



Full wwPDB EM Validation Report ⓘ

Apr 12, 2023 – 02:23 PM EDT

PDB ID : 8CWO
EMDB ID : EMD-27028
Title : Cutibacterium acnes 30S ribosomal subunit with Sarecycline bound, body domain only in the local refined map
Authors : Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on : 2022-05-19
Resolution : 2.84 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:

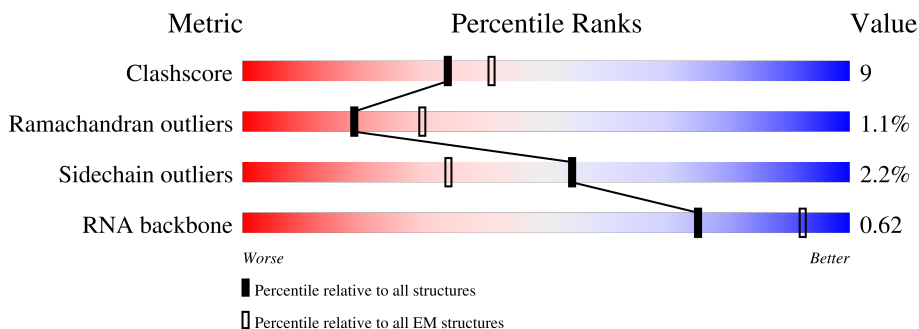
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

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 2.84 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.









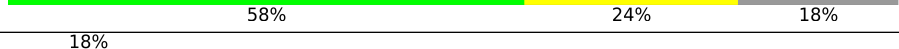
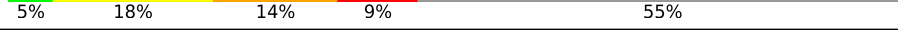
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1537	
2	D	201	
3	E	215	
4	F	96	
5	H	135	
6	K	135	
7	L	123	

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Mol	Chain	Length	Quality of chain
8	O	87	 69% 31%
9	Q	90	 68% 27% 6%
10	R	79	 66% 19% 15%
11	T	88	 84% 15%
12	P	147	 54% 25% 7% 13%
13	X	33	 52% 45% 27%
14	B	283	 58% 24% 18%
15	Y	22	 5% 18% 14% 9% 55%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 34342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1034	22250	9913	4077	7226	1034	0	0

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	200	1632	1021	313	297	1	0	0

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	115	827	507	157	159	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	96	785	496	134	149	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	134	1021	642	182	194	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	117	858	532	168	154	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	122	948	587	195	164	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	87	708	440	140	125	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	90	728	446	142	134	6	0	0

- Molecule 10 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	R	67	527	334	103	90	0	0

- Molecule 11 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	T	87	673	408	144	121	0	0

- Molecule 12 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	128	994	621	185	187	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein bS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	X	32	277	170	71	35	1	0	0

- Molecule 14 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	233	1836	1163	326	338	9	0	0

- Molecule 15 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	Y	10	211	95	35	71	10	0	0


- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

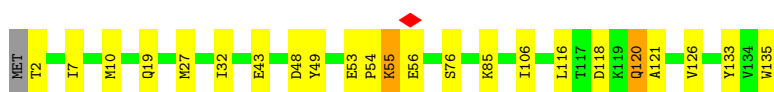
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
16	A	66	66	66	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
17	A	1	1	1	0

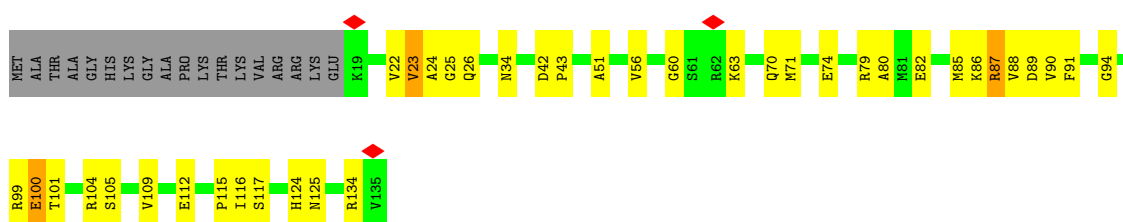
- Molecule 5: 30S ribosomal protein S8

Chain H:  82% 16% ..




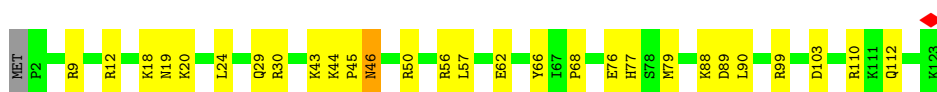
- Molecule 6: 30S ribosomal protein S11

Chain K:  58% 27% 13%



- Molecule 7: 30S ribosomal protein S12

Chain L:  76% 22% ..



- Molecule 8: 30S ribosomal protein S15

Chain O:  69% 31%



- Molecule 9: 30S ribosomal protein S17

Chain Q:  6% 68% 27% ..

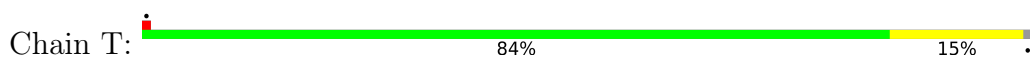


- Molecule 10: 30S ribosomal protein S18

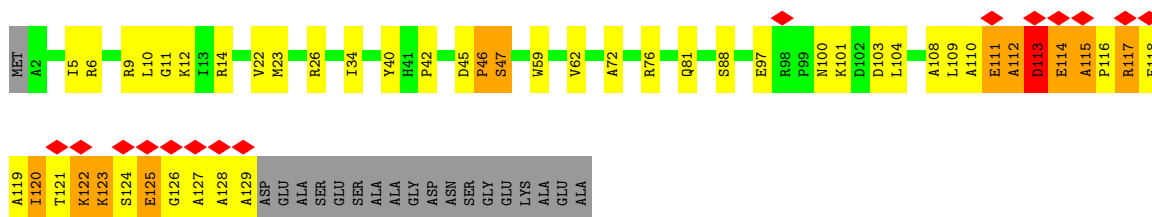
Chain R:  5% 66% 19% 15%



- Molecule 11: 30S ribosomal protein S20



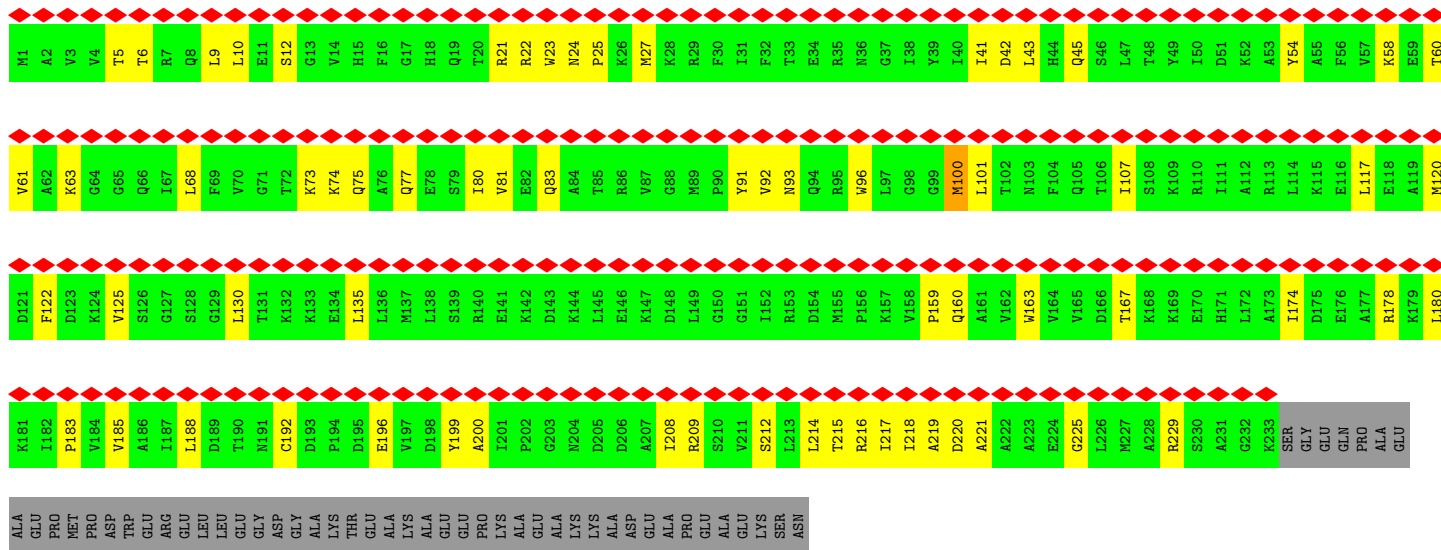
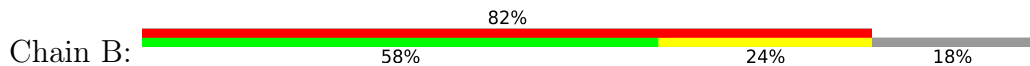
- Molecule 12: 30S ribosomal protein S16



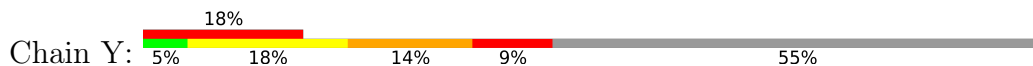
- Molecule 13: 30S ribosomal protein bS22



- Molecule 14: 30S ribosomal protein S2



- Molecule 15: mRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70853	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 ($e^-/\text{\AA}^2$)	30.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.313	Depositor
Minimum map value	-0.485	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.16	Depositor
Map size (\AA)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	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: G7M, 2MG, PSU, 5MC, MG, MA6, UR3, 4OC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/24662	0.72	14/38483 (0.0%)
2	D	0.33	0/1662	0.57	0/2239
3	E	0.33	0/835	0.60	0/1130
4	F	0.29	0/794	0.55	0/1069
5	H	0.31	0/1036	0.52	0/1395
6	K	0.30	0/874	0.59	0/1177
7	L	0.35	0/960	0.61	0/1283
8	O	0.27	0/718	0.56	0/959
9	Q	0.34	0/734	0.60	0/978
10	R	0.28	0/532	0.60	0/713
11	T	0.29	0/676	0.52	0/897
12	P	0.41	0/1013	0.66	0/1370
13	X	0.23	0/277	0.63	0/355
14	B	0.25	0/1864	0.52	0/2509
15	Y	0.53	0/235	1.19	4/363 (1.1%)
All	All	0.41	0/36872	0.69	18/54920 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	U	P-O3'-C3'	-10.51	107.09	119.70
1	A	810	A	P-O3'-C3'	-9.51	108.29	119.70
1	A	432	A	P-O3'-C3'	-9.48	108.32	119.70
15	Y	18	G	P-O3'-C3'	-9.17	108.70	119.70
15	Y	19	U	P-O3'-C3'	-9.07	108.81	119.70
1	A	195	G	P-O3'-C3'	-8.98	108.92	119.70
1	A	196	C	P-O3'-C3'	-8.19	109.87	119.70
1	A	129	U	P-O3'-C3'	-8.12	109.95	119.70
15	Y	20	U	P-O3'-C3'	-7.99	110.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	809	U	P-O3'-C3'	-7.64	110.53	119.70
15	Y	21	U	P-O3'-C3'	-7.36	110.87	119.70
1	A	736	C	C2-N1-C1'	5.82	125.20	118.80
1	A	197	A	P-O3'-C3'	-5.72	112.83	119.70
1	A	130	A	P-O3'-C3'	-5.67	112.89	119.70
1	A	96	G	P-O3'-C3'	-5.61	112.97	119.70
1	A	95	U	P-O3'-C3'	-5.22	113.44	119.70
1	A	194	U	P-O3'-C3'	-5.07	113.62	119.70
1	A	808	C	P-O3'-C3'	-5.02	113.68	119.70

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	A	22250	0	11187	181	0
2	D	1632	0	1663	69	0
3	E	827	0	853	29	0
4	F	785	0	818	33	0
5	H	1021	0	1059	17	0
6	K	858	0	884	31	0
7	L	948	0	1031	26	0
8	O	708	0	737	19	0
9	Q	728	0	772	27	0
10	R	527	0	580	10	0
11	T	673	0	726	12	0
12	P	994	0	1008	80	0
13	X	277	0	338	14	0
14	B	1836	0	1902	47	0
15	Y	211	0	106	9	0
16	A	66	0	0	0	0
17	A	1	0	0	0	0
All	All	34342	0	23664	495	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 9.

All (495) 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)
12:P:114:GLU:HA	12:P:117:ARG:HB2	1.30	1.08
2:D:171:ASN:HB2	12:P:119:ALA:C	1.86	0.96
12:P:45:ASP:HB2	12:P:46:PRO:HD2	1.48	0.94
1:A:1480:A:H4'	15:Y:19:U:H1'	1.52	0.91
2:D:171:ASN:CB	12:P:119:ALA:HB1	2.06	0.85
12:P:108:ALA:HA	12:P:111:GLU:HB2	1.61	0.81
1:A:183:G:H21	1:A:226:G:H4'	1.47	0.79
1:A:824:U:H3	1:A:828:A:H61	1.31	0.77
9:Q:7:GLU:C	9:Q:9:THR:H	1.89	0.76
1:A:646:G:H22	1:A:723:G:H1	1.30	0.76
12:P:122:LYS:HA	12:P:125:GLU:HB2	1.68	0.75
2:D:49:GLN:HB3	2:D:198:LEU:HB2	1.69	0.74
1:A:805:G:HO2'	5:H:2:THR:N	1.86	0.74
12:P:112:ALA:O	12:P:115:ALA:N	2.20	0.73
3:E:171:GLU:HG3	3:E:176:VAL:HG22	1.70	0.73
14:B:23:TRP:HE1	14:B:27:MET:HB2	1.53	0.73
12:P:117:ARG:O	12:P:121:THR:HG23	1.88	0.73
4:F:15:GLU:O	4:F:17:ARG:NH1	2.22	0.72
12:P:116:PRO:HA	12:P:119:ALA:HB3	1.71	0.72
12:P:45:ASP:O	12:P:46:PRO:C	2.28	0.71
1:A:11:G:N7	3:E:120:ARG:NH1	2.38	0.71
12:P:116:PRO:HA	12:P:119:ALA:CB	2.21	0.71
2:D:178:HIS:CE1	12:P:109:LEU:HD11	2.25	0.71
1:A:700:A:C8	6:K:124:HIS:HD2	2.09	0.70
3:E:179:ARG:HG2	5:H:76:SER:HA	1.74	0.69
12:P:115:ALA:HB3	12:P:116:PRO:CD	2.20	0.69
1:A:476:A:H2'	1:A:478:A:H8	1.57	0.69
6:K:94:GLY:O	6:K:99:ARG:NH2	2.23	0.69
12:P:116:PRO:O	12:P:119:ALA:HB3	1.91	0.69
1:A:512:G:C2	15:Y:22:U:H5''	2.27	0.68
3:E:179:ARG:NH2	5:H:135:TRP:OXT	2.26	0.68
6:K:70:GLN:NE2	6:K:74:GLU:OE1	2.27	0.68
14:B:117:LEU:HA	14:B:120:MET:HG3	1.75	0.67
12:P:114:GLU:CA	12:P:117:ARG:HB2	2.18	0.67
8:O:45:LYS:O	8:O:51:ARG:NH2	2.29	0.66
2:D:171:ASN:C	12:P:119:ALA:HB1	2.17	0.65
12:P:125:GLU:O	12:P:129:ALA:N	2.27	0.65
7:L:45:PRO:O	7:L:46:ASN:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:25:GLY:HA2	6:K:43:PRO:HD3	1.78	0.65
2:D:171:ASN:HB2	12:P:119:ALA:HB1	1.77	0.65
2:D:171:ASN:HB2	12:P:119:ALA:O	1.96	0.65
12:P:124:SER:O	12:P:127:ALA:HB3	1.98	0.64
4:F:16:GLU:O	4:F:18:GLN:N	2.30	0.64
3:E:203:ALA:HB1	3:E:207:ARG:NH2	2.12	0.64
2:D:18:ASP:OD1	2:D:24:LYS:NZ	2.27	0.64
9:Q:9:THR:O	9:Q:10:THR:C	2.36	0.64
1:A:657:A:H1'	6:K:124:HIS:ND1	2.12	0.64
14:B:100:MET:HA	14:B:107:ILE:HG13	1.80	0.64
2:D:171:ASN:HB2	12:P:119:ALA:CA	2.28	0.64
1:A:1386:C:H4'	1:A:1387:5MC:H3'	1.80	0.64
3:E:157:ILE:HG22	3:E:161:HIS:CE1	2.33	0.64
8:O:34:ILE:HG23	8:O:54:LEU:HD11	1.80	0.63
12:P:111:GLU:OE2	12:P:114:GLU:HG3	1.97	0.63
1:A:179:G:OP1	11:T:56:ARG:NH2	2.30	0.63
1:A:1500:A:OP2	13:X:18:ARG:NH2	2.30	0.63
11:T:15:GLU:OE2	11:T:19:GLN:NE2	2.31	0.63
12:P:116:PRO:C	12:P:119:ALA:HB3	2.18	0.63
2:D:171:ASN:CG	12:P:119:ALA:HB1	2.19	0.63
12:P:112:ALA:O	12:P:116:PRO:HD2	1.99	0.63
1:A:177:C:H2'	1:A:178:G:H5''	1.80	0.63
1:A:793:U:O2'	1:A:885:A:N1	2.30	0.63
2:D:103:ALA:O	2:D:160:ARG:NH1	2.32	0.63
2:D:171:ASN:HB2	12:P:119:ALA:CB	2.29	0.62
2:D:169:ARG:NH1	12:P:112:ALA:HA	2.14	0.62
4:F:27:LEU:HD11	4:F:40:VAL:HG21	1.82	0.62
14:B:188:LEU:HB2	14:B:192:CYS:HB2	1.81	0.62
1:A:192:G:H21	9:Q:1:MET:H3	1.47	0.62
2:D:171:ASN:OD1	12:P:119:ALA:HB1	1.99	0.62
14:B:125:VAL:HG23	14:B:135:LEU:HD21	1.80	0.61
12:P:111:GLU:O	12:P:112:ALA:C	2.37	0.61
2:D:168:VAL:O	2:D:170:PRO:HD3	2.00	0.61
4:F:68:GLU:HB2	4:F:71:THR:HG23	1.82	0.61
1:A:47:C:OP1	12:P:14:ARG:NH2	2.33	0.61
3:E:193:LEU:HB3	3:E:197:LYS:NZ	2.16	0.61
1:A:75:A:N1	1:A:99:C:O2'	2.31	0.61
3:E:172:GLU:O	3:E:175:GLU:HG2	2.00	0.61
1:A:1428:G:H8	1:A:1447:A:H62	1.47	0.61
1:A:439:U:H5''	2:D:147:LEU:HD22	1.82	0.61
4:F:11:ASP:OD1	4:F:55:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:24:LEU:O	7:L:30:ARG:NH2	2.33	0.61
1:A:406:G:OP2	2:D:110:ARG:NH2	2.34	0.60
3:E:207:ARG:O	3:E:210:GLU:HG2	2.00	0.60
3:E:104:ILE:HD12	3:E:170:LEU:HD11	1.84	0.60
8:O:24:ASP:OD2	8:O:75:HIS:NE2	2.34	0.59
12:P:112:ALA:O	12:P:113:ASP:C	2.40	0.59
1:A:9:U:O2'	1:A:10:G:O5'	2.20	0.59
14:B:185:VAL:HG12	14:B:199:TYR:HB2	1.85	0.59
9:Q:7:GLU:C	9:Q:9:THR:N	2.55	0.59
7:L:43:LYS:HE2	7:L:89:ASP:HA	1.84	0.58
1:A:659:U:H3	1:A:695:G:H22	1.50	0.58
2:D:172:LYS:HB2	12:P:119:ALA:HB2	1.85	0.58
1:A:326:G:N1	1:A:329:A:OP2	2.36	0.58
1:A:1506:MA6:H5'	13:X:12:MET:HE1	1.86	0.58
2:D:182:THR:O	2:D:186:ILE:HD12	2.03	0.58
3:E:209:GLU:O	3:E:210:GLU:C	2.40	0.58
12:P:120:ILE:HA	12:P:123:LYS:HB3	1.85	0.58
14:B:188:LEU:HD21	14:B:200:ALA:HB1	1.86	0.58
1:A:192:G:H1'	9:Q:1:MET:SD	2.44	0.58
2:D:105:THR:HG23	2:D:108:GLN:H	1.67	0.58
14:B:24:ASN:ND2	14:B:192:CYS:O	2.36	0.58
8:O:21:GLY:O	8:O:26:GLN:NE2	2.36	0.58
12:P:116:PRO:CA	12:P:119:ALA:HB3	2.33	0.58
1:A:210:G:OP1	11:T:56:ARG:NH1	2.37	0.58
14:B:80:ILE:O	14:B:83:GLN:NE2	2.36	0.57
1:A:563:G:OP1	8:O:63:ARG:NH1	2.35	0.57
8:O:14:ALA:HB1	8:O:19:ASP:HB3	1.87	0.57
14:B:101:LEU:HB3	14:B:180:LEU:HD21	1.87	0.57
1:A:634:U:O4	1:A:734:G:O2'	2.22	0.57
4:F:26:TYR:OH	4:F:82:ASP:OD2	2.23	0.56
4:F:47:ARG:HA	4:F:57:GLU:HG2	1.88	0.56
1:A:299:G:N2	1:A:302:A:OP2	2.36	0.56
1:A:202:G:H1'	9:Q:1:MET:HG2	1.87	0.56
1:A:10:G:H2'	3:E:147:LEU:HD21	1.87	0.56
1:A:1479:A:H4'	1:A:1480:A:C6	2.41	0.56
14:B:61:VAL:HG11	14:B:225:GLY:HA3	1.87	0.56
9:Q:16:GLU:OE2	9:Q:67:ARG:NH2	2.39	0.56
1:A:12:A:N6	2:D:197:GLU:O	2.38	0.56
1:A:268:G:H3'	9:Q:76:ALA:HB2	1.88	0.56
1:A:257:G:OP1	9:Q:78:LYS:NZ	2.35	0.56
1:A:544:U:H1'	7:L:12:ARG:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:100:ASN:OD1	12:P:101:LYS:N	2.40	0.55
14:B:209:ARG:HA	14:B:212:SER:HB2	1.87	0.55
2:D:171:ASN:CA	12:P:119:ALA:HB1	2.37	0.55
15:Y:21:U:H2'	15:Y:22:U:H4'	1.88	0.55
1:A:505:A:N6	7:L:89:ASP:OD1	2.28	0.55
1:A:751:G:H4'	1:A:1500:A:H4'	1.88	0.55
14:B:92:VAL:HG11	14:B:96:TRP:HD1	1.70	0.55
6:K:91:PHE:HA	6:K:117:SER:HB2	1.89	0.55
10:R:21:VAL:HG21	10:R:54:LYS:HB3	1.88	0.55
10:R:42:ARG:HA	10:R:45:THR:HG22	1.89	0.55
1:A:668:G:N2	1:A:668:G:OP2	2.39	0.54
11:T:32:VAL:HG22	11:T:79:ILE:HD11	1.90	0.54
9:Q:24:MET:HG3	9:Q:27:THR:HB	1.88	0.54
12:P:103:ASP:OD1	12:P:104:LEU:N	2.39	0.54
1:A:54:A:O2'	1:A:362:G:N2	2.40	0.54
1:A:94:G:N2	1:A:97:C:OP2	2.40	0.54
12:P:115:ALA:HB3	12:P:116:PRO:HD2	1.88	0.54
14:B:75:GLN:HG3	14:B:208:ILE:HG13	1.89	0.54
1:A:334:G:H4'	11:T:7:GLN:HG2	1.89	0.54
1:A:845:G:HO2'	1:A:858:G:HO2'	1.54	0.54
5:H:7:ILE:HD11	5:H:32:ILE:HD13	1.88	0.54
1:A:810:A:H61	1:A:842:G:H1'	1.72	0.54
6:K:80:ALA:HB1	6:K:85:MET:HE2	1.90	0.54
2:D:73:GLU:OE2	2:D:131:ARG:NH2	2.35	0.53
11:T:33:ARG:HH11	11:T:33:ARG:HG2	1.73	0.53
3:E:171:GLU:OE2	3:E:175:GLU:HG3	2.07	0.53
12:P:81:GLN:OE1	12:P:81:GLN:N	2.41	0.53
1:A:874:G:OP2	13:X:10:LYS:NZ	2.41	0.53
1:A:1480:A:C4'	15:Y:19:U:H1'	2.33	0.53
2:D:178:HIS:HE1	12:P:109:LEU:HD11	1.70	0.53
7:L:30:ARG:HB3	7:L:57:LEU:HD23	1.90	0.53
1:A:638:G:H4'	8:O:60:GLN:HE22	1.73	0.53
1:A:483:C:H2'	1:A:484:A:C8	2.44	0.53
1:A:643:G:O2'	1:A:819:G:OP1	2.26	0.53
1:A:824:U:H3	1:A:828:A:N6	2.03	0.53
2:D:180:LEU:HD12	2:D:181:PRO:HD2	1.89	0.53
3:E:157:ILE:HG22	3:E:161:HIS:HE1	1.72	0.53
8:O:37:LEU:HB3	8:O:54:LEU:HD13	1.91	0.53
14:B:77:GLN:NE2	14:B:93:ASN:OD1	2.42	0.53
15:Y:13:A:O2'	15:Y:14:A:H8	1.92	0.53
1:A:10:G:H4'	1:A:300:A:H4'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:70:GLN:HG2	6:K:105:SER:OG	2.09	0.52
7:L:50:ARG:NH1	7:L:89:ASP:OD2	2.42	0.52
14:B:163:TRP:HE3	14:B:185:VAL:HG23	1.74	0.52
1:A:32:G:O2'	1:A:298:U:OP1	2.22	0.52
4:F:52:ILE:HD11	10:R:66:ALA:HB2	1.90	0.52
1:A:683:C:OP1	1:A:684:A:O2'	2.20	0.52
1:A:893:A:OP1	7:L:18:LYS:NZ	2.42	0.52
1:A:1422:G:H2'	1:A:1423:C:C6	2.44	0.52
8:O:7:LYS:O	8:O:11:GLU:HG3	2.10	0.52
9:Q:35:ARG:NH1	9:Q:46:THR:OG1	2.42	0.52
1:A:392:U:H2'	1:A:393:G:C8	2.44	0.52
2:D:145:LYS:HD3	12:P:122:LYS:HG3	1.92	0.52
12:P:23:MET:HA	12:P:34:ILE:HD12	1.92	0.52
2:D:108:GLN:O	2:D:112:MET:HG3	2.10	0.51
6:K:99:ARG:HG3	6:K:100:GLU:H	1.73	0.51
1:A:828:A:O3'	10:R:17:HIS:NE2	2.43	0.51
7:L:44:LYS:HA	7:L:45:PRO:C	2.31	0.51
1:A:12:A:C6	2:D:201:LYS:HB3	2.45	0.51
1:A:317:A:N7	1:A:330:U:H5	2.07	0.51
1:A:865:G:P	7:L:9:ARG:HH22	2.34	0.51
4:F:27:LEU:HD22	4:F:37:VAL:HG21	1.91	0.51
8:O:1:MET:N	8:O:5:GLU:OE2	2.31	0.51
2:D:40:ARG:HG3	2:D:42:LYS:NZ	2.25	0.51
13:X:26:ILE:O	13:X:30:ARG:HG2	2.10	0.51
1:A:600:C:O2	12:P:12:LYS:NZ	2.44	0.51
11:T:33:ARG:O	11:T:37:ARG:HG3	2.10	0.51
5:H:10:MET:HG3	5:H:27:MET:SD	2.51	0.51
11:T:43:ASP:OD1	11:T:44:VAL:N	2.43	0.51
3:E:189:PRO:HG2	3:E:192:MET:HB3	1.92	0.50
4:F:79:LEU:HB3	4:F:88:THR:HG21	1.93	0.50
1:A:512:G:HO2'	15:Y:22:U:H6	1.59	0.50
1:A:657:A:H1'	6:K:124:HIS:CE1	2.46	0.50
9:Q:7:GLU:O	9:Q:9:THR:N	2.43	0.50
9:Q:8:ARG:O	9:Q:10:THR:N	2.44	0.50
11:T:15:GLU:O	11:T:19:GLN:HG2	2.12	0.50
1:A:655:G:H5''	4:F:87:ARG:NH1	2.26	0.50
2:D:44:SER:O	2:D:48:LEU:HG	2.11	0.50
2:D:172:LYS:N	12:P:119:ALA:HB1	2.26	0.50
4:F:33:GLU:O	4:F:33:GLU:HG2	2.11	0.50
12:P:40:TYR:CZ	12:P:42:PRO:HB3	2.47	0.50
12:P:59:TRP:HA	12:P:62:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:C:O2'	11:T:84:ASN:ND2	2.38	0.50
1:A:511:G:O6	7:L:46:ASN:HA	2.11	0.50
1:A:415:G:O2'	1:A:430:G:N2	2.44	0.50
1:A:467:G:H4'	1:A:468:U:O5'	2.12	0.50
1:A:382:G:N2	1:A:385:A:OP2	2.36	0.50
1:A:639:G:H4'	8:O:26:GLN:HG2	1.94	0.50
2:D:90:GLU:OE1	2:D:95:ASN:ND2	2.38	0.50
2:D:148:PRO:O	2:D:152:ILE:HG12	2.12	0.50
4:F:48:LEU:HD13	4:F:52:ILE:HD12	1.94	0.50
1:A:1399:C:H2'	1:A:1400:A:C8	2.47	0.49
6:K:89:ASP:OD1	6:K:115:PRO:HD2	2.12	0.49
6:K:101:THR:HG22	6:K:104:ARG:HH22	1.76	0.49
13:X:22:LYS:HZ1	13:X:25:ARG:HH12	1.59	0.49
12:P:110:ALA:O	12:P:111:GLU:C	2.50	0.49
12:P:116:PRO:O	12:P:120:ILE:HG12	2.12	0.49
12:P:125:GLU:O	12:P:128:ALA:N	2.46	0.49
14:B:178:ARG:NH1	14:B:178:ARG:HB2	2.27	0.49
3:E:188:ALA:HB3	3:E:193:LEU:HD21	1.93	0.49
6:K:116:ILE:H	6:K:116:ILE:HD12	1.76	0.49
3:E:122:ALA:HB2	3:E:147:LEU:HD13	1.94	0.49
1:A:410:G:OP1	2:D:105:THR:HG21	2.13	0.49
2:D:15:LEU:HD11	2:D:54:GLN:HB2	1.95	0.49
2:D:171:ASN:CB	12:P:119:ALA:CB	2.83	0.49
14:B:74:LYS:HE2	14:B:77:GLN:HG3	1.93	0.49
12:P:81:GLN:HE21	12:P:88:SER:HB3	1.77	0.48
3:E:172:GLU:O	3:E:176:VAL:HG23	2.13	0.48
3:E:194:ARG:HA	3:E:197:LYS:HE2	1.94	0.48
14:B:68:LEU:HD23	14:B:159:PRO:HB3	1.95	0.48
6:K:105:SER:O	6:K:109:VAL:HG23	2.14	0.48
10:R:73:THR:OG1	10:R:74:ALA:N	2.46	0.48
3:E:157:ILE:CG2	3:E:161:HIS:HE1	2.25	0.48
14:B:41:ILE:HG22	14:B:43:LEU:H	1.78	0.48
1:A:183:G:H2'	1:A:184:G:H2'	1.94	0.48
1:A:438:C:H4'	2:D:148:PRO:HG2	1.96	0.48
2:D:90:GLU:HG3	2:D:186:ILE:HG12	1.95	0.48
1:A:822:C:H2'	1:A:823:A:C8	2.49	0.48
4:F:12:PRO:O	4:F:45:LYS:NZ	2.47	0.48
12:P:122:LYS:HE3	12:P:125:GLU:HG2	1.94	0.48
1:A:201:U:H2'	1:A:202:G:H8	1.78	0.48
13:X:3:SER:C	13:X:5:ILE:H	2.17	0.48
1:A:1391:5MC:O2	1:A:1506:MA6:O2'	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:193:LEU:HB3	3:E:197:LYS:HZ3	1.78	0.48
8:O:74:GLU:O	8:O:78:GLU:HG3	2.14	0.48
1:A:96:G:H2'	1:A:97:C:C6	2.48	0.48
1:A:354:C:O2	1:A:357:C:N4	2.47	0.48
1:A:739:U:H2'	1:A:740:G:O4'	2.14	0.48
1:A:1505:MA6:H8	1:A:1505:MA6:O5'	2.13	0.48
2:D:172:LYS:N	12:P:119:ALA:CB	2.76	0.48
1:A:460:A:C5	1:A:461:G:H1'	2.49	0.47
1:A:521:A:H2'	1:A:522:G:C8	2.49	0.47
1:A:569:G:N1	1:A:736:C:OP2	2.47	0.47
2:D:54:GLN:HE21	2:D:58:TYR:HE2	1.62	0.47
1:A:1479:A:H4'	1:A:1480:A:C5	2.49	0.47
7:L:44:LYS:HA	7:L:45:PRO:O	2.14	0.47
1:A:519:G:H5''	7:L:110:ARG:NH1	2.30	0.47
2:D:94:ASP:OD1	2:D:95:ASN:N	2.46	0.47
14:B:9:LEU:HD13	14:B:43:LEU:HD22	1.95	0.47
4:F:14:VAL:HG11	4:F:19:VAL:HB	1.96	0.47
4:F:74:GLU:HA	4:F:77:ARG:HG2	1.97	0.47
7:L:56:ARG:CZ	7:L:62:GLU:HB2	2.44	0.47
1:A:38:C:O4'	7:L:29:GLN:NE2	2.48	0.47
1:A:69:A:C2	1:A:220:G:H8	2.33	0.47
2:D:171:ASN:OD1	12:P:119:ALA:CB	2.63	0.47
6:K:42:ASP:OD1	6:K:43:PRO:HD2	2.15	0.47
6:K:51:ALA:HB2	6:K:79:ARG:HH22	1.79	0.47
10:R:29:LEU:HD22	10:R:59:ILE:HG13	1.97	0.47
6:K:87:ARG:HB2	6:K:112:GLU:HB2	1.97	0.47
12:P:42:PRO:HA	12:P:47:SER:HB2	1.97	0.47
14:B:5:THR:OG1	14:B:6:THR:N	2.48	0.47
1:A:699:C:H4'	6:K:125:ASN:OD1	2.15	0.47
1:A:865:G:OP2	7:L:9:ARG:NH2	2.48	0.47
2:D:171:ASN:C	12:P:119:ALA:CB	2.82	0.47
1:A:561:U:H2'	1:A:562:C:C6	2.50	0.46
4:F:14:VAL:HG13	4:F:18:GLN:HG2	1.97	0.46
9:Q:12:ARG:HD3	9:Q:70:GLU:O	2.16	0.46
4:F:9:ILE:HG12	4:F:60:TYR:CE1	2.50	0.46
1:A:111:G:HO2'	1:A:391:A:HO2'	1.61	0.46
1:A:463:G:O2'	1:A:465:C:N4	2.45	0.46
1:A:527:C:H5'	2:D:64:GLU:HB2	1.96	0.46
4:F:9:ILE:HD11	10:R:65:LEU:HD12	1.97	0.46
1:A:721:C:P	4:F:2:ARG:HH22	2.38	0.46
2:D:40:ARG:HG3	2:D:42:LYS:HZ1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:17:ARG:HG2	4:F:18:GLN:N	2.31	0.46
1:A:157:C:H2'	1:A:158:A:H8	1.79	0.46
1:A:882:G:N2	1:A:885:A:OP2	2.44	0.46
3:E:187:ILE:HG13	3:E:188:ALA:N	2.30	0.46
14:B:130:LEU:HD23	14:B:135:LEU:HB2	1.97	0.46
1:A:161:A:H1'	1:A:346:A:N7	2.31	0.46
12:P:9:ARG:O	12:P:10:LEU:HD23	2.16	0.46
12:P:126:GLY:HA2	12:P:129:ALA:HB3	1.97	0.46
14:B:216:ARG:NH1	14:B:220:ASP:OD2	2.39	0.46
1:A:129:U:H4'	1:A:131:A:OP1	2.15	0.46
1:A:378:G:H5''	12:P:6:ARG:HB2	1.97	0.46
1:A:454:A:O3'	12:P:76:ARG:NH2	2.48	0.46
1:A:765:C:H2'	1:A:766:A:C8	2.51	0.46
2:D:163:PRO:HB2	2:D:165:TRP:CD1	2.51	0.46
4:F:39:ASN:OD1	4:F:40:VAL:N	2.49	0.46
12:P:117:ARG:HD3	12:P:117:ARG:HA	1.32	0.46
1:A:1518:A:H2'	1:A:1519:U:C6	2.51	0.46
2:D:14:ARG:HA	2:D:32:PRO:HB3	1.97	0.46
1:A:296:C:OP1	1:A:592:U:O2'	2.24	0.46
1:A:606:C:O3'	12:P:11:GLY:HA2	2.16	0.46
1:A:1503:2MG:HM21	1:A:1506:MA6:N7	2.31	0.45
4:F:26:TYR:O	4:F:29:VAL:HG12	2.16	0.45
4:F:30:ILE:HD11	4:F:75:LEU:HD22	1.98	0.45
12:P:115:ALA:CB	12:P:116:PRO:CD	2.91	0.45
1:A:109:A:C6	1:A:328:G:C6	3.04	0.45
1:A:1400:A:H2	1:A:1474:G:H22	1.63	0.45
1:A:1441:U:H2'	1:A:1442:G:C8	2.51	0.45
3:E:200:ASP:O	3:E:203:ALA:HB3	2.16	0.45
5:H:53:GLU:HG2	5:H:54:PRO:HD2	1.99	0.45
14:B:73:LYS:O	14:B:77:GLN:HG2	2.16	0.45
4:F:20:ASP:O	4:F:24:GLU:HG3	2.17	0.45
1:A:66:U:O2'	1:A:381:C:O2	2.31	0.45
1:A:505:A:C2	7:L:88:LYS:HB3	2.52	0.45
2:D:4:TYR:HE2	2:D:11:LYS:HG3	1.79	0.45
4:F:9:ILE:HG22	4:F:86:MET:HE3	1.99	0.45
6:K:51:ALA:HB2	6:K:79:ARG:NH2	2.31	0.45
2:D:191:ASN:OD1	2:D:194:ALA:N	2.40	0.45
5:H:43:GLU:HG3	5:H:106:ILE:HD13	1.98	0.45
3:E:118:MET:O	3:E:148:ALA:HA	2.17	0.45
14:B:100:MET:HG2	14:B:107:ILE:HG13	1.97	0.45
1:A:403:C:O2'	1:A:603:A:N3	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:H4'	13:X:12:MET:HE2	1.98	0.45
15:Y:19:U:H4'	15:Y:19:U:OP1	2.16	0.45
1:A:256:G:O2'	9:Q:25:ASN:O	2.35	0.45
1:A:378:G:O3'	12:P:6:ARG:NH1	2.49	0.45
7:L:19:ASN:OD1	7:L:20:LYS:N	2.49	0.45
12:P:115:ALA:HB3	12:P:116:PRO:HD3	1.96	0.45
7:L:90:LEU:HD23	7:L:90:LEU:HA	1.83	0.45
12:P:5:ILE:HG12	12:P:22:VAL:HG22	1.99	0.45
1:A:90:U:O2'	1:A:91:G:O5'	2.28	0.44
1:A:78:G:H2'	1:A:79:C:C6	2.51	0.44
2:D:168:VAL:C	2:D:170:PRO:HD3	2.37	0.44
1:A:96:G:H2'	1:A:97:C:H6	1.83	0.44
1:A:718:U:H2'	1:A:719:C:C6	2.52	0.44
14:B:130:LEU:HD23	14:B:135:LEU:HD13	1.99	0.44
1:A:692:G:H5''	4:F:54:LYS:NZ	2.32	0.44
1:A:806:U:H2'	1:A:807:A:C8	2.52	0.44
1:A:1418:C:H2'	1:A:1419:G:O4'	2.16	0.44
2:D:145:LYS:HB3	12:P:122:LYS:HD2	1.98	0.44
2:D:171:ASN:O	12:P:119:ALA:HA	2.18	0.44
5:H:121:ALA:HB1	5:H:126:VAL:O	2.16	0.44
1:A:157:C:H2'	1:A:158:A:C8	2.52	0.44
7:L:110:ARG:NH2	7:L:112:GLN:O	2.51	0.44
14:B:174:ILE:HG21	14:B:196:GLU:HB3	1.98	0.44
1:A:25:G:H2'	1:A:26:G:C8	2.53	0.44
9:Q:1:MET:HB2	9:Q:2:SER:H	1.52	0.44
1:A:816:G:H5''	10:R:49:VAL:HG21	1.99	0.44
2:D:42:LYS:HD3	2:D:42:LYS:HA	1.77	0.44
6:K:26:GLN:HA	6:K:88:VAL:HG13	2.00	0.44
12:P:117:ARG:O	12:P:120:ILE:HG13	2.17	0.44
12:P:123:LYS:HG3	12:P:124:SER:N	2.31	0.44
1:A:798:A:OP1	1:A:1513:G:O2'	2.27	0.44
1:A:831:G:H5'	1:A:832:G:OP2	2.18	0.44
14:B:75:GLN:HA	14:B:208:ILE:HG13	2.00	0.44
14:B:215:THR:HA	14:B:218:ILE:HG12	1.99	0.44
1:A:1497:C:OP1	13:X:11:ARG:HB2	2.18	0.44
9:Q:23:LYS:HB3	9:Q:23:LYS:HE3	1.70	0.44
9:Q:88:LYS:HG3	9:Q:90:LYS:HG3	1.99	0.44
14:B:54:TYR:O	14:B:58:LYS:HG2	2.18	0.44
1:A:392:U:H2'	1:A:393:G:H8	1.83	0.43
1:A:407:U:O4	2:D:2:ALA:N	2.51	0.43
1:A:813:U:H5''	14:B:21:ARG:HD2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:68:ILE:HG22	8:O:76:TYR:HB2	1.99	0.43
1:A:278:G:OP1	9:Q:21:SER:OG	2.29	0.43
1:A:528:G:H4'	1:A:530:G:O3'	2.19	0.43
1:A:845:G:H4'	5:H:19:GLN:NE2	2.33	0.43
1:A:455:G:N2	1:A:455:G:OP2	2.50	0.43
1:A:563:G:N1	1:A:741:A:OP2	2.39	0.43
1:A:700:A:C5	6:K:124:HIS:CD2	3.05	0.43
5:H:55:LYS:NZ	5:H:56:GLU:OE2	2.37	0.43
1:A:1509:U:OP1	6:K:134:ARG:NH1	2.51	0.43
9:Q:6:ALA:C	9:Q:8:ARG:H	2.22	0.43
1:A:77:G:H1	1:A:97:C:H42	1.65	0.43
1:A:406:G:N7	2:D:2:ALA:HB3	2.33	0.43
1:A:512:G:C4	15:Y:22:U:H3'	2.53	0.43
2:D:54:GLN:NE2	2:D:58:TYR:HE2	2.15	0.43
14:B:12:SER:HB2	14:B:209:ARG:HE	1.83	0.43
14:B:77:GLN:O	14:B:93:ASN:ND2	2.41	0.43
1:A:721:C:O2'	8:O:40:HIS:ND1	2.35	0.43
14:B:60:THR:HA	14:B:63:LYS:HE2	1.99	0.43
14:B:167:THR:OG1	14:B:174:ILE:HD12	2.19	0.43
1:A:90:U:H4'	1:A:91:G:OP1	2.19	0.43
2:D:169:ARG:HH11	12:P:115:ALA:HB3	1.83	0.43
9:Q:6:ALA:O	9:Q:8:ARG:N	2.46	0.43
12:P:117:ARG:C	12:P:119:ALA:N	2.72	0.43
2:D:182:THR:OG1	2:D:184:ASP:OD2	2.30	0.43
3:E:171:GLU:HG2	3:E:179:ARG:NH1	2.33	0.43
5:H:48:ASP:OD2	5:H:49:TYR:N	2.45	0.43
6:K:79:ARG:HA	6:K:82:GLU:CD	2.39	0.43
7:L:68:PRO:O	7:L:99:ARG:NH1	2.52	0.43
2:D:99:ARG:NH2	2:D:106:ARG:HH22	2.17	0.43
3:E:180:ARG:NH2	5:H:43:GLU:OE1	2.52	0.43
4:F:23:MET:SD	4:F:61:VAL:HG11	2.59	0.43
12:P:109:LEU:HD23	12:P:109:LEU:HA	1.85	0.43
1:A:500:C:O2'	1:A:512:G:N2	2.52	0.42
1:A:504:C:OP2	7:L:66:TYR:OH	2.30	0.42
1:A:528:G:O2'	1:A:530:G:O2'	2.32	0.42
11:T:33:ARG:HG2	11:T:33:ARG:NH1	2.33	0.42
14:B:42:ASP:OD1	14:B:45:GLN:NE2	2.45	0.42
14:B:58:LYS:NZ	14:B:221:ALA:O	2.30	0.42
2:D:20:VAL:HG21	2:D:105:THR:OG1	2.18	0.42
9:Q:8:ARG:HG3	9:Q:10:THR:OG1	2.19	0.42
12:P:45:ASP:HB2	12:P:46:PRO:CD	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:U:H2'	1:A:730:U:O4'	2.19	0.42
6:K:90:VAL:HG13	6:K:116:ILE:HA	2.00	0.42
7:L:79:MET:N	7:L:103:ASP:OD2	2.48	0.42
4:F:67:CYS:SG	4:F:71:THR:OG1	2.78	0.42
12:P:122:LYS:CE	12:P:125:GLU:HG2	2.50	0.42
1:A:673:G:OP2	6:K:34:ASN:ND2	2.52	0.42
1:A:861:C:OP1	5:H:85:LYS:HE2	2.19	0.42
5:H:118:ASP:OD2	5:H:118:ASP:N	2.52	0.42
15:Y:22:U:H6	15:Y:22:U:H2'	1.72	0.42
1:A:639:G:H21	8:O:20:THR:HG23	1.85	0.42
1:A:874:G:O2'	1:A:890:A:N6	2.52	0.42
7:L:43:LYS:O	7:L:45:PRO:O	2.38	0.42
1:A:1516:G:N7	13:X:7:LYS:HE3	2.34	0.42
8:O:30:LEU:O	8:O:34:ILE:HG13	2.20	0.42
14:B:160:GLN:O	14:B:183:PRO:HG2	2.19	0.42
1:A:405:C:H5''	2:D:128:PRO:HD2	2.00	0.42
1:A:810:A:N3	14:B:25:PRO:HG2	2.34	0.42
1:A:868:U:H4'	1:A:869:G:H5''	2.02	0.42
1:A:700:A:C4	6:K:124:HIS:CD2	3.07	0.42
1:A:737:G:OP2	8:O:63:ARG:HD2	2.20	0.42
1:A:765:C:H2'	1:A:766:A:H8	1.84	0.42
1:A:92:G:O2'	1:A:93:G:H5'	2.19	0.42
3:E:104:ILE:O	3:E:121:PRO:HB3	2.20	0.42
6:K:23:VAL:O	6:K:86:LYS:N	2.51	0.42
6:K:56:VAL:HG23	6:K:56:VAL:O	2.20	0.42
13:X:16:LYS:HA	13:X:16:LYS:HD2	1.86	0.42
1:A:421:C:OP1	1:A:495:A:O2'	2.33	0.41
6:K:60:GLY:O	6:K:63:LYS:HG2	2.19	0.41
10:R:23:TYR:HE2	10:R:65:LEU:HD23	1.85	0.41
14:B:6:THR:HG22	14:B:10:LEU:HG	2.02	0.41
14:B:83:GLN:OE1	14:B:219:ALA:HB2	2.19	0.41
1:A:403:C:H5''	2:D:69:ARG:HD2	2.02	0.41
4:F:8:ILE:HG22	4:F:10:ILE:HG13	2.01	0.41
5:H:133:TYR:O	5:H:135:TRP:HE3	2.03	0.41
1:A:161:A:H2'	1:A:162:A:O4'	2.20	0.41
1:A:201:U:H4'	9:Q:4:ASN:ND2	2.35	0.41
2:D:91:SER:HB3	2:D:180:LEU:HD11	2.02	0.41
2:D:169:ARG:NH2	12:P:109:LEU:O	2.52	0.41
3:E:100:VAL:HG21	3:E:192:MET:HG3	2.01	0.41
12:P:45:ASP:O	12:P:47:SER:N	2.52	0.41
1:A:123:C:OP1	1:A:313:C:O2'	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:U:H2'	1:A:429:U:C6	2.56	0.41
5:H:116:LEU:HD22	5:H:120:GLN:HB3	2.01	0.41
11:T:31:TYR:CE2	11:T:57:GLN:HG3	2.56	0.41
1:A:246:U:O4	1:A:890:A:H1'	2.20	0.41
1:A:695:G:H2'	1:A:696:G:C8	2.55	0.41
2:D:148:PRO:HA	2:D:151:VAL:HG22	2.02	0.41
4:F:14:VAL:CG2	4:F:84:LYS:HE3	2.51	0.41
4:F:69:PRO:HA	4:F:72:ILE:HG22	2.03	0.41
14:B:229:ARG:HE	14:B:229:ARG:HB3	1.72	0.41
1:A:406:G:O2'	1:A:480:A:N1	2.43	0.41
9:Q:9:THR:OG1	9:Q:10:THR:N	2.52	0.41
13:X:22:LYS:NZ	13:X:25:ARG:HH12	2.19	0.41
14:B:81:VAL:HG23	14:B:91:TYR:CE2	2.55	0.41
14:B:122:PHE:HA	14:B:125:VAL:HG12	2.03	0.41
1:A:478:A:H2	1:A:480:A:H62	1.66	0.41
1:A:485:C:O2'	1:A:492:A:N1	2.41	0.41
1:A:537:C:H2'	1:A:538:C:C6	2.56	0.41
1:A:729:U:C4	1:A:730:U:C5	3.09	0.41
1:A:845:G:H4'	5:H:19:GLN:HE22	1.85	0.41
1:A:1503:2MG:HM21	1:A:1506:MA6:C8	2.50	0.41
2:D:171:ASN:CG	12:P:119:ALA:CB	2.88	0.41
8:O:81:ALA:HA	8:O:85:LEU:HD12	2.03	0.41
14:B:54:TYR:CE2	14:B:221:ALA:HB2	2.56	0.41
2:D:174:ARG:HD3	2:D:176:LEU:HD21	2.03	0.41
9:Q:15:ARG:HD2	9:Q:32:VAL:HG11	2.02	0.41
12:P:72:ALA:O	12:P:76:ARG:HD3	2.21	0.41
1:A:546:U:P	7:L:12:ARG:HH21	2.44	0.40
9:Q:21:SER:HB3	9:Q:29:THR:HB	2.03	0.40
12:P:108:ALA:HA	12:P:111:GLU:CB	2.43	0.40
1:A:91:G:O2'	1:A:92:G:H8	2.04	0.40
1:A:1392:G:H4'	13:X:12:MET:CE	2.52	0.40
2:D:52:GLU:OE1	2:D:191:ASN:N	2.54	0.40
6:K:22:VAL:O	6:K:24:ALA:N	2.54	0.40
8:O:37:LEU:HD23	8:O:54:LEU:HB2	2.03	0.40
9:Q:44:VAL:O	9:Q:44:VAL:HG13	2.21	0.40
13:X:18:ARG:O	13:X:22:LYS:HG2	2.22	0.40
14:B:214:LEU:HA	14:B:217:ILE:HG12	2.03	0.40
1:A:91:G:O2'	1:A:92:G:H5'	2.21	0.40
1:A:545:A:O2'	1:A:548:G:O3'	2.38	0.40
1:A:619:U:H2'	1:A:620:C:C6	2.56	0.40
10:R:22:ASP:O	10:R:25:ASP:N	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:TYR:HA	2:D:32:PRO:HD3	1.96	0.40
3:E:157:ILE:CG2	3:E:161:HIS:CE1	3.01	0.40
7:L:76:GLU:HB3	7:L:77:HIS:ND1	2.36	0.40
13:X:20:LEU:O	13:X:24:THR:OG1	2.35	0.40
4:F:27:LEU:HD22	4:F:37:VAL:HG11	2.04	0.40
6:K:71:MET:O	6:K:74:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	198/201 (98%)	187 (94%)	10 (5%)	1 (0%)	29	51
3	E	113/215 (53%)	107 (95%)	6 (5%)	0	100	100
4	F	94/96 (98%)	91 (97%)	2 (2%)	1 (1%)	14	30
5	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
6	K	115/135 (85%)	99 (86%)	15 (13%)	1 (1%)	17	34
7	L	120/123 (98%)	110 (92%)	9 (8%)	1 (1%)	19	38
8	O	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
9	Q	88/90 (98%)	79 (90%)	5 (6%)	4 (4%)	2	4
10	R	65/79 (82%)	58 (89%)	7 (11%)	0	100	100
11	T	85/88 (97%)	85 (100%)	0	0	100	100
12	P	126/147 (86%)	111 (88%)	9 (7%)	6 (5%)	2	4
13	X	30/33 (91%)	29 (97%)	0	1 (3%)	4	8
14	B	231/283 (82%)	214 (93%)	16 (7%)	1 (0%)	34	56
All	All	1482/1712 (87%)	1377 (93%)	89 (6%)	16 (1%)	18	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	17	ARG
12	P	46	PRO
12	P	47	SER
13	X	4	VAL
9	Q	10	THR
12	P	97	GLU
12	P	112	ALA
12	P	113	ASP
9	Q	5	THR
9	Q	9	THR
7	L	46	ASN
9	Q	8	ARG
14	B	100	MET
12	P	115	ALA
2	D	170	PRO
6	K	23	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	175/176 (99%)	170 (97%)	5 (3%)	42	67
3	E	83/155 (54%)	81 (98%)	2 (2%)	49	72
4	F	89/89 (100%)	88 (99%)	1 (1%)	73	86
5	H	108/109 (99%)	106 (98%)	2 (2%)	57	77
6	K	88/101 (87%)	86 (98%)	2 (2%)	50	73
7	L	103/104 (99%)	103 (100%)	0	100	100
8	O	74/74 (100%)	73 (99%)	1 (1%)	67	83
9	Q	81/81 (100%)	77 (95%)	4 (5%)	25	47
10	R	55/65 (85%)	55 (100%)	0	100	100
11	T	68/69 (99%)	68 (100%)	0	100	100
12	P	103/115 (90%)	93 (90%)	10 (10%)	8	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	X	28/29 (97%)	28 (100%)	0	100	100
14	B	197/234 (84%)	196 (100%)	1 (0%)	88	94
All	All	1252/1401 (89%)	1224 (98%)	28 (2%)	54	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	42	LYS
2	D	45	GLU
2	D	47	SER
2	D	171	ASN
2	D	172	LYS
3	E	207	ARG
3	E	210	GLU
4	F	17	ARG
5	H	55	LYS
5	H	120	GLN
6	K	87	ARG
6	K	100	GLU
8	O	86	ARG
9	Q	1	MET
9	Q	7	GLU
9	Q	8	ARG
9	Q	11	ARG
12	P	26	ARG
12	P	111	GLU
12	P	113	ASP
12	P	114	GLU
12	P	117	ARG
12	P	118	GLU
12	P	120	ILE
12	P	122	LYS
12	P	123	LYS
12	P	125	GLU
14	B	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	178	HIS

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Mol	Chain	Res	Type
3	E	161	HIS
6	K	124	HIS
14	B	24	ASN
14	B	94	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1029/1537 (66%)	131 (12%)	6 (0%)
15	Y	9/22 (40%)	7 (77%)	0
All	All	1038/1559 (66%)	138 (13%)	6 (0%)

All (138) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	U
1	A	10	G
1	A	13	G
1	A	36	A
1	A	43	G
1	A	51	C
1	A	52	U
1	A	55	A
1	A	75	A
1	A	78	G
1	A	82	U
1	A	91	G
1	A	92	G
1	A	93	G
1	A	95	U
1	A	100	G
1	A	121	C
1	A	130	A
1	A	143	C
1	A	145	U
1	A	164	C
1	A	174	U
1	A	178	G
1	A	183	G
1	A	184	G

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Mol	Chain	Res	Type
1	A	185	A
1	A	195	G
1	A	197	A
1	A	214	G
1	A	218	C
1	A	220	G
1	A	222	G
1	A	226	G
1	A	242	C
1	A	247	C
1	A	249	G
1	A	252	U
1	A	253	G
1	A	268	G
1	A	269	C
1	A	291	G
1	A	323	A
1	A	330	U
1	A	331	A
1	A	349	G
1	A	354	C
1	A	356	G
1	A	369	U
1	A	374	C
1	A	375	A
1	A	386	G
1	A	408	G
1	A	413	A
1	A	414	U
1	A	415	G
1	A	416	A
1	A	423	U
1	A	424	C
1	A	426	G
1	A	431	U
1	A	432	A
1	A	441	U
1	A	461	G
1	A	463	G
1	A	467	G
1	A	468	U
1	A	478	A

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Mol	Chain	Res	Type
1	A	493	C
1	A	500	C
1	A	503	G
1	A	509	G7M
1	A	513	U
1	A	529	A
1	A	541	A
1	A	544	U
1	A	546	U
1	A	554	A
1	A	555	A
1	A	558	G
1	A	559	G
1	A	600	C
1	A	614	U
1	A	635	U
1	A	647	G
1	A	703	A
1	A	704	G
1	A	716	G
1	A	729	U
1	A	730	U
1	A	737	G
1	A	759	A
1	A	775	U
1	A	776	A
1	A	791	G
1	A	797	A
1	A	799	C
1	A	803	G
1	A	811	G
1	A	825	U
1	A	826	C
1	A	827	C
1	A	828	A
1	A	831	G
1	A	832	G
1	A	871	G
1	A	874	G
1	A	886	G
1	A	898	A
1	A	1382	C

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Mol	Chain	Res	Type
1	A	1384	C
1	A	1387	5MC
1	A	1388	G
1	A	1406	G
1	A	1409	G
1	A	1414	C
1	A	1416	C
1	A	1429	G
1	A	1433	A
1	A	1438	U
1	A	1440	G
1	A	1479	A
1	A	1480	A
1	A	1484	G
1	A	1486	A
1	A	1490	A
1	A	1493	U
1	A	1504	G
1	A	1516	G
1	A	1517	G
1	A	1521	A
15	Y	14	A
15	Y	15	A
15	Y	16	A
15	Y	19	U
15	Y	20	U
15	Y	21	U
15	Y	22	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	90	U
1	A	94	G
1	A	466	G
1	A	467	G
1	A	1387	5MC

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

10 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	MA6	A	1505	1	19,26,27	1.06	2 (10%)	18,38,41	5.16	3 (16%)
1	5MC	A	1387	1	18,22,23	0.57	0	26,32,35	0.65	0
1	G7M	A	509	1	20,26,27	2.72	7 (35%)	17,39,42	1.07	1 (5%)
1	2MG	A	1503	1	18,26,27	1.15	3 (16%)	16,38,41	1.01	1 (6%)
1	UR3	A	1485	1,16	19,22,23	2.72	8 (42%)	26,32,35	1.29	1 (3%)
1	MA6	A	1506	1	19,26,27	1.00	1 (5%)	18,38,41	5.30	3 (16%)
1	5MC	A	1391	1	18,22,23	0.63	0	26,32,35	0.55	0
1	5MC	A	1394	1	18,22,23	0.55	0	26,32,35	0.58	0
1	PSU	A	498	1,16	18,21,22	1.06	1 (5%)	22,30,33	1.84	5 (22%)
1	4OC	A	1389	1	20,23,24	3.10	8 (40%)	26,32,35	0.90	1 (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
1	MA6	A	1505	1	-	0/7/29/30	0/3/3/3
1	5MC	A	1387	1	-	3/7/25/26	0/2/2/2
1	G7M	A	509	1	-	2/3/25/26	0/3/3/3
1	2MG	A	1503	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1485	1,16	-	0/7/25/26	0/2/2/2
1	MA6	A	1506	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1391	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1394	1	-	0/7/25/26	0/2/2/2
1	PSU	A	498	1,16	-	0/7/25/26	0/2/2/2
1	4OC	A	1389	1	-	1/9/29/30	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1485	UR3	C2-N1	6.91	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1389	4OC	C4-N3	6.86	1.44	1.32
1	A	509	G7M	C2-N2	6.44	1.49	1.34
1	A	1389	4OC	C6-C5	6.23	1.49	1.35
1	A	1485	UR3	C6-C5	6.14	1.49	1.35
1	A	1389	4OC	C2-N3	5.96	1.48	1.36
1	A	509	G7M	C2-N3	5.63	1.46	1.33
1	A	509	G7M	C4-N3	5.02	1.49	1.37
1	A	1485	UR3	C2-N3	5.01	1.48	1.39
1	A	1389	4OC	C4-N4	4.54	1.45	1.35
1	A	509	G7M	C6-N1	4.17	1.44	1.37
1	A	1389	4OC	C2-N1	3.94	1.48	1.40
1	A	1389	4OC	C5-C4	3.90	1.49	1.40
1	A	509	G7M	C5-C6	3.24	1.53	1.45
1	A	498	PSU	C6-C5	3.16	1.39	1.35
1	A	1389	4OC	C6-N1	3.08	1.45	1.38
1	A	1485	UR3	C6-N1	2.92	1.45	1.38
1	A	509	G7M	C2-N1	2.84	1.44	1.37
1	A	1389	4OC	O2-C2	-2.78	1.18	1.23
1	A	1506	MA6	C5-C4	-2.74	1.33	1.40
1	A	1503	2MG	C8-N7	-2.74	1.30	1.35
1	A	1505	MA6	C5-C4	-2.72	1.33	1.40
1	A	509	G7M	O6-C6	-2.29	1.18	1.23
1	A	1503	2MG	C5-C6	-2.28	1.42	1.47
1	A	1485	UR3	O4-C4	-2.23	1.18	1.23
1	A	1485	UR3	O2-C2	-2.18	1.18	1.22
1	A	1485	UR3	C5-C4	2.17	1.49	1.43
1	A	1505	MA6	C2-N3	2.16	1.35	1.32
1	A	1485	UR3	C4-N3	2.13	1.45	1.40
1	A	1503	2MG	C5-C4	-2.02	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1506	MA6	N1-C6-N6	-19.36	96.68	117.06
1	A	1505	MA6	N1-C6-N6	-18.48	97.60	117.06
1	A	1505	MA6	C1'-N9-C4	-10.22	108.69	126.64
1	A	1506	MA6	C1'-N9-C4	-9.82	109.40	126.64
1	A	1506	MA6	N3-C2-N1	-5.49	120.10	128.68
1	A	1505	MA6	N3-C2-N1	-5.36	120.30	128.68
1	A	498	PSU	C4-N3-C2	-4.81	119.41	126.34
1	A	1485	UR3	C4-N3-C2	-4.69	120.14	124.56
1	A	498	PSU	N1-C2-N3	4.54	120.27	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	G7M	C2-N1-C6	-3.08	119.42	125.10
1	A	498	PSU	O2-C2-N1	-2.58	119.95	122.79
1	A	1503	2MG	O6-C6-C5	2.29	128.85	124.37
1	A	1389	4OC	C6-C5-C4	2.22	119.67	116.96
1	A	498	PSU	C6-N1-C2	-2.12	120.52	122.68
1	A	498	PSU	O4'-C1'-C2'	2.05	108.04	105.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1387	5MC	O4'-C4'-C5'-O5'
1	A	1506	MA6	O4'-C4'-C5'-O5'
1	A	1387	5MC	C3'-C4'-C5'-O5'
1	A	1506	MA6	C3'-C4'-C5'-O5'
1	A	509	G7M	C3'-C4'-C5'-O5'
1	A	1387	5MC	C4'-C5'-O5'-P
1	A	1389	4OC	O4'-C4'-C5'-O5'
1	A	509	G7M	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1505	MA6	1	0
1	A	1387	5MC	1	0
1	A	1503	2MG	2	0
1	A	1506	MA6	4	0
1	A	1391	5MC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 66 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

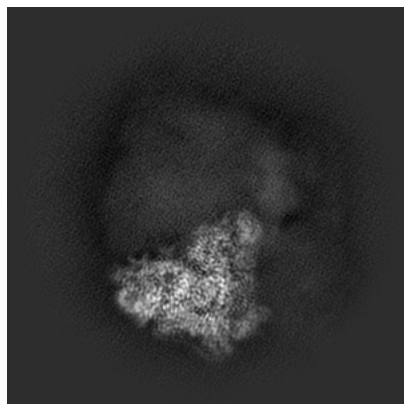
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27028. These allow visual inspection of the internal detail of the map and identification of artifacts.

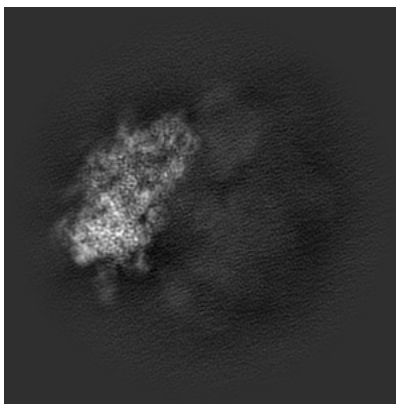
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

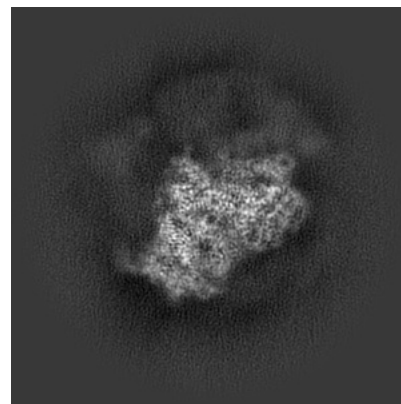
6.1.1 Primary map



X

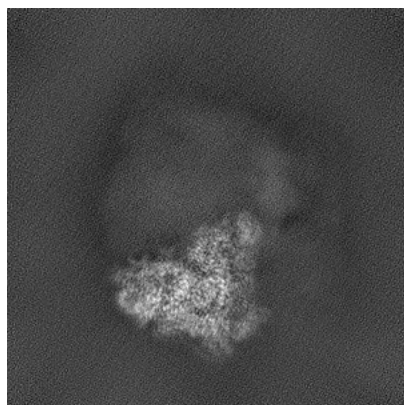


Y

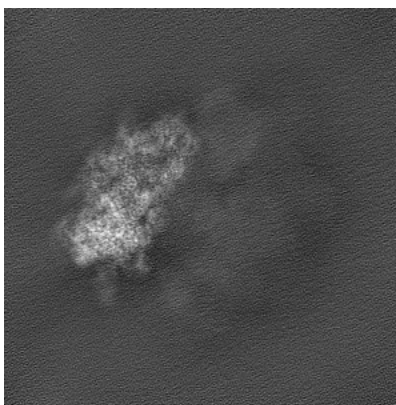


Z

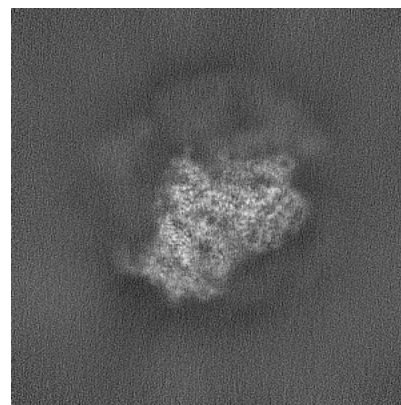
6.1.2 Raw map



X



Y

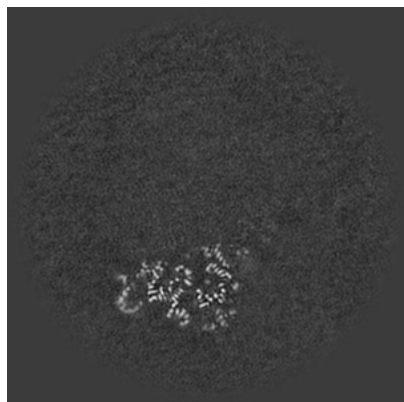


Z

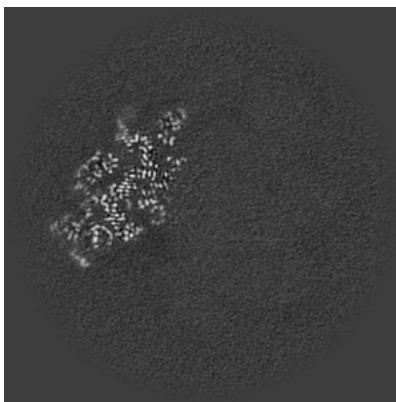
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

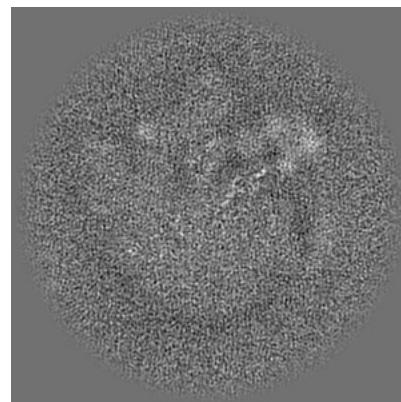
6.2.1 Primary map



X Index: 170

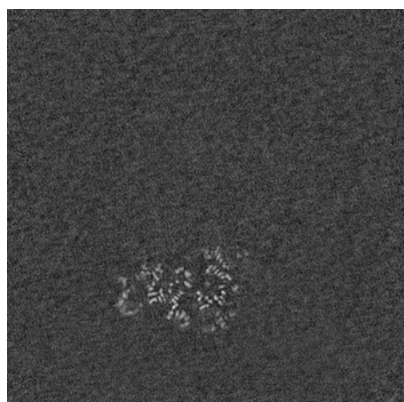


Y Index: 170

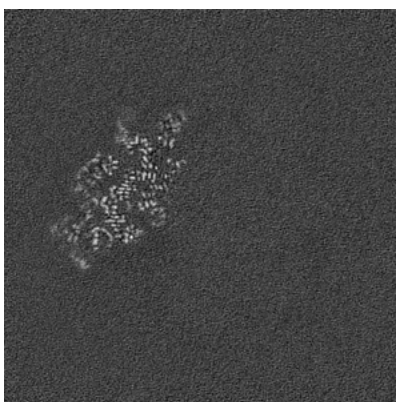


Z Index: 170

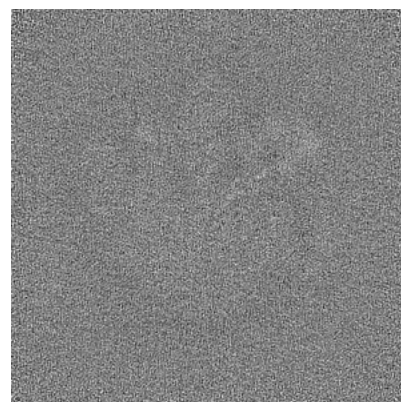
6.2.2 Raw map



X Index: 170



Y Index: 170

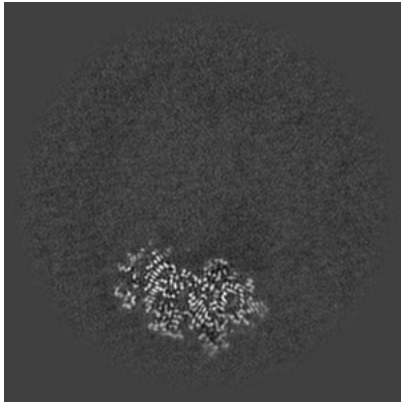


Z Index: 170

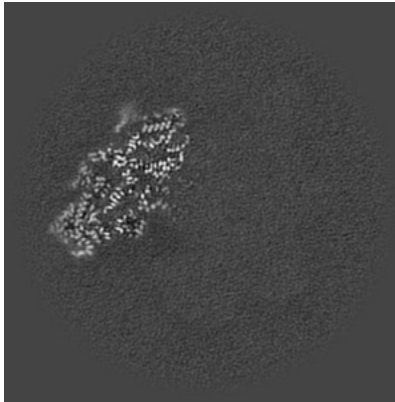
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

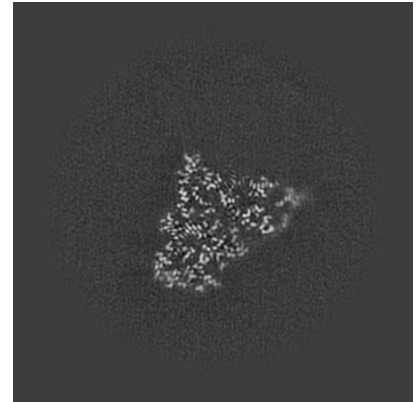
6.3.1 Primary map



X Index: 147

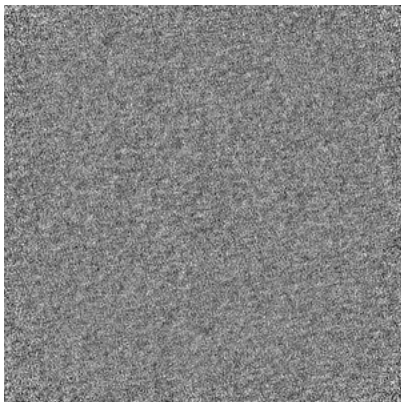


Y Index: 176

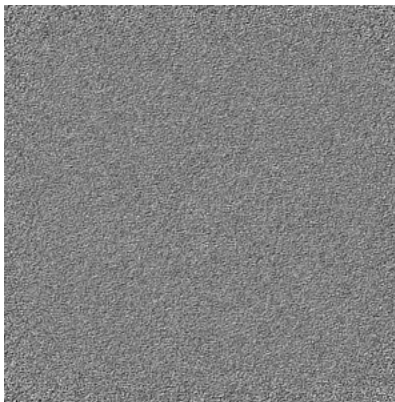


Z Index: 99

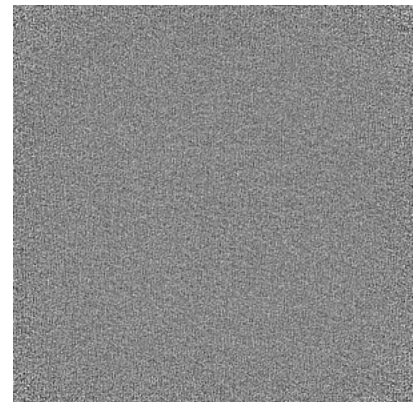
6.3.2 Raw map



X Index: 0



Y Index: 0

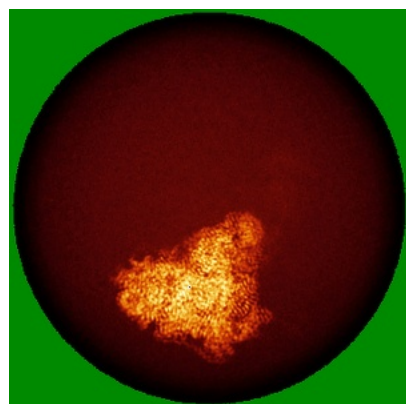


Z Index: 0

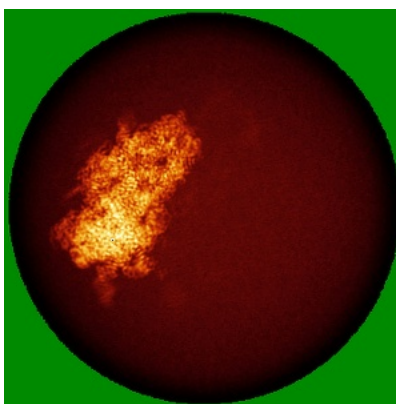
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

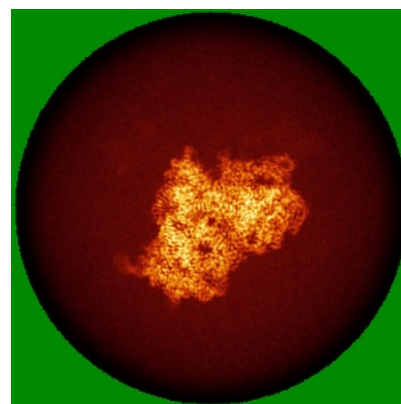
6.4.1 Primary map



X

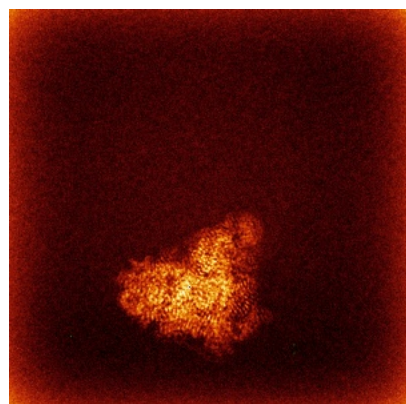


Y

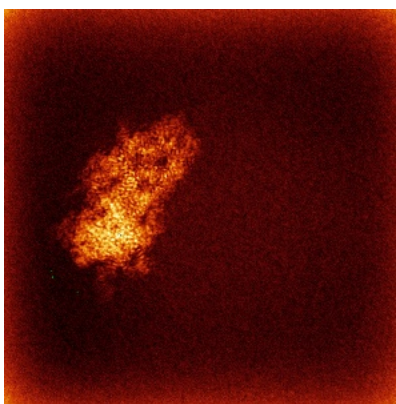


Z

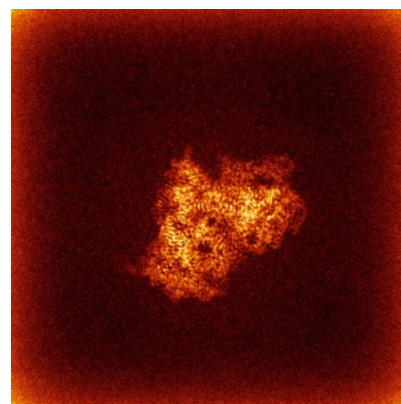
6.4.2 Raw map



X



Y

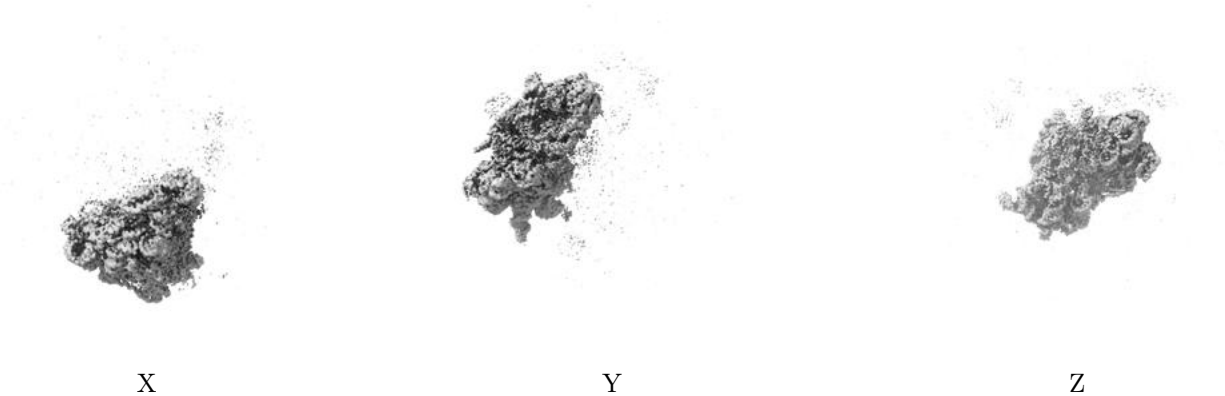


Z

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.

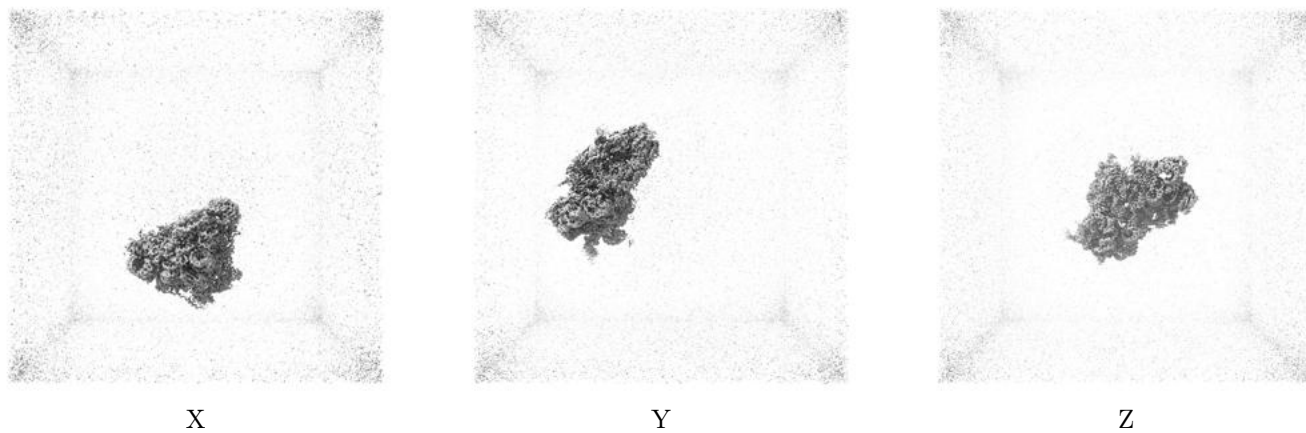
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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



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.

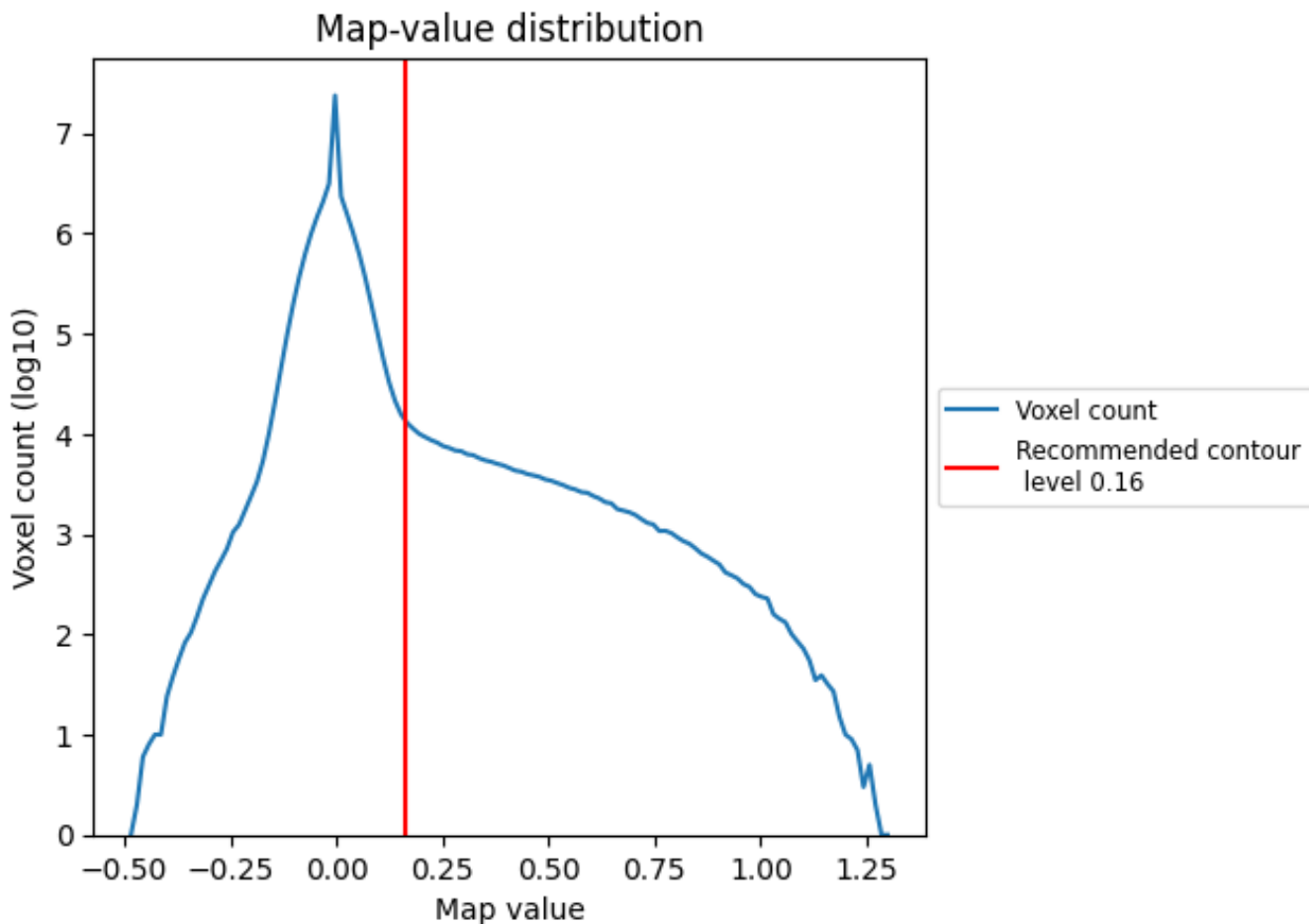
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

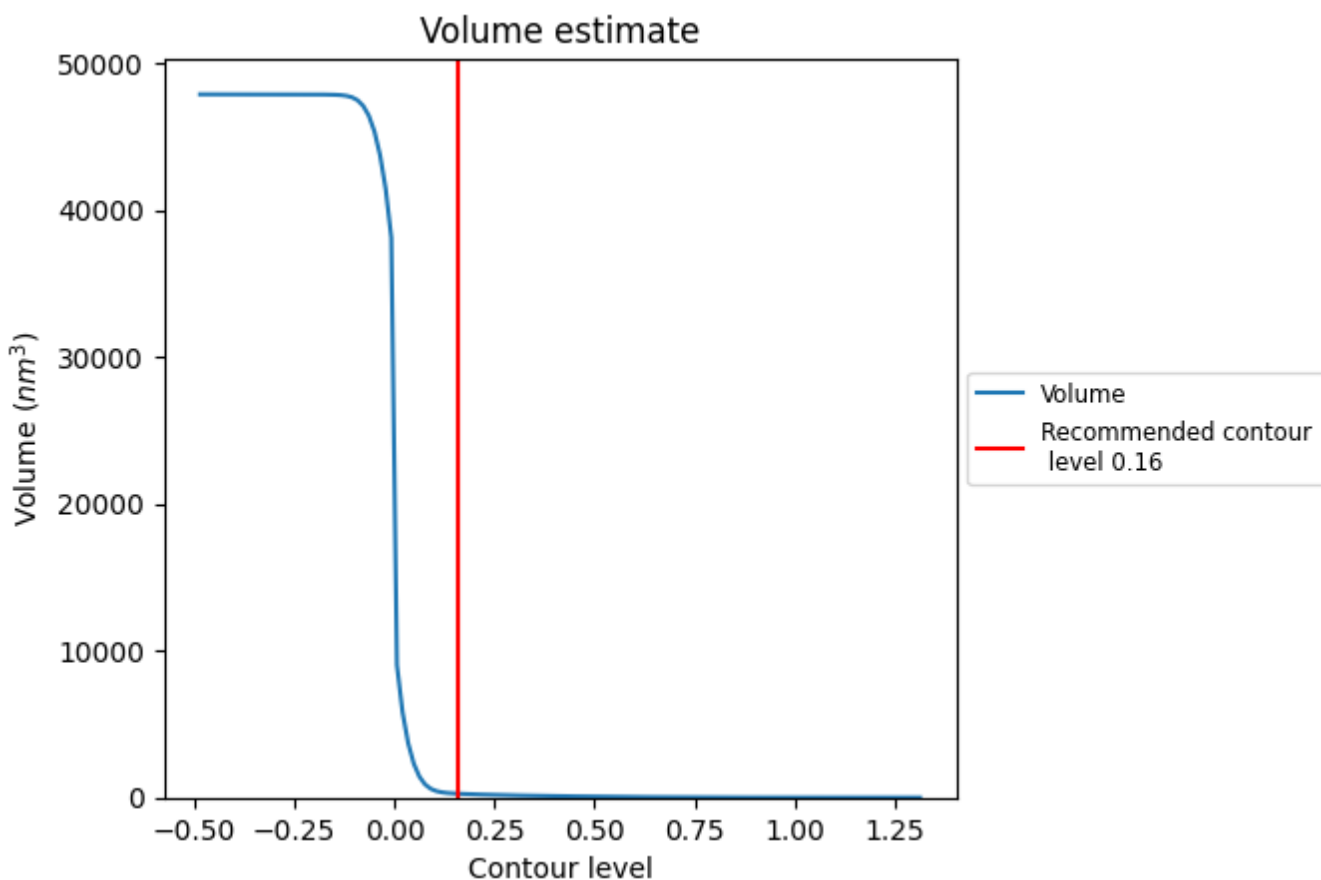
This section contains the results of statistical analysis of the map.

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.

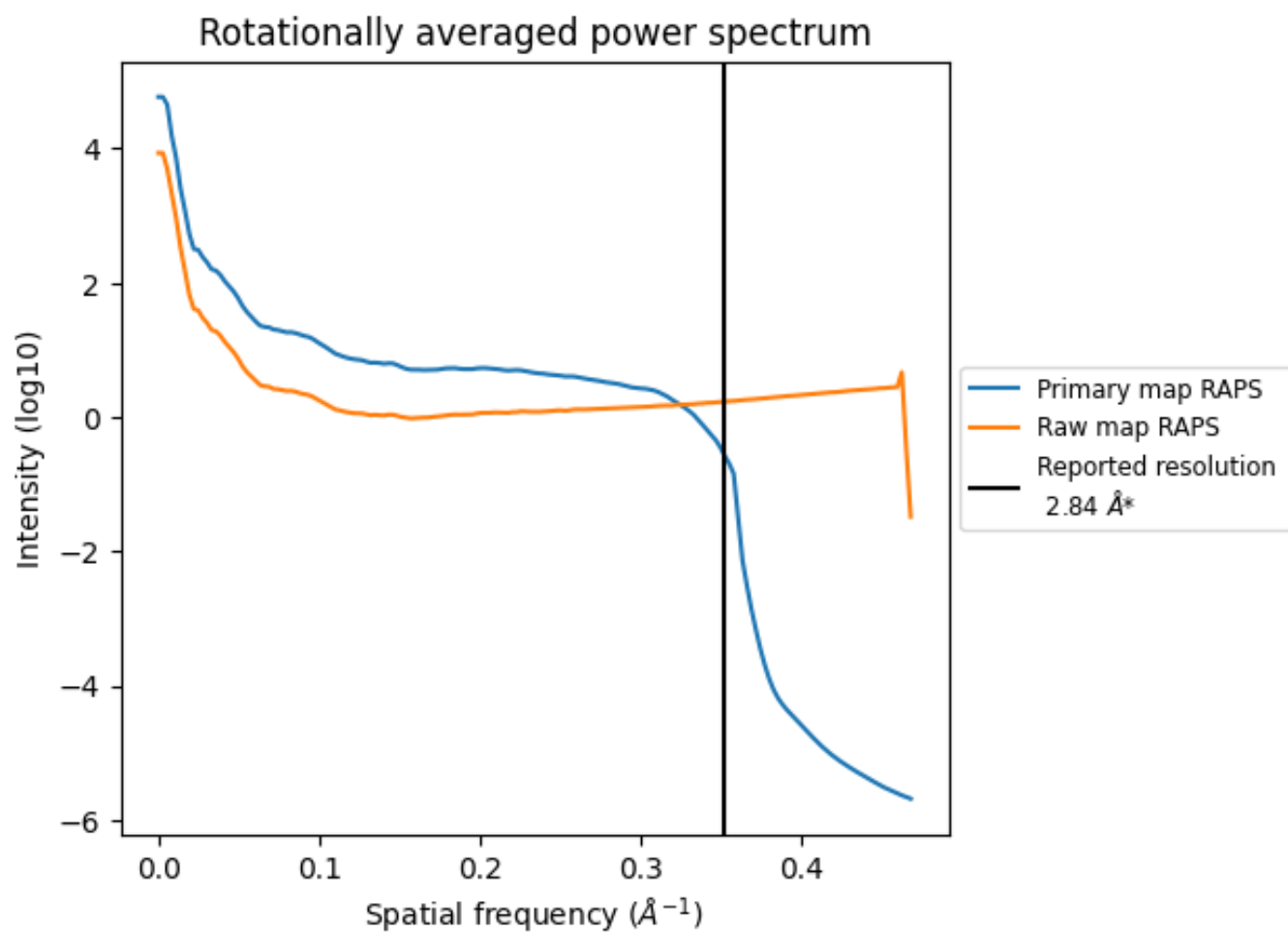
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 236 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

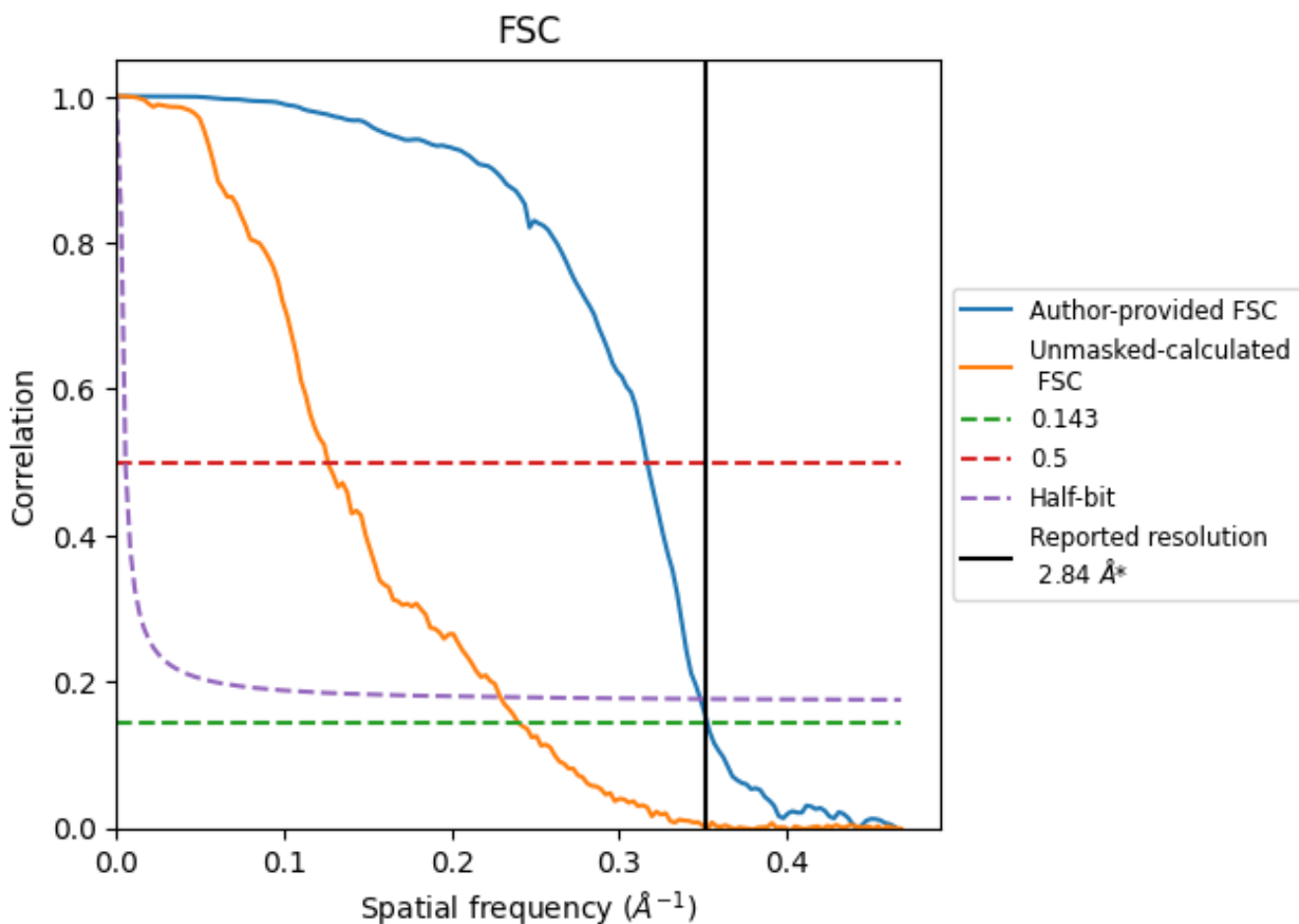


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

8.2 Resolution estimates [i](#)

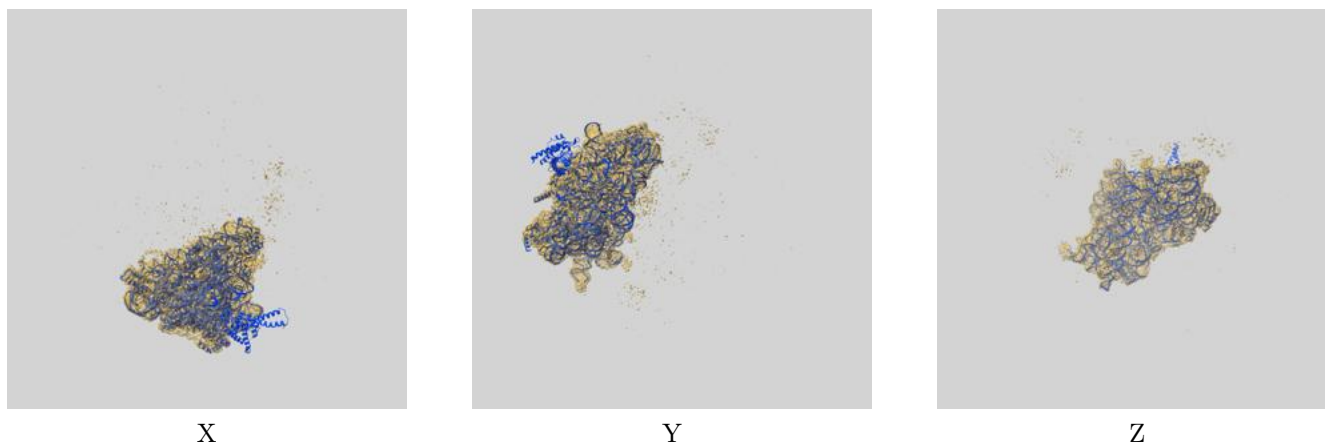
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.16	2.87
Unmasked-calculated*	4.16	7.92	4.36

*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 4.16 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

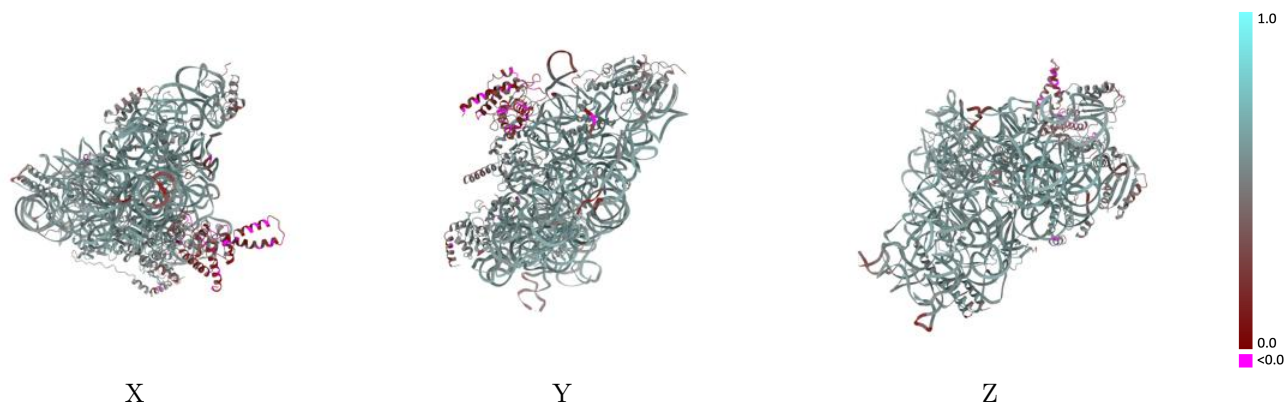
This section contains information regarding the fit between EMDB map EMD-27028 and PDB model 8CWO. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



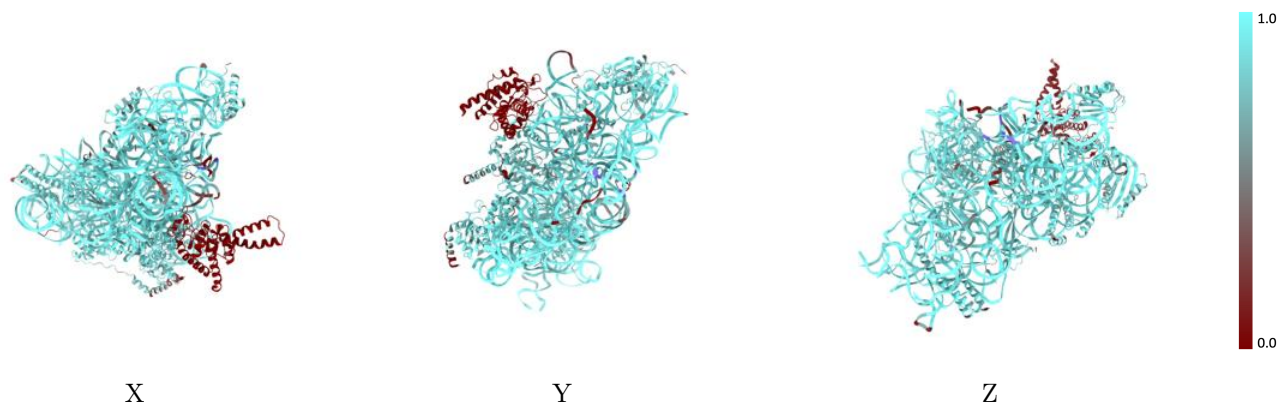
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



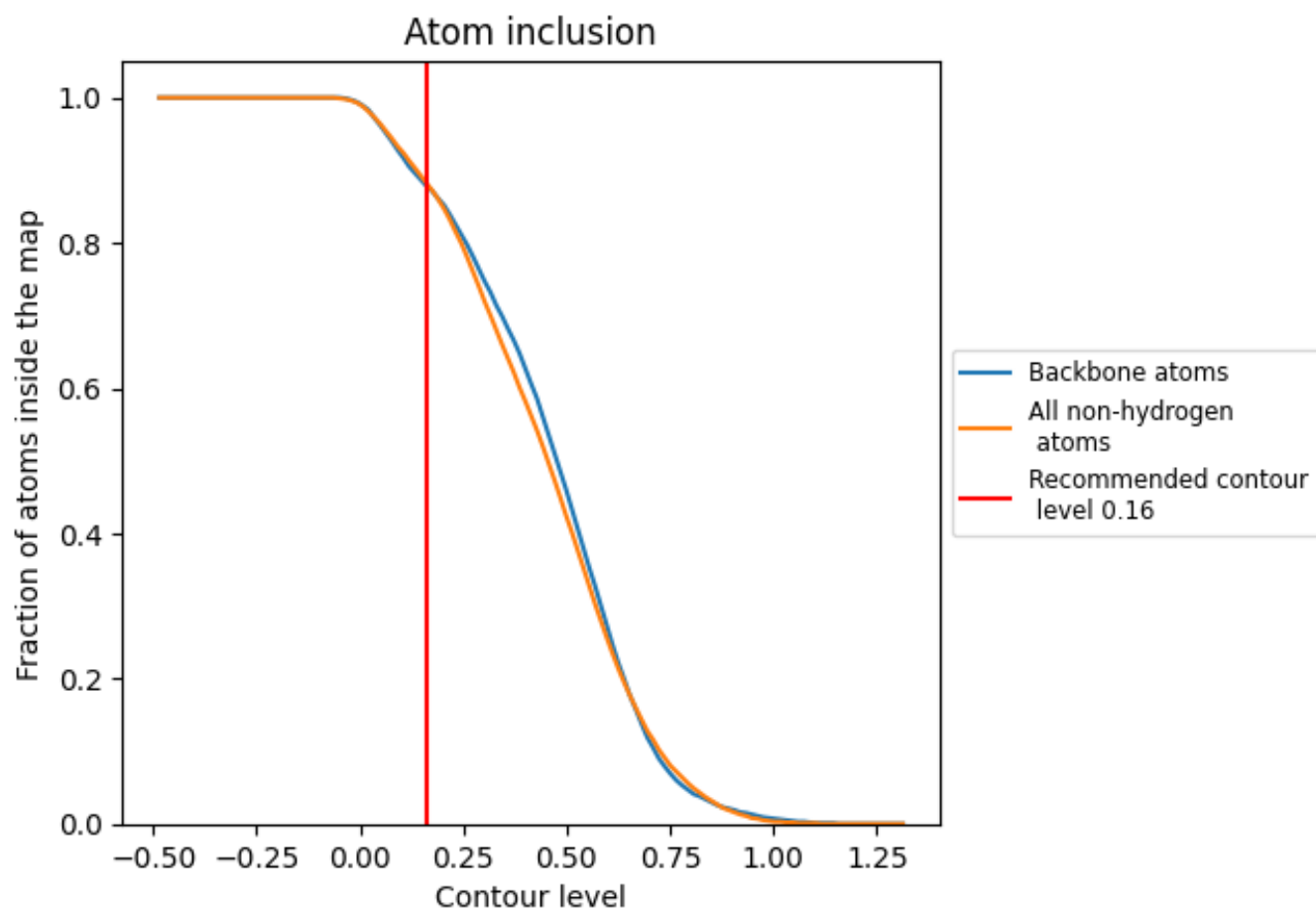
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.16).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5420
A	 0.9660	 0.5740
B	 0.0150	 0.2100
D	 0.8860	 0.5270
E	 0.7650	 0.5190
F	 0.8460	 0.4980
H	 0.9310	 0.5640
K	 0.8500	 0.4990
L	 0.9310	 0.5770
O	 0.8560	 0.5360
P	 0.8300	 0.5110
Q	 0.8680	 0.5500
R	 0.8430	 0.5130
T	 0.9290	 0.5570
X	 0.6560	 0.5420
Y	 0.6210	 0.4020

