Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 08:24 AM JST

PDB ID	:	6LXE
EMDB ID	:	EMD-30006
Title	:	DROSHA-DGCR8 complex
Authors	:	Jin, W.; Wang, J.; Liu, C.P.; Wang, H.W.; Xu, R.M.
Deposited on	:	2020-02-10
Resolution	:	4.20 Å(reported)
Based on initial model	:	5B16

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

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

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

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

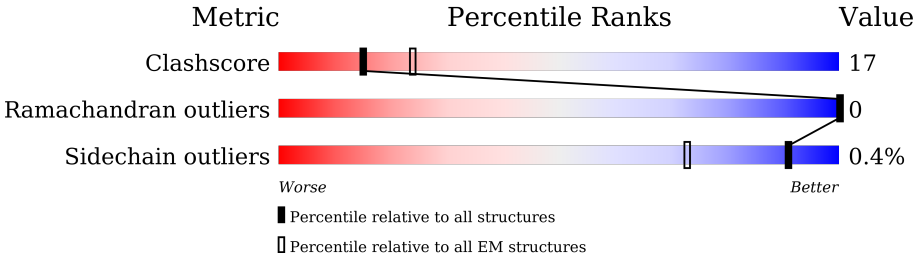
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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

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

Mol	Chain	Length	Quality of chain
1	A	990	51% 27% 22%
2	B	773	97%
2	C	773	97%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6519 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 Ribonuclease 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	768	6133	3910	1073	1111	39	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1045	GLN	GLU	engineered mutation	UNP Q9NRR4
A	1222	GLN	GLU	engineered mutation	UNP Q9NRR4
A	1375	HIS	-	expression tag	UNP Q9NRR4
A	1376	HIS	-	expression tag	UNP Q9NRR4
A	1377	HIS	-	expression tag	UNP Q9NRR4
A	1378	HIS	-	expression tag	UNP Q9NRR4
A	1379	HIS	-	expression tag	UNP Q9NRR4
A	1380	HIS	-	expression tag	UNP Q9NRR4

- Molecule 2 is a protein called Microprocessor complex subunit DGCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	24	205	125	39	40	1	0	0
2	C	21	179	110	32	36	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

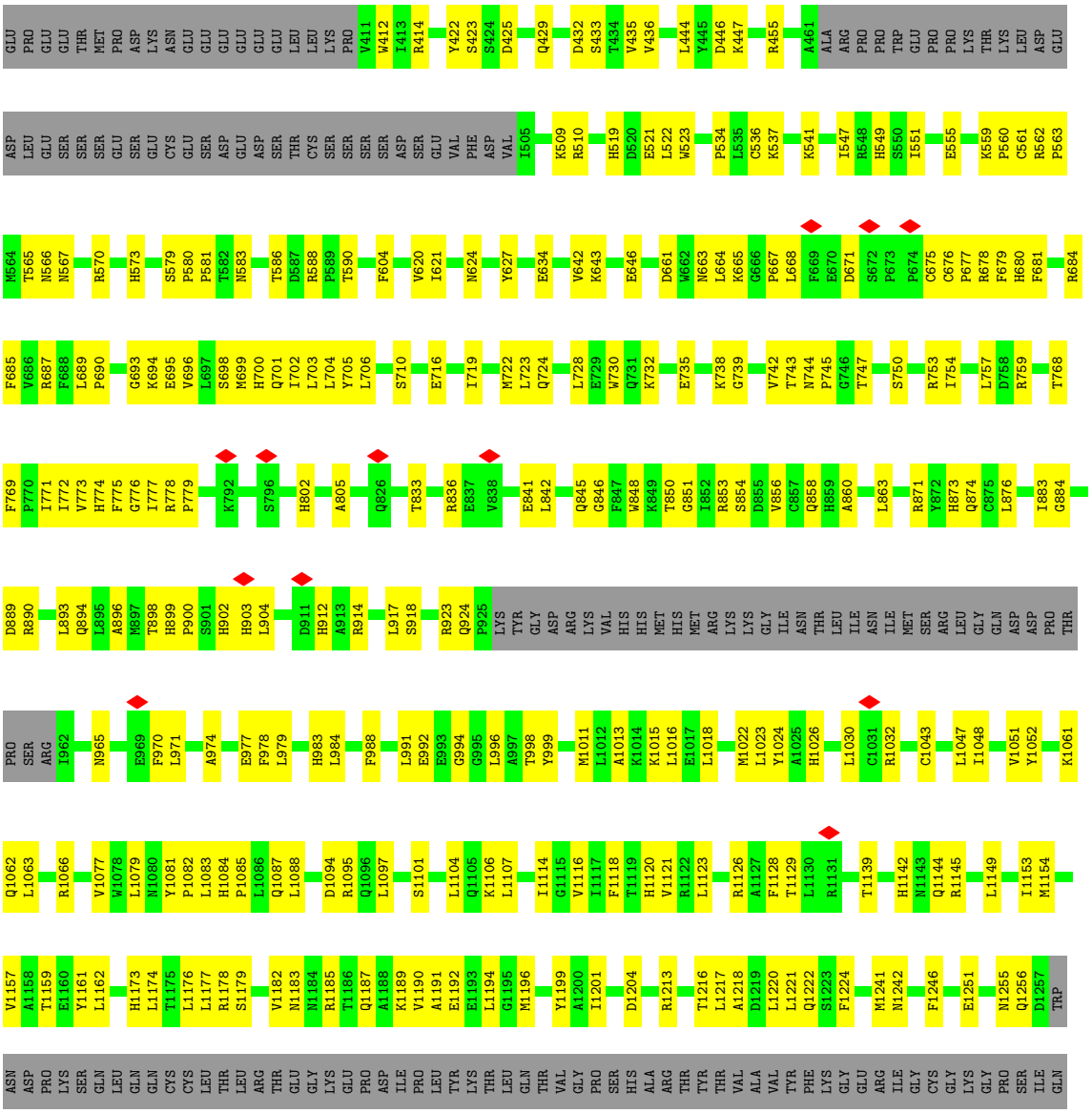
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	2	2	2	0

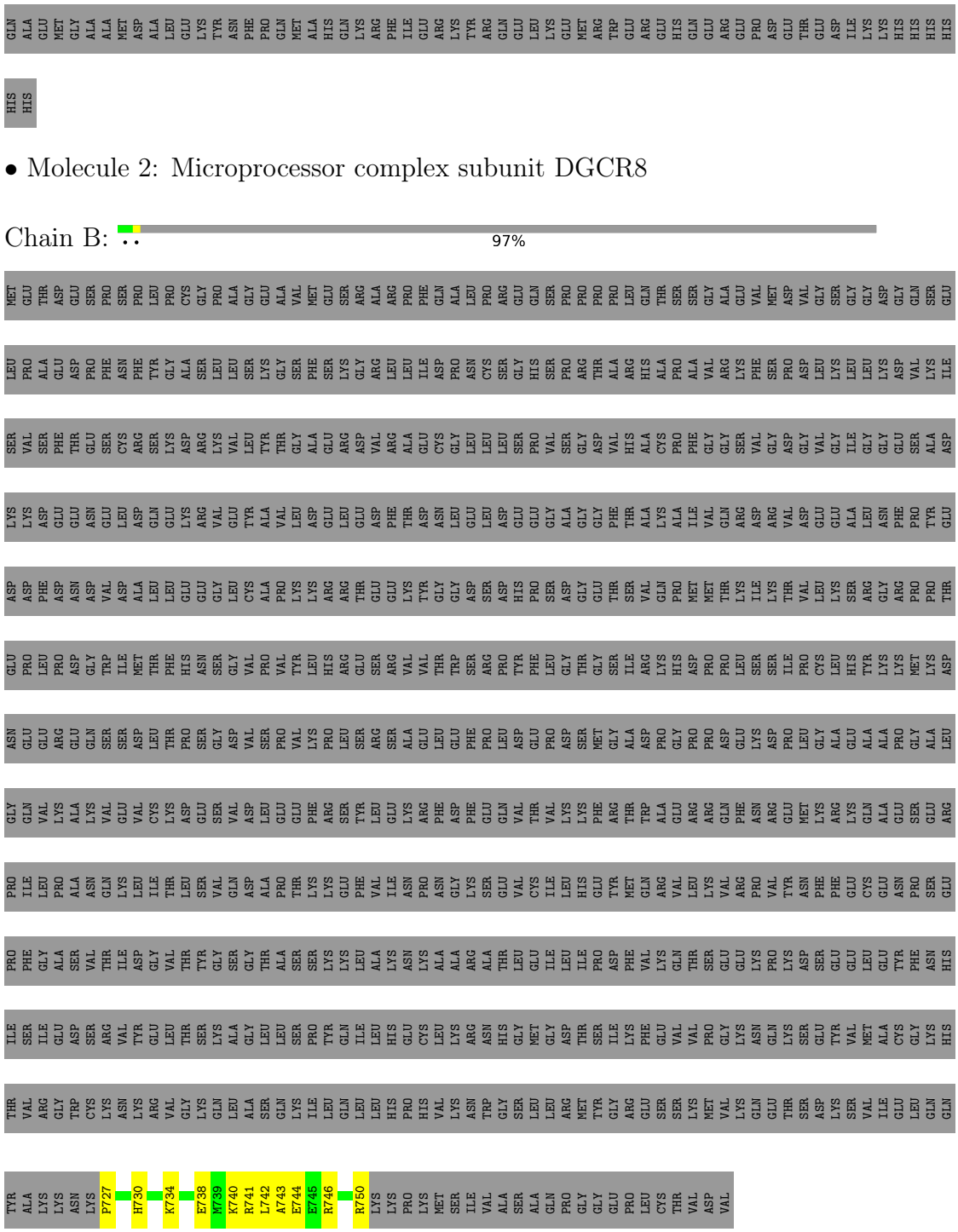
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribonuclease 3

Chain A: 51% 27% 22%



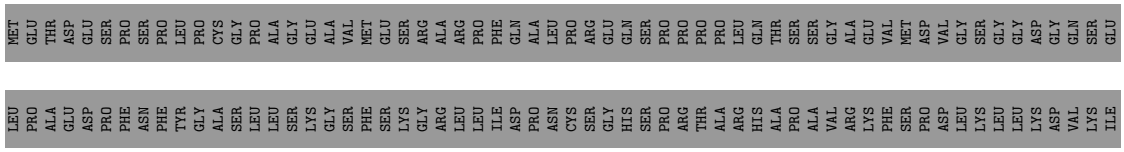


• Molecule 2: Microprocessor complex subunit DGCR8

Chain B: 97%

• Molecule 2: Microprocessor complex subunit DGCR8

Chain C: 97%



SER VAL SER PHE THR GLU SER CYS ARG SER LYS ASP ARG LYS VAL LEU TYR THR GLY ALA GLU ARG ASP VAL ARG ALA GLU CYS GLY LEU LEU LEU SER PRO VAL SER GLY ASP VAL HIS ALA CYS PRO PHE GLY GLY SER VAL GLY ASP GLY VAL GLY ILE GLY GLY GLU SER ALA ASP
LYS LYS ASP GLU GLU ASN GLU LEU ASP GLN GLU LYS ARG VAL GLU TYR ALA VAL LEU ASP GLU LEU GLU ASP PHE THR ASP ASN LEU GLU LEU ASP GLU GLU GLY ALA GLY GLY PHE THR ALA LYS ALA ILE VAL GLN ARG ASP ARG VAL ASP GLU GLU ALA LEU ASN PHE PRO TYR GLU
ASP ASP PHE ASP ASN ASP VAL ASP ALA LEU LEU GLU GLU LEU ASP ALA PRO LYS LYS ARG ARG THR GLU GLU LYS TYR GLY GLY ASP SER ASP HIS PRO SER ASP GLY GLU THR SER VAL GLN PRO MET MET THR LYS ILE LYS THR VAL LEU LYS SER ARG GLY ARG PRO THR
GLU PRO LEU PRO ASP GLY TRP ILE MET THR PHE HIS ASN SER GLY VAL PRO VAL TYR LEU HIS ARG GLU SER ARG VAL VAL THR TRP SER ARG PRO TYR PHE LEU GLY THR GLY SER ILE ARG LYS HIS ASP PRO PRO LEU SER LEU CYS LEU HIS TYR LYS LYS MET LYS ASP
ASN GLU GLU ARG GLU GLN SER SER ASP LEU THR PRO SER GLY ASP VAL SER PRO VAL LYS LEU PRO LEU SER ARG SER ALA GLU LEU GLU PHE PRO LEU ASP GLU GLU LYS ASP PRO LEU GLY ALA GLU ALA ALA ARG PRO PRO ASP GLY ALA ASP LEU
GLY GLN VAL LYS ALA LYS VAL GLU VAL CYS LYS ASP VAL GLU GLU LYS ARG PHE ASP PHE GLU GLN VAL THR VAL LYS LYS PHE ARG THR TRP ALA GLU ARG ARG GLN PHE ASN ARG GLU MET LYS ARG LYS GLN ALA GLU SER GLU ARG
PRO ILE LEU PRO ALA ASN GLN LYS LEU ILE THR LEU SER VAL GLN ASP ALA PRO THR LYS LYS GLU PHE VAL ILE ASN PRO ASN GLY LYS SER GLU VAL CYS ILE LEU HIS GLU TYR MET GLN ARG VAL LEU LYS VAL ARG PRO VAL TYR ASN PHE PHE GLU CYS GLU ASN PRO SER GLU
PRO PHE GLY ALA SER VAL THR ILE ASP GLY VAL THR TYR GLY SER GLY THR ALA SER SER LYS LYS LEU ALA LYS ASN LYS ALA ALA ARG ALA THR LEU GLU ILE LEU ILE PRO ASP PHE VAL LYS GLN THR SER GLU GLU LYS PRO LYS ASP SER GLU GLU GLU LEU GLU TYR PHE ASN HIS
ILE SER ILE GLU ASP SER ARG VAL TYR GLU LEU THR SER LYS ALA GLY LEU LEU SER PRO TYR GLN ILE LEU HIS GLU CYS LEU LYS ARG ASN HIS GLY MET GLY ASP THR SER ILE LYS PHE GLU VAL VAL PRO GLY LYS ASN GLN LYS SER GLU TYR VAL MET ALA CYS GLU GLY LYS HIS
THR VAL ARG GLY TRP CYS LYS ASN LYS ARG VAL GLY LYS GLN LEU ALA SER GLN LYS ILE LEU GLN LEU LEU HIS PRO HIS VAL LYS ASN TRP GLY SER LEU LEU ARG MET TYR GLY ARG GLU SER SER LYS MET VAL LYS GLN GLU THR SER ASP LYS SER VAL ILE GLU LEU GLN GLN
TYR ALA LYS LYS ASN LYS PRO ASN L729 H730 I731 L732 S733 Q736 K740 R741 L742 T749 ARG LYS LYS PRO LYS MET SER ILE VAL ALA SER ALA GLN PRO GLY GLY GLU PRO LEU CYS THR VAL ASP VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109333	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	174.56, 174.56, 174.56	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: ZN

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	0.24	0/6284	0.43	0/8521
2	B	0.21	0/206	0.36	0/272
2	C	0.22	0/179	0.49	0/236
All	All	0.24	0/6669	0.43	0/9029

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6133	0	5916	204	0
2	B	205	0	210	8	0
2	C	179	0	183	5	0
3	A	2	0	0	1	0
All	All	6519	0	6309	214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:SER:OG	1:A:565:THR:HG21	1.32	1.26
1:A:435:VAL:O	1:A:565:THR:HG23	1.49	1.09
1:A:562:ARG:O	1:A:642:VAL:HG21	1.52	1.07
1:A:560:PRO:HA	1:A:676:CYS:HB2	1.30	1.06
1:A:433:SER:OG	1:A:565:THR:CG2	2.03	1.06
1:A:562:ARG:NH2	1:A:567:ASN:HD21	1.60	0.99
1:A:562:ARG:HH21	1:A:567:ASN:HD21	1.05	0.99
1:A:560:PRO:CA	1:A:676:CYS:HB2	2.00	0.91
1:A:536:CYS:SG	1:A:1026:HIS:NE2	2.49	0.85
1:A:562:ARG:CD	1:A:565:THR:HB	2.05	0.85
1:A:560:PRO:HA	1:A:676:CYS:CB	2.08	0.83
1:A:562:ARG:HD3	1:A:565:THR:HB	1.60	0.83
1:A:562:ARG:HH21	1:A:567:ASN:ND2	1.77	0.80
1:A:562:ARG:O	1:A:642:VAL:CG2	2.28	0.80
1:A:565:THR:HG22	1:A:566:ASN:N	1.98	0.76
1:A:1144:GLN:HG3	1:A:1145:ARG:HD2	1.66	0.75
1:A:559:LYS:H	1:A:559:LYS:HD2	1.50	0.75
2:B:746:ARG:HB3	2:B:750:ARG:HE	1.50	0.74
1:A:1187:GLN:HG3	1:A:1221:LEU:HD12	1.69	0.73
1:A:433:SER:HG	1:A:565:THR:HG21	1.54	0.70
1:A:559:LYS:HD2	1:A:559:LYS:N	2.07	0.69
1:A:455:ARG:NH2	1:A:747:THR:O	2.26	0.69
1:A:739:GLY:N	1:A:754:ILE:O	2.25	0.69
1:A:1174:LEU:HB3	1:A:1178:ARG:HH12	1.58	0.69
1:A:1251:GLU:O	1:A:1255:ASN:ND2	2.26	0.69
1:A:1157:VAL:HG21	1:A:1241:MET:HG3	1.75	0.68
1:A:742:VAL:HA	1:A:850:THR:HG21	1.78	0.66
1:A:1217:LEU:HA	1:A:1220:LEU:HD12	1.77	0.66
2:B:727:PRO:HB2	2:B:730:HIS:HB2	1.78	0.66
1:A:573:HIS:HE1	1:A:634:GLU:HB3	1.62	0.64
2:C:741:ARG:HE	2:C:742:LEU:HD22	1.61	0.64
1:A:536:CYS:SG	3:A:1402:ZN:ZN	1.86	0.64
1:A:854:SER:O	1:A:858:GLN:NE2	2.31	0.63
1:A:565:THR:CG2	1:A:566:ASN:N	2.62	0.62
1:A:562:ARG:HB3	1:A:565:THR:O	1.99	0.62
1:A:423:SER:O	1:A:429:GLN:NE2	2.33	0.62
1:A:735:GLU:O	1:A:738:LYS:NZ	2.32	0.62
1:A:1062:GLN:HA	1:A:1079:LEU:HD11	1.81	0.62
1:A:884:GLY:HA3	1:A:1066:ARG:HH12	1.66	0.61
1:A:898:THR:O	1:A:965:ASN:ND2	2.34	0.61
1:A:436:VAL:HG22	1:A:565:THR:OG1	2.01	0.61
1:A:565:THR:HG22	1:A:566:ASN:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ARG:HE	1:A:567:ASN:CG	2.03	0.60
2:B:738:GLU:OE2	2:B:741:ARG:NH2	2.34	0.60
1:A:565:THR:CG2	1:A:566:ASN:H	2.15	0.59
1:A:663:ASN:HD21	1:A:667:PRO:HD3	1.67	0.59
1:A:991:LEU:O	1:A:1145:ARG:NH2	2.34	0.59
1:A:579:SER:O	1:A:581:PRO:HD3	2.02	0.59
1:A:560:PRO:HG3	1:A:675:CYS:O	2.02	0.58
1:A:1061:LYS:NZ	1:A:1079:LEU:O	2.30	0.58
1:A:890:ARG:HH22	1:A:893:LEU:HD13	1.68	0.58
1:A:883:ILE:O	1:A:1066:ARG:NH2	2.37	0.57
1:A:1077:VAL:HG11	2:B:743:ALA:HB2	1.86	0.57
1:A:412:TRP:H	1:A:693:GLY:HA3	1.70	0.57
1:A:716:GLU:HB2	1:A:719:ILE:HG12	1.87	0.56
1:A:444:LEU:HD11	1:A:704:LEU:HD11	1.86	0.56
1:A:1083:LEU:HD22	1:A:1088:LEU:HB3	1.88	0.56
1:A:1204:ASP:OD1	1:A:1204:ASP:N	2.38	0.56
1:A:896:ALA:O	1:A:965:ASN:ND2	2.29	0.56
1:A:1126:ARG:HG3	1:A:1139:THR:HG23	1.86	0.56
1:A:1191:ALA:HB2	1:A:1217:LEU:HD22	1.88	0.56
2:C:731:ILE:HG13	2:C:732:LEU:HD12	1.87	0.56
1:A:536:CYS:SG	1:A:549:HIS:NE2	2.77	0.56
1:A:698:SER:OG	1:A:699:MET:N	2.38	0.56
1:A:1082:PRO:HD3	2:B:746:ARG:HH22	1.71	0.56
1:A:1213:ARG:O	1:A:1216:THR:OG1	2.20	0.55
1:A:562:ARG:CZ	1:A:567:ASN:HD21	2.19	0.55
1:A:1104:LEU:HA	1:A:1107:LEU:HD13	1.88	0.55
1:A:754:ILE:HG12	1:A:772:ILE:HG21	1.89	0.55
1:A:860:ALA:HA	1:A:863:LEU:HD23	1.88	0.54
1:A:999:TYR:OH	2:B:734:LYS:NZ	2.35	0.54
1:A:536:CYS:SG	1:A:1026:HIS:CE1	3.00	0.54
1:A:745:PRO:HD3	1:A:848:TRP:CD1	2.43	0.54
1:A:583:ASN:HB3	1:A:924:GLN:HE22	1.71	0.54
1:A:994:GLY:O	1:A:998:THR:HG23	2.07	0.54
1:A:1242:ASN:HA	1:A:1246:PHE:HB2	1.88	0.54
1:A:722:MET:HG3	1:A:730:TRP:HZ2	1.72	0.54
1:A:898:THR:HA	1:A:1023:LEU:HD13	1.90	0.54
2:C:741:ARG:HH21	2:C:742:LEU:HD13	1.71	0.54
1:A:1201:ILE:HG13	1:A:1220:LEU:HD21	1.89	0.54
1:A:902:HIS:CE1	1:A:1023:LEU:HB3	2.44	0.53
2:C:736:GLN:O	2:C:740:LYS:HG2	2.09	0.53
1:A:1094:ASP:HB3	1:A:1121:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:LYS:HD3	1:A:1199:TYR:HD1	1.74	0.53
1:A:1194:LEU:HD22	1:A:1196:MET:HB2	1.91	0.53
1:A:551:ILE:HD11	1:A:667:PRO:HG2	1.91	0.52
1:A:1129:THR:HG21	1:A:1139:THR:HG21	1.91	0.52
1:A:522:LEU:HD12	1:A:778:ARG:HG2	1.91	0.52
1:A:560:PRO:HD3	1:A:675:CYS:CA	2.40	0.52
1:A:1084:HIS:HE1	1:A:1126:ARG:HH12	1.57	0.52
1:A:1114:ILE:HG22	1:A:1116:VAL:HG13	1.92	0.52
1:A:547:ILE:HG22	1:A:1024:TYR:HB3	1.91	0.52
1:A:586:THR:HG23	1:A:588:ARG:H	1.74	0.52
1:A:971:LEU:HA	1:A:1159:THR:HG21	1.92	0.52
1:A:1173:HIS:O	1:A:1177:LEU:HG	2.10	0.52
1:A:590:THR:HG22	1:A:853:ARG:HB2	1.92	0.51
1:A:1011:MET:O	1:A:1015:LYS:NZ	2.40	0.51
1:A:979:LEU:HD11	1:A:1061:LYS:HG3	1.90	0.51
1:A:970:PHE:CE2	1:A:1159:THR:HG23	2.46	0.51
1:A:536:CYS:HA	1:A:1026:HIS:CD2	2.46	0.51
1:A:1085:PRO:HA	1:A:1088:LEU:HG	1.93	0.51
1:A:664:LEU:HD23	1:A:679:PHE:H	1.76	0.50
1:A:560:PRO:N	1:A:676:CYS:HB2	2.26	0.50
1:A:580:PRO:HG2	1:A:627:TYR:HA	1.93	0.50
1:A:604:PHE:HZ	1:A:856:VAL:HG13	1.77	0.50
1:A:700:HIS:NE2	1:A:701:GLN:OE1	2.45	0.49
1:A:971:LEU:HD21	1:A:1052:TYR:HD2	1.77	0.49
1:A:723:LEU:O	1:A:759:ARG:NH1	2.45	0.49
1:A:1048:ILE:HA	1:A:1051:VAL:HG22	1.94	0.49
1:A:774:HIS:HB3	1:A:842:LEU:HD13	1.93	0.49
1:A:722:MET:O	1:A:730:TRP:NE1	2.41	0.49
1:A:802:HIS:HA	1:A:1030:LEU:HD22	1.93	0.49
1:A:668:LEU:HG	1:A:671:ASP:HB2	1.95	0.49
1:A:992:GLU:HA	1:A:1145:ARG:HH12	1.78	0.49
1:A:1179:SER:O	1:A:1183:ASN:ND2	2.46	0.49
1:A:735:GLU:HA	1:A:738:LYS:HG3	1.96	0.48
1:A:739:GLY:CA	1:A:754:ILE:O	2.61	0.48
1:A:1142:HIS:H	1:A:1144:GLN:NE2	2.11	0.48
1:A:774:HIS:CE1	1:A:776:GLY:HA3	2.49	0.48
1:A:1022:MET:SD	1:A:1023:LEU:N	2.87	0.48
1:A:773:VAL:HG13	1:A:841:GLU:HA	1.95	0.48
1:A:777:ILE:N	1:A:923:ARG:HH22	2.12	0.48
1:A:634:GLU:OE1	1:A:684:ARG:NH2	2.44	0.48
1:A:661:ASP:OD2	1:A:912:HIS:ND1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:HIS:CE1	1:A:1081:TYR:HB3	2.49	0.47
1:A:414:ARG:HH21	1:A:689:LEU:HD23	1.79	0.47
1:A:562:ARG:CD	1:A:565:THR:CB	2.87	0.47
1:A:573:HIS:CE1	1:A:634:GLU:HB3	2.45	0.47
1:A:974:ALA:O	1:A:977:GLU:HG3	2.14	0.47
2:B:742:LEU:O	2:B:746:ARG:HG2	2.14	0.47
1:A:562:ARG:HB2	1:A:567:ASN:OD1	2.14	0.47
1:A:705:TYR:OH	1:A:851:GLY:O	2.26	0.47
1:A:579:SER:HB2	1:A:580:PRO:HD3	1.97	0.47
1:A:1087:GLN:HE22	1:A:1123:LEU:HD22	1.79	0.46
1:A:1097:LEU:O	1:A:1101:SER:OG	2.27	0.46
2:C:733:SER:O	2:C:736:GLN:HG3	2.15	0.46
1:A:414:ARG:HH12	1:A:693:GLY:H	1.63	0.46
1:A:914:ARG:HA	1:A:917:LEU:HG	1.97	0.46
1:A:665:LYS:HE2	1:A:677:PRO:HD3	1.97	0.46
1:A:1190:VAL:O	1:A:1194:LEU:HB2	2.15	0.46
1:A:432:ASP:HB3	1:A:570:ARG:HE	1.80	0.46
1:A:677:PRO:HG2	1:A:680:HIS:NE2	2.31	0.46
1:A:699:MET:O	1:A:702:ILE:HG22	2.16	0.46
1:A:779:PRO:HB3	1:A:914:ARG:HG2	1.98	0.46
1:A:560:PRO:HG3	1:A:675:CYS:C	2.35	0.46
2:B:740:LYS:O	2:B:744:GLU:HG2	2.16	0.45
1:A:422:TYR:CG	1:A:435:VAL:HG13	2.51	0.45
1:A:687:ARG:HB2	1:A:695:GLU:H	1.81	0.45
1:A:743:THR:HG23	1:A:848:TRP:NE1	2.32	0.45
1:A:1047:LEU:O	1:A:1051:VAL:HG13	2.15	0.45
1:A:1218:ALA:O	1:A:1222:GLN:HG2	2.17	0.45
1:A:1013:ALA:HB1	1:A:1018:LEU:HD21	1.99	0.45
1:A:643:LYS:O	1:A:646:GLU:HG2	2.17	0.45
1:A:699:MET:O	1:A:703:LEU:HG	2.17	0.45
1:A:833:THR:HG22	1:A:836:ARG:NH2	2.32	0.44
1:A:1173:HIS:CD2	1:A:1176:LEU:HD22	2.52	0.44
1:A:446:ASP:OD1	1:A:447:LYS:N	2.50	0.44
1:A:768:THR:OG1	1:A:769:PHE:N	2.48	0.44
1:A:1149:LEU:O	1:A:1153:ILE:HG13	2.18	0.44
1:A:687:ARG:HB3	1:A:694:LYS:HA	1.99	0.44
1:A:706:LEU:O	1:A:710:SER:HB3	2.18	0.44
1:A:871:ARG:HA	1:A:874:GLN:HG2	1.99	0.44
1:A:771:ILE:HD12	1:A:845:GLN:HB2	1.98	0.44
1:A:425:ASP:O	1:A:429:GLN:HG2	2.18	0.44
1:A:433:SER:OG	1:A:565:THR:HG22	2.09	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:LEU:O	1:A:732:LYS:HG2	2.18	0.44
1:A:1154:MET:HG2	1:A:1182:VAL:HG22	2.00	0.44
1:A:1063:LEU:HA	1:A:1066:ARG:HE	1.83	0.43
1:A:805:ALA:HB3	1:A:1032:ARG:HH11	1.83	0.43
1:A:988:PHE:HB3	1:A:991:LEU:HB3	2.00	0.43
1:A:534:PRO:HG2	1:A:537:LYS:HG2	2.01	0.43
1:A:759:ARG:HD2	1:A:759:ARG:HA	1.81	0.43
1:A:509:LYS:HE2	1:A:510:ARG:HE	1.83	0.43
1:A:519:HIS:ND1	1:A:521:GLU:HG2	2.34	0.43
1:A:685:PHE:HB2	1:A:696:VAL:HG13	2.00	0.43
1:A:773:VAL:HG12	1:A:775:PHE:HD2	1.84	0.43
1:A:914:ARG:O	1:A:918:SER:OG	2.22	0.43
1:A:873:HIS:NE2	1:A:894:GLN:OE1	2.52	0.43
1:A:978:PHE:HE1	1:A:1153:ILE:HG12	1.84	0.43
1:A:1018:LEU:HD13	1:A:1043:CYS:SG	2.58	0.43
1:A:744:ASN:HD21	1:A:846:GLY:HA2	1.84	0.42
1:A:984:LEU:HD13	1:A:996:LEU:HD22	2.00	0.42
1:A:1126:ARG:HA	1:A:1139:THR:HG23	2.01	0.42
1:A:883:ILE:HG22	1:A:1016:LEU:HD23	2.02	0.42
1:A:1063:LEU:HD12	1:A:1066:ARG:HH21	1.84	0.42
1:A:724:GLN:HA	1:A:759:ARG:NH1	2.35	0.42
1:A:1189:LYS:HA	1:A:1192:GLU:HG3	2.01	0.42
1:A:560:PRO:HA	1:A:676:CYS:SG	2.59	0.42
1:A:536:CYS:SG	1:A:549:HIS:CE1	3.13	0.41
1:A:1094:ASP:HB2	1:A:1120:HIS:HA	2.02	0.41
1:A:1128:PHE:HE1	1:A:1224:PHE:HE1	1.68	0.41
1:A:899:HIS:ND1	1:A:900:PRO:HD2	2.35	0.41
1:A:978:PHE:CE1	1:A:1153:ILE:HG12	2.55	0.41
1:A:1173:HIS:HD2	1:A:1176:LEU:HD22	1.86	0.41
1:A:681:PHE:CZ	1:A:863:LEU:HD12	2.56	0.41
1:A:1161:TYR:HD2	1:A:1162:LEU:HD12	1.85	0.41
1:A:757:LEU:HD13	1:A:772:ILE:HG23	2.02	0.41
1:A:555:GLU:OE1	1:A:678:ARG:NH1	2.40	0.41
1:A:743:THR:OG1	1:A:750:SER:HB3	2.20	0.41
1:A:522:LEU:HD22	1:A:523:TRP:CE3	2.56	0.41
1:A:562:ARG:HE	1:A:567:ASN:ND2	2.18	0.41
1:A:689:LEU:HD12	1:A:690:PRO:HD2	2.02	0.41
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.84	0.41
1:A:889:ASP:OD1	1:A:890:ARG:N	2.54	0.41
1:A:563:PRO:O	1:A:643:LYS:HB2	2.21	0.41
1:A:1185:ARG:HH22	1:A:1256:GLN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:HG23	1:A:627:TYR:HB2	2.02	0.41
1:A:677:PRO:HG2	1:A:680:HIS:CD2	2.56	0.40
1:A:562:ARG:NE	1:A:567:ASN:OD1	2.46	0.40
1:A:1095:ARG:NH1	1:A:1118:PHE:O	2.35	0.40
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.79	0.40
1:A:621:ILE:HD11	1:A:624:ASN:HA	2.03	0.40
1:A:899:HIS:CG	1:A:900:PRO:HD2	2.57	0.40
1:A:903:HIS:ND1	1:A:904:LEU:HG	2.37	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	762/990 (77%)	692 (91%)	70 (9%)	0	100	100
2	B	22/773 (3%)	22 (100%)	0	0	100	100
2	C	19/773 (2%)	19 (100%)	0	0	100	100
All	All	803/2536 (32%)	733 (91%)	70 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	651/894 (73%)	648 (100%)	3 (0%)	88 93
2	B	23/673 (3%)	23 (100%)	0	100 100
2	C	20/673 (3%)	20 (100%)	0	100 100
All	All	694/2240 (31%)	691 (100%)	3 (0%)	91 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	541	LYS
1	A	561	CYS
1	A	753	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	531	ASN
1	A	567	ASN
1	A	663	ASN
1	A	724	GLN
1	A	761	GLN
1	A	858	GLN
1	A	868	HIS
1	A	899	HIS
1	A	924	GLN
1	A	1038	HIS
1	A	1087	GLN
1	A	1144	GLN
1	A	1173	HIS
1	A	1222	GLN
1	A	1255	ASN
2	C	730	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

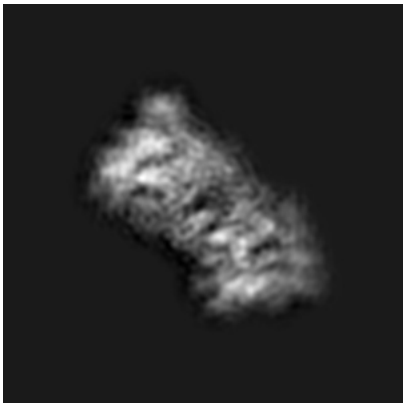
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30006. These allow visual inspection of the internal detail of the map and identification of artifacts.

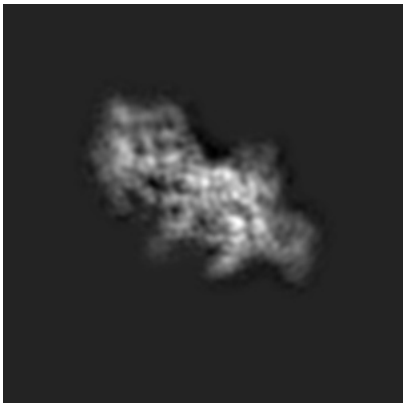
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

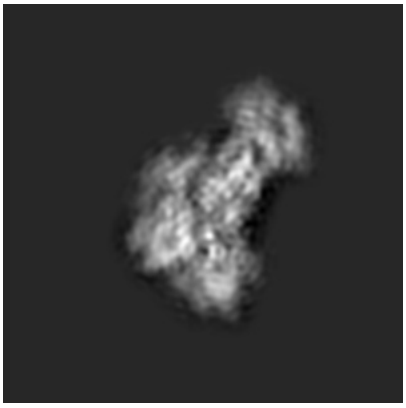
6.1.1 Primary map



X



Y

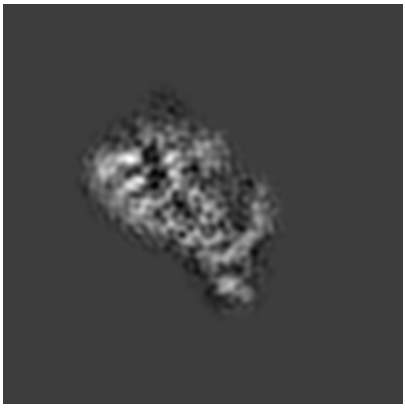


Z

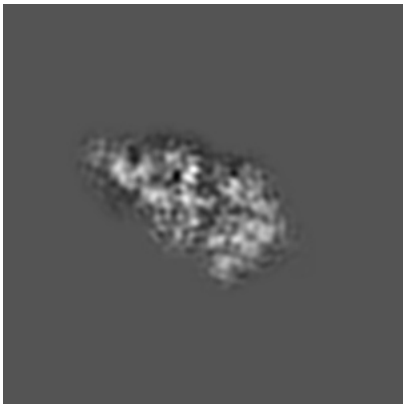
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 80



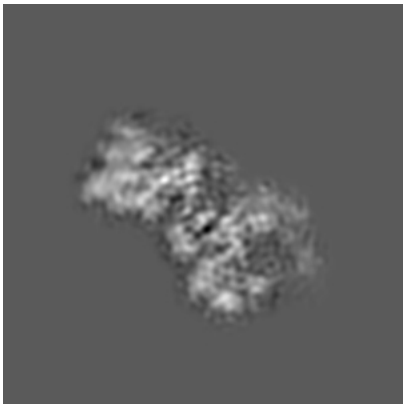
Y Index: 80

Z Index: 80

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

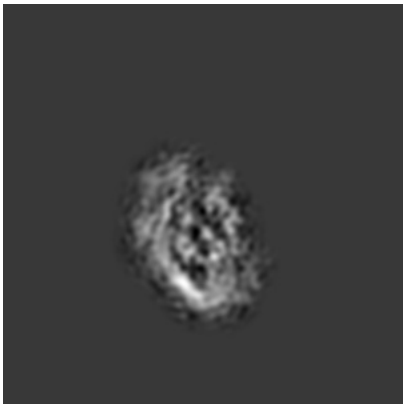
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 91

Y Index: 59



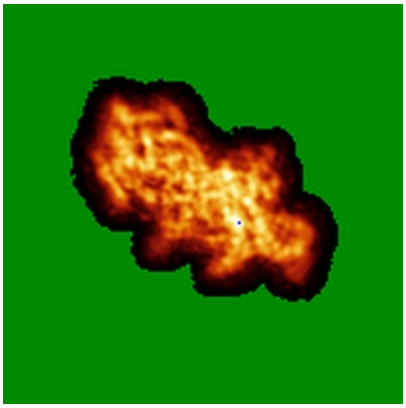
Z Index: 93

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

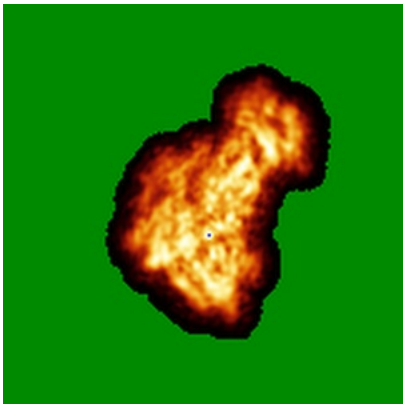
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

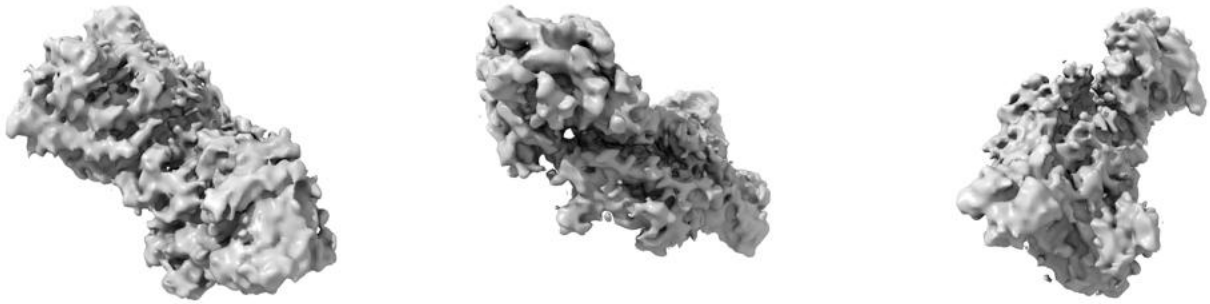


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

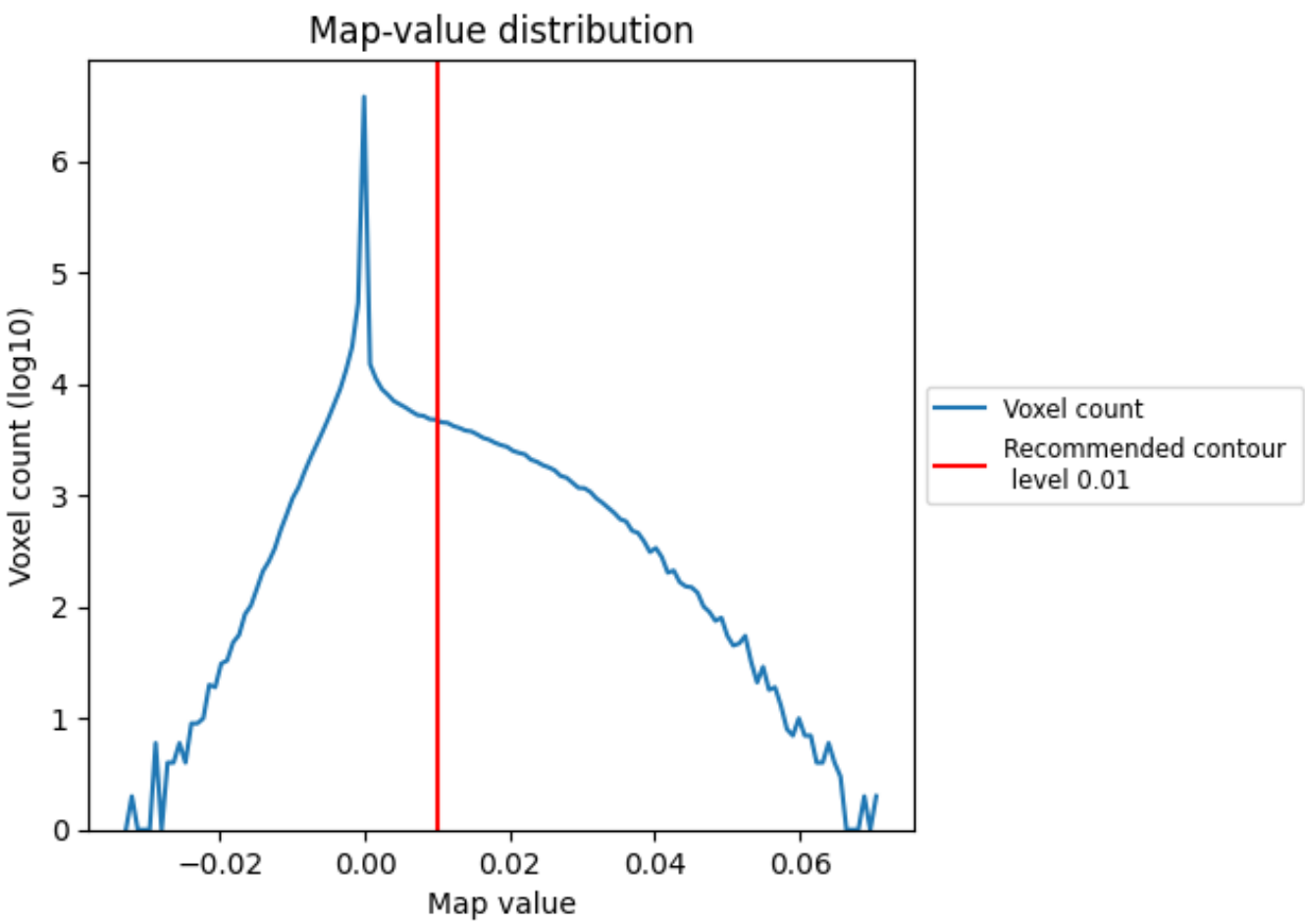
6.6 Mask visualisation (i)

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

7 Map analysis (i)

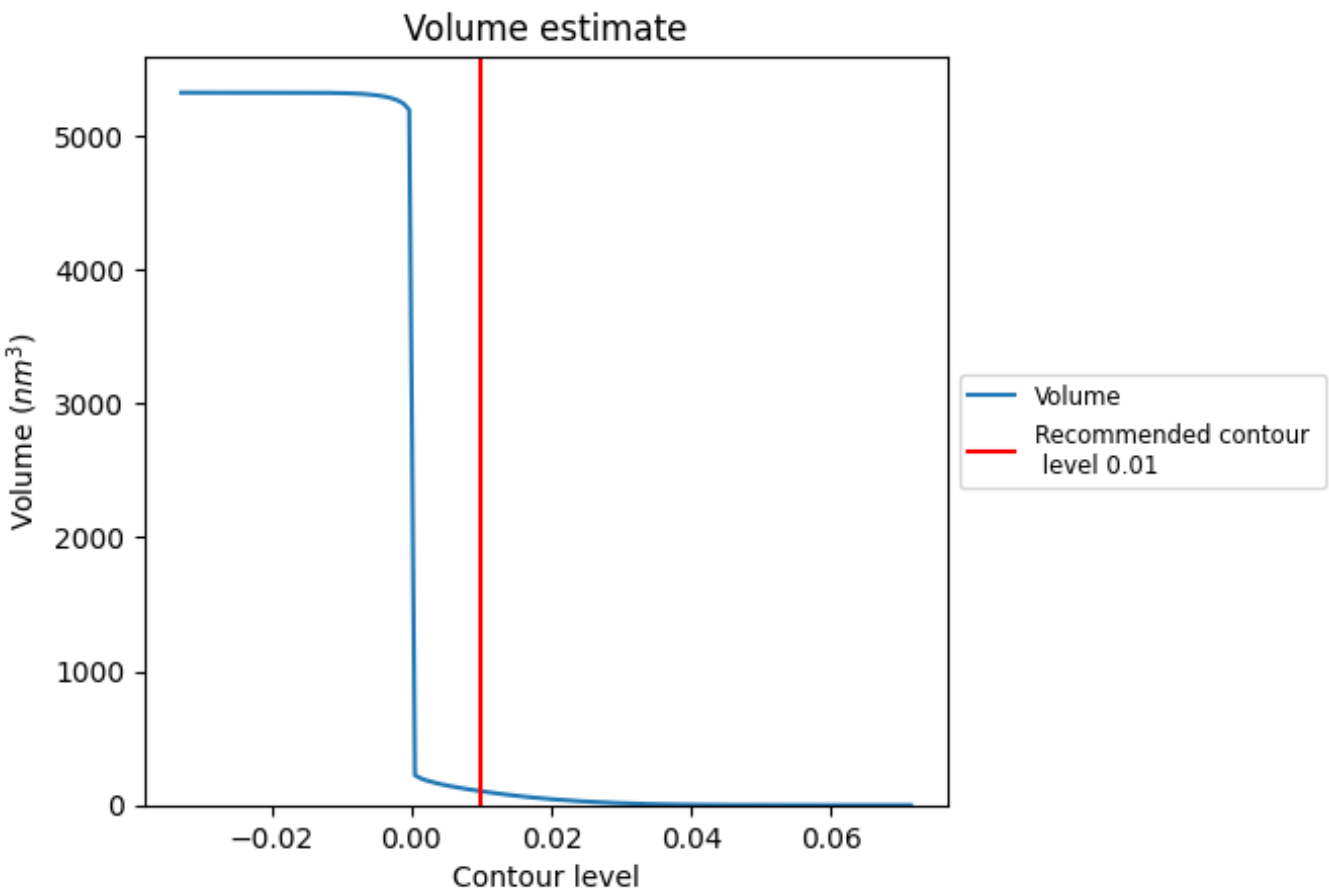
This section contains the results of statistical analysis of the map.

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.

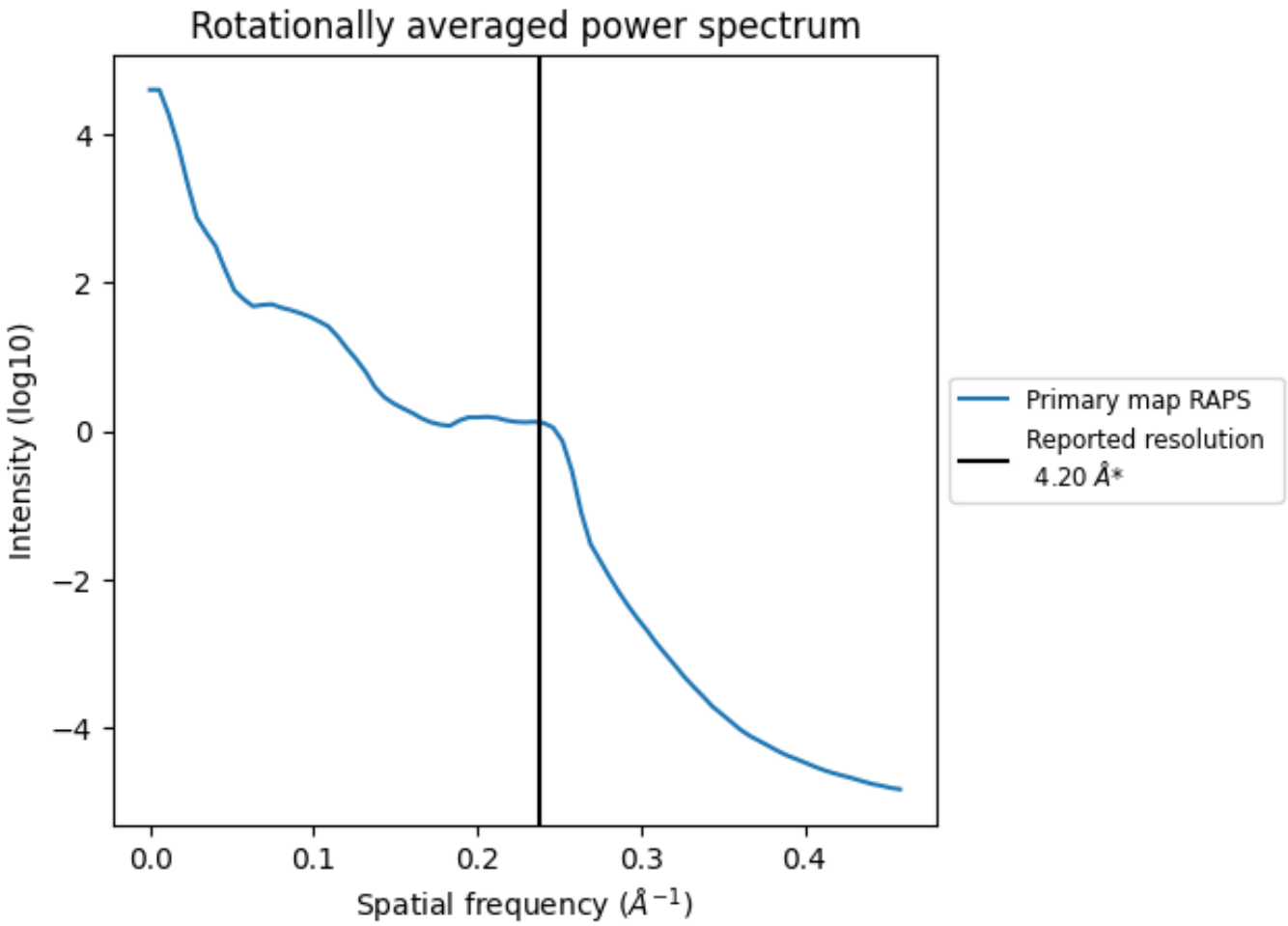
7.2 Volume estimate (i)



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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 0.238 Å^{-1}

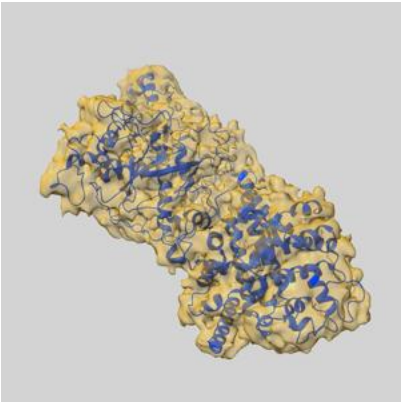
8 Fourier-Shell correlation (i)

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

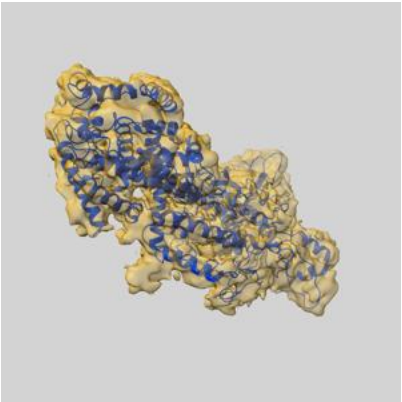
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30006 and PDB model 6LXE. Per-residue inclusion information can be found in section 3 on page 4.

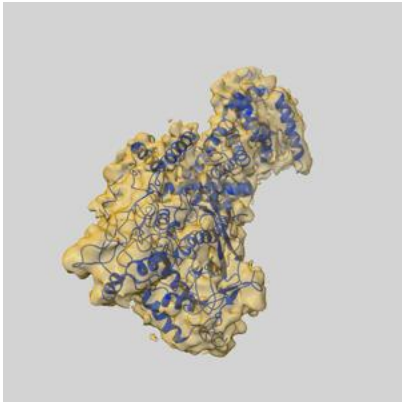
9.1 Map-model overlay (i)



X



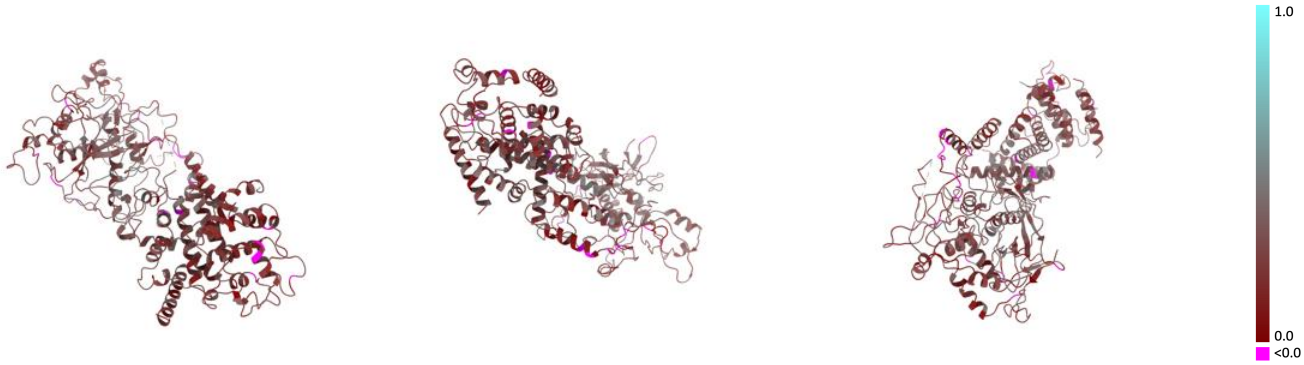
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

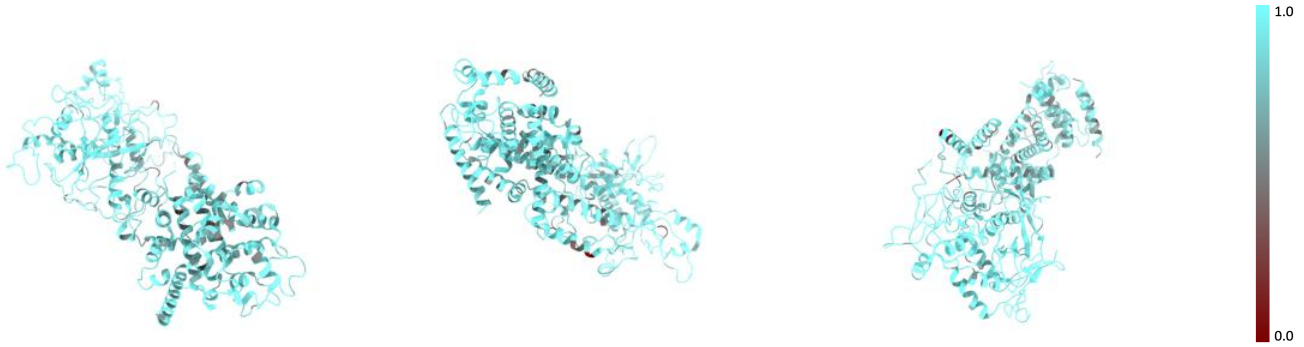
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

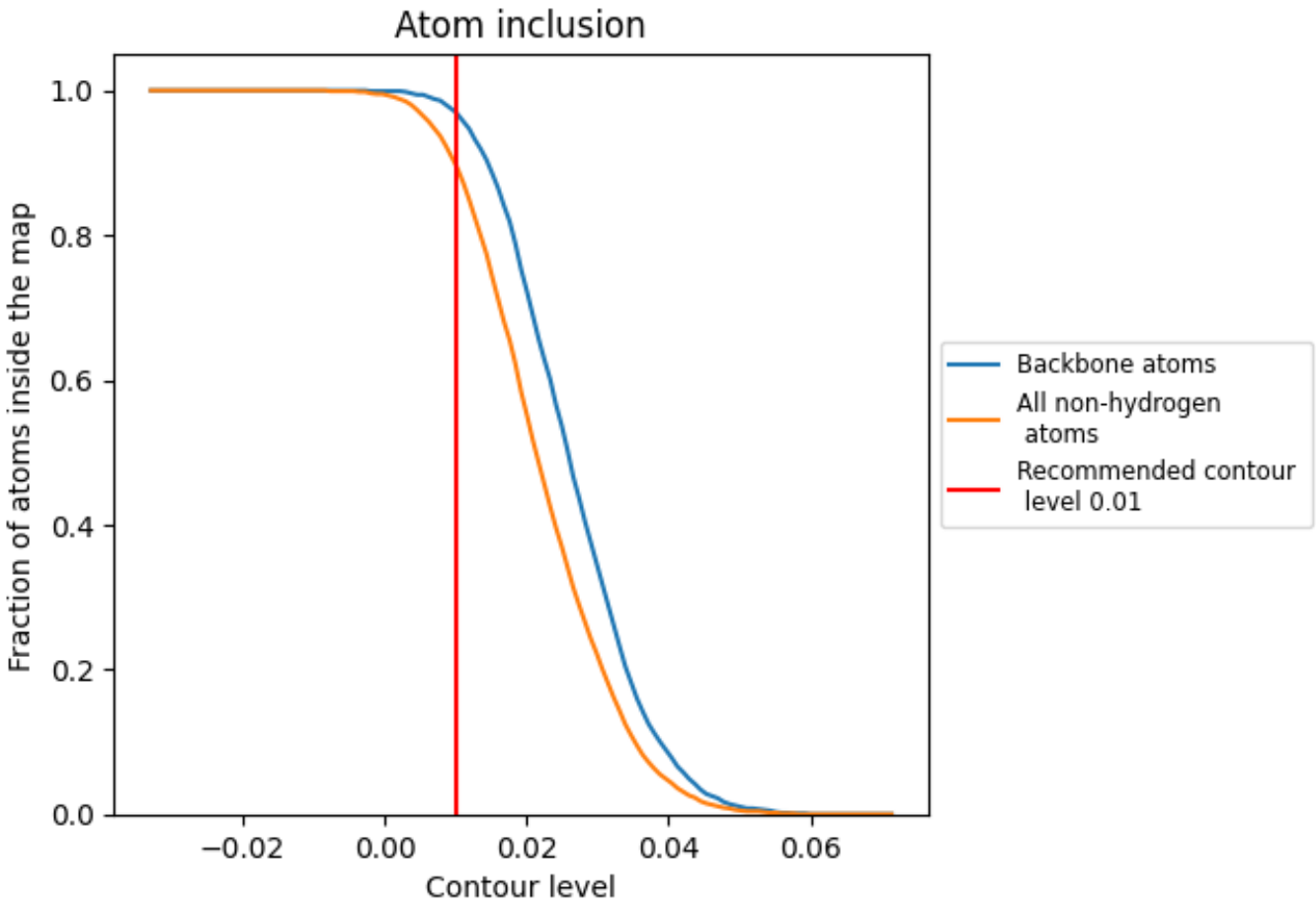
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.2630
A	0.9000	0.2660
B	0.9090	0.2440
C	0.7660	0.1980