Full wwPDB EM Map/Model Validation Report ⓘ

May 31, 2020 – 11:12 am BST

PDB ID	:	6KLB
EMDB ID	:	EMD-0705
Title	:	Structure of LbCas12a-crRNA complex bound to AcrVA4 (form B complex)
Authors	:	Peng, R.; Li, Z.; Xu, Y.; He, S.; Peng, Q.; Shi, Y.; Gao, G.F.
Deposited on	:	2019-07-30
Resolution	:	4.10 Å(reported)
Based on initial model	:	6KL9

This is a Full wwPDB EM Map/Model 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 following versions of software and data (see references ①) were used in the production of this report:

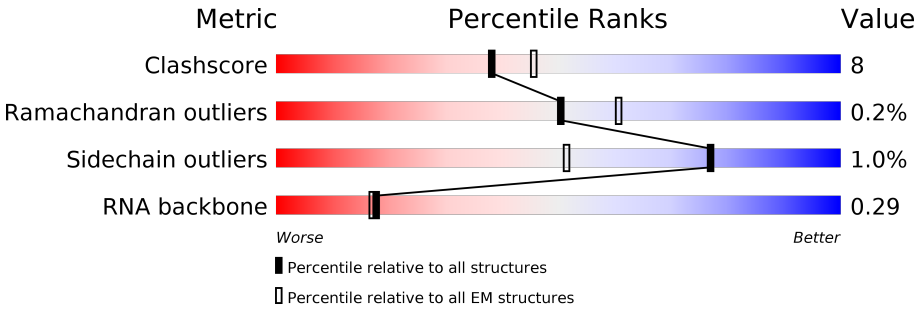
EMDB validation analysis	:	0.0.0.dev33
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1228	14% 73% 18% 9%
1	D	1228	17% 75% 15% 9%
2	B	234	38% 12% 50%
2	C	234	33% 16% • 50%
3	E	42	14% 43% • 40%
3	G	42	26% 26% 7% 40%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called LbCas12a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1118	Total	C	N	O	S	1	0
			9206	5923	1508	1750	25		
1	D	1115	Total	C	N	O	S	1	0
			9171	5896	1504	1746	25		

- Molecule 2 is a protein called AcrVA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	117	Total	C	N	O	S	0	0
			967	613	163	185	6		
2	C	117	Total	C	N	O	S	0	0
			967	613	163	185	6		

- Molecule 3 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	25	Total	C	N	O	P	0	0
			529	237	90	177	25		
3	G	25	Total	C	N	O	P	0	0
			529	237	90	177	25		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	E	2	Total	Mg	0
			2	2	

- Molecule 5 is water.

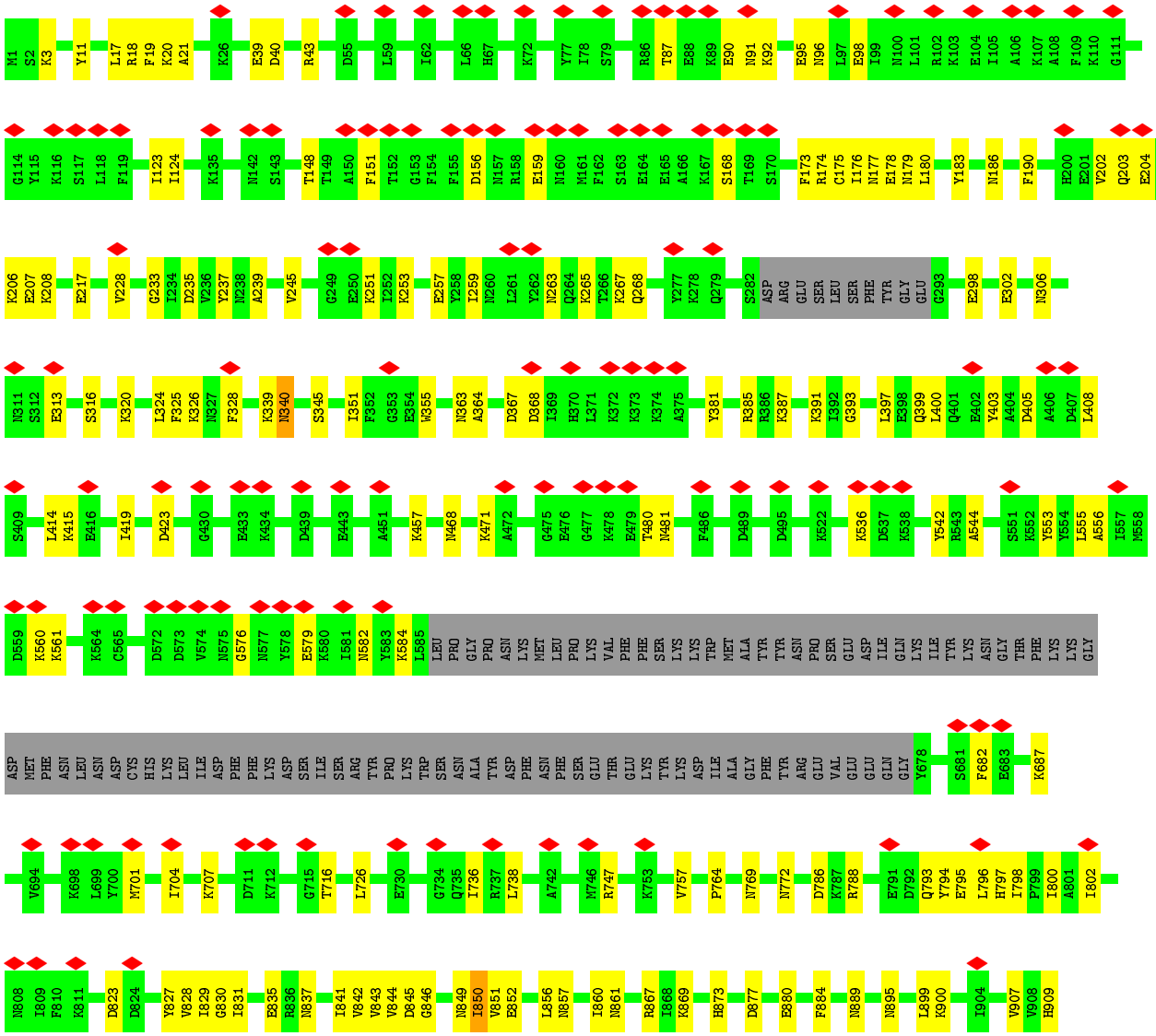
Mol	Chain	Residues	Atoms	AltConf
5	E	6	Total O 6 6	0
5	G	5	Total O 5 5	0

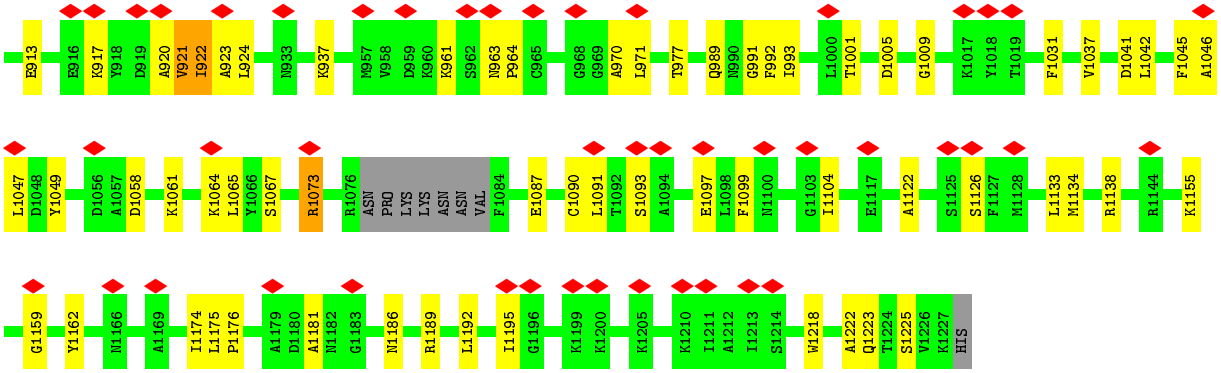
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: LbCas12a

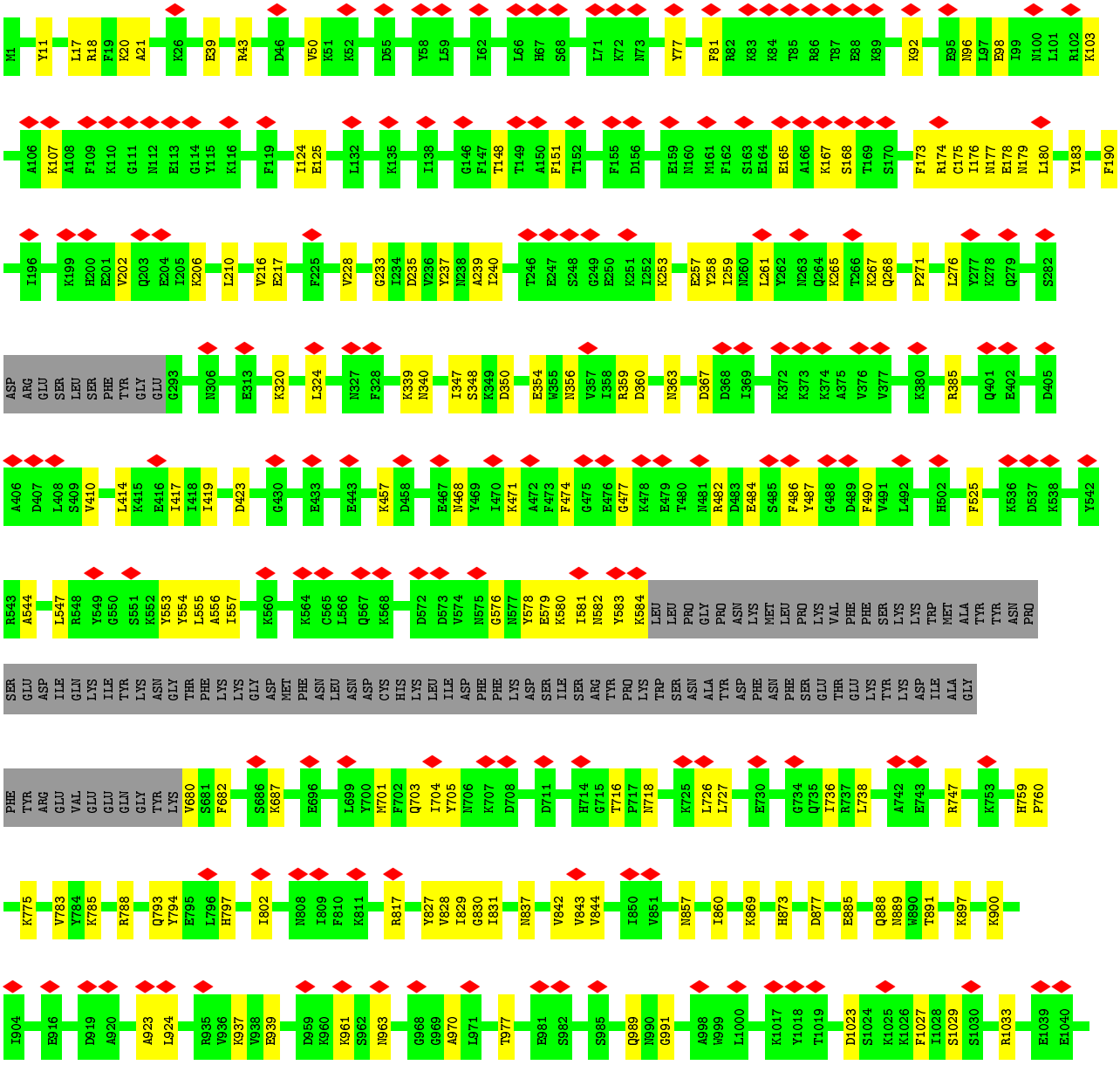
Chain A:

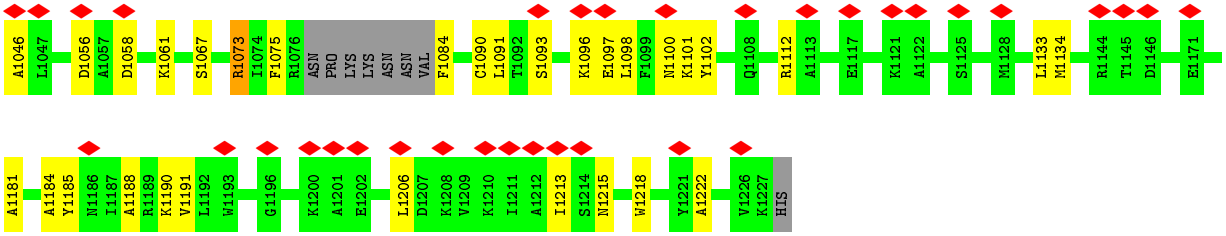




- Molecule 1: LbCas12a

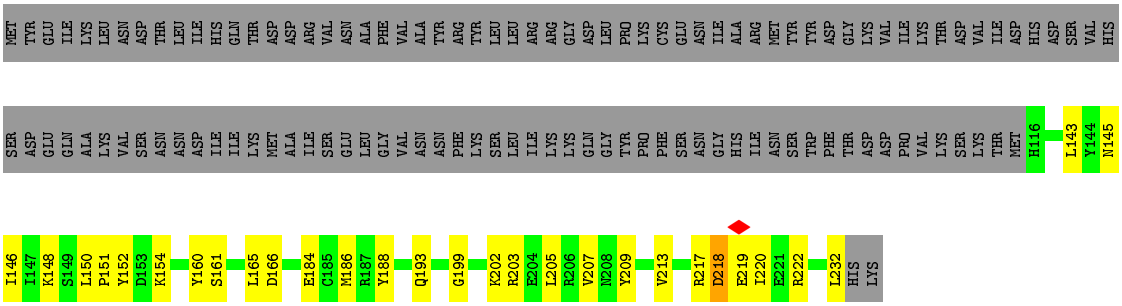
Chain D:





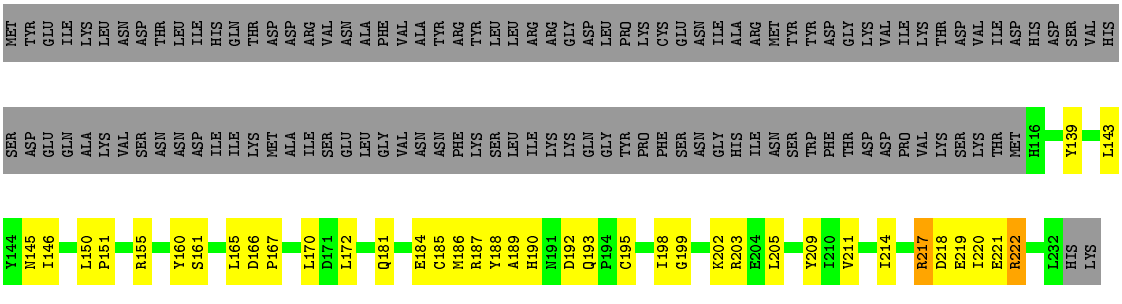
- Molecule 2: AcrVA4

Chain B:



- Molecule 2: AcrVA4

Chain C:



- Molecule 3: crRNA

Chain E:

- Molecule 3: crRNA

Chain G:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	Depositor
Map dimensions	400, 400, 400	Depositor
Map angles (°)	90.0, 90.0, 90.0	Depositor
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.27	0/9388	0.53	0/12610
1	D	0.28	0/9351	0.53	0/12561
2	B	0.30	0/986	0.61	0/1341
2	C	0.29	0/986	0.63	0/1341
3	E	0.28	0/590	0.94	0/916
3	G	0.30	0/590	0.99	0/916
All	All	0.28	0/21891	0.57	0/29685

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9206	0	9168	157	0
1	D	9171	0	9128	122	0
2	B	967	0	953	16	0
2	C	967	0	953	32	0
3	E	529	0	267	21	0
3	G	529	0	267	6	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2	0	0	0	0
4	G	1	0	0	0	0
5	E	6	0	0	0	0
5	G	5	0	0	0	0
All	All	21384	0	20736	337	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 8.

All (337) 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)
2:C:185:CYS:HA	2:C:195:CYS:O	1.39	1.19
2:C:187:ARG:HA	2:C:193:GLN:O	1.53	1.08
1:A:828:VAL:HA	1:A:923:ALA:HB3	1.34	1.04
1:A:176:ILE:O	1:A:180:LEU:HB3	1.68	0.93
1:A:21:ALA:O	1:A:794:TYR:HB2	1.69	0.92
1:D:176:ILE:O	1:D:180:LEU:HB3	1.69	0.92
1:D:21:ALA:O	1:D:794:TYR:HB2	1.70	0.92
1:A:202:VAL:O	1:A:206:LYS:HB3	1.72	0.90
2:C:188:TYR:N	2:C:193:GLN:H	1.72	0.88
2:C:217:ARG:NH2	1:D:885:GLU:HB3	1.88	0.88
1:A:843:VAL:HB	1:A:852:GLU:O	1.75	0.86
1:A:844:VAL:HG23	1:A:850:ILE:HG22	1.54	0.86
1:A:203:GLN:O	1:A:207:GLU:HB3	1.76	0.86
1:A:844:VAL:CG2	1:A:850:ILE:HG22	2.05	0.86
1:A:1073:ARG:O	1:A:1087:GLU:HB2	1.74	0.85
1:D:174:ARG:O	1:D:178:GLU:HB2	1.76	0.85
3:E:21:C:C5	3:E:22:G:C4	2.63	0.85
1:A:922:ILE:HG12	1:A:992:PHE:HB3	1.58	0.84
1:A:174:ARG:O	1:A:178:GLU:HB2	1.77	0.83
1:A:830:GLY:O	1:A:841:ILE:HA	1.77	0.83
1:D:1093:SER:O	1:D:1097:GLU:HB2	1.78	0.81
2:C:185:CYS:CA	2:C:195:CYS:O	2.27	0.81
1:A:1045:PHE:O	1:A:1065:LEU:HB2	1.80	0.80
1:D:829:ILE:HA	1:D:842:VAL:O	1.81	0.80
2:B:188:TYR:HB3	2:B:193:GLN:O	1.83	0.78
1:A:922:ILE:HG13	1:A:992:PHE:C	2.05	0.77
3:E:21:C:C6	3:E:22:G:C4	2.75	0.74
1:A:92:LYS:O	1:A:96:ASN:HB2	1.88	0.74
2:C:187:ARG:CA	2:C:193:GLN:O	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ALA:HA	1:D:703:GLN:O	1.87	0.74
1:D:544:ALA:HA	1:D:556:ALA:O	1.88	0.73
1:A:555:LEU:O	1:A:701:MET:HA	1.89	0.72
1:D:555:LEU:O	1:D:701:MET:HA	1.89	0.72
3:E:21:C:C5	3:E:22:G:C2	2.79	0.71
1:A:922:ILE:CG1	1:A:992:PHE:HB3	2.21	0.70
1:D:457:LYS:HE3	1:D:889:ASN:HB2	1.71	0.70
3:E:21:C:H5	3:E:22:G:C2	2.10	0.69
1:D:20:LYS:HB3	1:D:705:TYR:O	1.92	0.69
1:D:173:PHE:O	1:D:177:ASN:HB2	1.93	0.69
1:D:92:LYS:O	1:D:96:ASN:HB2	1.94	0.68
1:A:576:GLY:HA3	1:A:687:LYS:HB2	1.76	0.68
1:D:827:TYR:HA	1:D:844:VAL:O	1.94	0.67
1:A:457:LYS:HE3	1:A:889:ASN:HB2	1.76	0.67
1:D:175:CYS:O	1:D:179:ASN:HB2	1.94	0.67
2:C:217:ARG:HH21	1:D:885:GLU:HB3	1.57	0.67
1:A:387:LYS:O	1:A:391:LYS:HB2	1.95	0.67
1:A:320:LYS:O	1:A:324:LEU:HB2	1.95	0.66
1:A:18:ARG:HA	1:A:796:LEU:O	1.96	0.66
1:A:175:CYS:O	1:A:179:ASN:HB2	1.96	0.65
1:A:364:ALA:O	1:A:368:ASP:HB2	1.96	0.65
1:A:828:VAL:HA	1:A:923:ALA:CB	2.21	0.64
1:A:39:GLU:O	1:A:43:ARG:HB2	1.97	0.64
1:D:77:TYR:O	1:D:81:PHE:HB2	1.98	0.64
1:D:39:GLU:O	1:D:43:ARG:HB2	1.98	0.64
1:A:263:ASN:H	1:A:268:GLN:HE22	1.44	0.63
1:A:17:LEU:O	1:A:797:HIS:HA	1.99	0.63
2:C:187:ARG:HE	1:D:760:PRO:HG3	1.63	0.63
2:C:219:GLU:O	2:C:219:GLU:HG3	1.96	0.63
3:E:21:C:C5	3:E:22:G:C5	2.86	0.63
1:A:363:ASN:O	1:A:367:ASP:HB2	1.99	0.62
3:E:9:C:N3	3:E:10:U:C4	2.67	0.62
1:A:921:VAL:HG23	1:A:992:PHE:HD1	1.65	0.61
1:A:325:PHE:HA	1:A:328:PHE:HB3	1.82	0.61
1:A:173:PHE:O	1:A:177:ASN:HB2	2.01	0.61
1:A:204:GLU:O	1:A:208:LYS:HB2	2.00	0.61
1:A:235:ASP:O	1:A:239:ALA:HB2	2.00	0.61
3:E:21:C:C5	3:E:22:G:N3	2.68	0.60
1:A:381:TYR:O	1:A:385:ARG:HB2	2.02	0.60
1:A:1031:PHE:HA	1:A:1047:LEU:HD13	1.82	0.60
1:A:736:ILE:HG12	1:A:802:ILE:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:155:ARG:HB2	2:C:181:GLN:HE21	1.66	0.59
1:D:576:GLY:HA3	1:D:687:LYS:HB2	1.83	0.59
1:D:579:GLU:HB3	1:D:682:PHE:HB3	1.85	0.59
1:D:259:ILE:O	1:D:268:GLN:NE2	2.36	0.59
3:E:21:C:C4	3:E:22:G:C6	2.90	0.59
1:A:351:ILE:HD11	1:A:414:LEU:HB2	1.85	0.59
1:A:845:ASP:H	1:A:851:VAL:HG23	1.68	0.58
1:D:235:ASP:O	1:D:239:ALA:HB2	2.03	0.58
1:A:302:GLU:OE2	1:A:306:ASN:ND2	2.37	0.58
1:A:17:LEU:HB2	1:A:798:ILE:HB	1.86	0.58
1:A:922:ILE:CG1	1:A:992:PHE:C	2.72	0.57
1:A:769:ASN:HB3	1:A:772:ASN:HB2	1.86	0.57
1:A:845:ASP:N	1:A:851:VAL:HG23	2.20	0.57
1:D:873:HIS:O	1:D:877:ASP:HB2	2.04	0.57
1:A:747:ARG:NH2	1:A:793:GLN:OE1	2.38	0.57
1:A:203:GLN:O	1:A:207:GLU:CB	2.52	0.56
1:A:339:LYS:NZ	1:A:471:LYS:O	2.37	0.56
2:B:213:VAL:HG21	2:B:220:ILE:HD12	1.86	0.56
1:A:726:LEU:HD12	1:A:970:ALA:HB3	1.87	0.56
1:D:320:LYS:O	1:D:324:LEU:HB2	2.05	0.56
1:A:922:ILE:CG1	1:A:992:PHE:CB	2.83	0.56
2:C:199:GLY:HA3	2:C:203:ARG:HD3	1.88	0.56
1:D:888:GLN:NE2	1:D:891:THR:OG1	2.37	0.56
1:A:707:LYS:NZ	3:G:3:U:O2	2.39	0.56
1:A:989:GLN:NE2	1:A:991:GLY:O	2.39	0.56
1:D:583:TYR:O	1:D:680:VAL:N	2.40	0.55
1:D:50:VAL:HG11	1:D:151:PHE:HE1	1.72	0.55
1:D:1190:LYS:HD3	1:D:1213:ILE:HG21	1.88	0.55
1:D:176:ILE:O	1:D:180:LEU:CB	2.50	0.55
1:D:759:HIS:HB2	1:D:783:VAL:HB	1.88	0.55
1:A:419:ILE:O	1:A:423:ASP:HB2	2.06	0.55
1:A:259:ILE:O	1:A:268:GLN:NE2	2.34	0.55
1:D:1033:ARG:HB3	1:D:1046:ALA:HB3	1.89	0.55
1:A:828:VAL:HB	1:A:844:VAL:HG13	1.87	0.54
2:C:186:MET:O	2:C:195:CYS:N	2.40	0.54
1:A:860:ILE:HG12	1:A:869:LYS:HG2	1.88	0.54
1:D:98:GLU:OE2	1:D:177:ASN:ND2	2.40	0.54
1:A:1058:ASP:O	1:A:1061:LYS:NZ	2.39	0.54
1:D:39:GLU:O	1:D:43:ARG:CB	2.56	0.54
1:D:900:LYS:NZ	1:D:937:LYS:O	2.41	0.54
2:B:199:GLY:HA3	2:B:203:ARG:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:OG	1:A:174:ARG:NH1	2.40	0.54
2:C:188:TYR:N	2:C:193:GLN:N	2.51	0.54
1:A:1218:TRP:O	1:A:1222:ALA:HB2	2.08	0.54
1:D:356:ASN:O	1:D:360:ASP:N	2.36	0.54
1:D:747:ARG:NH2	1:D:793:GLN:OE1	2.40	0.54
1:A:298:GLU:O	1:A:302:GLU:HB2	2.08	0.53
1:D:356:ASN:O	1:D:359:ARG:HB3	2.08	0.53
1:A:253:LYS:HD2	1:A:257:GLU:HG2	1.89	0.53
1:A:340:ASN:HB2	1:A:393:GLY:HA2	1.90	0.53
1:A:176:ILE:O	1:A:180:LEU:CB	2.50	0.53
2:B:152:TYR:HE1	2:B:184:GLU:H	1.56	0.53
1:A:186:ASN:ND2	1:A:237:TYR:OH	2.42	0.53
1:A:179:ASN:O	1:A:183:TYR:HB2	2.08	0.53
1:D:989:GLN:NE2	1:D:991:GLY:O	2.41	0.53
1:A:228:VAL:HA	1:A:233:GLY:HA3	1.91	0.53
1:A:20:LYS:HG3	1:A:793:GLN:HE21	1.74	0.53
1:D:1098:LEU:O	1:D:1101:LYS:O	2.27	0.53
1:A:837:ASN:OD1	1:A:857:ASN:ND2	2.42	0.53
1:D:419:ILE:O	1:D:423:ASP:HB2	2.08	0.53
3:E:21:C:O2	3:E:21:C:H2'	2.08	0.53
1:D:174:ARG:HD3	1:D:178:GLU:HG3	1.91	0.53
2:C:187:ARG:C	2:C:193:GLN:H	2.12	0.52
1:D:923:ALA:HB2	1:D:1191:VAL:HG21	1.91	0.52
1:A:716:THR:OG1	1:A:961:LYS:NZ	2.36	0.52
1:D:860:ILE:HG12	1:D:869:LYS:HG2	1.91	0.52
1:A:1001:THR:O	1:A:1186:ASN:ND2	2.42	0.52
1:D:1073:ARG:HB2	1:D:1133:LEU:HD21	1.91	0.52
1:D:897:LYS:NZ	1:D:939:GLU:OE2	2.43	0.52
2:B:160:TYR:HB2	2:B:207:VAL:HG21	1.92	0.52
1:D:1097:GLU:O	1:D:1101:LYS:CB	2.58	0.52
1:D:168:SER:OG	1:D:174:ARG:NH1	2.43	0.52
1:A:1192:LEU:HD23	1:A:1195:ILE:HD12	1.91	0.52
1:D:788:ARG:NH2	3:E:6:C:OP2	2.41	0.52
2:C:188:TYR:H	2:C:192:ASP:HA	1.75	0.51
1:A:846:GLY:HA3	1:A:1192:LEU:HD21	1.93	0.51
1:A:880:GLU:O	1:A:884:PHE:HB2	2.09	0.51
1:D:1090:CYS:SG	1:D:1091:LEU:N	2.81	0.51
1:D:1096:LYS:O	1:D:1100:ASN:HB2	2.10	0.51
1:A:345:SER:HB3	1:A:355:TRP:HB3	1.93	0.51
1:A:922:ILE:HG13	1:A:993:ILE:N	2.26	0.51
1:A:1093:SER:O	1:A:1097:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:21:C:N4	3:E:22:G:C6	2.78	0.51
1:A:895:ASN:ND2	2:B:202:LYS:O	2.43	0.50
1:D:1056:ASP:HA	1:D:1061:LYS:HE3	1.92	0.50
1:A:1005:ASP:HB3	1:A:1009:GLY:H	1.77	0.50
2:C:184:GLU:O	2:C:195:CYS:O	2.28	0.50
1:A:39:GLU:O	1:A:43:ARG:CB	2.59	0.50
1:A:233:GLY:O	1:A:237:TYR:HB2	2.11	0.50
3:E:16:U:H2'	3:E:17:A:H8	1.77	0.50
1:A:900:LYS:NZ	1:A:937:LYS:O	2.43	0.50
2:C:186:MET:O	2:C:193:GLN:O	2.28	0.50
1:A:265:LYS:HD2	1:A:267:LYS:HE2	1.93	0.49
1:A:579:GLU:HB3	1:A:682:PHE:HB3	1.93	0.49
1:A:835:GLU:OE1	1:A:1138:ARG:NH2	2.44	0.49
1:A:922:ILE:CG1	1:A:992:PHE:O	2.60	0.49
1:A:764:PRO:O	2:B:148:LYS:NZ	2.37	0.49
2:B:161:SER:O	2:B:209:TYR:HB2	2.11	0.49
1:D:1181:ALA:O	1:D:1185:TYR:CB	2.60	0.49
1:A:1037:VAL:O	1:A:1041:ASP:HA	2.12	0.49
1:A:845:ASP:O	1:A:849:ASN:O	2.30	0.49
1:A:842:VAL:HG21	1:A:1181:ALA:HA	1.94	0.49
2:C:172:LEU:HD11	2:C:222:ARG:HA	1.95	0.49
1:D:1067:SER:OG	1:D:1134:MET:SD	2.70	0.49
1:A:204:GLU:O	1:A:208:LYS:CB	2.61	0.49
1:A:921:VAL:HG23	1:A:992:PHE:CD1	2.48	0.49
1:D:477:GLY:HA2	1:D:482:ARG:HH12	1.78	0.49
1:D:265:LYS:HD2	1:D:267:LYS:HE2	1.95	0.48
1:A:1162:TYR:OH	1:A:1176:PRO:O	2.31	0.48
1:D:190:PHE:HZ	1:D:217:GLU:HG2	1.79	0.48
2:C:165:LEU:O	2:C:166:ASP:OD1	2.30	0.48
1:D:553:TYR:HB2	1:D:704:ILE:HB	1.95	0.48
1:D:785:LYS:HG3	3:E:1:A:H5"	1.95	0.48
1:A:844:VAL:HA	1:A:851:VAL:H	1.79	0.47
1:A:18:ARG:HG2	1:A:797:HIS:CD2	2.49	0.47
1:D:179:ASN:O	1:D:183:TYR:HB2	2.13	0.47
1:D:830:GLY:HA3	1:D:1184:ALA:HB1	1.95	0.47
1:A:553:TYR:HB2	1:A:704:ILE:HB	1.96	0.47
1:D:1181:ALA:O	1:D:1185:TYR:HB3	2.15	0.47
1:A:190:PHE:HZ	1:A:217:GLU:HG2	1.80	0.47
1:D:716:THR:OG1	1:D:961:LYS:NZ	2.47	0.47
1:A:235:ASP:O	1:A:239:ALA:CB	2.63	0.47
1:A:922:ILE:HG22	1:A:924:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:C:C2	3:E:10:U:C5	3.02	0.47
1:A:913:GLU:O	1:A:917:LYS:HB2	2.15	0.47
1:D:77:TYR:O	1:D:81:PHE:CB	2.61	0.47
1:A:1073:ARG:HB2	1:A:1133:LEU:HD21	1.96	0.47
1:A:1218:TRP:O	1:A:1222:ALA:CB	2.63	0.47
1:A:87:THR:HA	1:A:90:GLU:HB3	1.96	0.47
2:B:143:LEU:HA	2:B:146:ILE:HG22	1.97	0.47
1:D:829:ILE:HG12	1:D:843:VAL:HG22	1.97	0.47
1:A:827:TYR:HB2	1:A:920:ALA:HB1	1.97	0.46
1:D:547:LEU:HB2	1:D:554:TYR:O	2.15	0.46
1:A:726:LEU:HD13	1:A:971:LEU:HG	1.97	0.46
2:B:154:LYS:HG3	2:B:232:LEU:HD13	1.97	0.46
2:C:139:TYR:O	2:C:143:LEU:CB	2.63	0.46
1:A:924:LEU:HD21	1:A:993:ILE:HG23	1.98	0.46
1:D:324:LEU:HD11	1:D:486:PHE:HA	1.98	0.46
1:D:487:TYR:HA	1:D:490:PHE:HB3	1.97	0.46
1:A:536:LYS:HD2	1:A:542:TYR:HE2	1.80	0.46
2:C:188:TYR:O	2:C:190:HIS:N	2.35	0.46
1:D:253:LYS:HD2	1:D:257:GLU:HG2	1.97	0.46
1:A:786:ASP:H	3:G:2:A:H5"	1.80	0.46
1:A:245:VAL:HG23	1:A:251:LYS:HG2	1.98	0.46
1:A:419:ILE:O	1:A:423:ASP:CB	2.64	0.46
3:E:21:C:O2'	3:E:22:G:H5"	2.16	0.46
1:A:1174:ILE:HG23	1:A:1175:LEU:HG	1.98	0.46
1:D:206:LYS:HE3	1:D:216:VAL:HG21	1.98	0.46
1:D:1075:PHE:HB2	1:D:1084:PHE:HD1	1.81	0.46
1:D:580:LYS:O	1:D:682:PHE:HA	2.16	0.46
1:D:228:VAL:HA	1:D:233:GLY:HA3	1.98	0.46
1:D:17:LEU:O	1:D:797:HIS:HA	2.15	0.46
2:B:188:TYR:CB	2:B:193:GLN:O	2.58	0.45
1:D:727:LEU:HD21	1:D:738:LEU:HD21	1.98	0.45
1:A:544:ALA:HA	1:A:556:ALA:O	2.16	0.45
1:D:525:PHE:HD2	1:D:557:ILE:HG21	1.82	0.45
1:A:844:VAL:HG23	1:A:850:ILE:HA	1.97	0.45
1:A:873:HIS:O	1:A:877:ASP:HB2	2.16	0.45
1:D:410:VAL:O	1:D:414:LEU:CB	2.64	0.45
1:D:828:VAL:O	1:D:843:VAL:HA	2.16	0.45
1:D:1067:SER:HB3	1:D:1091:LEU:HD13	1.97	0.45
1:D:547:LEU:HD22	1:D:578:TYR:HB3	1.99	0.45
3:E:21:C:C4	3:E:22:G:C5	3.03	0.45
2:C:161:SER:O	2:C:209:TYR:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:C:N4	3:E:10:U:O4	2.49	0.45
1:A:313:GLU:HA	1:A:316:SER:HB3	1.99	0.45
2:C:217:ARG:HH21	1:D:885:GLU:CB	2.27	0.45
1:A:1099:PHE:HA	1:A:1104:ILE:HD11	1.98	0.45
2:B:165:LEU:O	2:B:166:ASP:OD1	2.35	0.45
1:A:1067:SER:OG	1:A:1134:MET:SD	2.72	0.44
1:D:11:TYR:OH	1:D:977:THR:O	2.34	0.44
1:A:1090:CYS:SG	1:A:1091:LEU:N	2.90	0.44
1:A:844:VAL:HG23	1:A:850:ILE:CG2	2.38	0.44
1:A:91:ASN:O	1:A:95:GLU:HB3	2.17	0.44
1:D:1097:GLU:O	1:D:1101:LYS:HB2	2.18	0.44
2:C:202:LYS:NZ	3:E:7:U:OP1	2.39	0.44
2:B:202:LYS:NZ	3:G:7:U:OP1	2.38	0.44
1:A:397:LEU:HD23	1:A:400:LEU:HD12	1.99	0.44
1:A:3:LYS:NZ	1:A:823:ASP:OD2	2.40	0.44
1:D:339:LYS:N	1:D:474:PHE:O	2.49	0.44
1:A:1058:ASP:OD1	1:A:1223:GLN:NE2	2.43	0.44
1:A:156:ASP:HA	1:A:159:GLU:HG2	1.99	0.44
1:D:1029:SER:O	1:D:1112:ARG:NH1	2.51	0.44
2:B:150:LEU:HA	2:B:151:PRO:HD3	1.83	0.43
1:D:1215:ASN:HA	1:D:1218:TRP:HB3	2.00	0.43
1:D:736:ILE:HG12	1:D:802:ILE:HG12	2.00	0.43
1:D:18:ARG:HG2	1:D:797:HIS:CD2	2.52	0.43
1:D:363:ASN:O	1:D:367:ASP:N	2.40	0.43
2:C:165:LEU:C	2:C:166:ASP:OD1	2.57	0.43
1:D:348:SER:OG	1:D:354:GLU:O	2.31	0.43
3:E:9:C:C4	3:E:10:U:C4	3.06	0.43
1:D:817:ARG:NH1	1:D:1206:LEU:O	2.44	0.43
1:D:419:ILE:O	1:D:423:ASP:CB	2.65	0.43
1:D:237:TYR:HE2	1:D:276:LEU:HD13	1.83	0.43
1:A:399:GLN:NE2	1:A:403:TYR:OH	2.46	0.43
2:C:150:LEU:HA	2:C:151:PRO:HD3	1.85	0.43
2:C:214:ILE:HB	2:C:221:GLU:HB2	2.00	0.43
1:A:174:ARG:HD3	1:A:178:GLU:HG3	2.00	0.43
1:D:206:LYS:O	1:D:210:LEU:HB2	2.19	0.43
1:D:359:ARG:HH21	1:D:385:ARG:HG2	1.83	0.43
1:D:468:ASN:HA	1:D:471:LYS:HG2	2.01	0.43
1:D:339:LYS:NZ	1:D:471:LYS:O	2.52	0.43
1:A:91:ASN:O	1:A:95:GLU:CB	2.66	0.42
1:D:1023:ASP:O	1:D:1027:PHE:HB2	2.19	0.42
1:A:830:GLY:HA3	1:A:842:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:LEU:HD12	1:D:970:ALA:HB3	2.01	0.42
1:D:103:LYS:O	1:D:107:LYS:HB2	2.19	0.42
1:D:837:ASN:OD1	1:D:857:ASN:ND2	2.40	0.42
1:A:148:THR:HA	1:A:151:PHE:HB2	2.00	0.42
1:A:40:ASP:OD1	1:A:43:ARG:NH1	2.53	0.42
1:D:235:ASP:O	1:D:239:ALA:CB	2.66	0.42
1:D:828:VAL:HG11	1:D:1188:ALA:HA	2.01	0.42
2:C:139:TYR:O	2:C:143:LEU:HB3	2.19	0.42
1:D:165:GLU:HG2	1:D:167:LYS:HG2	2.01	0.42
3:E:21:C:C5	3:E:22:G:C6	3.07	0.42
1:A:381:TYR:O	1:A:385:ARG:CB	2.66	0.42
1:D:124:ILE:HG13	1:D:125:GLU:HG3	2.02	0.42
1:A:98:GLU:OE2	1:A:177:ASN:ND2	2.53	0.42
1:D:831:ILE:HB	1:D:924:LEU:HB2	2.02	0.42
1:A:829:ILE:HG22	1:A:831:ILE:HG13	2.02	0.42
1:D:258:TYR:HA	1:D:261:LEU:HB3	2.01	0.42
2:C:143:LEU:HA	2:C:146:ILE:HG22	2.01	0.42
1:D:202:VAL:HA	1:D:206:LYS:HE2	2.02	0.42
1:A:738:LEU:HD23	1:A:800:ILE:HG22	2.02	0.41
1:D:1058:ASP:O	1:D:1061:LYS:NZ	2.37	0.41
1:D:148:THR:HA	1:D:151:PHE:HD2	1.85	0.41
1:A:1037:VAL:HG23	1:A:1042:LEU:H	1.85	0.41
2:C:167:PRO:HG3	2:C:211:VAL:HG22	2.02	0.41
1:D:1218:TRP:O	1:D:1222:ALA:HB2	2.20	0.41
1:A:861:ASN:O	1:A:867:ARG:HA	2.21	0.41
1:D:271:PRO:HA	1:D:484:GLU:HB3	2.02	0.41
1:A:922:ILE:HB	1:A:993:ILE:HA	2.02	0.41
1:D:1097:GLU:O	1:D:1101:LYS:HB3	2.20	0.41
1:A:788:ARG:NH2	3:G:6:C:OP2	2.51	0.41
1:A:909:HIS:CE1	3:G:18:G:H4'	2.55	0.41
1:A:123:ILE:HG23	1:A:124:ILE:HG23	2.02	0.41
1:A:856:LEU:HD13	1:A:907:VAL:HG22	2.02	0.41
1:A:405:ASP:HB2	1:A:408:LEU:HD12	2.03	0.41
1:A:895:ASN:O	1:A:899:LEU:HB2	2.20	0.41
1:D:206:LYS:HD2	1:D:240:ILE:HG23	2.03	0.41
1:D:581:ILE:HD11	1:D:680:VAL:HG13	2.02	0.41
1:A:1046:ALA:HB2	1:A:1064:LYS:HD3	2.03	0.41
1:A:913:GLU:O	1:A:917:LYS:CB	2.69	0.41
1:A:20:LYS:HB2	3:G:4:U:H5'	2.01	0.41
1:A:468:ASN:HA	1:A:471:LYS:HG2	2.03	0.41
1:A:560:LYS:HG3	1:A:561:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:TYR:N	1:A:1061:LYS:O	2.49	0.41
1:A:1122:ALA:O	1:A:1126:SER:OG	2.34	0.41
1:A:480:THR:OG1	1:A:481:ASN:N	2.54	0.41
1:A:11:TYR:OH	1:A:977:THR:O	2.33	0.41
1:D:347:ILE:HD12	1:D:350:ASP:HB2	2.02	0.41
1:D:350:ASP:HB3	1:D:417:ILE:HD13	2.03	0.41
1:A:895:ASN:O	1:A:899:LEU:CB	2.69	0.41
1:D:775[A]:LYS:HD3	1:D:775[A]:LYS:HA	1.83	0.41
1:A:1189:ARG:NH2	1:A:1225:SER:OG	2.45	0.40
1:A:19:PHE:O	1:A:795:GLU:HA	2.21	0.40
1:D:20:LYS:HG3	1:D:793:GLN:HE21	1.85	0.40
1:D:828:VAL:HB	1:D:844:VAL:HG12	2.03	0.40
1:A:726:LEU:HD11	1:A:964:PRO:HB3	2.04	0.40
1:D:718:ASN:ND2	3:E:4:U:O4	2.55	0.40
1:A:757:VAL:HG12	2:B:186:MET:HE2	2.04	0.40
2:B:165:LEU:C	2:B:166:ASP:OD1	2.59	0.40
2:C:160:TYR:HB3	2:C:198:ILE:HD13	2.03	0.40
1:A:1155:LYS:HD2	1:A:1159:GLY:HA2	2.04	0.40
1:A:326:LYS:HA	1:A:415:LYS:HZ2	1.86	0.40
2:C:170:LEU:HD22	2:C:211:VAL:HG11	2.03	0.40
1:D:1218:TRP:O	1:D:1222:ALA:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1111/1228 (90%)	1019 (92%)	92 (8%)	0	100 100
1	D	1108/1228 (90%)	1020 (92%)	87 (8%)	1 (0%)	51 84
2	B	115/234 (49%)	94 (82%)	19 (16%)	2 (2%)	9 42
2	C	115/234 (49%)	90 (78%)	22 (19%)	3 (3%)	5 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2449/2924 (84%)	2223 (91%)	220 (9%)	6 (0%)	50 80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1102	TYR
2	C	189	ALA
2	B	218	ASP
2	B	219	GLU
2	C	218	ASP
2	C	220	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1010/1115 (91%)	1002 (99%)	8 (1%)	81 88
1	D	1006/1115 (90%)	1001 (100%)	5 (0%)	88 93
2	B	110/217 (51%)	105 (96%)	5 (4%)	27 54
2	C	110/217 (51%)	106 (96%)	4 (4%)	35 60
All	All	2236/2664 (84%)	2214 (99%)	22 (1%)	77 85

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	582	ASN
1	A	584	LYS
1	A	850	ILE
1	A	921	VAL
1	A	922	ILE
1	A	963	ASN
1	A	1073	ARG
2	B	145	ASN

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Mol	Chain	Res	Type
2	B	205	LEU
2	B	217	ARG
2	B	218	ASP
2	B	222	ARG
2	C	145	ASN
2	C	205	LEU
2	C	217	ARG
2	C	222	ARG
1	D	340	ASN
1	D	582	ASN
1	D	584	LYS
1	D	963	ASN
1	D	1073	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	186	ASN
1	A	340	ASN
1	A	399	GLN
1	A	582	ASN
1	A	797	HIS
1	A	803	ASN
1	A	813	ASN
1	A	963	ASN
1	A	989	GLN
1	A	1186	ASN
2	B	145	ASN
2	C	145	ASN
2	C	181	GLN
1	D	63	ASN
1	D	340	ASN
1	D	582	ASN
1	D	718	ASN
1	D	803	ASN
1	D	813	ASN
1	D	864	ASN
1	D	963	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	24/42 (57%)	10 (41%)	1 (4%)
3	G	24/42 (57%)	11 (45%)	1 (4%)
All	All	48/84 (57%)	21 (43%)	2 (4%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	2	A
3	E	3	U
3	E	12	A
3	E	14	U
3	E	15	G
3	E	18	G
3	E	20	U
3	E	21	C
3	E	23	G
3	E	24	U
3	G	2	A
3	G	3	U
3	G	9	C
3	G	11	A
3	G	12	A
3	G	14	U
3	G	15	G
3	G	18	G
3	G	21	C
3	G	23	G
3	G	24	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	23	G
3	G	23	G

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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.

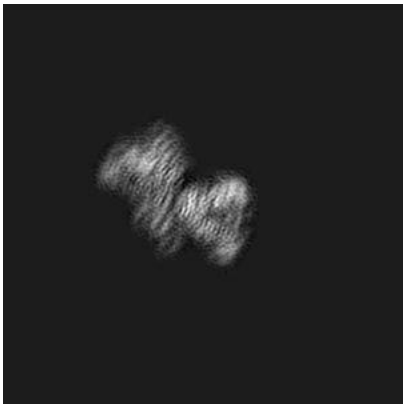
5.8 Polymer linkage issues

There are no chain breaks in this entry.

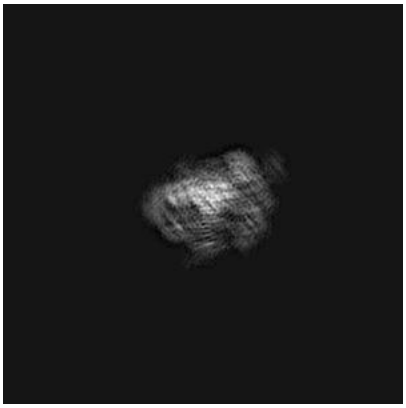
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0705. These are intended to permit visual inspection of the internal detail of the map and identification of artifacts.

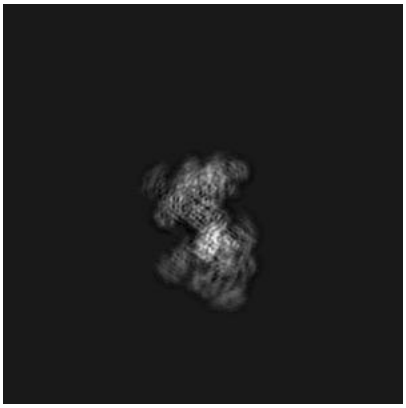
6.1 Orthogonal projections



X



Y

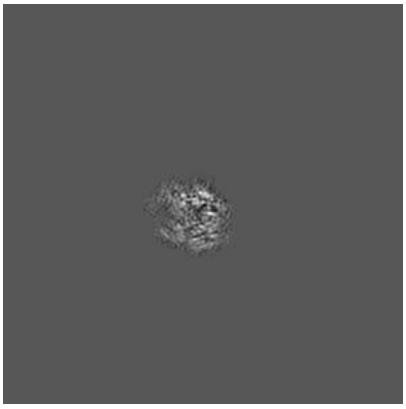


Z

The images above show the map projected in three orthogonal projections, in greyscale.

6.2 Central slices

X



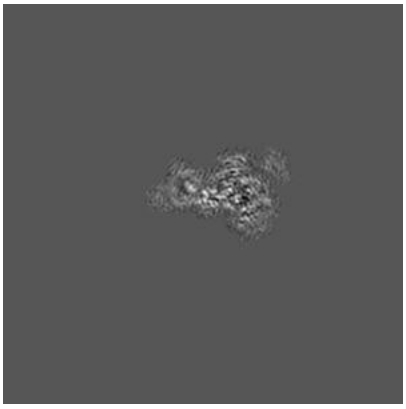
Y

Z

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

6.3 Largest variance slices (i)

X Index: 211

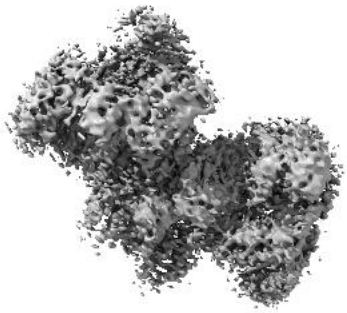


Y Index: 156

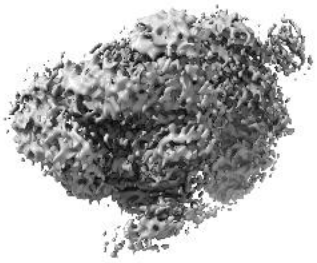
Z Index: 205

The images above show the highest variance slices of the map in three orthogonal directions, in greyscale.

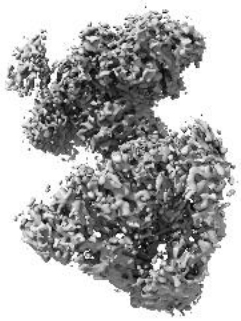
6.4 Orthogonal surface views (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. This in conjunction with the slice images can indicate whether an appropriate contour level has been selected.

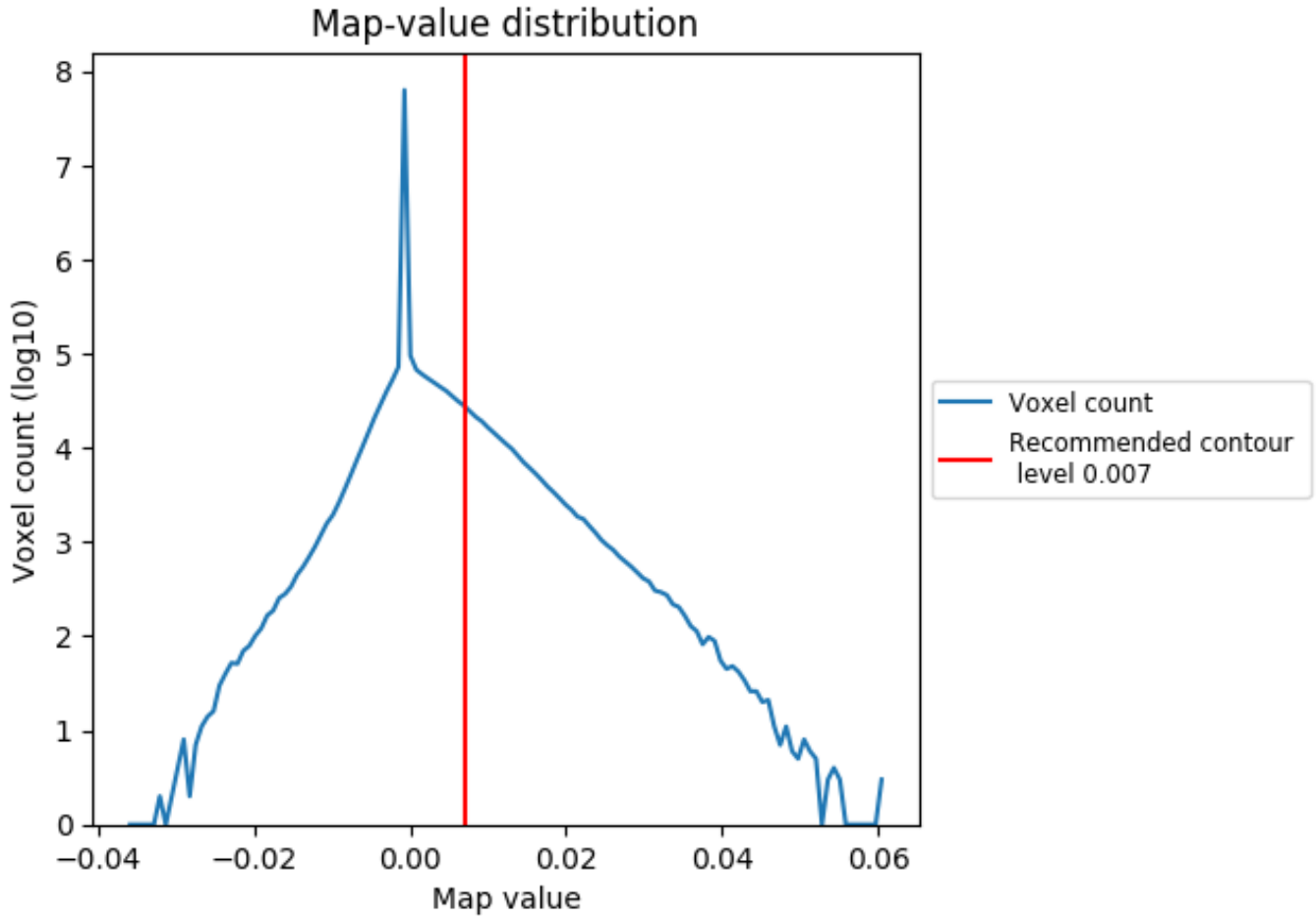
6.5 Mask visualisation (i)

This section was not generated. No masks were provided.

7 Map analysis

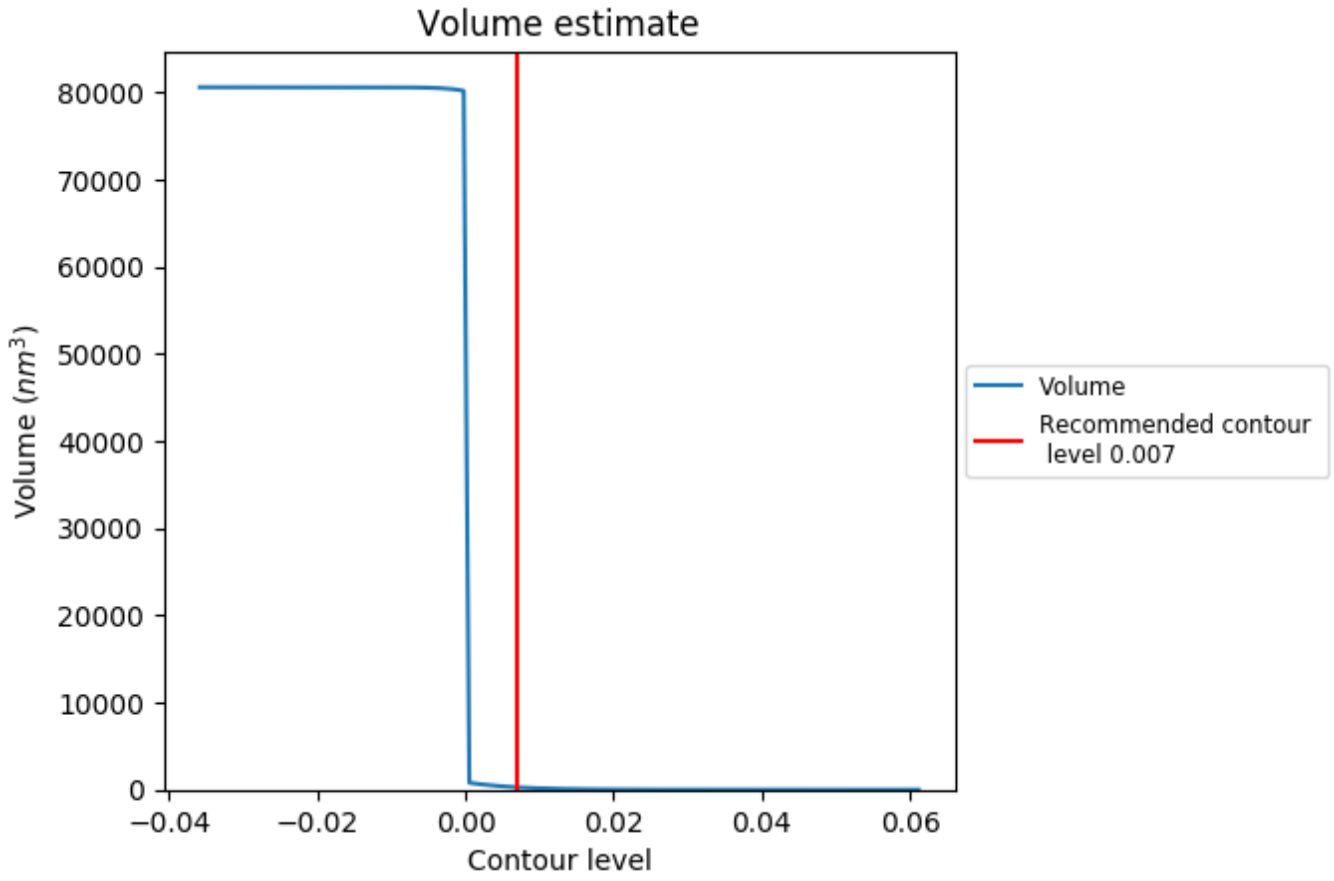
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

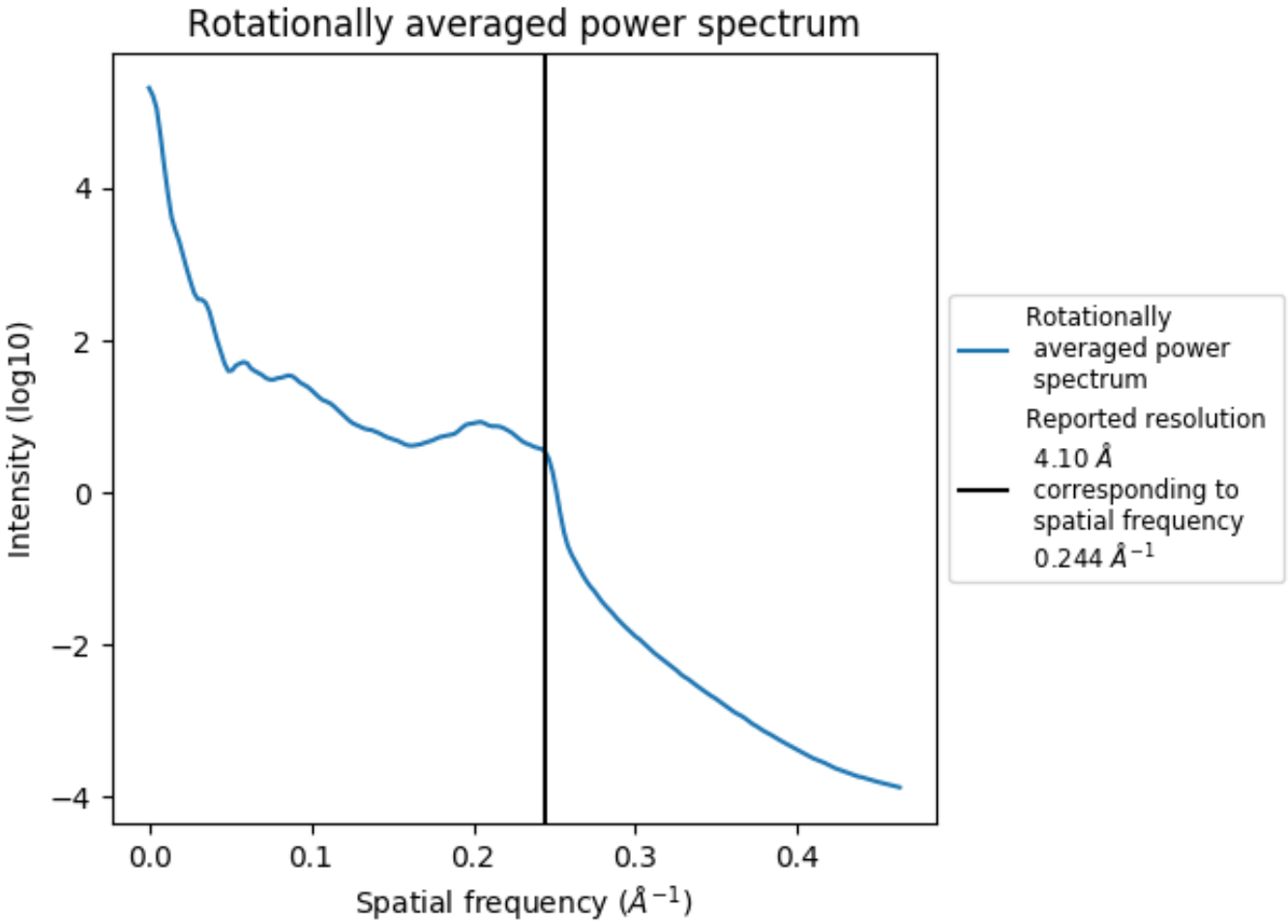
7.2 Volume estimate



The volume at the recommended contour level is 272 nm^3; this corresponds to an approximate mass of 245 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)



8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution for single-particle and subtomogram-averaging methods. 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. Curves are displayed for 3σ, 1-bit and 1/2-bit in addition to lines showing the 0.143 gold standard cut-off, 0.333 cut-off and legacy 0.5 cut-off.

8.1 Resolution estimates

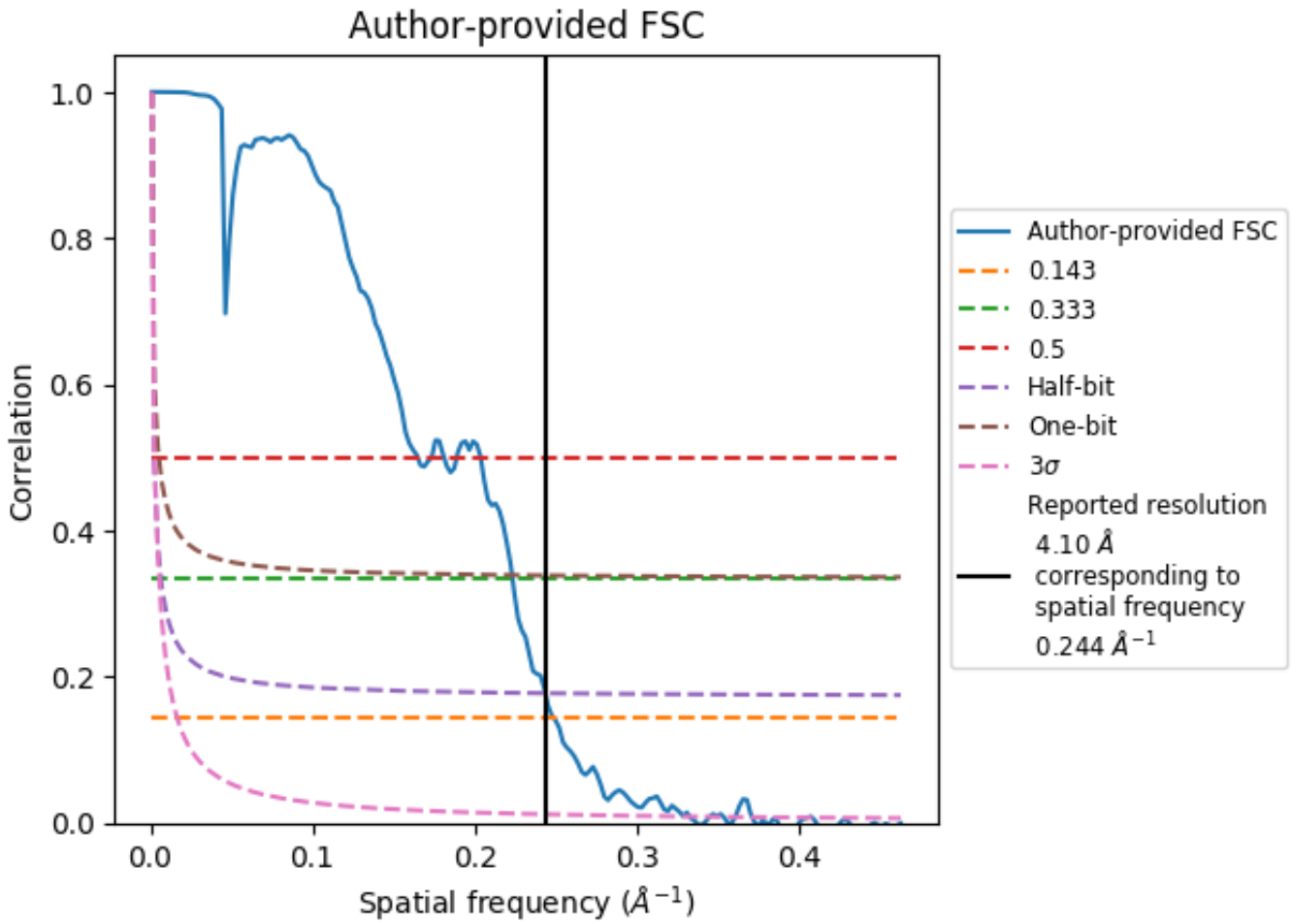
These are global values for the map.

Source	Criterion	Resolution estimate (Å)
Reported value	FSC 0.143 CUT-OFF	4.10
Author-provided FSC	FSC 0.5 CUT-OFF	6.15
Author-provided FSC	FSC 1 BIT CUT-OFF	4.53
Author-provided FSC	FSC 0.33 CUT-OFF	4.52
Author-provided FSC	FSC 1/2 BIT CUT-OFF	4.14
Author-provided FSC	FSC 0.143 CUT-OFF	4.06
Author-provided FSC	FSC 3 SIGMA CUT-OFF	3.03

8.2 Calculated FSC

This section was not generated. Half-maps were not provided.

8.3 Author-provided FSC (i)

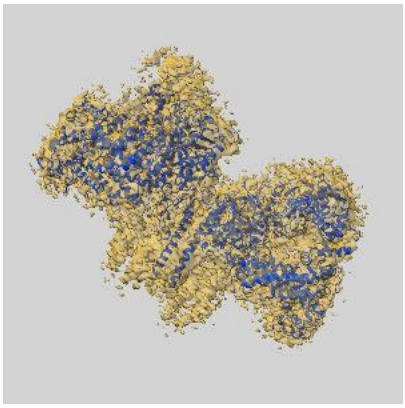


This FSC information was provided by the depositor.

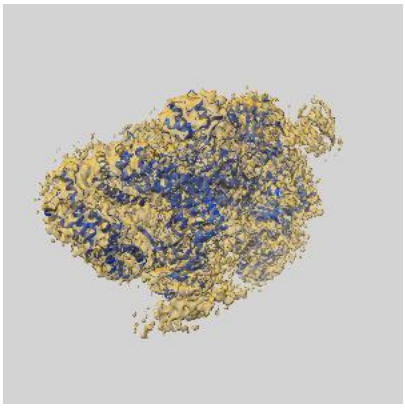
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0705 and PDB model 6KLB. Per-residue inclusion information can be found in section 3 on page 5.

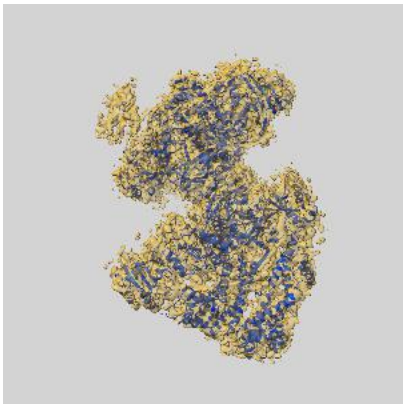
9.1 Map-model overlay



X



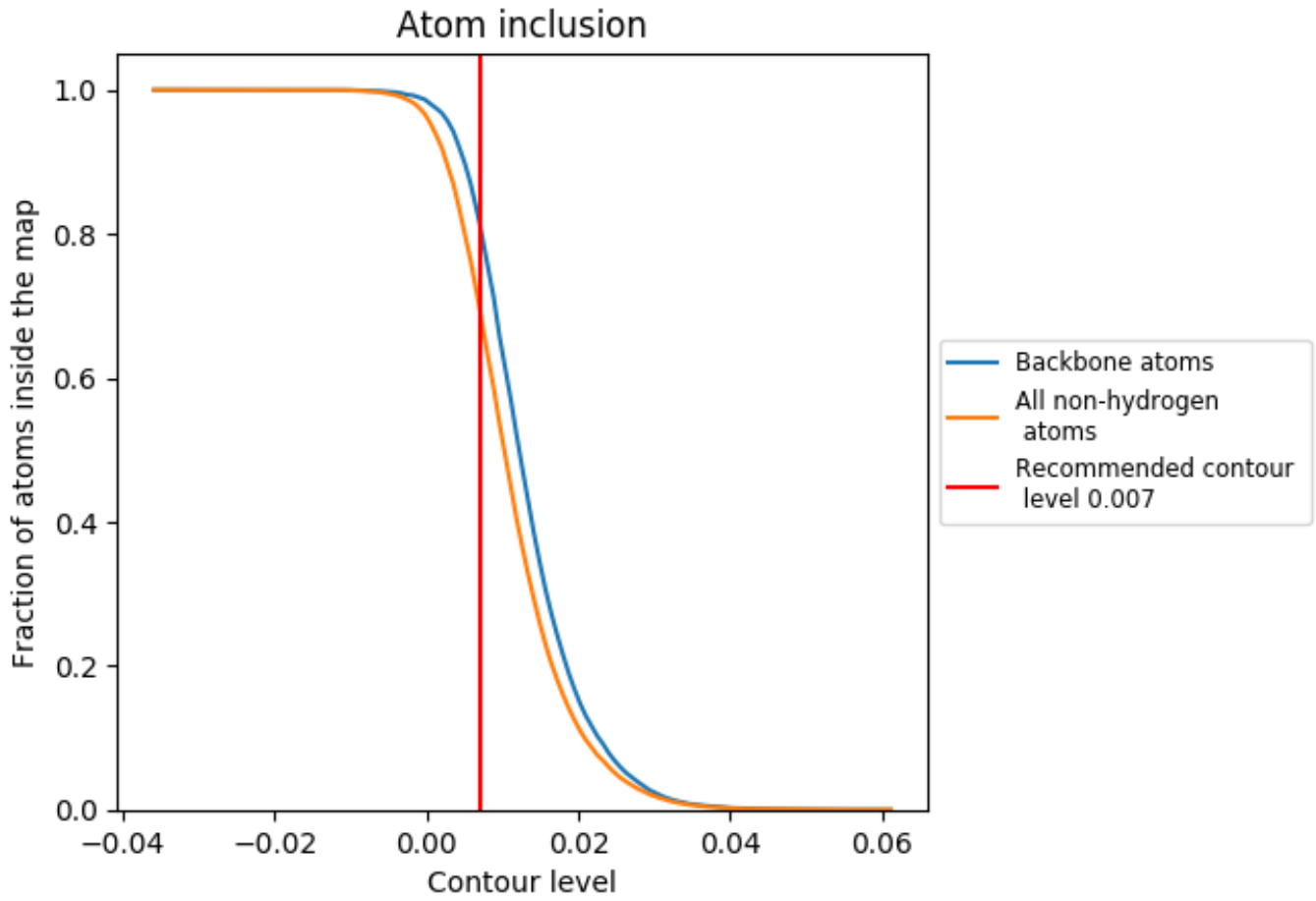
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.