Full wwPDB EM Validation Report

Apr 20, 2024 – 03:07 pm BST

PDB ID	:	8R57
EMDB ID	:	EMD-18903
Title	:	CryoEM structure of wheat 40S ribosomal subunit, head domain
Authors	:	Kravchenko, O.V.; Baymukhametov, T.N.; Afonina, Z.A.; Vasilenko, K.S.
Deposited on	:	2023-11-16
Resolution	:	2.55 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

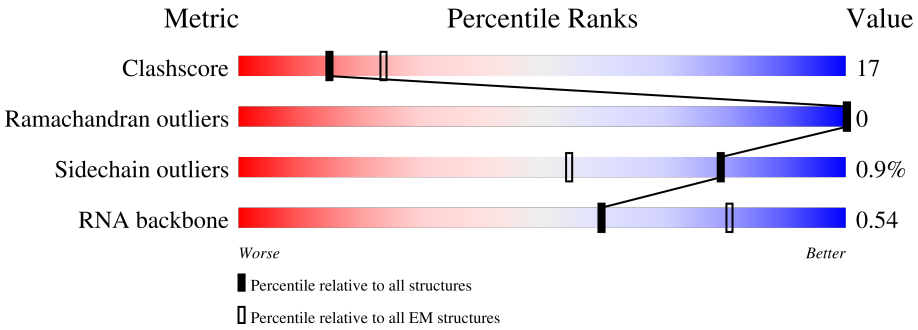
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.55 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	K	188	23% 21% 56%
2	M	144	24% 42% 38% 18%
3	F	227	67% 25% 7%
4	P	200	64% 28% 8%
5	Q	149	66% 31%
6	U	127	57% 24% 19%
7	T	155	76% 14% 10%

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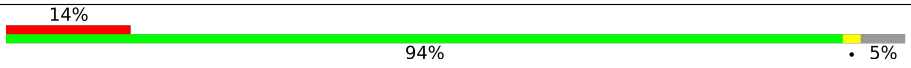
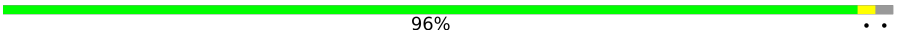
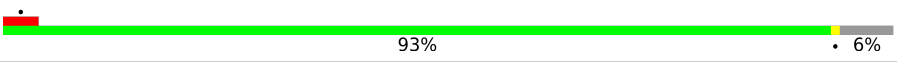
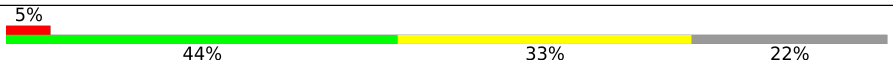
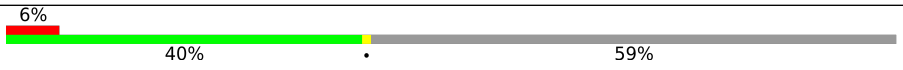
Mol	Chain	Length	Quality of chain
8	Z	108	
9	c	65	
10	d	56	
11	g	332	
12	S	152	
13	R	153	
14	h	143	
15	A	1810	
16	f	155	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 25048 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 Plectin/eS10 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	83	718	472	119	124	3	0	0

- Molecule 2 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	118	887	556	153	170	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	211	1652	1048	300	295	9	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	183	1453	908	272	266	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Q	145	1153	735	220	193	5	0	0

- Molecule 6 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	U	103	806	504	147	151	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	140	Total	C	N	O	S	0	0
			1099	691	208	196	4		

- Molecule 8 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	71	Total	C	N	O	S	0	0
			570	359	106	103	2		

- Molecule 9 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	62	Total	C	N	O	S	0	0
			498	306	102	88	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	55	Total	C	N	O	S	0	0
			436	268	89	73	6		

- Molecule 11 is a protein called Ribosomal protein RACK1 subfamily. WD repeat G protein beta family.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	313	Total	C	N	O	S	0	0
			2424	1528	420	465	11		

- Molecule 12 is a protein called Putative ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	140	Total	C	N	O	S	0	0
			1147	716	227	198	6		

- Molecule 13 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	119	Total	C	N	O	S	0	0
			953	608	176	162	7		

- Molecule 14 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	71	Total	C	N	O	S	0	0
			587	368	119	98	2		

- Molecule 15 is a RNA chain called RNA (458-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	458	Total	C	N	O	P	0	0
			9766	4369	1720	3219	458		

- Molecule 16 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	64	Total	C	N	O	S	0	0
			514	327	96	86	5		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	P	1	Total	Mg	0
			1	1	
17	A	19	Total	Mg	0
			19	19	

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	d	1	Total	Zn	0
			1	1	
18	f	1	Total	Zn	0
			1	1	

- Molecule 19 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
19	d	1	Total	K	0
			1	1	
19	A	5	Total	K	0
			5	5	

- Molecule 20 is water.

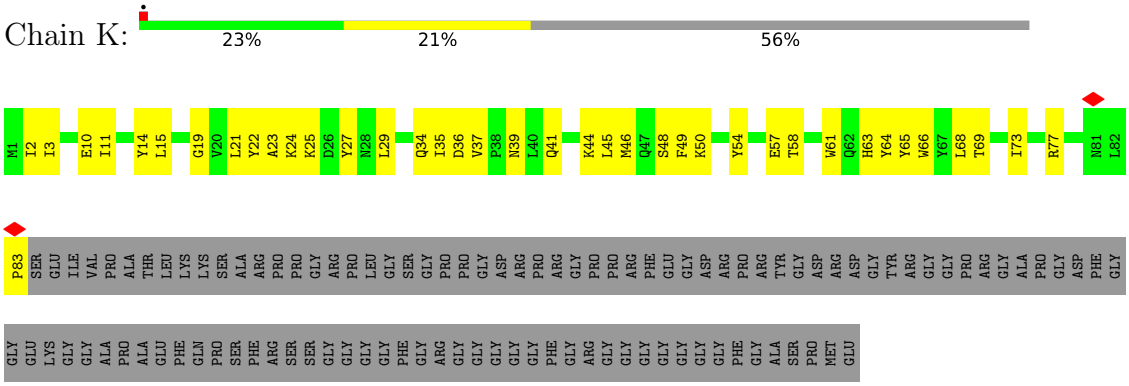
Mol	Chain	Residues	Atoms	AltConf
20	F	1	Total O 1 1	0
20	P	7	Total O 7 7	0
20	Q	14	Total O 14 14	0
20	U	4	Total O 4 4	0
20	T	16	Total O 16 16	0
20	d	2	Total O 2 2	0
20	S	2	Total O 2 2	0
20	R	3	Total O 3 3	0
20	A	308	Total O 308 308	0

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.

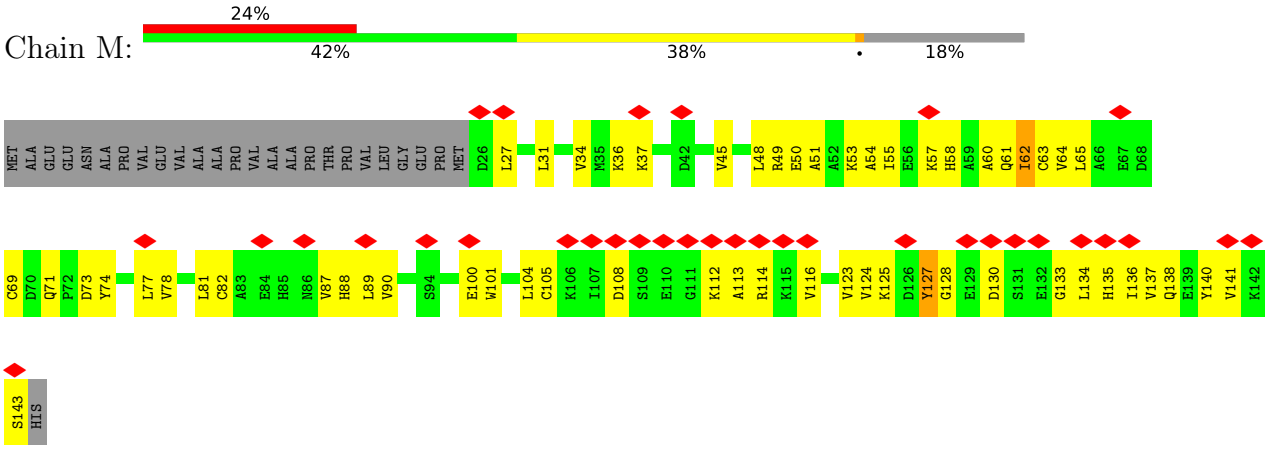
• Molecule 1: Plectin/eS10 N-terminal domain-containing protein

Chain K:



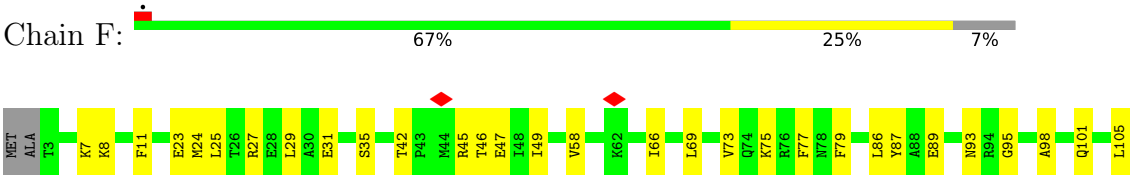
• Molecule 2: 40S ribosomal protein S12

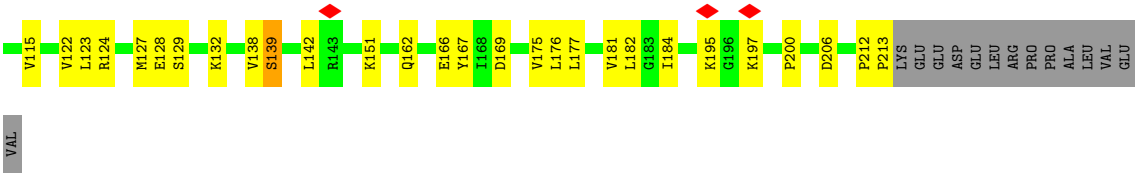
Chain M:



• Molecule 3: 40S ribosomal protein S3

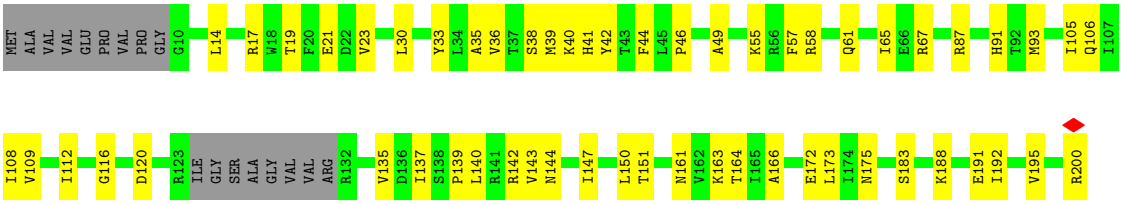
Chain F:





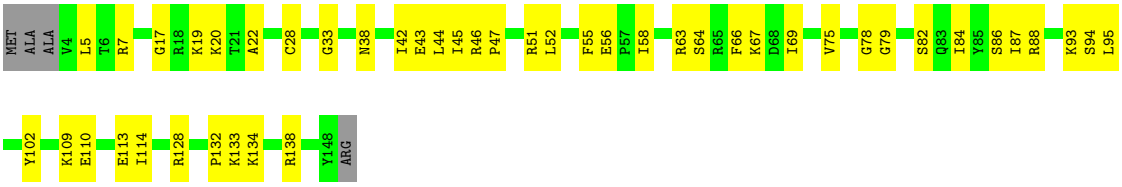
• Molecule 4: Small ribosomal subunit protein uS7c

Chain P:



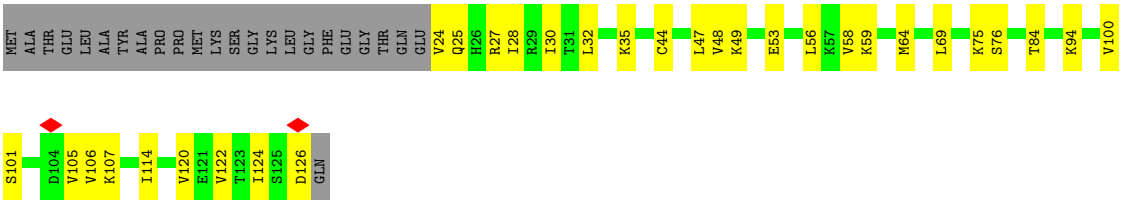
• Molecule 5: 40S ribosomal protein S16

Chain Q:



• Molecule 6: Ribosomal protein S20

Chain U:

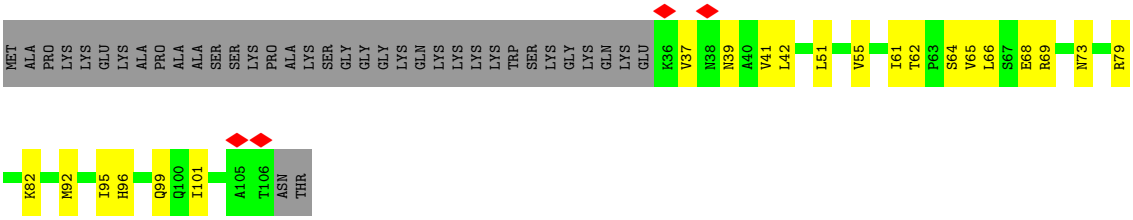


• Molecule 7: 40S ribosomal protein S19

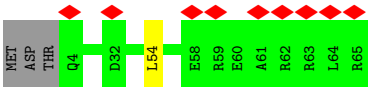
Chain T:

• Molecule 8: 40S ribosomal protein S25

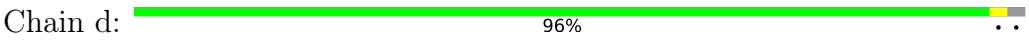
Chain Z:

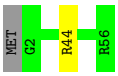


• Molecule 9: 40S ribosomal protein S28

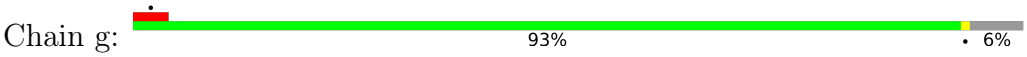


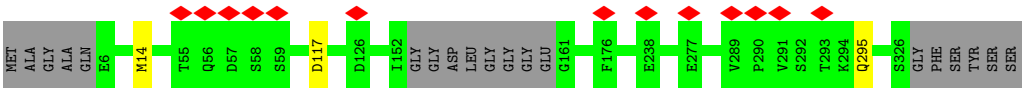
• Molecule 10: Small ribosomal subunit protein uS14



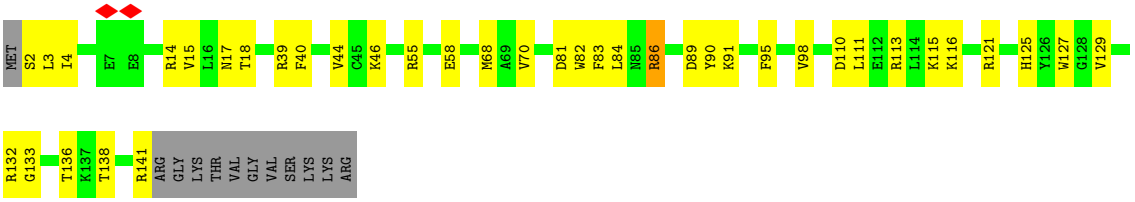


• Molecule 11: Ribosomal protein RACK1 subfamily. WD repeat G protein beta family

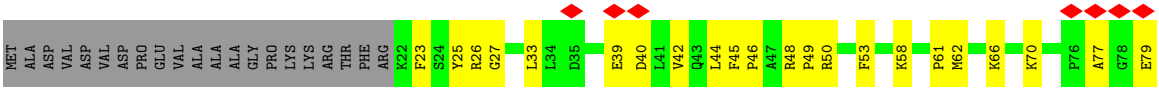




• Molecule 12: Putative ribosomal protein S18

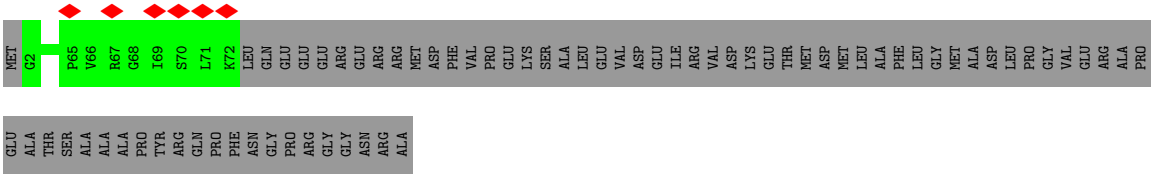


• Molecule 13: 40S ribosomal protein S15



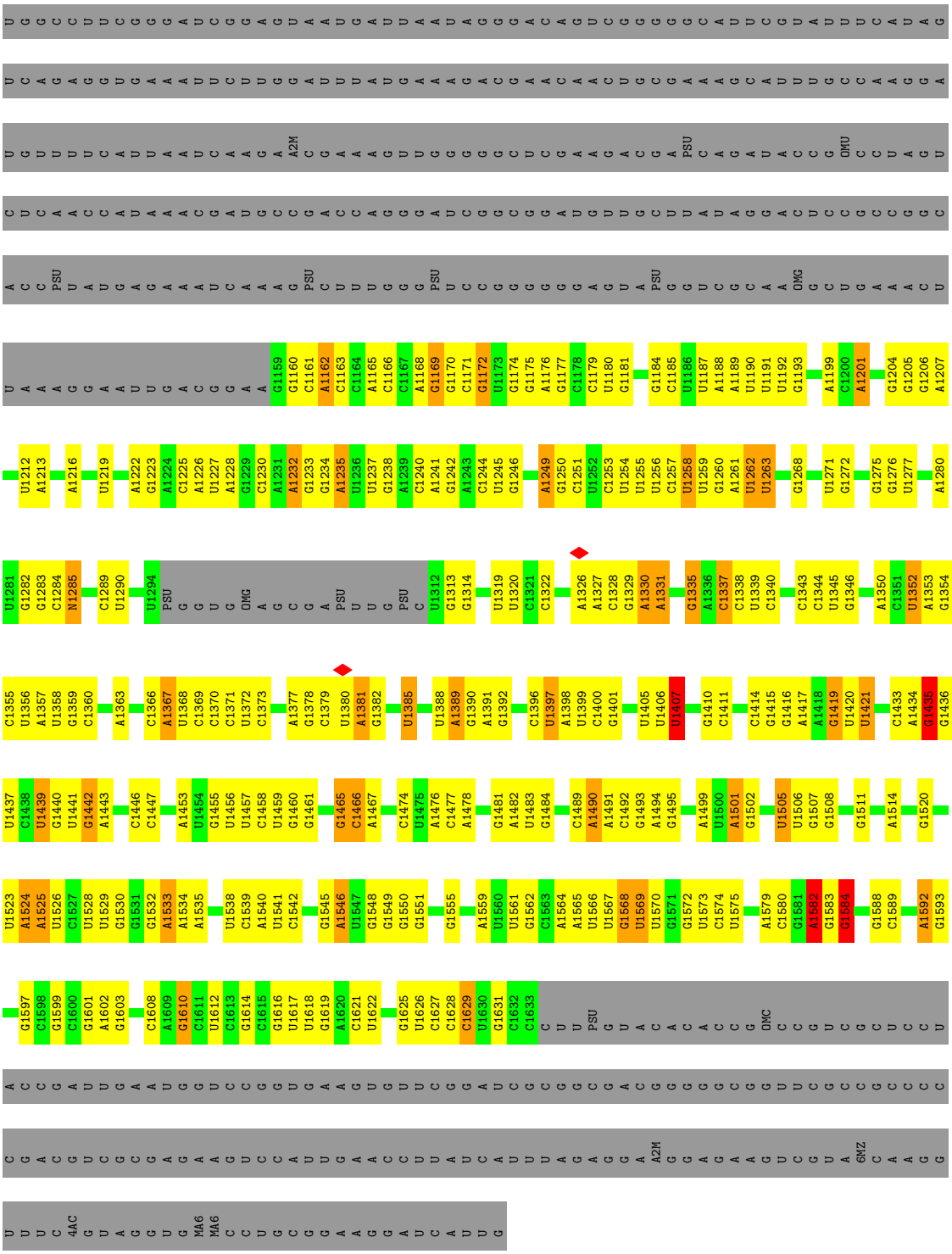
• Molecule 14: 40S ribosomal protein S17

Chain h:



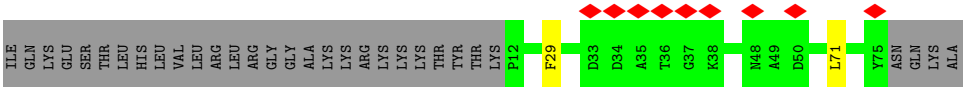
• Molecule 15: RNA (458-MER)

Chain A:



• Molecule 16: Ubiquitin-like domain-containing protein

Chain f:


ILE
GLN
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LYS
LYS
ARG
LYS
LYS
LYS
THR
TYR
THR
LYS
P12
F29
D33
D34
A35
T36
G37
K38
N48
A49
D50
L71
Y75
ASN
GLN
LYS
ALA

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	9.428	Depositor
Minimum map value	-5.602	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.5	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMG, OMU, K, A2M, MG, PSU, ZN, 7MG, 4AC

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	K	0.36	0/738	0.55	0/995
2	M	0.40	0/898	0.57	0/1210
3	F	0.32	0/1677	0.57	0/2255
4	P	0.32	0/1473	0.57	0/1981
5	Q	0.31	0/1173	0.60	0/1569
6	U	0.27	0/815	0.56	0/1098
7	T	0.27	0/1122	0.51	0/1509
8	Z	0.24	0/576	0.55	0/774
9	c	0.32	0/499	0.66	0/664
10	d	0.49	0/446	0.77	0/593
11	g	0.32	0/2480	0.57	0/3376
12	S	0.31	0/1165	0.61	0/1555
13	R	0.27	0/973	0.58	0/1302
14	h	0.23	0/593	0.56	0/788
15	A	0.33	0/10237	0.76	0/15952
16	f	0.58	0/526	0.69	0/701
All	All	0.33	0/25391	0.66	0/36322

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

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	K	718	0	719	32	0
2	M	887	0	908	70	0
3	F	1652	0	1734	44	0
4	P	1453	0	1494	41	0
5	Q	1153	0	1228	35	0
6	U	806	0	863	24	0
7	T	1099	0	1118	19	0
8	Z	570	0	605	15	0
9	c	498	0	540	0	0
10	d	436	0	420	0	0
11	g	2424	0	2366	0	0
12	S	1147	0	1180	34	0
13	R	953	0	998	48	0
14	h	587	0	643	0	0
15	A	9766	0	4956	216	0
16	f	514	0	520	0	0
17	A	19	0	0	0	0
17	P	1	0	0	0	0
18	d	1	0	0	0	0
18	f	1	0	0	0	0
19	A	5	0	0	0	0
19	d	1	0	0	0	0
20	A	308	0	0	16	0
20	F	1	0	0	0	0
20	P	7	0	0	1	0
20	Q	14	0	0	0	0
20	R	3	0	0	0	0
20	S	2	0	0	0	0
20	T	16	0	0	1	0
20	U	4	0	0	1	0
20	d	2	0	0	0	0
All	All	25048	0	20292	523	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 17.

All (523) 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)
3:F:162:GLN:HB3	15:A:1337:OMC:HM23	1.55	0.88
15:A:1597:G:H1	15:A:1617:U:H3	1.26	0.84
7:T:129:ASP:HB3	7:T:135:LEU:HD23	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:120:ASP:HB2	4:P:137:ILE:HD11	1.63	0.80
2:M:133:GLY:HA2	2:M:136:ILE:HD13	1.65	0.79
15:A:1237:U:H2'	15:A:1238:G:C8	2.19	0.78
1:K:11:ILE:HD11	1:K:37:VAL:HG11	1.66	0.76
2:M:31:LEU:HG	2:M:137:VAL:HB	1.69	0.75
15:A:1465:G:H5"	15:A:1466:C:H5	1.51	0.75
2:M:34:VAL:HG21	2:M:134:LEU:HB2	1.68	0.75
2:M:124:VAL:HG12	2:M:127:TYR:HA	1.68	0.75
2:M:65:LEU:HD12	2:M:89:LEU:HD21	1.69	0.74
5:Q:45:ILE:HD11	5:Q:87:ILE:HD13	1.69	0.74
2:M:87:VAL:HG23	2:M:88:HIS:H	1.51	0.74
6:U:56:LEU:HD11	6:U:105:VAL:HG11	1.70	0.73
15:A:1176:A:H2'	15:A:1177:G:C8	2.24	0.73
15:A:1377:A:H2'	15:A:1378:G:C8	2.23	0.73
6:U:24:VAL:HG12	6:U:25:GLN:HG3	1.71	0.71
15:A:1465:G:H5"	15:A:1466:C:C5	2.25	0.71
4:P:30:LEU:HD21	4:P:142:ARG:HG2	1.73	0.71
12:S:116:LYS:HE3	13:R:118:GLU:HG2	1.73	0.70
15:A:1225:C:H2'	15:A:1226:A:H8	1.55	0.70
13:R:89:ARG:HB3	13:R:125:ALA:HB2	1.74	0.69
15:A:1381:A:H2'	15:A:1382:G:C8	2.27	0.69
15:A:1344:C:O2'	15:A:1346:G:N7	2.26	0.69
7:T:48:ASP:HB2	12:S:46:LYS:HD2	1.75	0.68
15:A:1249:A:C8	15:A:1249:A:H3'	2.27	0.68
1:K:77:ARG:HG3	1:K:83:PRO:HA	1.75	0.68
1:K:61:TRP:CD1	3:F:23:GLU:HG2	2.30	0.67
15:A:1562:G:N2	15:A:1564:A:H3'	2.10	0.67
3:F:7:LYS:HG2	15:A:1524:A:OP2	1.94	0.66
8:Z:79:ARG:HB3	12:S:2:SER:HB2	1.78	0.66
15:A:1570:PSU:H4'	15:A:1608:C:H4'	1.77	0.66
2:M:77:LEU:HD23	2:M:81:LEU:HD11	1.76	0.66
2:M:27:LEU:HD13	2:M:136:ILE:HG22	1.78	0.65
15:A:1533:A:H2'	15:A:1534:A:C8	2.32	0.64
2:M:108:ASP:OD2	2:M:114:ARG:HA	1.97	0.64
13:R:105:TYR:OH	15:A:1216:A:N3	2.30	0.64
13:R:48:ARG:NH2	15:A:1561:U:O4	2.27	0.64
1:K:45:LEU:HG	1:K:49:PHE:CE2	2.33	0.64
4:P:120:ASP:CB	4:P:137:ILE:HD11	2.27	0.64
15:A:1245:U:H1'	15:A:1249:A:H62	1.63	0.64
2:M:36:LYS:HZ3	2:M:101:TRP:HA	1.63	0.64
15:A:1249:A:H5'	15:A:1249:A:H8	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1389:A:HO2'	15:A:1390:G:H8	1.45	0.64
15:A:1237:U:H2'	15:A:1238:G:H8	1.61	0.63
15:A:1161:C:H2'	15:A:1162:A:C8	2.34	0.63
15:A:1460:G:H5'	20:A:2115:HOH:O	1.98	0.63
4:P:164:THR:HG22	4:P:166:ALA:H	1.63	0.63
15:A:1481:G:H2'	15:A:1482:A:C8	2.34	0.63
4:P:120:ASP:O	4:P:135:VAL:N	2.27	0.63
15:A:1174:G:C2	15:A:1584:7MG:HM72	2.33	0.63
15:A:1400:C:H2'	15:A:1401:G:C8	2.34	0.63
2:M:136:ILE:HD12	2:M:136:ILE:H	1.64	0.63
13:R:85:ARG:NH2	15:A:1246:G:OP1	2.31	0.63
2:M:78:VAL:HA	2:M:81:LEU:HD12	1.81	0.62
15:A:1249:A:C8	15:A:1249:A:C3'	2.83	0.62
6:U:107:LYS:HD3	6:U:107:LYS:N	2.14	0.62
13:R:101:VAL:HG11	13:R:112:GLN:HE21	1.65	0.62
15:A:1225:C:H2'	15:A:1226:A:C8	2.34	0.61
4:P:87:ARG:HD2	8:Z:96:HIS:CE1	2.35	0.61
2:M:45:VAL:HG11	2:M:54:ALA:HB2	1.82	0.61
6:U:28:ILE:HG21	6:U:106:VAL:HG11	1.81	0.61
4:P:192:ILE:O	4:P:195:VAL:HG22	2.01	0.60
2:M:62:ILE:HG12	2:M:124:VAL:HG23	1.84	0.60
15:A:1476:A:N7	20:A:2003:HOH:O	2.31	0.60
3:F:98:ALA:N	3:F:169:ASP:OD2	2.35	0.59
3:F:138:VAL:HG13	3:F:182:LEU:HD21	1.84	0.59
5:Q:56:GLU:OE1	5:Q:88:ARG:NH1	2.35	0.59
6:U:44:CYS:O	6:U:48:VAL:HG23	2.01	0.59
13:R:42:VAL:HG23	13:R:53:PHE:HD2	1.67	0.59
3:F:206:ASP:OD2	15:A:1335:G:N2	2.31	0.59
15:A:1400:C:H2'	15:A:1401:G:H8	1.66	0.59
15:A:1259:U:H2'	15:A:1260:G:C8	2.37	0.59
15:A:1494:A:N7	20:A:2006:HOH:O	2.32	0.59
15:A:1240:C:H2'	15:A:1241:A:H8	1.67	0.59
15:A:1337:OMC:HM22	15:A:1338:C:H5'	1.83	0.59
15:A:1481:G:H2'	15:A:1482:A:H8	1.68	0.59
8:Z:61:ILE:HG23	8:Z:66:LEU:HD11	1.85	0.59
15:A:1465:G:N3	15:A:1465:G:H2'	2.17	0.59
15:A:1188:A:H2'	15:A:1189:A:C8	2.39	0.58
2:M:62:ILE:HG23	2:M:124:VAL:HB	1.85	0.58
15:A:1465:G:H5'	15:A:1466:C:OP2	2.04	0.58
8:Z:37:VAL:HG13	8:Z:39:ASN:H	1.68	0.58
2:M:138:GLN:O	2:M:141:VAL:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:49:PHE:O	1:K:54:TYR:HB2	2.03	0.58
15:A:1533:A:N6	20:A:2020:HOH:O	2.36	0.57
4:P:23:VAL:HG11	4:P:36:VAL:HG21	1.87	0.57
5:Q:66:PHE:HD1	5:Q:69:ILE:HD11	1.67	0.57
15:A:1592:A:H62	15:A:1621:C:H5	1.51	0.57
1:K:35:ILE:HG22	1:K:37:VAL:HG23	1.85	0.57
12:S:86:ARG:HD2	12:S:98:VAL:HG21	1.87	0.57
5:Q:19:LYS:HD3	20:A:2272:HOH:O	2.04	0.57
5:Q:45:ILE:HG22	5:Q:51:ARG:HG3	1.86	0.57
2:M:100:GLU:HG2	2:M:116:VAL:HG21	1.87	0.57
5:Q:132:PRO:O	5:Q:134:LYS:NZ	2.34	0.57
15:A:1322:C:O2'	15:A:1407:PSU:O4	2.22	0.57
5:Q:82:SER:HB3	20:A:2272:HOH:O	2.05	0.57
13:R:66:LYS:O	13:R:70:LYS:HG3	2.04	0.57
3:F:29:LEU:HD21	3:F:69:LEU:HD11	1.86	0.56
3:F:166:GLU:O	3:F:200:PRO:HG3	2.05	0.56
4:P:39:MET:HA	4:P:42:TYR:CE2	2.40	0.56
3:F:162:GLN:CB	15:A:1337:OMC:HM23	2.34	0.56
15:A:1179:C:O2'	15:A:1201:A:N6	2.39	0.56
12:S:132:ARG:NH1	15:A:1568:G:O6	2.39	0.56
12:S:138:THR:HA	12:S:141:ARG:HH21	1.71	0.56
15:A:1370:C:H2'	15:A:1371:OMC:C6	2.40	0.56
15:A:1397:U:H1'	15:A:1398:A:N7	2.20	0.56
3:F:49:ILE:HG23	3:F:89:GLU:HG2	1.87	0.56
4:P:38:SER:OG	4:P:40:LYS:HG2	2.05	0.56
12:S:86:ARG:NH2	12:S:110:ASP:OD2	2.36	0.56
5:Q:47:PRO:HD2	5:Q:84:ILE:HD12	1.86	0.56
6:U:27:ARG:HG3	6:U:100:VAL:HG23	1.87	0.56
2:M:34:VAL:CG2	2:M:134:LEU:HB2	2.36	0.56
12:S:133:GLY:HA3	15:A:1568:G:H5"	1.86	0.56
15:A:1176:A:H2'	15:A:1177:G:H8	1.70	0.56
2:M:138:GLN:HA	2:M:141:VAL:HB	1.87	0.56
13:R:58:LYS:O	13:R:61:PRO:HD2	2.05	0.56
15:A:1398:A:H2'	15:A:1399:U:H6	1.71	0.56
12:S:89:ASP:OD1	12:S:90:TYR:N	2.39	0.56
15:A:1573:U:H2'	15:A:1574:C:C6	2.41	0.56
15:A:1358:U:H2'	15:A:1359:G:H8	1.71	0.55
2:M:62:ILE:HG13	2:M:63:CYS:N	2.20	0.55
2:M:55:ILE:HD13	2:M:60:ALA:CB	2.35	0.55
15:A:1416:G:N2	15:A:1419:G:OP2	2.37	0.55
15:A:1505:U:HO2'	15:A:1528:U:HO2'	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:87:VAL:HG23	2:M:88:HIS:N	2.20	0.55
15:A:1457:U:H2'	15:A:1458:C:C6	2.41	0.55
2:M:134:LEU:HA	2:M:137:VAL:HG12	1.89	0.55
15:A:1381:A:H2'	15:A:1382:G:H8	1.69	0.54
12:S:15:VAL:HG13	12:S:68:MET:HE3	1.90	0.54
12:S:40:PHE:HA	12:S:83:PHE:HE1	1.72	0.54
12:S:55:ARG:HB2	12:S:58:GLU:HG3	1.89	0.54
2:M:137:VAL:O	2:M:141:VAL:N	2.39	0.54
13:R:25:TYR:HB3	13:R:33:LEU:HD11	1.89	0.54
13:R:90:ASN:ND2	15:A:1564:A:O2'	2.38	0.54
13:R:111:ASN:ND2	13:R:128:SER:OG	2.41	0.54
15:A:1327:A:H2'	15:A:1328:C:C6	2.42	0.54
7:T:46:TRP:HB2	7:T:50:VAL:HG13	1.90	0.54
6:U:64:MET:HB2	6:U:94:LYS:HB3	1.90	0.54
6:U:48:VAL:HG13	6:U:58:VAL:HG21	1.90	0.54
12:S:14:ARG:CZ	12:S:17:ASN:HA	2.38	0.54
15:A:1272:G:HO2'	15:A:1455:G:HO2'	1.56	0.54
2:M:31:LEU:CG	2:M:137:VAL:HB	2.38	0.53
15:A:1165:A:H2'	15:A:1166:C:C6	2.43	0.53
4:P:14:LEU:HD21	4:P:65:ILE:HG21	1.90	0.53
13:R:130:SER:OG	15:A:1461:G:O3'	2.20	0.53
15:A:1370:C:H2'	15:A:1371:OMC:H6	1.73	0.53
12:S:125:HIS:NE2	15:A:1555:G:OP1	2.35	0.53
3:F:7:LYS:O	3:F:11:PHE:HD2	1.91	0.53
8:Z:41:VAL:HG23	8:Z:73:ASN:HD22	1.73	0.53
8:Z:92:MET:SD	8:Z:95:ILE:HB	2.48	0.53
15:A:1282:G:H22	15:A:1441:PSU:HN3	1.56	0.53
2:M:74:TYR:O	2:M:78:VAL:HG12	2.09	0.53
8:Z:37:VAL:N	15:A:1545:G:OP1	2.41	0.53
15:A:1534:A:H2'	15:A:1535:A:C8	2.44	0.53
3:F:23:GLU:O	3:F:27:ARG:HG2	2.09	0.53
13:R:46:PRO:HD2	13:R:49:PRO:HG2	1.91	0.53
2:M:36:LYS:NZ	2:M:101:TRP:HA	2.23	0.53
15:A:1257:C:H2'	15:A:1258:U:O4'	2.08	0.52
1:K:22:TYR:OH	1:K:34:GLN:NE2	2.41	0.52
2:M:137:VAL:O	2:M:141:VAL:HG23	2.10	0.52
3:F:195:LYS:HB3	3:F:197:LYS:HE3	1.90	0.52
3:F:73:VAL:HG13	3:F:77:PHE:HD2	1.75	0.52
13:R:50:ARG:HH21	15:A:1559:A:P	2.32	0.52
15:A:1193:G:O2'	15:A:1437:U:OP1	2.26	0.52
15:A:1367:A:H2'	15:A:1367:A:N3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1367:A:OP1	15:A:1369:C:N4	2.42	0.52
5:Q:138:ARG:NH1	15:A:1474:C:OP1	2.43	0.52
6:U:107:LYS:HZ1	6:U:124:ILE:HD11	1.75	0.52
2:M:31:LEU:HD11	2:M:133:GLY:O	2.10	0.52
5:Q:22:ALA:HB2	5:Q:78:GLY:HA3	1.91	0.51
15:A:1180:PSU:H2'	15:A:1181:G:C8	2.45	0.51
15:A:1240:C:H2'	15:A:1241:A:C8	2.44	0.51
4:P:147:ILE:O	4:P:151:THR:HG23	2.10	0.51
8:Z:65:VAL:HG12	8:Z:69:ARG:HD2	1.92	0.51
3:F:31:GLU:O	3:F:31:GLU:HG2	2.10	0.51
12:S:136:THR:OG1	15:A:1465:G:H5'	2.10	0.51
15:A:1420:U:H4'	15:A:1421:U:OP2	2.10	0.51
15:A:1436:G:H2'	15:A:1437:U:C6	2.45	0.51
5:Q:52:LEU:O	5:Q:56:GLU:HG3	2.11	0.51
2:M:136:ILE:HD12	2:M:136:ILE:N	2.25	0.51
5:Q:110:GLU:O	5:Q:114:ILE:HG13	2.10	0.51
13:R:77:ALA:O	13:R:79:GLU:N	2.38	0.51
5:Q:43:GLU:HA	5:Q:55:PHE:HZ	1.75	0.51
13:R:42:VAL:HG23	13:R:53:PHE:CD2	2.46	0.51
15:A:1367:A:C5	15:A:1368:U:C5	2.99	0.51
15:A:1227:U:H2'	15:A:1228:A:H8	1.76	0.51
1:K:10:GLU:HG2	1:K:35:ILE:CG2	2.41	0.50
13:R:40:ASP:O	13:R:44:LEU:HD12	2.11	0.50
13:R:139:PRO:O	15:A:1184:G:O2'	2.28	0.50
4:P:35:ALA:HB1	4:P:41:HIS:CD2	2.45	0.50
5:Q:109:LYS:O	5:Q:113:GLU:HG3	2.11	0.50
15:A:1356:U:H2'	15:A:1357:A:H8	1.75	0.50
2:M:27:LEU:HA	2:M:31:LEU:HD23	1.94	0.50
2:M:77:LEU:HD23	2:M:81:LEU:CD1	2.41	0.50
3:F:11:PHE:CD1	6:U:35:LYS:HD2	2.46	0.50
3:F:123:LEU:O	3:F:127:MET:HG2	2.11	0.50
12:S:14:ARG:NH2	12:S:17:ASN:HA	2.27	0.50
3:F:24:MET:HG3	3:F:25:LEU:N	2.27	0.50
6:U:107:LYS:NZ	6:U:124:ILE:HD11	2.27	0.50
13:R:23:PHE:CZ	13:R:25:TYR:HB2	2.47	0.50
1:K:64:TYR:OH	15:A:1442:G:O6	2.21	0.50
13:R:66:LYS:HZ3	13:R:66:LYS:HB2	1.75	0.50
15:A:1235:A:N1	15:A:1262:U:H5	2.09	0.50
15:A:1343:C:H1'	15:A:1417:A:C4	2.47	0.50
13:R:98:ILE:HD12	13:R:117:PRO:HA	1.94	0.50
15:A:1180:PSU:H2'	15:A:1181:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1562:G:N1	15:A:1565:A:OP2	2.43	0.49
5:Q:42:ILE:C	5:Q:44:LEU:H	2.16	0.49
7:T:66:TYR:CZ	7:T:116:ILE:HG12	2.47	0.49
7:T:104:HIS:NE2	15:A:1610:G:OP2	2.43	0.49
13:R:104:ILE:HG12	13:R:124:LEU:HB3	1.95	0.49
15:A:1356:U:H2'	15:A:1357:A:C8	2.46	0.49
15:A:1175:G:C2	15:A:1176:A:C8	3.00	0.49
15:A:1357:A:H2	15:A:1378:G:H22	1.60	0.49
15:A:1358:U:H2'	15:A:1359:G:C8	2.46	0.49
4:P:91:HIS:HD2	8:Z:99:GLN:HB3	1.77	0.49
5:Q:46:ARG:HA	5:Q:47:PRO:C	2.33	0.49
2:M:73:ASP:N	2:M:73:ASP:OD1	2.45	0.49
3:F:175:VAL:HG23	3:F:184:ILE:HD11	1.95	0.49
4:P:55:LYS:HB2	4:P:58:ARG:HE	1.77	0.49
13:R:85:ARG:HH21	15:A:1246:G:P	2.36	0.49
15:A:1258:U:H2'	15:A:1259:U:C6	2.47	0.49
4:P:39:MET:HA	4:P:42:TYR:CD2	2.47	0.49
4:P:91:HIS:CD2	8:Z:99:GLN:HB3	2.48	0.49
4:P:93:MET:HE1	4:P:105:ILE:HG12	1.95	0.49
7:T:114:ARG:NH2	15:A:1511:G:N7	2.57	0.49
15:A:1538:PSU:H2'	15:A:1539:C:C6	2.47	0.49
2:M:55:ILE:HD13	2:M:60:ALA:HB2	1.95	0.49
2:M:108:ASP:OD2	2:M:113:ALA:O	2.31	0.49
13:R:138:ARG:O	15:A:1185:C:H4'	2.13	0.49
13:R:101:VAL:CG1	13:R:112:GLN:HE21	2.23	0.49
15:A:1359:G:H2'	15:A:1360:C:C6	2.48	0.49
6:U:114:ILE:HG12	6:U:120:VAL:HG21	1.94	0.48
13:R:106:ASN:OD1	13:R:109:CYS:O	2.31	0.48
15:A:1396:C:H2'	15:A:1397:U:H4'	1.93	0.48
15:A:1507:G:H2'	15:A:1508:G:H8	1.78	0.48
3:F:47:GLU:HB3	3:F:87:TYR:HE2	1.77	0.48
15:A:1355:C:H2'	15:A:1356:U:C6	2.48	0.48
15:A:1490:A:H2'	15:A:1491:A:C8	2.48	0.48
2:M:31:LEU:HD11	2:M:133:GLY:C	2.33	0.48
6:U:28:ILE:HG13	6:U:106:VAL:HG21	1.95	0.48
2:M:69:CYS:HA	15:A:1233:G:O6	2.14	0.48
15:A:1227:U:H2'	15:A:1228:A:C8	2.48	0.48
2:M:34:VAL:HG21	2:M:134:LEU:CB	2.41	0.48
4:P:106:GLN:HA	4:P:109:VAL:HG22	1.95	0.48
7:T:54:ARG:NH1	15:A:1514:A:OP1	2.44	0.48
15:A:1354:G:H2'	15:A:1355:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:39:GLU:O	13:R:42:VAL:HG12	2.14	0.48
15:A:1618:PSU:H2'	15:A:1619:G:O4'	2.13	0.48
12:S:121:ARG:HD3	15:A:1555:G:OP1	2.14	0.48
13:R:62:MET:O	13:R:66:LYS:HG3	2.14	0.48
13:R:95:PRO:HG3	13:R:120:ILE:HD13	1.94	0.48
15:A:1235:A:N1	15:A:1262:U:C5	2.82	0.48
1:K:10:GLU:HG2	1:K:35:ILE:HG23	1.95	0.48
1:K:61:TRP:HD1	3:F:23:GLU:HG2	1.79	0.48
3:F:175:VAL:HG23	3:F:184:ILE:CD1	2.44	0.48
15:A:1283:G:H2'	15:A:1284:C:O4'	2.14	0.48
4:P:188:LYS:O	4:P:192:ILE:HD13	2.13	0.47
13:R:49:PRO:HB3	13:R:92:ILE:HG21	1.97	0.47
15:A:1256:U:HO2'	15:A:1257:C:H6	1.55	0.47
15:A:1263:U:O2	15:A:1263:U:O4'	2.32	0.47
3:F:138:VAL:CG1	3:F:182:LEU:HD21	2.45	0.47
20:P:405:HOH:O	15:A:1621:C:H5"	2.14	0.47
2:M:64:VAL:O	2:M:65:LEU:HD23	2.14	0.47
4:P:19:THR:HG22	4:P:21:GLU:H	1.79	0.47
12:S:82:TRP:O	15:A:1573:U:O2'	2.31	0.47
15:A:1245:U:H1'	15:A:1249:A:N6	2.29	0.47
15:A:1546:A:C8	15:A:1549:G:C6	3.02	0.47
1:K:3:ILE:HA	1:K:41:GLN:NE2	2.30	0.47
2:M:48:LEU:HD12	2:M:74:TYR:CZ	2.49	0.47
2:M:82:CYS:SG	2:M:89:LEU:HD12	2.55	0.47
2:M:48:LEU:HD12	2:M:74:TYR:CE2	2.49	0.47
4:P:14:LEU:HD11	4:P:46:PRO:HD3	1.97	0.47
5:Q:64:SER:HA	5:Q:67:LYS:HE3	1.97	0.47
13:R:48:ARG:HB3	13:R:49:PRO:HD3	1.96	0.47
15:A:1232:A:N3	15:A:1232:A:H5'	2.29	0.47
1:K:46:MET:HG3	1:K:66:TRP:CE3	2.50	0.47
15:A:1235:A:C2	15:A:1262:U:H5	2.33	0.47
1:K:10:GLU:OE1	1:K:36:ASP:HB2	2.14	0.47
15:A:1494:A:C8	20:A:2006:HOH:O	2.66	0.47
7:T:95:ARG:HG3	15:A:1534:A:H4'	1.95	0.46
15:A:1338:C:H2'	15:A:1339:U:C6	2.50	0.46
2:M:105:CYS:HB3	2:M:116:VAL:HG22	1.96	0.46
2:M:134:LEU:HD23	2:M:134:LEU:C	2.36	0.46
3:F:73:VAL:HG13	3:F:77:PHE:CD2	2.50	0.46
15:A:1391:A:H2'	15:A:1392:G:O4'	2.15	0.46
15:A:1446:C:H2'	15:A:1447:C:H6	1.80	0.46
15:A:1528:U:H5	15:A:1529:U:HO2'	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:LYS:HE3	1:K:57:GLU:HB3	1.97	0.46
15:A:1389:A:O2'	15:A:1390:G:H8	1.99	0.46
15:A:1456:U:H2'	15:A:1457:U:C6	2.50	0.46
1:K:2:ILE:HA	15:A:1262:U:H2'	1.96	0.46
5:Q:33:GLY:O	5:Q:63:ARG:NH2	2.48	0.46
15:A:1169:G:H2'	15:A:1170:G:C8	2.50	0.46
15:A:1171:C:H2'	15:A:1172:G:O4'	2.16	0.46
15:A:1588:G:H2'	15:A:1589:C:C6	2.51	0.46
1:K:58:THR:CG2	1:K:65:TYR:HB2	2.46	0.46
5:Q:51:ARG:HG2	5:Q:55:PHE:CZ	2.51	0.46
8:Z:79:ARG:HA	8:Z:82:LYS:HE3	1.97	0.46
1:K:24:LYS:HG3	1:K:63:HIS:CE1	2.51	0.46
6:U:59:LYS:HB3	6:U:59:LYS:HE3	1.80	0.46
15:A:1346:G:H22	15:A:1391:A:H2	1.64	0.46
2:M:87:VAL:CG2	2:M:88:HIS:H	2.26	0.46
5:Q:133:LYS:NZ	15:A:1614:G:OP2	2.39	0.46
15:A:1542:C:H4'	15:A:1548:G:O6	2.16	0.46
3:F:11:PHE:HD1	6:U:35:LYS:HD2	1.80	0.46
13:R:58:LYS:C	13:R:61:PRO:HD2	2.37	0.46
15:A:1457:U:H2'	15:A:1458:C:H6	1.82	0.45
15:A:1465:G:N3	15:A:1465:G:C2'	2.80	0.45
3:F:42:THR:OG1	3:F:45:ARG:O	2.24	0.45
4:P:67:ARG:NH2	4:P:144:ASN:OD1	2.32	0.45
6:U:30:ILE:HG23	6:U:122:VAL:HG22	1.98	0.45
12:S:81:ASP:HB3	12:S:95:PHE:CD2	2.50	0.45
15:A:1256:U:O2'	15:A:1257:C:H6	2.00	0.45
2:M:55:ILE:O	2:M:58:HIS:N	2.47	0.45
3:F:105:LEU:HB2	3:F:122:VAL:HG21	1.97	0.45
12:S:14:ARG:NH1	12:S:17:ASN:C	2.69	0.45
15:A:1249:A:H8	15:A:1249:A:C5'	2.28	0.45
15:A:1313:G:H2'	15:A:1314:G:H8	1.82	0.45
6:U:49:LYS:O	6:U:53:GLU:HG3	2.16	0.45
12:S:84:LEU:HD12	12:S:95:PHE:HB3	1.99	0.45
15:A:1285:4AC:C2	15:A:1435:OMG:HN1	2.29	0.45
2:M:53:LYS:HG2	2:M:57:LYS:HE2	1.98	0.45
4:P:36:VAL:O	4:P:42:TYR:HE1	1.99	0.45
13:R:97:MET:O	13:R:100:SER:OG	2.34	0.45
15:A:1174:G:N3	15:A:1584:7MG:HM72	2.31	0.45
15:A:1339:U:H2'	15:A:1340:C:C6	2.52	0.45
12:S:90:TYR:O	13:R:26:ARG:N	2.43	0.45
15:A:1234:G:N2	15:A:1260:G:O2'	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:32:LEU:HD21	6:U:47:LEU:HD12	1.98	0.45
13:R:132:LYS:HD2	15:A:1187:U:H5"	1.99	0.45
1:K:54:TYR:O	1:K:68:LEU:HD12	2.17	0.45
6:U:76:SER:HB2	20:U:203:HOH:O	2.17	0.45
12:S:2:SER:OG	12:S:3:LEU:N	2.50	0.45
15:A:1506:U:C2	15:A:1507:G:C8	3.04	0.45
3:F:95:GLY:HA2	3:F:101:GLN:NE2	2.32	0.45
4:P:116:GLY:HA3	4:P:142:ARG:HG3	1.99	0.45
7:T:58:LEU:HD22	7:T:59:PRO:HD2	1.97	0.45
15:A:1191:U:H2'	15:A:1192:PSU:O4'	2.16	0.45
15:A:1213:A:C5'	20:A:2185:HOH:O	2.65	0.45
15:A:1476:A:H2'	15:A:1477:C:C6	2.52	0.45
15:A:1616:G:H2'	15:A:1617:U:H6	1.82	0.45
15:A:1168:A:N3	15:A:1622:U:O2'	2.43	0.45
15:A:1328:C:H2'	15:A:1329:G:C8	2.51	0.45
15:A:1410:G:H2'	15:A:1411:C:C6	2.52	0.45
15:A:1626:U:H2'	15:A:1627:C:C6	2.52	0.45
8:Z:64:SER:O	8:Z:68:GLU:HG2	2.17	0.44
15:A:1446:C:H2'	15:A:1447:C:C6	2.52	0.44
2:M:127:TYR:HD1	2:M:128:GLY:N	2.15	0.44
4:P:49:ALA:HB2	20:A:2249:HOH:O	2.18	0.44
4:P:57:PHE:O	4:P:61:GLN:NE2	2.50	0.44
15:A:1372:PSU:H2'	15:A:1373:C:C6	2.52	0.44
15:A:1602:A:H2'	15:A:1603:G:C8	2.51	0.44
2:M:104:LEU:HD11	15:A:1232:A:C5	2.52	0.44
2:M:108:ASP:OD2	2:M:113:ALA:C	2.55	0.44
15:A:1483:U:H2'	15:A:1484:G:C8	2.53	0.44
4:P:150:LEU:HD22	4:P:173:LEU:HD23	1.99	0.44
4:P:175:ASN:HB2	4:P:183:SER:HB2	1.99	0.44
8:Z:51:LEU:O	8:Z:55:VAL:HB	2.18	0.44
12:S:127:TRP:HB2	12:S:129:VAL:HG22	1.99	0.44
1:K:2:ILE:HG13	15:A:1263:U:H4'	1.98	0.44
1:K:58:THR:HG22	1:K:65:TYR:HB2	1.99	0.44
6:U:126:ASP:OD1	6:U:126:ASP:N	2.51	0.44
13:R:105:TYR:HB2	13:R:110:PHE:CE2	2.52	0.44
15:A:1271:U:H2'	15:A:1272:G:C8	2.52	0.44
15:A:1313:G:H2'	15:A:1314:G:C8	2.52	0.44
2:M:37:LYS:HD2	2:M:130:ASP:OD2	2.18	0.44
7:T:19:VAL:HB	7:T:78:TYR:CE1	2.53	0.44
2:M:51:ALA:O	2:M:55:ILE:HG12	2.17	0.44
2:M:135:HIS:O	2:M:138:GLN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:33:TYR:HD2	4:P:140:LEU:HD13	1.83	0.44
13:R:117:PRO:O	13:R:120:ILE:HG13	2.18	0.44
15:A:1385:OMU:H1'	15:A:1385:OMU:HM23	1.61	0.44
15:A:1255:U:O2'	15:A:1256:U:H5'	2.17	0.44
3:F:115:VAL:HG21	3:F:142:LEU:HD22	2.00	0.44
4:P:14:LEU:HD23	4:P:93:MET:CE	2.48	0.44
13:R:95:PRO:O	13:R:98:ILE:HG12	2.17	0.44
1:K:69:THR:O	1:K:73:ILE:HG13	2.18	0.43
7:T:43:LEU:HG	7:T:47:VAL:HG21	1.99	0.43
1:K:21:LEU:HD11	1:K:35:ILE:HD11	1.99	0.43
2:M:112:LYS:O	2:M:114:ARG:HG2	2.18	0.43
12:S:44:VAL:HG22	12:S:70:VAL:HG12	2.00	0.43
4:P:35:ALA:HB1	4:P:41:HIS:CG	2.52	0.43
4:P:150:LEU:HD23	4:P:172:GLU:OE1	2.17	0.43
2:M:71:GLN:HB3	2:M:73:ASP:OD1	2.17	0.43
2:M:134:LEU:O	2:M:137:VAL:HG12	2.19	0.43
7:T:78:TYR:HB2	7:T:144:LEU:HD13	2.00	0.43
12:S:14:ARG:CZ	12:S:17:ASN:C	2.87	0.43
4:P:200:ARG:O	4:P:200:ARG:HG3	2.19	0.43
13:R:80:LYS:HB3	13:R:101:VAL:HG21	2.00	0.43
15:A:1161:C:H2'	15:A:1162:A:H8	1.82	0.43
15:A:1495:G:H3'	15:A:1524:A:H61	1.83	0.43
1:K:14:TYR:OH	3:F:75:LYS:HD3	2.19	0.43
3:F:93:ASN:OD1	3:F:129:SER:OG	2.36	0.43
5:Q:28:CYS:SG	5:Q:94:SER:HB3	2.59	0.43
6:U:24:VAL:N	6:U:101:SER:HA	2.33	0.43
12:S:111:LEU:HB3	12:S:115:LYS:NZ	2.34	0.43
15:A:1235:A:N6	15:A:1260:G:H1'	2.34	0.43
15:A:1540:A:H2'	15:A:1541:U:C6	2.53	0.43
3:F:132:LYS:HE3	3:F:132:LYS:HB3	1.84	0.43
12:S:116:LYS:CE	13:R:118:GLU:HG2	2.45	0.43
1:K:25:LYS:NZ	1:K:27:TYR:OH	2.46	0.43
5:Q:128:ARG:HB3	15:A:1593:G:C8	2.54	0.43
1:K:44:LYS:HA	1:K:44:LYS:HD3	1.85	0.43
3:F:212:PRO:HA	3:F:213:PRO:HD2	1.71	0.43
15:A:1476:A:H4'	15:A:1550:G:H4'	2.01	0.43
2:M:87:VAL:O	2:M:88:HIS:HB2	2.19	0.42
2:M:140:TYR:HA	2:M:143:SER:O	2.19	0.42
5:Q:38:ASN:HD21	5:Q:75:VAL:HG12	1.83	0.42
8:Z:62:THR:HG22	8:Z:101:ILE:HA	2.01	0.42
15:A:1161:C:O2'	15:A:1162:A:H5'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1249:A:H3'	15:A:1249:A:H8	1.82	0.42
5:Q:20:LYS:HB2	20:A:2090:HOH:O	2.20	0.42
7:T:129:ASP:OD1	7:T:129:ASP:N	2.34	0.42
15:A:1569:U:H2'	15:A:1570:PSU:O4'	2.18	0.42
2:M:77:LEU:O	2:M:81:LEU:HD12	2.19	0.42
2:M:88:HIS:CD2	2:M:90:VAL:HG23	2.54	0.42
4:P:108:ILE:O	4:P:112:ILE:HG13	2.19	0.42
4:P:139:PRO:O	4:P:143:VAL:HG22	2.20	0.42
5:Q:58:ILE:H	5:Q:58:ILE:HG13	1.66	0.42
15:A:1213:A:H4'	15:A:1275:G:P	2.59	0.42
3:F:151:LYS:HE2	3:F:151:LYS:HB2	1.73	0.42
5:Q:17:GLY:O	5:Q:86:SER:OG	2.36	0.42
12:S:15:VAL:HG13	12:S:68:MET:CE	2.48	0.42
15:A:1206:G:H2'	20:A:2076:HOH:O	2.19	0.42
2:M:134:LEU:O	2:M:138:GLN:N	2.42	0.42
3:F:46:THR:O	3:F:46:THR:OG1	2.32	0.42
3:F:139:SER:HB3	20:A:2063:HOH:O	2.19	0.42
4:P:191:GLU:O	4:P:195:VAL:HG13	2.20	0.42
5:Q:43:GLU:HA	5:Q:55:PHE:CZ	2.53	0.42
5:Q:93:LYS:HB3	5:Q:93:LYS:HE2	1.77	0.42
15:A:1439:U:H4'	15:A:1440:G:H5"	2.02	0.42
1:K:21:LEU:HD12	1:K:21:LEU:HA	1.84	0.42
1:K:48:SER:C	1:K:50:LYS:H	2.23	0.42
3:F:176:LEU:HD13	3:F:181:VAL:HG22	2.02	0.42
13:R:117:PRO:HD2	13:R:118:GLU:OE1	2.20	0.42
15:A:1491:A:H2'	15:A:1492:C:C6	2.54	0.42
2:M:77:LEU:CD2	2:M:81:LEU:HD11	2.44	0.42
15:A:1458:C:H2'	15:A:1459:U:C6	2.54	0.42
1:K:15:LEU:O	1:K:19:GLY:N	2.42	0.42
3:F:175:VAL:HG12	3:F:177:LEU:HG	2.01	0.42
8:Z:42:LEU:HB3	12:S:4:ILE:O	2.20	0.42
15:A:1165:A:H2'	15:A:1166:C:H6	1.84	0.42
15:A:1592:A:H1'	20:A:2042:HOH:O	2.20	0.42
2:M:125:LYS:O	2:M:127:TYR:N	2.49	0.42
5:Q:66:PHE:CE1	5:Q:95:LEU:HD13	2.54	0.42
15:A:1277:U:O2'	15:A:1280:A:OP2	2.27	0.42
15:A:1616:G:H2'	15:A:1617:U:C6	2.55	0.42
1:K:29:LEU:HB3	1:K:39:ASN:HB2	2.01	0.41
3:F:124:ARG:O	3:F:128:GLU:HG3	2.20	0.41
5:Q:7:ARG:HG2	5:Q:102:TYR:O	2.20	0.41
7:T:95:ARG:HD2	15:A:1599:G:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1213:A:H5”	20:A:2185:HOH:O	2.20	0.41
15:A:1574:C:H2’	15:A:1575:U:O4’	2.20	0.41
15:A:1582:A2M:H4’	15:A:1583:G:C4	2.55	0.41
15:A:1601:G:H2’	15:A:1602:A:H8	1.85	0.41
5:Q:79:GLY:HA3	15:A:1617:U:O3’	2.20	0.41
6:U:75:LYS:HD2	6:U:84:THR:HG22	2.02	0.41
12:S:113:ARG:HH12	13:R:122:HIS:HE2	1.67	0.41
13:R:45:PHE:HB3	13:R:49:PRO:HB2	2.02	0.41
13:R:85:ARG:HB3	13:R:110:PHE:CD2	2.55	0.41
1:K:23:ALA:O	1:K:64:TYR:N	2.43	0.41
5:Q:110:GLU:HA	5:Q:110:GLU:OE1	2.20	0.41
7:T:114:ARG:HD3	20:T:214:HOH:O	2.20	0.41
12:S:111:LEU:HB3	12:S:115:LYS:HE2	2.02	0.41
1:K:21:LEU:HB3	1:K:66:TRP:HE3	1.84	0.41
2:M:54:ALA:HB1	2:M:123:VAL:HG11	2.02	0.41
15:A:1169:G:H2’	15:A:1170:G:H8	1.85	0.41
15:A:1227:U:C2	15:A:1228:A:C8	3.08	0.41
15:A:1338:C:H2’	15:A:1339:U:H6	1.86	0.41
15:A:1601:G:H2’	15:A:1602:A:C8	2.55	0.41
3:F:8:LYS:HG2	6:U:69:LEU:HD11	2.03	0.41
12:S:91:LYS:O	13:R:27:GLY:N	2.51	0.41
15:A:1388:U:O2’	15:A:1389:A:H5’	2.21	0.41
15:A:1414:C:H2’	15:A:1415:G:O4’	2.21	0.41
15:A:1579:A:H2’	15:A:1580:C:O4’	2.20	0.41
15:A:1628:C:H2’	15:A:1629:C:H6	1.84	0.41
7:T:58:LEU:HD23	7:T:58:LEU:HA	1.94	0.41
7:T:128:VAL:HG12	7:T:134:ARG:HG3	2.02	0.41
13:R:45:PHE:CD2	13:R:53:PHE:HE2	2.38	0.41
15:A:1261:A:H4’	15:A:1262:U:O5’	2.20	0.41
15:A:1592:A:N6	15:A:1621:C:H5	2.17	0.41
4:P:17:ARG:HG2	4:P:17:ARG:O	2.21	0.41
5:Q:20:LYS:HE3	20:A:2272:HOH:O	2.20	0.41
15:A:1253:C:H2’	15:A:1254:U:H6	1.85	0.41
15:A:1525:A:O2’	15:A:1526:U:H5’	2.20	0.41
2:M:45:VAL:HG12	2:M:50:GLU:HB3	2.02	0.41
2:M:48:LEU:HA	2:M:51:ALA:HB3	2.02	0.41
4:P:44:PHE:CD2	5:Q:56:GLU:HG2	2.55	0.41
4:P:161:ASN:ND2	4:P:163:LYS:HB2	2.36	0.41
15:A:1285:4AC:O2	15:A:1435:OMG:N2	2.45	0.41
15:A:1354:G:H2’	15:A:1355:C:H6	1.85	0.41
15:A:1357:A:H2’	15:A:1358:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1367:A:OP2	15:A:1367:A:C8	2.74	0.41
15:A:1546:A:H2'	15:A:1546:A:N3	2.36	0.41
2:M:105:CYS:HB2	2:M:114:ARG:HB2	2.03	0.41
2:M:136:ILE:H	2:M:136:ILE:CD1	2.34	0.41
12:S:14:ARG:NH1	12:S:18:THR:N	2.69	0.41
15:A:1241:A:H2'	15:A:1242:G:C8	2.55	0.41
3:F:66:ILE:HD11	3:F:86:LEU:O	2.20	0.40
5:Q:20:LYS:HD2	20:A:2090:HOH:O	2.20	0.40
15:A:1249:A:C8	15:A:1249:A:H5'	2.50	0.40
6:U:94:LYS:HE2	15:A:1352:U:O4	2.20	0.40
15:A:1244:C:H2'	15:A:1245:U:O4'	2.21	0.40
15:A:1253:C:H2'	15:A:1254:U:C6	2.57	0.40
2:M:61:GLN:OE1	2:M:127:TYR:HB2	2.21	0.40
3:F:77:PHE:HB2	3:F:79:PHE:CE1	2.56	0.40
4:P:163:LYS:HB3	4:P:163:LYS:NZ	2.36	0.40
7:T:48:ASP:C	7:T:49:ILE:HD13	2.41	0.40
15:A:1206:G:N2	15:A:1608:C:H2'	2.37	0.40
15:A:1367:A:O5'	15:A:1368:U:H5	2.04	0.40
15:A:1499:A:N6	15:A:1501:A:O2'	2.51	0.40
3:F:29:LEU:HD22	3:F:58:VAL:HG23	2.03	0.40
3:F:167:TYR:CD1	3:F:200:PRO:HG2	2.56	0.40
7:T:142:ARG:NH1	15:A:1363:A:OP1	2.54	0.40
13:R:25:TYR:OH	13:R:46:PRO:HD3	2.21	0.40
15:A:1330:A:H2'	15:A:1331:A2M:H8	2.04	0.40
15:A:1353:A:H2'	15:A:1354:G:O4'	2.21	0.40
2:M:48:LEU:O	2:M:49:ARG:C	2.60	0.40
15:A:1249:A:C8	15:A:1249:A:C4'	3.05	0.40
15:A:1621:C:H2'	15:A:1622:U:O4'	2.22	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	K	81/188 (43%)	73 (90%)	8 (10%)	0	100	100
2	M	116/144 (81%)	89 (77%)	27 (23%)	0	100	100
3	F	209/227 (92%)	202 (97%)	7 (3%)	0	100	100
4	P	179/200 (90%)	172 (96%)	7 (4%)	0	100	100
5	Q	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
6	U	101/127 (80%)	95 (94%)	6 (6%)	0	100	100
7	T	138/155 (89%)	133 (96%)	5 (4%)	0	100	100
8	Z	69/108 (64%)	68 (99%)	1 (1%)	0	100	100
9	c	60/65 (92%)	58 (97%)	2 (3%)	0	100	100
10	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
11	g	309/332 (93%)	279 (90%)	30 (10%)	0	100	100
12	S	138/152 (91%)	131 (95%)	7 (5%)	0	100	100
13	R	117/153 (76%)	109 (93%)	8 (7%)	0	100	100
14	h	69/143 (48%)	61 (88%)	8 (12%)	0	100	100
16	f	62/155 (40%)	50 (81%)	12 (19%)	0	100	100
All	All	1844/2354 (78%)	1711 (93%)	133 (7%)	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	K	79/143 (55%)	79 (100%)	0	100	100
2	M	97/116 (84%)	95 (98%)	2 (2%)	53	68
3	F	178/192 (93%)	176 (99%)	2 (1%)	73	83
4	P	157/169 (93%)	157 (100%)	0	100	100
5	Q	118/120 (98%)	117 (99%)	1 (1%)	81	88
6	U	97/115 (84%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	T	115/124 (93%)	115 (100%)	0	100 100
8	Z	64/92 (70%)	64 (100%)	0	100 100
9	c	55/58 (95%)	54 (98%)	1 (2%)	59 74
10	d	46/47 (98%)	45 (98%)	1 (2%)	52 66
11	g	271/281 (96%)	268 (99%)	3 (1%)	73 83
12	S	123/133 (92%)	121 (98%)	2 (2%)	62 77
13	R	103/130 (79%)	102 (99%)	1 (1%)	76 84
14	h	66/124 (53%)	66 (100%)	0	100 100
16	f	54/134 (40%)	52 (96%)	2 (4%)	34 46
All	All	1623/1978 (82%)	1608 (99%)	15 (1%)	79 86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	62	ILE
2	M	127	TYR
3	F	35	SER
3	F	139	SER
5	Q	5	LEU
9	c	54	LEU
10	d	44	ARG
11	g	14	MET
11	g	117	ASP
11	g	295	GLN
12	S	39	ARG
12	S	86	ARG
13	R	91	MET
16	f	29	PHE
16	f	71	LEU

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

Mol	Chain	Res	Type
1	K	28	ASN
1	K	34	GLN
7	T	96	GLN
11	g	127	ASN
11	g	193	ASN

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Mol	Chain	Res	Type
13	R	111	ASN
13	R	112	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	A	455/1810 (25%)	86 (18%)	1 (0%)

All (86) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	A	1160	G
15	A	1162	A
15	A	1163	C
15	A	1169	G
15	A	1172	G
15	A	1190	U
15	A	1199	A
15	A	1201	A
15	A	1204	G
15	A	1205	G
15	A	1207	A
15	A	1212	U
15	A	1219	PSU
15	A	1222	A
15	A	1223	G
15	A	1230	C
15	A	1232	A
15	A	1235	A
15	A	1249	A
15	A	1250	G
15	A	1251	C
15	A	1258	U
15	A	1262	U
15	A	1263	U
15	A	1268	G
15	A	1289	C
15	A	1290	U
15	A	1319	U
15	A	1320	U
15	A	1326	A

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Mol	Chain	Res	Type
15	A	1330	A
15	A	1335	G
15	A	1350	A
15	A	1352	U
15	A	1366	C
15	A	1367	A
15	A	1379	C
15	A	1380	U
15	A	1381	A
15	A	1385	OMU
15	A	1389	A
15	A	1397	U
15	A	1405	U
15	A	1406	U
15	A	1407	PSU
15	A	1419	G
15	A	1421	U
15	A	1433	C
15	A	1434	A
15	A	1435	OMG
15	A	1439	U
15	A	1442	G
15	A	1443	A
15	A	1453	A
15	A	1465	G
15	A	1466	C
15	A	1467	A
15	A	1478	A
15	A	1489	C
15	A	1490	A
15	A	1493	G
15	A	1501	A
15	A	1502	G
15	A	1505	U
15	A	1520	G
15	A	1523	U
15	A	1524	A
15	A	1525	A
15	A	1530	G
15	A	1532	G
15	A	1533	A
15	A	1546	A

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Mol	Chain	Res	Type
15	A	1551	G
15	A	1566	U
15	A	1567	U
15	A	1568	G
15	A	1569	U
15	A	1572	G
15	A	1582	A2M
15	A	1584	7MG
15	A	1592	A
15	A	1610	G
15	A	1612	PSU
15	A	1625	G
15	A	1629	C
15	A	1631	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	A	1345	U

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

29 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	$\#\|Z\| > 2$
15	OMU	A	1449	15	19,22,23	0.33	0	26,31,34	0.40	0
15	PSU	A	1607	15	18,21,22	0.52	0	22,30,33	0.64	0
15	PSU	A	1618	15	18,21,22	0.52	0	22,30,33	0.61	0
15	OMU	A	1267	15	19,22,23	0.33	0	26,31,34	0.48	0
15	A2M	A	1331	15	18,25,26	0.73	0	18,36,39	1.09	2 (11%)
15	OMC	A	1220	15	19,22,23	0.31	0	26,31,34	0.43	0
15	OMU	A	1274	17,15	19,22,23	0.30	0	26,31,34	0.50	0
15	PSU	A	1180	15	18,21,22	0.52	0	22,30,33	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	PSU	A	1315	15	18,21,22	0.50	0	22,30,33	0.60	0
15	OMU	A	1265	15	19,22,23	0.31	0	26,31,34	0.44	0
15	PSU	A	1480	17,15	18,21,22	0.53	0	22,30,33	0.54	0
15	PSU	A	1192	15	18,21,22	0.49	0	22,30,33	0.58	0
15	PSU	A	1612	15	18,21,22	0.54	0	22,30,33	0.64	0
15	PSU	A	1441	19,15	18,21,22	0.50	0	22,30,33	0.56	0
15	A2M	A	1582	15	18,25,26	0.98	0	18,36,39	1.68	4 (22%)
15	PSU	A	1538	15	18,21,22	0.51	0	22,30,33	0.59	0
15	PSU	A	1570	15	18,21,22	0.52	0	22,30,33	0.57	0
15	OMC	A	1371	15	19,22,23	0.31	0	26,31,34	0.45	0
15	PSU	A	1407	15	18,21,22	0.52	0	22,30,33	0.68	1 (4%)
15	PSU	A	1219	15	18,21,22	0.54	0	22,30,33	0.60	0
15	OMU	A	1236	15	19,22,23	0.33	0	26,31,34	0.50	0
15	PSU	A	1536	15	18,21,22	0.47	0	22,30,33	0.66	0
15	OMC	A	1337	15	19,22,23	0.40	0	26,31,34	1.02	1 (3%)
15	PSU	A	1372	15	18,21,22	0.50	0	22,30,33	0.59	0
15	7MG	A	1584	15	22,26,27	1.17	1 (4%)	29,39,42	0.81	1 (3%)
15	OMU	A	1385	17,15	19,22,23	0.34	0	26,31,34	0.45	0
15	4AC	A	1285	15	21,24,25	1.42	3 (14%)	29,34,37	1.54	5 (17%)
15	OMG	A	1276	19,15	18,26,27	0.99	3 (16%)	19,38,41	0.64	0
15	OMG	A	1435	17,15	18,26,27	1.22	1 (5%)	19,38,41	1.34	3 (15%)

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
15	OMU	A	1449	15	-	1/9/27/28	0/2/2/2
15	PSU	A	1607	15	-	0/7/25/26	0/2/2/2
15	PSU	A	1618	15	-	0/7/25/26	0/2/2/2
15	OMU	A	1267	15	-	0/9/27/28	0/2/2/2
15	A2M	A	1331	15	-	0/5/27/28	0/3/3/3
15	OMC	A	1220	15	-	0/9/27/28	0/2/2/2
15	OMU	A	1274	17,15	-	0/9/27/28	0/2/2/2
15	PSU	A	1180	15	-	0/7/25/26	0/2/2/2
15	PSU	A	1315	15	-	0/7/25/26	0/2/2/2
15	OMU	A	1265	15	-	0/9/27/28	0/2/2/2
15	PSU	A	1480	17,15	-	0/7/25/26	0/2/2/2
15	PSU	A	1192	15	-	1/7/25/26	0/2/2/2
15	PSU	A	1612	15	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PSU	A	1441	19,15	-	0/7/25/26	0/2/2/2
15	A2M	A	1582	15	-	0/5/27/28	0/3/3/3
15	PSU	A	1538	15	-	0/7/25/26	0/2/2/2
15	PSU	A	1570	15	-	0/7/25/26	0/2/2/2
15	OMC	A	1371	15	-	0/9/27/28	0/2/2/2
15	PSU	A	1407	15	-	3/7/25/26	0/2/2/2
15	PSU	A	1219	15	-	2/7/25/26	0/2/2/2
15	OMU	A	1236	15	-	0/9/27/28	0/2/2/2
15	PSU	A	1536	15	-	0/7/25/26	0/2/2/2
15	OMC	A	1337	15	-	1/9/27/28	0/2/2/2
15	PSU	A	1372	15	-	0/7/25/26	0/2/2/2
15	7MG	A	1584	15	-	0/7/37/38	0/3/3/3
15	OMU	A	1385	17,15	-	1/9/27/28	0/2/2/2
15	4AC	A	1285	15	-	0/11/29/30	0/2/2/2
15	OMG	A	1276	19,15	-	0/5/27/28	0/3/3/3
15	OMG	A	1435	17,15	-	2/5/27/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1584	7MG	C5-N7	4.84	1.41	1.35
15	A	1285	4AC	C4-N4	-4.11	1.33	1.39
15	A	1435	OMG	C6-N1	-3.61	1.32	1.37
15	A	1285	4AC	C7-N4	-2.69	1.32	1.37
15	A	1276	OMG	C5-C6	-2.45	1.42	1.47
15	A	1276	OMG	C5-C4	-2.11	1.37	1.43
15	A	1285	4AC	C2-N3	-2.04	1.32	1.36
15	A	1276	OMG	C8-N7	-2.03	1.31	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1285	4AC	O2-C2-N3	-3.98	115.85	122.33
15	A	1582	A2M	O4'-C1'-C2'	-3.29	100.89	106.59
15	A	1582	A2M	N3-C2-N1	-3.25	123.61	128.68
15	A	1285	4AC	O2-C2-N1	2.90	124.88	118.89
15	A	1337	OMC	C1'-N1-C2	2.80	124.67	118.42
15	A	1435	OMG	O6-C6-C5	-2.77	118.97	124.37
15	A	1582	A2M	O2'-C2'-C1'	2.75	114.55	109.09
15	A	1435	OMG	C5-C6-N1	2.52	118.40	113.95
15	A	1285	4AC	C3'-C2'-C1'	2.32	105.83	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1584	7MG	C5-C4-N9	2.28	109.30	106.35
15	A	1331	A2M	C5-C6-N6	2.27	123.81	120.35
15	A	1331	A2M	C3'-C2'-C1'	-2.22	98.71	102.89
15	A	1285	4AC	C2'-C3'-C4'	-2.15	98.47	102.64
15	A	1435	OMG	C8-N7-C5	2.10	106.99	102.99
15	A	1407	PSU	O4'-C1'-C2'	2.06	108.06	105.14
15	A	1285	4AC	O7-C7-N4	2.05	125.13	121.82
15	A	1582	A2M	CM'-O2'-C2'	-2.01	109.25	114.52

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	1219	PSU	C3'-C4'-C5'-O5'
15	A	1385	OMU	C1'-C2'-O2'-CM2
15	A	1407	PSU	C3'-C4'-C5'-O5'
15	A	1407	PSU	O4'-C4'-C5'-O5'
15	A	1449	OMU	C1'-C2'-O2'-CM2
15	A	1612	PSU	C3'-C4'-C5'-O5'
15	A	1612	PSU	O4'-C4'-C5'-O5'
15	A	1219	PSU	O4'-C4'-C5'-O5'
15	A	1435	OMG	O4'-C4'-C5'-O5'
15	A	1435	OMG	C4'-C5'-O5'-P
15	A	1407	PSU	C4'-C5'-O5'-P
15	A	1192	PSU	O4'-C4'-C5'-O5'
15	A	1337	OMC	C2'-C1'-N1-C2

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1618	PSU	1	0
15	A	1331	A2M	1	0
15	A	1180	PSU	2	0
15	A	1192	PSU	1	0
15	A	1441	PSU	1	0
15	A	1582	A2M	1	0
15	A	1538	PSU	1	0
15	A	1570	PSU	2	0
15	A	1371	OMC	2	0
15	A	1407	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1337	OMC	3	0
15	A	1372	PSU	1	0
15	A	1584	7MG	2	0
15	A	1385	OMU	1	0
15	A	1285	4AC	2	0
15	A	1435	OMG	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 28 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.

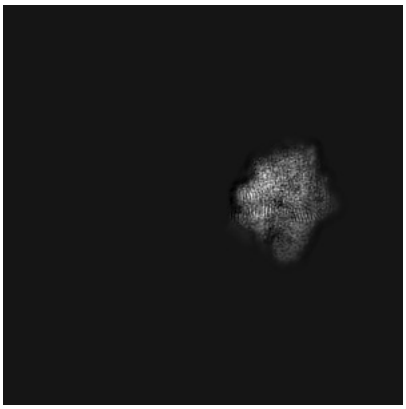
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18903. These allow visual inspection of the internal detail of the map and identification of artifacts.

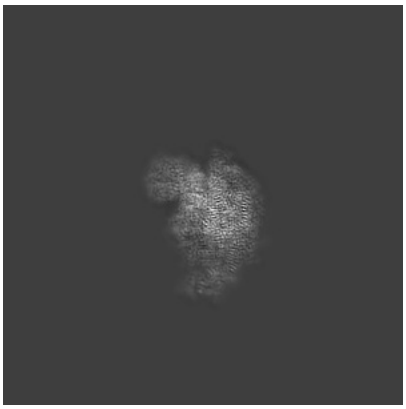
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

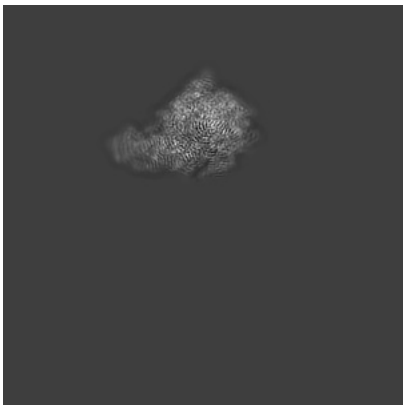
6.1.1 Primary map



X

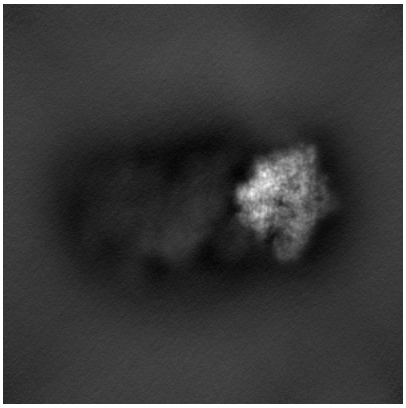


Y

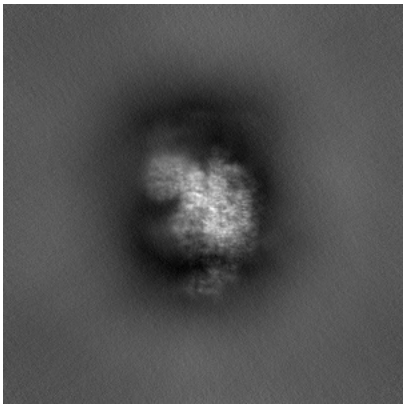


Z

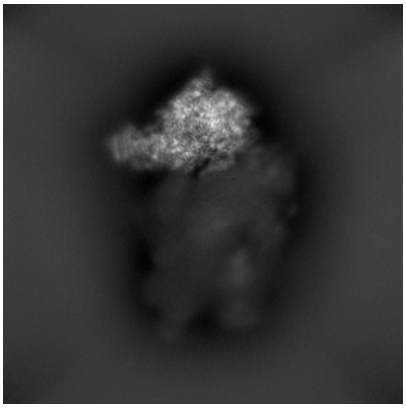
6.1.2 Raw map



X



Y



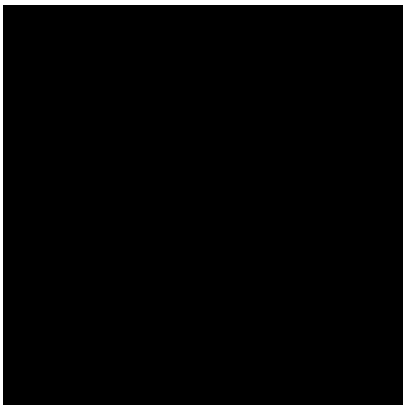
Z

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

6.2 Central slices (i)

6.2.1 Primary map

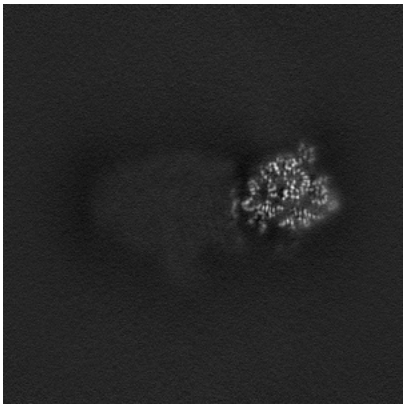
X Index: 240



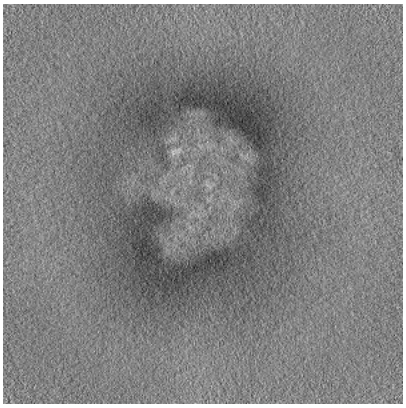
Y Index: 240

Z Index: 240

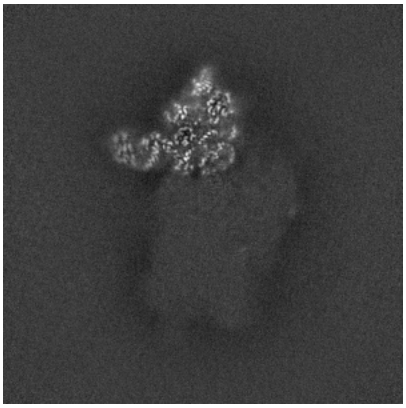
6.2.2 Raw map



X Index: 240



Y Index: 240



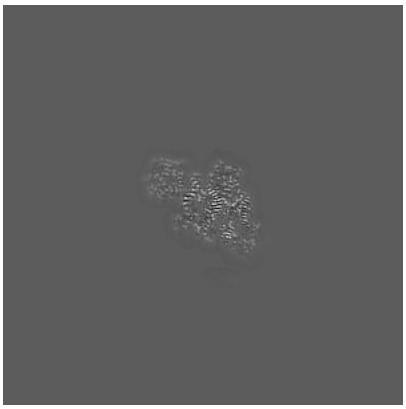
Z Index: 240

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

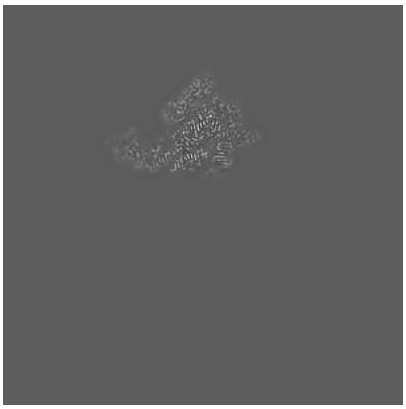
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 238

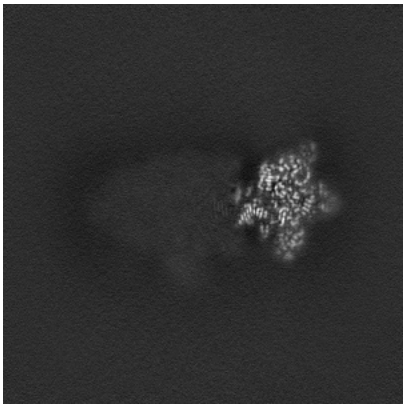


Y Index: 338

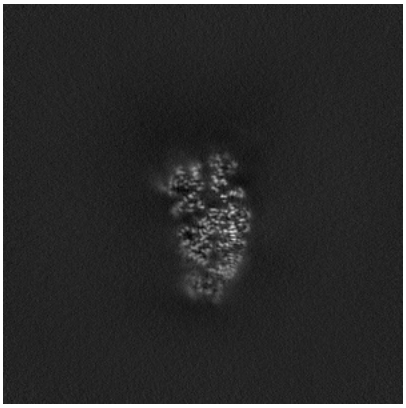


Z Index: 252

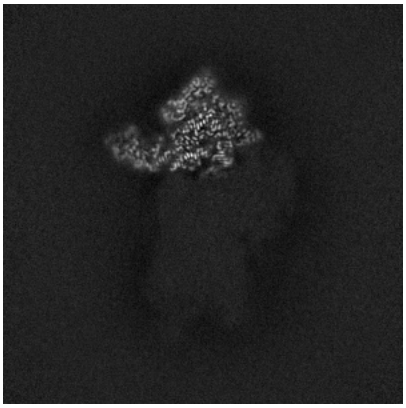
6.3.2 Raw map



X Index: 251



Y Index: 313

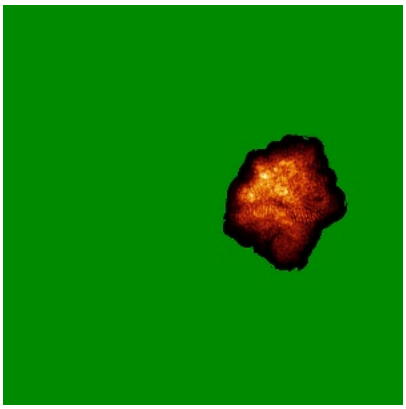


Z Index: 252

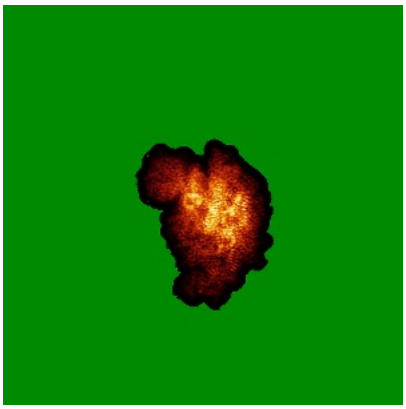
The images above show the largest variance slices of the map in three orthogonal directions.

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

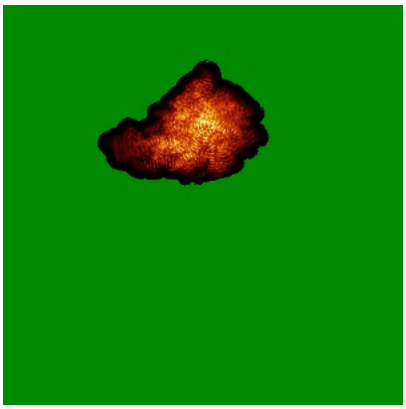
6.4.1 Primary map



X

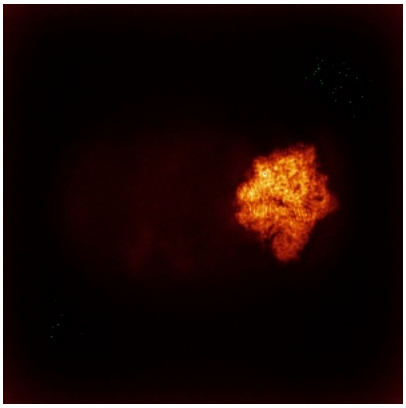


Y

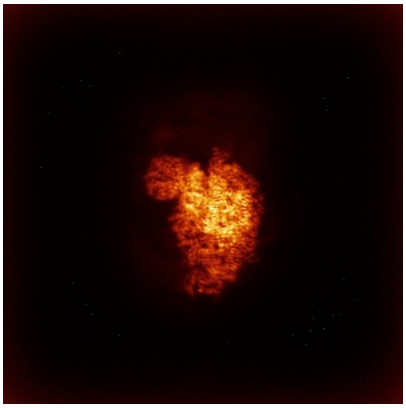


Z

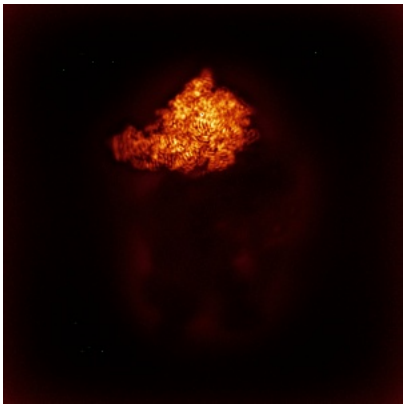
6.4.2 Raw map



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 0.5. 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.

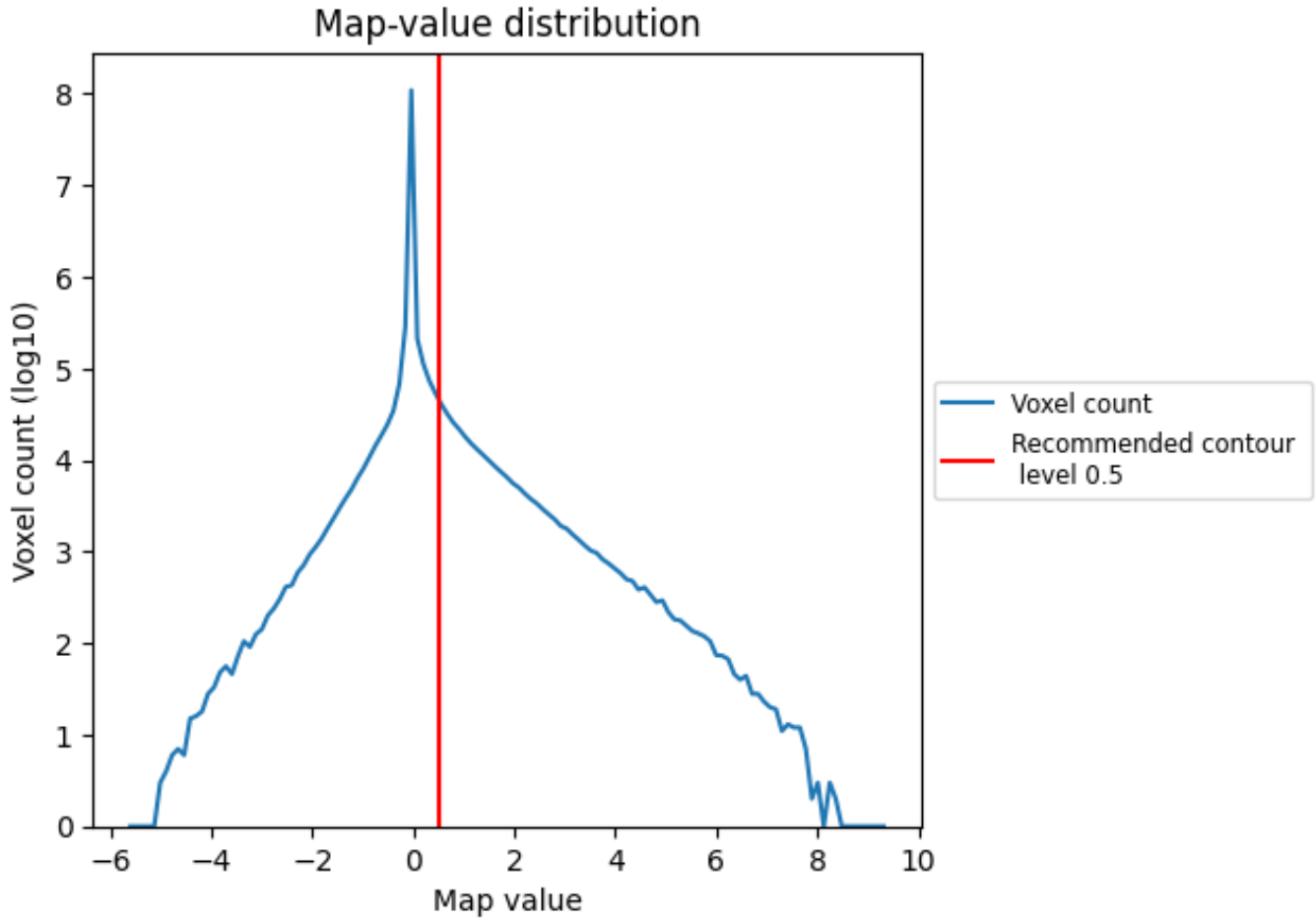
6.6 Mask visualisation (i)

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

7 Map analysis

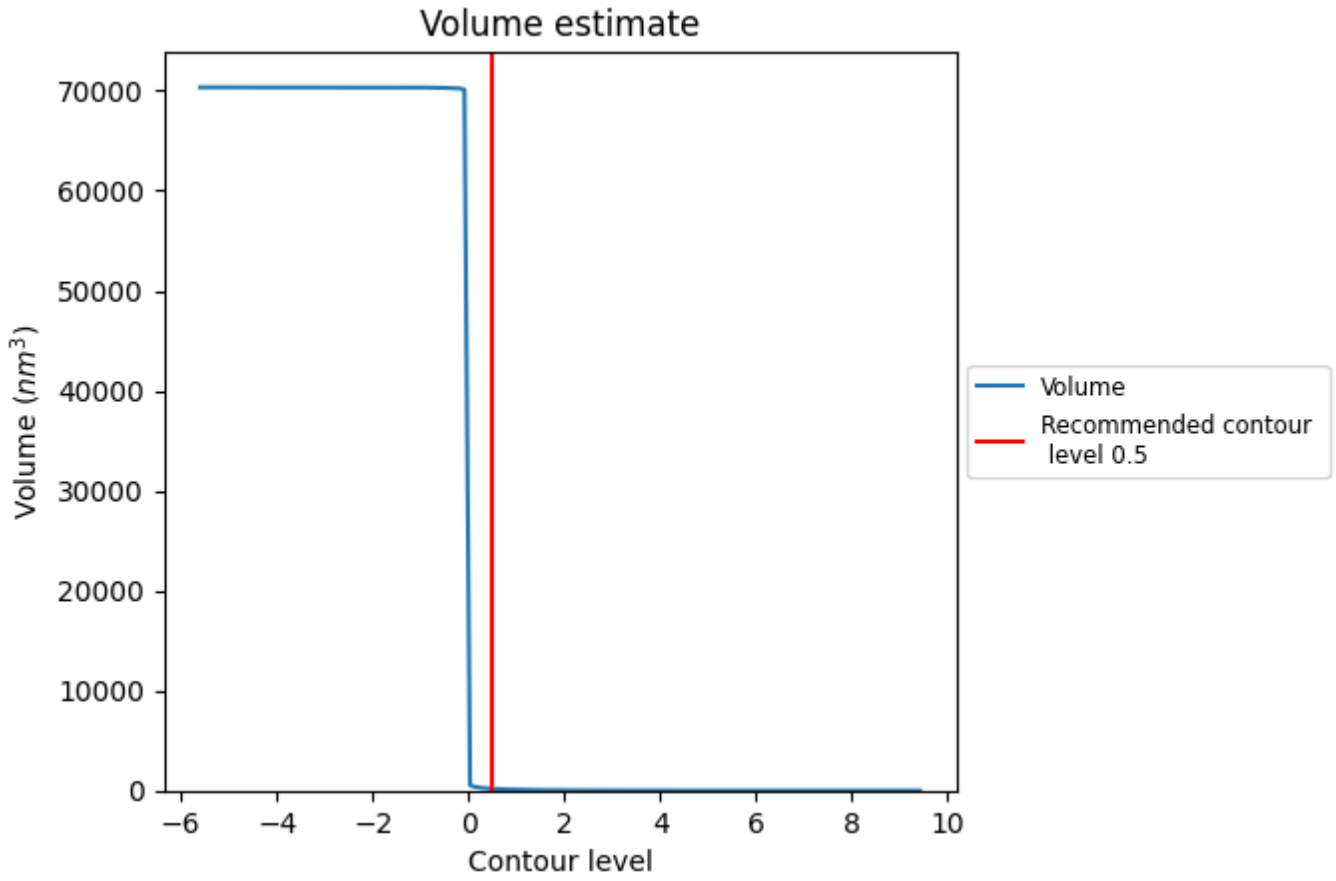
This section contains the results of statistical analysis of the map.

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.

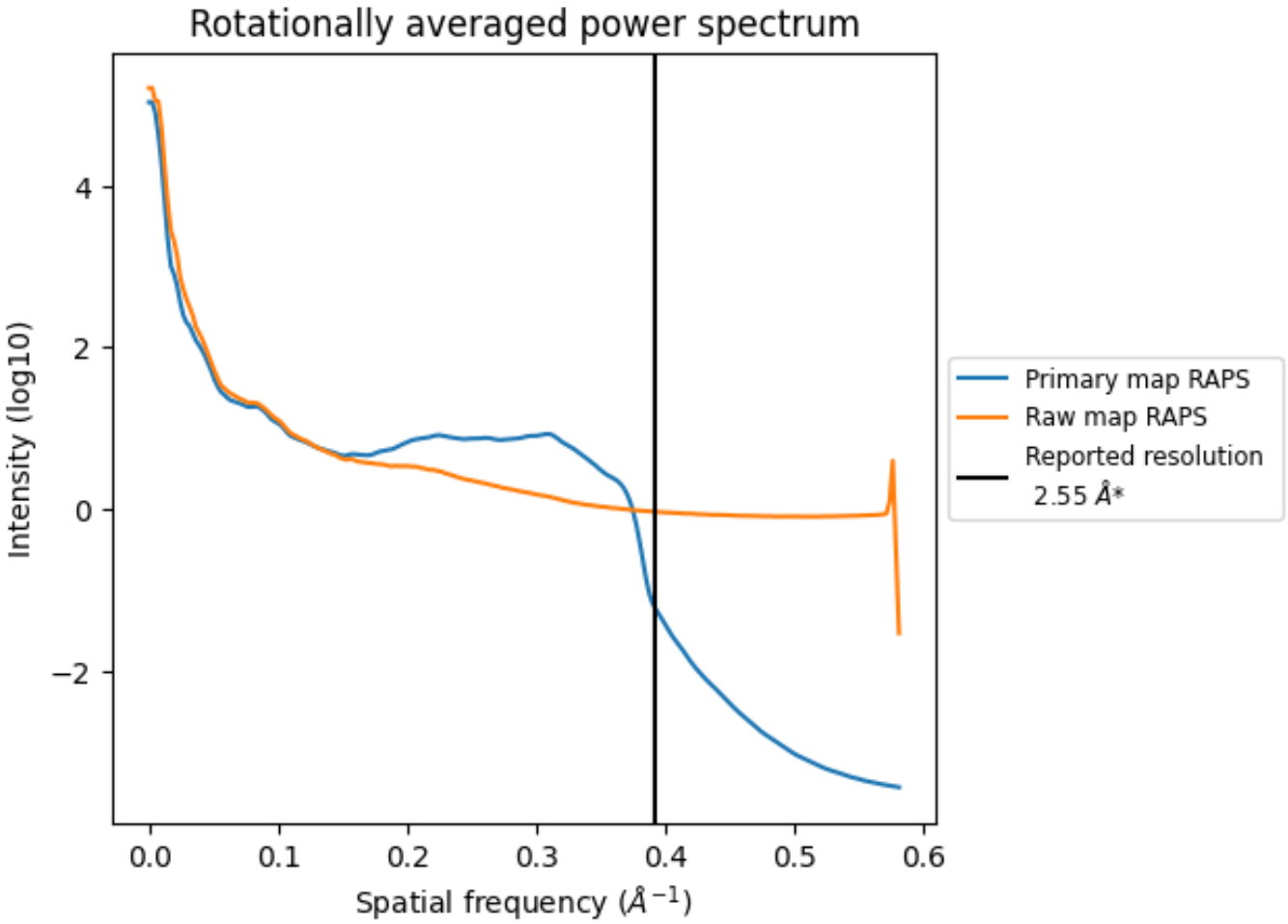
7.2 Volume estimate



The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 160 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)

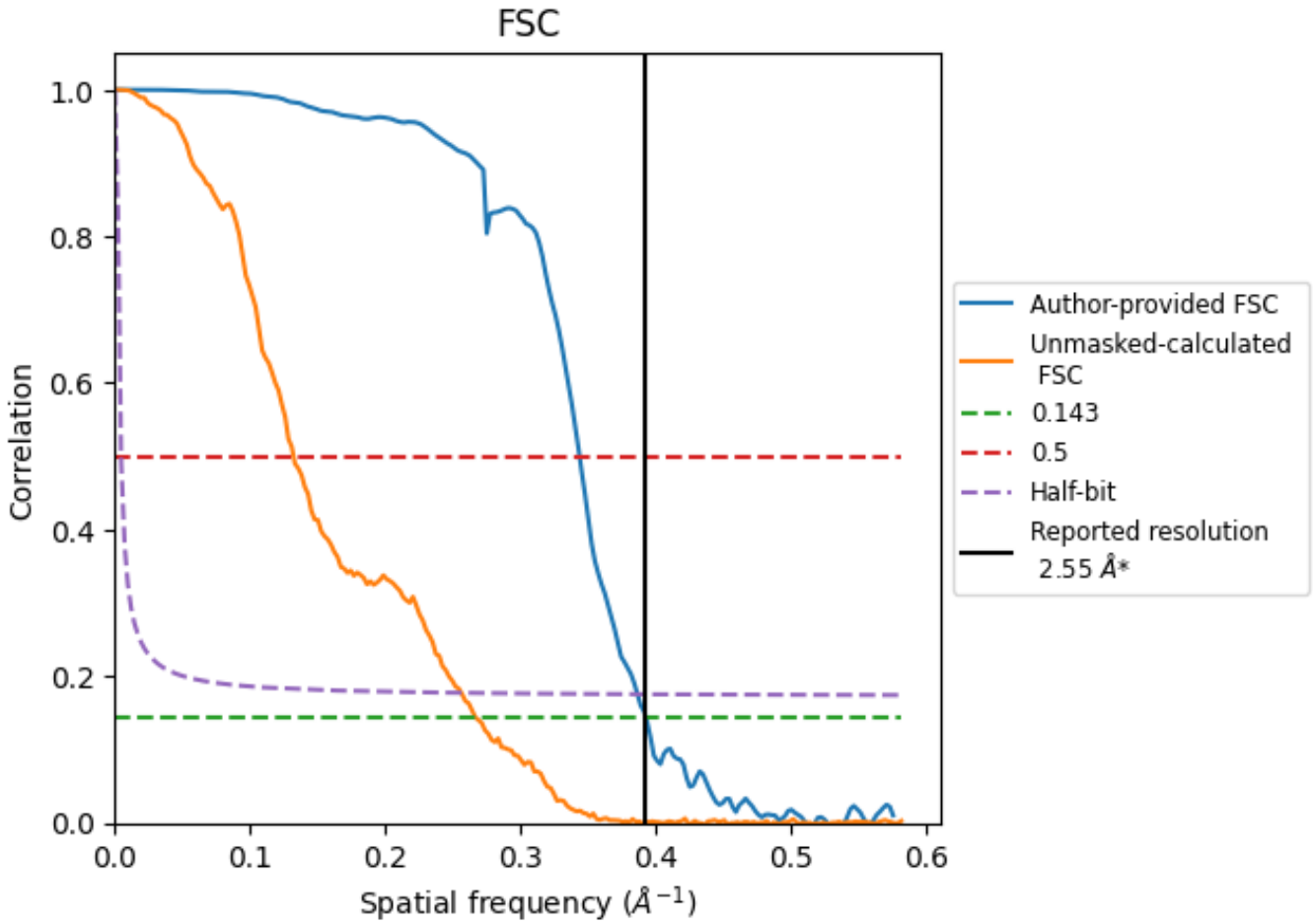


*Reported resolution corresponds to spatial frequency of 0.392 Å^{-1}

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 0.392 Å^{-1}

8.2 Resolution estimates (i)

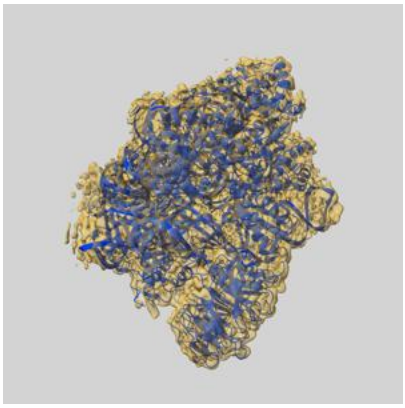
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.91	2.59
Unmasked-calculated*	3.75	7.56	3.90

*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 3.75 differs from the reported value 2.55 by more than 10 %

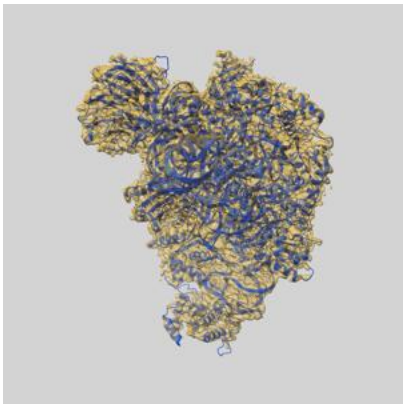
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18903 and PDB model 8R57. Per-residue inclusion information can be found in section 3 on page 8.

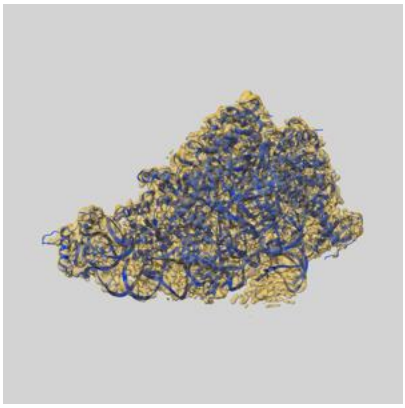
9.1 Map-model overlay



X



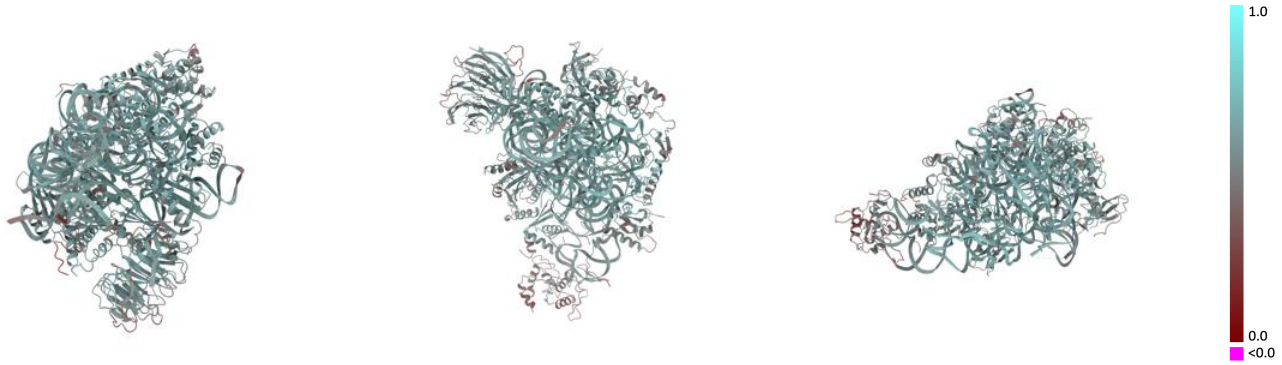
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

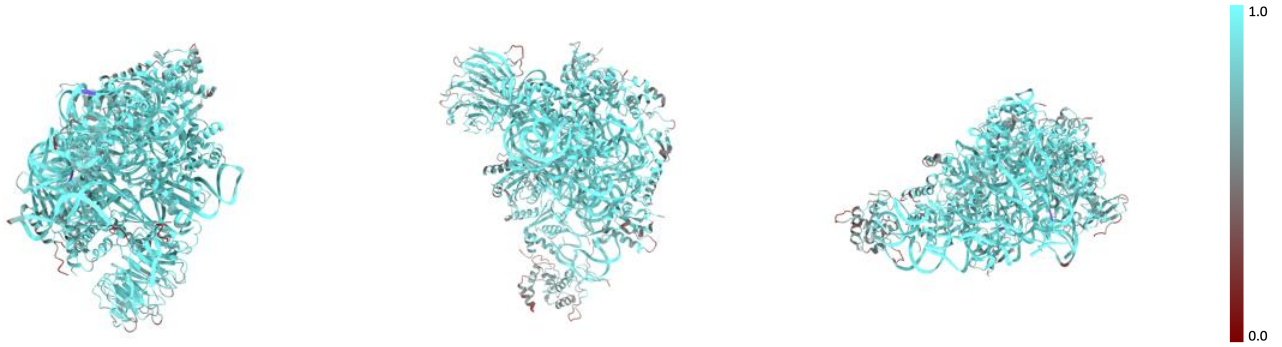
9.2 Q-score mapped to coordinate model (i)



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.

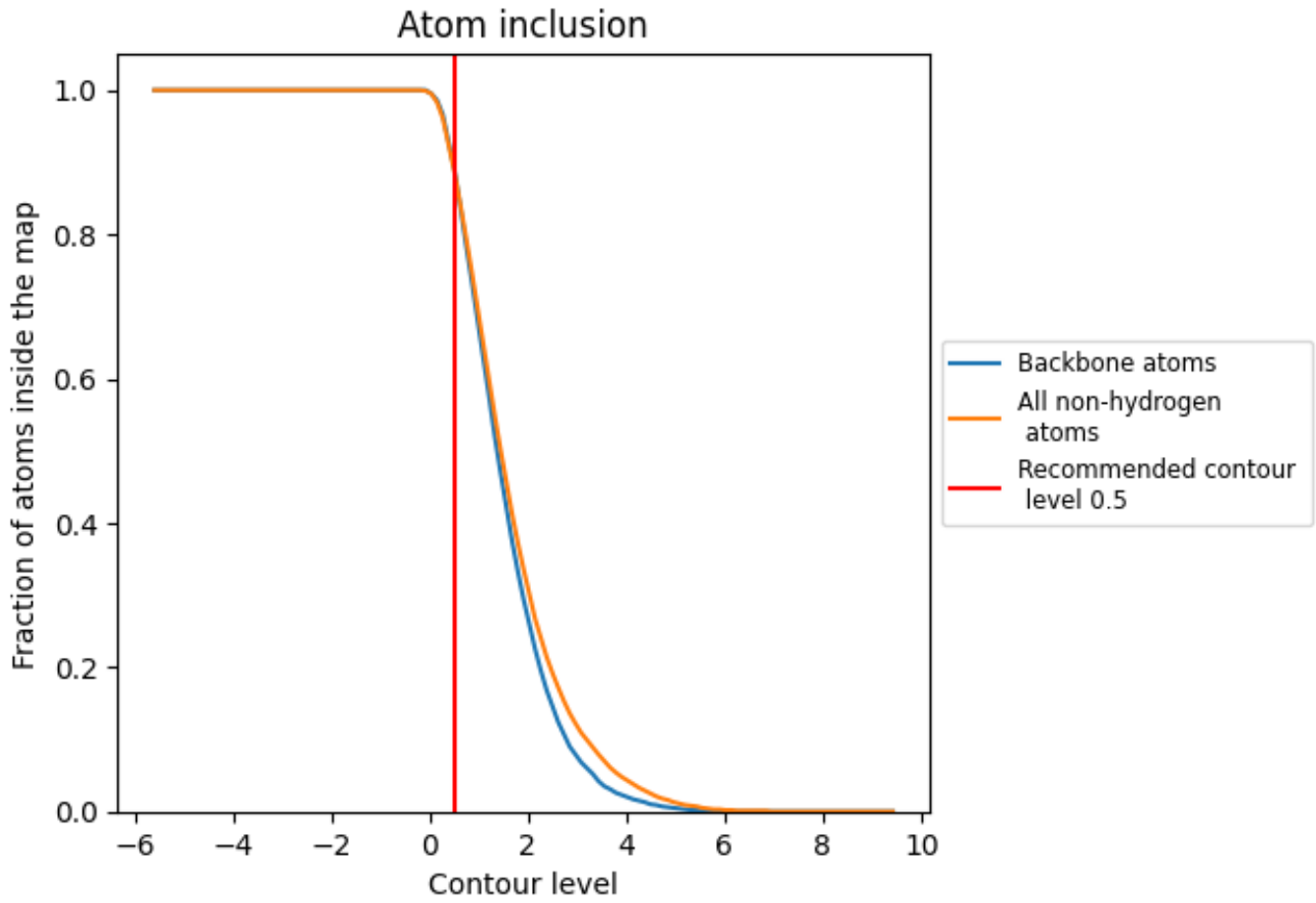
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.5800
A	0.9740	0.6170
F	0.8400	0.5600
K	0.8800	0.5670
M	0.5040	0.3690
P	0.9160	0.5950
Q	0.9600	0.6330
R	0.8110	0.5470
S	0.8590	0.5780
T	0.9470	0.6190
U	0.8360	0.5720
Z	0.8030	0.5360
c	0.7130	0.5170
d	0.9360	0.6230
f	0.6180	0.4350
g	0.8420	0.5410
h	0.8530	0.5670