C:H6	1.82	0.44
21:A:1662:C:H2'	21:A:1663:G:O4'	2.17	0.44
3:E:194:VAL:HG11	3:E:232:THR:HG22	1.99	0.44
9:B:59:GLU:OE1	9:B:59:GLU:N	2.49	0.44
9:B:97:LEU:HB3	9:B:232:HIS:NE2	2.32	0.44
12:J:33:VAL:HG13	12:J:38:LEU:HB2	2.00	0.44
14:G:53:MET:HG3	14:G:114:VAL:CG2	2.45	0.44
20:I:26:LYS:HG2	20:I:29:LEU:HD23	2.00	0.44
1:Y:63:VAL:HB	1:Y:66:PHE:CE2	2.53	0.44
5:W:49:GLU:HB2	5:W:64:GLU:HG2	2.00	0.44
12:J:80:ARG:NH1	21:A:769:G:OP1	2.51	0.44
18:N:23:PRO:HG2	18:N:26:VAL:HG23	2.00	0.44
20:I:23:LYS:HE3	21:A:395:A:OP2	2.18	0.44
21:A:638:G:N1	21:A:970:U:OP2	2.40	0.44
21:A:994:U:H2'	21:A:995:C:O4'	2.17	0.44
21:A:1753:U:H3'	21:A:1754:U:C5	2.52	0.44
21:A:1776:A:N6	25:A:2077:HOH:O	2.39	0.44
1:Y:51:LYS:HE2	1:Y:51:LYS:HB2	1.72	0.44
21:A:786:U:O2	21:A:786:U:C2'	2.66	0.44
21:A:823:A:C2	21:A:824:U:C2	3.06	0.44
21:A:1654:G:N3	21:A:1654:G:H2'	2.33	0.44
21:A:1749:U:H2'	21:A:1750:C:C6	2.53	0.44
3:E:196:LYS:HZ3	3:E:211:GLU:HB3	1.82	0.44
14:G:135:ARG:HD2	21:A:164:C:O2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:124:VAL:HG12	17:L:143:VAL:HG22	2.00	0.44
21:A:1635:U:H2'	21:A:1636:U:C6	2.53	0.44
3:E:202:LYS:NZ	21:A:249:G:H4'	2.33	0.43
5:W:54:ASP:HB3	15:H:139:LYS:HB3	1.99	0.43
9:B:36:LEU:HA	9:B:41:ARG:HH11	1.81	0.43
9:B:125:VAL:HG21	9:B:169:VAL:HG13	2.00	0.43
9:B:133:TYR:CD1	9:B:181:LEU:HD11	2.53	0.43
13:C:89:GLU:HA	13:C:89:GLU:OE1	2.18	0.43
21:A:247:A:H2'	21:A:248:U:C6	2.53	0.43
21:A:338:G:H4'	25:A:2051:HOH:O	2.17	0.43
21:A:342:C:H2'	21:A:343:C:C6	2.52	0.43
21:A:344:U:H2'	21:A:345:A:H8	1.83	0.43
21:A:952:U:H2'	21:A:953:G:C8	2.53	0.43
21:A:1755:A:H2'	21:A:1756:G:O4'	2.18	0.43
21:A:492:G:H1	21:A:503:U:H3	1.66	0.43
2:X:7:MET:HA	17:L:100:ARG:HD2	2.00	0.43
2:X:38:LYS:HA	2:X:38:LYS:HD3	1.84	0.43
9:B:136:ARG:HD2	9:B:138:PHE:CZ	2.52	0.43
21:A:204:U:H2'	21:A:205:U:C6	2.53	0.43
21:A:647:G:H2'	21:A:648:C:H6	1.84	0.43
21:A:820:A:H2'	21:A:822:G:O4'	2.19	0.43
21:A:1304:G:H2'	21:A:1305:A:C8	2.53	0.43
21:A:1650:C:H2'	21:A:1651:G:H8	1.82	0.43
9:B:109:LYS:O	9:B:113:LEU:HG	2.18	0.43
14:G:59:GLN:OE1	14:G:72:ARG:NH1	2.47	0.43
17:L:56:ASP:HB3	17:L:59:CYS:HB2	2.01	0.43
21:A:196:G:H2'	21:A:197:G:H8	1.84	0.43
21:A:388:G:H2'	21:A:389:A:C8	2.54	0.43
21:A:437:C:H1'	25:A:2256:HOH:O	2.18	0.43
21:A:825:U:C2	21:A:858:G:C2	3.07	0.43
13:C:98:LYS:HD2	21:A:1306:PSU:H5"	1.99	0.43
21:A:69:A:H2'	21:A:70:C:C6	2.53	0.43
21:A:285:G:H2'	21:A:286:C:C6	2.53	0.43
21:A:297:U:H2'	21:A:298:C:C6	2.53	0.43
21:A:967:C:H2'	21:A:968:A:O4'	2.18	0.43
21:A:1634:C:H2'	21:A:1635:U:H6	1.83	0.43
21:A:1781:U:H2'	21:A:1782:U:C6	2.54	0.43
14:G:178:PRO:O	21:A:79:A:O2'	2.26	0.43
20:I:11:ARG:NH1	20:I:15:GLY:O	2.51	0.43
21:A:991:G:H2'	21:A:992:G:O4'	2.19	0.43
21:A:1008:A:H1'	21:A:1010:A:N7	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:204:ILE:O	21:A:1069:G:O2'	2.36	0.43
18:N:124:ARG:HH21	21:A:632:G:P	2.41	0.43
21:A:647:G:N2	21:A:693:C:C2	2.87	0.43
21:A:820:A:O4'	21:A:863:G:N2	2.51	0.43
21:A:826:C:H2'	21:A:827:C:H6	1.84	0.43
3:E:45:ILE:HG13	3:E:61:VAL:HG21	2.00	0.43
4:O:43:HIS:HE1	21:A:900:G:N2	2.16	0.43
14:G:172:LYS:NZ	21:A:72:A:H62	2.17	0.43
15:H:51:GLN:OE1	15:H:59:LYS:HE2	2.18	0.43
21:A:901:U:H2'	21:A:902:C:C6	2.54	0.43
1:Y:87:SER:HA	1:Y:90:LYS:HZ2	1.83	0.43
15:H:12:LYS:O	15:H:14:VAL:HG23	2.19	0.43
21:A:589:A:H2'	21:A:590:G:H8	1.83	0.43
21:A:855:G:N1	21:A:856:G:C5	2.87	0.43
21:A:898:U:O4	21:A:899:A:N6	2.52	0.43
2:X:25:LYS:HD2	21:A:1114:G:OP2	2.18	0.43
5:W:55:ASP:OD1	5:W:55:ASP:N	2.52	0.43
14:G:94:ARG:NH1	21:A:1683:U:OP1	2.52	0.43
20:I:46:ARG:HG3	20:I:56:TRP:CH2	2.53	0.43
21:A:492:G:N2	21:A:503:U:H3	2.16	0.43
21:A:1048:A:H2	25:A:2293:HOH:O	2.01	0.43
1:Y:15:ARG:HE	21:A:786:U:H3	1.67	0.42
15:H:31:GLU:HA	15:H:41:LEU:CD1	2.41	0.42
15:H:36:GLU:HG3	15:H:79:ARG:HH11	1.84	0.42
21:A:58:U:OP1	21:A:460:G:O2'	2.35	0.42
21:A:1087:U:O2'	21:A:1088:G:H5'	2.18	0.42
21:A:1634:C:H2'	21:A:1635:U:C6	2.54	0.42
1:Y:94:LYS:HE3	1:Y:98:ILE:HD11	2.01	0.42
3:E:247:THR:OG1	3:E:250:GLU:HG3	2.19	0.42
5:W:51:GLU:OE2	15:H:140:ARG:HB3	2.19	0.42
13:C:123:LEU:HD21	13:C:222:LYS:HG3	2.00	0.42
21:A:419:C:O2'	21:A:422:G:O6	2.29	0.42
21:A:855:G:C2	21:A:856:G:C5	3.07	0.42
21:A:1027:C:O2'	21:A:1130:A:N1	2.43	0.42
21:A:1108:PSU:H2'	21:A:1109:U:C6	2.54	0.42
10:V:50:THR:HG21	10:V:72:TRP:HZ3	1.85	0.42
15:H:68:ARG:O	15:H:68:ARG:HG2	2.18	0.42
21:A:53:G:H2'	21:A:54:C:C6	2.55	0.42
21:A:347:C:H2'	21:A:348:A:C8	2.54	0.42
21:A:389:A:H2'	21:A:390:G:C8	2.54	0.42
21:A:647:G:H2'	21:A:648:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:793:G:H2'	21:A:794:G:O4'	2.19	0.42
21:A:1651:G:H2'	21:A:1652:U:H6	1.84	0.42
9:B:229:MET:HA	9:B:229:MET:CE	2.50	0.42
13:C:179:MET:SD	13:C:198:LEU:HD21	2.59	0.42
21:A:824:U:O2	21:A:858:G:N2	2.48	0.42
21:A:1791:G:H2'	21:A:1792:MA6:H8	2.02	0.42
9:B:198:GLU:HG3	9:B:210:VAL:HG21	2.01	0.42
12:J:145:VAL:HG11	21:A:774:C:H1'	2.00	0.42
15:H:69:LEU:H	15:H:69:LEU:CD2	2.31	0.42
17:L:23:ASP:OD1	17:L:25:ALA:N	2.52	0.42
21:A:383:U:H5"	25:A:2307:HOH:O	2.19	0.42
12:J:133:GLN:HB2	12:J:135:HIS:CD2	2.54	0.42
14:G:58:LYS:HA	14:G:109:SER:OG	2.19	0.42
21:A:155:A:O2'	21:A:156:U:H5'	2.20	0.42
21:A:400:G:N2	21:A:402:G:H3'	2.35	0.42
21:A:1681:A:H2'	21:A:1682:G:H8	1.85	0.42
1:Y:67:ARG:NH1	21:A:534:C:O2	2.43	0.42
3:E:101:LEU:HD23	3:E:101:LEU:HA	1.86	0.42
5:W:100:GLY:HA2	5:W:130:TYR:HB3	2.02	0.42
15:H:77:HIS:O	15:H:81:VAL:HG23	2.20	0.42
21:A:464:A:H3'	21:A:465:G:C8	2.52	0.42
21:A:955:C:H2'	21:A:956:A:C8	2.55	0.42
21:A:1013:G:H2'	21:A:1014:OMU:H6	2.01	0.42
21:A:1738:A:N7	25:A:2045:HOH:O	2.36	0.42
9:B:231:VAL:HG12	9:B:231:VAL:O	2.19	0.42
12:J:126:HIS:HA	12:J:129:VAL:HG22	2.01	0.42
14:G:135:ARG:HH22	21:A:147:C:H1'	1.85	0.42
15:H:156:ASP:OD1	15:H:157:PRO:HD2	2.20	0.42
21:A:1675:C:H2'	21:A:1676:G:C8	2.54	0.42
3:E:44:LEU:HD23	3:E:44:LEU:HA	1.92	0.42
3:E:127:ARG:NH2	3:E:142:TYR:HA	2.35	0.42
9:B:163:GLN:HB3	9:B:204:ILE:HD13	2.01	0.42
10:V:15:ARG:NE	13:C:68:LEU:O	2.53	0.42
21:A:853:U:H2'	21:A:854:C:C6	2.55	0.42
21:A:981:G:N1	21:A:1028:A:O2'	2.42	0.42
1:Y:15:ARG:NE	21:A:786:U:H3	2.17	0.42
3:E:108:ARG:HE	3:E:108:ARG:HB2	1.60	0.42
10:V:17:CYS:HB2	10:V:55:SER:HB2	2.01	0.42
20:I:74:THR:O	20:I:75:ARG:HD3	2.20	0.42
21:A:594:C:H2'	21:A:595:A:H8	1.85	0.42
21:A:648:C:H2'	21:A:649:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1137:A:H2'	21:A:1138:A:C8	2.54	0.42
21:A:1754:U:O3'	21:A:1755:A:H8	2.03	0.42
4:O:66:ARG:NH2	21:A:910:A:H4'	2.35	0.41
9:B:39:THR:OG1	9:B:40:SER:N	2.52	0.41
12:J:112:GLN:OE1	12:J:128:ARG:HD2	2.20	0.41
17:L:70:ARG:HG3	21:A:308:PSU:O2'	2.20	0.41
21:A:509:A:H2'	21:A:511:U:C5	2.55	0.41
21:A:855:G:C2	21:A:856:G:C8	3.08	0.41
21:A:1147:A:H2'	21:A:1148:A:C8	2.55	0.41
21:A:1733:A:H2'	21:A:1734:G:O4'	2.20	0.41
21:A:1797:G:H2'	21:A:1798:C:C6	2.55	0.41
9:B:82:ARG:NH1	9:B:212:VAL:O	2.51	0.41
13:C:236:THR:OG1	13:C:238:ASP:OD1	2.38	0.41
21:A:52:U:H2'	21:A:53:G:H8	1.81	0.41
21:A:316:A:C2	21:A:318:C:H2'	2.55	0.41
21:A:822:G:N1	21:A:860:A:C6	2.88	0.41
21:A:912:A:H2'	21:A:913:U:H6	1.85	0.41
21:A:1683:U:H2'	21:A:1684:G:C8	2.56	0.41
4:O:32:HIS:CD2	21:A:923:U:H4'	2.55	0.41
10:V:50:THR:HG21	10:V:72:TRP:CZ3	2.56	0.41
12:J:80:ARG:NH2	21:A:770:U:OP1	2.51	0.41
13:C:68:LEU:HD12	13:C:68:LEU:HA	1.90	0.41
14:G:205:LYS:O	14:G:209:GLU:HG3	2.21	0.41
15:H:165:TYR:CZ	15:H:166:LYS:HE3	2.55	0.41
21:A:31:C:O2'	21:A:551:U:OP1	2.36	0.41
21:A:96:G:HO2'	21:A:464:A:HO2'	1.67	0.41
21:A:491:G:N2	21:A:505:U:O2	2.53	0.41
21:A:570:C:H2'	21:A:571:A:O4'	2.20	0.41
21:A:775:A:H2'	21:A:776:A:C8	2.56	0.41
21:A:818:A:N6	21:A:864:A:OP2	2.54	0.41
20:I:191:ARG:HD3	25:I:301:HOH:O	2.19	0.41
21:A:30:G:H2'	21:A:31:C:H6	1.86	0.41
21:A:432:A:H2'	21:A:433:G:O4'	2.20	0.41
21:A:894:U:H2'	21:A:895:U:C6	2.55	0.41
21:A:999:G:H2'	21:A:1000:A:C8	2.55	0.41
4:O:71:PRO:HB3	4:O:114:SER:HB2	2.03	0.41
20:I:217:LYS:HB2	20:I:217:LYS:HE3	1.85	0.41
21:A:415:C:H2'	21:A:416:A:O4'	2.21	0.41
21:A:417:U:H2'	21:A:418:OMC:H6	1.86	0.41
21:A:973:U:H2'	21:A:974:C:O4'	2.21	0.41
1:Y:99:ARG:NH1	25:Y:204:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:61:LEU:HG	9:B:96:VAL:HG21	2.02	0.41
15:H:160:ARG:HE	15:H:160:ARG:HB2	1.77	0.41
18:N:102:LEU:HD21	18:N:111:SER:HB2	2.03	0.41
21:A:819:U:H1'	21:A:821:G:C4	2.55	0.41
21:A:1657:C:H2'	21:A:1658:C:C6	2.56	0.41
3:E:80:LYS:H	3:E:80:LYS:HG2	1.70	0.41
4:O:57:THR:HB	4:O:60:MET:HB2	2.03	0.41
12:J:13:THR:HG23	21:A:476:U:H5"	2.01	0.41
13:C:151:ARG:HE	13:C:151:ARG:HB2	1.69	0.41
21:A:1138:A:H2'	21:A:1139:C:O4'	2.21	0.41
2:X:107:LYS:HD2	2:X:107:LYS:N	2.35	0.41
5:W:28:ARG:HD3	5:W:60:LYS:HZ2	1.85	0.41
9:B:27:LYS:HA	9:B:49:SER:HA	2.03	0.41
15:H:79:ARG:HA	15:H:82:ARG:HD2	2.03	0.41
20:I:84:TYR:HB3	20:I:102:ILE:HB	2.03	0.41
21:A:179:A:H2'	21:A:180:A:O4'	2.20	0.41
21:A:614:G:N3	21:A:614:G:H2'	2.35	0.41
21:A:850:G:H2'	21:A:851:G:C8	2.56	0.41
21:A:1076:C:H2'	21:A:1077:C:C6	2.55	0.41
21:A:1663:G:N2	21:A:1756:G:H2'	2.35	0.41
1:Y:30:LEU:HD22	1:Y:49:LEU:HD11	2.03	0.41
1:Y:117:LYS:HE3	1:Y:117:LYS:HB3	1.90	0.41
9:B:28:GLN:HB2	9:B:30:TYR:HE1	1.85	0.41
9:B:48:VAL:HG21	9:B:61:LEU:HD22	2.03	0.41
14:G:26:ASN:ND2	14:G:40:LEU:HB3	2.36	0.41
14:G:30:LYS:HE3	14:G:36:VAL:HG22	2.03	0.41
14:G:172:LYS:HZ2	21:A:72:A:H62	1.69	0.41
14:G:199:LYS:HB3	21:A:176:A:N6	2.35	0.41
15:H:31:GLU:HG2	15:H:41:LEU:CD2	2.50	0.41
15:H:84:LEU:O	15:H:87:LYS:HB2	2.21	0.41
21:A:129:U:H5	21:A:201:G:H5'	1.86	0.41
21:A:492:G:H22	21:A:503:U:H3	1.69	0.41
21:A:635:G:H2'	21:A:636:PSU:H6	1.86	0.41
21:A:830:U:H2'	21:A:831:C:C6	2.56	0.41
21:A:1752:U:H2'	21:A:1753:U:C6	2.56	0.41
21:A:305:A:H2'	21:A:306:PSU:O4'	2.21	0.41
9:B:222:LYS:HA	9:B:222:LYS:HD2	1.90	0.40
13:C:63:MET:HG2	13:C:82:LEU:HB2	2.02	0.40
17:L:57:LYS:HG3	17:L:58:LYS:HG3	2.04	0.40
21:A:45:U:O2	21:A:438:G:H1'	2.21	0.40
21:A:824:U:H2'	21:A:825:U:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:825:U:H2'	21:A:826:C:H6	1.86	0.40
21:A:1656:U:H2'	21:A:1657:C:H6	1.85	0.40
21:A:1722:A:H2'	21:A:1723:C:C6	2.56	0.40
18:N:128:TYR:HE1	21:A:969:U:H5"	1.86	0.40
21:A:193:G:H2'	21:A:194:G:O4'	2.20	0.40
21:A:417:U:C2	21:A:418:OMC:C5	3.10	0.40
21:A:644:U:N3	21:A:645:G:N7	2.69	0.40
21:A:692:C:H2'	21:A:693:C:H6	1.75	0.40
21:A:958:G:H1'	25:A:2511:HOH:O	2.20	0.40
2:X:56:ILE:HD11	2:X:114:ILE:HG23	2.03	0.40
9:B:145:ARG:NH2	9:B:151:LYS:O	2.47	0.40
10:V:33:GLN:HG3	10:V:53:ALA:HB2	2.02	0.40
15:H:39:SER:HA	15:H:42:LYS:HE3	2.03	0.40
21:A:330:G:H2'	21:A:331:U:C6	2.57	0.40
21:A:378:U:H2'	21:A:379:U:C6	2.57	0.40
21:A:812:A:H2'	21:A:813:A:C8	2.52	0.40
21:A:824:U:C2	21:A:825:U:C5	3.09	0.40
2:X:47:LYS:HG3	21:A:439:C:H5"	2.04	0.40
2:X:104:PHE:O	2:X:111:VAL:HG21	2.21	0.40
15:H:45:TYR:H	15:H:69:LEU:HD11	1.86	0.40
18:N:43:LYS:HD2	18:N:43:LYS:H	1.87	0.40
21:A:862:U:C2'	21:A:863:G:H5'	2.52	0.40
21:A:999:G:H2'	21:A:1000:A:H8	1.86	0.40
21:A:1068:G:C2	21:A:1069:G:C8	3.09	0.40
21:A:1661:C:H2'	21:A:1662:C:C6	2.56	0.40
21:A:1669:A:N1	21:A:1753:U:C2	2.90	0.40
3:E:36:HIS:CG	3:E:85:GLY:HA3	2.56	0.40
9:B:179:CYS:HB3	9:B:183:GLU:CG	2.51	0.40
18:N:100:LYS:O	18:N:104:ARG:HG3	2.21	0.40
21:A:161:G:OP2	21:A:161:G:N2	2.43	0.40
21:A:928:A:H2'	21:A:929:A:C8	2.56	0.40
21:A:1695:G:C6	21:A:1696:G:N7	2.90	0.40
21:A:1726:C:O2'	21:A:1727:G:O5'	2.33	0.40
21:A:1766:A:H3'	21:A:1767:A:H5"	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
2	X	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
3	E	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
4	O	126/151 (83%)	123 (98%)	3 (2%)	0	100	100
5	W	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
6	b	81/86 (94%)	72 (89%)	9 (11%)	0	100	100
7	e	44/62 (71%)	42 (96%)	2 (4%)	0	100	100
8	k	197/308 (64%)	192 (98%)	5 (2%)	0	100	100
9	B	208/263 (79%)	203 (98%)	5 (2%)	0	100	100
10	V	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
11	a	96/139 (69%)	94 (98%)	2 (2%)	0	100	100
12	J	179/195 (92%)	177 (99%)	2 (1%)	0	100	100
13	C	212/275 (77%)	206 (97%)	6 (3%)	0	100	100
14	G	228/250 (91%)	225 (99%)	3 (1%)	0	100	100
15	H	182/192 (95%)	170 (93%)	12 (7%)	0	100	100
16	h	25/143 (18%)	23 (92%)	2 (8%)	0	100	100
17	L	144/159 (91%)	143 (99%)	1 (1%)	0	100	100
18	N	139/151 (92%)	136 (98%)	3 (2%)	0	100	100
19	n	21/25 (84%)	21 (100%)	0	0	100	100
20	I	182/224 (81%)	176 (97%)	6 (3%)	0	100	100
All	All	2788/3378 (82%)	2712 (97%)	76 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	108/117 (92%)	108 (100%)	0	100	100
2	X	111/113 (98%)	110 (99%)	1 (1%)	78	87
3	E	222/224 (99%)	222 (100%)	0	100	100
4	O	101/120 (84%)	101 (100%)	0	100	100
5	W	111/112 (99%)	111 (100%)	0	100	100
6	b	76/78 (97%)	76 (100%)	0	100	100
7	e	39/49 (80%)	39 (100%)	0	100	100
8	k	170/233 (73%)	169 (99%)	1 (1%)	86	92
9	B	189/228 (83%)	188 (100%)	1 (0%)	88	93
10	V	65/65 (100%)	65 (100%)	0	100	100
11	a	85/108 (79%)	84 (99%)	1 (1%)	71	82
12	J	154/162 (95%)	153 (99%)	1 (1%)	86	92
13	C	181/219 (83%)	178 (98%)	3 (2%)	60	72
14	G	202/215 (94%)	201 (100%)	1 (0%)	88	93
15	H	164/171 (96%)	160 (98%)	4 (2%)	49	59
16	h	22/124 (18%)	21 (96%)	1 (4%)	27	34
17	L	125/132 (95%)	123 (98%)	2 (2%)	62	74
18	N	123/131 (94%)	122 (99%)	1 (1%)	81	89
19	n	22/24 (92%)	21 (96%)	1 (4%)	27	34
20	I	160/179 (89%)	160 (100%)	0	100	100
All	All	2430/2804 (87%)	2412 (99%)	18 (1%)	84	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	104	PHE
8	k	103	ILE
9	B	103	MET

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Mol	Chain	Res	Type
11	a	95	ARG
12	J	142	ILE
13	C	59	ARG
13	C	220	PHE
13	C	232	TYR
14	G	41	LEU
15	H	20	GLU
15	H	52	MET
15	H	113	ARG
15	H	156	ASP
16	h	108	PHE
17	L	47	ARG
17	L	68	ARG
18	N	3	ARG
19	n	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
6	b	51	HIS
8	k	81	GLN
18	N	123	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1159/1810 (64%)	205 (17%)	0

All (205) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	14	C
21	A	25	C
21	A	26	A
21	A	34	G
21	A	42	G
21	A	47	A
21	A	59	G
21	A	68	A
21	A	83	U

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Mol	Chain	Res	Type
21	A	105	A
21	A	112	U
21	A	115	A
21	A	116	G
21	A	128	G
21	A	129	U
21	A	139	U
21	A	151	A
21	A	156	U
21	A	158	C
21	A	164	C
21	A	176	A
21	A	177	C
21	A	189	U
21	A	191	U
21	A	192	G
21	A	201	G
21	A	252	U
21	A	253	C
21	A	260	A
21	A	264	G
21	A	266	C
21	A	275	C
21	A	278	C
21	A	291	G
21	A	303	A
21	A	318	C
21	A	320	A
21	A	326	G
21	A	341	G
21	A	342	C
21	A	365	C
21	A	370	A
21	A	374	A
21	A	377	G
21	A	384	U
21	A	394	G
21	A	397	C
21	A	404	A
21	A	405	A
21	A	406	C
21	A	408	G

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Mol	Chain	Res	Type
21	A	420	A
21	A	421	A
21	A	423	G
21	A	427	G
21	A	428	C
21	A	430	G
21	A	438	G
21	A	443	U
21	A	448	C
21	A	449	A
21	A	457	C
21	A	458	A
21	A	472	A
21	A	473	C
21	A	481	A
21	A	486	U
21	A	490	G
21	A	491	G
21	A	504	C
21	A	505	U
21	A	509	A
21	A	510	A
21	A	511	U
21	A	512	U
21	A	514	G
21	A	515	A
21	A	523	C
21	A	531	A
21	A	538	A
21	A	542	A
21	A	546	U
21	A	553	G
21	A	559	A
21	A	572	G
21	A	575	G
21	A	582	U
21	A	583	A
21	A	586	U
21	A	598	A
21	A	610	A
21	A	623	A2M
21	A	624	A

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Mol	Chain	Res	Type
21	A	626	A
21	A	627	A
21	A	628	G
21	A	642	C
21	A	643	U
21	A	645	G
21	A	749	G
21	A	772	C
21	A	777	A
21	A	784	C
21	A	785	A
21	A	786	U
21	A	787	C
21	A	788	G
21	A	791	C
21	A	792	U
21	A	795	A
21	A	816	U
21	A	818	A
21	A	819	U
21	A	820	A
21	A	821	G
21	A	822	G
21	A	823	A
21	A	825	U
21	A	828	G
21	A	861	A
21	A	862	U
21	A	863	G
21	A	865	U
21	A	867	A
21	A	868	A
21	A	881	G
21	A	911	A
21	A	919	G
21	A	931	A
21	A	938	A
21	A	940	U
21	A	947	G
21	A	950	U
21	A	965	U
21	A	971	A

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Mol	Chain	Res	Type
21	A	975	A
21	A	976	A
21	A	978	A
21	A	1003	A
21	A	1006	A
21	A	1008	A
21	A	1009	U
21	A	1010	A
21	A	1016	C
21	A	1031	A
21	A	1033	C
21	A	1035	A
21	A	1043	C
21	A	1058	G
21	A	1061	G
21	A	1062	C
21	A	1063	U
21	A	1070	A
21	A	1072	U
21	A	1075	G
21	A	1081	A
21	A	1087	U
21	A	1094	U
21	A	1097	A
21	A	1099	G
21	A	1102	U
21	A	1103	U
21	A	1118	A
21	A	1131	OMG
21	A	1143	A
21	A	1155	G
21	A	1156	A
21	A	1640	A
21	A	1643	C
21	A	1644	A
21	A	1645	C
21	A	1646	C
21	A	1647	G
21	A	1655	C
21	A	1656	U
21	A	1664	A
21	A	1666	U

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Mol	Chain	Res	Type
21	A	1667	G
21	A	1671	G
21	A	1673	U
21	A	1674	C
21	A	1676	G
21	A	1677	G
21	A	1689	G
21	A	1695	G
21	A	1697	C
21	A	1726	C
21	A	1727	G
21	A	1753	U
21	A	1754	U
21	A	1761	A2M
21	A	1766	A
21	A	1767	A
21	A	1771	G
21	A	1773	A
21	A	1777	A
21	A	1780	U
21	A	1791	G
21	A	1803	G
21	A	1804	G
21	A	1805	A
21	A	1806	U
21	A	1807	C
21	A	1809	U
21	A	1810	U

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	OMG	A	599	21	18,26,27	1.01	3 (16%)	19,38,41	0.69	0
21	PSU	A	1004	21	18,21,22	0.49	0	22,30,33	0.59	0
21	PSU	A	255	21,23	18,21,22	0.50	0	22,30,33	0.60	0
21	OMG	A	1131	21	18,26,27	1.02	3 (16%)	19,38,41	0.62	0
21	OMU	A	168	21	19,22,23	0.41	0	26,31,34	0.88	1 (3%)
21	PSU	A	606	21	18,21,22	0.53	0	22,30,33	0.59	0
10	AME	V	1	10	9,10,11	1.37	1 (11%)	9,11,13	1.62	2 (22%)
21	OMU	A	615	21	19,22,23	1.70	4 (21%)	26,31,34	1.83	6 (23%)
21	PSU	A	1122	21	18,21,22	0.50	0	22,30,33	0.61	0
21	OMG	A	434	21	18,26,27	1.02	3 (16%)	19,38,41	0.63	0
21	A2M	A	979	21	18,25,26	0.73	1 (5%)	18,36,39	1.03	1 (5%)
21	A2M	A	424	21	18,25,26	0.72	1 (5%)	18,36,39	0.97	1 (5%)
21	PSU	A	607	21	18,21,22	0.53	0	22,30,33	0.56	0
21	PSU	A	35	21	18,21,22	0.52	0	22,30,33	0.58	0
21	4AC	A	1784	21	21,24,25	0.43	0	29,34,37	0.60	0
21	PSU	A	103	21	18,21,22	0.52	0	22,30,33	0.56	0
21	PSU	A	306	21	18,21,22	0.54	0	22,30,33	0.57	0
21	PSU	A	308	21	18,21,22	0.56	0	22,30,33	0.57	0
21	MA6	A	1792	21	18,26,27	0.83	1 (5%)	19,38,41	0.71	1 (5%)
21	A2M	A	162	21	18,25,26	0.71	0	18,36,39	0.95	1 (5%)
21	PSU	A	1306	21	18,21,22	0.57	0	22,30,33	0.55	0
21	OMC	A	38	21	19,22,23	0.33	0	26,31,34	0.51	0
21	PSU	A	806	21	18,21,22	0.48	0	22,30,33	0.61	0
21	OMU	A	1014	21	19,22,23	0.34	0	26,31,34	0.50	0
21	PSU	A	1108	21	18,21,22	0.53	0	22,30,33	0.57	0
21	PSU	A	1310	21	18,21,22	0.53	0	22,30,33	0.40	0
21	PSU	A	1637	21	18,21,22	0.52	0	22,30,33	0.57	0
21	A2M	A	545	21	18,25,26	0.72	1 (5%)	18,36,39	0.90	1 (5%)
21	A2M	A	1761	21	18,25,26	0.70	0	18,36,39	0.82	1 (5%)
21	PSU	A	636	21	18,21,22	0.55	0	22,30,33	0.58	0
21	PSU	A	121	21	18,21,22	0.50	0	22,30,33	0.76	0
21	A2M	A	440	21	18,25,26	0.70	1 (5%)	18,36,39	0.79	1 (5%)
21	OMG	A	246	21	18,26,27	0.99	2 (11%)	19,38,41	0.61	0
21	UY1	A	604	21	19,22,23	0.50	0	22,31,34	0.61	0
21	PSU	A	765	21	18,21,22	0.48	0	22,30,33	0.59	0
21	PSU	A	208	21	18,21,22	0.50	0	22,30,33	0.59	0
21	MA6	A	1793	21	18,26,27	0.76	1 (5%)	19,38,41	0.95	1 (5%)
21	PSU	A	1100	21	18,21,22	0.54	0	22,30,33	0.55	0
21	A2M	A	28	21	18,25,26	0.73	1 (5%)	18,36,39	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	IAS	O	138	4	6,7,8	0.82	0	6,8,10	1.06	0
21	A2M	A	802	21	18,25,26	0.70	0	18,36,39	0.94	1 (5%)
21	OMC	A	418	21	19,22,23	0.30	0	26,31,34	0.47	0
21	OMU	A	123	21	19,22,23	0.36	0	26,31,34	0.46	0
21	PSU	A	1295	21	18,21,22	0.46	0	22,30,33	0.60	0
21	6MZ	A	1774	24,21,23	18,25,26	0.78	1 (5%)	16,36,39	1.12	2 (12%)
21	PSU	A	258	21	18,21,22	0.50	0	22,30,33	0.59	0
21	PSU	A	300	21	18,21,22	0.50	0	22,30,33	0.56	0
21	PSU	A	811	21	18,21,22	0.51	0	22,30,33	0.59	0
21	OMC	A	1648	21	19,22,23	0.33	0	26,31,34	0.50	0
21	A2M	A	468	21	18,25,26	0.70	0	18,36,39	1.04	1 (5%)
21	PSU	A	362	21	18,21,22	0.50	0	22,30,33	0.63	0
21	OMG	A	1300	21	18,26,27	1.00	3 (16%)	19,38,41	0.68	0
21	PSU	A	111	24,21	18,21,22	0.52	0	22,30,33	0.59	0
21	A2M	A	623	21,23	18,25,26	0.72	0	18,36,39	0.82	1 (5%)
21	OMG	A	392	21	18,26,27	1.01	3 (16%)	19,38,41	0.66	0
21	PSU	A	1084	21	18,21,22	0.48	0	22,30,33	0.63	0
21	PSU	A	764	21	18,21,22	0.50	0	22,30,33	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	OMG	A	599	21	-	1/5/27/28	0/3/3/3
21	PSU	A	1004	21	-	0/7/25/26	0/2/2/2
21	PSU	A	255	21,23	-	0/7/25/26	0/2/2/2
21	OMG	A	1131	21	-	1/5/27/28	0/3/3/3
21	OMU	A	168	21	-	0/9/27/28	0/2/2/2
21	PSU	A	606	21	-	0/7/25/26	0/2/2/2
10	AME	V	1	10	-	2/9/10/12	-
21	OMU	A	615	21	-	1/9/27/28	0/2/2/2
21	PSU	A	1122	21	-	0/7/25/26	0/2/2/2
21	OMG	A	434	21	-	0/5/27/28	0/3/3/3
21	A2M	A	979	21	-	0/5/27/28	0/3/3/3
21	A2M	A	424	21	-	0/5/27/28	0/3/3/3
21	PSU	A	607	21	-	0/7/25/26	0/2/2/2
21	PSU	A	35	21	-	0/7/25/26	0/2/2/2
21	4AC	A	1784	21	-	0/11/29/30	0/2/2/2
21	PSU	A	103	21	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PSU	A	306	21	-	0/7/25/26	0/2/2/2
21	PSU	A	308	21	-	0/7/25/26	0/2/2/2
21	MA6	A	1792	21	-	0/7/29/30	0/3/3/3
21	A2M	A	162	21	-	0/5/27/28	0/3/3/3
21	PSU	A	1306	21	-	0/7/25/26	0/2/2/2
21	OMC	A	38	21	-	0/9/27/28	0/2/2/2
21	PSU	A	806	21	-	0/7/25/26	0/2/2/2
21	OMU	A	1014	21	-	0/9/27/28	0/2/2/2
21	PSU	A	1108	21	-	0/7/25/26	0/2/2/2
21	PSU	A	1310	21	-	2/7/25/26	0/2/2/2
21	PSU	A	1637	21	-	0/7/25/26	0/2/2/2
21	A2M	A	545	21	-	0/5/27/28	0/3/3/3
21	A2M	A	1761	21	-	2/5/27/28	0/3/3/3
21	PSU	A	636	21	-	0/7/25/26	0/2/2/2
21	PSU	A	121	21	-	0/7/25/26	0/2/2/2
21	A2M	A	440	21	-	0/5/27/28	0/3/3/3
21	OMG	A	246	21	-	2/5/27/28	0/3/3/3
21	UY1	A	604	21	-	0/9/27/28	0/2/2/2
21	PSU	A	765	21	-	0/7/25/26	0/2/2/2
21	PSU	A	208	21	-	0/7/25/26	0/2/2/2
21	MA6	A	1793	21	-	2/7/29/30	0/3/3/3
21	PSU	A	1100	21	-	0/7/25/26	0/2/2/2
21	A2M	A	28	21	-	0/5/27/28	0/3/3/3
4	IAS	O	138	4	-	1/7/7/8	-
21	A2M	A	802	21	-	0/5/27/28	0/3/3/3
21	OMC	A	418	21	-	0/9/27/28	0/2/2/2
21	OMU	A	123	21	-	1/9/27/28	0/2/2/2
21	PSU	A	1295	21	-	0/7/25/26	0/2/2/2
21	6MZ	A	1774	24,21,23	-	0/5/27/28	0/3/3/3
21	PSU	A	258	21	-	0/7/25/26	0/2/2/2
21	PSU	A	300	21	-	0/7/25/26	0/2/2/2
21	PSU	A	811	21	-	0/7/25/26	0/2/2/2
21	OMC	A	1648	21	-	2/9/27/28	0/2/2/2
21	A2M	A	468	21	-	2/5/27/28	0/3/3/3
21	PSU	A	362	21	-	0/7/25/26	0/2/2/2
21	OMG	A	1300	21	-	0/5/27/28	0/3/3/3
21	PSU	A	111	24,21	-	0/7/25/26	0/2/2/2
21	A2M	A	623	21,23	-	2/5/27/28	0/3/3/3
21	OMG	A	392	21	-	2/5/27/28	0/3/3/3
21	PSU	A	1084	21	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PSU	A	764	21	-	0/7/25/26	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	615	OMU	C4-N3	-4.31	1.30	1.38
21	A	615	OMU	C2-N3	-4.04	1.30	1.38
10	V	1	AME	CT1-N	3.31	1.45	1.34
21	A	615	OMU	C5-C4	-2.53	1.38	1.43
21	A	1131	OMG	C5-C6	-2.49	1.42	1.47
21	A	246	OMG	C5-C6	-2.48	1.42	1.47
21	A	599	OMG	C5-C6	-2.41	1.42	1.47
21	A	434	OMG	C5-C6	-2.39	1.42	1.47
21	A	392	OMG	C5-C6	-2.38	1.42	1.47
21	A	1300	OMG	C5-C6	-2.27	1.42	1.47
21	A	434	OMG	C8-N7	-2.26	1.31	1.35
21	A	1792	MA6	C8-N7	-2.26	1.30	1.34
21	A	1300	OMG	C5-C4	-2.25	1.37	1.43
21	A	392	OMG	C8-N7	-2.24	1.31	1.35
21	A	599	OMG	C8-N7	-2.18	1.31	1.35
21	A	434	OMG	C5-C4	-2.16	1.37	1.43
21	A	1131	OMG	C5-C4	-2.16	1.37	1.43
21	A	1300	OMG	C8-N7	-2.14	1.31	1.35
21	A	1131	OMG	C8-N7	-2.13	1.31	1.35
21	A	246	OMG	C5-C4	-2.13	1.37	1.43
21	A	1774	6MZ	C8-N7	-2.11	1.30	1.34
21	A	392	OMG	C5-C4	-2.10	1.37	1.43
21	A	599	OMG	C5-C4	-2.09	1.37	1.43
21	A	440	A2M	C8-N7	-2.08	1.31	1.34
21	A	615	OMU	C6-N1	-2.07	1.33	1.38
21	A	979	A2M	C8-N7	-2.06	1.31	1.34
21	A	424	A2M	C8-N7	-2.04	1.31	1.34
21	A	545	A2M	C8-N7	-2.03	1.31	1.34
21	A	28	A2M	C8-N7	-2.02	1.31	1.34
21	A	1793	MA6	C8-N7	-2.01	1.31	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	615	OMU	N3-C2-N1	4.45	120.80	114.89
21	A	615	OMU	C4-N3-C2	-4.42	120.75	126.58
21	A	615	OMU	C5-C4-N3	4.33	121.32	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1793	MA6	N1-C6-N6	-3.32	113.56	117.06
21	A	1774	6MZ	C9-N6-C6	3.27	125.69	122.87
21	A	615	OMU	O2-C2-N3	-2.75	116.37	121.50
21	A	1774	6MZ	C2-N1-C6	2.69	118.89	116.59
10	V	1	AME	CT2-CT1-N	2.64	120.56	116.10
10	V	1	AME	CE-SD-CG	2.63	109.43	100.40
21	A	468	A2M	C5-C6-N6	2.61	124.32	120.35
21	A	979	A2M	C5-C6-N6	2.54	124.22	120.35
21	A	440	A2M	C5-C6-N6	2.42	124.03	120.35
21	A	162	A2M	C5-C6-N6	2.38	123.97	120.35
21	A	623	A2M	C5-C6-N6	2.34	123.91	120.35
21	A	802	A2M	C5-C6-N6	2.34	123.91	120.35
21	A	28	A2M	C5-C6-N6	2.31	123.86	120.35
21	A	545	A2M	C5-C6-N6	2.26	123.79	120.35
21	A	1792	MA6	N1-C6-N6	-2.26	114.68	117.06
21	A	424	A2M	C5-C6-N6	2.23	123.75	120.35
21	A	1761	A2M	C5-C6-N6	2.20	123.70	120.35
21	A	615	OMU	C2'-C1'-N1	-2.14	110.07	114.22
21	A	615	OMU	O4-C4-C5	-2.13	121.41	125.16
21	A	168	OMU	O2'-C2'-C1'	2.13	113.23	109.08

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	246	OMG	O4'-C4'-C5'-O5'
21	A	615	OMU	C1'-C2'-O2'-CM2
21	A	623	A2M	O4'-C4'-C5'-O5'
21	A	1310	PSU	C2'-C1'-C5-C4
21	A	1648	OMC	O4'-C1'-N1-C2
21	A	1648	OMC	O4'-C1'-N1-C6
21	A	1761	A2M	O4'-C4'-C5'-O5'
21	A	1761	A2M	C3'-C4'-C5'-O5'
21	A	246	OMG	C3'-C4'-C5'-O5'
21	A	623	A2M	C3'-C4'-C5'-O5'
10	V	1	AME	CT2-CT1-N-CA
10	V	1	AME	OT-CT1-N-CA
21	A	468	A2M	O4'-C4'-C5'-O5'
21	A	1793	MA6	C3'-C4'-C5'-O5'
21	A	392	OMG	O4'-C4'-C5'-O5'
21	A	392	OMG	C3'-C4'-C5'-O5'
21	A	1793	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
21	A	123	OMU	C1'-C2'-O2'-CM2
21	A	599	OMG	C4'-C5'-O5'-P
21	A	1131	OMG	C4'-C5'-O5'-P
21	A	468	A2M	C3'-C4'-C5'-O5'
4	O	138	IAS	CA-CB-CG-OD1
21	A	1310	PSU	O4'-C1'-C5-C4

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	606	PSU	2	0
21	A	615	OMU	1	0
21	A	1122	PSU	2	0
21	A	607	PSU	2	0
21	A	306	PSU	1	0
21	A	308	PSU	2	0
21	A	1792	MA6	1	0
21	A	1306	PSU	1	0
21	A	38	OMC	1	0
21	A	1014	OMU	2	0
21	A	1108	PSU	1	0
21	A	1637	PSU	1	0
21	A	1761	A2M	1	0
21	A	636	PSU	2	0
21	A	208	PSU	2	0
21	A	1793	MA6	1	0
21	A	28	A2M	1	0
21	A	418	OMC	3	0
21	A	123	OMU	1	0
21	A	1774	6MZ	2	0
21	A	1648	OMC	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 47 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

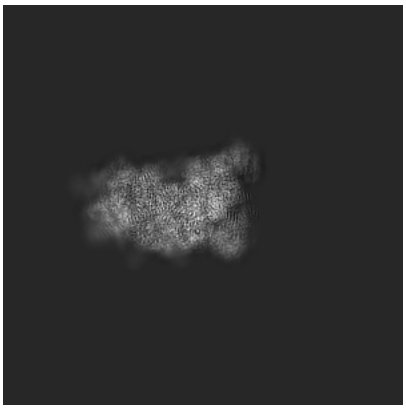
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18951. These allow visual inspection of the internal detail of the map and identification of artifacts.

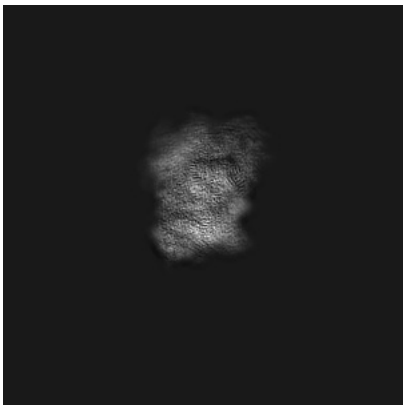
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

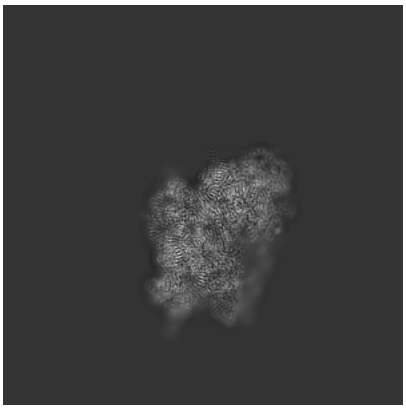
6.1.1 Primary map



X

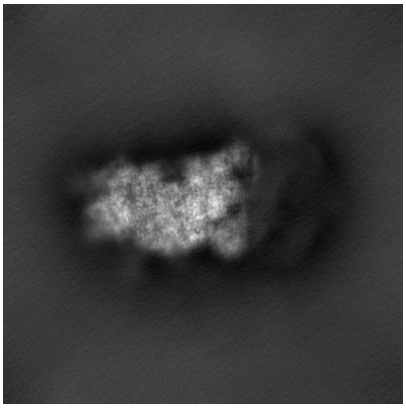


Y

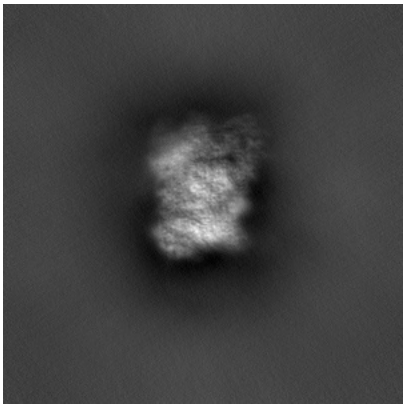


Z

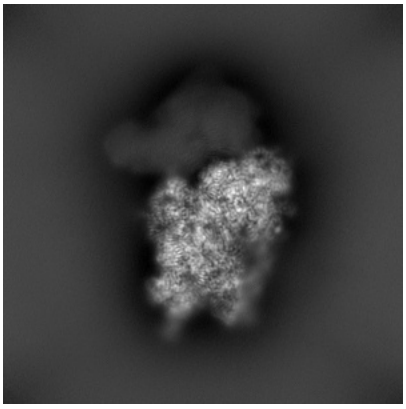
6.1.2 Raw map



X



Y

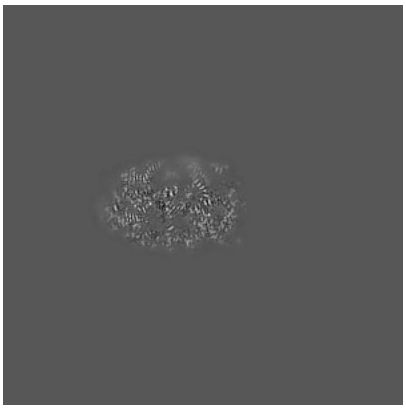


Z

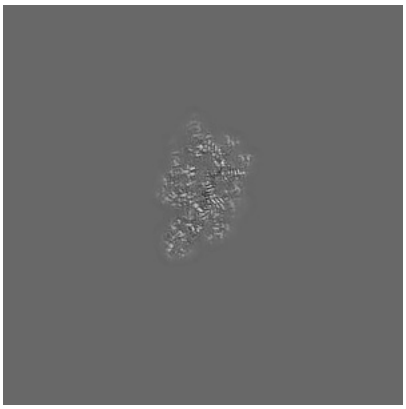
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

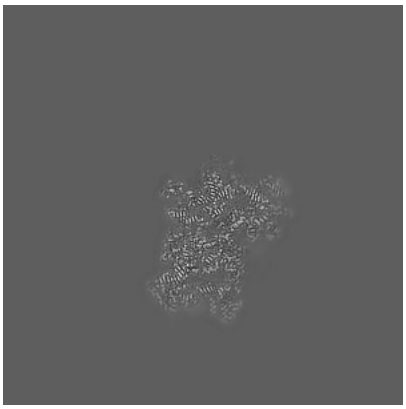
6.2.1 Primary map



X Index: 240

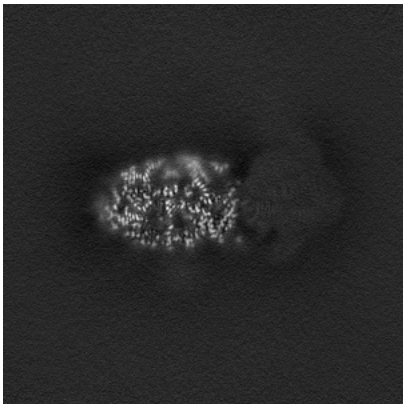


Y Index: 240

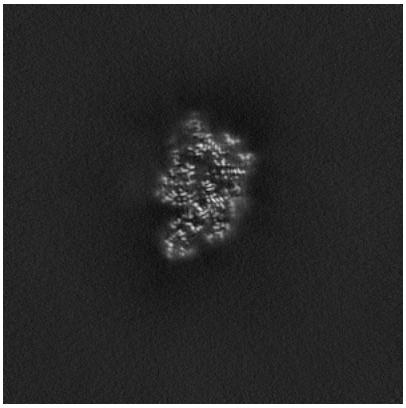


Z Index: 240

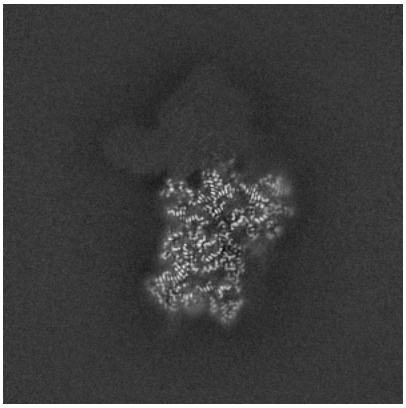
6.2.2 Raw map



X Index: 240



Y Index: 240

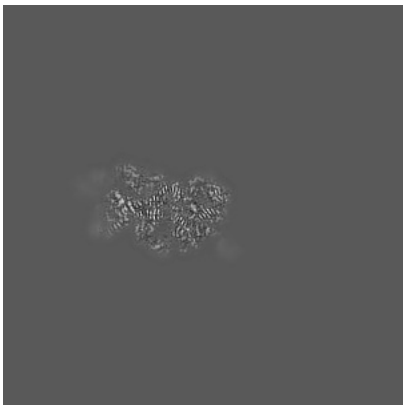


Z Index: 240

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

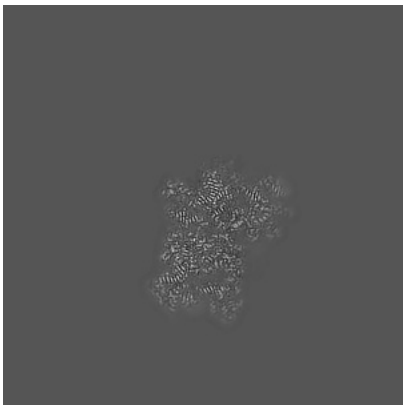
6.3 Largest variance slices (i)

6.3.1 Primary map



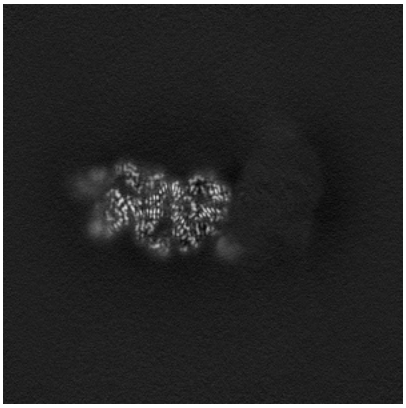
X Index: 210

Y Index: 229

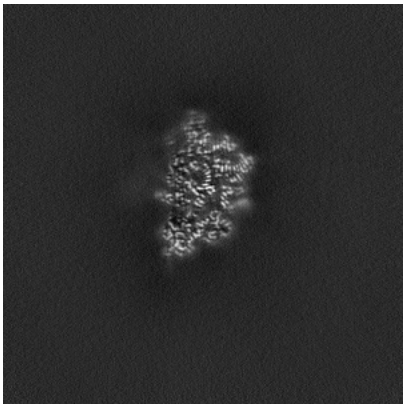


Z Index: 241

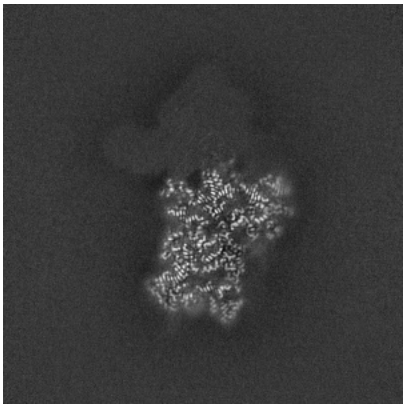
6.3.2 Raw map



X Index: 210



Y Index: 234

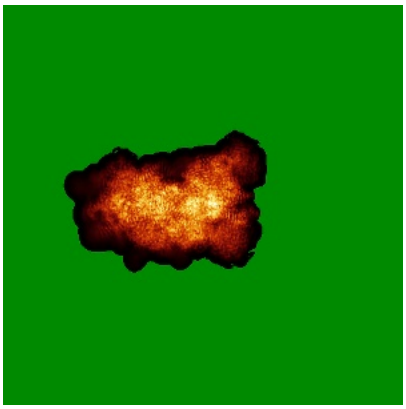


Z Index: 240

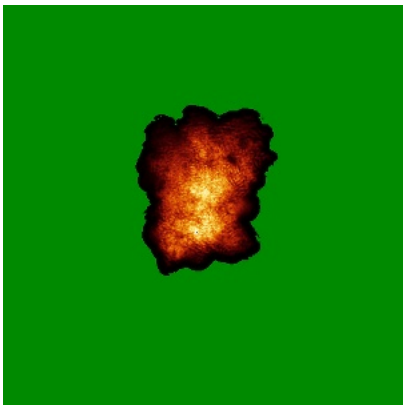
The images above show the largest variance slices of the map in three orthogonal directions.

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

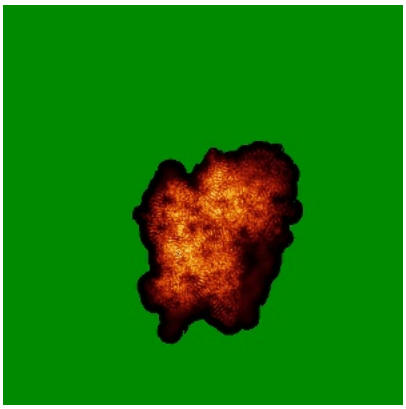
6.4.1 Primary map



X

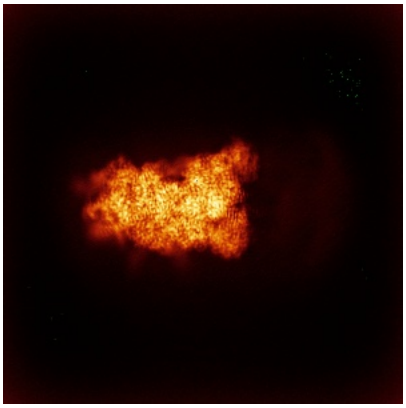


Y

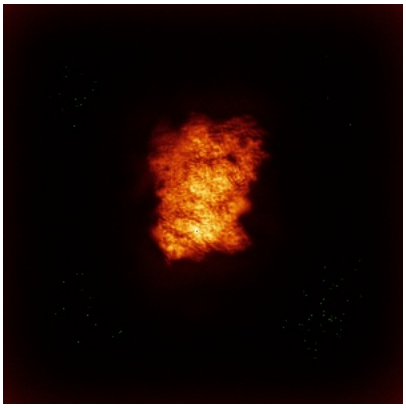


Z

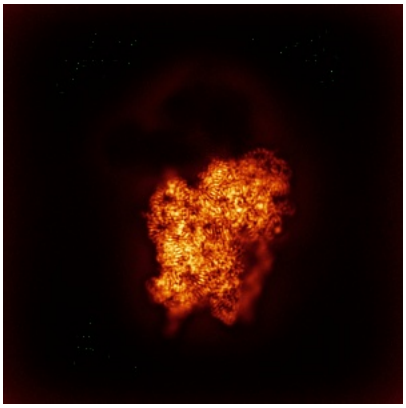
6.4.2 Raw map



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.

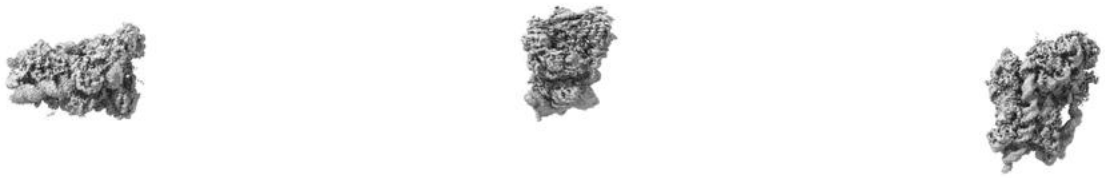
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

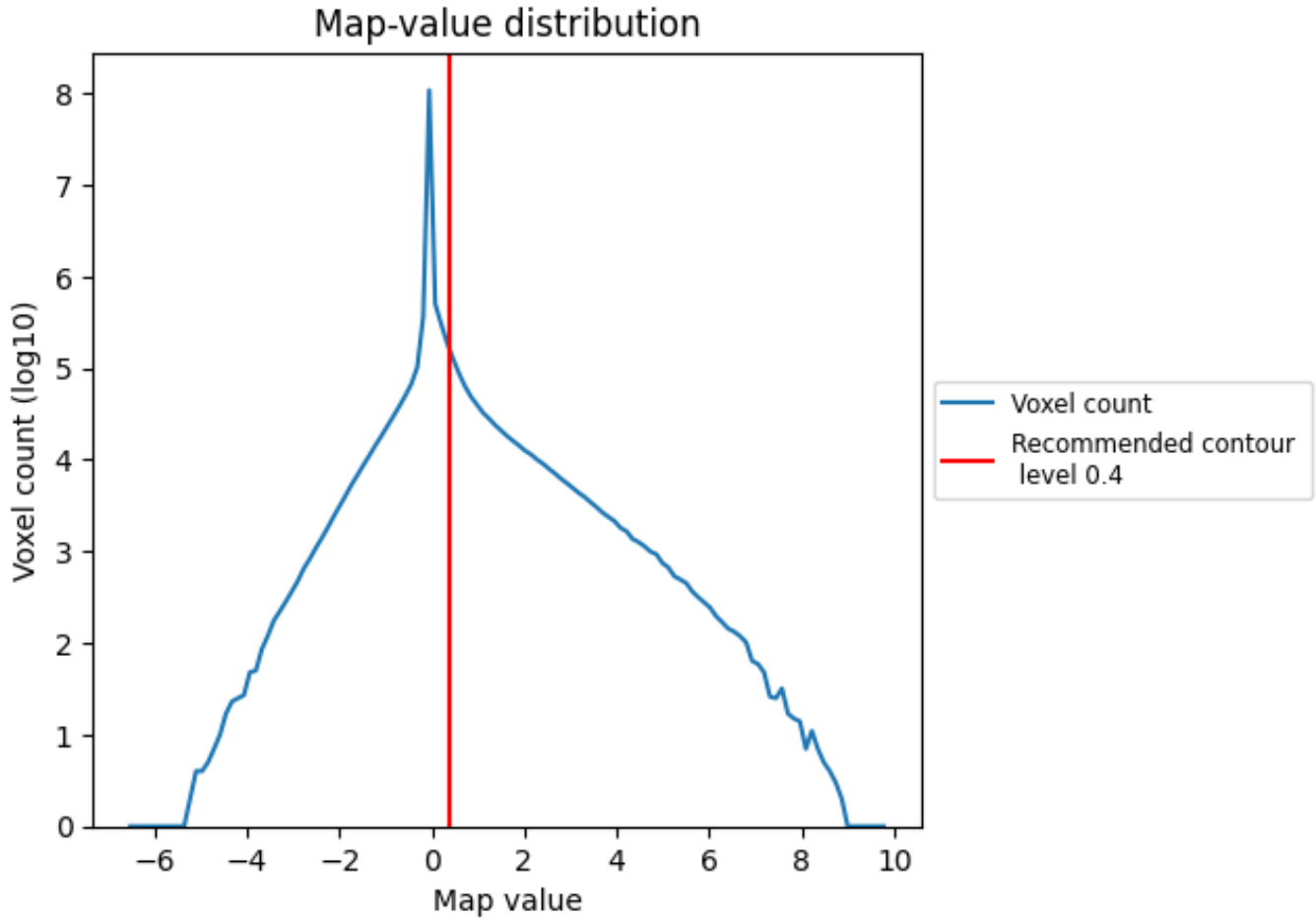
6.6 Mask visualisation (i)

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

7 Map analysis

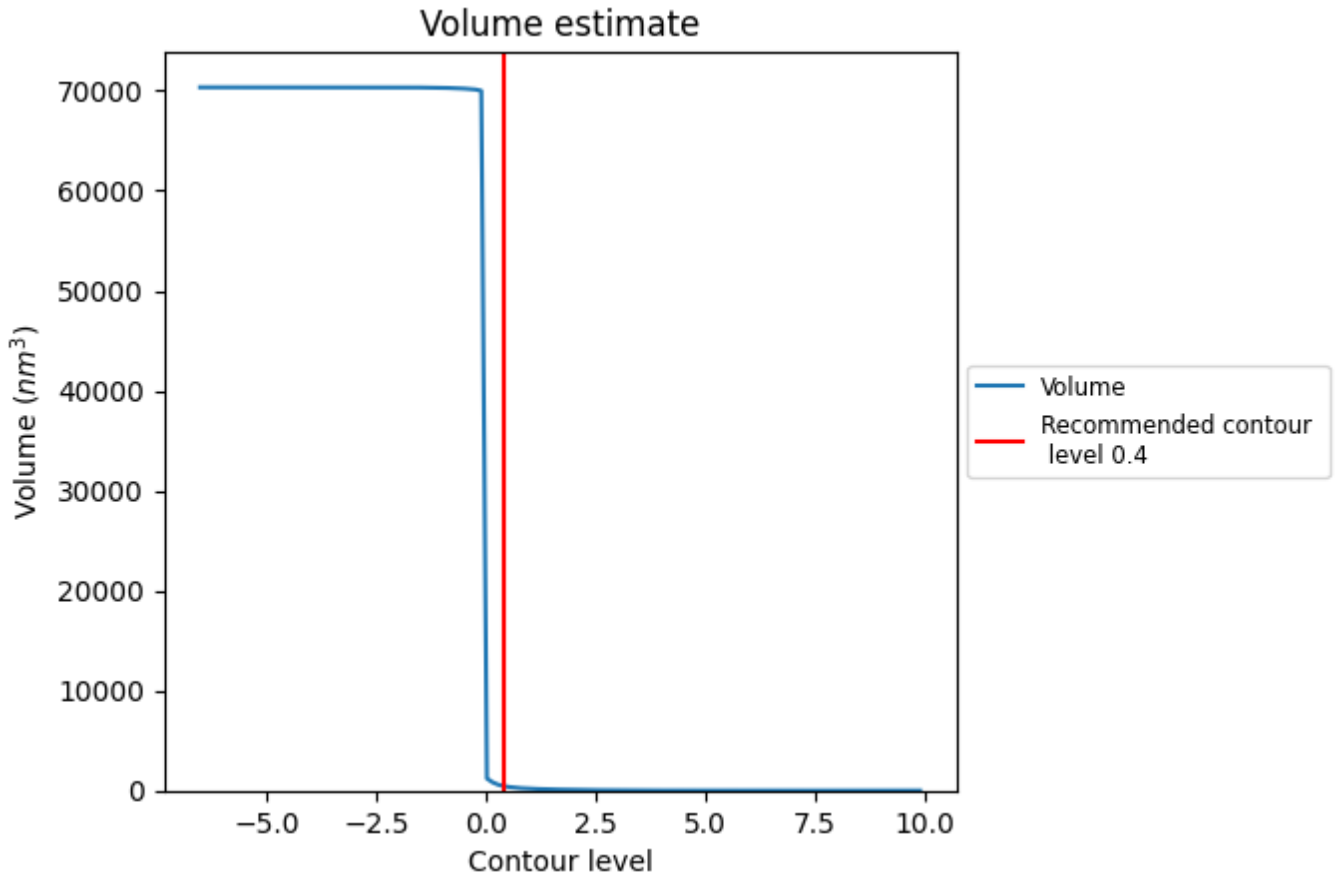
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

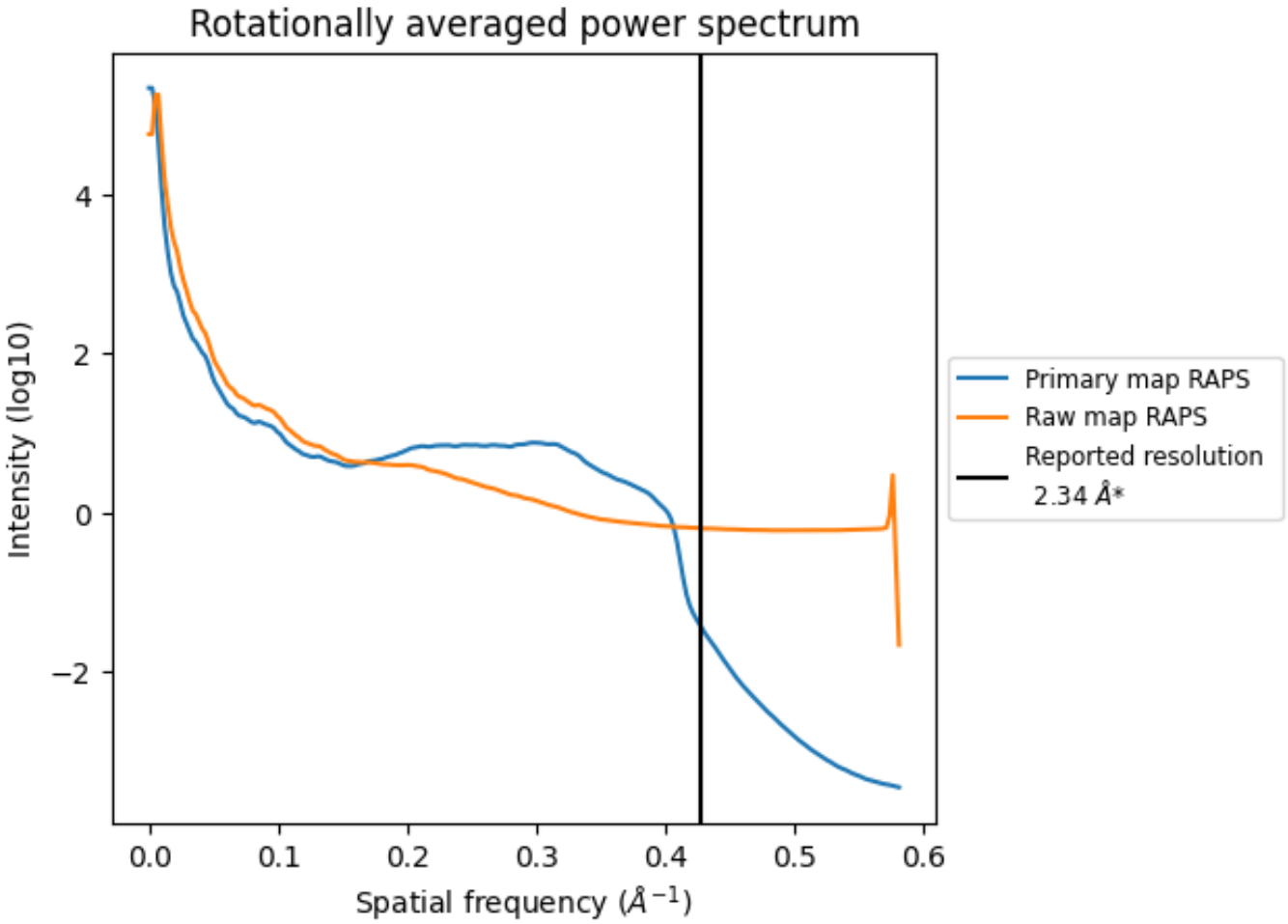
7.2 Volume estimate



The volume at the recommended contour level is 453 nm^3; this corresponds to an approximate mass of 409 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)

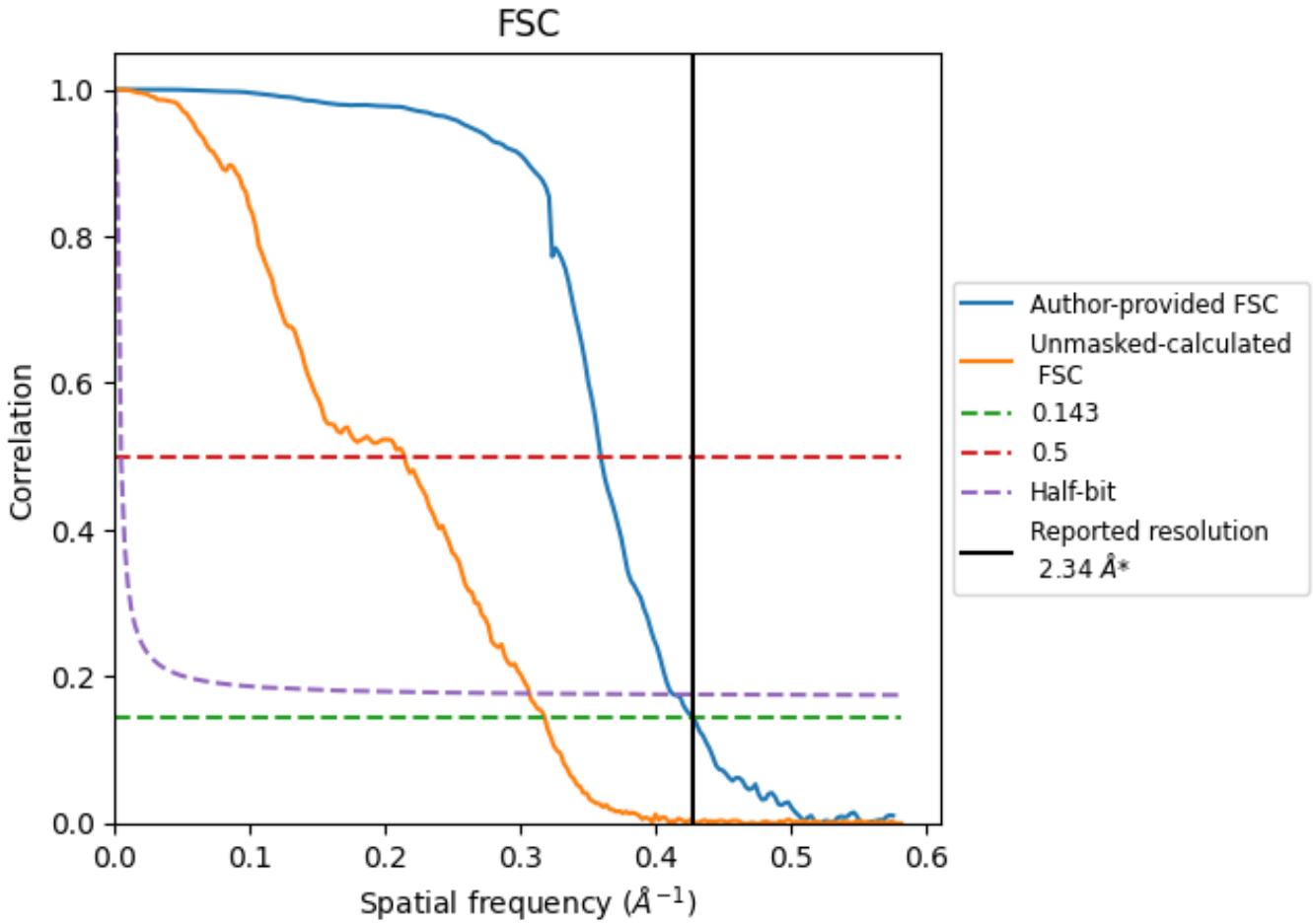


*Reported resolution corresponds to spatial frequency of 0.427 Å^{-1}

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 0.427 $Å^{-1}$

8.2 Resolution estimates (i)

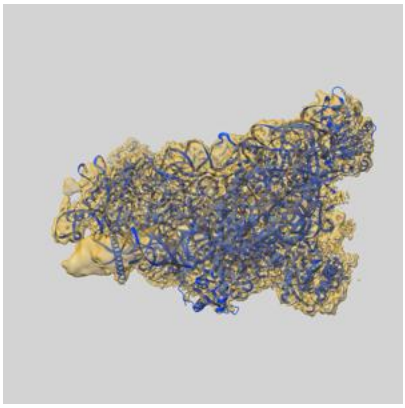
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	2.34	2.78	2.42
Unmasked-calculated*	3.15	4.68	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.34 by more than 10 %

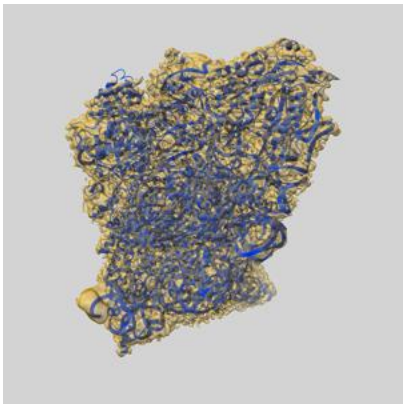
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18951 and PDB model 8R6F. Per-residue inclusion information can be found in section 3 on page 9.

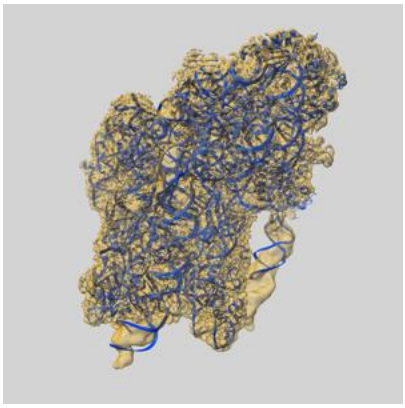
9.1 Map-model overlay



X



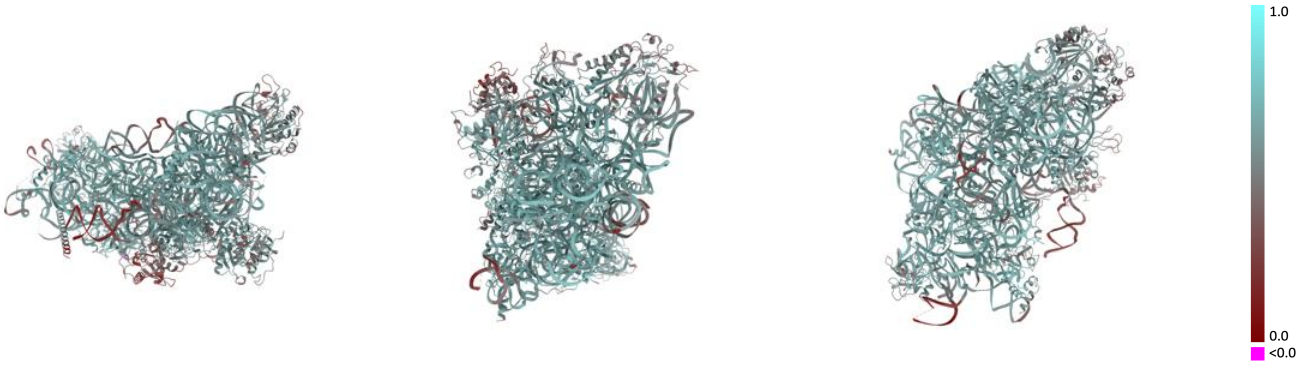
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

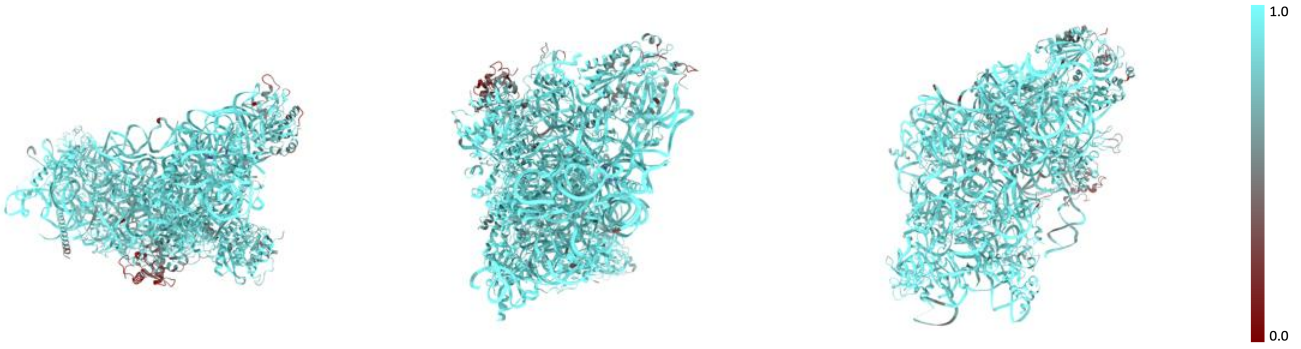
9.2 Q-score mapped to coordinate model (i)



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.

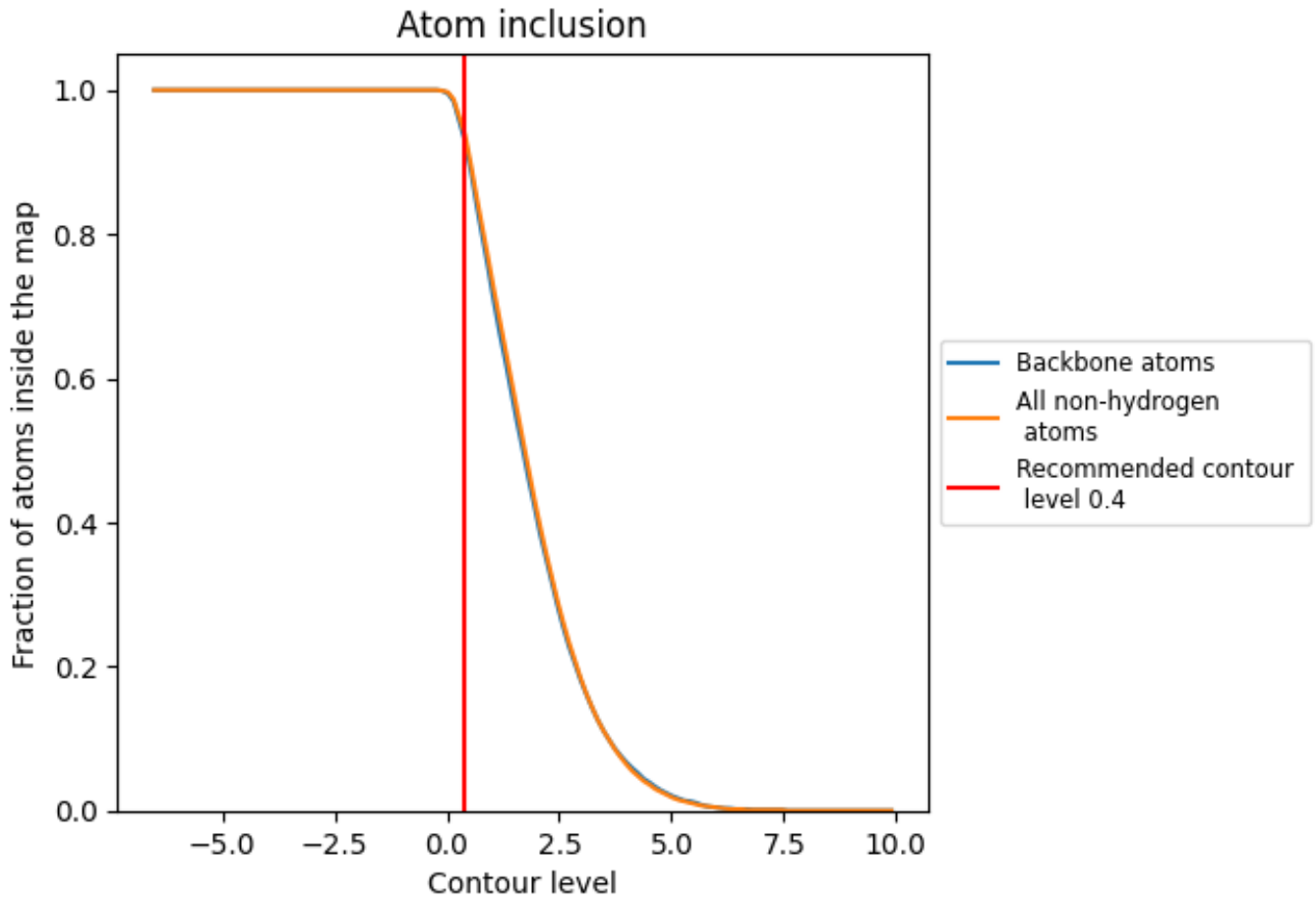
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.6000
A	0.9700	0.6060
B	0.8370	0.5260
C	0.9620	0.6410
E	0.9620	0.6430
G	0.9280	0.5700
H	0.5400	0.4000
I	0.9670	0.6380
J	0.9670	0.6490
L	0.9750	0.6630
N	0.9430	0.5980
O	0.8410	0.5460
V	0.9450	0.6060
W	0.9820	0.6700
X	0.9710	0.6460
Y	0.9610	0.6320
a	0.8850	0.6060
b	0.8410	0.5120
e	0.9180	0.6070
h	0.6030	0.3810
k	0.9410	0.5810
n	0.9310	0.5990