Full wwPDB EM Validation Report ⓘ

Jan 29, 2024 – 06:40 pm GMT

PDB ID	:	8CDE
EMDB ID	:	EMD-16570
Title	:	PfCyRPA-PfRIPR complex from Plasmodium falciparum bound to antibody Cy.003
Authors	:	Farrell, B.; Higgins, M.K.
Deposited on	:	2023-01-30
Resolution	:	3.10 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:

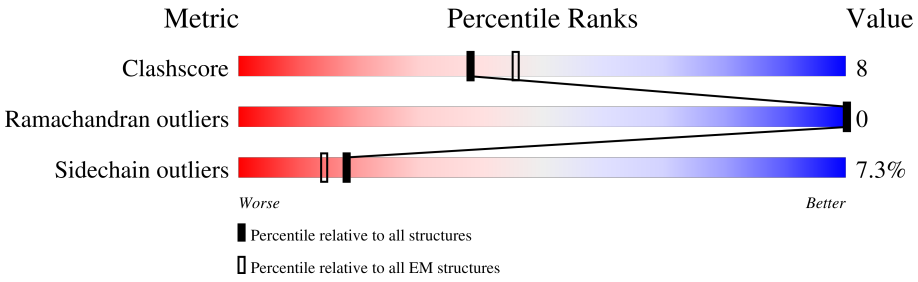
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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

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	1070	44% 11% 45%
2	B	342	69% 18% 10%
3	C	207	71% 25%
4	D	226	71% 22% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10464 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 Rh5-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	589	Total	C	N	O	S	0	0
			4785	3009	799	925	52		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLN	ASN	conflict	UNP O97302
A	144	GLN	ASN	conflict	UNP O97302
A	228	GLN	ASN	conflict	UNP O97302
A	334	GLN	ASN	conflict	UNP O97302
A	480	GLN	ASN	conflict	UNP O97302
A	498	GLN	ASN	conflict	UNP O97302
A	506	GLN	ASN	conflict	UNP O97302
A	526	GLN	ASN	conflict	UNP O97302
A	646	GLN	ASN	conflict	UNP O97302
A	647	GLN	ASN	conflict	UNP O97302
A	964	GLN	ASN	conflict	UNP O97302
A	1021	GLN	ASN	conflict	UNP O97302
A	1087	GLU	-	expression tag	UNP O97302
A	1088	PRO	-	expression tag	UNP O97302
A	1089	GLU	-	expression tag	UNP O97302
A	1090	ALA	-	expression tag	UNP O97302

- Molecule 2 is a protein called Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	307	Total	C	N	O	S	0	0
			2559	1654	406	486	13		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	ALA	SER	conflict	UNP Q8IFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q8IFM8
B	340	ALA	THR	conflict	UNP Q8IFM8
B	363	GLY	-	expression tag	UNP Q8IFM8
B	364	GLY	-	expression tag	UNP Q8IFM8
B	365	GLY	-	expression tag	UNP Q8IFM8
B	366	GLY	-	expression tag	UNP Q8IFM8
B	367	SER	-	expression tag	UNP Q8IFM8
B	368	GLU	-	expression tag	UNP Q8IFM8
B	369	PRO	-	expression tag	UNP Q8IFM8
B	370	GLU	-	expression tag	UNP Q8IFM8
B	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 3 is a protein called Cy.003 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1552	963	263	322	4		

- Molecule 4 is a protein called Cy.003.

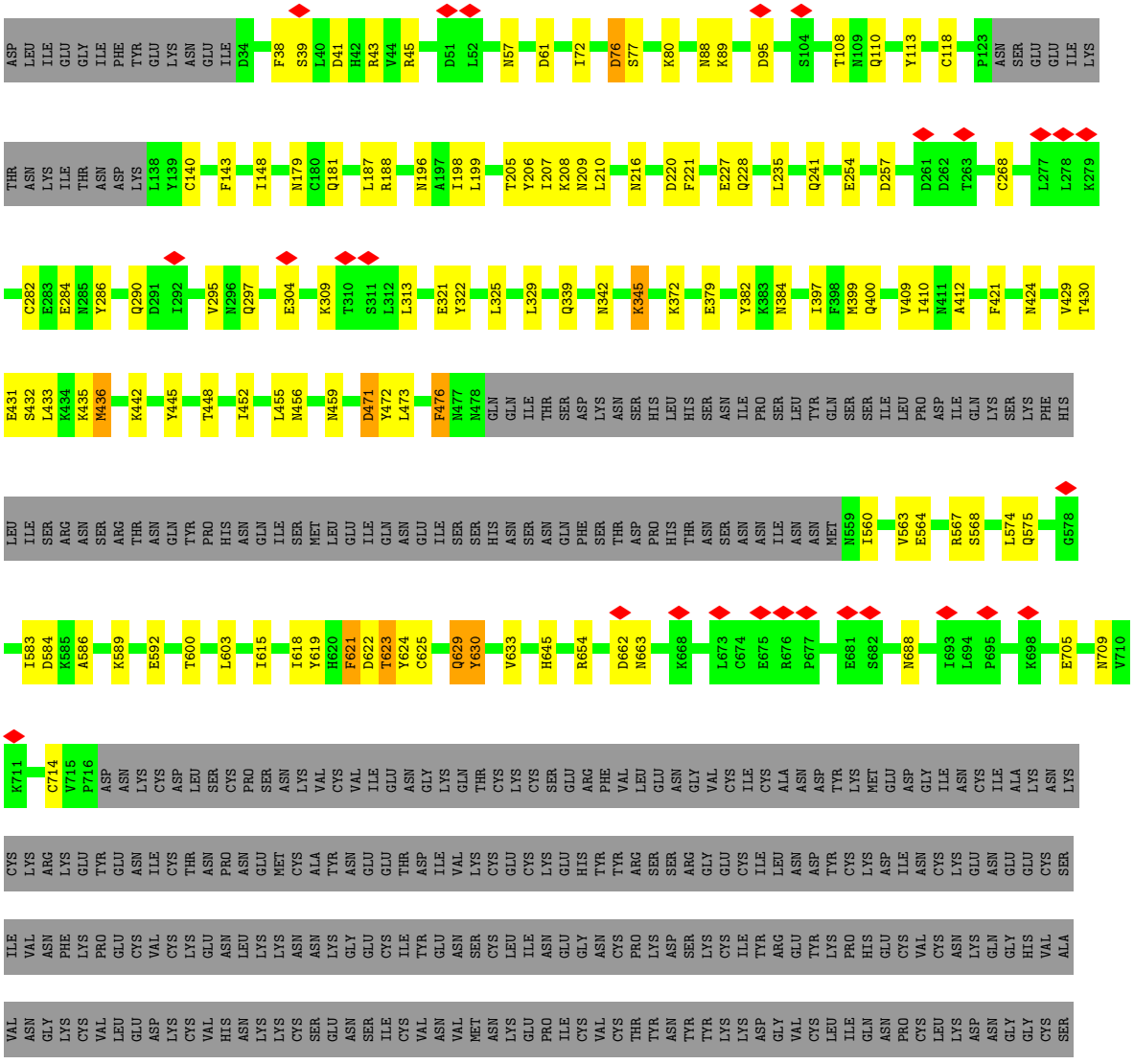
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	214	Total	C	N	O	S	0	0
			1568	982	268	311	7		

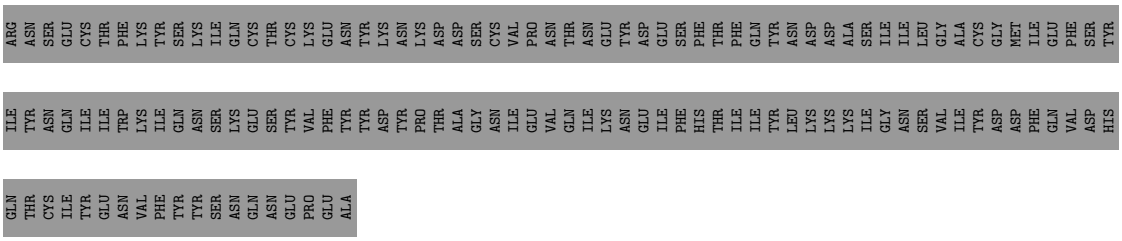
3 Residue-property plots (i)

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: Rh5-interacting protein

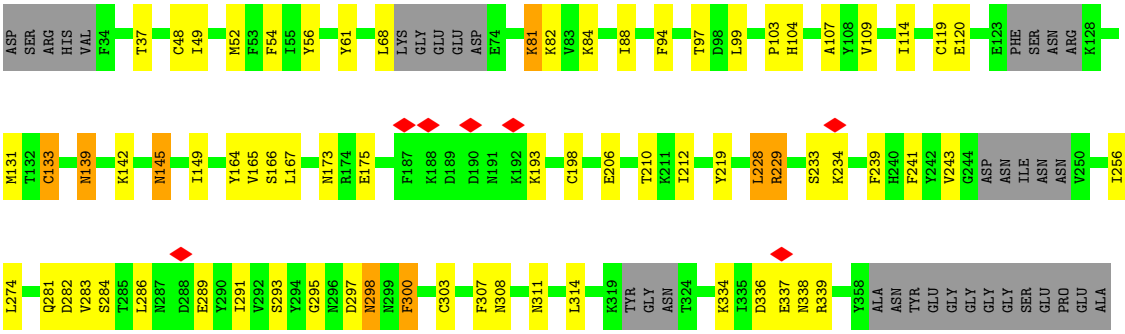
Chain A:





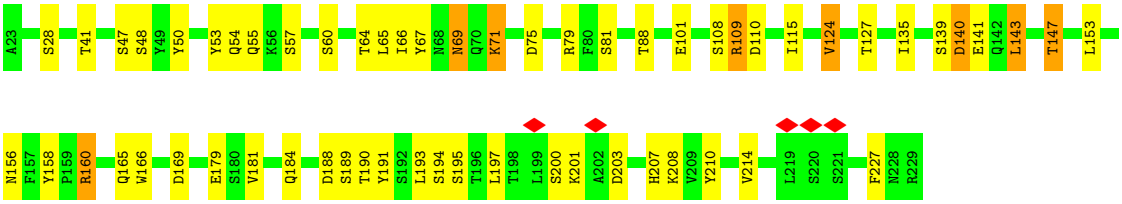
• Molecule 2: Cysteine-rich protective antigen

Chain B:



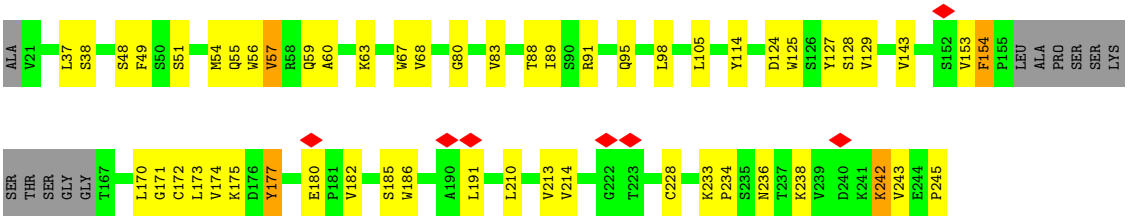
• Molecule 3: Cy.003 light chain

Chain C:



• Molecule 4: Cy.003

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	506797	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 ($e^-/Å^2$)	48.97	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	78.612	Depositor
Minimum map value	-30.952	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.130	Depositor
Recommended contour level	10.0	Depositor
Map size (Å)	346.112, 346.112, 346.112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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	0.26	0/4880	0.54	0/6577
2	B	0.27	0/2615	0.53	0/3525
3	C	0.27	0/1584	0.51	0/2153
4	D	0.27	0/1604	0.56	0/2184
All	All	0.27	0/10683	0.54	0/14439

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	4785	0	4574	71	0
2	B	2559	0	2474	39	0
3	C	1552	0	1499	32	0
4	D	1568	0	1514	28	0
All	All	10464	0	10061	164	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 (164) 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:B:52:MET:HG2	2:B:165:VAL:HG23	1.62	0.81
2:B:119:CYS:HA	2:B:133:CYS:HB2	1.64	0.78
1:A:295:VAL:O	1:A:309:LYS:NZ	2.23	0.71
3:C:141:GLU:N	3:C:141:GLU:OE1	2.23	0.71
4:D:191:LEU:HD11	4:D:214:VAL:HG21	1.74	0.70
3:C:179:GLU:OE1	3:C:179:GLU:N	2.25	0.69
2:B:107:ALA:HB3	2:B:165:VAL:HG22	1.75	0.68
4:D:54:MET:HB3	4:D:98:LEU:HD11	1.76	0.68
4:D:49:PHE:O	4:D:91:ARG:NH2	2.28	0.65
2:B:336:ASP:OD1	2:B:337:GLU:N	2.29	0.65
1:A:284:GLU:HG3	1:A:286:TYR:CZ	2.33	0.63
3:C:110:ASP:HB3	3:C:115:ILE:HD13	1.79	0.63
2:B:289:GLU:OE1	2:B:308:ASN:ND2	2.32	0.62
4:D:57:VAL:HG23	4:D:114:TYR:HB2	1.81	0.61
1:A:220:ASP:OD1	1:A:221:PHE:N	2.34	0.61
1:A:412:ALA:H	1:A:430:THR:HG22	1.66	0.60
2:B:175:GLU:OE1	2:B:175:GLU:N	2.34	0.60
4:D:124:ASP:OD1	4:D:125:TRP:N	2.35	0.60
1:A:187:LEU:HD21	1:A:207:ILE:HG22	1.84	0.59
1:A:429:VAL:HG12	1:A:432:SER:HB2	1.84	0.59
3:C:101:GLU:OE1	3:C:191:TYR:OH	2.21	0.59
3:C:165:GLN:NE2	3:C:166:TRP:O	2.36	0.59
3:C:47:SER:HB2	3:C:109:ARG:HB3	1.84	0.58
2:B:97:THR:HG22	2:B:99:LEU:H	1.68	0.58
2:B:337:GLU:N	2:B:337:GLU:OE1	2.35	0.58
1:A:397:ILE:HG21	1:A:433:LEU:HD11	1.85	0.58
2:B:145:ASN:OD1	2:B:145:ASN:N	2.35	0.58
4:D:55:GLN:NE2	4:D:128:SER:O	2.33	0.58
1:A:76:ASP:N	1:A:76:ASP:OD1	2.35	0.58
1:A:442:LYS:HA	1:A:442:LYS:HE2	1.85	0.57
1:A:564:GLU:OE1	1:A:564:GLU:N	2.37	0.57
3:C:53:TYR:OH	4:D:129:VAL:O	2.13	0.57
1:A:424:ASN:ND2	1:A:592:GLU:OE2	2.34	0.57
3:C:169:ASP:OD2	3:C:207:HIS:ND1	2.33	0.57
1:A:198:ILE:H	1:A:198:ILE:HD12	1.70	0.56
1:A:436:MET:SD	1:A:436:MET:N	2.78	0.56
4:D:95:GLN:OE1	4:D:95:GLN:N	2.38	0.56
3:C:50:TYR:N	3:C:69:ASN:OD1	2.36	0.56
1:A:241:GLN:NE2	2:B:37:THR:O	2.31	0.56
2:B:164:TYR:HB2	2:B:229:ARG:HG3	1.88	0.55
3:C:47:SER:OG	3:C:48:SER:N	2.40	0.54
4:D:68:VAL:O	4:D:80:GLY:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:ND2	1:A:216:ASN:OD1	2.41	0.54
1:A:322:TYR:CZ	1:A:618:ILE:HG22	2.43	0.53
1:A:429:VAL:HG11	1:A:455:LEU:HD22	1.90	0.53
1:A:372:LYS:O	1:A:663:ASN:ND2	2.41	0.53
1:A:471:ASP:OD2	1:A:630:TYR:OH	2.26	0.53
1:A:574:LEU:H	1:A:574:LEU:HD23	1.73	0.53
2:B:228:LEU:HD22	2:B:229:ARG:H	1.73	0.53
2:B:241:PHE:HE1	2:B:256:ILE:HD13	1.74	0.53
1:A:181:GLN:OE1	1:A:181:GLN:N	2.40	0.53
1:A:654:ARG:O	1:A:654:ARG:NE	2.42	0.53
2:B:198:CYS:HB2	2:B:212:ILE:HB	1.91	0.52
3:C:160:ARG:HH12	3:C:181:VAL:HG21	1.73	0.52
4:D:170:LEU:HD21	4:D:245:PRO:HD3	1.91	0.52
1:A:38:PHE:HA	1:A:623:THR:O	2.09	0.52
1:A:309:LYS:HB2	1:A:313:LEU:HD13	1.92	0.51
1:A:705:GLU:OE1	1:A:705:GLU:N	2.40	0.51
1:A:88:ASN:ND2	1:A:95:ASP:OD2	2.44	0.51
1:A:583:ILE:HD13	1:A:603:LEU:HD23	1.93	0.51
4:D:48:SER:OG	4:D:51:SER:OG	2.25	0.51
2:B:228:LEU:HD23	2:B:241:PHE:HB3	1.91	0.51
4:D:56:TRP:HD1	4:D:89:ILE:HD12	1.76	0.51
1:A:205:THR:O	1:A:209:ASN:ND2	2.44	0.51
2:B:286:LEU:HD13	2:B:291:ILE:HD12	1.92	0.51
4:D:37:LEU:HB2	4:D:105:LEU:HD11	1.92	0.50
3:C:55:GLN:NE2	3:C:60:SER:O	2.44	0.50
1:A:456:ASN:O	1:A:459:ASN:ND2	2.45	0.50
3:C:139:SER:OG	3:C:140:ASP:N	2.44	0.49
1:A:254:GLU:HA	1:A:268:CYS:HA	1.94	0.49
1:A:227:GLU:N	1:A:227:GLU:OE1	2.45	0.49
1:A:448:THR:HG21	1:A:452:ILE:HD11	1.95	0.49
1:A:148:ILE:HG13	1:A:148:ILE:O	2.12	0.49
2:B:339:ARG:HB2	2:B:339:ARG:NH1	2.28	0.49
4:D:143:VAL:O	4:D:143:VAL:HG23	2.13	0.49
1:A:586:ALA:HB1	1:A:633:VAL:HG12	1.95	0.48
1:A:622:ASP:HA	1:A:629:GLN:NE2	2.28	0.48
1:A:431:GLU:N	1:A:431:GLU:OE1	2.46	0.48
3:C:184:GLN:NE2	3:C:189:SER:O	2.47	0.48
4:D:60:ALA:HB3	4:D:63:LYS:HB3	1.95	0.48
2:B:139:ASN:O	2:B:139:ASN:ND2	2.47	0.47
3:C:141:GLU:HB2	4:D:154:PHE:HB2	1.96	0.47
4:D:172:CYS:HB3	4:D:243:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLN:NE2	1:A:304:GLU:O	2.44	0.47
1:A:382:TYR:CG	1:A:563:VAL:HB	2.49	0.47
3:C:181:VAL:HG12	3:C:193:LEU:HG	1.97	0.47
1:A:39:SER:HB2	1:A:297:GLN:O	2.15	0.46
1:A:384:ASN:ND2	1:A:584:ASP:OD2	2.49	0.46
2:B:297:ASP:OD1	2:B:298:ASN:N	2.47	0.46
1:A:400:GLN:O	1:A:472:TYR:OH	2.26	0.46
3:C:156:ASN:HA	3:C:190:THR:OG1	2.16	0.46
1:A:72:ILE:HG21	1:A:235:LEU:HD11	1.97	0.46
1:A:108:THR:HG22	1:A:110:GLN:HE21	1.81	0.46
2:B:228:LEU:HD11	2:B:239:PHE:HD2	1.81	0.46
4:D:177:TYR:CZ	4:D:182:VAL:HG21	2.51	0.46
2:B:120:GLU:OE1	2:B:120:GLU:N	2.49	0.46
2:B:282:ASP:OD1	2:B:283:VAL:N	2.48	0.45
1:A:113:TYR:HA	1:A:143:PHE:CD2	2.51	0.45
2:B:49:ILE:HD11	2:B:68:LEU:H	1.81	0.45
1:A:339:GLN:OE1	1:A:342:ASN:N	2.50	0.45
2:B:99:LEU:HD22	2:B:120:GLU:HB3	1.99	0.45
3:C:153:LEU:HD22	4:D:213:VAL:HG11	1.99	0.45
4:D:153:VAL:HA	4:D:174:VAL:HG12	1.98	0.45
2:B:339:ARG:HB2	2:B:339:ARG:HH11	1.82	0.45
3:C:65:LEU:O	3:C:66:ILE:HD13	2.16	0.45
2:B:228:LEU:HD11	2:B:239:PHE:CD2	2.52	0.45
1:A:72:ILE:HD13	1:A:235:LEU:HD11	1.99	0.44
2:B:61:TYR:CE2	2:B:81:LYS:HG3	2.53	0.44
3:C:41:THR:HG23	3:C:88:THR:HG23	2.00	0.44
2:B:228:LEU:HD21	2:B:239:PHE:HB3	2.00	0.44
1:A:435:LYS:HA	1:A:435:LYS:HE2	2.00	0.44
1:A:476:PHE:HD2	1:A:560:ILE:HG21	1.82	0.44
2:B:281:GLN:NE2	2:B:293:SER:OG	2.50	0.44
3:C:160:ARG:HH22	3:C:181:VAL:HG21	1.83	0.44
2:B:88:ILE:HD12	2:B:88:ILE:O	2.17	0.44
1:A:208:LYS:HD2	2:B:314:LEU:HD11	2.00	0.44
1:A:379:GLU:OE1	1:A:379:GLU:N	2.51	0.44
3:C:55:GLN:HE22	4:D:59:GLN:HE22	1.65	0.44
3:C:124:VAL:O	3:C:158:TYR:OH	2.28	0.44
2:B:99:LEU:HD13	2:B:103:PRO:HB3	2.00	0.43
1:A:196:ASN:HB3	1:A:199:LEU:HD12	1.99	0.43
3:C:143:LEU:HD12	3:C:201:LYS:HE3	2.00	0.43
4:D:238:LYS:N	4:D:238:LYS:HD2	2.33	0.43
1:A:603:LEU:HB2	1:A:619:TYR:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:233:LYS:HB2	4:D:234:PRO:HD3	1.99	0.43
1:A:615:ILE:HG13	1:A:621:PHE:HZ	1.83	0.43
1:A:325:LEU:HD13	1:A:329:LEU:HD23	2.01	0.43
4:D:83:VAL:HG12	4:D:83:VAL:O	2.19	0.43
2:B:233:SER:OG	2:B:234:LYS:N	2.52	0.43
2:B:149:ILE:HG12	2:B:206:GLU:HG2	2.01	0.42
1:A:88:ASN:OD1	1:A:89:LYS:N	2.52	0.42
1:A:589:LYS:HE3	1:A:589:LYS:HB2	1.81	0.42
2:B:54:PHE:HB2	2:B:109:VAL:HG21	2.02	0.42
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.87	0.42
1:A:412:ALA:N	1:A:430:THR:HG22	2.34	0.42
3:C:75:ASP:N	3:C:75:ASP:OD1	2.50	0.42
1:A:345:LYS:HB2	1:A:345:LYS:HE3	1.48	0.42
4:D:170:LEU:HD13	4:D:171:GLY:N	2.35	0.42
1:A:399:MET:HG2	1:A:472:TYR:CE1	2.55	0.42
4:D:57:VAL:HG12	4:D:67:TRP:HA	2.02	0.42
1:A:257:ASP:OD1	1:A:257:ASP:N	2.53	0.42
3:C:53:TYR:HD1	3:C:64:THR:HA	1.83	0.42
4:D:173:LEU:HD11	4:D:175:LYS:HD2	2.02	0.42
1:A:688:ASN:ND2	1:A:714:CYS:O	2.48	0.42
3:C:147:THR:O	3:C:147:THR:OG1	2.35	0.42
1:A:709:ASN:HA	1:A:714:CYS:HA	2.02	0.41
1:A:118:CYS:HA	1:A:140:CYS:HA	2.01	0.41
1:A:284:GLU:HG3	1:A:286:TYR:CE1	2.56	0.41
1:A:567:ARG:HE	1:A:567:ARG:HB2	1.66	0.41
1:A:321:GLU:OE1	1:A:322:TYR:N	2.37	0.41
1:A:206:TYR:CZ	1:A:210:LEU:HD22	2.56	0.41
4:D:242:LYS:HE3	4:D:242:LYS:HB3	1.90	0.41
1:A:586:ALA:O	1:A:600:THR:OG1	2.25	0.41
2:B:56:TYR:CD2	2:B:114:ILE:HD11	2.56	0.41
3:C:188:ASP:OD1	3:C:190:THR:N	2.50	0.41
3:C:208:LYS:HA	3:C:208:LYS:HD3	1.97	0.41
1:A:188:ARG:HA	1:A:188:ARG:HD3	1.87	0.40
2:B:104:HIS:N	2:B:119:CYS:O	2.54	0.40
1:A:41:ASP:OD1	1:A:43:ARG:N	2.55	0.40
1:A:409:VAL:O	1:A:410:ILE:HD13	2.20	0.40
3:C:67:TYR:CZ	3:C:71:LYS:HB3	2.57	0.40
2:B:291:ILE:HG13	2:B:307:PHE:CD1	2.57	0.40
2:B:295:GLY:HA3	2:B:300:PHE:CZ	2.57	0.40
3:C:47:SER:HB3	3:C:108:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/1070 (54%)	541 (93%)	42 (7%)	0	100	100
2	B	297/342 (87%)	254 (86%)	43 (14%)	0	100	100
3	C	205/207 (99%)	197 (96%)	8 (4%)	0	100	100
4	D	210/226 (93%)	202 (96%)	8 (4%)	0	100	100
All	All	1295/1845 (70%)	1194 (92%)	101 (8%)	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	554/1011 (55%)	529 (96%)	25 (4%)	27	60
2	B	289/316 (92%)	262 (91%)	27 (9%)	9	32
3	C	177/177 (100%)	155 (88%)	22 (12%)	4	19
4	D	173/181 (96%)	160 (92%)	13 (8%)	13	42
All	All	1193/1685 (71%)	1106 (93%)	87 (7%)	18	43

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	57	ASN

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Mol	Chain	Res	Type
1	A	61	ASP
1	A	76	ASP
1	A	77	SER
1	A	80	LYS
1	A	228	GLN
1	A	282	CYS
1	A	345	LYS
1	A	421	PHE
1	A	436	MET
1	A	445	TYR
1	A	471	ASP
1	A	473	LEU
1	A	476	PHE
1	A	568	SER
1	A	575	GLN
1	A	621	PHE
1	A	623	THR
1	A	624	TYR
1	A	625	CYS
1	A	629	GLN
1	A	630	TYR
1	A	645	HIS
1	A	662	ASP
2	B	48	CYS
2	B	81	LYS
2	B	82	LYS
2	B	84	LYS
2	B	94	PHE
2	B	131	MET
2	B	133	CYS
2	B	139	ASN
2	B	142	LYS
2	B	145	ASN
2	B	166	SER
2	B	167	LEU
2	B	173	ASN
2	B	193	LYS
2	B	210	THR
2	B	219	TYR
2	B	228	LEU
2	B	229	ARG
2	B	243	VAL

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Mol	Chain	Res	Type
2	B	274	LEU
2	B	284	SER
2	B	298	ASN
2	B	300	PHE
2	B	303	CYS
2	B	311	ASN
2	B	334	LYS
2	B	338	ASN
3	C	28	SER
3	C	54	GLN
3	C	57	SER
3	C	69	ASN
3	C	71	LYS
3	C	79	ARG
3	C	81	SER
3	C	109	ARG
3	C	124	VAL
3	C	127	THR
3	C	135	ILE
3	C	140	ASP
3	C	143	LEU
3	C	147	THR
3	C	160	ARG
3	C	194	SER
3	C	195	SER
3	C	200	SER
3	C	203	ASP
3	C	210	TYR
3	C	214	VAL
3	C	227	PHE
4	D	38	SER
4	D	57	VAL
4	D	88	THR
4	D	127	TYR
4	D	154	PHE
4	D	177	TYR
4	D	180	GLU
4	D	185	SER
4	D	186	TRP
4	D	210	LEU
4	D	228	CYS
4	D	236	ASN

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Mol	Chain	Res	Type
4	D	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	243	GLN
1	A	280	ASN
1	A	318	ASN
1	A	319	ASN
1	A	358	ASN
1	A	459	ASN
2	B	134	HIS
2	B	139	ASN
2	B	191	ASN
2	B	218	ASN
2	B	240	HIS
2	B	281	GLN
2	B	352	ASN
3	C	54	GLN
3	C	70	GLN
3	C	217	GLN
4	D	59	GLN
4	D	203	GLN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

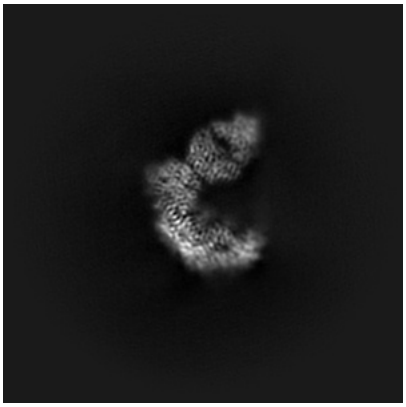
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16570. These allow visual inspection of the internal detail of the map and identification of artifacts.

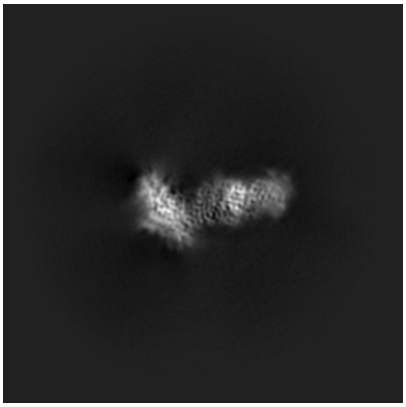
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

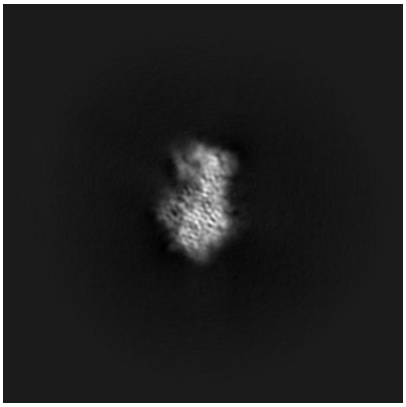
6.1.1 Primary map



X



Y

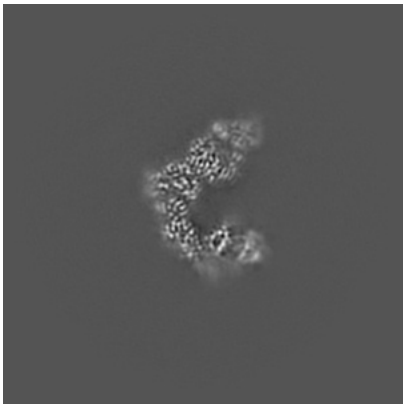


Z

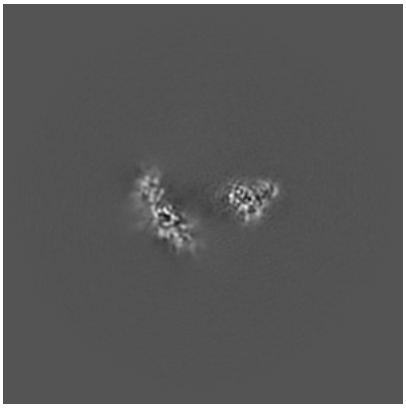
The images above show the map projected in three orthogonal directions.

6.2 Central slices

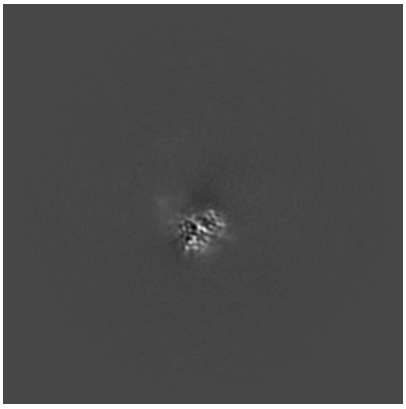
6.2.1 Primary map



X Index: 208



Y Index: 208

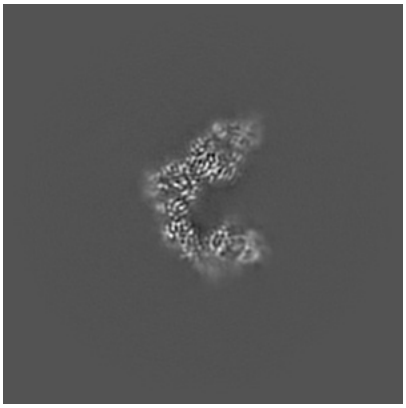


Z Index: 208

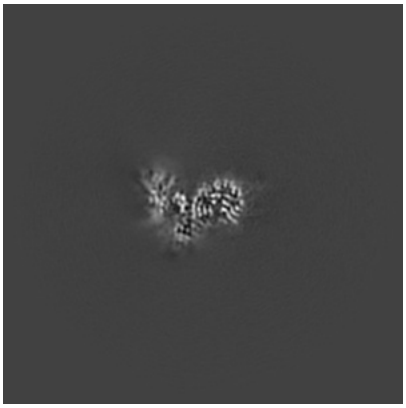
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

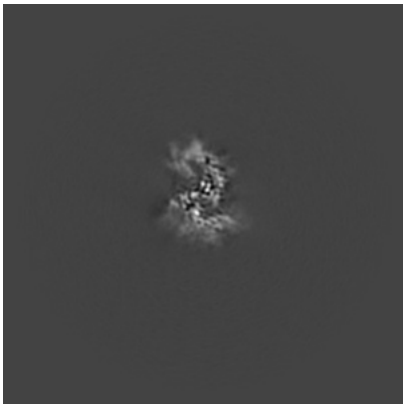
6.3.1 Primary map



X Index: 209



Y Index: 188

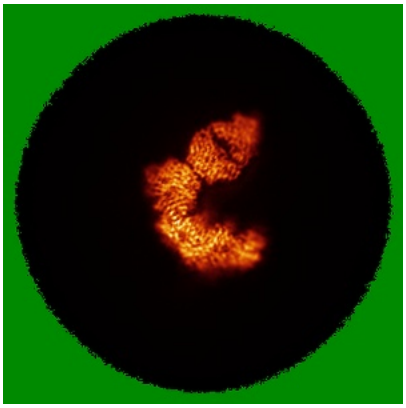


Z Index: 166

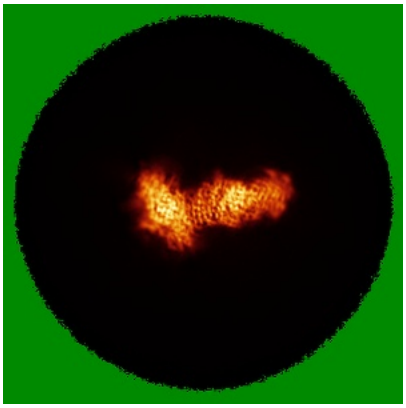
The images above show the largest variance slices of the map in three orthogonal directions.

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

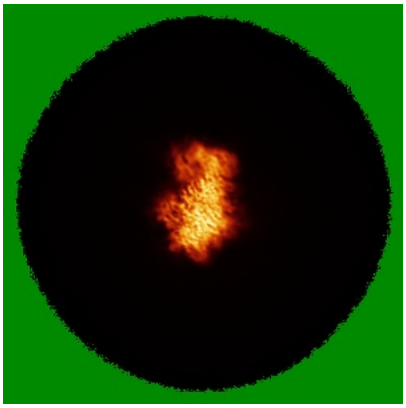
6.4.1 Primary map



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 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

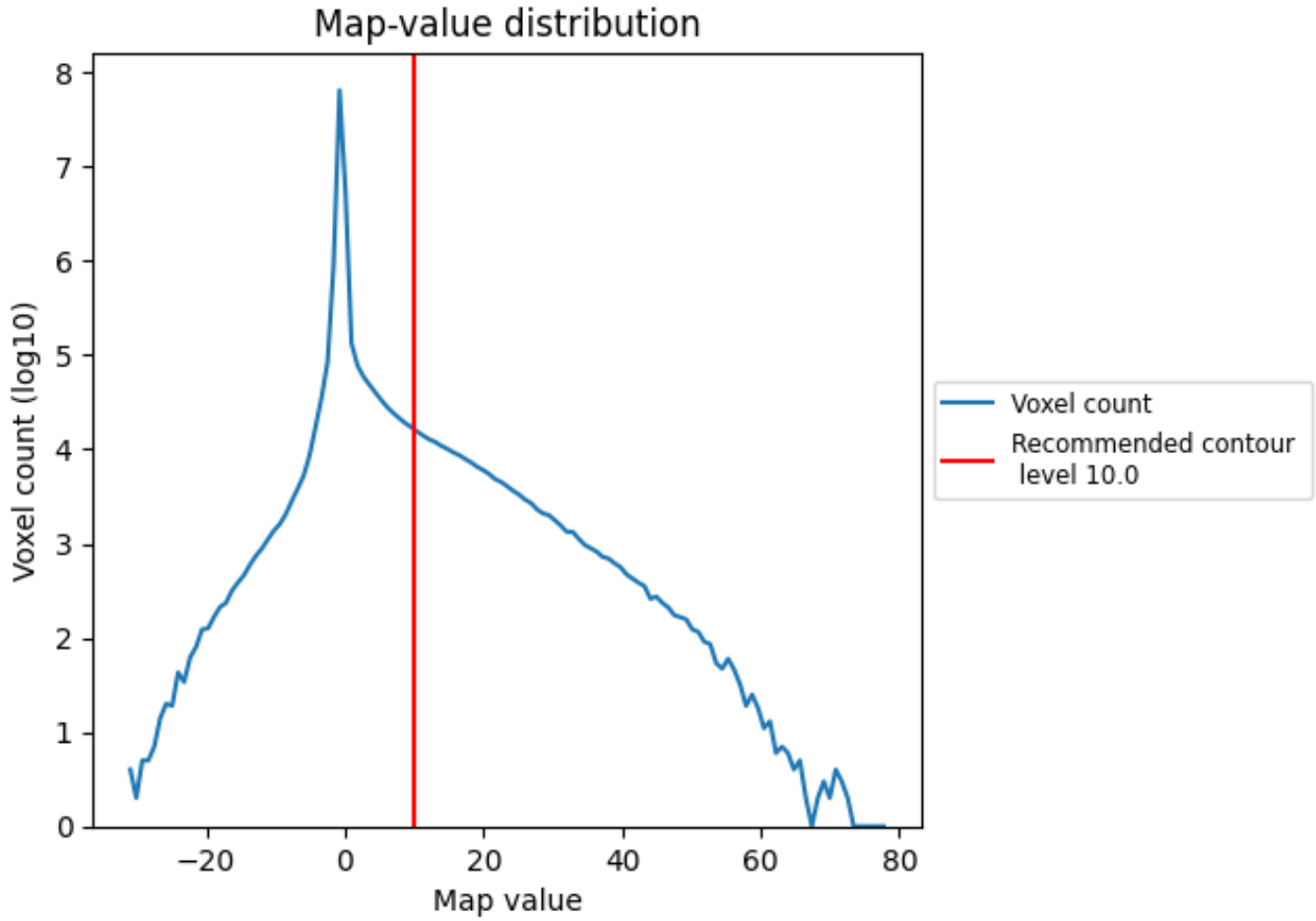
6.6 Mask visualisation (i)

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

7 Map analysis

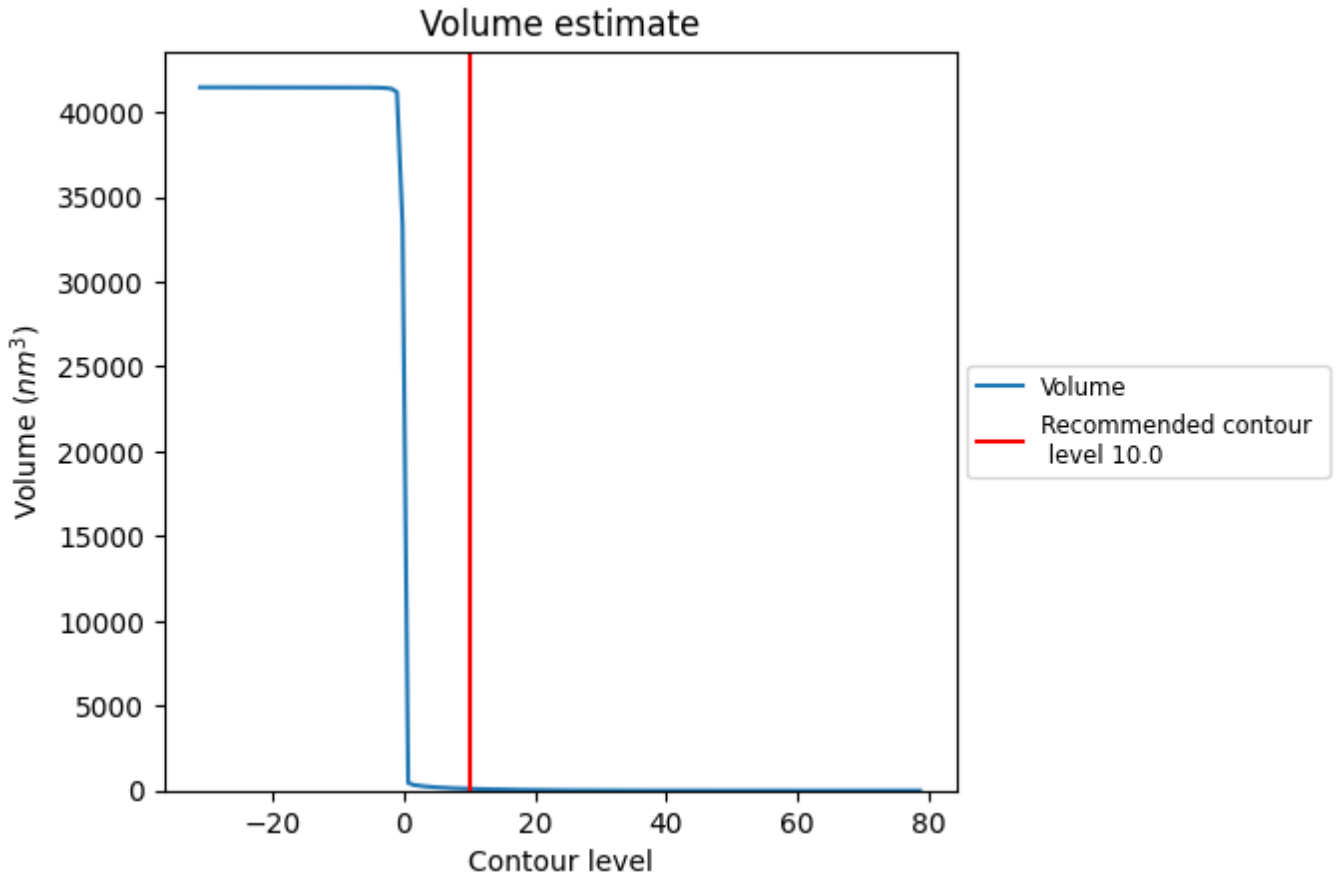
This section contains the results of statistical analysis of the map.

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.

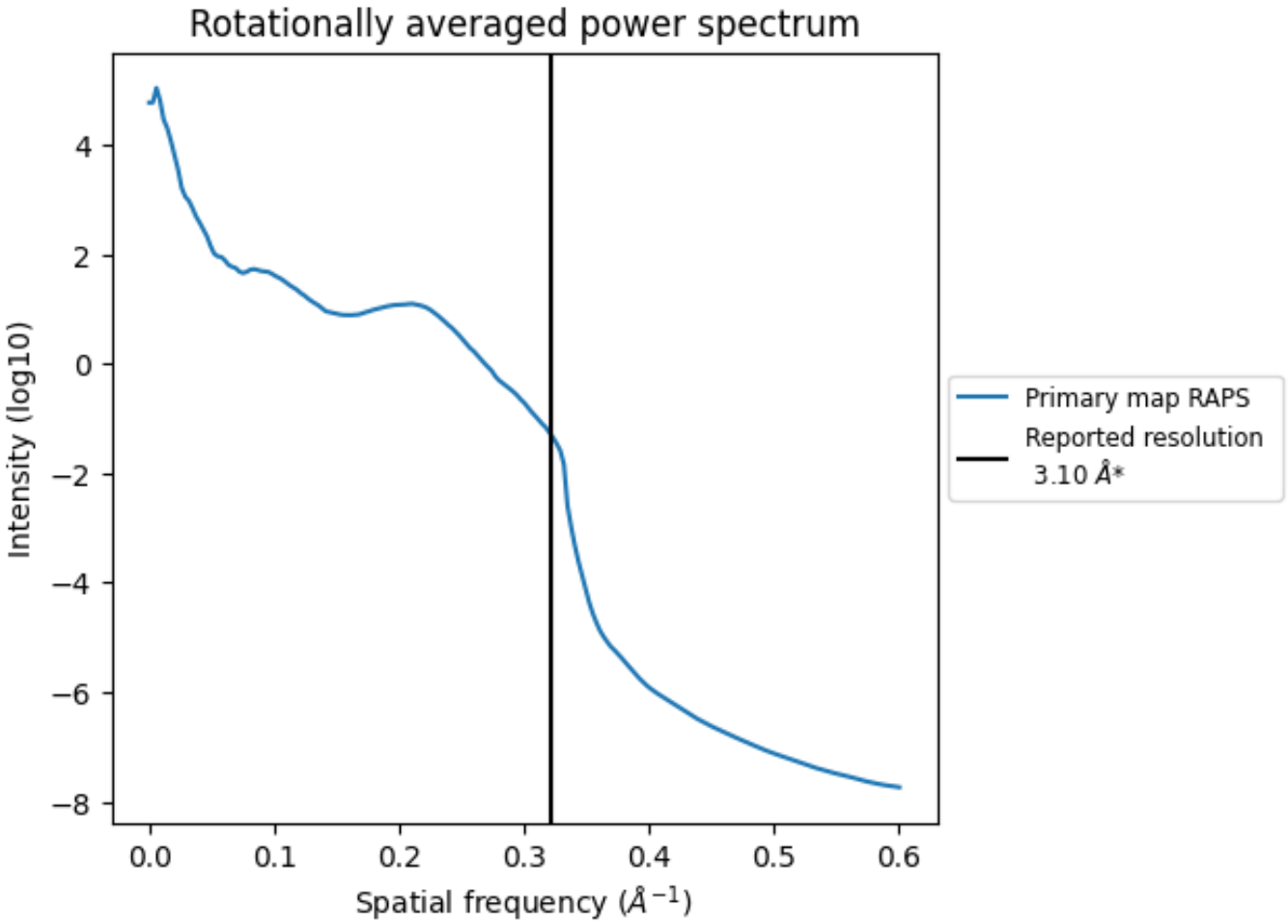
7.2 Volume estimate (i)



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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 0.323 Å^{-1}

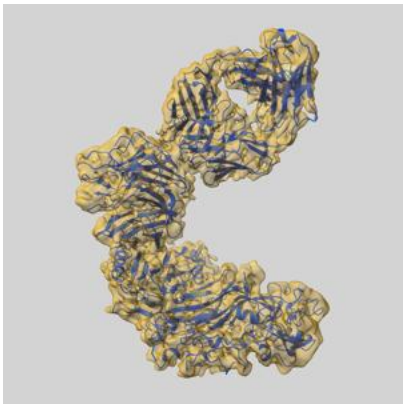
8 Fourier-Shell correlation (i)

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

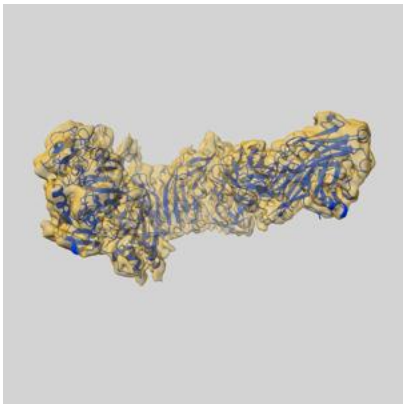
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16570 and PDB model 8CDE. Per-residue inclusion information can be found in section 3 on page 5.

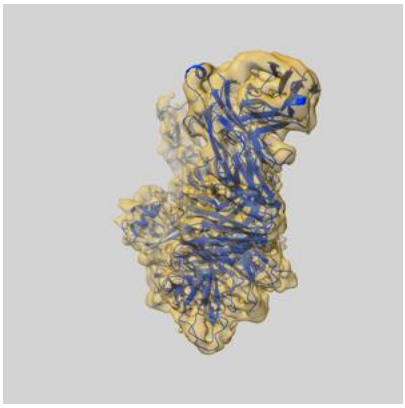
9.1 Map-model overlay



X



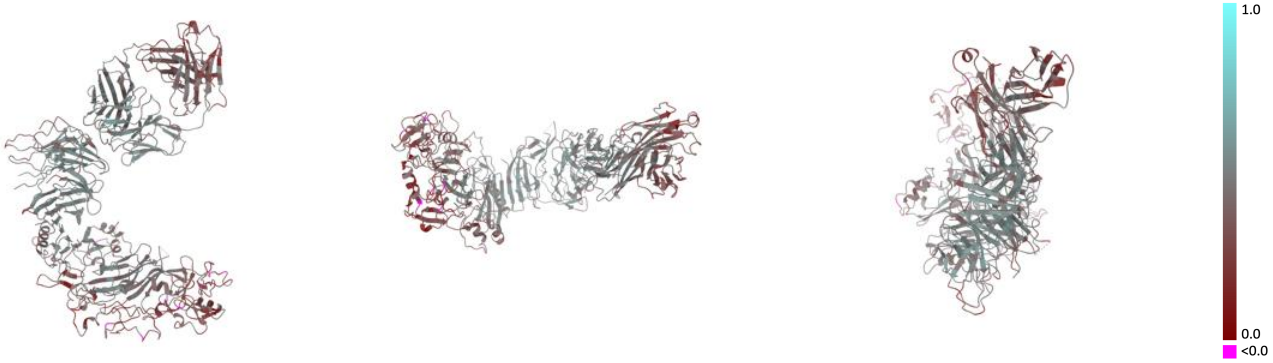
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 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.

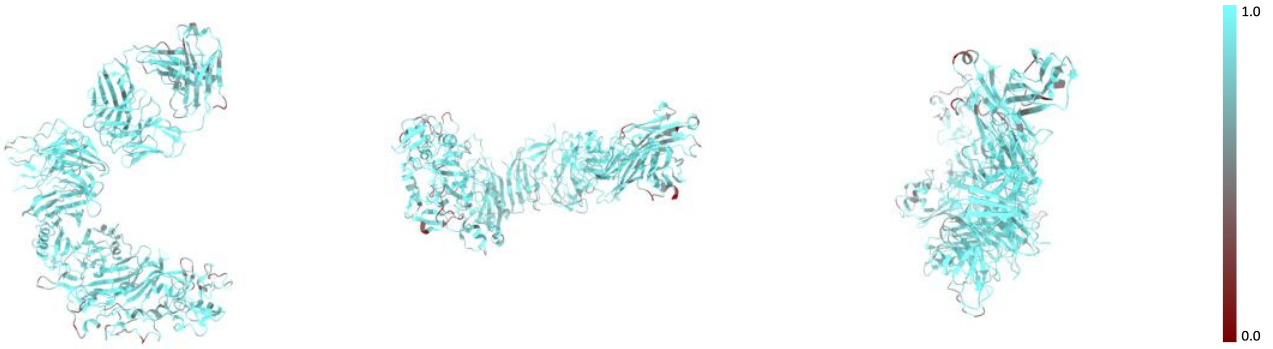
9.2 Q-score mapped to coordinate model (i)



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.

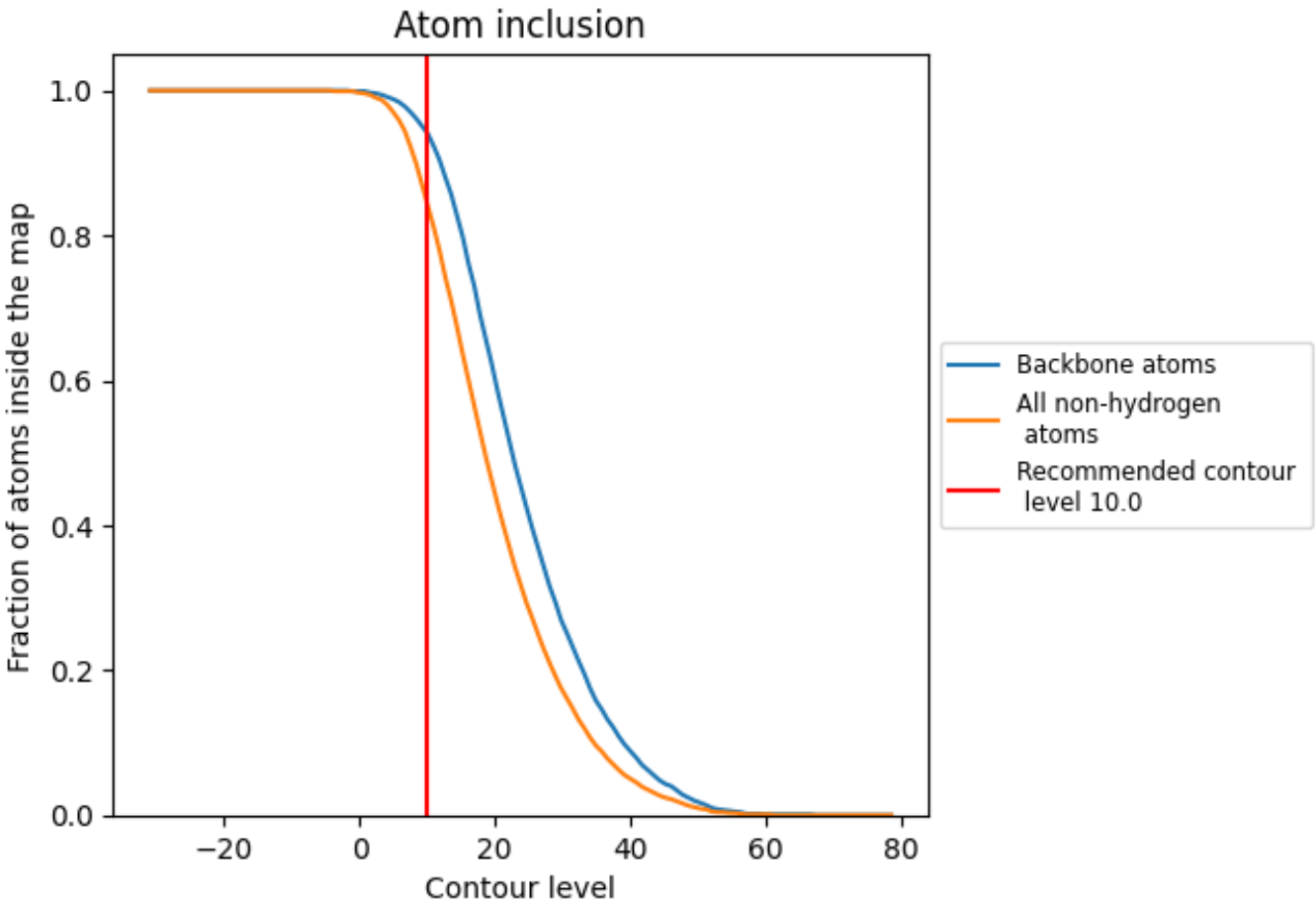
9.3 Atom inclusion mapped to coordinate model (i)



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 (10.0).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.4090
A	0.8330	0.3660
B	0.8610	0.4700
C	0.8430	0.4280
D	0.8580	0.4230