Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 08:18 AM EST

PDB ID	:	6PCS
EMDB ID	:	EMD-20306
Title	:	E. coli 50S ribosome bound to compound 40e
Authors	:	Pellegrino, J.; Lee, D.J.; Fraser, J.S.; Seiple, I.B.
Deposited on	:	2019-06-18
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

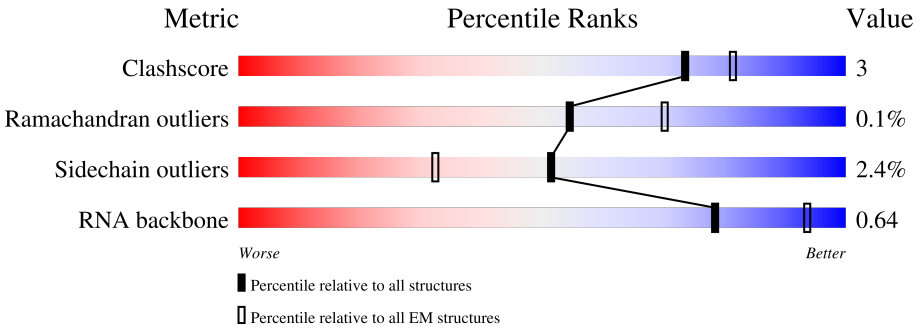
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	I	2904	5%, 77%, 20%, •
2	J	118	•, 86%, 14%
3	K	271	•, 82%, 17%, •
4	L	144	•, 85%, 13%, •
5	M	201	88%, 12%
6	N	209	•, 90%, 10%
7	O	142	89%, 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 72169 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	I	2897	62206	27757	11443	20109	2897	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	J	118	2529	1126	464	821	118	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	271	2083	1288	423	365	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	144	1053	654	207	190	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	201	1552	974	283	290	5	0	0

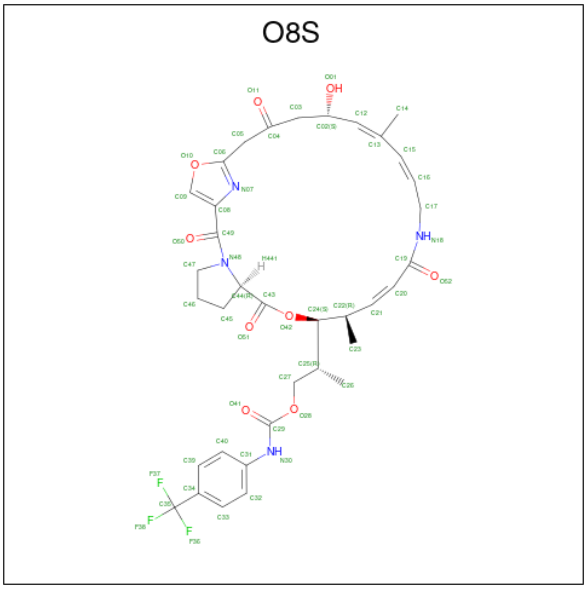
- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	209	1565	979	288	294	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	O	142	1129	714	212	199	4	0	0

- Molecule 8 is (2R)-2-[(3S,4R,5E,10E,12E,14S,26aR)-14-hydroxy-4,12-dimethyl-1,7,16,22-tetraoxo-4,7,8,9,14,15,16,17,24,25,26,26a-dodecahydro-1H,3H,22H-21,18-(azeno)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosin-3-yl]propyl [4-(trifluoromethyl)phenyl]carbamate (three-letter code: O8S) (formula: $C_{36}H_{41}F_3N_4O_9$) (labeled as "Ligand of Interest" by depositor).



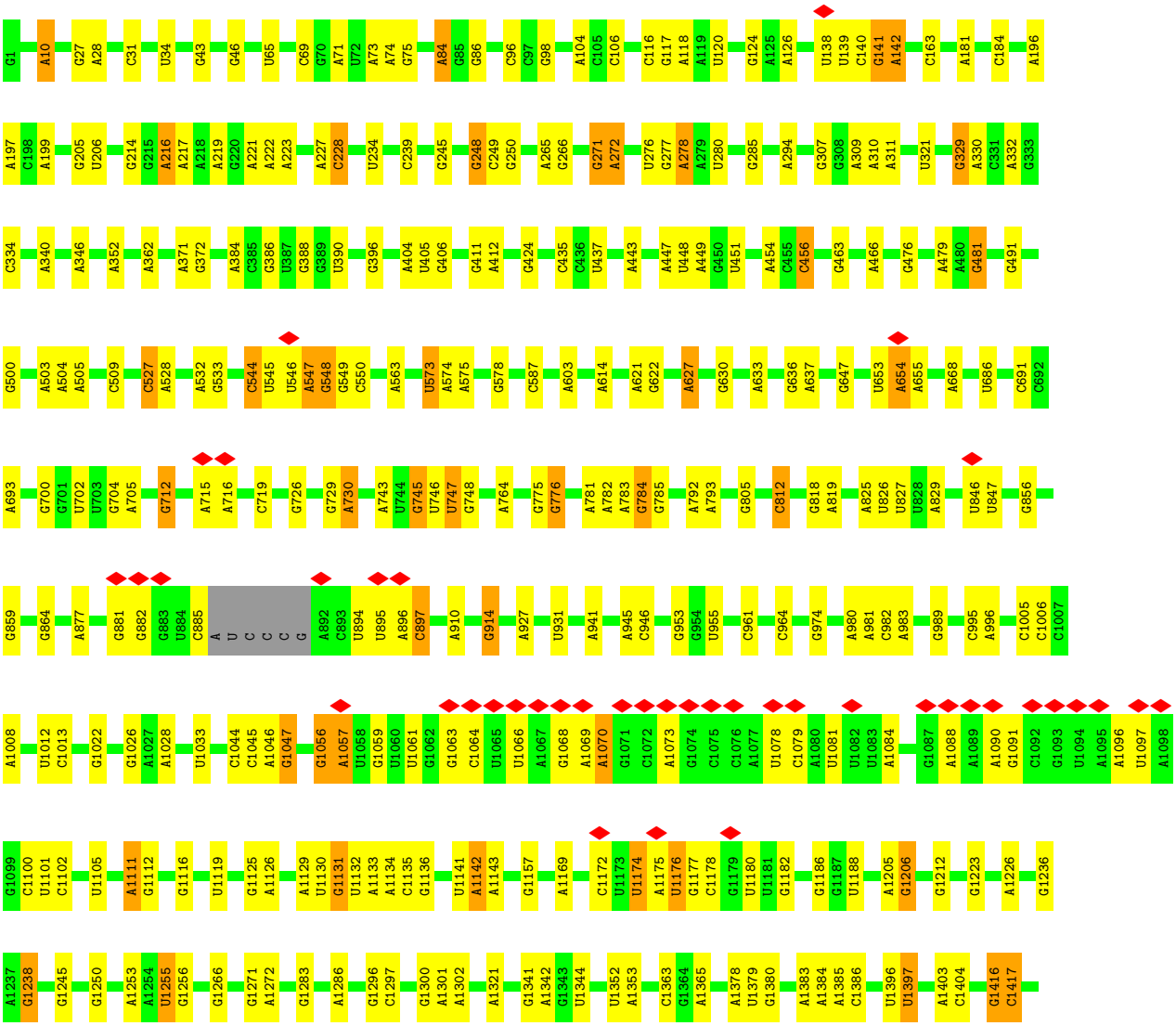
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
8	I	1	52	36	3	4	9	0

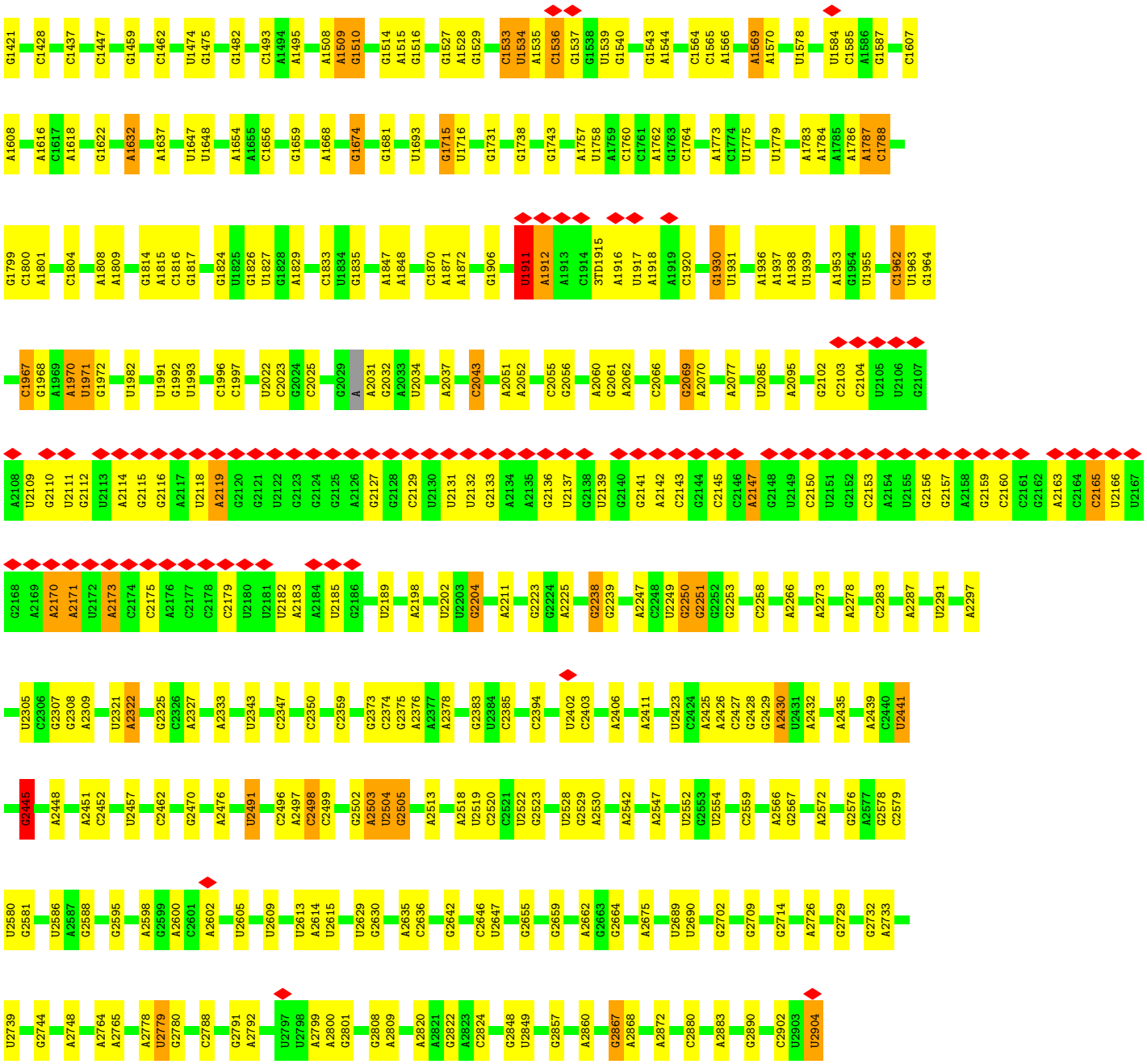
3 Residue-property plots (i)

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: 23S ribosomal RNA

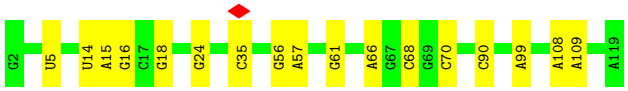
Chain I:





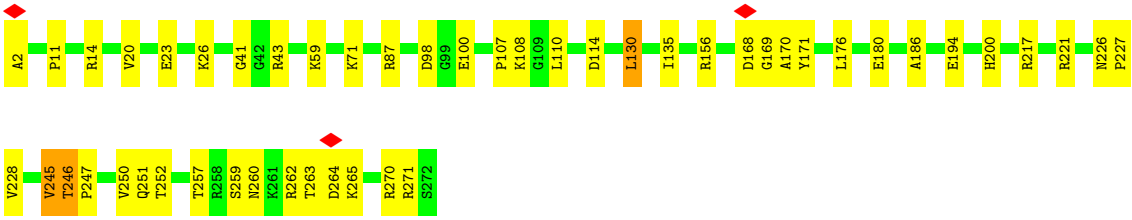
- Molecule 2: 5S ribosomal RNA

Chain J:



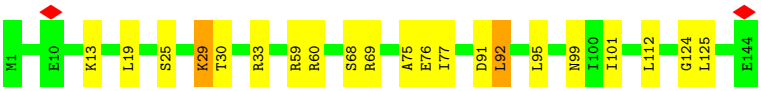
- Molecule 3: 50S ribosomal protein L2

Chain K:



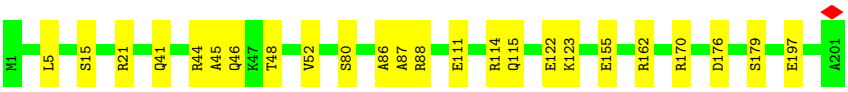
• Molecule 4: 50S ribosomal protein L15

Chain L:



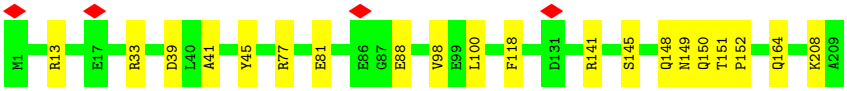
• Molecule 5: 50S ribosomal protein L4

Chain M:



• Molecule 6: 50S ribosomal protein L3

Chain N:



• Molecule 7: 50S ribosomal protein L13

Chain O:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20644	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	34.251	Depositor
Minimum map value	-19.011	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	1.420	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	496.98, 496.98, 496.98	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8283, 0.8283, 0.8283	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, 2MG, 3TD, 1MG, G7M, OMU, PSU, OMC, O8S, 6MZ, 5MC, 5MU, OMG

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	I	0.25	0/69165	0.67	0/107896
2	J	0.21	0/2828	0.66	0/4410
3	K	0.28	0/2122	0.46	0/2852
4	L	0.27	0/1062	0.46	0/1413
5	M	0.30	0/1571	0.42	0/2113
6	N	0.31	0/1586	0.49	0/2134
7	O	0.28	0/1152	0.42	0/1551
All	All	0.25	0/79486	0.65	0/122369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	62206	0	31305	252	0
2	J	2529	0	1281	7	0
3	K	2083	0	2154	38	0
4	L	1053	0	1129	16	0
5	M	1552	0	1618	18	0
6	N	1565	0	1616	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	1129	0	1162	12	0
8	I	52	0	0	0	0
All	All	72169	0	40265	313	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 3.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2032:G:N3	6:N:150:GLN:NE2	1.66	1.42
1:I:2032:G:C4	6:N:150:GLN:NE2	1.93	1.33
1:I:2032:G:C2	6:N:150:GLN:NE2	2.26	1.01
1:I:1084:A:HO2'	1:I:1105:U:HO2'	1.09	0.97
1:I:1656:C:OP1	6:N:141:ARG:NH1	2.05	0.89
1:I:1084:A:O2'	1:I:1105:U:O2'	1.91	0.88
1:I:1174:U:OP1	1:I:1177:G:N2	2.08	0.86
1:I:895:U:O2	1:I:897:C:N4	2.09	0.86
1:I:1090:A:N6	1:I:1101:U:O2	2.09	0.86
3:K:2:ALA:N	3:K:20:VAL:O	2.10	0.84
1:I:2848:G:O2'	1:I:2867:G:N2	2.12	0.82
1:I:1693:U:O2'	3:K:14:ARG:NH2	2.13	0.82
1:I:1715:G:O2'	1:I:1743:G:O6	1.99	0.81
1:I:1826:G:O2'	1:I:1971:U:OP2	2.01	0.79
1:I:65:U:O2'	1:I:456:C:N3	2.16	0.78
1:I:1911:PSU:O2'	1:I:1912:A:OP1	2.02	0.78
2:J:16:G:O6	2:J:68:C:N4	2.15	0.78
5:M:21:ARG:O	5:M:114:ARG:NH2	2.17	0.78
1:I:745:1MG:O2'	1:I:748:G:O2'	2.02	0.78
1:I:1245:G:OP1	4:L:13:LYS:NZ	2.17	0.78
1:I:1779:U:OP2	1:I:1784:A:N6	2.17	0.77
1:I:712:G:O6	1:I:719:C:N4	2.17	0.77
1:I:463:G:N2	1:I:466:A:OP2	2.16	0.77
1:I:1607:C:N4	1:I:1622:G:OP2	2.16	0.77
1:I:2266:A:N6	1:I:2273:A:OP2	2.18	0.77
1:I:1378:A:O2'	1:I:1380:G:OP2	2.02	0.77
1:I:2439:A:O2'	1:I:2600:A:OP1	2.03	0.77
1:I:1091:G:N2	1:I:1100:C:O2	2.17	0.77
1:I:2576:G:O2'	1:I:2579:C:OP2	2.03	0.76
1:I:574:A:N6	1:I:2034:U:OP1	2.18	0.76
1:I:2503:2MA:O2'	1:I:2505:G:OP2	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1788:C:OP2	3:K:221:ARG:NH1	2.19	0.76
1:I:621:A:OP2	4:L:99:ASN:ND2	2.20	0.75
1:I:1799:G:OP2	3:K:270:ARG:NH1	2.19	0.75
1:I:2291:U:O2'	1:I:2374:C:O2	2.05	0.75
1:I:1044:C:O2'	1:I:1111:A:N1	2.19	0.74
1:I:781:A:OP1	3:K:217:ARG:NH2	2.21	0.74
1:I:2902:C:OP2	1:I:2904:U:O3'	2.06	0.73
1:I:1799:G:O2'	3:K:180:GLU:OE2	2.03	0.73
1:I:1475:G:O2'	1:I:1514:G:O6	2.07	0.73
1:I:1936:A:OP2	1:I:1962:5MC:N4	2.22	0.73
1:I:1417:C:O5'	1:I:1587:G:N2	2.22	0.73
3:K:251:GLN:O	3:K:252:THR:OG1	2.07	0.73
1:I:1130:U:O4	6:N:151:THR:O	2.07	0.72
1:I:449:A:OP1	5:M:80:SER:HA	1.91	0.71
3:K:71:LYS:NZ	3:K:98:ASP:OD2	2.23	0.71
1:I:745:1MG:HO2'	1:I:748:G:HO2'	1.38	0.71
5:M:46:GLN:O	5:M:88:ARG:NH1	2.24	0.71
1:I:1462:C:O2'	1:I:2702:G:O2'	2.03	0.71
1:I:2822:G:OP1	6:N:164:GLN:NE2	2.24	0.71
1:I:1066:U:O2'	1:I:1068:G:N7	2.21	0.71
1:I:691:C:OP1	3:K:217:ARG:NH1	2.23	0.70
1:I:578:G:OP1	1:I:1255:U:O2'	2.10	0.70
1:I:544:C:N4	1:I:548:G:OP2	2.26	0.69
3:K:170:ALA:O	3:K:186:ALA:N	2.25	0.68
1:I:1069:A:N6	1:I:1096:A:OP1	2.26	0.68
1:I:1787:A:O2'	1:I:1788:C:OP1	2.10	0.68
1:I:1437:C:O2'	1:I:1516:G:O2'	2.12	0.68
1:I:2202:U:O2'	1:I:2204:G:OP1	2.08	0.68
1:I:1283:G:N1	1:I:1286:A:OP2	2.27	0.67
1:I:1911:PSU:O3'	1:I:1918:A:N6	2.19	0.67
1:I:2085:U:OP1	3:K:259:SER:OG	2.12	0.67
1:I:743:A:O2'	1:I:1659:G:OP1	2.13	0.66
1:I:248:G:O2'	1:I:2432:A:OP1	2.09	0.66
1:I:1296:G:OP1	1:I:2709:G:O2'	2.13	0.66
1:I:2051:A:O2'	1:I:2614:A:N6	2.29	0.66
1:I:573:U:N3	1:I:2031:A:OP1	2.28	0.65
1:I:271:G:O2'	1:I:272:A:O5'	2.06	0.65
1:I:1363:C:O2'	1:I:1809:A:N3	2.28	0.65
1:I:730:A:OP1	1:I:1775:U:O2'	2.07	0.65
6:N:148:GLN:N	6:N:148:GLN:OE1	2.30	0.65
1:I:1992:G:N2	1:I:1996:C:O2'	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:125:TYR:OH	7:O:132:HIS:NE2	2.31	0.64
1:I:1008:A:OP2	7:O:37:ARG:NH1	2.31	0.64
1:I:2646:C:OP2	1:I:2732:G:O2'	2.14	0.64
1:I:500:G:N1	1:I:503:A:OP2	2.30	0.64
1:I:2522:U:O2'	1:I:2647:U:OP1	2.09	0.64
1:I:2581:G:OP2	1:I:2581:G:N2	2.31	0.64
1:I:2788:C:O2'	1:I:2809:A:N3	2.28	0.64
1:I:784:G:O4'	3:K:226:ASN:ND2	2.32	0.63
1:I:1385:A:O2'	1:I:1396:U:O2	2.17	0.63
1:I:1930:G:O2'	1:I:1968:G:O6	2.14	0.62
3:K:71:LYS:NZ	3:K:100:GLU:OE1	2.32	0.61
1:I:1654:A:O2'	6:N:118:PHE:O	2.18	0.61
1:I:1528:A:OP2	1:I:1543:G:N2	2.33	0.61
1:I:2116:G:O6	1:I:2165:C:N4	2.33	0.61
3:K:226:ASN:O	3:K:228:VAL:N	2.33	0.61
1:I:2822:G:O2'	1:I:2824:C:OP2	2.12	0.61
1:I:309:A:N3	1:I:329:G:O2'	2.32	0.61
1:I:527:C:N4	1:I:2779:U:OP2	2.34	0.60
1:I:249:C:OP2	1:I:2394:C:O2'	2.10	0.60
1:I:2406:A:OP2	1:I:2411:A:N6	2.33	0.59
1:I:2109:U:O4	1:I:2179:C:N4	2.35	0.59
1:I:106:C:O2	1:I:294:A:O2'	2.19	0.59
1:I:69:C:O2	1:I:73:A:O2'	2.15	0.59
1:I:307:G:N1	1:I:310:A:OP2	2.35	0.59
1:I:2523:G:HO2'	1:I:2764:A:HO2'	1.51	0.59
1:I:1101:U:O2'	1:I:1102:C:O4'	2.21	0.59
1:I:1417:C:HO2'	1:I:1587:G:HO2'	1.47	0.58
1:I:1130:U:C4	6:N:151:THR:O	2.57	0.58
1:I:2451:A:OP1	1:I:2497:A:N6	2.36	0.58
1:I:2642:G:OP1	7:O:78:THR:OG1	2.10	0.58
1:I:2359:C:O2	4:L:60:ARG:NH2	2.37	0.58
1:I:630:G:N2	1:I:633:A:OP2	2.33	0.58
6:N:151:THR:OG1	6:N:152:PRO:CD	2.52	0.57
1:I:1871:A:O2'	1:I:1872:A:N7	2.32	0.57
6:N:88:GLU:N	6:N:88:GLU:OE1	2.37	0.57
1:I:864:G:O2'	1:I:914:G:O6	2.22	0.57
1:I:2223:G:OP1	3:K:171:TYR:OH	2.13	0.57
1:I:1056:G:O2'	1:I:1057:A:O5'	2.23	0.57
1:I:1174:U:O2'	1:I:1176:U:OP2	2.22	0.56
1:I:2143:C:N3	1:I:2147:A:N6	2.52	0.56
1:I:2052:A:H4'	6:N:148:GLN:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1297:C:O2'	1:I:1302:A:N1	2.33	0.56
1:I:1341:G:OP1	1:I:1397:U:N3	2.38	0.56
3:K:246:THR:HG22	3:K:247:PRO:HD2	1.87	0.56
1:I:476:G:N1	1:I:479:A:OP2	2.35	0.56
1:I:1509:A:O2'	1:I:1510:G:OP2	2.21	0.55
1:I:2799:A:O2'	1:I:2801:G:OP2	2.24	0.55
1:I:278:A:N6	1:I:362:A:N7	2.54	0.55
1:I:443:A:OP1	5:M:41:GLN:N	2.40	0.55
1:I:2166:U:N3	1:I:2170:A:N1	2.54	0.55
3:K:263:THR:OG1	3:K:264:ASP:N	2.40	0.55
1:I:1824:G:O2'	3:K:246:THR:HG23	2.07	0.55
1:I:881:G:N2	1:I:882:G:O6	2.39	0.55
1:I:221:A:N1	1:I:265:A:O2'	2.40	0.54
1:I:2051:A:N6	1:I:2614:A:O2'	2.40	0.53
1:I:2595:G:N2	1:I:2598:A:OP2	2.37	0.53
3:K:107:PRO:HD2	3:K:110:LEU:HD22	1.89	0.53
1:I:27:G:O2'	1:I:28:A:OP2	2.25	0.53
1:I:2077:A:OP1	1:I:2238:G:N2	2.32	0.53
1:I:197:A:N6	1:I:2430:A:O2'	2.42	0.53
1:I:2343:U:HO2'	1:I:2373:G:HO2'	1.55	0.53
1:I:964:C:O2'	1:I:2273:A:N3	2.33	0.53
5:M:46:GLN:HB2	5:M:86:ALA:HB1	1.91	0.52
1:I:86:G:HO2'	1:I:104:A:HO2'	1.57	0.52
5:M:5:LEU:HD23	5:M:122:GLU:OE1	2.10	0.52
3:K:108:LYS:N	3:K:194:GLU:O	2.42	0.52
1:I:818:G:N1	1:I:1188:U:OP2	2.33	0.52
5:M:5:LEU:HD23	5:M:122:GLU:OE2	2.10	0.52
1:I:1064:C:N4	1:I:1070:A:OP2	2.43	0.52
1:I:704:G:O2'	1:I:726:G:N2	2.35	0.52
5:M:15:SER:N	5:M:197:GLU:OE2	2.40	0.52
1:I:704:G:O2'	1:I:705:A:OP2	2.25	0.52
1:I:1817:G:OP1	3:K:87:ARG:NH2	2.43	0.52
2:J:24:G:O2'	2:J:56:G:N7	2.33	0.52
1:I:1681:G:O2'	1:I:1762:A:N3	2.37	0.51
1:I:84:A:N1	1:I:98:G:O2'	2.36	0.51
1:I:729:G:N2	3:K:11:PRO:O	2.43	0.51
1:I:1569:A:O4'	3:K:59:LYS:NZ	2.38	0.51
1:I:2659:G:N2	1:I:2662:A:OP2	2.42	0.51
1:I:449:A:OP1	5:M:80:SER:N	2.43	0.51
1:I:449:A:OP1	5:M:80:SER:CA	2.57	0.51
1:I:2114:A:H61	1:I:2119:A:H62	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:227:A:O2'	1:I:228:C:OP2	2.24	0.51
1:I:1787:A:HO2'	1:I:1788:C:P	2.33	0.51
1:I:2258:C:O2'	1:I:2427:C:OP2	2.26	0.51
3:K:168:ASP:OD1	3:K:169:GLY:N	2.44	0.51
7:O:81:ILE:H	7:O:81:ILE:HD12	1.74	0.51
1:I:276:U:O2'	1:I:278:A:N7	2.45	0.50
1:I:1916:A:OP2	1:I:1918:A:N6	2.44	0.50
1:I:2066:C:O2	1:I:2445:2MG:HM22	2.12	0.50
6:N:45:TYR:OH	6:N:81:GLU:OE2	2.24	0.50
1:I:1565:C:O2'	1:I:1566:A:OP2	2.26	0.50
1:I:239:C:HO2'	1:I:622:G:HO2'	1.55	0.50
1:I:2635:A:O2'	6:N:81:GLU:OE1	2.11	0.50
1:I:1786:A:O2'	1:I:1938:A:N6	2.45	0.49
1:I:1380:G:N2	1:I:1570:A:N1	2.60	0.49
1:I:1223:G:N2	1:I:1226:A:OP2	2.42	0.49
1:I:2780:G:OP2	7:O:120:ARG:NE	2.45	0.49
6:N:151:THR:OG1	6:N:152:PRO:HD3	2.12	0.49
1:I:31:C:O2'	1:I:1238:G:OP1	2.30	0.49
1:I:447:A:N1	1:I:454:A:O2'	2.32	0.49
1:I:980:A:N3	1:I:2037:A:O2'	2.40	0.49
1:I:1804:C:OP1	3:K:257:THR:OG1	2.30	0.49
1:I:141:G:O2'	1:I:142:A:P	2.71	0.49
5:M:176:ASP:OD1	5:M:179:SER:N	2.38	0.49
7:O:82:GLY:O	7:O:84:ILE:N	2.39	0.49
1:I:1005:C:O2'	7:O:30:THR:HG21	2.12	0.49
1:I:2430:A:N3	1:I:2430:A:H2'	2.28	0.49
1:I:1779:U:C2'	1:I:1783:A:H62	2.25	0.49
1:I:388:G:O6	1:I:390:U:O2'	2.20	0.48
1:I:2249:U:N3	1:I:2253:G:OP2	2.46	0.48
1:I:2655:G:O2'	1:I:2664:G:O6	2.28	0.48
1:I:981:A:OP2	1:I:982:C:N4	2.38	0.48
1:I:1101:U:HO2'	1:I:1102:C:H6	1.59	0.48
1:I:2732:G:OP1	6:N:208:LYS:NZ	2.43	0.48
3:K:23:GLU:N	3:K:23:GLU:OE1	2.46	0.48
1:I:1091:G:N1	1:I:1100:C:N3	2.61	0.48
1:I:1964:G:O2'	1:I:1967:C:OP2	2.25	0.48
1:I:2462:C:O2	1:I:2491:U:N3	2.44	0.48
1:I:2857:G:N2	1:I:2860:A:OP2	2.43	0.48
6:N:39:ASP:OD1	6:N:41:ALA:N	2.47	0.48
1:I:1069:A:O2'	1:I:1073:A:N6	2.43	0.48
2:J:66:A:H2	2:J:68:C:H41	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:214:G:N2	1:I:216:A:N3	2.60	0.47
1:I:1068:G:O2'	1:I:1070:A:N6	2.46	0.47
5:M:111:GLU:OE1	5:M:115:GLN:NE2	2.44	0.47
1:I:141:G:O2'	1:I:142:A:OP2	2.27	0.47
1:I:2250:G:O2'	1:I:2496:C:OP1	2.33	0.47
1:I:2375:G:N2	1:I:2378:A:OP2	2.40	0.47
3:K:246:THR:N	3:K:250:VAL:O	2.40	0.47
1:I:2808:G:O2'	1:I:2890:G:O6	2.14	0.47
1:I:219:A:N3	1:I:234:U:O2'	2.37	0.47
1:I:1061:U:HO2'	1:I:1063:G:P	2.38	0.47
1:I:2572:A:H2'	6:N:149:ASN:HD22	1.80	0.46
1:I:2171:A:O2'	1:I:2173:A:OP1	2.23	0.46
1:I:1026:G:OP2	1:I:1134:A:O2'	2.16	0.46
1:I:1911:PSU:O2'	1:I:1912:A:P	2.73	0.46
1:I:2904:U:O3'	1:I:2904:U:OP1	2.34	0.46
1:I:1447:C:O2'	1:I:1544:A:N3	2.42	0.46
7:O:11:VAL:HG21	7:O:50:THR:HG22	1.98	0.46
1:I:1911:PSU:HO2'	1:I:1912:A:P	2.32	0.45
1:I:812:C:O2'	1:I:1226:A:O2'	2.32	0.45
1:I:989:G:OP1	1:I:1157:G:O2'	2.33	0.45
1:I:1787:A:O2'	1:I:1788:C:P	2.74	0.45
1:I:1799:G:C5	3:K:176:LEU:HD22	2.50	0.45
5:M:170:ARG:NH1	5:M:179:SER:OG	2.44	0.45
3:K:260:ASN:OD1	3:K:262:ARG:N	2.41	0.45
1:I:1174:U:HO2'	1:I:1176:U:P	2.39	0.45
1:I:1474:U:O4	1:I:1475:G:N1	2.50	0.45
1:I:184:C:O2'	1:I:217:A:N3	2.44	0.45
1:I:693:A:O2'	1:I:1353:A:N3	2.40	0.45
1:I:1384:A:O2'	1:I:1404:C:O2	2.33	0.45
3:K:176:LEU:HD12	3:K:176:LEU:H	1.82	0.45
3:K:130:LEU:HB2	3:K:135:ILE:HD11	2.00	0.44
1:I:1564:C:OP2	3:K:26:LYS:NZ	2.28	0.44
1:I:2141:G:HO2'	1:I:2142:A:H8	1.60	0.44
1:I:2182:U:O2'	1:I:2183:A:O4'	2.36	0.44
1:I:2636:C:O2'	6:N:45:TYR:OH	2.34	0.44
4:L:124:GLY:O	4:L:125:LEU:HD12	2.18	0.44
1:I:995:C:O2	7:O:3:THR:OG1	2.20	0.44
1:I:2441:U:OP2	1:I:2586:U:O2'	2.34	0.44
3:K:41:GLY:O	3:K:43:ARG:NH1	2.51	0.44
1:I:1814:G:OP2	1:I:1815:A:O2'	2.22	0.44
1:I:2182:U:HO2'	1:I:2183:A:P	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1342:A:HO2'	1:I:1344:U:P	2.38	0.43
1:I:2528:U:O2'	1:I:2530:A:OP1	2.34	0.43
1:I:1141:U:H4'	1:I:1142:A:O4'	2.18	0.43
7:O:13:ARG:NH1	7:O:49:ASP:O	2.51	0.43
1:I:1061:U:O2'	1:I:1063:G:OP2	2.28	0.43
2:J:66:A:O4'	2:J:108:A:N6	2.51	0.43
1:I:141:G:HO2'	1:I:142:A:P	2.42	0.43
1:I:1539:U:N3	1:I:1540:G:N7	2.67	0.43
5:M:5:LEU:HD23	5:M:122:GLU:CD	2.38	0.43
1:I:250:G:H4'	4:L:59:ARG:HD3	2.01	0.42
1:I:1417:C:O2'	1:I:1587:G:O2'	2.21	0.42
1:I:1668:A:O2'	1:I:1674:G:N7	2.48	0.42
1:I:704:G:HO2'	1:I:705:A:P	2.40	0.42
1:I:2519:U:O4'	1:I:2542:A:N6	2.52	0.42
1:I:479:A:HO2'	1:I:481:G:H8	1.64	0.42
1:I:1212:G:O2'	1:I:1236:G:N2	2.45	0.42
3:K:176:LEU:HD12	3:K:176:LEU:N	2.34	0.42
1:I:776:G:N7	1:I:793:A:O2'	2.44	0.42
1:I:1205:A:O2'	1:I:1206:G:OP1	2.33	0.42
1:I:1245:G:H5"	4:L:13:LYS:HZ3	1.83	0.42
1:I:1421:G:N2	1:I:1495:A:N1	2.68	0.42
1:I:1953:A:O2'	1:I:2559:C:O2	2.32	0.42
1:I:124:G:N2	1:I:126:A:O2'	2.52	0.42
1:I:1141:U:OP2	7:O:65:THR:OG1	2.34	0.42
1:I:1437:C:HO2'	1:I:1516:G:HO2'	1.37	0.42
1:I:700:G:O2'	1:I:1632:A:N3	2.40	0.42
4:L:75:ALA:HB3	4:L:101:ILE:HD11	2.02	0.42
1:I:528:A:C2	1:I:2043:C:H4'	2.54	0.42
1:I:587:C:O2	4:L:33:ARG:NH2	2.53	0.42
1:I:1827:U:O2'	1:I:1970:A:N3	2.50	0.42
6:N:148:GLN:N	6:N:148:GLN:CD	2.73	0.42
1:I:1028:A:OP2	1:I:1126:A:N6	2.48	0.42
1:I:1057:A:N6	1:I:1081:U:O4	2.53	0.42
1:I:1416:G:O2'	1:I:1417:C:OP2	2.27	0.41
2:J:5:U:OP1	2:J:61:G:O2'	2.31	0.41
4:L:124:GLY:C	4:L:125:LEU:HD12	2.39	0.41
1:I:1817:G:O5'	3:K:156:ARG:NH2	2.53	0.41
2:J:24:G:N7	2:J:56:G:O2'	2.30	0.41
3:K:130:LEU:HD13	3:K:135:ILE:CD1	2.50	0.41
5:M:45:ALA:HA	5:M:87:ALA:O	2.19	0.41
1:I:1533:C:O2'	1:I:1534:U:OP1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1045:C:O2	1:I:1047:G:N1	2.53	0.41
1:I:1637:A:H5'	1:I:1760:C:HO2'	1.86	0.41
4:L:19:LEU:N	4:L:19:LEU:HD12	2.36	0.41
4:L:29:LYS:C	4:L:30:THR:HG23	2.41	0.41
3:K:245:VAL:HA	3:K:250:VAL:O	2.21	0.41
5:M:48:THR:O	5:M:52:VAL:HG23	2.19	0.41
1:I:825:A:H2'	1:I:826:U:O4'	2.21	0.41
1:I:829:A:N7	1:I:2247:A:O2'	2.54	0.41
1:I:1536:C:O4'	1:I:1537:G:N2	2.54	0.41
1:I:321:U:O3'	5:M:162:ARG:NH1	2.48	0.41
1:I:636:G:N1	4:L:76:GLU:OE1	2.48	0.41
1:I:1715:G:O2'	1:I:1716:U:OP2	2.38	0.41
3:K:263:THR:O	3:K:265:LYS:N	2.54	0.41
1:I:276:U:H2'	1:I:277:G:O4'	2.21	0.40
1:I:1527:G:N2	1:I:1544:A:OP2	2.52	0.40
1:I:340:A:O2'	5:M:162:ARG:NH1	2.54	0.40
1:I:547:A:H3'	1:I:547:A:N3	2.36	0.40
1:I:1006:C:O4'	7:O:30:THR:HG23	2.21	0.40
1:I:1131:G:O2'	1:I:2025:C:O2'	2.23	0.40
1:I:2646:C:N4	1:I:2675:A:N1	2.69	0.40
4:L:68:SER:O	4:L:69:ARG:HB2	2.22	0.40
4:L:77:ILE:HD11	4:L:95:LEU:HD13	2.03	0.40
4:L:91:ASP:OD1	4:L:92:LEU:N	2.53	0.40
1:I:245:G:O2'	1:I:384:A:N1	2.37	0.40
1:I:1125:G:OP2	1:I:1126:A:O2'	2.29	0.40
1:I:2321:U:H5'	1:I:2322:A:OP2	2.22	0.40
1:I:2867:G:O2'	1:I:2868:A:OP2	2.37	0.40
6:N:98:VAL:HG22	6:N:98:VAL:O	2.21	0.40
1:I:10:A:H2	1:I:2800:A:HO2'	1.68	0.40
1:I:116:C:H2'	1:I:117:G:O4'	2.22	0.40
1:I:653:U:H3'	1:I:654:A:C5'	2.51	0.40
1:I:205:G:O2'	1:I:206:U:OP2	2.39	0.40
1:I:332:A:HO2'	1:I:334:C:P	2.44	0.40
1:I:627:A:N6	4:L:112:LEU:O	2.41	0.40
1:I:745:1MG:HN21	1:I:745:1MG:HM11	1.71	0.40
2:J:14:U:OP2	2:J:70:C:O2'	2.36	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	
3	K	269/271 (99%)	241 (90%)	27 (10%)	1 (0%)	34	66
4	L	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
5	M	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
6	N	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	O	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
All	All	957/967 (99%)	901 (94%)	55 (6%)	1 (0%)	54	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	227	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	216/216 (100%)	210 (97%)	6 (3%)	43	77
4	L	103/103 (100%)	100 (97%)	3 (3%)	42	76
5	M	165/165 (100%)	162 (98%)	3 (2%)	59	86
6	N	164/164 (100%)	159 (97%)	5 (3%)	41	75
7	O	116/116 (100%)	115 (99%)	1 (1%)	78	94
All	All	764/764 (100%)	746 (98%)	18 (2%)	51	81

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

Mol	Chain	Res	Type
3	K	114	ASP
3	K	130	LEU
3	K	200	HIS
3	K	245	VAL
3	K	246	THR
3	K	271	ARG
4	L	25	SER
4	L	29	LYS
4	L	92	LEU
5	M	44	ARG
5	M	123	LYS
5	M	155	GLU
6	N	13	ARG
6	N	33	ARG
6	N	77	ARG
6	N	100	LEU
6	N	145	SER
7	O	71	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	L	99	ASN
7	O	67	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2891/2904 (99%)	352 (12%)	9 (0%)
2	J	117/118 (99%)	7 (5%)	0
All	All	3008/3022 (99%)	359 (11%)	9 (0%)

All (359) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	34	U
1	I	43	G
1	I	46	G

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Mol	Chain	Res	Type
1	I	71	A
1	I	74	A
1	I	75	G
1	I	84	A
1	I	96	C
1	I	118	A
1	I	120	U
1	I	138	U
1	I	139	U
1	I	140	C
1	I	141	G
1	I	142	A
1	I	163	C
1	I	181	A
1	I	196	A
1	I	199	A
1	I	216	A
1	I	222	A
1	I	223	A
1	I	228	C
1	I	248	G
1	I	266	G
1	I	272	A
1	I	278	A
1	I	280	U
1	I	285	G
1	I	311	A
1	I	329	G
1	I	330	A
1	I	346	A
1	I	352	A
1	I	371	A
1	I	372	G
1	I	386	G
1	I	396	G
1	I	405	U
1	I	406	G
1	I	411	G
1	I	412	A
1	I	424	G
1	I	435	C
1	I	437	U

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Mol	Chain	Res	Type
1	I	448	U
1	I	451	U
1	I	456	C
1	I	481	G
1	I	491	G
1	I	504	A
1	I	505	A
1	I	509	C
1	I	527	C
1	I	532	A
1	I	533	G
1	I	544	C
1	I	545	U
1	I	546	U
1	I	547	A
1	I	548	G
1	I	549	G
1	I	550	C
1	I	563	A
1	I	573	U
1	I	575	A
1	I	603	A
1	I	614	A
1	I	627	A
1	I	637	A
1	I	647	G
1	I	654	A
1	I	655	A
1	I	668	A
1	I	686	U
1	I	702	U
1	I	712	G
1	I	715	A
1	I	716	A
1	I	730	A
1	I	747	5MU
1	I	764	A
1	I	775	G
1	I	776	G
1	I	782	A
1	I	783	A
1	I	784	G

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Mol	Chain	Res	Type
1	I	785	G
1	I	792	A
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	846	U
1	I	847	U
1	I	856	G
1	I	859	G
1	I	877	A
1	I	885	C
1	I	894	U
1	I	896	A
1	I	897	C
1	I	910	A
1	I	914	G
1	I	927	A
1	I	931	U
1	I	941	A
1	I	945	A
1	I	946	C
1	I	953	G
1	I	961	C
1	I	974	G
1	I	983	A
1	I	996	A
1	I	1012	U
1	I	1013	C
1	I	1022	G
1	I	1033	U
1	I	1046	A
1	I	1047	G
1	I	1056	G
1	I	1057	A
1	I	1059	G
1	I	1070	A
1	I	1078	U
1	I	1079	C
1	I	1088	A
1	I	1097	U
1	I	1111	A

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Mol	Chain	Res	Type
1	I	1112	G
1	I	1116	G
1	I	1119	U
1	I	1129	A
1	I	1131	G
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1143	A
1	I	1169	A
1	I	1172	C
1	I	1174	U
1	I	1175	A
1	I	1176	U
1	I	1178	C
1	I	1180	U
1	I	1182	G
1	I	1186	G
1	I	1206	G
1	I	1238	G
1	I	1250	G
1	I	1253	A
1	I	1255	U
1	I	1256	G
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1300	G
1	I	1301	A
1	I	1321	A
1	I	1352	U
1	I	1365	A
1	I	1379	U
1	I	1383	A
1	I	1386	C
1	I	1397	U
1	I	1403	A
1	I	1416	G
1	I	1417	C
1	I	1428	C

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Mol	Chain	Res	Type
1	I	1459	G
1	I	1482	G
1	I	1493	C
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A
1	I	1529	G
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1569	A
1	I	1578	U
1	I	1584	U
1	I	1585	C
1	I	1608	A
1	I	1616	A
1	I	1632	A
1	I	1647	U
1	I	1648	U
1	I	1674	G
1	I	1715	G
1	I	1731	G
1	I	1738	G
1	I	1758	U
1	I	1764	C
1	I	1773	A
1	I	1788	C
1	I	1800	C
1	I	1801	A
1	I	1808	A
1	I	1816	C
1	I	1829	A
1	I	1833	C
1	I	1847	A
1	I	1848	A
1	I	1870	C
1	I	1906	G
1	I	1912	A
1	I	1920	C
1	I	1930	G
1	I	1931	U

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Mol	Chain	Res	Type
1	I	1937	A
1	I	1955	U
1	I	1963	U
1	I	1967	C
1	I	1970	A
1	I	1971	U
1	I	1972	G
1	I	1982	U
1	I	1991	U
1	I	1993	U
1	I	1997	C
1	I	2022	U
1	I	2023	C
1	I	2043	C
1	I	2055	C
1	I	2056	G
1	I	2060	A
1	I	2061	G
1	I	2062	A
1	I	2069	G7M
1	I	2070	A
1	I	2095	A
1	I	2102	G
1	I	2103	C
1	I	2104	C
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2115	G
1	I	2118	U
1	I	2119	A
1	I	2127	G
1	I	2129	C
1	I	2131	U
1	I	2132	U
1	I	2133	G
1	I	2136	G
1	I	2137	U
1	I	2139	U
1	I	2145	C
1	I	2147	A
1	I	2150	C

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Mol	Chain	Res	Type
1	I	2153	C
1	I	2156	G
1	I	2157	G
1	I	2159	G
1	I	2160	C
1	I	2163	A
1	I	2165	C
1	I	2170	A
1	I	2171	A
1	I	2173	A
1	I	2175	C
1	I	2185	U
1	I	2189	U
1	I	2198	A
1	I	2204	G
1	I	2211	A
1	I	2225	A
1	I	2238	G
1	I	2239	G
1	I	2250	G
1	I	2251	OMG
1	I	2278	A
1	I	2283	C
1	I	2287	A
1	I	2297	A
1	I	2305	U
1	I	2307	G
1	I	2308	G
1	I	2309	A
1	I	2322	A
1	I	2325	G
1	I	2327	A
1	I	2333	A
1	I	2347	C
1	I	2350	C
1	I	2376	A
1	I	2383	G
1	I	2385	C
1	I	2402	U
1	I	2403	C
1	I	2423	U
1	I	2425	A

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Mol	Chain	Res	Type
1	I	2426	A
1	I	2428	G
1	I	2429	G
1	I	2430	A
1	I	2435	A
1	I	2441	U
1	I	2445	2MG
1	I	2448	A
1	I	2452	C
1	I	2470	G
1	I	2476	A
1	I	2491	U
1	I	2498	OMC
1	I	2499	C
1	I	2502	G
1	I	2504	PSU
1	I	2505	G
1	I	2513	A
1	I	2518	A
1	I	2520	C
1	I	2529	G
1	I	2547	A
1	I	2554	U
1	I	2566	A
1	I	2567	G
1	I	2578	G
1	I	2588	G
1	I	2602	A
1	I	2609	U
1	I	2613	U
1	I	2615	U
1	I	2629	U
1	I	2630	G
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2726	A
1	I	2729	G
1	I	2733	A
1	I	2739	U
1	I	2744	G
1	I	2748	A

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Mol	Chain	Res	Type
1	I	2765	A
1	I	2778	A
1	I	2779	U
1	I	2791	G
1	I	2792	A
1	I	2820	A
1	I	2849	U
1	I	2867	G
1	I	2872	A
1	I	2880	C
1	I	2883	A
1	I	2904	U
2	J	15	A
2	J	18	G
2	J	35	C
2	J	57	A
2	J	90	C
2	J	99	A
2	J	109	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	271	G
1	I	404	A
1	I	784	G
1	I	1056	G
1	I	1533	C
1	I	1757	A
1	I	1787	A
1	I	1911	PSU
1	I	2425	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	I	955	1	18,21,22	0.92	0	22,30,33	1.80	4 (18%)
1	OMC	I	2498	1	19,22,23	0.87	1 (5%)	26,31,34	1.01	1 (3%)
1	5MU	I	1939	1	19,22,23	1.03	2 (10%)	28,32,35	2.10	6 (21%)
1	2MA	I	2503	1	17,25,26	0.83	1 (5%)	17,37,40	0.97	1 (5%)
1	PSU	I	2605	1	18,21,22	0.93	0	22,30,33	1.82	4 (18%)
1	PSU	I	1911	1	18,21,22	0.85	0	22,30,33	1.87	3 (13%)
1	2MG	I	2445	5,1	18,26,27	1.26	2 (11%)	16,38,41	1.23	2 (12%)
1	PSU	I	2504	1	18,21,22	0.95	0	22,30,33	1.81	4 (18%)
1	PSU	I	1917	1	18,21,22	0.89	0	22,30,33	1.80	3 (13%)
1	PSU	I	2580	1	18,21,22	0.97	1 (5%)	22,30,33	1.84	5 (22%)
1	5MC	I	1962	1	18,22,23	0.83	1 (5%)	26,32,35	1.14	2 (7%)
1	G7M	I	2069	1	20,26,27	0.92	1 (5%)	17,39,42	0.47	0
1	3TD	I	1915	1	18,22,23	0.95	1 (5%)	22,32,35	1.65	2 (9%)
1	1MG	I	745	1	18,26,27	1.23	2 (11%)	19,39,42	1.27	3 (15%)
1	2MG	I	1835	1	18,26,27	1.20	2 (11%)	16,38,41	1.25	2 (12%)
1	PSU	I	2457	1	18,21,22	0.93	0	22,30,33	1.81	4 (18%)
1	6MZ	I	1618	1	18,25,26	1.04	2 (11%)	16,36,39	1.91	4 (25%)
1	OMU	I	2552	1	19,22,23	0.94	1 (5%)	26,31,34	1.81	6 (23%)
1	PSU	I	746	1	18,21,22	0.98	1 (5%)	22,30,33	1.72	3 (13%)
1	5MU	I	747	1	19,22,23	1.03	2 (10%)	28,32,35	2.07	6 (21%)
1	OMG	I	2251	1	18,26,27	1.20	2 (11%)	19,38,41	1.41	4 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	OMC	I	2498	1	-	2/9/27/28	0/2/2/2
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	I	2503	1	-	2/3/25/26	0/3/3/3
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	I	2445	5,1	-	2/5/27/28	0/3/3/3
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	G7M	I	2069	1	-	1/3/25/26	0/3/3/3
1	3TD	I	1915	1	-	3/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
1	2MG	I	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	2/5/27/28	0/3/3/3
1	OMU	I	2552	1	-	2/9/27/28	0/2/2/2
1	PSU	I	746	1	-	1/7/25/26	0/2/2/2
1	5MU	I	747	1	-	2/7/25/26	0/2/2/2
1	OMG	I	2251	1	-	2/5/27/28	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2445	2MG	C5-C6	-2.84	1.41	1.47
1	I	2069	G7M	C8-N9	2.82	1.38	1.33
1	I	2251	OMG	C5-C6	-2.79	1.41	1.47
1	I	1835	2MG	C5-C6	-2.78	1.41	1.47
1	I	2251	OMG	C8-N7	-2.76	1.30	1.35
1	I	745	1MG	C8-N7	-2.75	1.30	1.35
1	I	2445	2MG	C8-N7	-2.70	1.30	1.35
1	I	1835	2MG	C8-N7	-2.68	1.30	1.35
1	I	1915	3TD	C4-N3	-2.43	1.35	1.40
1	I	2552	OMU	C2-N1	-2.42	1.34	1.38
1	I	2498	OMC	C2-N1	-2.41	1.34	1.40
1	I	747	5MU	C2-N1	-2.39	1.34	1.38
1	I	1618	6MZ	C8-N7	-2.37	1.30	1.34
1	I	1939	5MU	C2-N1	-2.36	1.34	1.38
1	I	1618	6MZ	C6-N6	2.30	1.38	1.35
1	I	2503	2MA	C8-N7	-2.27	1.31	1.35
1	I	1962	5MC	C2-N1	-2.27	1.35	1.40
1	I	745	1MG	C6-N1	-2.21	1.35	1.39
1	I	747	5MU	C4-N3	-2.06	1.35	1.38
1	I	1939	5MU	C4-N3	-2.06	1.35	1.38
1	I	746	PSU	C4-N3	-2.06	1.35	1.38
1	I	2580	PSU	C4-N3	-2.01	1.35	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1915	3TD	N1-C2-N3	5.93	120.82	116.14
1	I	1939	5MU	C4-N3-C2	-5.49	120.24	127.35
1	I	747	5MU	C4-N3-C2	-5.42	120.33	127.35
1	I	1911	PSU	N1-C2-N3	5.22	121.05	115.13
1	I	1618	6MZ	C2-N1-C6	5.20	121.05	116.59
1	I	2504	PSU	N1-C2-N3	5.17	120.99	115.13
1	I	2605	PSU	N1-C2-N3	5.14	120.96	115.13
1	I	2580	PSU	N1-C2-N3	5.14	120.96	115.13
1	I	2457	PSU	N1-C2-N3	5.12	120.93	115.13
1	I	955	PSU	N1-C2-N3	5.09	120.90	115.13
1	I	1917	PSU	N1-C2-N3	5.07	120.88	115.13
1	I	746	PSU	N1-C2-N3	4.99	120.79	115.13
1	I	2552	OMU	C4-N3-C2	-4.77	120.29	126.58
1	I	1939	5MU	N3-C2-N1	4.65	121.06	114.89
1	I	747	5MU	N3-C2-N1	4.61	121.01	114.89
1	I	747	5MU	C5-C4-N3	4.57	119.21	115.31
1	I	1939	5MU	C5-C4-N3	4.56	119.20	115.31
1	I	2552	OMU	N3-C2-N1	4.55	120.93	114.89
1	I	1911	PSU	C4-N3-C2	-4.38	120.02	126.34
1	I	955	PSU	C4-N3-C2	-4.23	120.25	126.34
1	I	2504	PSU	C4-N3-C2	-4.23	120.25	126.34
1	I	2605	PSU	C4-N3-C2	-4.22	120.26	126.34
1	I	1917	PSU	C4-N3-C2	-4.20	120.28	126.34
1	I	2580	PSU	C4-N3-C2	-4.18	120.31	126.34
1	I	746	PSU	C4-N3-C2	-4.18	120.32	126.34
1	I	2457	PSU	C4-N3-C2	-4.14	120.37	126.34
1	I	747	5MU	O4-C4-C5	-4.11	120.13	124.90
1	I	1939	5MU	O4-C4-C5	-4.06	120.20	124.90
1	I	1618	6MZ	N3-C2-N1	-3.85	122.66	128.68
1	I	1939	5MU	C5-C6-N1	-3.75	119.48	123.34
1	I	1915	3TD	C4-N3-C2	-3.75	120.54	124.61
1	I	747	5MU	C5-C6-N1	-3.54	119.70	123.34
1	I	1962	5MC	C5-C6-N1	-3.53	119.71	123.34
1	I	2251	OMG	C8-N7-C5	3.29	109.25	102.99
1	I	2445	2MG	C8-N7-C5	3.24	109.16	102.99
1	I	745	1MG	C8-N7-C5	3.22	109.13	102.99
1	I	1835	2MG	C8-N7-C5	3.22	109.12	102.99
1	I	2503	2MA	C8-N7-C5	3.13	108.95	102.99
1	I	2552	OMU	CM2-O2'-C2'	-3.06	106.50	114.52
1	I	2580	PSU	O2-C2-N1	-3.01	119.48	122.79
1	I	2498	OMC	CM2-O2'-C2'	-3.00	106.66	114.52
1	I	2552	OMU	C5-C4-N3	2.99	119.32	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1917	PSU	O2-C2-N1	-2.96	119.53	122.79
1	I	1911	PSU	O2-C2-N1	-2.93	119.56	122.79
1	I	2457	PSU	O2-C2-N1	-2.93	119.57	122.79
1	I	745	1MG	C5-C6-N1	2.92	118.29	113.90
1	I	2504	PSU	O2-C2-N1	-2.91	119.58	122.79
1	I	746	PSU	O2-C2-N1	-2.91	119.59	122.79
1	I	2605	PSU	O2-C2-N1	-2.90	119.60	122.79
1	I	1618	6MZ	C9-N6-C6	-2.88	120.39	122.87
1	I	955	PSU	O2-C2-N1	-2.78	119.73	122.79
1	I	2552	OMU	O4-C4-C5	-2.77	120.29	125.16
1	I	2251	OMG	C2-N1-C6	-2.72	120.08	125.10
1	I	747	5MU	O2-C2-N1	-2.56	119.38	122.79
1	I	2251	OMG	C5-C6-N1	2.50	118.37	113.95
1	I	2251	OMG	CM2-O2'-C2'	-2.50	107.96	114.52
1	I	2445	2MG	C5-C6-N1	2.48	118.33	113.95
1	I	2552	OMU	O2-C2-N1	-2.47	119.51	122.79
1	I	1835	2MG	C5-C6-N1	2.40	118.19	113.95
1	I	1939	5MU	O2-C2-N1	-2.39	119.61	122.79
1	I	1618	6MZ	C4-C5-N7	-2.34	106.96	109.40
1	I	745	1MG	O6-C6-C5	-2.13	120.43	124.19
1	I	2580	PSU	C6-N1-C2	-2.09	120.54	122.68
1	I	1962	5MC	O2-C2-N3	-2.08	118.94	122.33
1	I	2580	PSU	O4'-C1'-C2'	2.07	108.06	105.14
1	I	2457	PSU	C6-N1-C2	-2.06	120.58	122.68
1	I	2504	PSU	C6-N1-C2	-2.05	120.59	122.68
1	I	955	PSU	C6-N1-C2	-2.03	120.61	122.68
1	I	2605	PSU	C6-N1-C2	-2.02	120.62	122.68

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1618	6MZ	N1-C6-N6-C9
1	I	1915	3TD	C2'-C1'-C5-C4
1	I	1915	3TD	O4'-C1'-C5-C4
1	I	1915	3TD	O4'-C1'-C5-C6
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	2498	OMC	O4'-C4'-C5'-O5'
1	I	2251	OMG	O4'-C4'-C5'-O5'
1	I	2498	OMC	C3'-C4'-C5'-O5'
1	I	2503	2MA	O4'-C4'-C5'-O5'
1	I	2503	2MA	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2445	2MG	O4'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
1	I	1911	PSU	C3'-C4'-C5'-O5'
1	I	2251	OMG	C3'-C4'-C5'-O5'
1	I	1911	PSU	O4'-C4'-C5'-O5'
1	I	747	5MU	C3'-C4'-C5'-O5'
1	I	2069	G7M	O4'-C4'-C5'-O5'
1	I	2552	OMU	C3'-C2'-O2'-CM2
1	I	1618	6MZ	C5-C6-N6-C9
1	I	2552	OMU	C1'-C2'-O2'-CM2
1	I	747	5MU	O4'-C4'-C5'-O5'
1	I	746	PSU	O4'-C1'-C5-C6

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	2503	2MA	1	0
1	I	1911	PSU	4	0
1	I	2445	2MG	1	0
1	I	1962	5MC	1	0
1	I	745	1MG	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
8	O8S	I	3001	-	51,55,55	0.98	1 (1%)	64,77,77	1.00	2 (3%)

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
8	O8S	I	3001	-	-	4/57/73/73	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	3001	O8S	C08-C49	-3.01	1.45	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	3001	O8S	C24-O42-C43	2.33	121.78	117.78
8	I	3001	O8S	C31-N30-C29	2.03	129.70	126.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	3001	O8S	O11-C04-C05-C06
8	I	3001	O8S	C03-C04-C05-C06
8	I	3001	O8S	C20-C21-C22-C23
8	I	3001	O8S	C12-C02-C03-C04

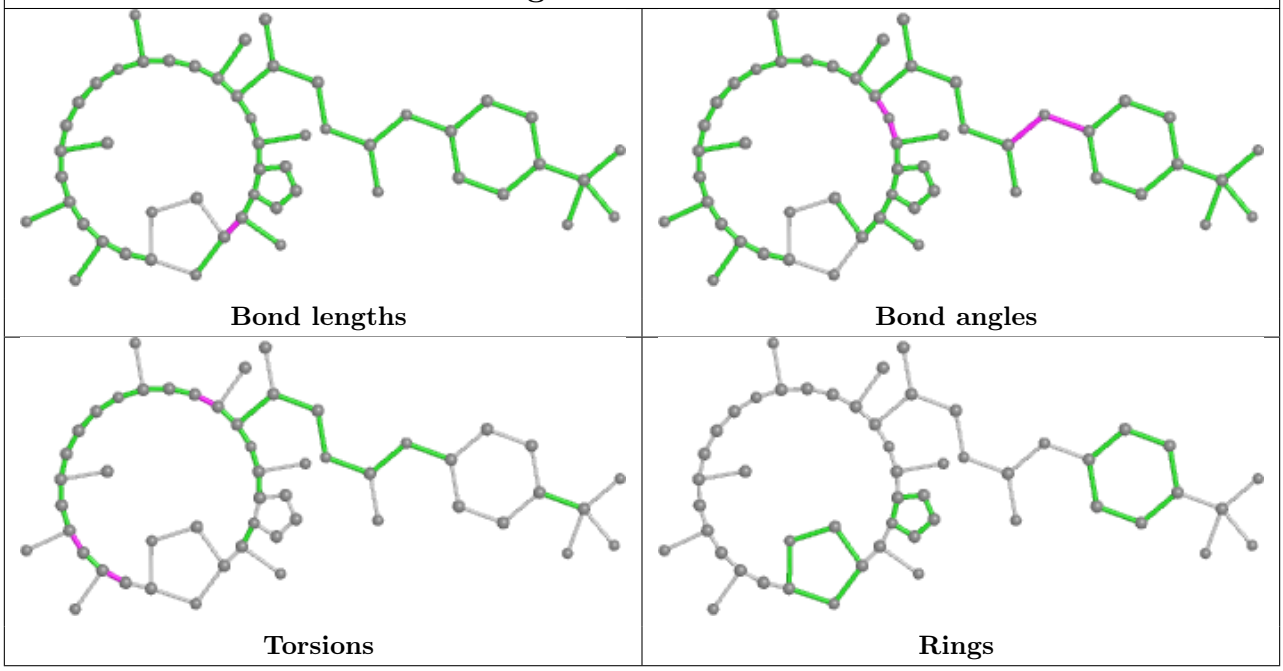
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand O8S I 3001



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.

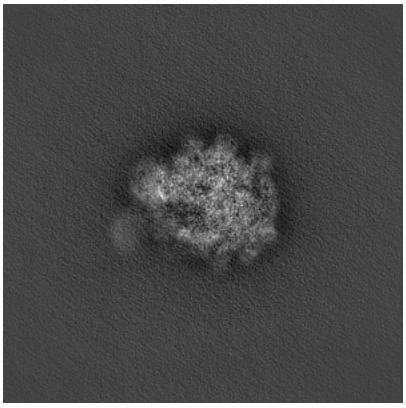
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20306. These allow visual inspection of the internal detail of the map and identification of artifacts.

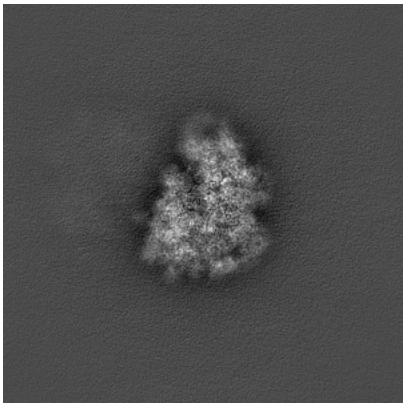
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

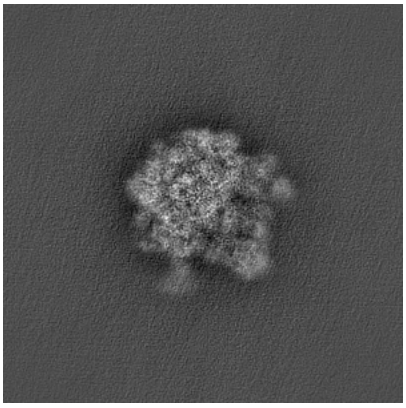
6.1.1 Primary map



X



Y

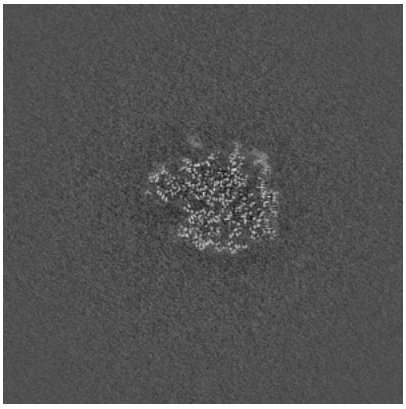


Z

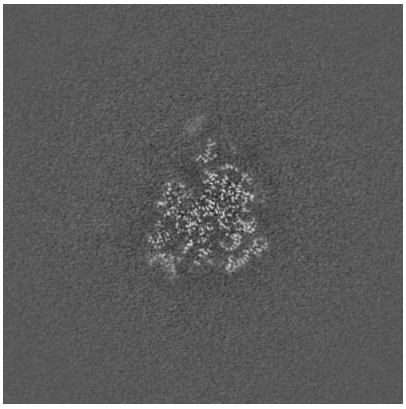
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

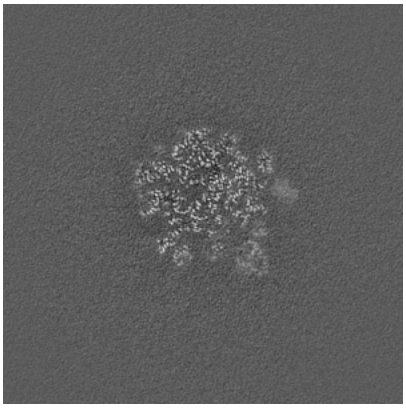
6.2.1 Primary map



X Index: 300



Y Index: 300

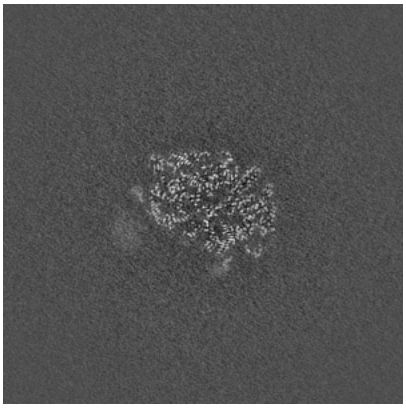


Z Index: 300

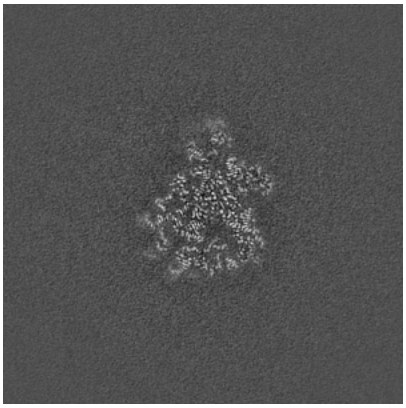
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

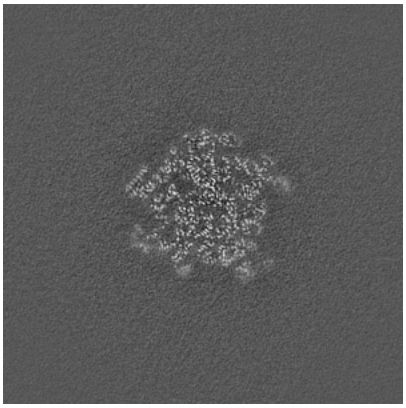
6.3.1 Primary map



X Index: 275



Y Index: 336



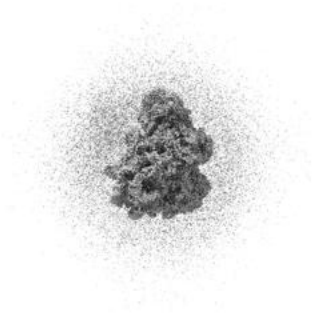
Z Index: 315

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

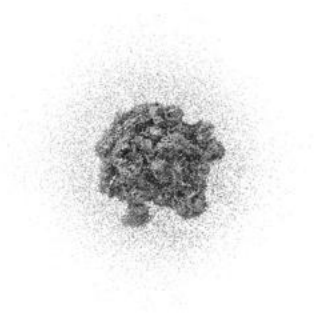
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

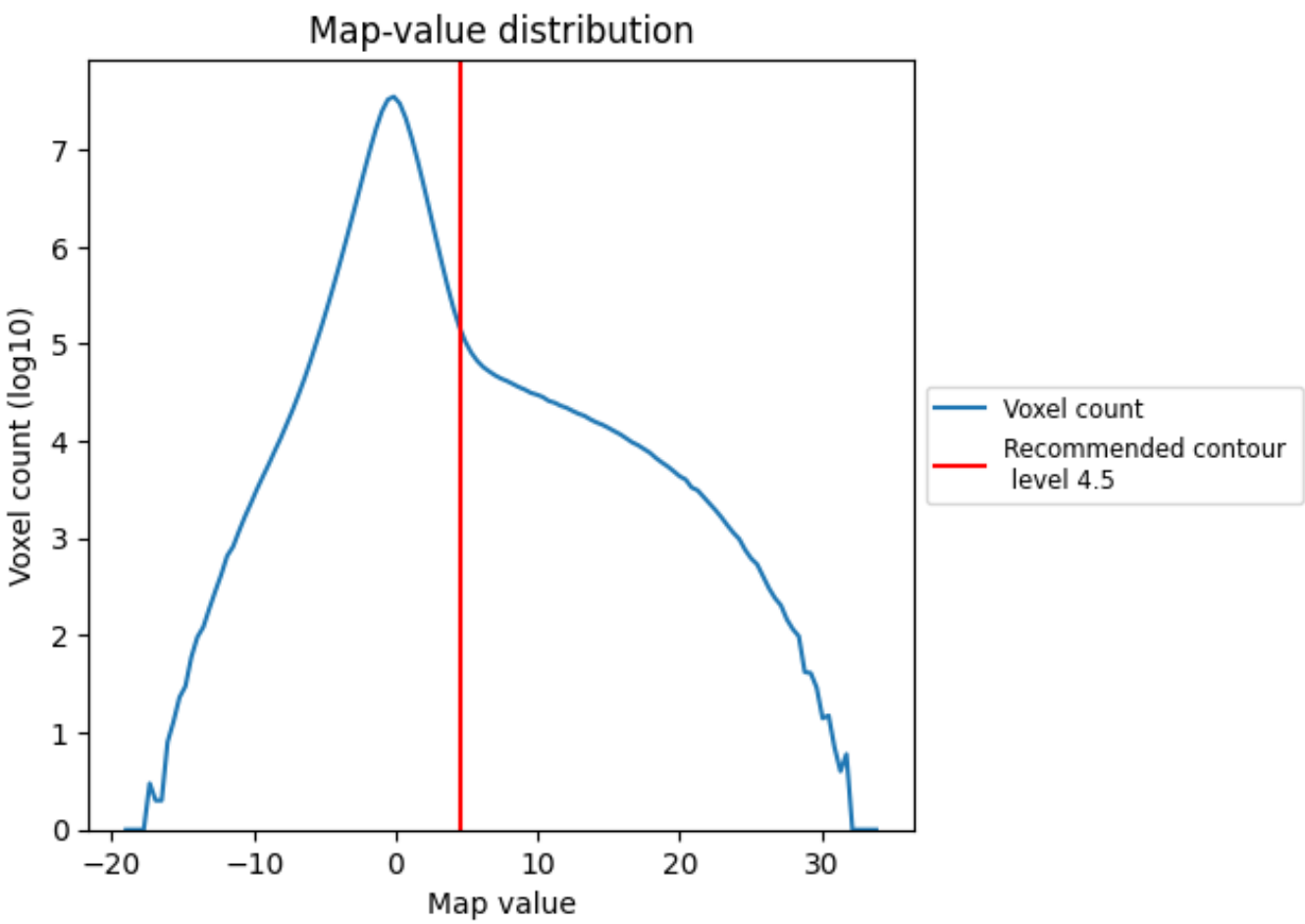
6.5 Mask visualisation (i)

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

7 Map analysis (i)

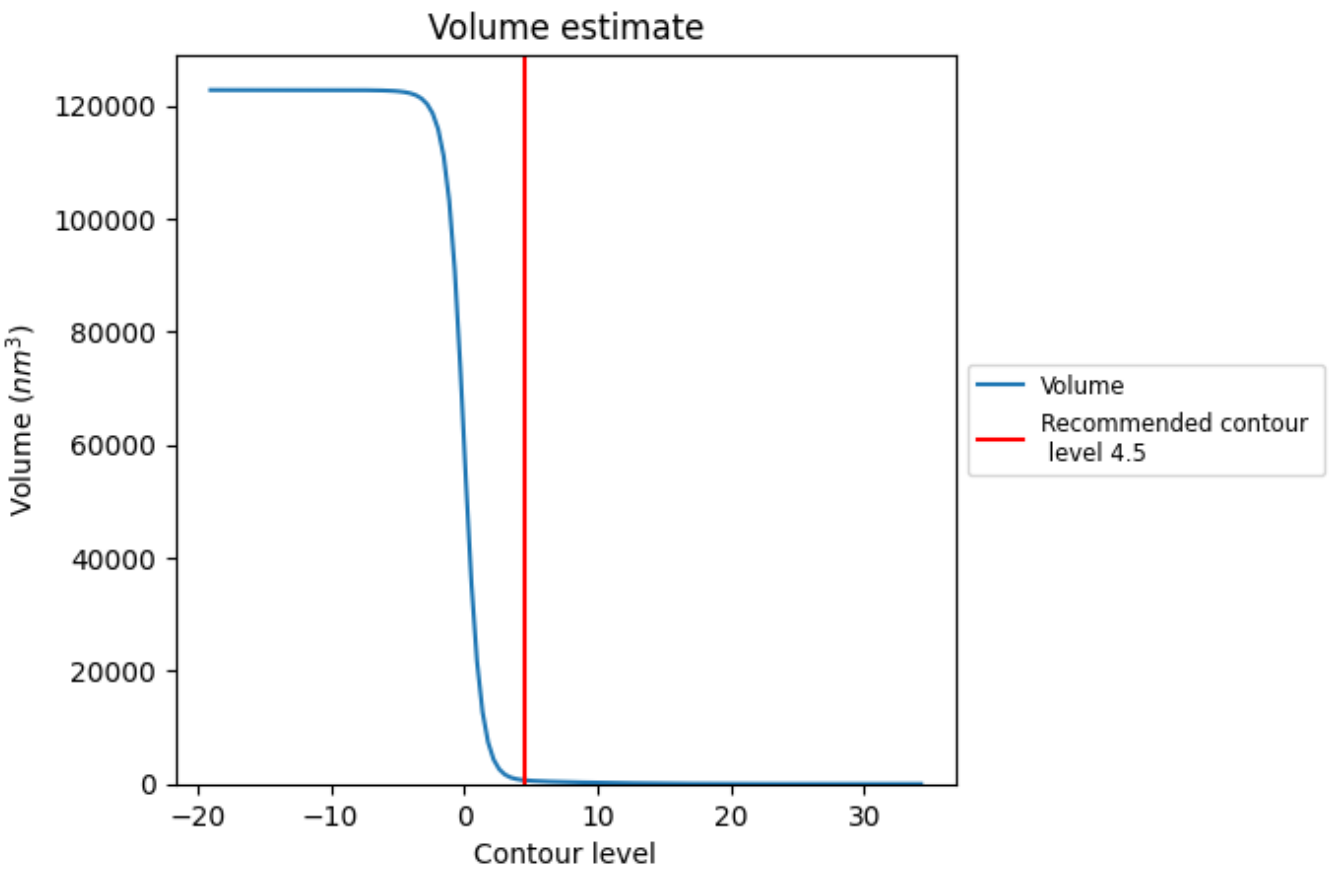
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

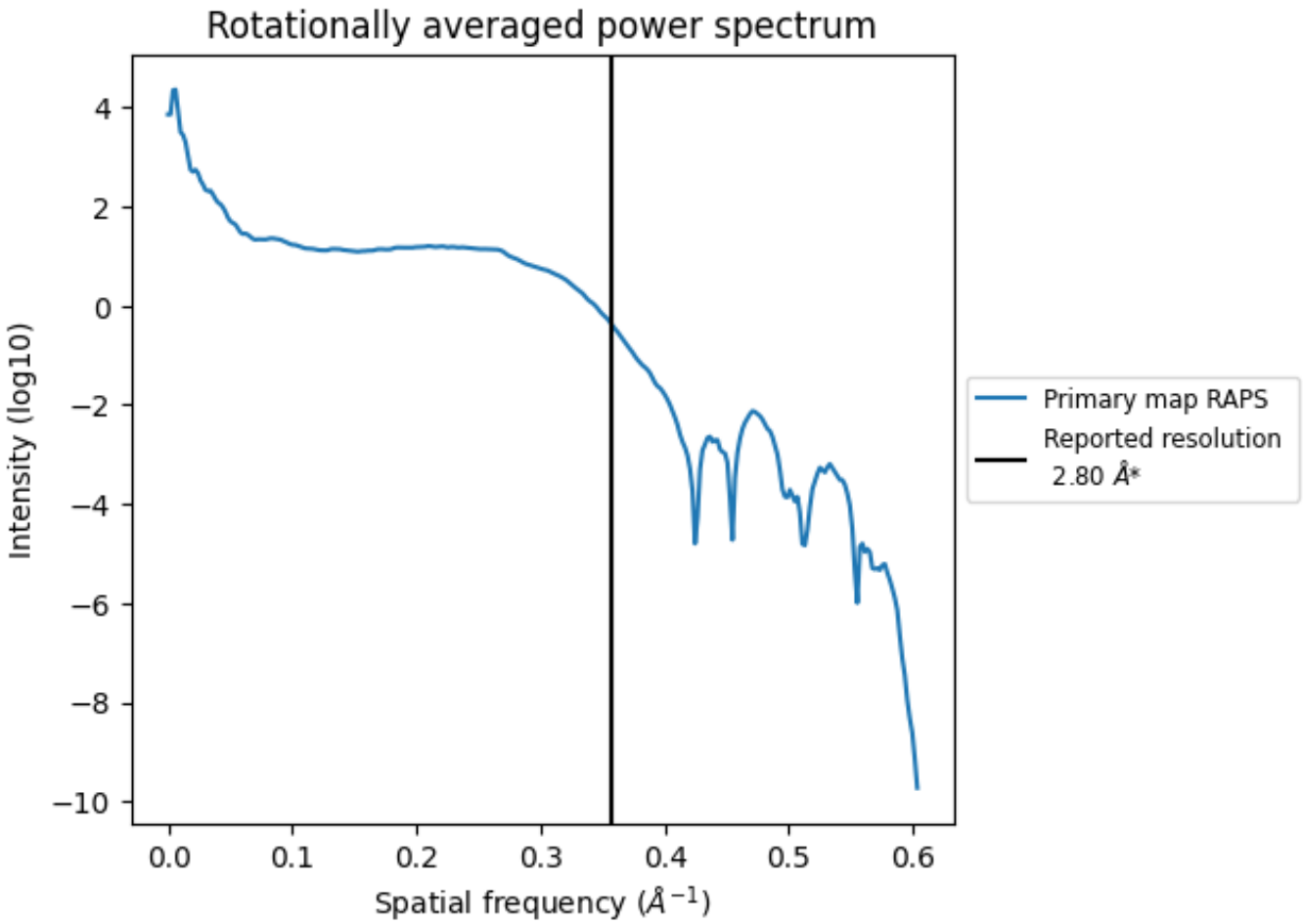
7.2 Volume estimate (i)



The volume at the recommended contour level is 672 nm^3; this corresponds to an approximate mass of 607 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 0.357 Å^{-1}

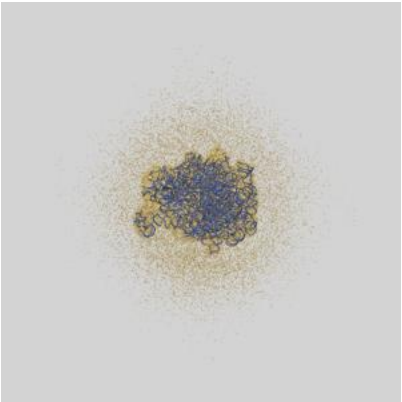
8 Fourier-Shell correlation (i)

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

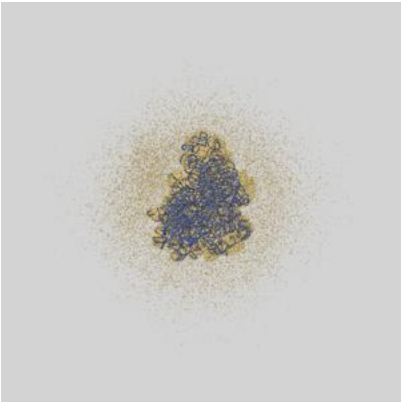
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20306 and PDB model 6PCS. Per-residue inclusion information can be found in section 3 on page 5.

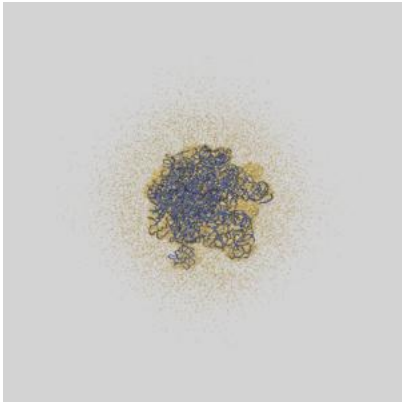
9.1 Map-model overlay (i)



X



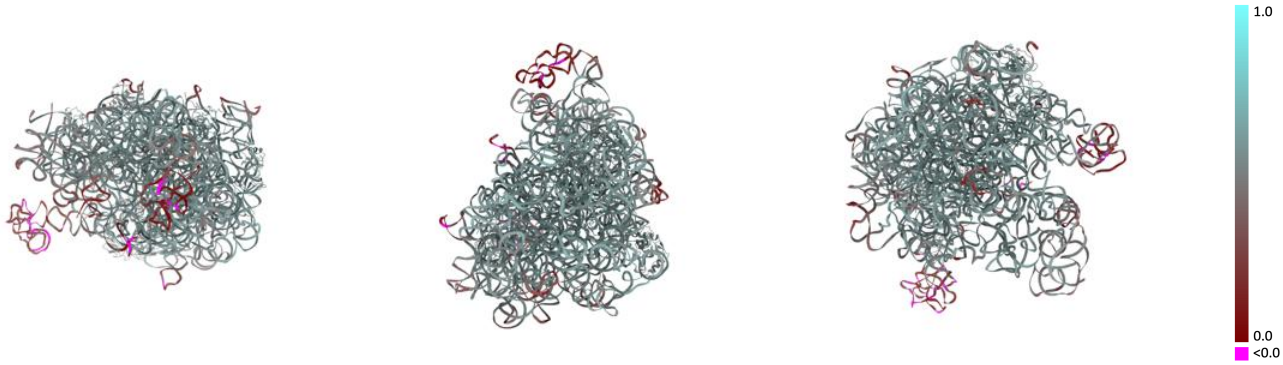
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

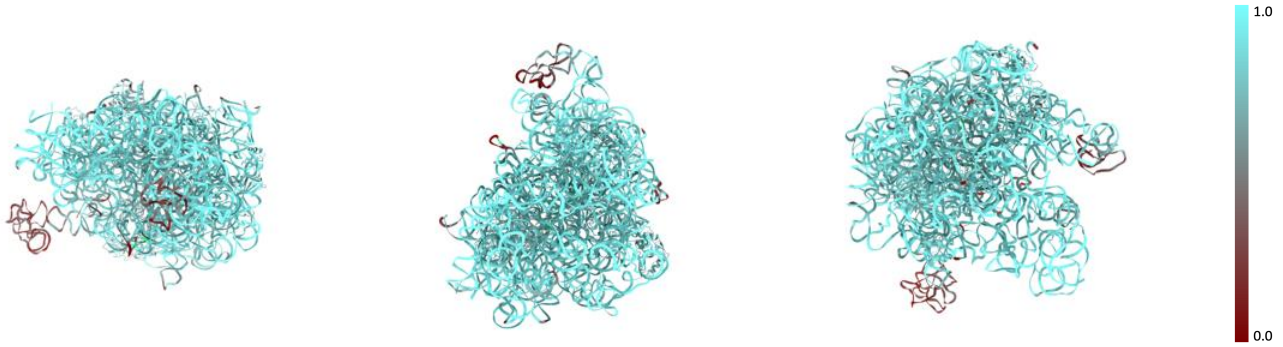
9.2 Q-score mapped to coordinate model (i)



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.

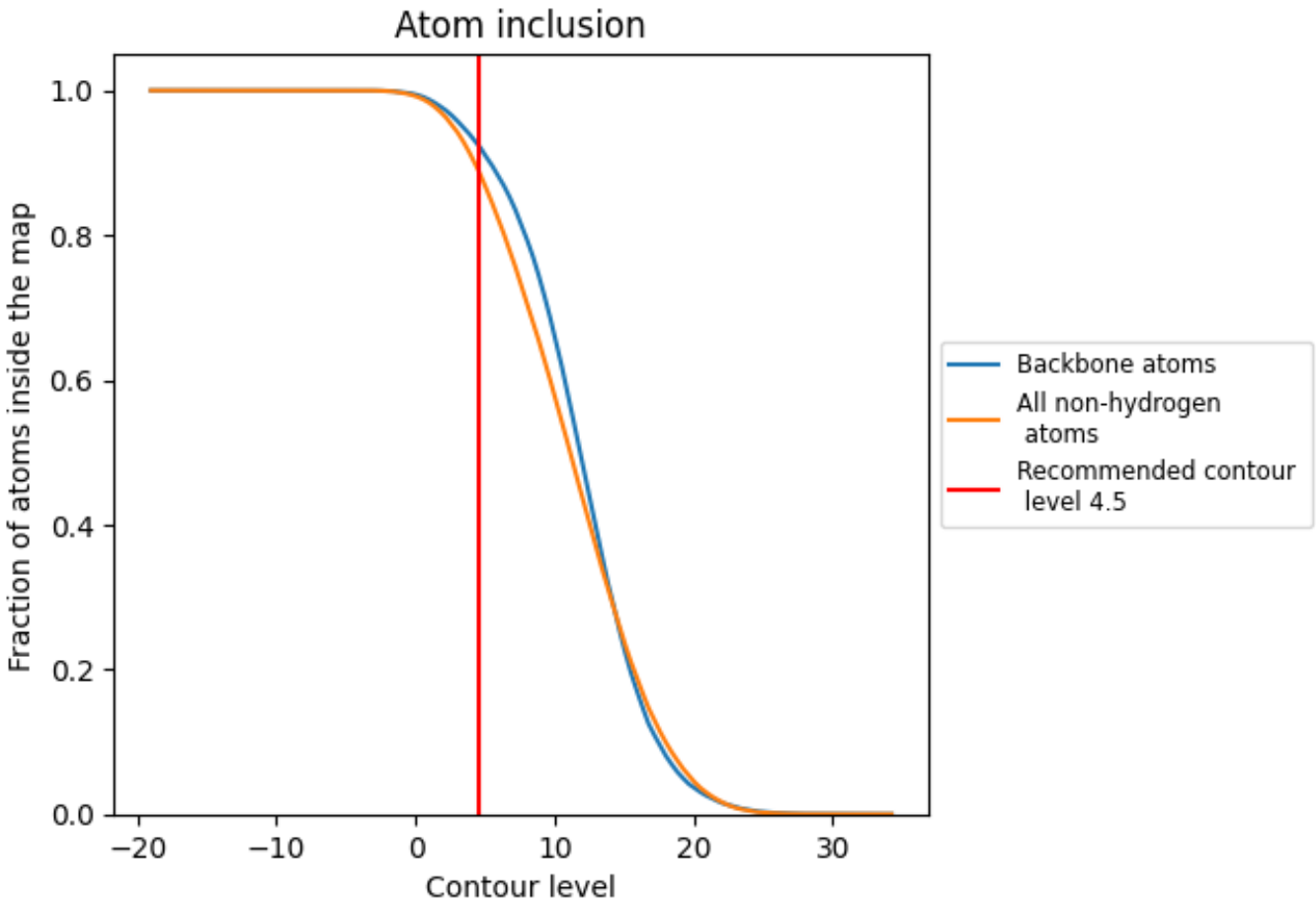
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.5250
I	0.8977	0.5230
J	0.9237	0.5000
K	0.8290	0.5490
L	0.8076	0.5450
M	0.7980	0.5360
N	0.8368	0.5600
O	0.8373	0.5550