Full wwPDB EM Validation Report ⓘ

Feb 13, 2024 – 12:46 PM EST

PDB ID	:	3J0D
EMDB ID	:	EMD-1915
Title	:	Models for the T. thermophilus ribosome recycling factor bound to the E. coli post-termination complex
Authors	:	Yokoyama, T.; Shaikh, T.R.; Iwakura, N.; Kaji, H.; Kaji, A.; Agrawal, R.K.
Deposited on	:	2011-06-29
Resolution	:	11.10 Å(reported)
Based on initial models	:	2AW4, 1EH1, 2AVY

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:

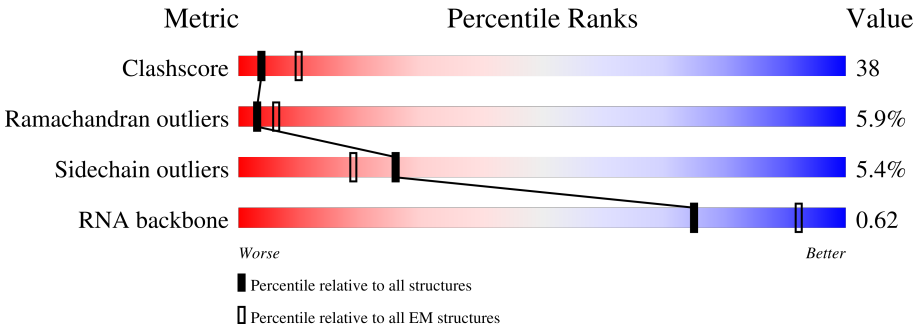
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 11.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	A	50	36% 56% · 6%
2	B	22	36% 55% 9%
3	C	17	35% 65%
4	D	13	54% 46%
5	E	19	5% 53% 47%
6	F	19	5% 32% 63% 5%
7	G	141	· 33% 62% ·

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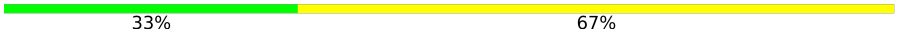
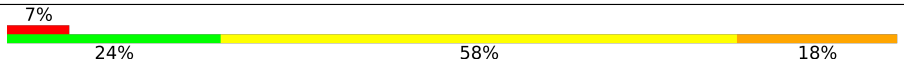
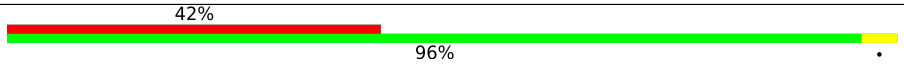
Mol	Chain	Length	Quality of chain
8	H	18	
9	h	19	
10	I	123	
11	J	185	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7260 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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	50	1070	479	196	345	50	0	0

- Molecule 2 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	22	463	208	81	152	22	0	0

- Molecule 3 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	17	364	162	65	120	17	0	0

- Molecule 4 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	13	283	125	53	92	13	0	0

- Molecule 5 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	19	407	182	75	131	19	0	0

- Molecule 6 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	19	411	183	79	130	19	0	0

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 8 is a RNA chain called ribosomal 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	18	Total	C	N	O	P	0	0
			386	172	71	125	18		

- Molecule 9 is a RNA chain called ribosomal 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	19	Total	C	N	O	P	0	0
			412	183	77	133	19		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	123	Total	C	N	O	S	0	0
			954	589	196	165	4		

- Molecule 11 is a protein called Ribosome-recycling factor.

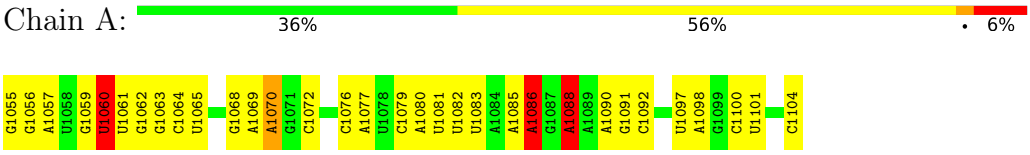
Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	185	Total	C	N	O	S	0	0
			1478	924	270	282	2		

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: ribosomal 23S RNA

Chain A:

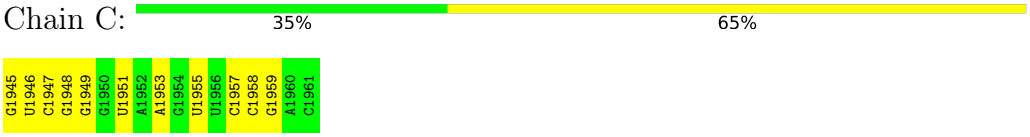


• Molecule 2: ribosomal 23S RNA

Chain B:

• Molecule 3: ribosomal 23S RNA

Chain C:

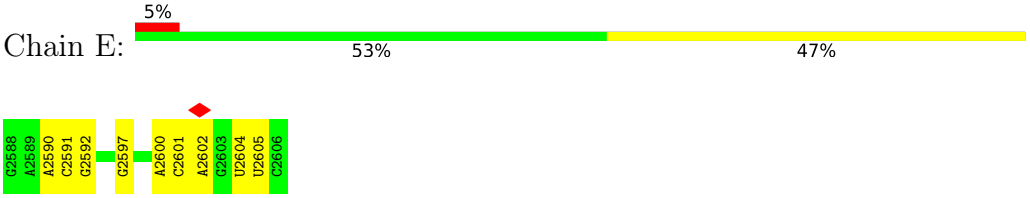


• Molecule 4: ribosomal 23S RNA

Chain D:

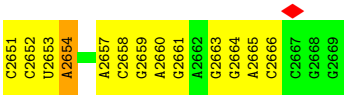
• Molecule 5: ribosomal 23S RNA

Chain E:



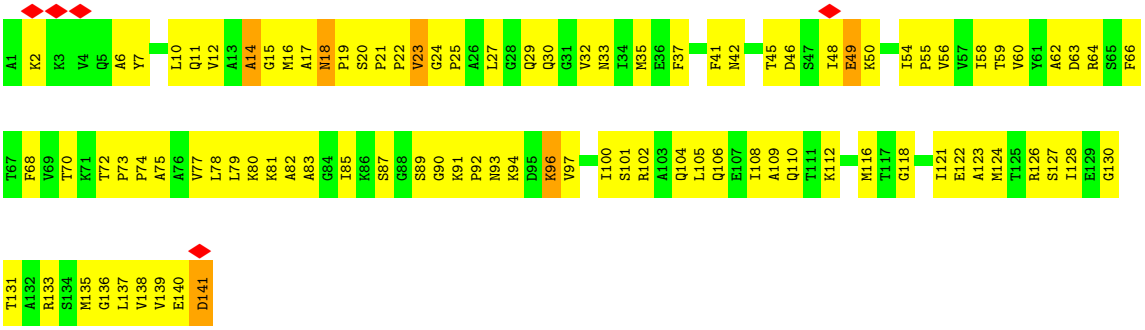
• Molecule 6: ribosomal 23S RNA

Chain F:



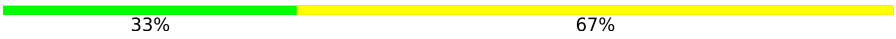
• Molecule 7: 50S ribosomal protein L11

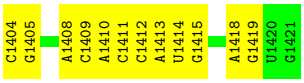
Chain G:



• Molecule 8: ribosomal 16S RNA

Chain H:



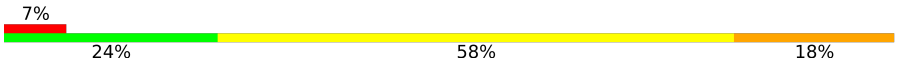


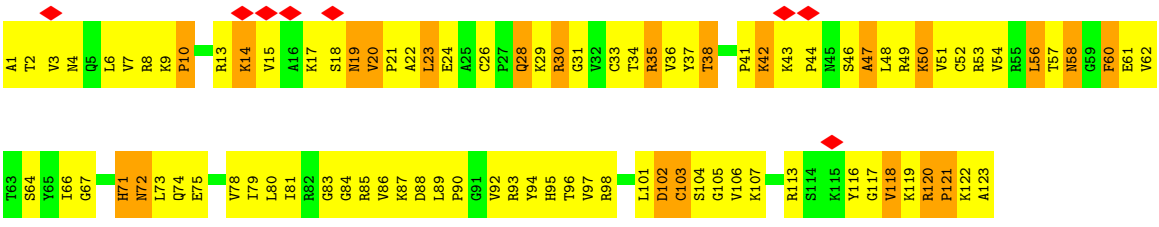
• Molecule 9: ribosomal 16S RNA

Chain h:

• Molecule 10: 30S ribosomal protein S12

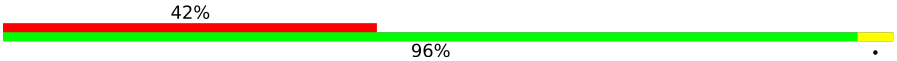
Chain I:

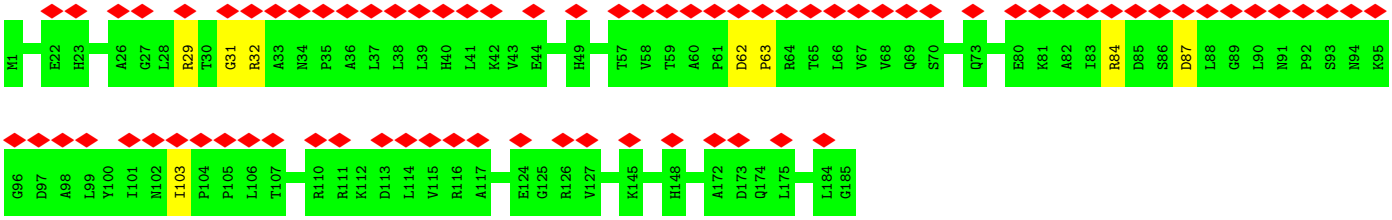




• Molecule 11: Ribosome-recycling factor

Chain J:




M1
E22
H23
A26
G27
L28
R29
T30
G31
R32
A33
N34
P35
A36
L37
L38
L39
H40
L41
K42
V43
E44
H49
T57
V58
T59
A60
P61
D62
P63
R64
T65
L66
V67
V68
Q69
S70
Q73
E80
K81
A82
I83
R84
D85
S86
D87
L88
G89
L90
N91
P92
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K95
G96
D97
A98
L99
Y100
I101
N102
I103
P104
P105
L106
T107
R110
R111
K112
D113
L114
V115
R116
A117
E124
G125
R126
V127
K145
H148
A172
D173
Q174
L175
L184
G185

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153927	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF CORRECTION OF 3D MAPS BY WIENER FILTRATION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	400.00	Depositor
Maximum defocus (nm)	4300.00	Depositor
Magnification	50310	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	2896.029	Depositor
Minimum map value	-898.730	Depositor
Average map value	30.563	Depositor
Map value standard deviation	271.777	Depositor
Recommended contour level	254.0	Depositor
Map size (Å)	361.4, 361.4, 361.4	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.78, 2.78, 2.78	Depositor

5 Model quality

5.1 Standard geometry

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	0.79	4/1198 (0.3%)	0.86	8/1865 (0.4%)
2	B	0.25	0/516	0.74	0/799
3	C	0.25	0/406	0.72	0/631
4	D	0.30	0/316	0.73	0/492
5	E	0.30	0/455	0.76	0/707
6	F	0.24	0/460	0.73	0/716
7	G	0.26	0/1046	0.58	0/1410
8	H	0.29	0/431	0.76	0/670
9	h	0.25	0/461	0.72	0/718
10	I	0.22	0/966	0.47	0/1295
11	J	0.96	0/1497	0.99	2/2017 (0.1%)
All	All	0.56	4/7752 (0.1%)	0.77	10/11320 (0.1%)

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
1	A	0	3
11	J	1	0
All	All	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1086	A	C5-C6	-17.67	1.25	1.41
1	A	1088	A	C6-N1	-10.45	1.28	1.35
1	A	1060	U	C2-N3	8.28	1.43	1.37
1	A	1086	A	N7-C5	-7.29	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1088	A	N1-C6-N6	-8.03	113.78	118.60
1	A	1060	U	C5-C4-O4	-7.43	121.44	125.90
1	A	1086	A	C4-C5-C6	6.93	120.47	117.00
1	A	1086	A	C6-C5-N7	-6.89	127.48	132.30
1	A	1088	A	C5-C6-N6	6.18	128.65	123.70
11	J	103	ILE	CA-CB-CG2	5.96	122.81	110.90
11	J	103	ILE	CG1-CB-CG2	5.57	123.66	111.40
1	A	1086	A	C2-N3-C4	-5.30	107.95	110.60
1	A	1060	U	N3-C2-O2	5.03	125.72	122.20
1	A	1060	U	N1-C2-O2	-5.02	119.28	122.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	J	103	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1060	U	Sidechain
1	A	1086	A	Sidechain
1	A	1088	A	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	1070	0	539	54	0
2	B	463	0	236	12	0
3	C	364	0	184	14	0
4	D	283	0	142	8	0
5	E	407	0	206	6	0
6	F	411	0	208	13	0
7	G	1032	0	1088	127	0
8	H	386	0	196	30	0
9	h	412	0	206	0	0
10	I	954	0	1011	111	0
11	J	1478	0	1521	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7260	0	5537	335	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 38.

All (335) 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)
8:H:1411:C:H5'	10:I:53:ARG:NH1	1.62	1.14
8:H:1411:C:H4'	10:I:53:ARG:HD2	1.45	0.98
1:A:1060:U:N3	1:A:1088:A:N7	2.17	0.92
7:G:105:LEU:HD11	7:G:139:VAL:HG11	1.54	0.89
7:G:27:LEU:HD23	7:G:27:LEU:H	1.37	0.88
10:I:8:ARG:HG3	10:I:9:LYS:H	1.40	0.87
7:G:25:PRO:O	7:G:29:GLN:HG2	1.75	0.86
1:A:1060:U:C2	1:A:1088:A:N7	2.46	0.83
10:I:56:LEU:HD11	10:I:81:ILE:HD12	1.61	0.83
10:I:48:LEU:HD23	10:I:48:LEU:H	1.42	0.83
7:G:55:PRO:HD3	7:G:74:PRO:HD3	1.60	0.82
8:H:1411:C:H4'	10:I:53:ARG:CD	2.09	0.82
10:I:1:ALA:CB	10:I:1:ALA:C	2.50	0.80
7:G:89:SER:HA	7:G:97:VAL:HG21	1.62	0.80
7:G:106:GLN:O	7:G:110:GLN:HG3	1.81	0.80
7:G:122:GLU:O	7:G:126:ARG:HG3	1.82	0.80
7:G:63:ASP:O	7:G:64:ARG:HG3	1.84	0.78
8:H:1411:C:C4'	10:I:53:ARG:HD2	2.13	0.77
10:I:1:ALA:CB	10:I:1:ALA:N	2.47	0.77
7:G:20:SER:HB3	7:G:21:PRO:HD3	1.67	0.76
8:H:1411:C:C5'	10:I:53:ARG:NH1	2.46	0.76
10:I:35:ARG:NH2	10:I:75:GLU:HB3	2.00	0.76
7:G:109:ALA:HB1	7:G:124:MET:HG3	1.66	0.76
7:G:89:SER:HB2	7:G:136:GLY:HA3	1.68	0.76
7:G:27:LEU:HD12	7:G:32:VAL:HG11	1.65	0.75
7:G:7:TYR:HB2	7:G:58:ILE:O	1.87	0.74
7:G:89:SER:HA	7:G:97:VAL:CG2	2.17	0.74
7:G:14:ALA:HA	7:G:45:THR:HG21	1.68	0.74
10:I:66:ILE:HD13	10:I:73:LEU:HD12	1.69	0.73
7:G:21:PRO:HB2	7:G:22:PRO:HD3	1.70	0.72
1:A:1060:U:C4	1:A:1088:A:N6	2.58	0.72
1:A:1083:U:H1'	1:A:1086:A:H61	1.55	0.72
8:H:1413:A:OP1	10:I:61:GLU:N	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:98:ARG:HE	10:I:98:ARG:HA	1.55	0.71
2:B:1913:A:H1'	2:B:1914:C:OP1	1.90	0.71
8:H:1413:A:OP1	10:I:61:GLU:HB2	1.90	0.71
7:G:32:VAL:HG22	7:G:60:VAL:HG21	1.73	0.70
10:I:35:ARG:HG3	10:I:36:VAL:H	1.56	0.70
7:G:135:MET:HG3	7:G:137:LEU:HG	1.73	0.70
10:I:28:GLN:HG3	10:I:80:LEU:HD21	1.73	0.70
10:I:20:VAL:HG13	10:I:94:TYR:HH	1.57	0.70
1:A:1082:U:N3	1:A:1086:A:C6	2.60	0.69
10:I:80:LEU:HD23	10:I:97:VAL:HG21	1.74	0.69
10:I:79:ILE:HD13	10:I:96:THR:HG22	1.74	0.69
10:I:24:GLU:HB3	10:I:26:CYS:SG	2.34	0.68
7:G:11:GLN:HA	7:G:55:PRO:HA	1.75	0.67
10:I:1:ALA:C	10:I:1:ALA:N	2.48	0.67
8:H:1411:C:O3'	10:I:53:ARG:NE	2.28	0.67
8:H:1412:C:H2'	8:H:1413:A:C8	2.29	0.67
3:C:1959:G:O2'	8:H:1418:A:O4'	2.12	0.66
1:A:1060:U:O2	1:A:1088:A:N7	2.27	0.66
2:B:1912:A:N6	8:H:1408:A:O2'	2.27	0.66
7:G:20:SER:O	7:G:25:PRO:HD2	1.96	0.66
3:C:1959:G:H1'	8:H:1418:A:H1'	1.80	0.64
7:G:91:LYS:HB2	7:G:94:LYS:HD2	1.78	0.64
1:A:1060:U:O4	1:A:1088:A:N6	2.31	0.64
7:G:77:VAL:HA	7:G:80:LYS:CE	2.29	0.63
7:G:100:ILE:O	7:G:139:VAL:HA	1.97	0.63
5:E:2591:C:H2'	5:E:2592:G:C8	2.33	0.63
10:I:20:VAL:HG13	10:I:94:TYR:OH	1.98	0.63
10:I:85:ARG:HA	10:I:93:ARG:HA	1.81	0.63
1:A:1097:U:H2'	1:A:1098:A:H5'	1.80	0.62
5:E:2591:C:H2'	5:E:2592:G:H8	1.64	0.62
10:I:43:LYS:N	10:I:44:PRO:HD2	2.14	0.62
1:A:1060:U:C5	7:G:131:THR:HG22	2.35	0.62
7:G:27:LEU:H	7:G:27:LEU:CD2	2.08	0.62
3:C:1959:G:O2'	8:H:1418:A:C1'	2.48	0.62
7:G:74:PRO:O	7:G:77:VAL:HG22	1.99	0.62
7:G:32:VAL:HG22	7:G:60:VAL:CG2	2.31	0.61
1:A:1060:U:OP2	7:G:74:PRO:HA	2.01	0.61
1:A:1064:C:H4'	7:G:90:GLY:HA2	1.82	0.61
1:A:1076:C:H4'	7:G:94:LYS:NZ	2.15	0.61
7:G:85:ILE:HD13	7:G:137:LEU:HD21	1.83	0.61
10:I:78:VAL:HG12	10:I:101:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:U:O4	1:A:1086:A:C2	2.54	0.60
7:G:11:GLN:O	7:G:11:GLN:HG3	2.00	0.60
10:I:64:SER:OG	10:I:96:THR:HG23	2.00	0.60
1:A:1082:U:C4	1:A:1086:A:C2	2.90	0.60
7:G:37:PHE:HB2	7:G:66:PHE:CZ	2.36	0.60
7:G:105:LEU:HD11	7:G:139:VAL:CG1	2.28	0.60
7:G:130:GLY:HA2	7:G:133:ARG:HH21	1.67	0.60
5:E:2600:A:O2'	5:E:2601:C:H5'	2.01	0.59
10:I:35:ARG:HE	10:I:35:ARG:HA	1.68	0.59
7:G:77:VAL:HA	7:G:80:LYS:HE2	1.84	0.59
1:A:1080:A:H2'	1:A:1081:U:H6	1.67	0.59
8:H:1411:C:H5'	10:I:53:ARG:HH11	1.60	0.59
8:H:1411:C:H5'	10:I:53:ARG:HH12	1.60	0.59
10:I:19:ASN:O	10:I:20:VAL:HG23	2.03	0.58
8:H:1411:C:C3'	10:I:53:ARG:HD2	2.33	0.58
7:G:79:LEU:HD23	7:G:108:ILE:CD1	2.33	0.58
10:I:42:LYS:HE3	10:I:90:PRO:HD3	1.84	0.58
4:D:2246:G:H2'	4:D:2247:A:C8	2.38	0.58
10:I:22:ALA:HB2	10:I:56:LEU:HD21	1.85	0.58
7:G:85:ILE:CD1	7:G:137:LEU:HD21	2.34	0.58
7:G:10:LEU:HD12	7:G:10:LEU:O	2.04	0.58
7:G:121:ILE:O	7:G:124:MET:HG2	2.04	0.58
10:I:19:ASN:HB2	10:I:93:ARG:NH1	2.18	0.58
1:A:1082:U:C4	1:A:1086:A:N1	2.71	0.57
1:A:1079:C:O2'	7:G:133:ARG:NH2	2.38	0.57
7:G:91:LYS:O	7:G:91:LYS:HG3	2.05	0.57
7:G:102:ARG:HD3	7:G:141:ASP:OD2	2.04	0.57
7:G:23:VAL:HG23	7:G:24:GLY:H	1.70	0.57
3:C:1951:U:H2'	3:C:1953:A:OP2	2.05	0.57
1:A:1083:U:H1'	1:A:1086:A:N6	2.19	0.56
4:D:2246:G:H2'	4:D:2247:A:H8	1.70	0.56
1:A:1061:U:O4'	1:A:1070:A:H1'	2.06	0.56
1:A:1060:U:H5	7:G:131:THR:HG22	1.70	0.56
7:G:49:GLU:CG	7:G:54:ILE:HD11	2.36	0.56
7:G:109:ALA:HB1	7:G:124:MET:CG	2.34	0.56
10:I:8:ARG:HG3	10:I:9:LYS:N	2.17	0.56
7:G:46:ASP:HA	7:G:50:LYS:HG3	1.87	0.56
1:A:1055:G:HO2'	1:A:1085:A:H2	1.50	0.56
10:I:105:GLY:HA3	10:I:117:GLY:HA3	1.88	0.56
7:G:10:LEU:HD13	7:G:12:VAL:HG13	1.87	0.56
7:G:138:VAL:HG12	7:G:139:VAL:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:48:LEU:H	10:I:48:LEU:CD2	2.18	0.55
7:G:124:MET:O	7:G:128:ILE:HG12	2.06	0.55
8:H:1411:C:O3'	10:I:53:ARG:HD2	2.06	0.55
10:I:37:TYR:HB2	10:I:51:VAL:HG23	1.88	0.55
10:I:3:VAL:O	10:I:7:VAL:HG23	2.06	0.55
1:A:1097:U:C2'	1:A:1098:A:H5'	2.36	0.55
10:I:83:GLY:HA2	10:I:94:TYR:HD1	1.70	0.55
4:D:2247:A:H2'	4:D:2248:C:C6	2.41	0.55
7:G:63:ASP:O	7:G:64:ARG:CG	2.53	0.55
7:G:102:ARG:HD3	7:G:141:ASP:CG	2.27	0.55
10:I:30:ARG:CB	10:I:30:ARG:HH11	2.19	0.55
6:F:2666:C:O2	6:F:2666:C:O4'	2.25	0.54
10:I:20:VAL:O	10:I:23:LEU:HG	2.08	0.54
1:A:1083:U:H2'	1:A:1085:A:OP2	2.08	0.54
3:C:1945:G:H2'	3:C:1946:U:C6	2.43	0.54
5:E:2590:A:H2'	5:E:2591:C:C6	2.43	0.54
8:H:1412:C:H2'	8:H:1413:A:H8	1.73	0.54
10:I:58:ASN:ND2	10:I:58:ASN:H	2.06	0.54
7:G:18:ASN:N	7:G:19:PRO:HD2	2.23	0.53
7:G:130:GLY:HA2	7:G:133:ARG:NH2	2.23	0.53
7:G:102:ARG:HD3	7:G:141:ASP:OD1	2.08	0.53
10:I:86:VAL:HG11	10:I:89:LEU:HD23	1.90	0.53
1:A:1060:U:O2	1:A:1088:A:C8	2.61	0.53
7:G:23:VAL:HG23	7:G:24:GLY:N	2.23	0.53
7:G:27:LEU:HB2	7:G:32:VAL:HG21	1.91	0.53
7:G:116:MET:HE2	7:G:124:MET:HA	1.90	0.53
3:C:1959:G:O2'	8:H:1418:A:H1'	2.08	0.53
7:G:83:ALA:N	7:G:100:ILE:HD11	2.24	0.53
7:G:122:GLU:CD	7:G:122:GLU:H	2.12	0.53
10:I:1:ALA:CB	10:I:2:THR:N	2.71	0.53
2:B:1912:A:N6	8:H:1408:A:HO2'	2.06	0.53
7:G:79:LEU:HD11	7:G:131:THR:OG1	2.08	0.53
1:A:1082:U:C2	1:A:1086:A:C6	2.97	0.53
10:I:22:ALA:HB2	10:I:56:LEU:CD2	2.39	0.53
10:I:30:ARG:HH11	10:I:30:ARG:HB3	1.74	0.53
1:A:1083:U:C2	1:A:1086:A:N1	2.77	0.52
10:I:20:VAL:O	10:I:20:VAL:HG12	2.08	0.52
10:I:35:ARG:CZ	10:I:75:GLU:HB3	2.39	0.52
10:I:56:LEU:HB3	10:I:58:ASN:ND2	2.24	0.52
8:H:1411:C:O3'	10:I:53:ARG:CD	2.57	0.52
1:A:1080:A:O2'	1:A:1081:U:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:116:MET:CE	7:G:127:SER:HB2	2.40	0.52
7:G:85:ILE:HD12	7:G:87:SER:O	2.10	0.51
10:I:106:VAL:CG2	10:I:116:TYR:HB3	2.40	0.51
6:F:2665:A:C2'	6:F:2666:C:H5'	2.40	0.51
2:B:1909:C:H2'	2:B:1910:G:H8	1.75	0.51
7:G:7:TYR:HB2	7:G:59:THR:HA	1.93	0.51
10:I:31:GLY:HA3	10:I:54:VAL:CG1	2.41	0.51
10:I:54:VAL:HG12	10:I:56:LEU:HD12	1.93	0.51
2:B:1923:U:H2'	2:B:1924:C:C6	2.45	0.51
10:I:103:CYS:SG	10:I:104:SER:N	2.83	0.51
10:I:113:ARG:HA	10:I:118:VAL:HG23	1.93	0.51
10:I:95:HIS:HD1	10:I:96:THR:N	2.09	0.50
1:A:1061:U:H4'	1:A:1070:A:O3'	2.11	0.50
10:I:3:VAL:HG23	10:I:4:ASN:OD1	2.11	0.50
10:I:20:VAL:HG22	10:I:94:TYR:CE1	2.46	0.50
6:F:2665:A:O2'	6:F:2666:C:H5'	2.13	0.49
1:A:1076:C:H4'	7:G:94:LYS:HE3	1.94	0.49
2:B:1917:U:H2'	2:B:1918:A:H5'	1.93	0.49
8:H:1411:C:C5'	10:I:53:ARG:HH11	2.18	0.49
1:A:1057:A:C8	1:A:1086:A:C8	3.01	0.49
3:C:1957:C:H2'	3:C:1958:C:H6	1.77	0.49
6:F:2657:A:H2'	6:F:2658:C:O4'	2.13	0.49
7:G:77:VAL:HA	7:G:80:LYS:HE3	1.92	0.49
7:G:19:PRO:HB2	7:G:22:PRO:HD2	1.95	0.49
7:G:75:ALA:CB	7:G:131:THR:HG21	2.43	0.49
4:D:2247:A:O2'	4:D:2248:C:H5'	2.12	0.49
10:I:35:ARG:O	10:I:52:CYS:HB2	2.13	0.49
1:A:1076:C:H4'	7:G:94:LYS:CE	2.43	0.49
6:F:2654:A:N1	6:F:2665:A:H5"	2.28	0.48
3:C:1948:G:O2'	3:C:1949:G:H5'	2.13	0.48
3:C:1957:C:H2'	3:C:1958:C:C6	2.48	0.48
7:G:49:GLU:HG2	7:G:54:ILE:HD11	1.94	0.48
3:C:1947:C:O2'	3:C:1948:G:H5'	2.14	0.48
1:A:1076:C:H4'	7:G:94:LYS:HZ2	1.78	0.48
7:G:48:ILE:O	7:G:49:GLU:HB3	2.14	0.48
2:B:1919:A:H2'	2:B:1920:C:H5'	1.95	0.47
7:G:81:LYS:HG3	7:G:82:ALA:N	2.29	0.47
10:I:80:LEU:O	10:I:97:VAL:HG23	2.14	0.47
10:I:90:PRO:C	10:I:92:VAL:H	2.17	0.47
10:I:106:VAL:HG22	10:I:117:GLY:H	1.79	0.47
7:G:77:VAL:HG23	7:G:78:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:G:O2'	1:A:1092:C:H5'	2.15	0.47
7:G:72:THR:HB	7:G:73:PRO:HD2	1.96	0.47
8:H:1414:U:H2'	8:H:1415:G:H8	1.79	0.47
1:A:1059:G:N2	7:G:130:GLY:HA3	2.30	0.47
10:I:35:ARG:HG3	10:I:36:VAL:N	2.26	0.47
7:G:14:ALA:HB1	7:G:50:LYS:HA	1.95	0.47
10:I:50:LYS:N	10:I:50:LYS:HE2	2.30	0.47
10:I:58:ASN:N	10:I:58:ASN:HD22	2.11	0.47
1:A:1080:A:H2'	1:A:1081:U:C6	2.48	0.47
1:A:1064:C:C4'	7:G:90:GLY:HA2	2.45	0.47
7:G:54:ILE:HG21	7:G:70:THR:CG2	2.45	0.47
2:B:1917:U:C2'	2:B:1918:A:H5'	2.45	0.46
8:H:1410:A:H2'	8:H:1411:C:C6	2.50	0.46
4:D:2250:G:O5'	4:D:2250:G:H8	1.98	0.46
8:H:1411:C:H4'	10:I:53:ARG:HH11	1.79	0.46
10:I:121:PRO:C	10:I:123:ALA:H	2.18	0.46
1:A:1081:U:C5'	7:G:126:ARG:HD2	2.44	0.46
2:B:1921:G:O2'	2:B:1922:G:H5'	2.16	0.46
1:A:1055:G:O2'	1:A:1085:A:C2	2.66	0.46
8:H:1411:C:O3'	10:I:53:ARG:CZ	2.64	0.46
1:A:1064:C:O2'	1:A:1065:U:H5'	2.16	0.46
1:A:1081:U:O2'	1:A:1082:U:H5'	2.16	0.46
7:G:12:VAL:HG23	7:G:41:PHE:CZ	2.50	0.46
10:I:98:ARG:CB	10:I:116:TYR:HA	2.46	0.46
7:G:12:VAL:HG23	7:G:41:PHE:CE2	2.51	0.46
7:G:37:PHE:CZ	7:G:58:ILE:HD11	2.51	0.46
7:G:27:LEU:HD23	7:G:27:LEU:N	2.17	0.46
1:A:1081:U:H5'	7:G:126:ARG:HD2	1.97	0.45
10:I:49:ARG:HH12	10:I:88:ASP:CB	2.29	0.45
1:A:1081:U:H4'	7:G:123:ALA:HB1	1.99	0.45
3:C:1946:U:H2'	3:C:1947:C:C6	2.52	0.45
8:H:1412:C:H5"	10:I:61:GLU:HB3	1.97	0.45
1:A:1062:G:H2'	1:A:1063:G:H8	1.81	0.45
7:G:116:MET:SD	7:G:124:MET:HB2	2.56	0.45
10:I:8:ARG:CG	10:I:9:LYS:H	2.21	0.45
1:A:1082:U:H2'	1:A:1083:U:O4'	2.16	0.45
7:G:14:ALA:CB	7:G:50:LYS:HA	2.47	0.45
7:G:79:LEU:CD1	7:G:131:THR:OG1	2.64	0.45
10:I:119:LYS:O	10:I:119:LYS:HG3	2.16	0.45
7:G:96:LYS:HG3	7:G:138:VAL:HG23	1.99	0.45
10:I:43:LYS:N	10:I:44:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:34:THR:HG21	10:I:53:ARG:CZ	2.47	0.45
7:G:140:GLU:OE1	7:G:140:GLU:HA	2.17	0.45
10:I:52:CYS:SG	10:I:66:ILE:HD11	2.58	0.45
7:G:17:ALA:C	7:G:19:PRO:HD2	2.37	0.44
10:I:71:HIS:CG	10:I:72:ASN:N	2.85	0.44
10:I:106:VAL:CG1	10:I:116:TYR:HB3	2.47	0.44
3:C:1959:G:C1'	8:H:1418:A:H1'	2.46	0.44
7:G:27:LEU:O	7:G:30:GLN:HB2	2.17	0.44
10:I:80:LEU:HD13	10:I:101:LEU:HD11	1.99	0.44
7:G:83:ALA:CA	7:G:100:ILE:HD11	2.46	0.44
6:F:2659:G:N2	6:F:2661:G:H5"	2.32	0.44
8:H:1410:A:H2'	8:H:1411:C:H6	1.81	0.44
1:A:1079:C:C2	1:A:1080:A:C8	3.06	0.44
4:D:2248:C:C2'	4:D:2249:U:H5'	2.47	0.44
7:G:92:PRO:O	7:G:93:ASN:HB2	2.17	0.44
8:H:1404:C:H2'	8:H:1405:G:C8	2.52	0.44
10:I:35:ARG:HH21	10:I:75:GLU:HB3	1.78	0.44
1:A:1082:U:N3	1:A:1086:A:C2	2.84	0.44
7:G:7:TYR:CB	7:G:59:THR:HA	2.47	0.44
7:G:64:ARG:HD2	7:G:64:ARG:C	2.38	0.44
7:G:121:ILE:HA	7:G:124:MET:HG2	1.99	0.44
7:G:7:TYR:C	7:G:7:TYR:CD1	2.91	0.43
7:G:29:GLN:HE21	7:G:29:GLN:HA	1.83	0.43
10:I:58:ASN:ND2	10:I:58:ASN:N	2.64	0.43
1:A:1079:C:O2'	7:G:133:ARG:CZ	2.67	0.43
6:F:2663:G:H2'	6:F:2664:G:C8	2.53	0.43
10:I:41:PRO:HD3	10:I:47:ALA:O	2.19	0.43
3:C:1958:C:O2'	3:C:1959:G:H5'	2.18	0.43
10:I:41:PRO:HG3	10:I:46:SER:O	2.18	0.43
1:A:1100:C:H2'	1:A:1101:U:H6	1.83	0.43
7:G:15:GLY:O	7:G:16:MET:HB2	2.19	0.43
10:I:35:ARG:HE	10:I:35:ARG:CA	2.30	0.43
10:I:38:THR:HA	10:I:49:ARG:O	2.19	0.43
7:G:74:PRO:HD2	7:G:77:VAL:HG21	2.01	0.43
1:A:1068:G:C6	1:A:1069:A:N6	2.87	0.43
10:I:22:ALA:HB1	10:I:29:LYS:HG3	2.00	0.43
10:I:117:GLY:O	10:I:118:VAL:HG13	2.19	0.43
10:I:56:LEU:HB2	10:I:60:PHE:O	2.19	0.42
5:E:2590:A:H2'	5:E:2591:C:H6	1.83	0.42
6:F:2653:U:H2'	6:F:2654:A:C8	2.54	0.42
10:I:14:LYS:NZ	10:I:17:LYS:HE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:34:THR:HB	10:I:53:ARG:HB2	2.02	0.42
1:A:1064:C:H2'	1:A:1065:U:O4'	2.20	0.42
7:G:17:ALA:O	7:G:18:ASN:CB	2.67	0.42
7:G:21:PRO:CB	7:G:22:PRO:HD3	2.46	0.42
10:I:83:GLY:HA2	10:I:94:TYR:CD1	2.52	0.42
7:G:18:ASN:N	7:G:19:PRO:CD	2.82	0.42
10:I:8:ARG:CZ	10:I:9:LYS:HE3	2.49	0.42
10:I:98:ARG:HA	10:I:98:ARG:NE	2.29	0.42
1:A:1072:C:N3	1:A:1092:C:N4	2.66	0.42
4:D:2247:A:H2'	4:D:2248:C:H6	1.83	0.42
6:F:2659:G:C2	6:F:2661:G:H5"	2.55	0.42
10:I:21:PRO:HD2	10:I:94:TYR:OH	2.20	0.42
2:B:1913:A:C1'	2:B:1914:C:OP1	2.65	0.42
7:G:46:ASP:HA	7:G:50:LYS:CG	2.49	0.42
4:D:2251:G:H8	4:D:2251:G:OP2	2.02	0.42
7:G:14:ALA:CA	7:G:45:THR:HG21	2.42	0.42
7:G:75:ALA:HB2	7:G:112:LYS:HE2	2.00	0.42
10:I:9:LYS:HG3	10:I:9:LYS:O	2.20	0.42
7:G:78:LEU:O	7:G:81:LYS:HG3	2.19	0.42
1:A:1056:G:N2	1:A:1104:C:N4	2.68	0.42
1:A:1076:C:O2'	1:A:1077:A:H5'	2.19	0.42
1:A:1081:U:O2'	7:G:118:GLY:HA2	2.20	0.42
6:F:2660:A:H2'	6:F:2661:G:O4'	2.20	0.42
7:G:138:VAL:CG1	7:G:139:VAL:N	2.83	0.42
5:E:2604:U:O2'	5:E:2605:U:H5'	2.20	0.41
7:G:62:ALA:C	7:G:64:ARG:H	2.24	0.41
7:G:100:ILE:HG22	7:G:101:SER:O	2.20	0.41
10:I:113:ARG:HD3	10:I:121:PRO:HD3	2.02	0.41
6:F:2651:C:O2'	6:F:2652:C:H5'	2.20	0.41
10:I:4:ASN:O	10:I:8:ARG:HG2	2.19	0.41
6:F:2653:U:H5	6:F:2654:A:HO2'	1.68	0.41
7:G:14:ALA:HA	7:G:45:THR:CG2	2.42	0.41
2:B:1922:G:H2'	2:B:1923:U:O4'	2.19	0.41
3:C:1946:U:H2'	3:C:1947:C:H6	1.85	0.41
6:F:2653:U:H3'	6:F:2654:A:H2'	2.02	0.41
7:G:56:VAL:CG2	7:G:68:PHE:HB2	2.50	0.41
10:I:30:ARG:HB3	10:I:57:THR:CG2	2.51	0.41
7:G:32:VAL:HG13	7:G:66:PHE:CD2	2.56	0.41
7:G:11:GLN:O	7:G:11:GLN:CG	2.69	0.41
10:I:6:LEU:O	10:I:10:PRO:HG3	2.19	0.41
10:I:42:LYS:HB3	10:I:43:LYS:H	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:42:LYS:HB3	10:I:44:PRO:HD2	2.03	0.41
10:I:87:LYS:HA	10:I:87:LYS:HZ3	1.86	0.41
10:I:120:ARG:HA	10:I:121:PRO:HD2	1.87	0.41
2:B:1918:A:H1'	2:B:1919:A:N7	2.36	0.40
7:G:6:ALA:O	7:G:7:TYR:HB3	2.21	0.40
7:G:56:VAL:HG22	7:G:68:PHE:HB2	2.03	0.40
7:G:75:ALA:HB3	7:G:131:THR:HG21	2.03	0.40
7:G:78:LEU:HA	7:G:81:LYS:HG2	2.02	0.40
10:I:80:LEU:HD13	10:I:101:LEU:CD1	2.51	0.40
7:G:16:MET:N	7:G:42:ASN:OD1	2.55	0.40
10:I:56:LEU:HB3	10:I:58:ASN:HD21	1.83	0.40
7:G:32:VAL:HG12	7:G:33:ASN:N	2.37	0.40
7:G:35:MET:SD	7:G:35:MET:C	3.00	0.40
7:G:100:ILE:CG2	7:G:104:GLN:HB2	2.52	0.40
10:I:101:LEU:HB3	10:I:102:ASP:H	1.61	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
7	G	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	4 29
10	I	121/123 (98%)	75 (62%)	29 (24%)	17 (14%)	0 4
11	J	183/185 (99%)	169 (92%)	9 (5%)	5 (3%)	5 31
All	All	443/449 (99%)	368 (83%)	49 (11%)	26 (6%)	3 17

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	18	ASN
10	I	10	PRO

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Mol	Chain	Res	Type
10	I	23	LEU
11	J	84	ARG
10	I	19	ASN
10	I	72	ASN
10	I	84	GLY
7	G	23	VAL
10	I	13	ARG
10	I	60	PHE
10	I	122	LYS
11	J	31	GLY
11	J	87	ASP
7	G	49	GLU
10	I	14	LYS
10	I	15	VAL
10	I	47	ALA
10	I	56	LEU
10	I	67	GLY
10	I	120	ARG
7	G	14	ALA
10	I	42	LYS
10	I	121	PRO
11	J	32	ARG
11	J	63	PRO
10	I	62	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	109/109 (100%)	106 (97%)	3 (3%)	43 65
10	I	103/103 (100%)	88 (85%)	15 (15%)	3 15
11	J	157/157 (100%)	155 (99%)	2 (1%)	69 81
All	All	369/369 (100%)	349 (95%)	20 (5%)	26 47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	2	LYS
7	G	96	LYS
7	G	141	ASP
10	I	18	SER
10	I	20	VAL
10	I	28	GLN
10	I	30	ARG
10	I	33	CYS
10	I	35	ARG
10	I	38	THR
10	I	50	LYS
10	I	58	ASN
10	I	71	HIS
10	I	74	GLN
10	I	102	ASP
10	I	103	CYS
10	I	107	LYS
10	I	118	VAL
11	J	29	ARG
11	J	62	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
7	G	11	GLN
7	G	29	GLN
7	G	30	GLN
7	G	33	ASN
7	G	93	ASN
10	I	58	ASN
10	I	72	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	49/50 (98%)	3 (6%)	0
2	B	20/22 (90%)	2 (10%)	1 (5%)
3	C	16/17 (94%)	1 (6%)	0
4	D	12/13 (92%)	0	0
5	E	17/19 (89%)	2 (11%)	0
6	F	18/19 (94%)	1 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	H	17/18 (94%)	2 (11%)	0
9	h	18/19 (94%)	3 (16%)	0
All	All	167/177 (94%)	14 (8%)	1 (0%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1070	A
1	A	1088	A
1	A	1090	A
2	B	1906	G
2	B	1914	C
3	C	1955	U
5	E	2597	G
5	E	2602	A
6	F	2654	A
8	H	1409	C
8	H	1419	G
9	h	1490	U
9	h	1493	A
9	h	1497	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1913	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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.

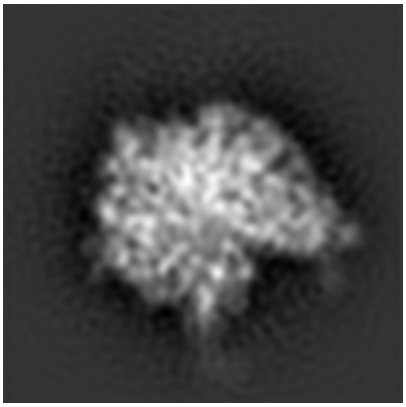
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1915. These allow visual inspection of the internal detail of the map and identification of artifacts.

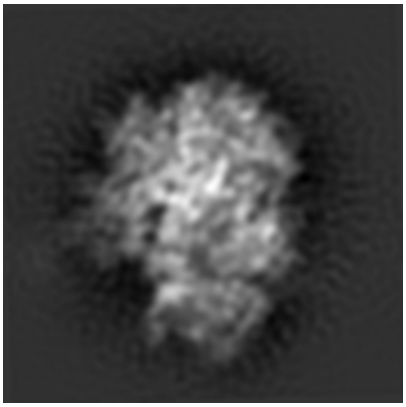
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

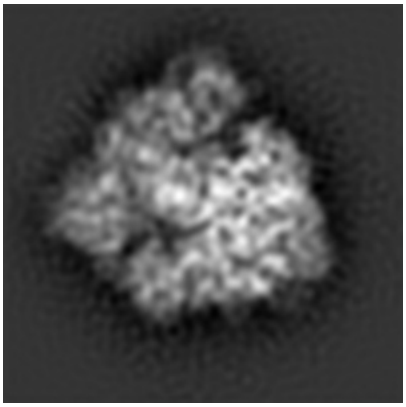
6.1.1 Primary map



X



Y

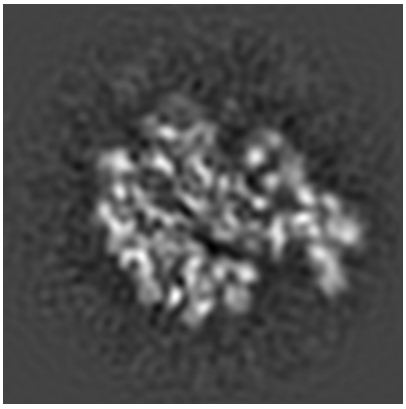


Z

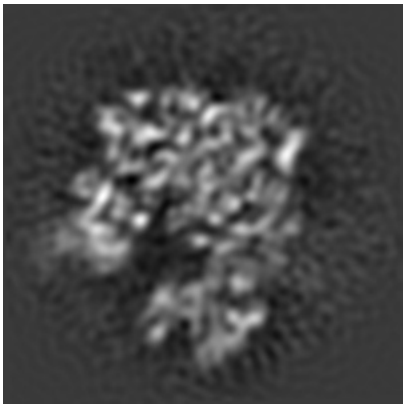
The images above show the map projected in three orthogonal directions.

6.2 Central slices

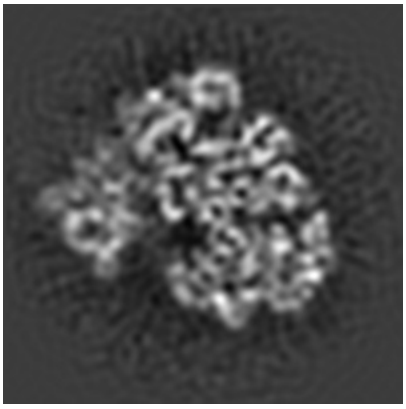
6.2.1 Primary map



X Index: 65



Y Index: 65

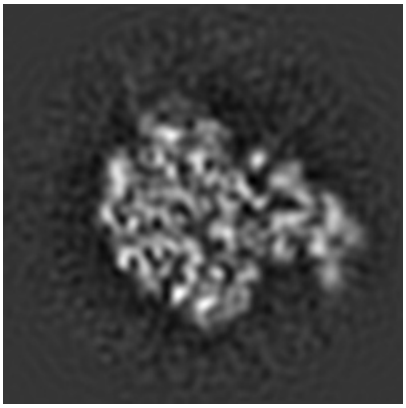


Z Index: 65

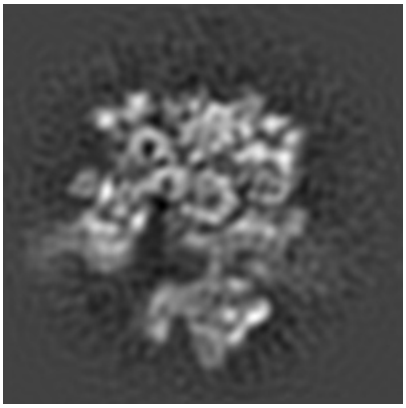
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

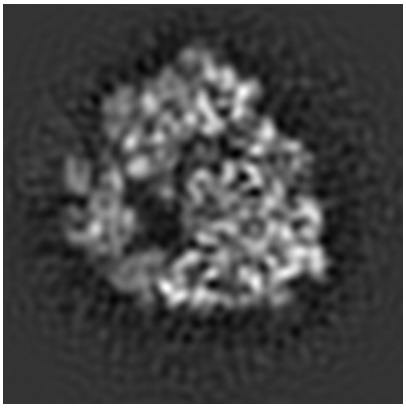
6.3.1 Primary map



X Index: 67



Y Index: 67

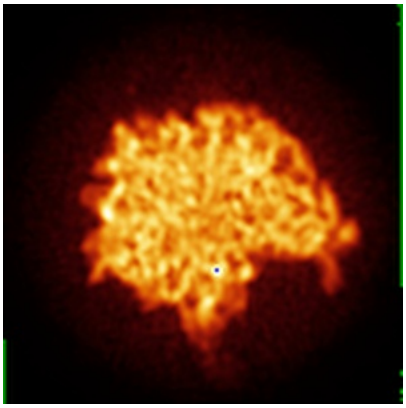


Z Index: 59

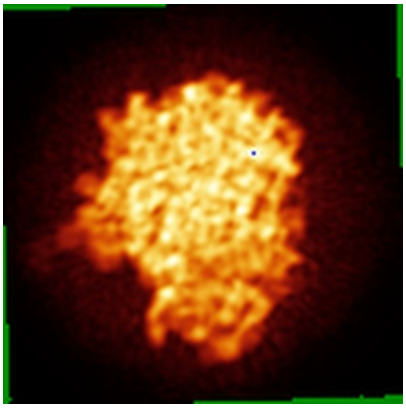
The images above show the largest variance slices of the map in three orthogonal directions.

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

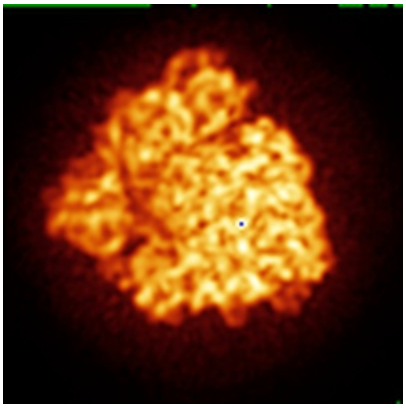
6.4.1 Primary map



X



Y

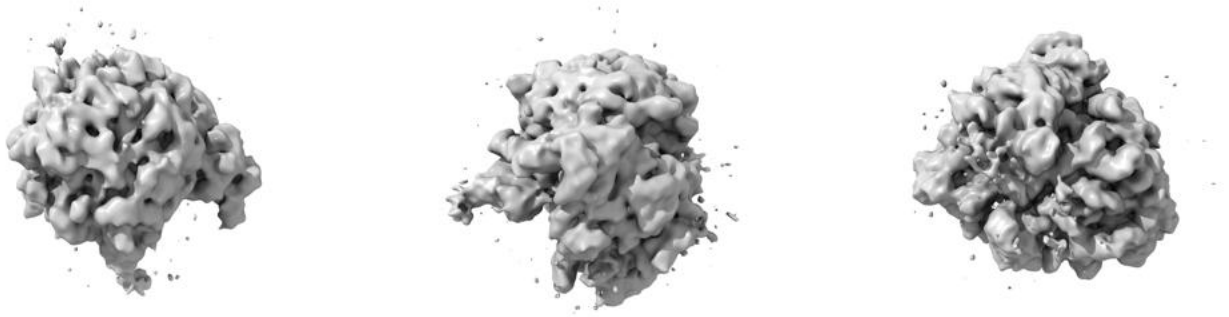


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 254.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

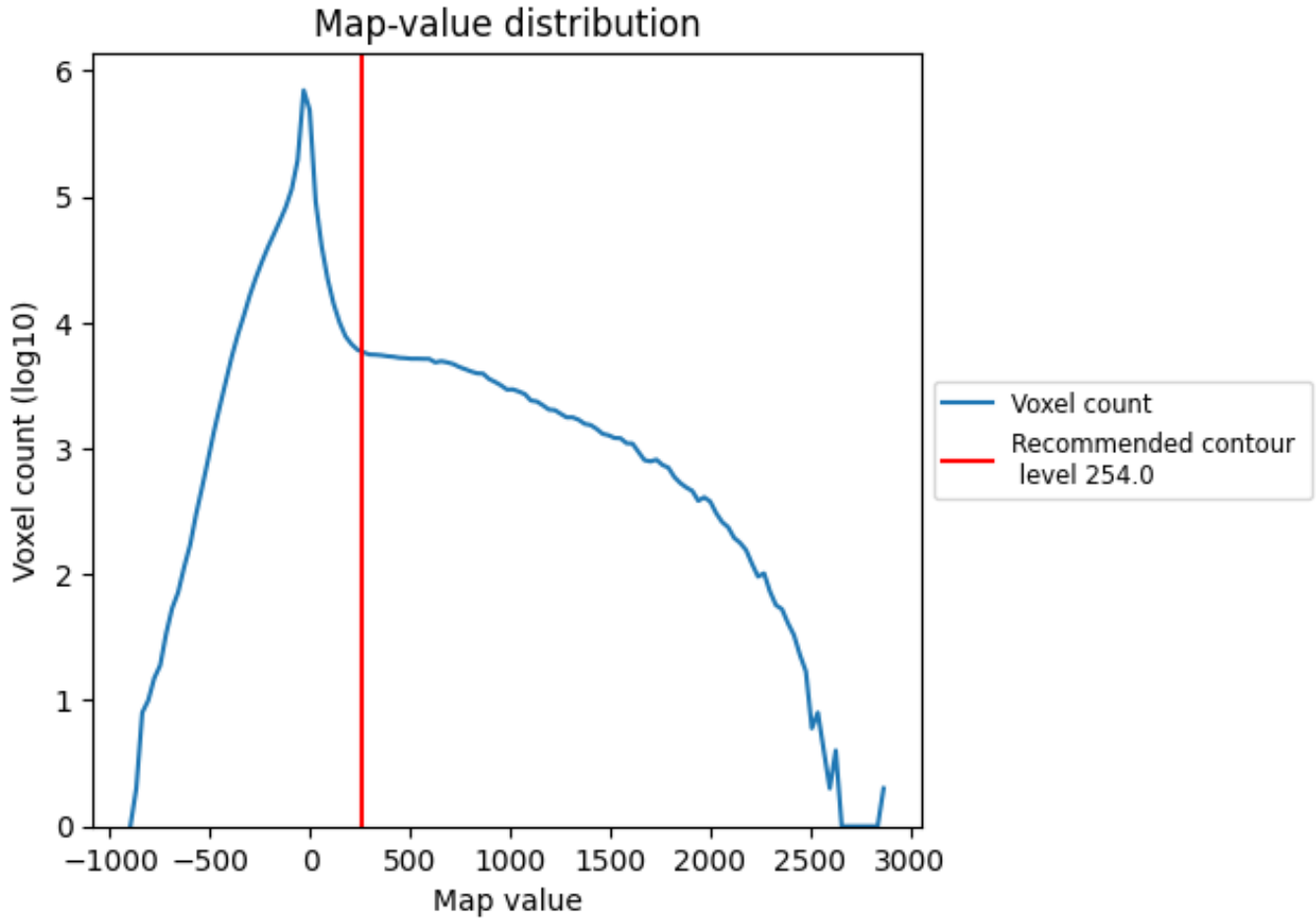
6.6 Mask visualisation (i)

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

7 Map analysis

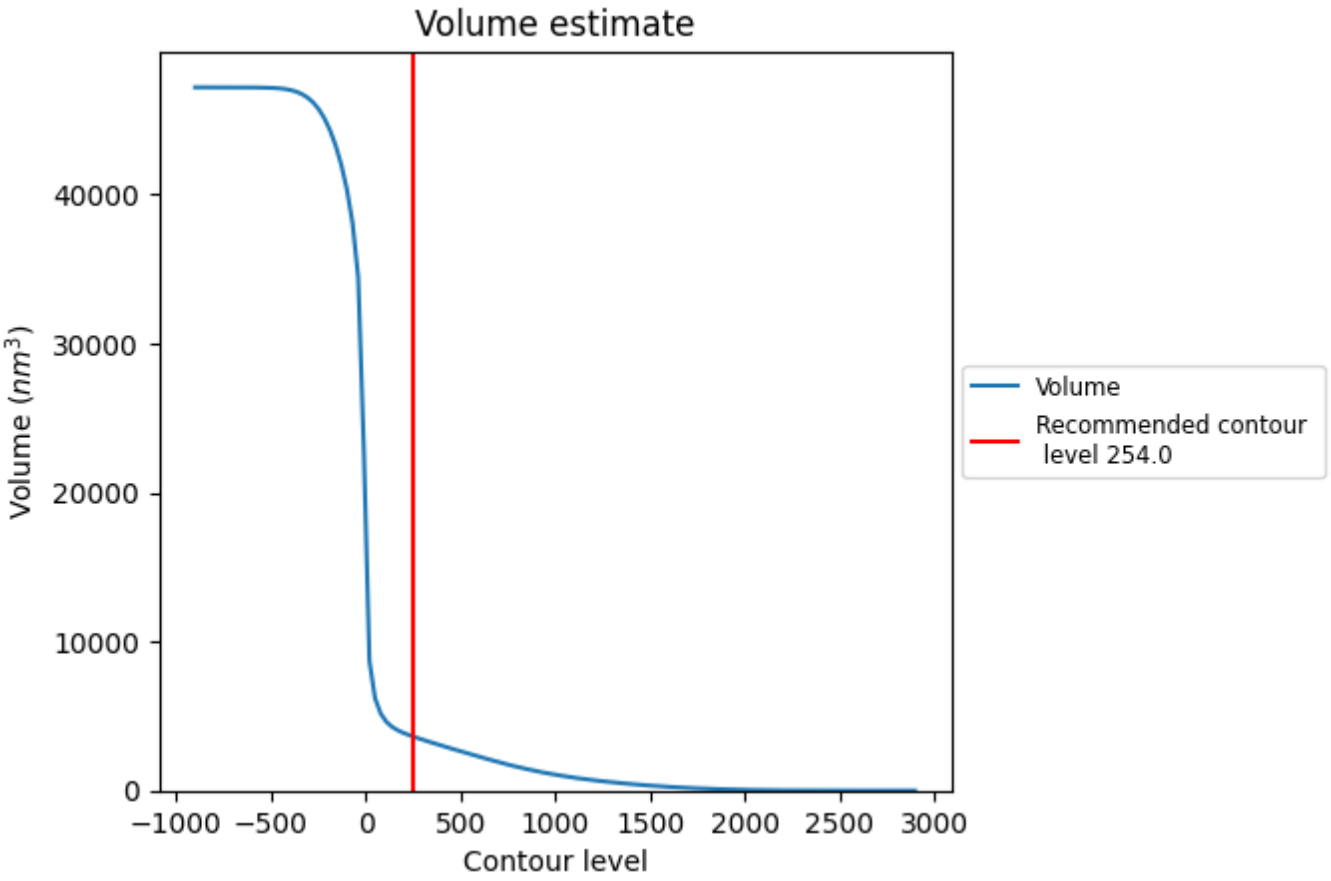
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

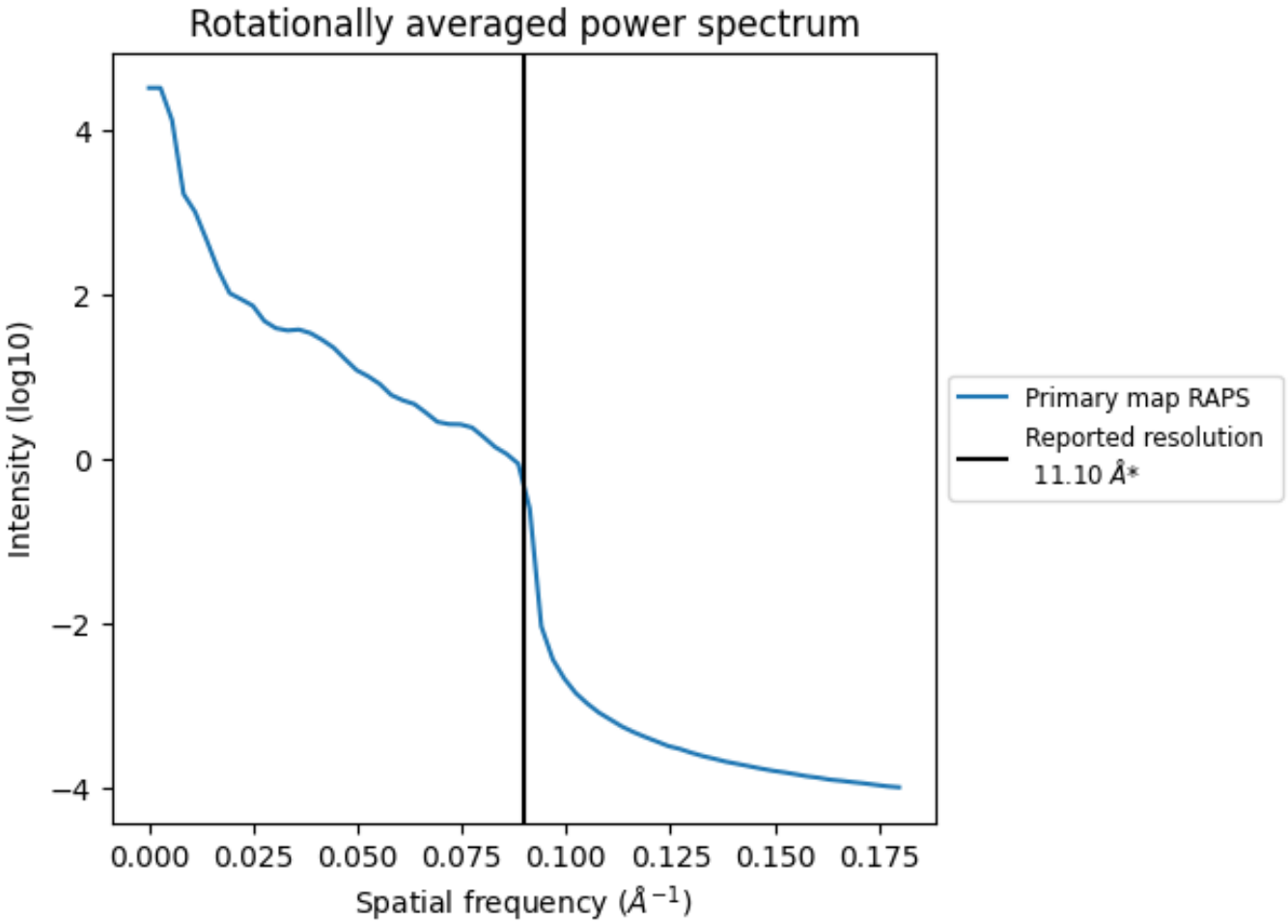
7.2 Volume estimate



The volume at the recommended contour level is 3609 nm^3; this corresponds to an approximate mass of 3260 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 0.090 Å^{-1}

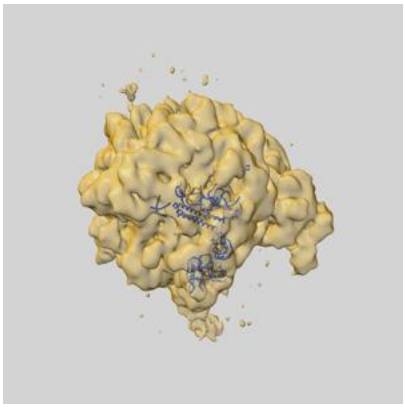
8 Fourier-Shell correlation (i)

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

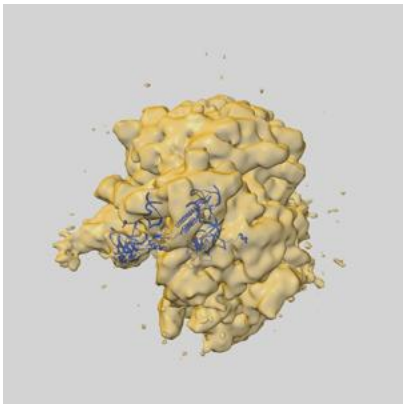
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1915 and PDB model 3J0D. Per-residue inclusion information can be found in section 3 on page 6.

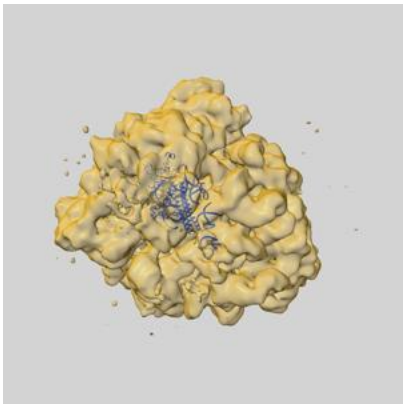
9.1 Map-model overlay



X



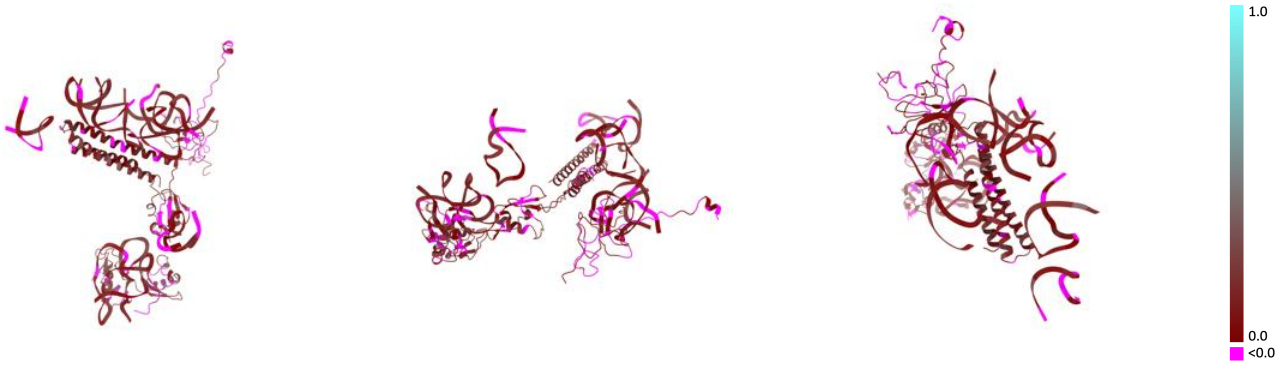
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 254.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

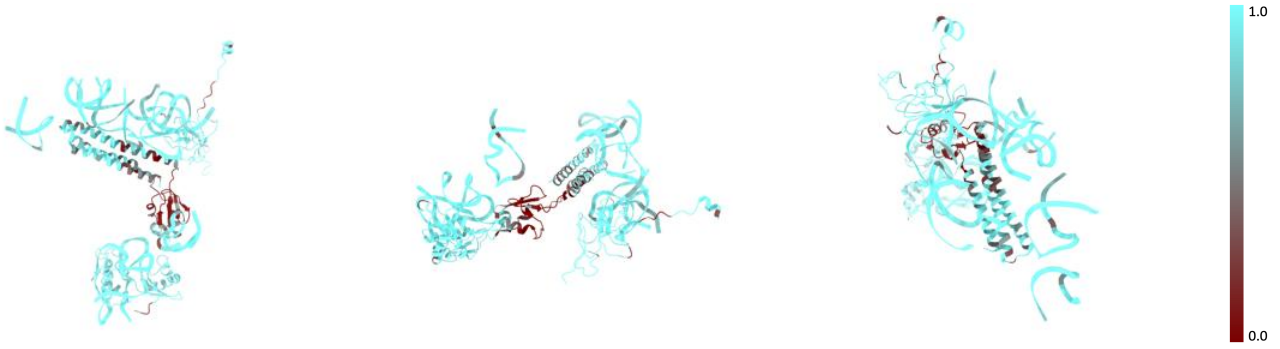
9.2 Q-score mapped to coordinate model



X Y Z

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

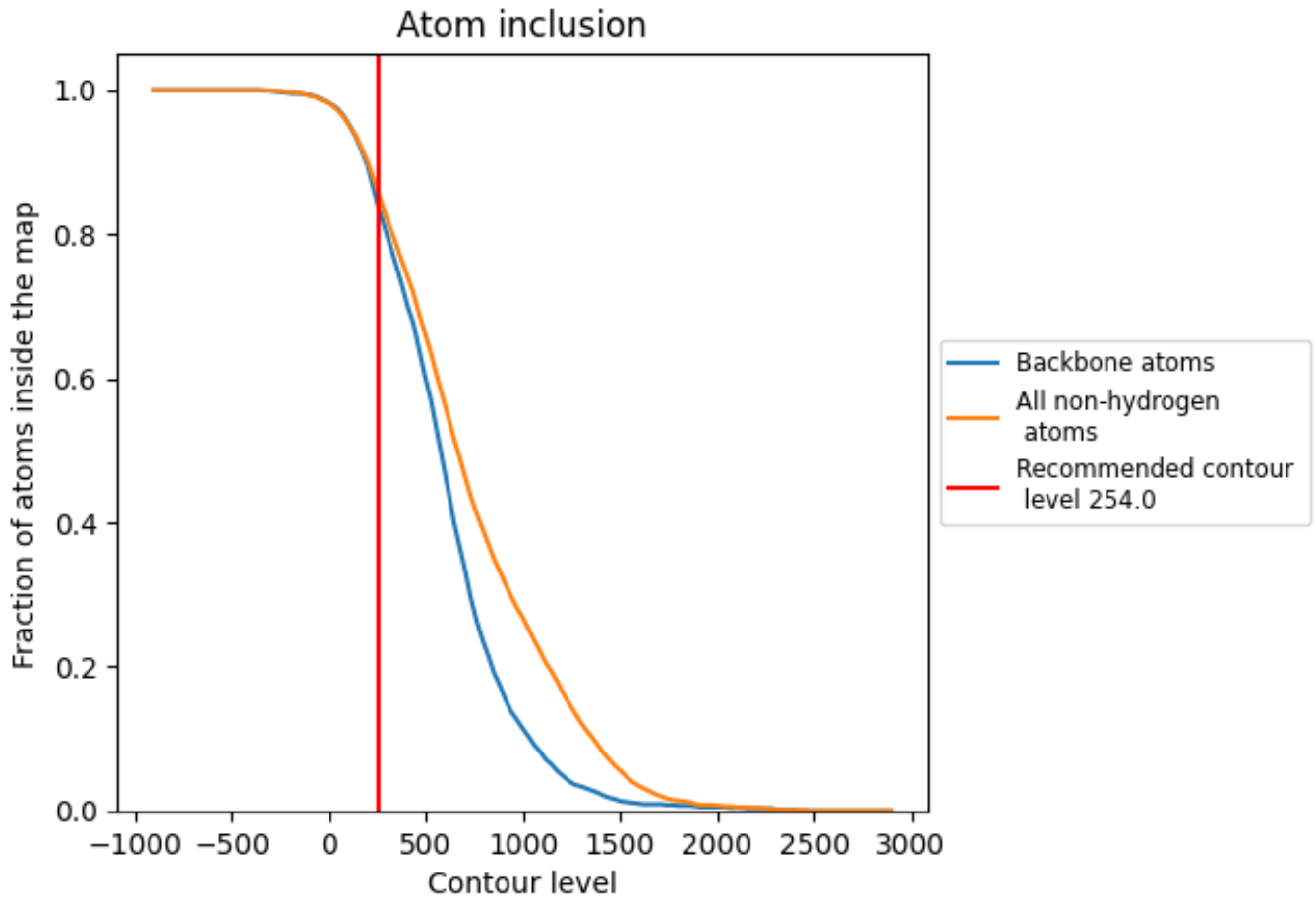
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (254.0).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 86% 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 (254.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8570	0.0830
A	0.9990	0.0940
B	0.9420	0.1040
C	0.9920	0.1030
D	0.8900	0.0530
E	0.9020	0.1120
F	0.8760	0.0490
G	0.9510	0.0760
H	0.8550	0.0640
I	0.9040	0.0160
J	0.5350	0.1160
h	0.9810	0.1120