Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:11 PM EDT

PDB ID	:	9O7S / pdb_00009o7s
EMDB ID	:	EMD-70207
Title	:	Cryo-EM structure of KCa2.2/calmodulin channel in complex with NS309
Deposited on	:	2025-04-15
Resolution	:	2.71 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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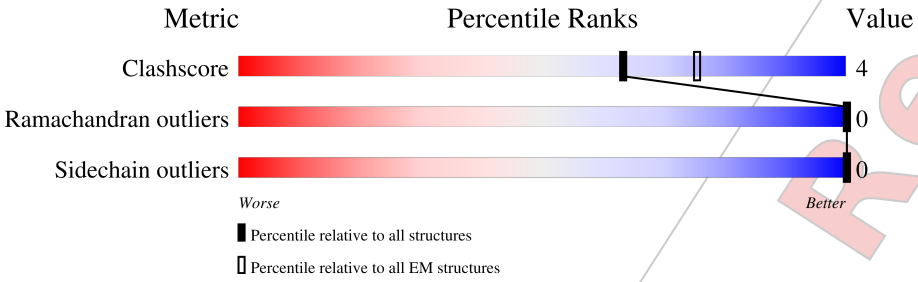
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.71 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	361	93% 7%
1	B	361	89% 11%
1	C	361	91% 9%
1	D	361	92% 8%
2	E	145	88% 12%
2	F	145	85% 15%
2	G	145	90% 10%

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Mol	Chain	Length	Quality of chain
2	H	145	

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2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15539 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 Small conductance calcium-activated potassium channel protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total 2884	C 1876	N 496	O 490	S 22	0	0
1	B	361	Total 2884	C 1876	N 496	O 490	S 22	0	0
1	C	361	Total 2884	C 1876	N 496	O 490	S 22	0	0
1	D	361	Total 2884	C 1876	N 496	O 490	S 22	0	0

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	145	Total 982	C 612	N 167	O 195	S 8	0	0
2	F	145	Total 982	C 612	N 167	O 195	S 8	0	0
2	G	145	Total 986	C 615	N 168	O 195	S 8	0	0
2	H	145	Total 982	C 612	N 167	O 195	S 8	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	K 2	0
3	C	1	Total 1	K 1	0

- Molecule 4 is (3E)-6,7-dichloro-3-(hydroxyimino)-1,3-dihydro-2H-indol-2-one (CCD ID: 1KP) (formula: $C_8H_4Cl_2N_2O_2$) (labeled as "Ligand of Interest" by depositor).

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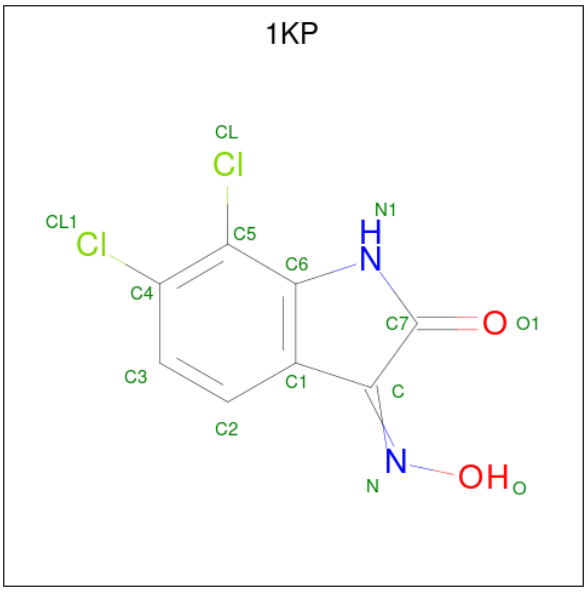

Mol	Chain	Residues	Atoms	AltConf
4	E	1	Total C Cl N O 14 8 2 2 2	0
4	F	1	Total C Cl N O 14 8 2 2 2	0
4	G	1	Total C Cl N O 14 8 2 2 2	0
4	H	1	Total C Cl N O 14 8 2 2 2	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	E	2	Total Ca 2 2	0
5	F	2	Total Ca 2 2	0
5	G	2	Total Ca 2 2	0
5	H	2	Total Ca 2 2	0

- Molecule 6 is water.

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

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Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total O 1 1	0
6	C	1	Total O 1 1	0
6	D	1	Total O 1 1	0

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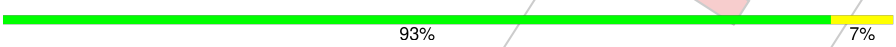
3 Residue-property plots (i)

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.

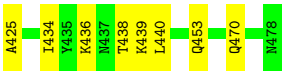
- Molecule 1: Small conductance calcium-activated potassium channel protein 2

Chain A:



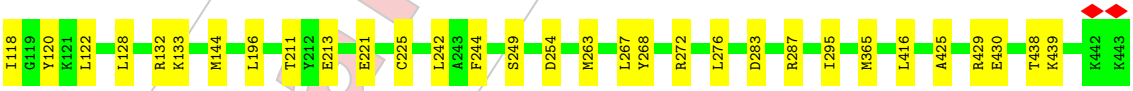
- Molecule 1: Small conductance calcium-activated potassium channel protein 2

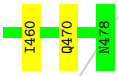
Chain B:



- Molecule 1: Small conductance calcium-activated potassium channel protein 2

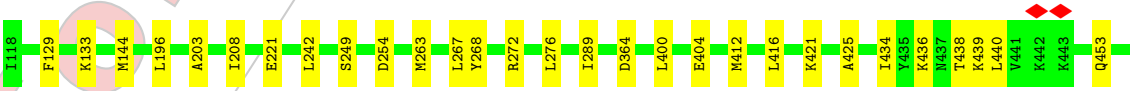
Chain C:





- Molecule 1: Small conductance calcium-activated potassium channel protein 2

Chain D:



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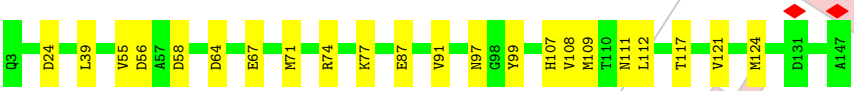
• Molecule 2: Calmodulin-1

Chain E:

• Molecule 2: Calmodulin-1

Chain F:



• Molecule 2: Calmodulin-1

Chain G:

• Molecule 2: Calmodulin-1

Chain H:

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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	56.624	Depositor
Minimum map value	-37.547	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	364.80002, 364.80002, 364.80002	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7296, 0.7296, 0.7296	Depositor

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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: CA, 1KP, K

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	0/2943	0.34	0/3980
1	B	0.26	0/2943	0.33	0/3980
1	C	0.26	0/2943	0.33	0/3980
1	D	0.26	0/2943	0.32	0/3980
2	E	0.17	0/992	0.28	0/1347
2	F	0.17	0/992	0.28	0/1347
2	G	0.17	0/996	0.35	0/1351
2	H	0.17	0/992	0.32	0/1347
All	All	0.24	0/15744	0.32	0/21312

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	2884	0	3009	18	0
1	B	2884	0	3010	27	0
1	C	2884	0	3009	23	0
1	D	2884	0	3010	18	0
2	E	982	0	845	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	982	0	845	15	0
2	G	986	0	856	12	0
2	H	982	0	844	16	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	E	14	0	4	0	0
4	F	14	0	4	1	0
4	G	14	0	4	3	0
4	H	14	0	4	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	15539	0	15444	125	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 4.

All (125) 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:G:57:ALA:O	2:G:58:ASP:OD1	1.57	1.22
2:F:109:MET:HG3	2:F:124:MET:HE1	1.62	0.80
2:G:109:MET:HG3	2:G:124:MET:HE1	1.68	0.76
1:A:118:ILE:HG22	1:A:121:LYS:HG2	1.71	0.71
2:H:28:THR:HG23	2:H:30:LYS:H	1.58	0.69
2:F:97:ASN:ND2	2:F:99:TYR:O	2.24	0.69
1:B:118:ILE:HG23	1:B:120:TYR:H	1.63	0.63
1:B:289:ILE:HG23	2:H:39:LEU:HD11	1.81	0.62
2:F:56:ASP:OD1	2:F:58:ASP:O	2.18	0.62
1:B:438:THR:HG22	1:B:439:LYS:HG3	1.85	0.59
2:F:58:ASP:O	2:F:58:ASP:OD1	2.21	0.58
2:F:107:HIS:ND1	2:F:111:ASN:OD1	2.37	0.58
1:B:144:MET:HE1	1:B:267:LEU:HD23	1.86	0.57
2:H:22:ASP:CG	2:H:31:GLU:OE2	2.42	0.57
1:A:281:PHE:O	1:A:287:ARG:NH1	2.38	0.57
1:A:209:ALA:HB1	1:A:214:ARG:HH11	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HB3	1:B:196:LEU:HD12	1.88	0.56
1:C:225:CYS:HG	1:C:268:TYR:HH	1.49	0.56
1:C:118:ILE:HG13	1:C:120:TYR:H	1.71	0.54
2:G:63:ILE:HG13	4:G:201:1KP:CL1	2.45	0.54
2:G:71:MET:HE1	4:G:201:1KP:C1	2.37	0.54
1:D:438:THR:HG22	1:D:439:LYS:HG3	1.89	0.53
1:C:438:THR:HG22	1:C:439:LYS:HD3	1.91	0.53
1:D:425:ALA:HB2	2:H:112:LEU:HD12	1.90	0.53
1:C:144:MET:HE1	1:C:267:LEU:HD23	1.91	0.53
1:D:144:MET:HE1	1:D:267:LEU:HD23	1.91	0.53
2:G:36:MET:HE3	2:G:43:PRO:HG3	1.92	0.52
2:H:24:ASP:OD1	2:H:26:THR:O	2.28	0.51
1:A:407:VAL:HG23	1:B:293:ASN:HD22	1.76	0.51
2:G:107:HIS:ND1	2:G:111:ASN:OD1	2.40	0.51
1:C:429:ARG:NH1	1:C:430:GLU:OE2	2.43	0.51
2:H:20:ASP:HA	2:H:31:GLU:OE1	2.11	0.51
1:C:122:LEU:HD11	2:E:12:PHE:CZ	2.47	0.50
2:H:74:ARG:HA	2:H:77:LYS:HE2	1.94	0.50
2:F:108:VAL:HG13	2:F:112:LEU:HD11	1.94	0.49
1:D:221:GLU:OE2	1:D:272:ARG:NH1	2.46	0.49
1:B:211:THR:C	1:B:213:GLU:H	2.21	0.49
1:B:425:ALA:HB2	2:F:112:LEU:HD12	1.95	0.48
1:C:211:THR:C	1:C:213:GLU:H	2.20	0.48
2:G:57:ALA:O	2:G:67:GLU:OE2	2.32	0.48
1:C:221:GLU:OE2	1:C:272:ARG:NH1	2.47	0.48
1:B:132:ARG:HH11	1:B:196:LEU:HD13	1.80	0.47
1:C:460:ILE:HD12	2:G:84:GLU:HB3	1.97	0.47
2:E:74:ARG:HA	2:E:77:LYS:HE2	1.96	0.47
2:F:71:MET:HE1	4:F:201:1KP:C	2.44	0.47
1:B:364:ASP:HB3	1:C:244:PHE:CD1	2.49	0.47
1:B:221:GLU:OE2	1:B:272:ARG:NH1	2.48	0.47
1:A:121:LYS:C	1:A:123:GLY:H	2.24	0.46
1:D:421:LYS:HD3	2:H:112:LEU:HD22	1.97	0.46
1:A:244:PHE:CD1	1:D:364:ASP:HB3	2.49	0.46
1:D:436:LYS:HG3	1:D:440:LEU:HD22	1.96	0.46
1:C:132:ARG:HH11	1:C:196:LEU:HD13	1.80	0.46
1:A:242:LEU:CD1	1:A:249:SER:HB2	2.46	0.46
1:C:242:LEU:CD1	1:C:249:SER:HB2	2.45	0.46
1:D:129:PHE:HE1	1:D:196:LEU:HD21	1.80	0.46
1:A:211:THR:C	1:A:213:GLU:H	2.23	0.45
1:B:416:LEU:HD13	1:B:470:GLN:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HD12	1:B:329:THR:HG23	1.97	0.45
1:A:144:MET:HE1	1:A:267:LEU:HD23	1.98	0.45
1:A:133:LYS:HA	1:A:276:LEU:HD23	1.97	0.45
1:C:133:LYS:HA	1:C:276:LEU:HD23	1.99	0.45
1:B:242:LEU:CD1	1:B:249:SER:HB2	2.47	0.45
1:D:412:MET:O	1:D:416:LEU:HD23	2.17	0.45
1:D:242:LEU:CD1	1:D:249:SER:HB2	2.47	0.45
2:G:71:MET:HE1	4:G:201:1KP:C	2.46	0.45
2:E:131:ASP:O	2:E:135:GLN:N	2.49	0.45
2:F:55:VAL:HG13	2:F:71:MET:HB3	1.99	0.44
2:H:108:VAL:HG13	2:H:112:LEU:HD11	1.98	0.44
1:B:133:LYS:HA	1:B:276:LEU:HD23	2.00	0.44
2:E:53:ASN:C	2:E:55:VAL:H	2.26	0.44
1:A:126:ARG:HD3	1:A:126:ARG:HA	1.84	0.44
1:B:263:MET:HE2	1:B:263:MET:HB3	1.80	0.44
2:H:76:MET:HE3	2:H:76:MET:HB3	1.92	0.44
2:H:122:ASP:HA	2:H:125:ILE:HD13	1.98	0.44
1:C:416:LEU:HD13	1:C:470:GLN:HA	2.00	0.44
2:E:53:ASN:O	2:E:54:GLU:HB3	2.18	0.44
2:E:107:HIS:ND1	2:E:111:ASN:OD1	2.51	0.44
1:A:407:VAL:HG21	1:B:295:ILE:HG13	2.00	0.43
1:D:434:ILE:HD11	1:D:453:GLN:HA	2.00	0.43
1:D:263:MET:HE2	1:D:263:MET:HB3	1.83	0.43
1:D:400:LEU:HD22	1:D:404:GLU:HB3	1.99	0.43
1:C:254:ASP:OD1	1:C:254:ASP:N	2.51	0.43
1:C:283:ASP:O	1:C:287:ARG:HG2	2.19	0.43
2:F:87:GLU:O	2:F:91:VAL:HG23	2.18	0.43
1:C:128:LEU:HB3	1:C:196:LEU:HD12	2.00	0.43
1:D:133:LYS:HA	1:D:276:LEU:HD23	1.99	0.43
2:E:27:ILE:HB	2:E:63:ILE:HB	2.00	0.43
2:E:71:MET:HE2	2:E:71:MET:HB2	1.86	0.42
2:E:131:ASP:HA	2:E:136:VAL:HA	1.99	0.42
2:F:74:ARG:HA	2:F:77:LYS:HE2	2.01	0.42
2:G:28:THR:HA	2:G:62:THR:HG22	2.01	0.42
1:C:365:MET:HE3	1:C:365:MET:HB3	1.94	0.42
1:B:122:LEU:HB2	2:H:4:LEU:HD11	2.01	0.42
1:D:221:GLU:HG3	1:D:268:TYR:OH	2.19	0.42
2:E:65:PHE:HB3	2:E:66:PRO:HD3	2.02	0.42
1:B:434:ILE:HD11	1:B:453:GLN:HA	2.02	0.42
1:A:254:ASP:OD1	1:A:254:ASP:N	2.52	0.42
1:A:400:LEU:HD22	1:A:404:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ALA:HB2	2:G:112:LEU:HD12	2.01	0.42
2:F:64:ASP:N	2:F:67:GLU:OE1	2.48	0.42
2:H:5:THR:OG1	2:H:6:GLU:N	2.53	0.42
1:A:203:ALA:HB1	1:A:208:ILE:HD12	2.00	0.42
1:B:254:ASP:OD1	1:B:254:ASP:N	2.52	0.41
1:B:407:VAL:HG21	1:C:295:ILE:HG13	2.01	0.41
2:H:69:LEU:HD23	2:H:69:LEU:HA	1.96	0.41
1:B:436:LYS:HG3	1:B:440:LEU:HD22	2.02	0.41
1:C:221:GLU:HG3	1:C:268:TYR:OH	2.19	0.41
1:C:263:MET:HE2	1:C:263:MET:HB3	1.80	0.41
2:E:117:THR:O	2:E:121:VAL:HG23	2.21	0.41
1:C:225:CYS:SG	1:C:268:TYR:OH	2.60	0.41
2:F:117:THR:O	2:F:121:VAL:HG23	2.21	0.41
1:B:126:ARG:HD3	1:B:126:ARG:HA	1.81	0.41
1:B:285:SER:HB3	2:H:18:LEU:HD12	2.03	0.41
1:D:254:ASP:N	1:D:254:ASP:OD1	2.51	0.41
2:G:57:ALA:C	2:G:58:ASP:OD1	2.52	0.41
1:A:128:LEU:HD21	1:A:195:GLN:HG2	2.02	0.41
1:B:400:LEU:HD22	1:B:404:GLU:HB3	2.02	0.41
1:B:242:LEU:HD11	1:B:249:SER:HB2	2.04	0.40
2:H:20:ASP:OD1	2:H:24:ASP:OD1	2.39	0.40
1:B:221:GLU:HG3	1:B:268:TYR:OH	2.21	0.40
2:F:24:ASP:OD1	2:F:24:ASP:N	2.52	0.40
1:A:283:ASP:O	1:A:287:ARG:HG3	2.21	0.40
1:D:203:ALA:HB1	1:D:208:ILE:HD12	2.04	0.40
1:A:242:LEU:HD11	1:A:249:SER:HB2	2.04	0.40
1:D:289:ILE:HG23	2:F:39:LEU:HD11	2.02	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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/361 (99%)	344 (96%)	15 (4%)	0	100	100
1	B	359/361 (99%)	347 (97%)	12 (3%)	0	100	100
1	C	359/361 (99%)	344 (96%)	15 (4%)	0	100	100
1	D	359/361 (99%)	348 (97%)	11 (3%)	0	100	100
2	E	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
2	F	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
2	G	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
2	H	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
All	All	2008/2024 (99%)	1921 (96%)	87 (4%)	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	312/312 (100%)	312 (100%)	0	100	100
1	B	312/312 (100%)	312 (100%)	0	100	100
1	C	312/312 (100%)	312 (100%)	0	100	100
1	D	312/312 (100%)	312 (100%)	0	100	100
2	E	82/124 (66%)	82 (100%)	0	100	100
2	F	82/124 (66%)	82 (100%)	0	100	100
2	G	83/124 (67%)	83 (100%)	0	100	100
2	H	82/124 (66%)	82 (100%)	0	100	100
All	All	1577/1744 (90%)	1577 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

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Mol	Chain	Res	Type
1	A	201	ASN
1	A	345	ASN
1	A	453	GLN
1	C	345	ASN
1	C	461	HIS
1	D	345	ASN
2	F	42	ASN
2	F	49	GLN
2	G	49	GLN
2	H	53	ASN
2	H	107	HIS
2	H	111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	1KP	F	201	-	15,15,15	0.93	1 (6%)	20,22,22	1.33	5 (25%)
4	1KP	E	201	-	15,15,15	0.92	1 (6%)	20,22,22	1.28	3 (15%)

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	1KP	G	201	-	15,15,15	0.94	1 (6%)	20,22,22	1.37	4 (20%)
4	1KP	H	201	-	15,15,15	0.93	1 (6%)	20,22,22	1.32	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1KP	F	201	-	-	2/2/14/14	0/2/2/2
4	1KP	E	201	-	-	2/2/14/14	0/2/2/2
4	1KP	G	201	-	-	2/2/14/14	0/2/2/2
4	1KP	H	201	-	-	2/2/14/14	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	201	1KP	O-N	-2.24	1.33	1.40
4	E	201	1KP	O-N	-2.23	1.33	1.40
4	F	201	1KP	O-N	-2.22	1.33	1.40
4	H	201	1KP	O-N	-2.22	1.33	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	201	1KP	C5-C4-CL1	-2.62	118.10	120.51
4	H	201	1KP	C5-C4-CL1	-2.34	118.36	120.51
4	E	201	1KP	C1-C6-N1	2.33	111.12	108.13
4	F	201	1KP	C5-C4-CL1	-2.32	118.37	120.51
4	H	201	1KP	C1-C6-N1	2.32	111.11	108.13
4	F	201	1KP	C1-C6-N1	2.27	111.05	108.13
4	G	201	1KP	C1-C6-N1	2.27	111.04	108.13
4	F	201	1KP	O1-C7-C	2.23	128.69	126.80
4	E	201	1KP	O1-C7-C	2.23	128.69	126.80
4	G	201	1KP	O1-C7-C	2.21	128.67	126.80
4	H	201	1KP	O1-C7-C	2.17	128.64	126.80
4	G	201	1KP	C-C7-N1	-2.10	105.01	106.06
4	F	201	1KP	C-C7-N1	-2.09	105.01	106.06
4	E	201	1KP	C5-C4-CL1	-2.08	118.60	120.51
4	H	201	1KP	C-C7-N1	-2.04	105.04	106.06
4	F	201	1KP	C1-C-C7	2.03	107.34	106.31

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There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	1KP	C1-C-N-O
4	E	201	1KP	C7-C-N-O
4	F	201	1KP	C1-C-N-O
4	F	201	1KP	C7-C-N-O
4	G	201	1KP	C1-C-N-O
4	G	201	1KP	C7-C-N-O
4	H	201	1KP	C1-C-N-O
4	H	201	1KP	C7-C-N-O

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	201	1KP	1	0
4	G	201	1KP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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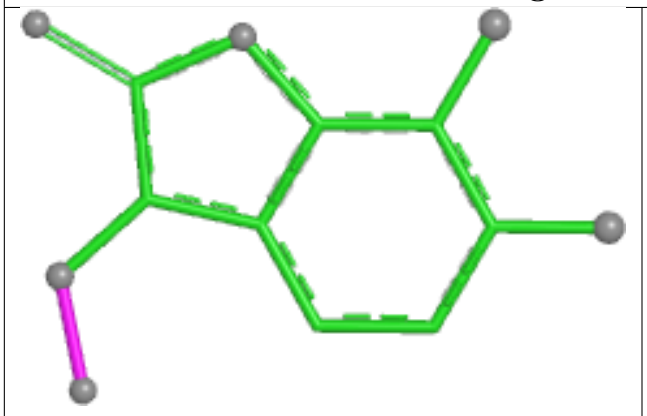
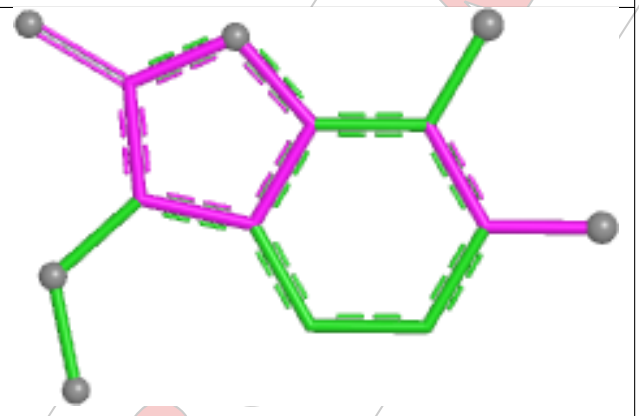
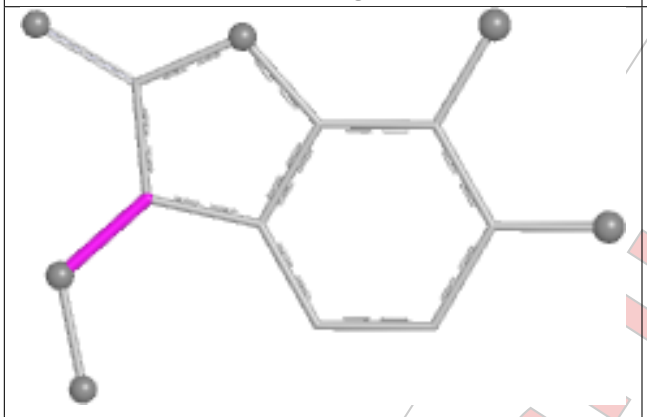
Ligand 1KP F 201



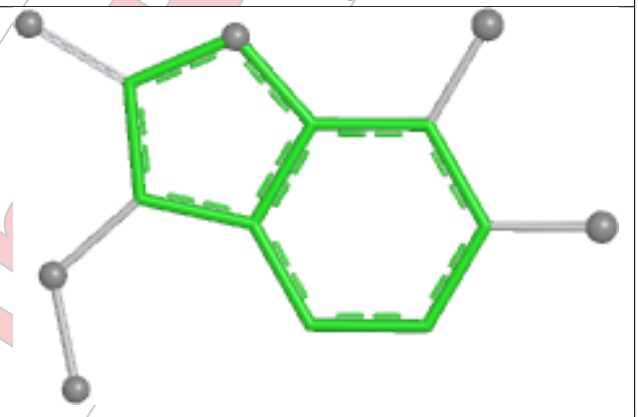
Bond lengths



Bond angles



Torsions



Rings

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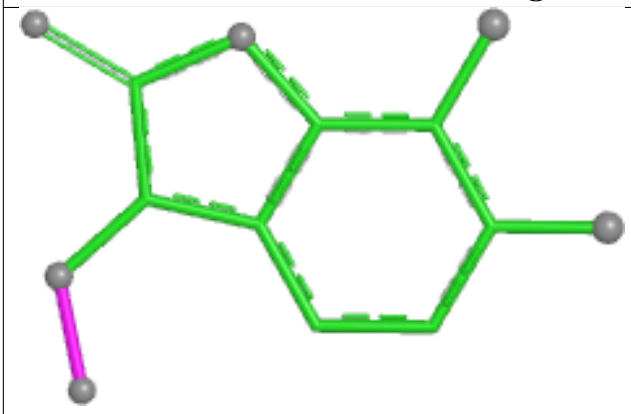
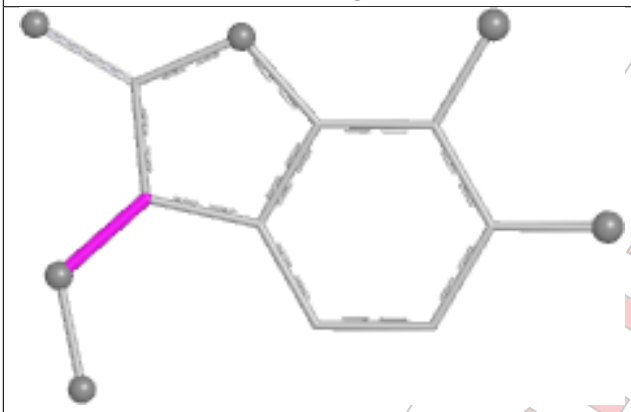
Ligand 1KP E 201

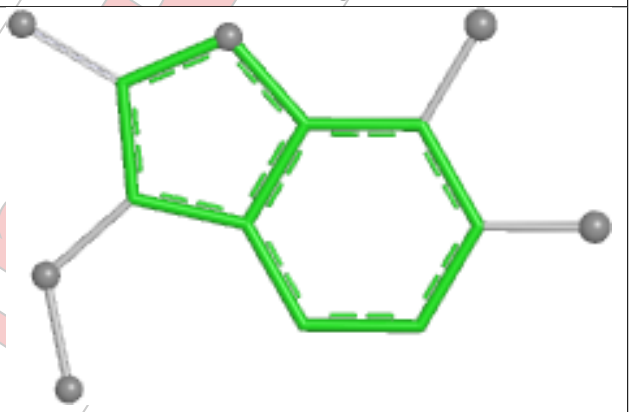


Bond lengths

Bond angles



Torsions



Rings

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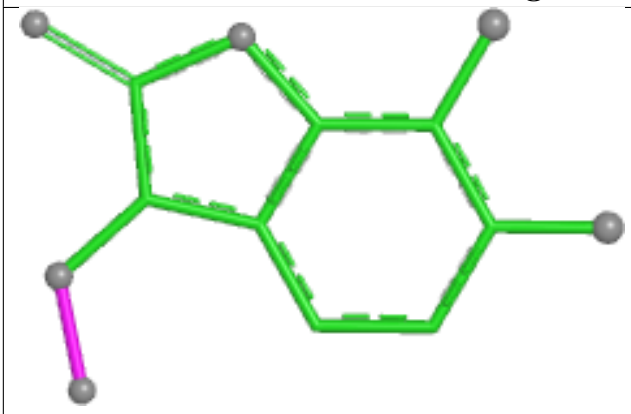
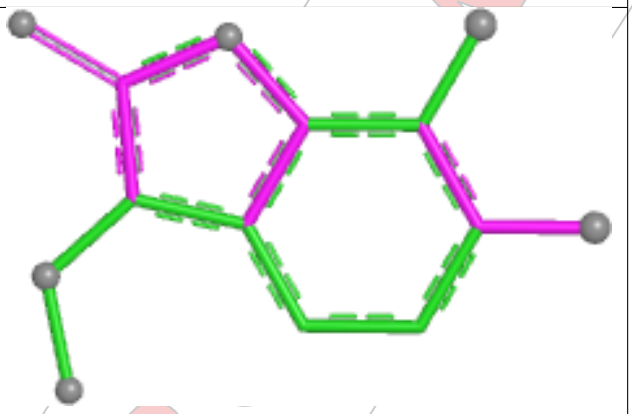
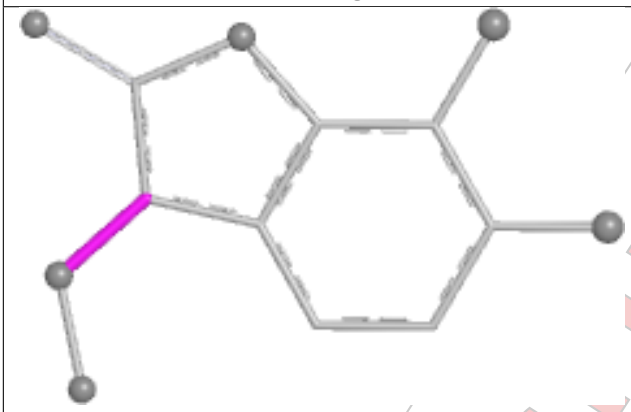
Ligand 1KP G 201



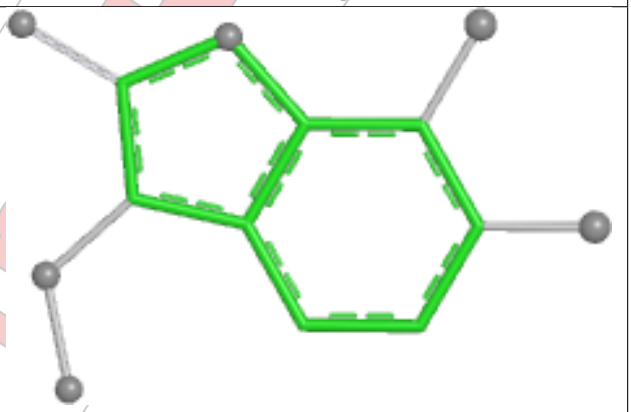
Bond lengths



Bond angles



Torsions



Rings

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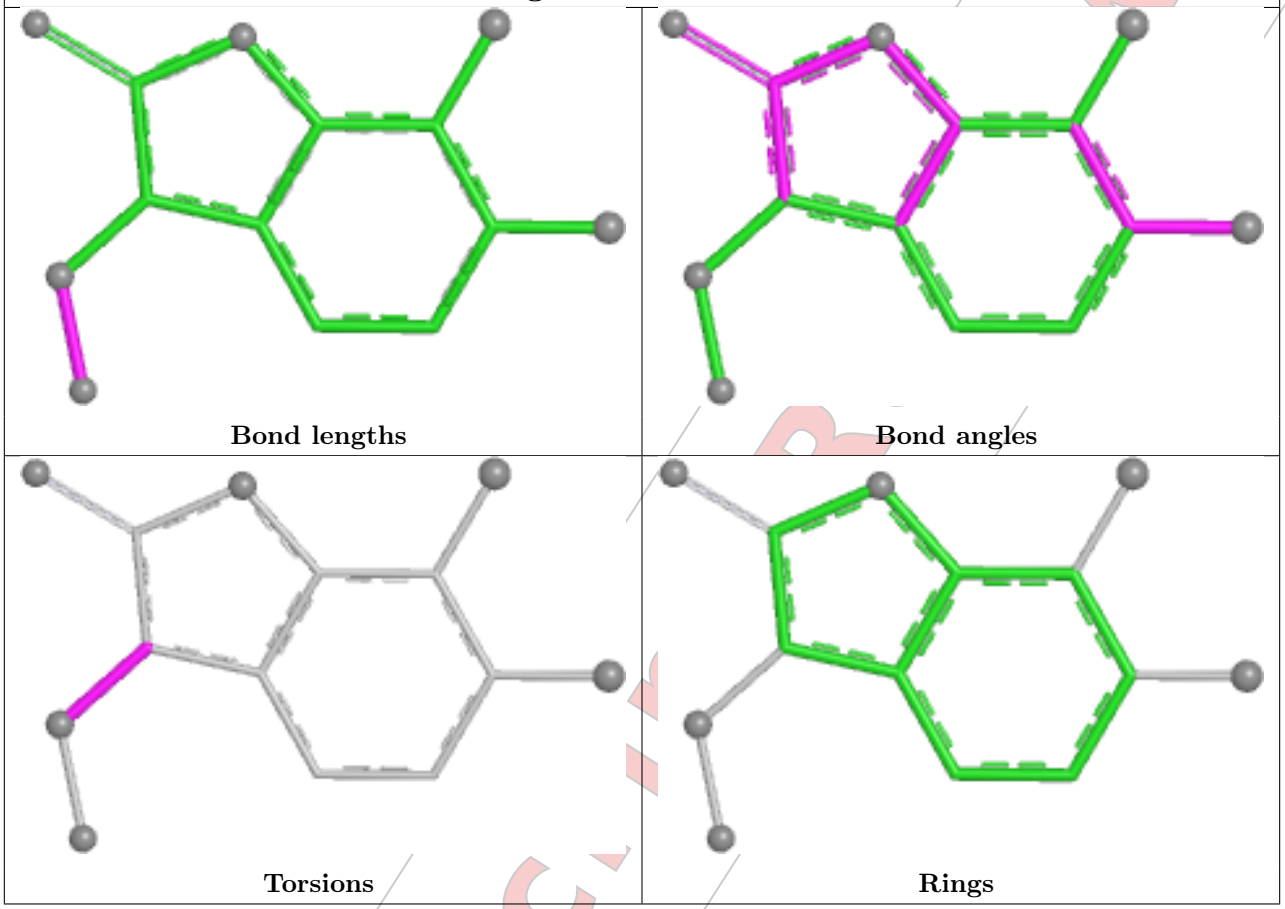
Ligand 1KP H 201



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.

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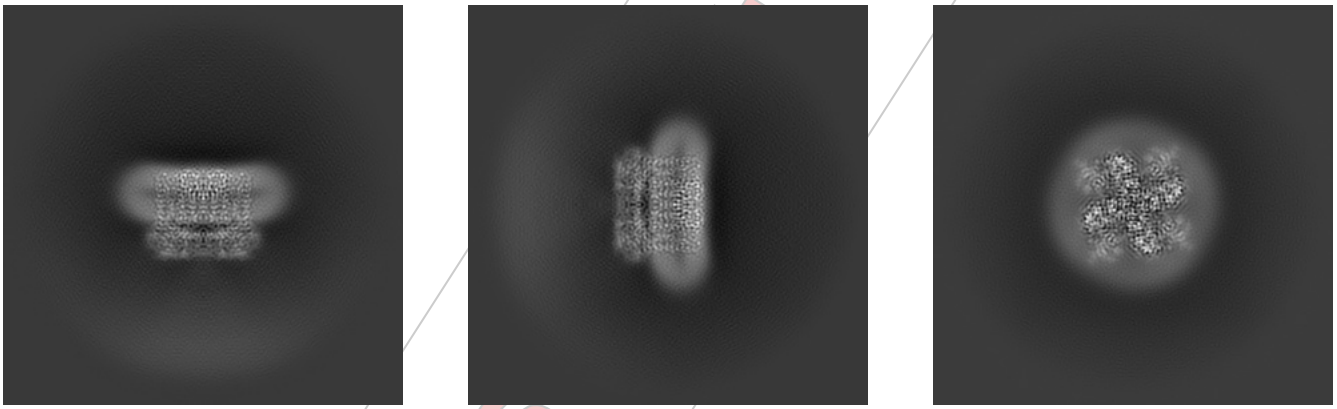
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70207. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

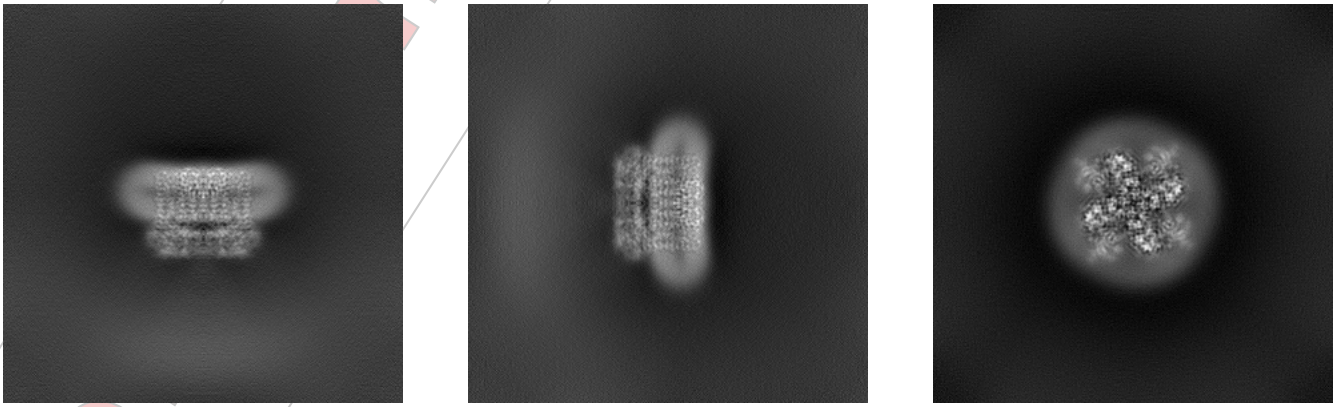
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



X Y Z

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

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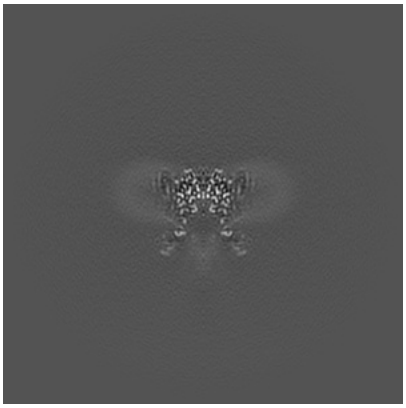
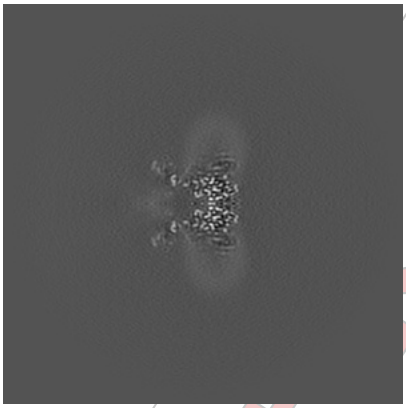
6.2 Central slices (i)

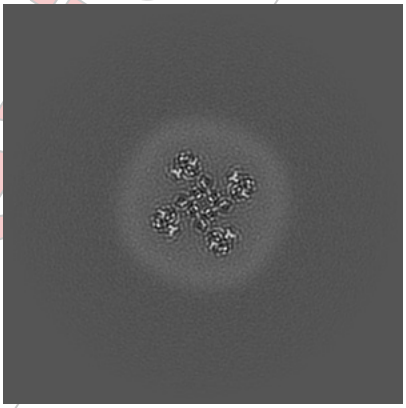
6.2.1 Primary map



X Index: 250

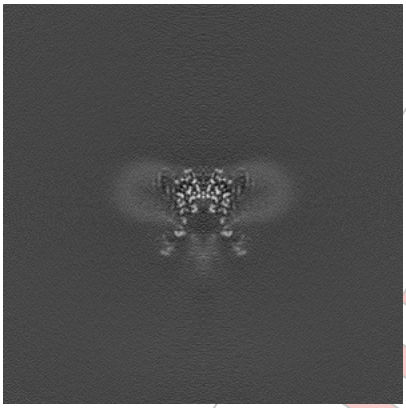


Y Index: 250

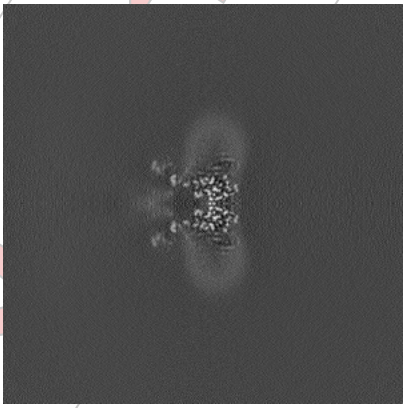


Z Index: 250

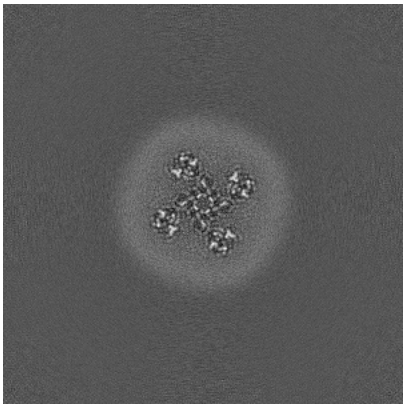
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

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

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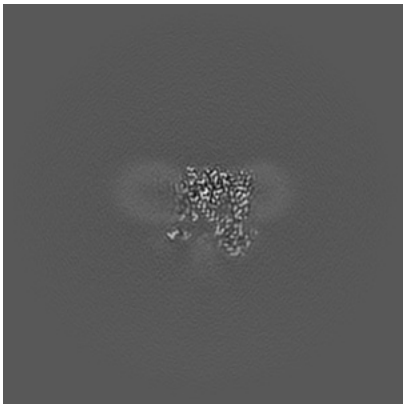
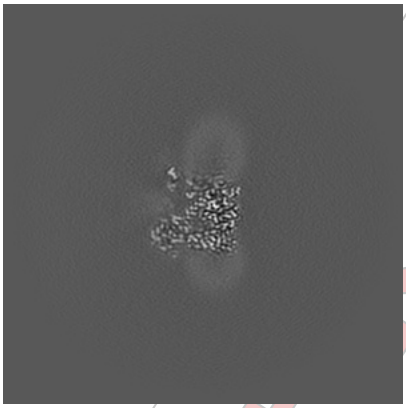
6.3 Largest variance slices (i)

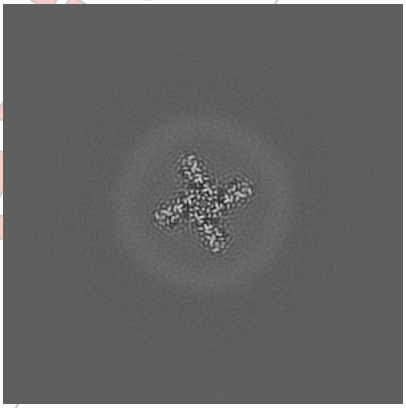
6.3.1 Primary map



X Index: 239

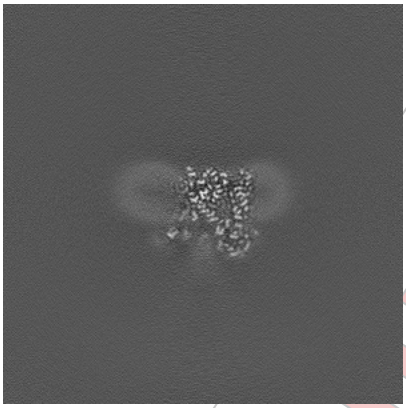


Y Index: 239

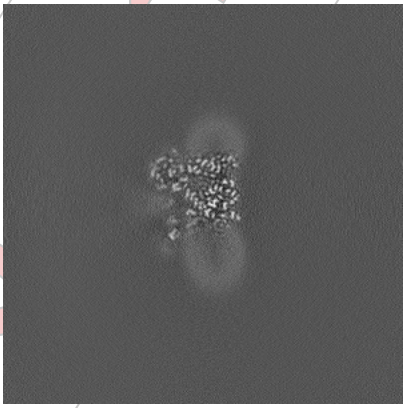


Z Index: 269

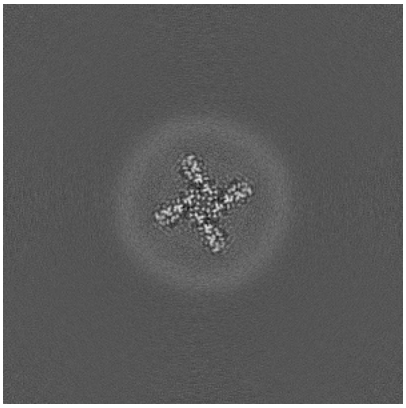
6.3.2 Raw map



X Index: 238



Y Index: 262



Z Index: 269

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

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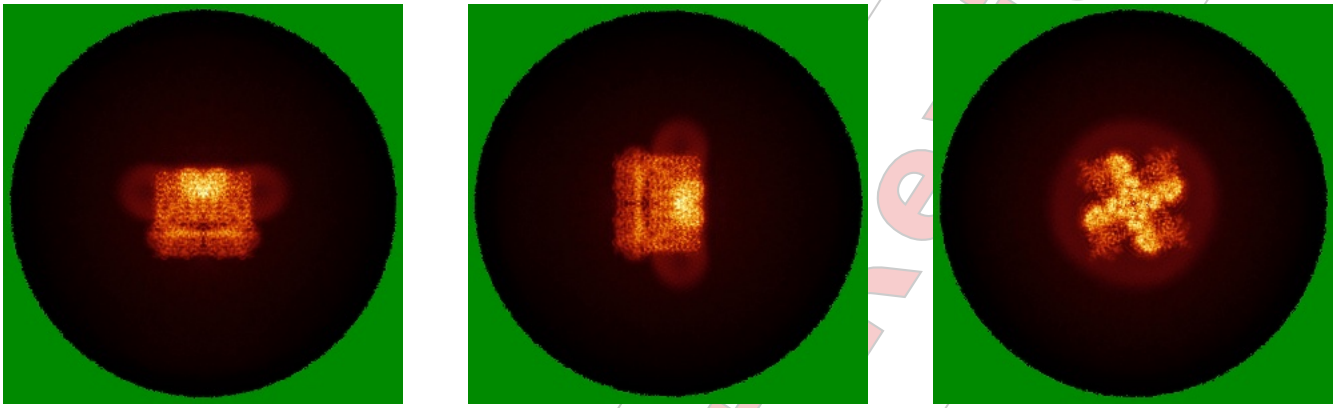
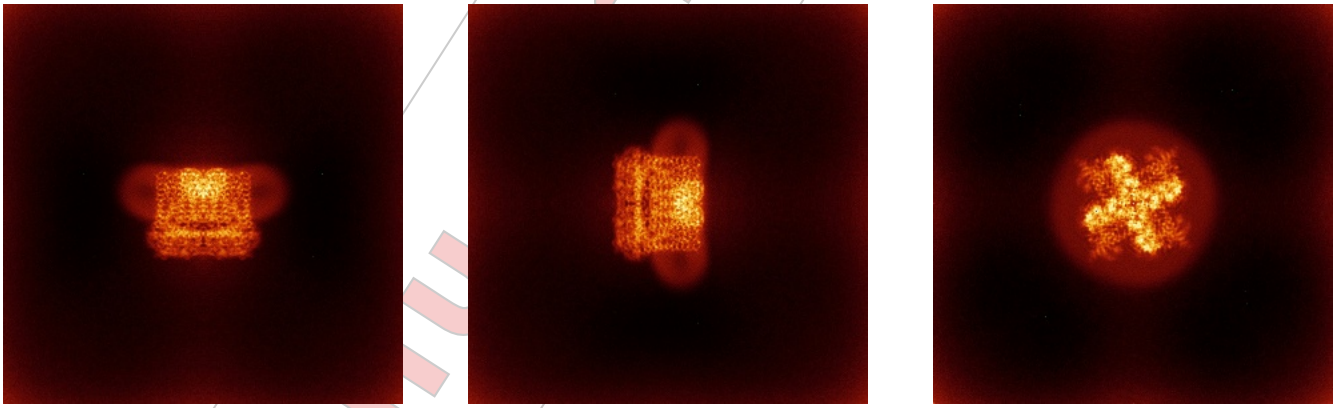
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

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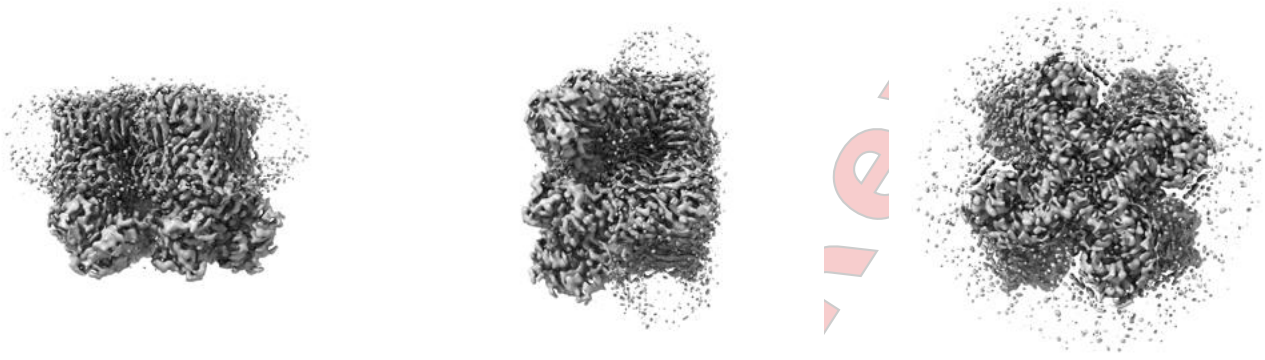
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

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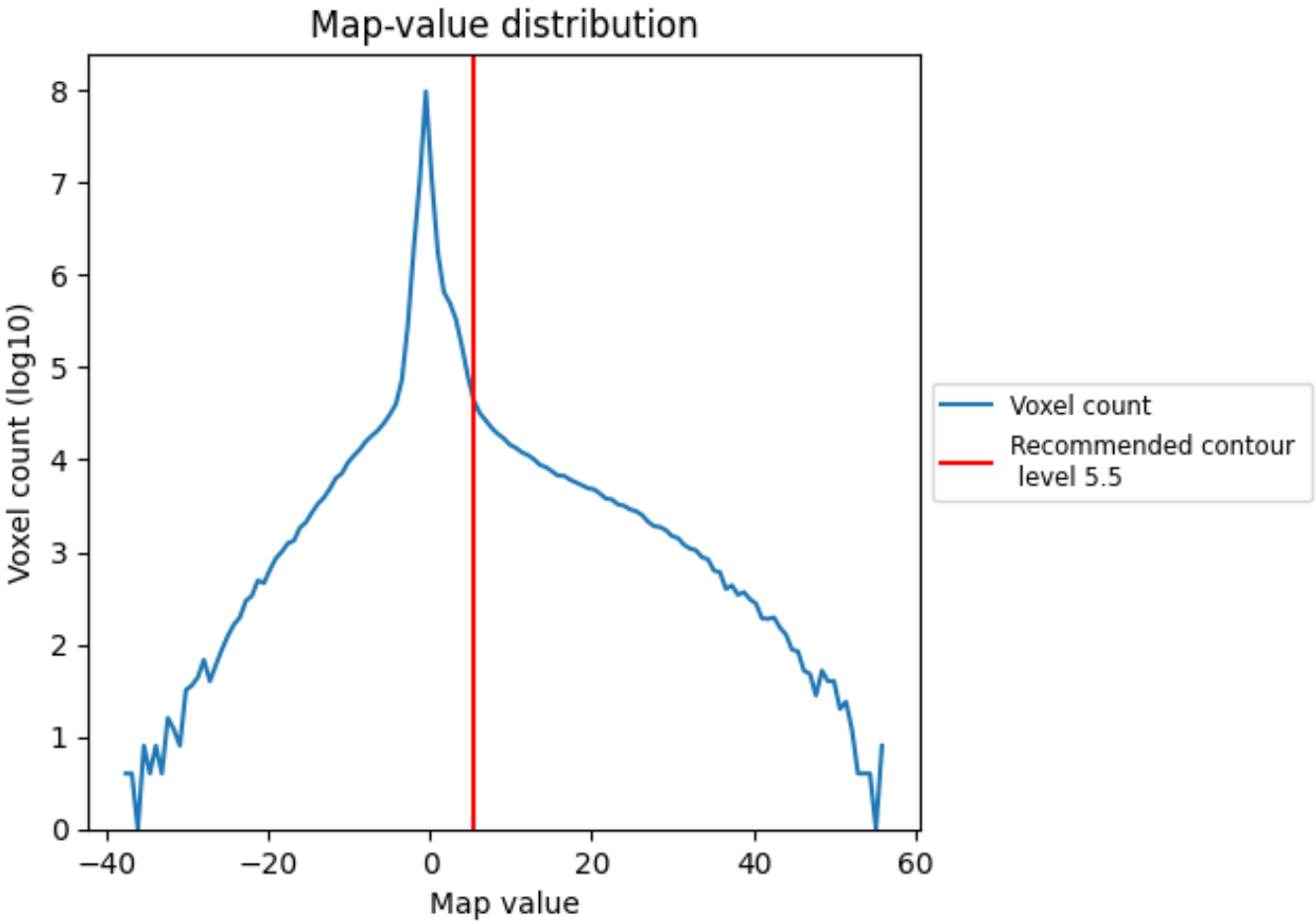
7 Map analysis

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.

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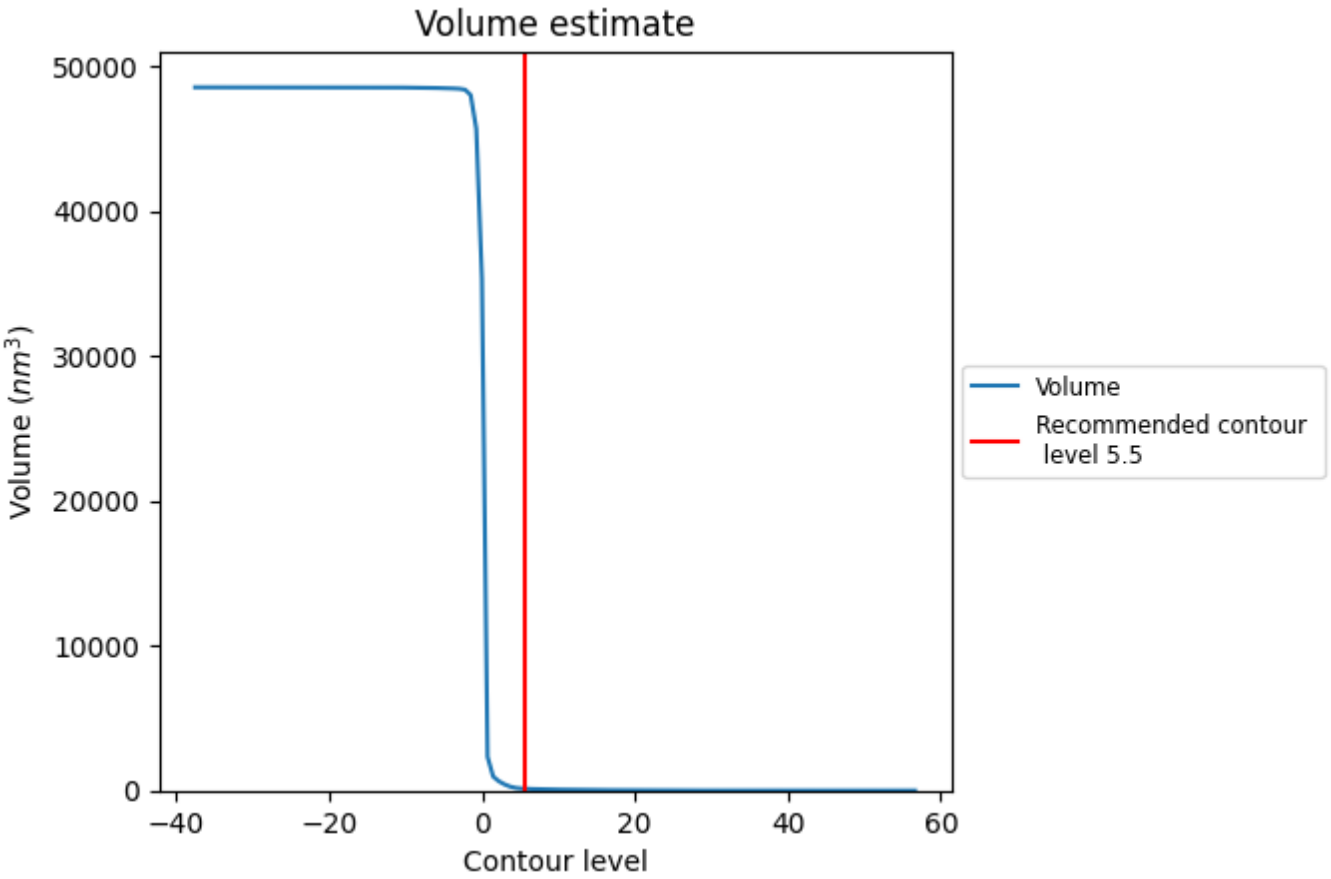
7.2 Volume estimate (i)

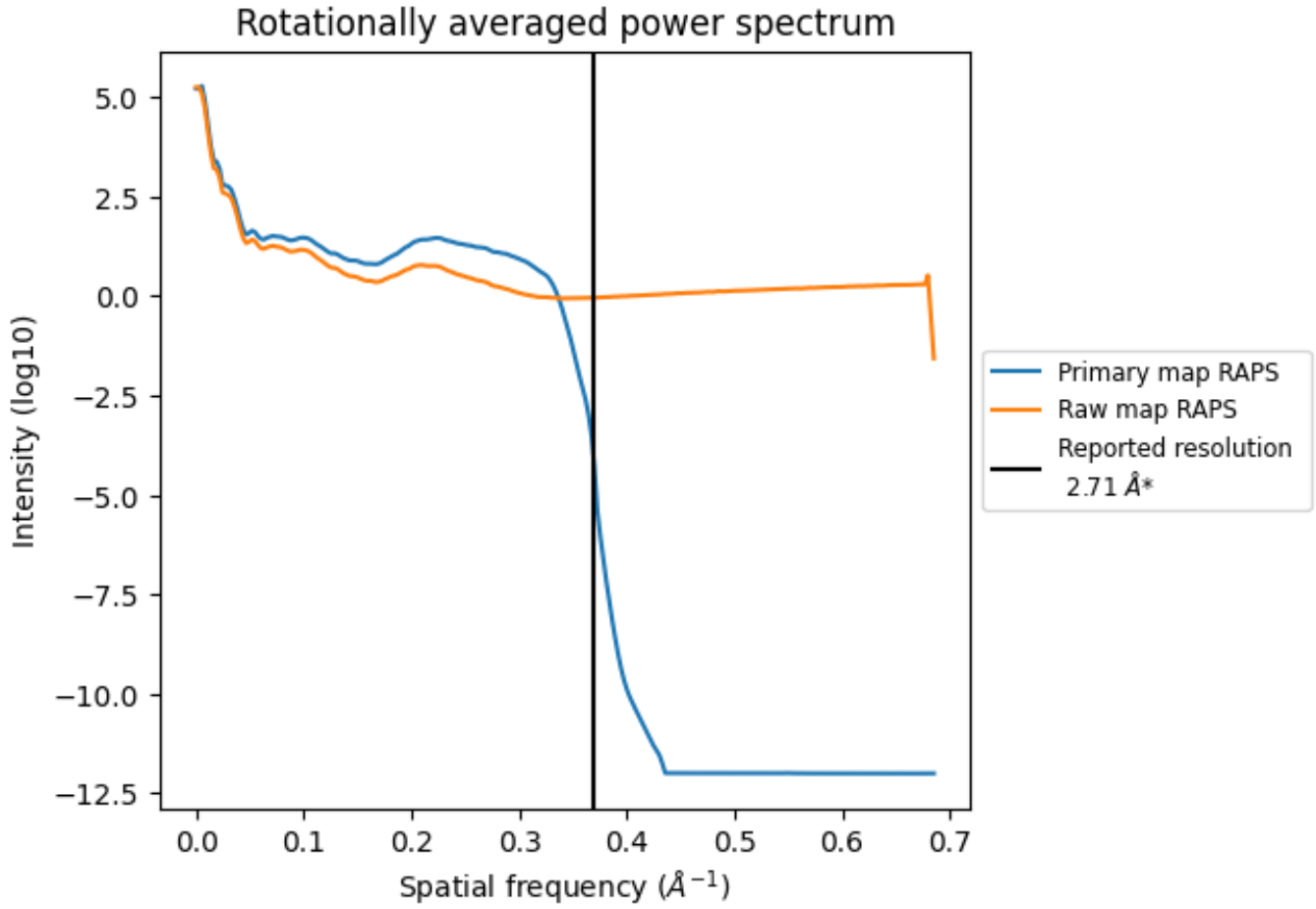


The volume at the recommended contour level is 130 nm^3; this corresponds to an approximate mass of 117 kDa.

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.

For Manus

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.369 Å^{-1}

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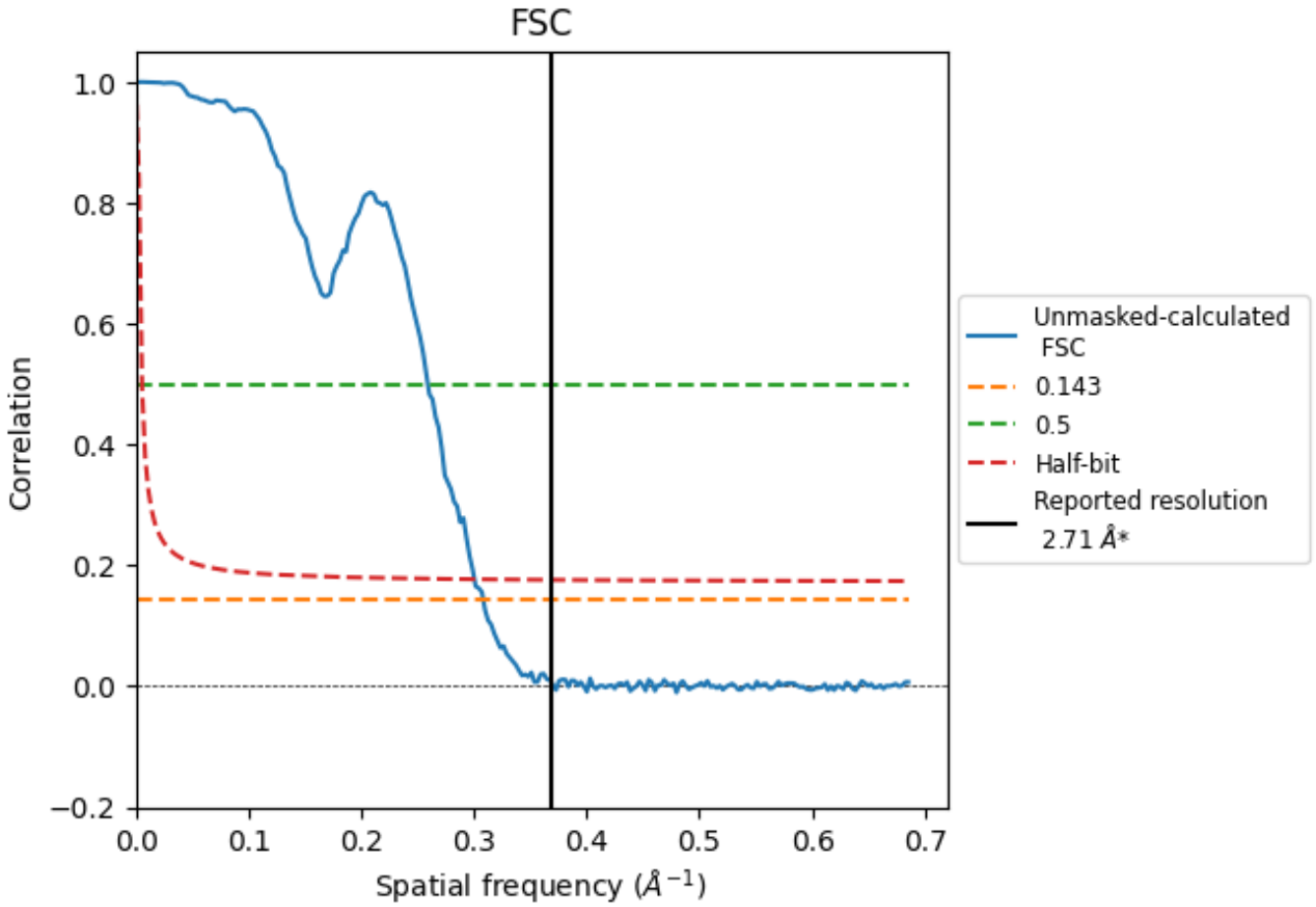
8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.369 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.24	3.86	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.24 differs from the reported value 2.71 by more than 10 %

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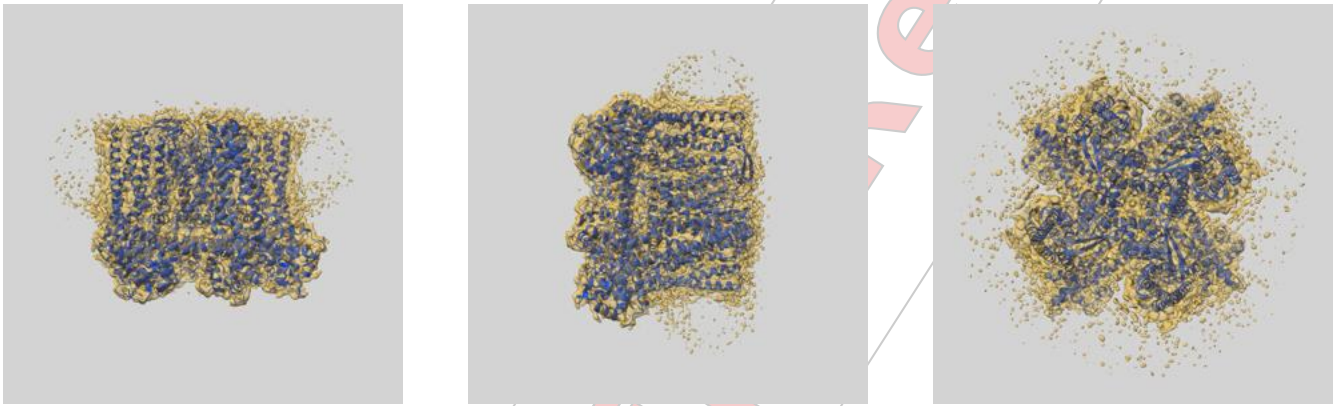
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70207 and PDB model 9O7S. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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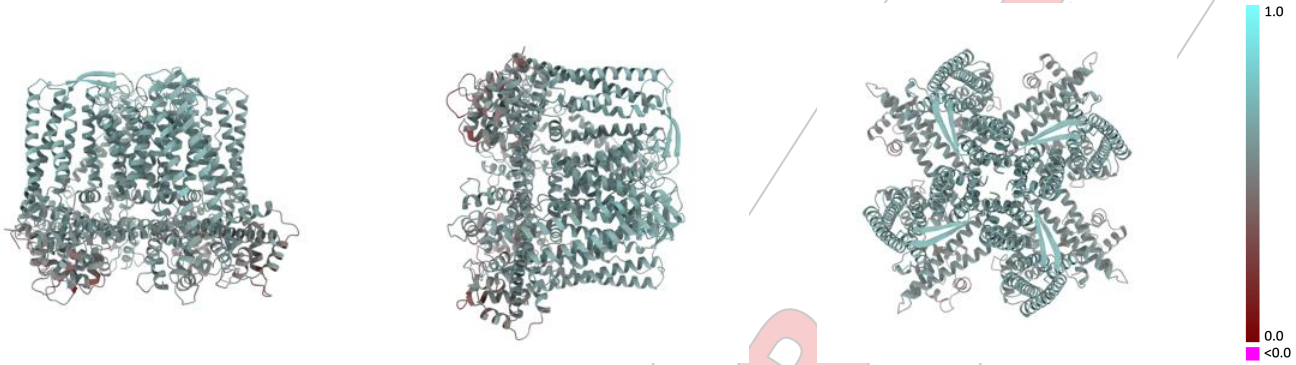
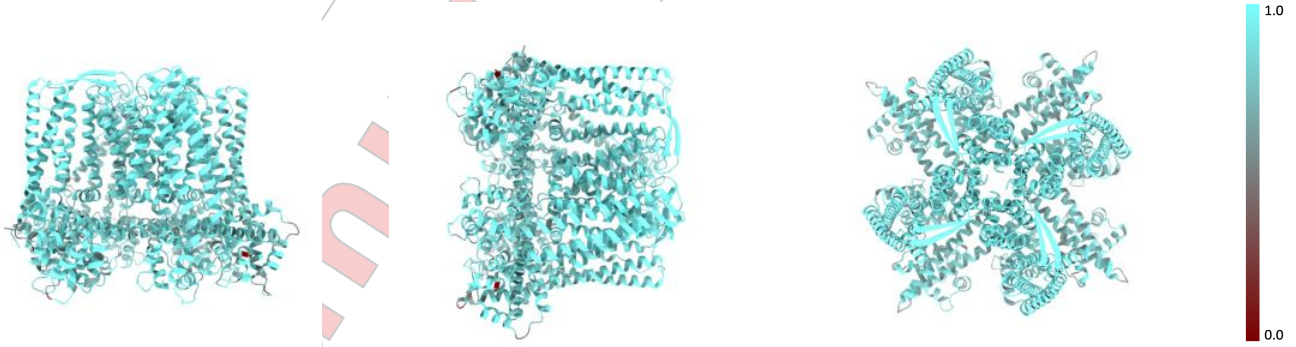
9.2 Q-score mapped to coordinate model (i)



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 (5.5).

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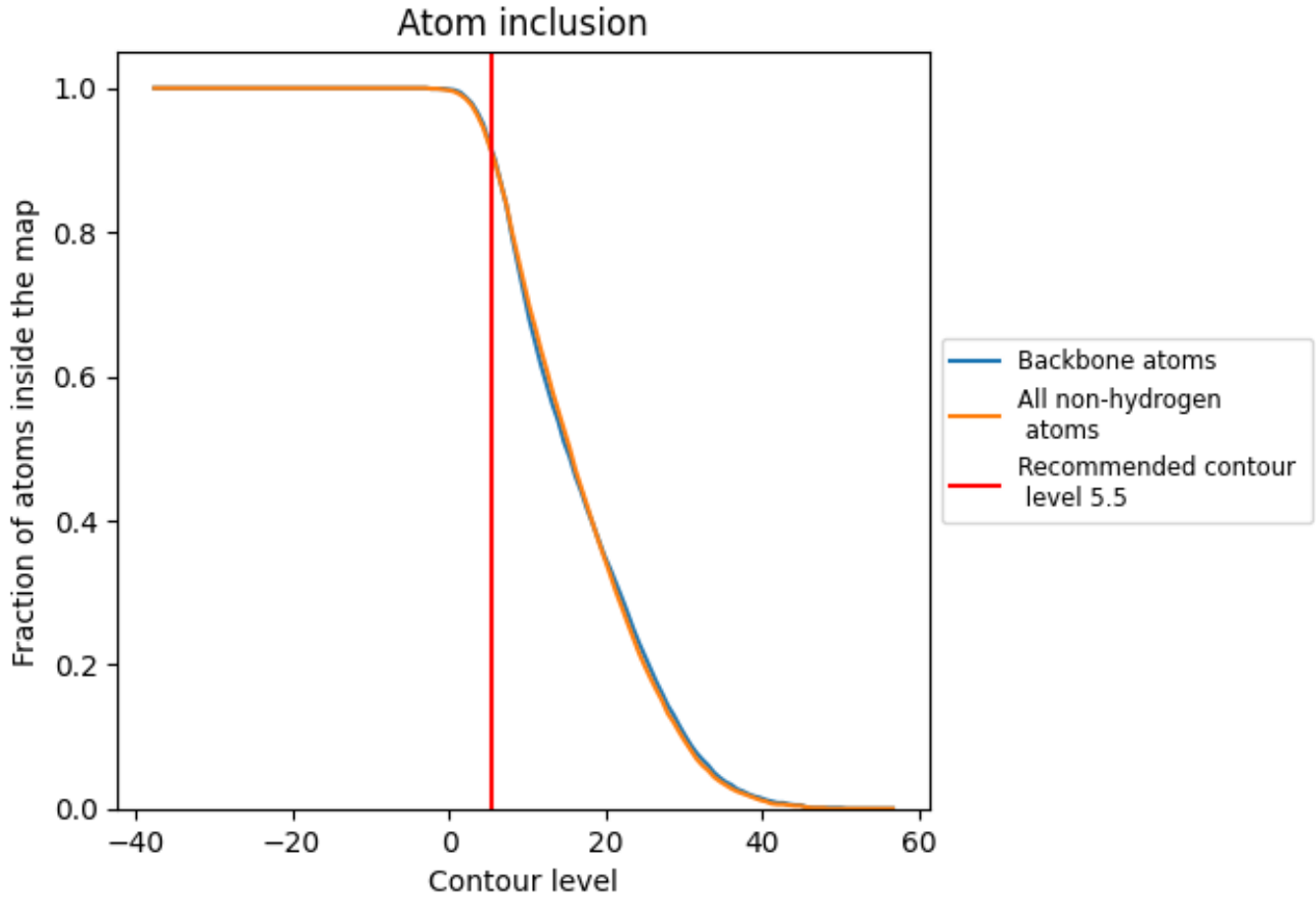
9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9090	0.5730
A	0.9330	0.5960
B	0.9320	0.5960
C	0.9280	0.5960
D	0.9310	0.5970
E	0.8610	0.5100
F	0.8640	0.5060
G	0.8600	0.5100
H	0.8530	0.5060

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Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 03:23 PM EDT

PDB ID	:	9OA8 / pdb_00009oa8
EMDB ID	:	EMD-70275
Title	:	Cryo-EM structure of KCa3.1/calmodulin channel in complex with NS309
Deposited on	:	2025-04-19
Resolution	:	3.59 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

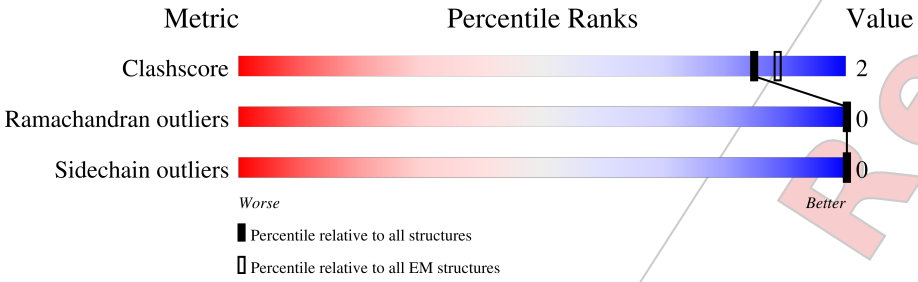
For Manuscript Review

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 3.59 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	378	90% 5% 5%
1	B	378	93% • 5%
1	C	378	94% • 5%
1	D	378	88% 8% 5%
2	E	146	92% 8%
2	F	146	93% 7%
2	G	146	88% 12%

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Mol	Chain	Length	Quality of chain
2	H	146	

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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15255 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 Intermediate conductance calcium-activated potassium channel protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	360	Total	C	N	O	S	0	0
			2758	1789	504	447	18		
1	B	360	Total	C	N	O	S	0	0
			2754	1788	503	445	18		
1	C	360	Total	C	N	O	S	0	0
			2754	1788	503	445	18		
1	D	360	Total	C	N	O	S	0	0
			2754	1788	503	445	18		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	146	Total	C	N	O	S	0	0
			1042	642	173	219	8		
2	F	146	Total	C	N	O	S	0	0
			1042	642	173	219	8		
2	G	146	Total	C	N	O	S	0	0
			1042	642	173	219	8		
2	H	146	Total	C	N	O	S	0	0
			1042	642	173	219	8		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	K	0
			3	3	

- Molecule 4 is (3E)-6,7-dichloro-3-(hydroxyimino)-1,3-dihydro-2H-indol-2-one (CCD ID: 1KP) (formula: $C_8H_4Cl_2N_2O_2$) (labeled as "Ligand of Interest" by depositor).

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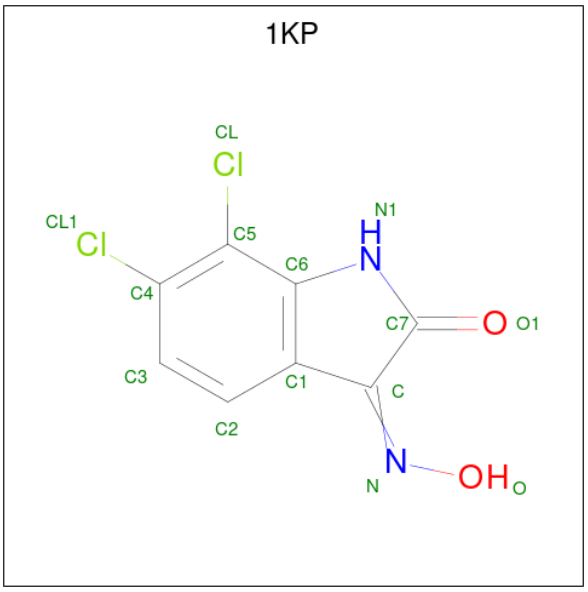

Mol	Chain	Residues	Atoms	AltConf
4	E	1	Total C Cl N O 14 8 2 2 2	0
4	F	1	Total C Cl N O 14 8 2 2 2	0
4	G	1	Total C Cl N O 14 8 2 2 2	0
4	H	1	Total C Cl N O 14 8 2 2 2	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	E	2	Total Ca 2 2	0
5	F	2	Total Ca 2 2	0
5	G	2	Total Ca 2 2	0
5	H	2	Total Ca 2 2	0

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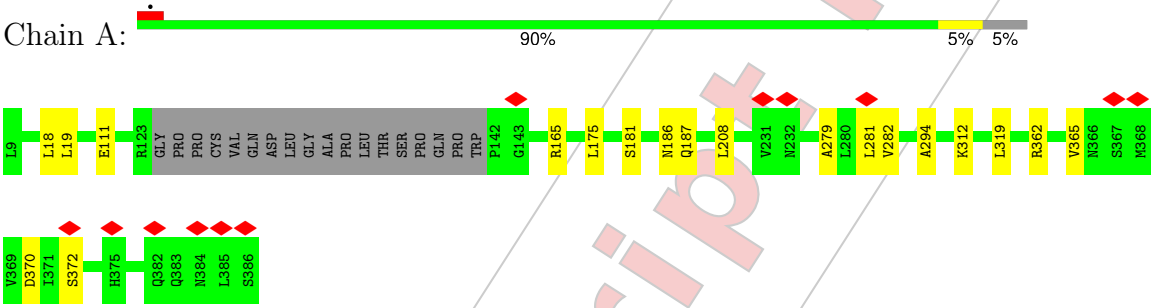
3 Residue-property plots (i)

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.

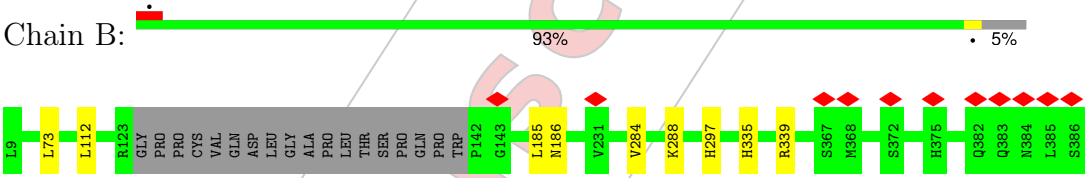
• Molecule 1: Intermediate conductance calcium-activated potassium channel protein 4

Chain A:



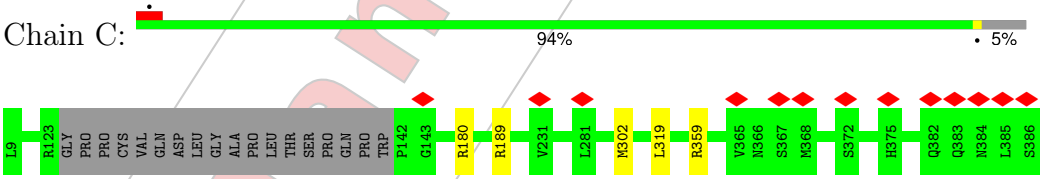
• Molecule 1: Intermediate conductance calcium-activated potassium channel protein 4

Chain B:



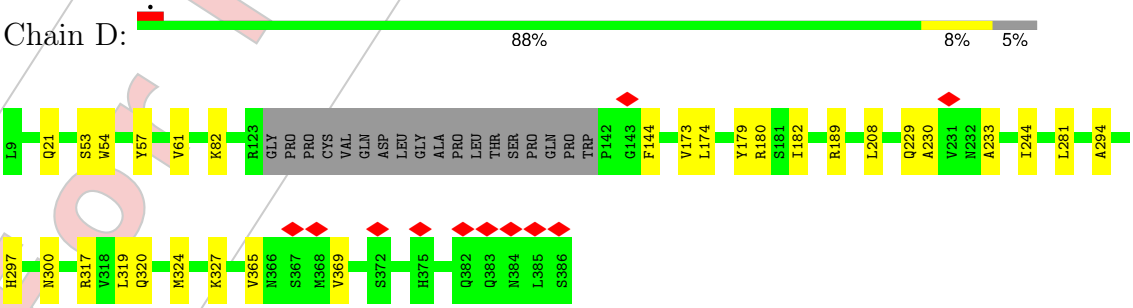
• Molecule 1: Intermediate conductance calcium-activated potassium channel protein 4

Chain C:



• Molecule 1: Intermediate conductance calcium-activated potassium channel protein 4

Chain D:



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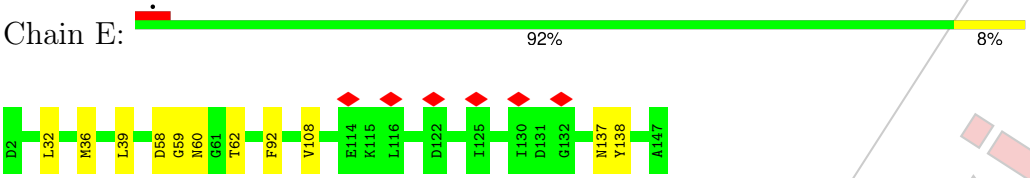
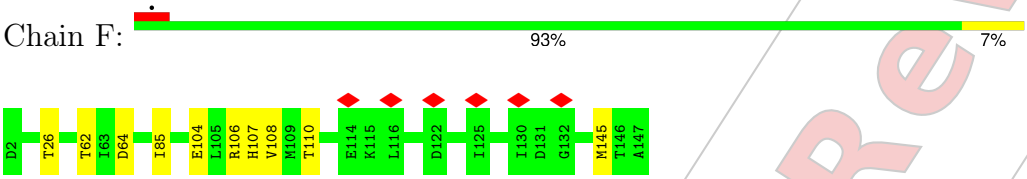
• Molecule 2: Calmodulin-1

Chain E:



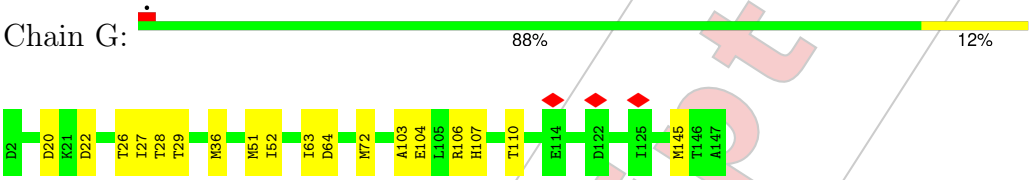
• Molecule 2: Calmodulin-1

Chain F:



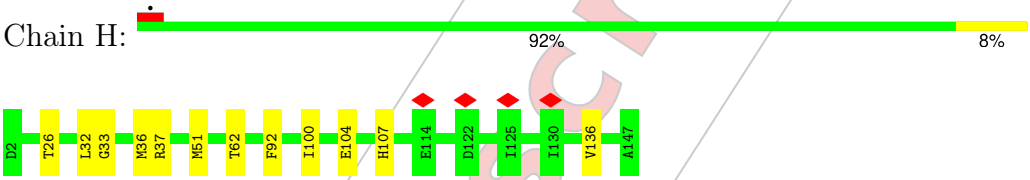
• Molecule 2: Calmodulin-1

Chain G:



• Molecule 2: Calmodulin-1

Chain H:



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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119846	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	65.515	Depositor
Minimum map value	-51.493	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.4	Depositor
Map size (Å)	430.0, 430.0, 430.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

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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: K, CA, 1KP

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	0.14	0/2815	0.27	0/3815
1	B	0.13	0/2811	0.24	0/3810
1	C	0.14	0/2811	0.27	0/3810
1	D	0.13	0/2811	0.26	0/3810
2	E	0.12	0/1053	0.25	0/1424
2	F	0.11	0/1053	0.23	0/1424
2	G	0.12	0/1053	0.32	0/1424
2	H	0.13	0/1053	0.31	0/1424
All	All	0.13	0/15460	0.27	0/20941

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	2758	0	2810	13	0
1	B	2754	0	2803	6	0
1	C	2754	0	2803	4	0
1	D	2754	0	2803	18	0
2	E	1042	0	902	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1042	0	902	6	0
2	G	1042	0	901	11	0
2	H	1042	0	901	9	0
3	A	3	0	0	0	0
4	E	14	0	4	0	0
4	F	14	0	4	0	0
4	G	14	0	4	0	0
4	H	14	0	4	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
All	All	15255	0	14841	63	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 2.

All (63) 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:G:104:GLU:HA	2:G:107:HIS:CE1	2.30	0.67
2:H:104:GLU:HA	2:H:107:HIS:CE1	2.31	0.66
1:D:21:GLN:OE1	1:D:82:LYS:NZ	2.28	0.66
1:D:229:GLN:HB3	1:D:233:ALA:HA	1.76	0.65
1:A:111:GLU:OE2	1:A:165:ARG:NH2	2.30	0.65
1:D:324:MET:SD	1:D:327:LYS:NZ	2.70	0.64
2:G:20:ASP:OD2	2:G:22:ASP:OD1	2.16	0.62
1:A:362:ARG:HA	1:A:365:VAL:HG22	1.82	0.62
1:A:181:SER:HB3	2:G:72:MET:HE1	1.89	0.54
2:H:32:LEU:HD11	2:H:36:MET:HE3	1.89	0.54
1:A:370:ASP:O	1:A:372:SER:N	2.40	0.54
2:F:85:ILE:HD12	2:F:145:MET:SD	2.47	0.54
2:F:106:ARG:O	2:F:110:THR:OG1	2.21	0.53
2:E:32:LEU:HD11	2:E:36:MET:HE3	1.91	0.52
1:A:187:GLN:HB2	1:C:359:ARG:HH21	1.74	0.52
2:E:58:ASP:OD1	2:E:59:GLY:N	2.43	0.52
1:A:208:LEU:HD22	1:A:281:LEU:HD13	1.91	0.51
1:C:180:ARG:HH21	1:C:189:ARG:HH12	1.59	0.51
1:D:173:VAL:HG13	1:D:174:LEU:HD12	1.95	0.49
2:F:104:GLU:O	2:F:108:VAL:HG12	2.12	0.49
2:H:100:ILE:HB	2:H:136:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD13	2:E:92:PHE:CE2	2.49	0.48
2:G:64:ASP:OD1	2:G:64:ASP:N	2.46	0.48
1:C:302:MET:HE3	1:D:182:ILE:HG13	1.97	0.47
1:B:73:LEU:HD22	1:B:112:LEU:HD22	1.97	0.47
2:F:64:ASP:OD1	2:F:64:ASP:N	2.46	0.47
2:G:36:MET:HE1	2:G:51:MET:HE1	1.97	0.47
1:D:319:LEU:HD12	2:H:92:PHE:CE2	2.50	0.46
1:C:319:LEU:HD13	2:G:145:MET:HE3	1.98	0.46
1:A:186:ASN:ND2	1:D:294:ALA:O	2.49	0.46
1:D:300:ASN:HD22	1:D:365:VAL:HG22	1.80	0.46
2:E:60:ASN:ND2	2:E:62:THR:OG1	2.38	0.45
2:H:26:THR:HB	2:H:62:THR:HB	1.99	0.45
1:A:294:ALA:O	1:B:186:ASN:ND2	2.50	0.45
1:A:312:LYS:HE2	2:E:108:VAL:HG23	1.98	0.45
1:B:335:HIS:HB3	1:B:339:ARG:HH21	1.82	0.44
1:D:180:ARG:HH21	1:D:189:ARG:HH12	1.65	0.44
2:G:28:THR:OG1	2:G:29:THR:N	2.51	0.44
2:F:104:GLU:O	2:F:107:HIS:ND1	2.51	0.43
1:D:144:PHE:HZ	1:D:230:ALA:HB2	1.83	0.43
1:B:284:VAL:O	1:B:288:LYS:HG2	2.19	0.43
1:D:297:HIS:CE1	1:D:369:VAL:HG23	2.54	0.43
1:D:317:ARG:HA	1:D:320:GLN:HG2	2.00	0.43
2:G:26:THR:O	2:G:27:ILE:HG13	2.19	0.43
1:D:57:TYR:O	1:D:61:VAL:HG23	2.18	0.43
2:E:137:ASN:OD1	2:E:138:TYR:N	2.49	0.43
1:D:53:SER:HG	1:D:54:TRP:CD1	2.37	0.42
1:A:279:ALA:HA	1:A:282:VAL:HG22	2.02	0.42
1:B:297:HIS:ND1	2:E:39:LEU:O	2.41	0.41
1:D:208:LEU:HD22	1:D:281:LEU:HD13	2.01	0.41
1:D:244:ILE:HD13	1:D:244:ILE:HA	1.93	0.41
1:D:173:VAL:HG23	1:D:179:TYR:CD2	2.56	0.41
2:H:104:GLU:HA	2:H:107:HIS:HE1	1.81	0.41
1:D:82:LYS:HD3	1:D:82:LYS:HA	1.90	0.41
2:F:26:THR:HB	2:F:62:THR:HB	2.02	0.41
2:H:36:MET:HE1	2:H:51:MET:SD	2.61	0.41
2:G:103:ALA:O	2:G:107:HIS:ND1	2.47	0.41
1:A:19:LEU:HD23	1:A:175:LEU:HD21	2.02	0.41
1:B:185:LEU:HD22	2:H:36:MET:HE2	2.01	0.41
2:G:52:ILE:HG23	2:G:63:ILE:HD11	2.03	0.41
2:G:106:ARG:O	2:G:110:THR:OG1	2.13	0.40
2:H:33:GLY:O	2:H:37:ARG:HD3	2.21	0.40

Continued on next page...

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Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.92	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	356/378 (94%)	340 (96%)	16 (4%)	0	100	100
1	B	356/378 (94%)	345 (97%)	11 (3%)	0	100	100
1	C	356/378 (94%)	342 (96%)	14 (4%)	0	100	100
1	D	356/378 (94%)	336 (94%)	20 (6%)	0	100	100
2	E	144/146 (99%)	144 (100%)	0	0	100	100
2	F	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	H	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
All	All	2000/2096 (95%)	1930 (96%)	70 (4%)	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/316 (86%)	271 (100%)	0	100	100
1	B	269/316 (85%)	269 (100%)	0	100	100
1	C	269/316 (85%)	269 (100%)	0	100	100
1	D	269/316 (85%)	269 (100%)	0	100	100
2	E	95/125 (76%)	95 (100%)	0	100	100
2	F	95/125 (76%)	95 (100%)	0	100	100
2	G	95/125 (76%)	95 (100%)	0	100	100
2	H	95/125 (76%)	95 (100%)	0	100	100
All	All	1458/1764 (83%)	1458 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	229	GLN
1	D	80	HIS
1	D	300	ASN
1	D	306	GLN
2	F	8	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	1KP	E	201	-	15,15,15	0.89	1 (6%)	20,22,22	1.21	1 (5%)
4	1KP	G	201	-	15,15,15	0.90	1 (6%)	20,22,22	1.22	1 (5%)
4	1KP	F	201	-	15,15,15	0.89	1 (6%)	20,22,22	1.23	1 (5%)
4	1KP	H	201	-	15,15,15	0.89	1 (6%)	20,22,22	1.20	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1KP	E	201	-	-	2/2/14/14	0/2/2/2
4	1KP	G	201	-	-	2/2/14/14	0/2/2/2
4	1KP	F	201	-	-	2/2/14/14	0/2/2/2
4	1KP	H	201	-	-	2/2/14/14	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	201	1KP	O-N	-2.23	1.33	1.40
4	F	201	1KP	O-N	-2.20	1.33	1.40
4	H	201	1KP	O-N	-2.18	1.34	1.40
4	E	201	1KP	O-N	-2.18	1.34	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	201	1KP	C1-C6-N1	2.08	110.80	108.13
4	F	201	1KP	C1-C6-N1	2.08	110.80	108.13
4	H	201	1KP	C1-C6-N1	2.07	110.79	108.13
4	E	201	1KP	C1-C6-N1	2.07	110.79	108.13

There are no chirality outliers.

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All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	1KP	C1-C-N-O
4	E	201	1KP	C7-C-N-O
4	F	201	1KP	C1-C-N-O
4	F	201	1KP	C7-C-N-O
4	G	201	1KP	C1-C-N-O
4	G	201	1KP	C7-C-N-O
4	H	201	1KP	C1-C-N-O
4	H	201	1KP	C7-C-N-O

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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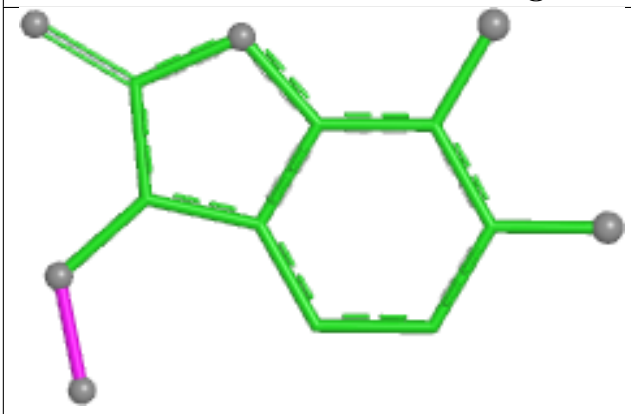
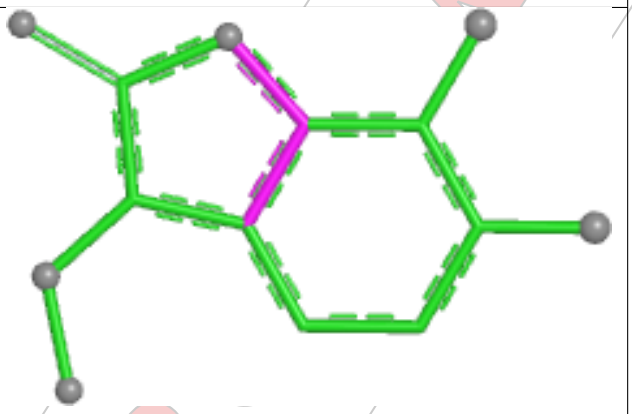
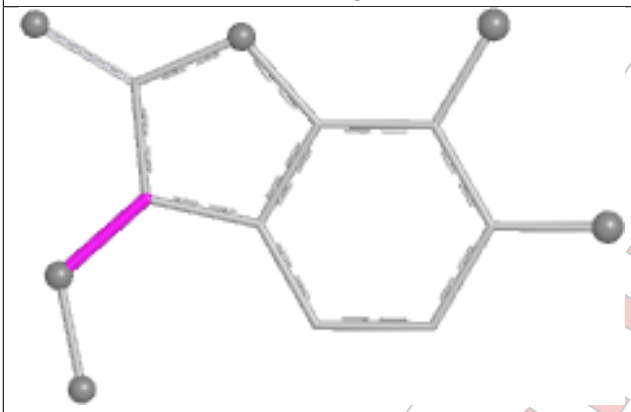
Ligand 1KP E 201



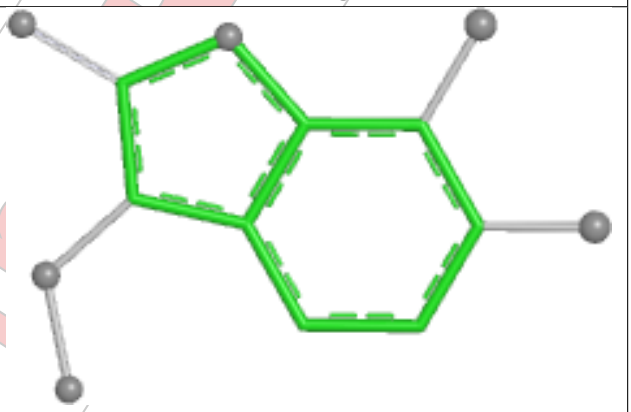
Bond lengths



Bond angles



Torsions



Rings

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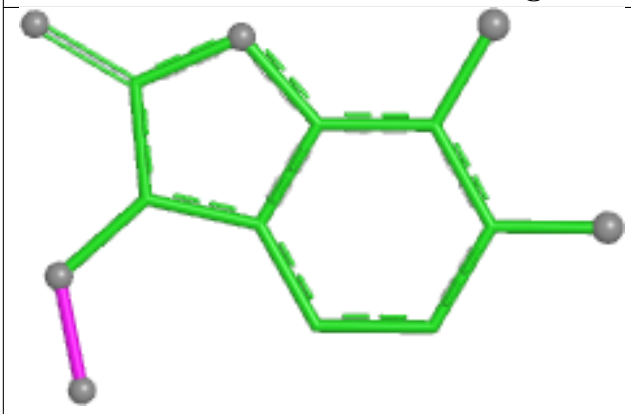
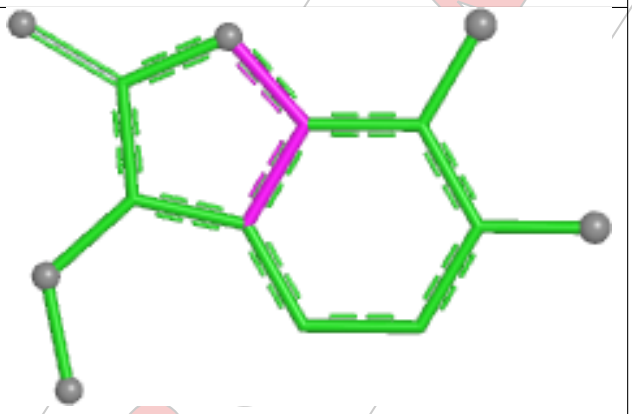
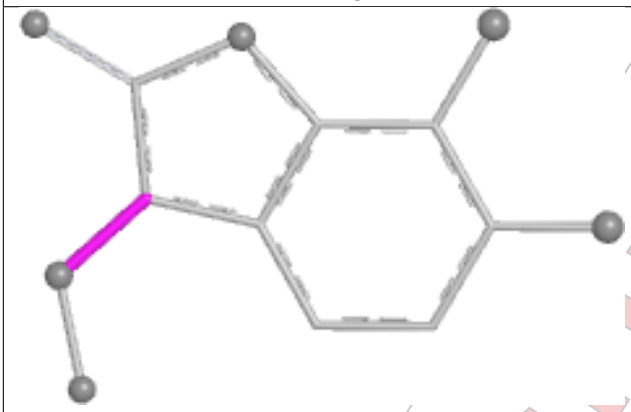
Ligand 1KP G 201



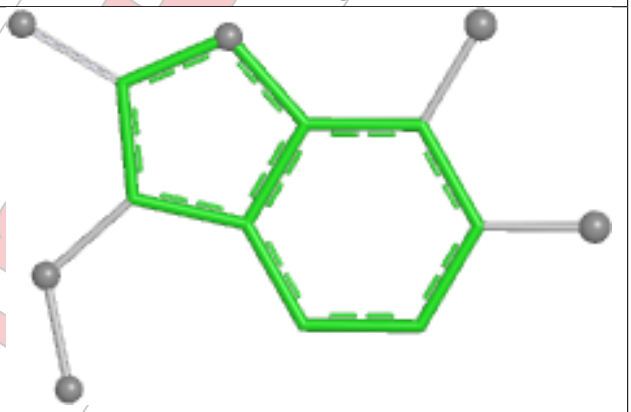
Bond lengths



Bond angles



Torsions



Rings

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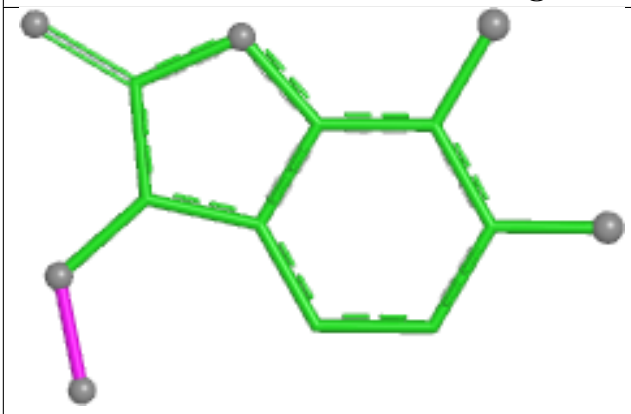
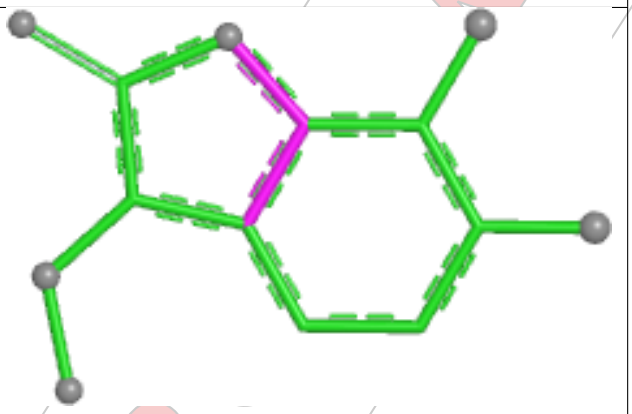
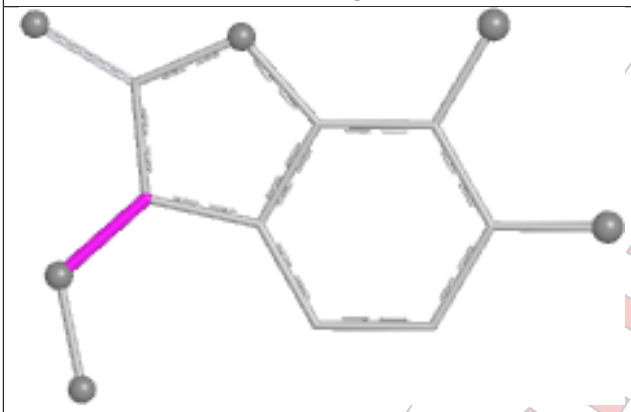
Ligand 1KP F 201



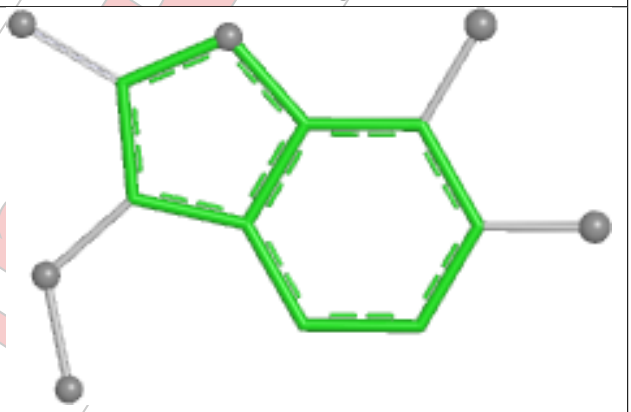
Bond lengths



Bond angles



Torsions



Rings

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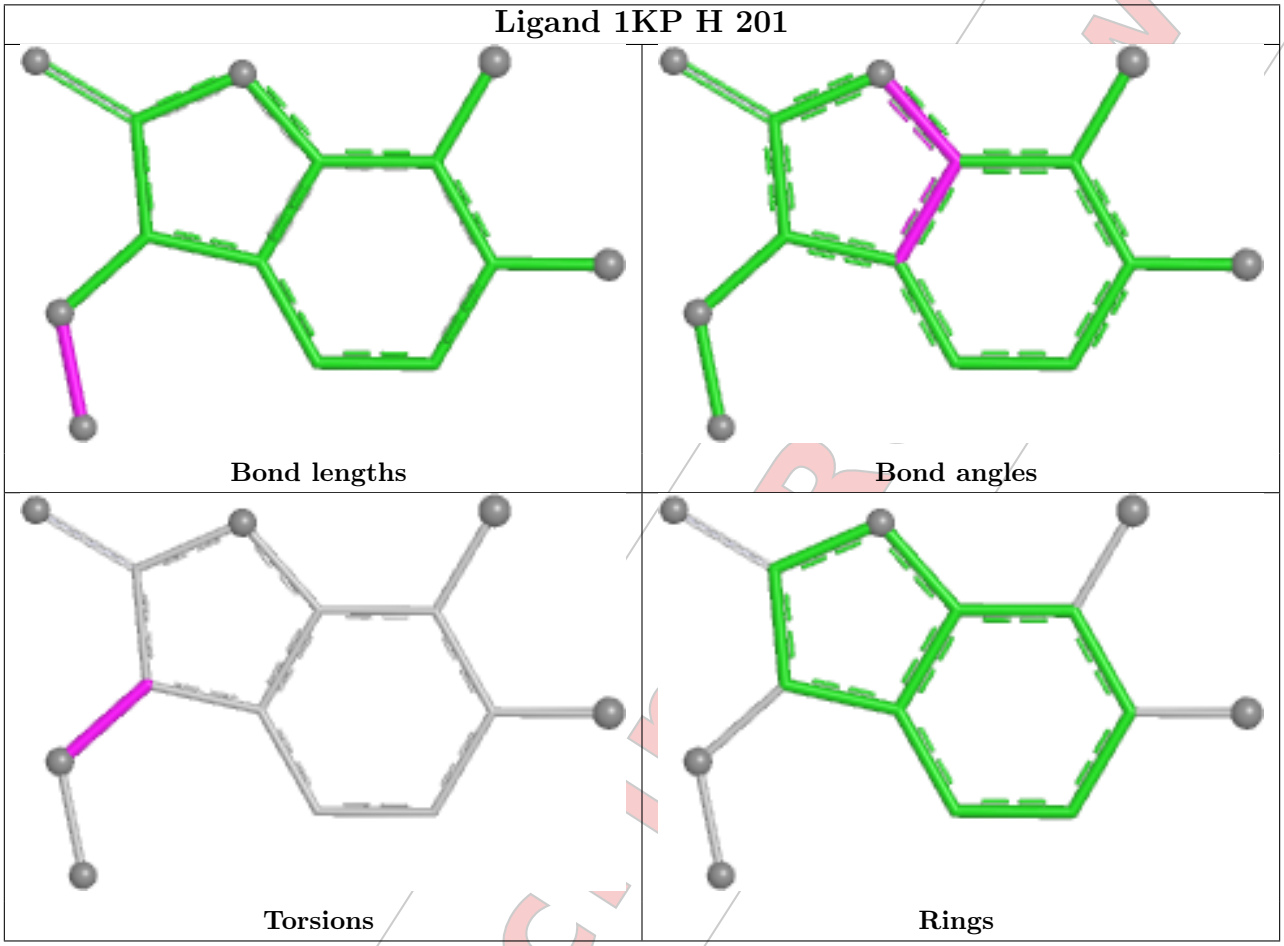

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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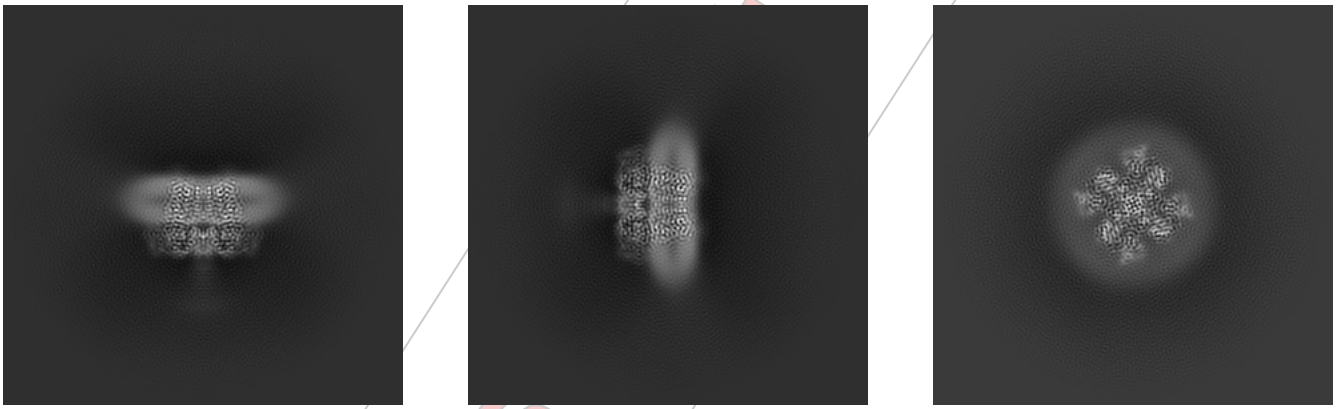
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70275. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

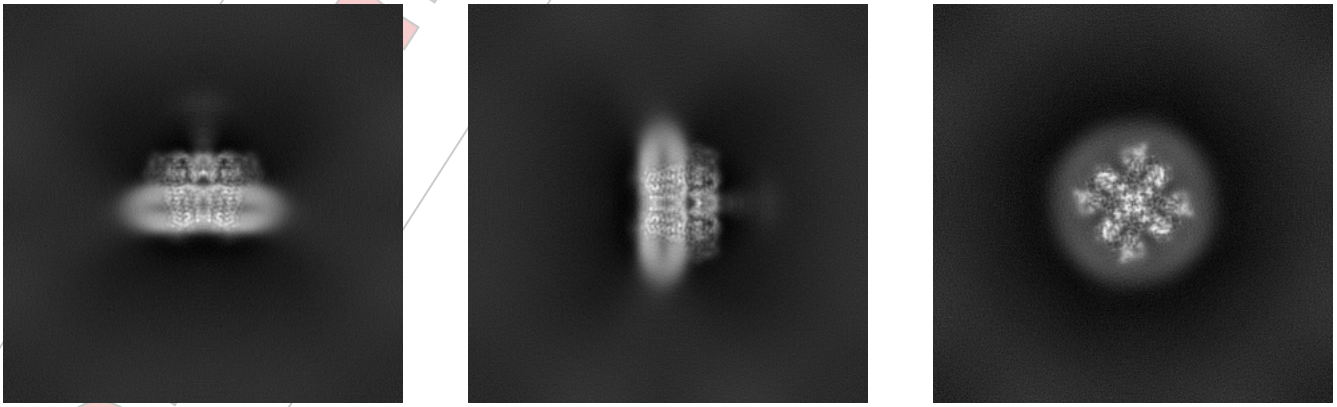
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



X Y Z

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

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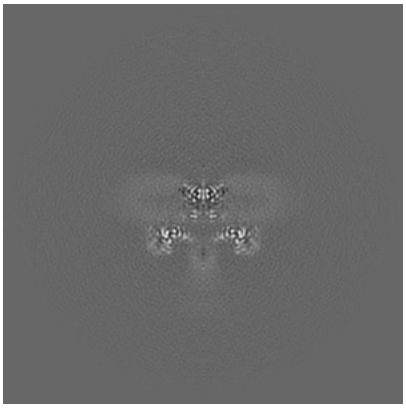
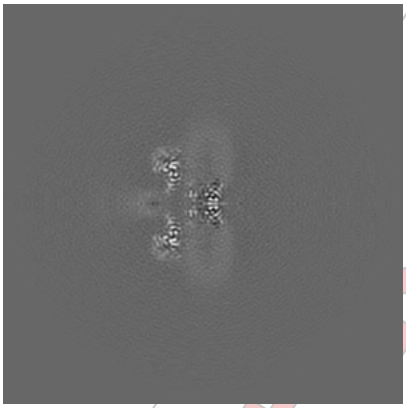
6.2 Central slices (i)

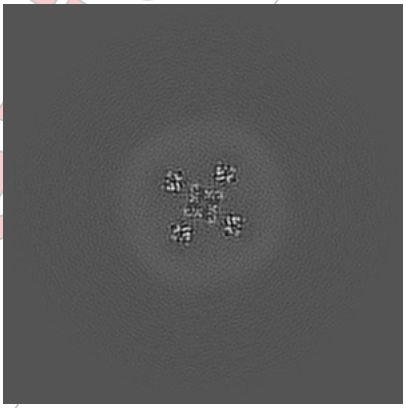
6.2.1 Primary map



X Index: 250

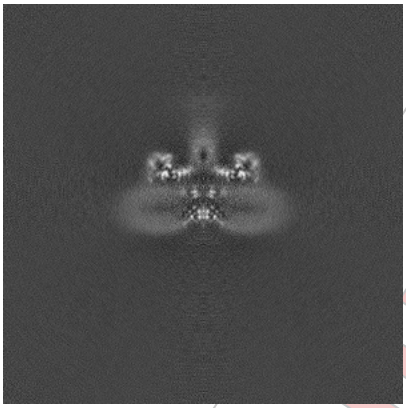


Y Index: 250

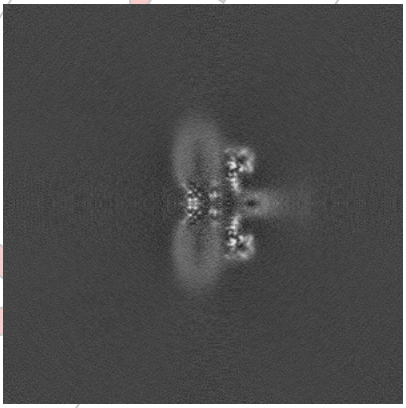


Z Index: 250

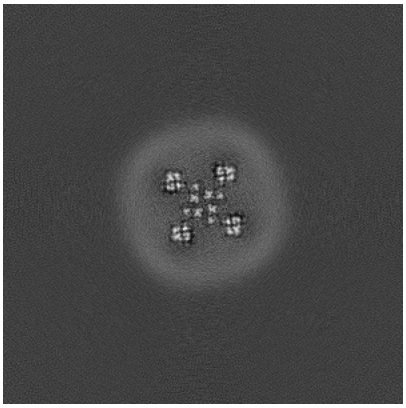
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

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

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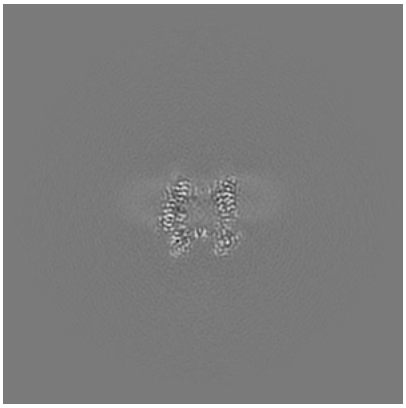
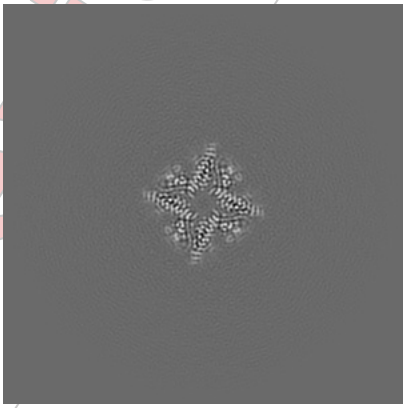
6.3 Largest variance slices (i)

6.3.1 Primary map



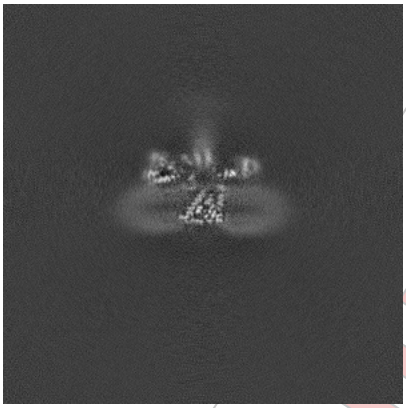
X Index: 221

Y Index: 221

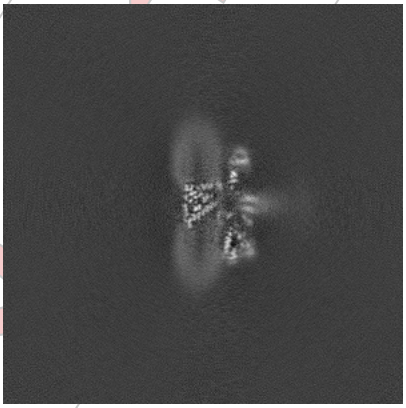


Z Index: 213

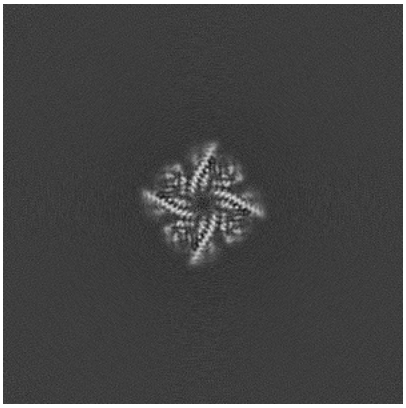
6.3.2 Raw map



X Index: 242



Y Index: 258



Z Index: 287

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

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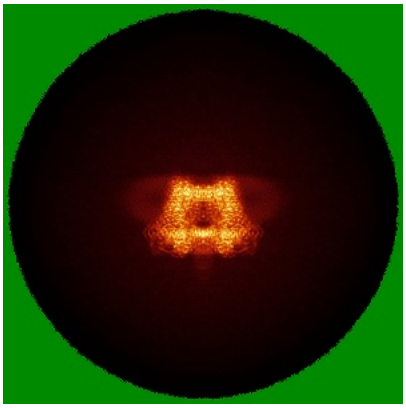
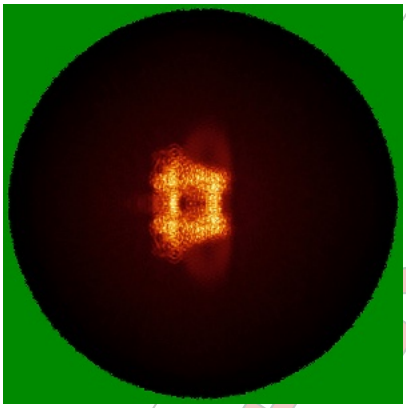
6.4 Orthogonal standard-deviation projections (False-color)

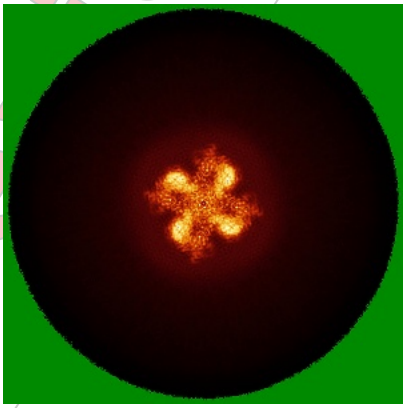
6.4.1 Primary map



X

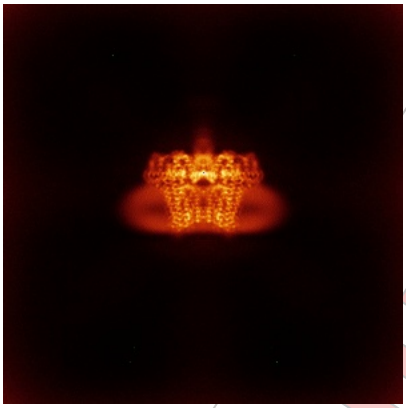


Y

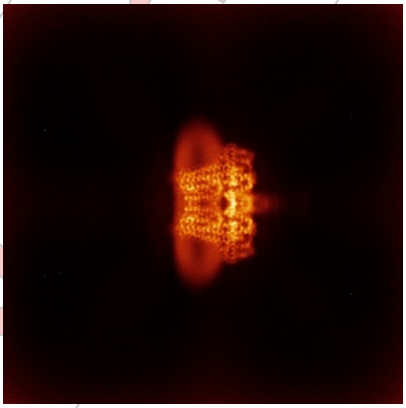


Z

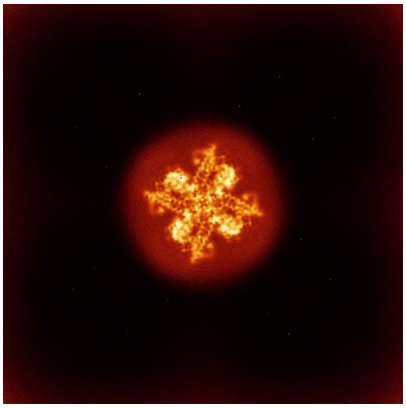
6.4.2 Raw map



X



Y



Z

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

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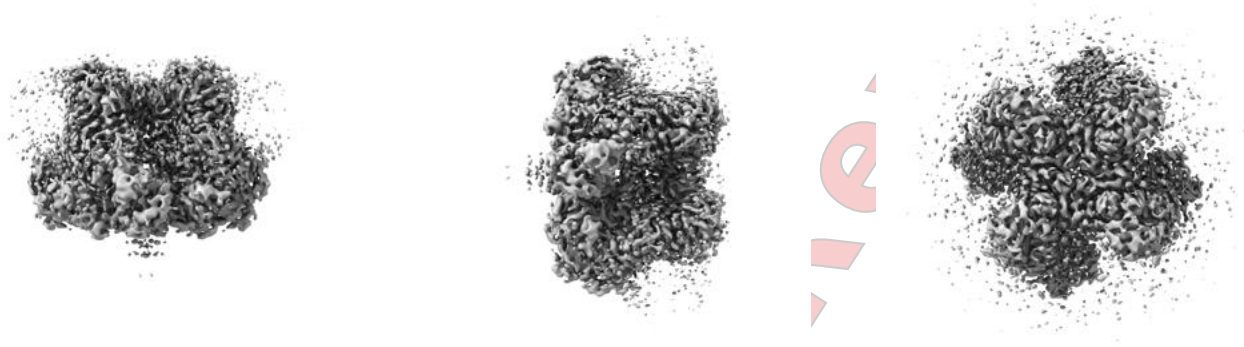
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

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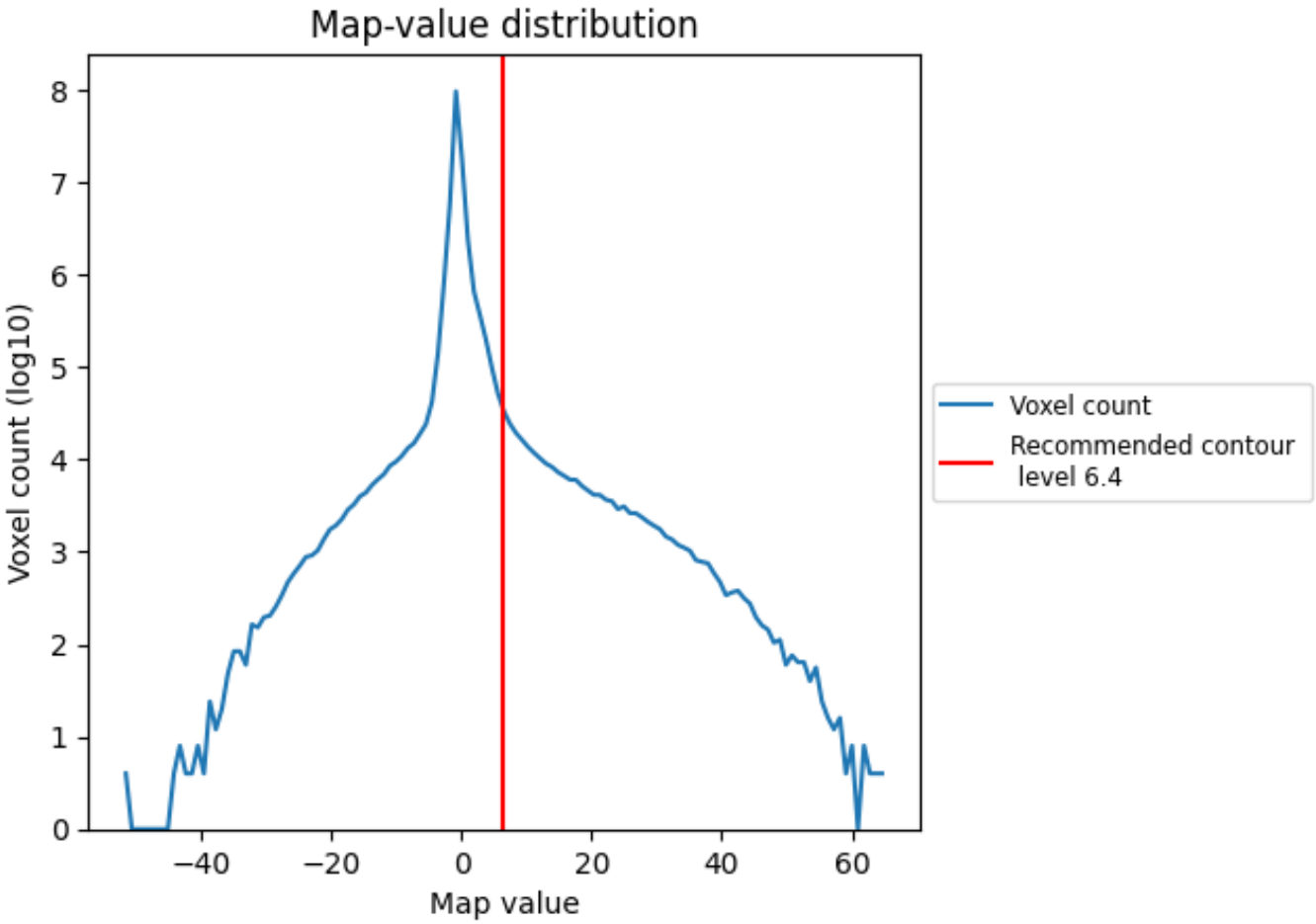
7 Map analysis

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.

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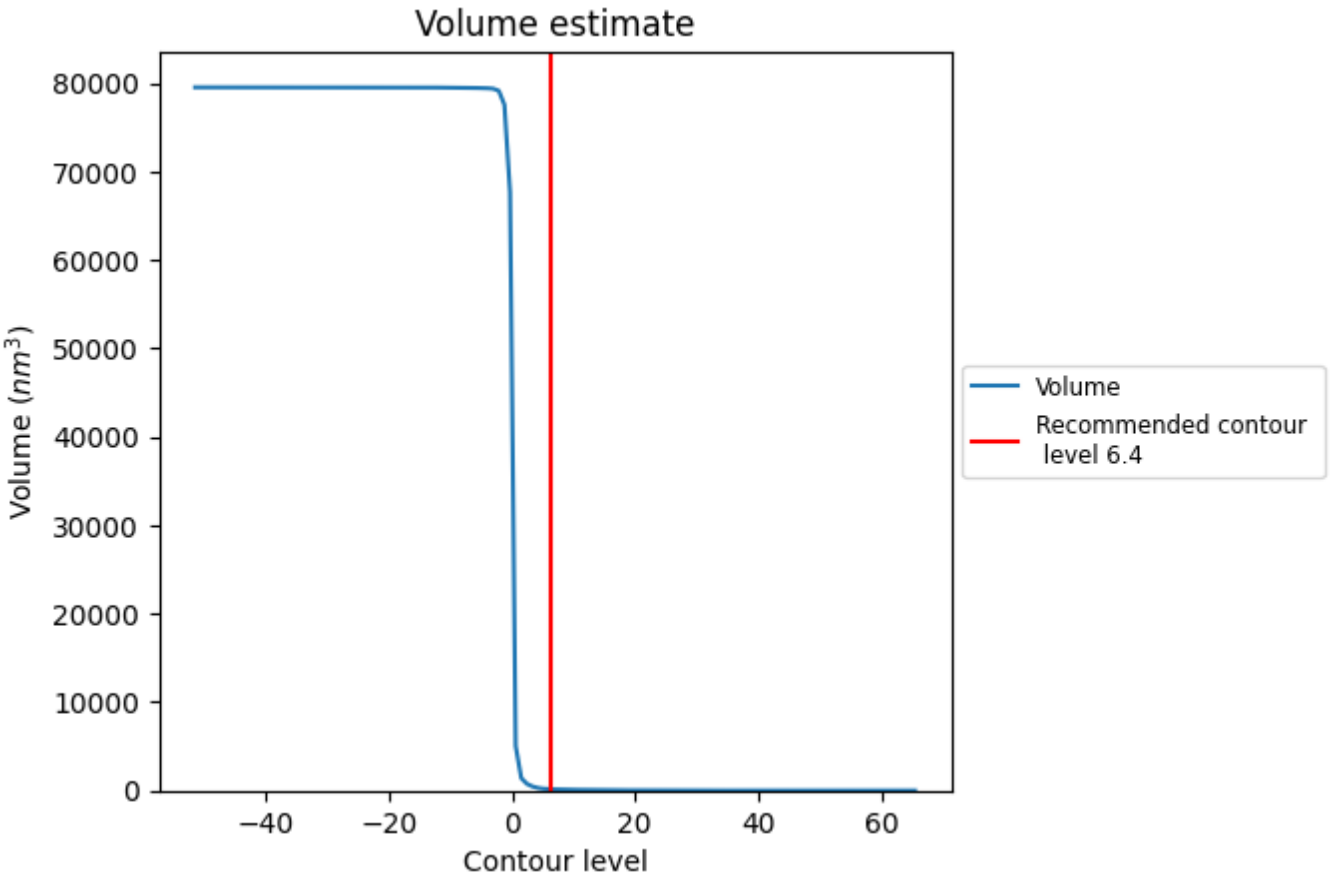
7.2 Volume estimate

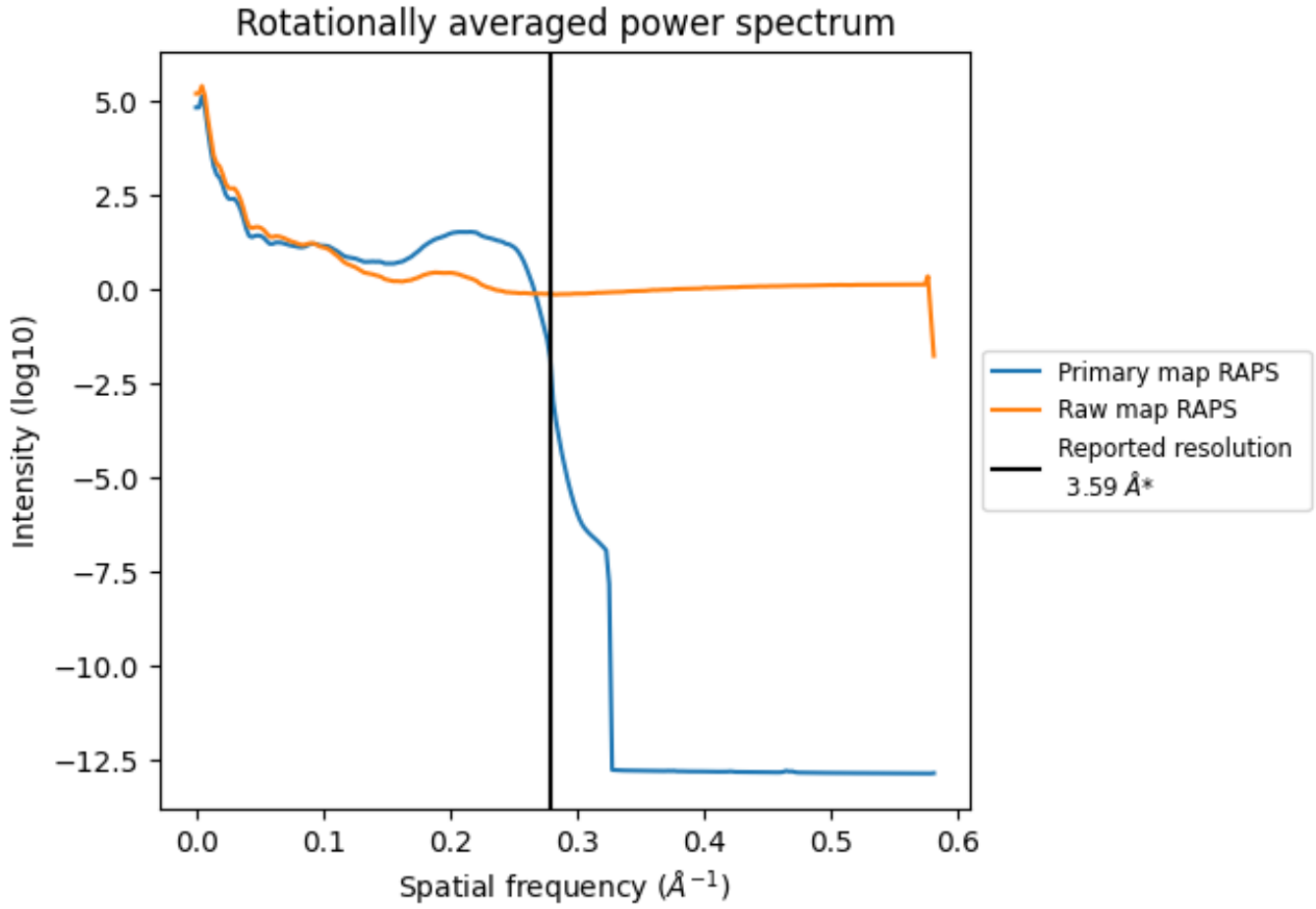


The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 137 kDa.

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.

For Manus

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

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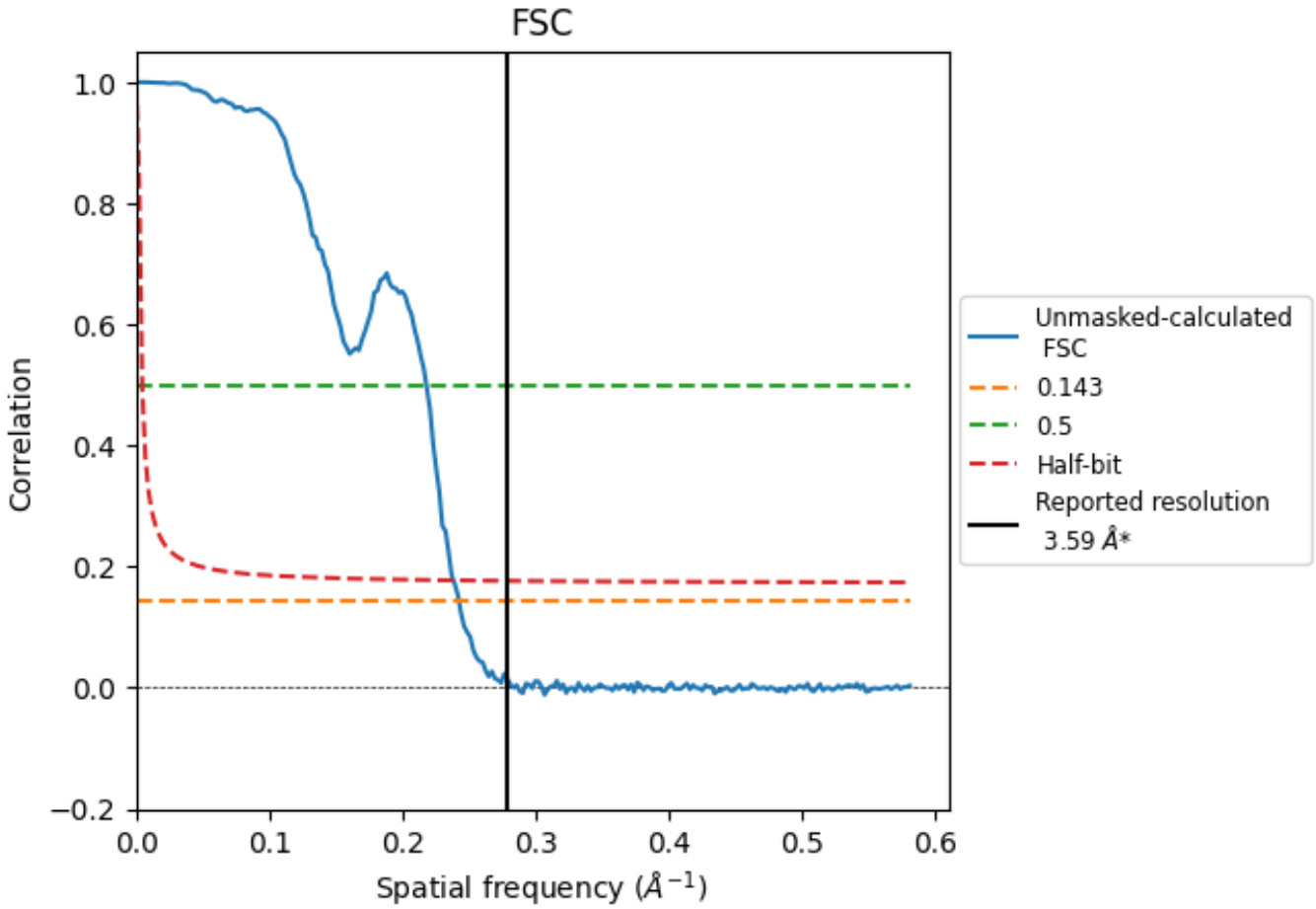
8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	4.58	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.59 by more than 10 %

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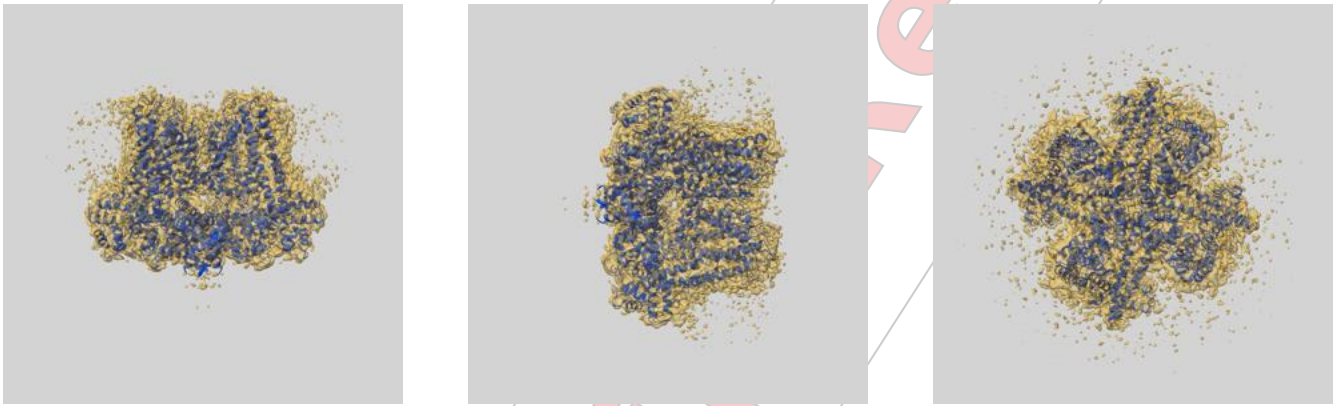
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70275 and PDB model 9OA8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.4 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.

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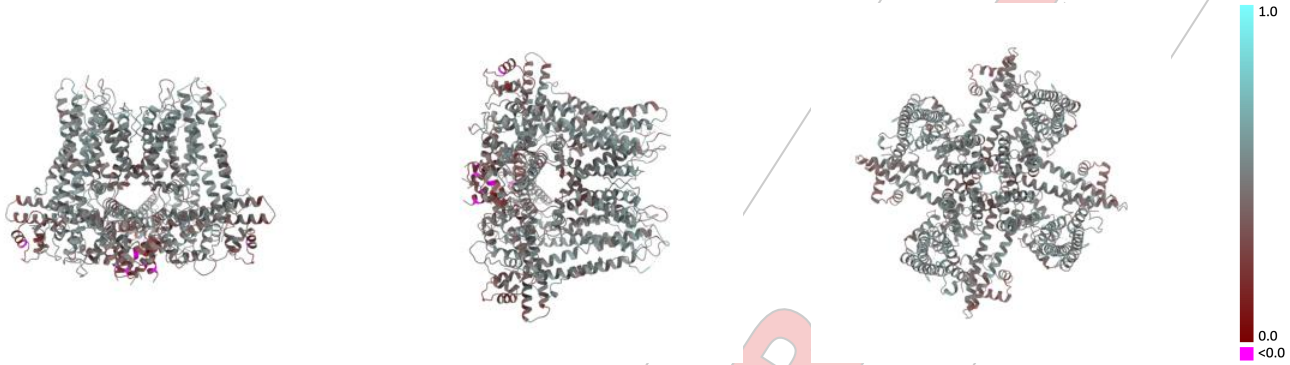
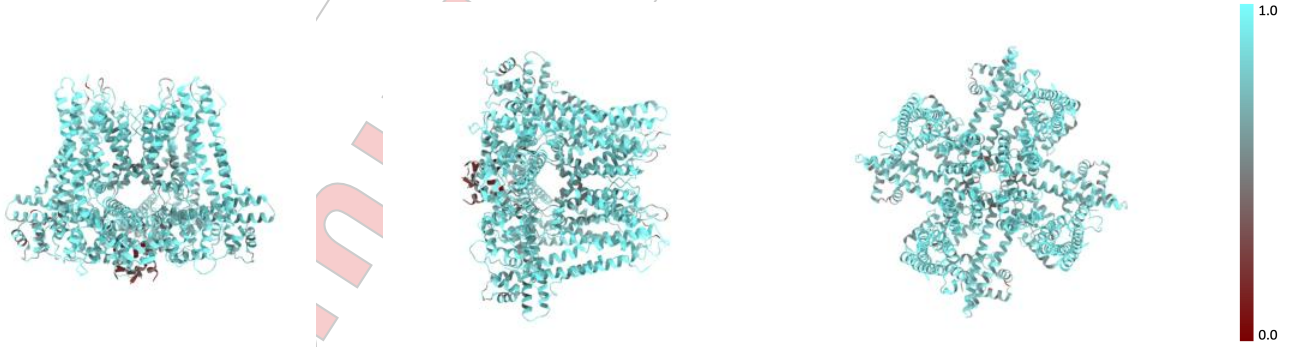
9.2 Q-score mapped to coordinate model



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



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 (6.4).

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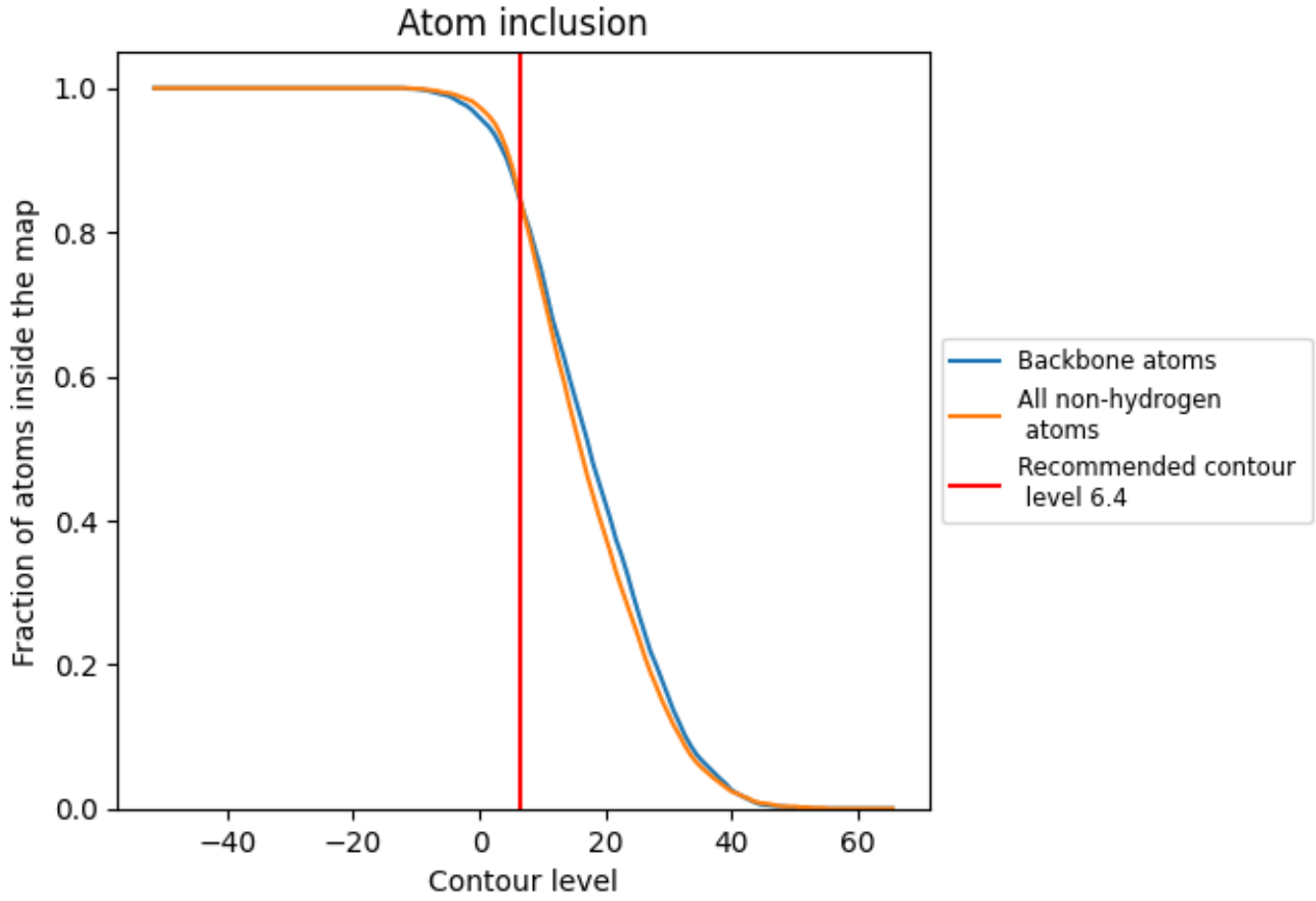
9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (6.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.4740
A	0.8630	0.4860
B	0.8560	0.4880
C	0.8500	0.4880
D	0.8590	0.4840
E	0.8260	0.4460
F	0.8280	0.4440
G	0.8330	0.4390
H	0.8190	0.4380

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Full wwPDB EM Validation Report (i)

May 14, 2025 – 03:24 PM EDT

PDB ID	:	9O93 / pdb_00009o93
EMDB ID	:	EMD-70240
Title	:	Cryo-EM structure of KCa2.2_II/calmodulin channel in complex with rimtuzalcap
Deposited on	:	2025-04-17
Resolution	:	2.96 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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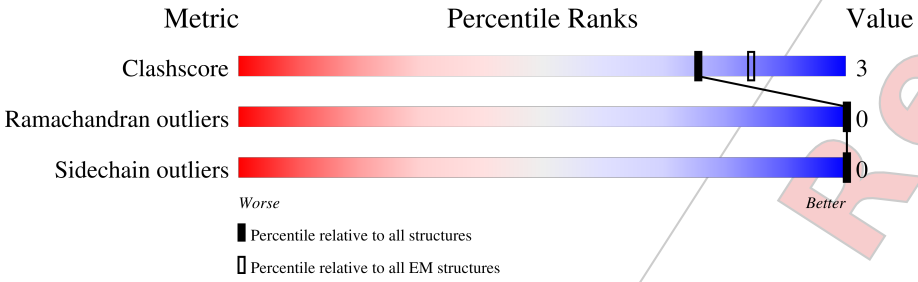
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.96 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	380	97%
1	B	380	95% 5%
1	C	380	92% 8%
1	D	380	95% 5%
2	E	144	87% 13%
2	F	144	84% 16%
2	G	144	87% 13%

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For Manuscript Review

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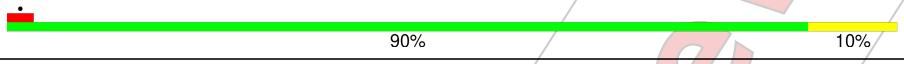
Mol	Chain	Length	Quality of chain
2	H	144	

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2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16057 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 Small conductance calcium-activated potassium channel protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total 2973	C 1927	N 512	O 511	S 23	0	0
1	B	380	Total 2973	C 1927	N 512	O 511	S 23	0	0
1	C	380	Total 2973	C 1927	N 512	O 511	S 23	0	0
1	D	380	Total 2973	C 1927	N 512	O 511	S 23	0	0

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	144	Total 1012	C 629	N 167	O 207	S 9	0	0
2	F	144	Total 1014	C 630	N 167	O 208	S 9	0	0
2	G	144	Total 1014	C 630	N 167	O 208	S 9	0	0
2	H	144	Total 1011	C 629	N 167	O 206	S 9	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is N-(4,4-difluorocyclohexyl)-2-(3-methyl-1H-pyrazol-1-yl)-6-(morpholin-4-yl)pyrimidin-4-amine (CCD ID: A1B92) (formula: $C_{18}H_{24}F_2N_6O$) (labeled as "Ligand of Interest" by depositor).

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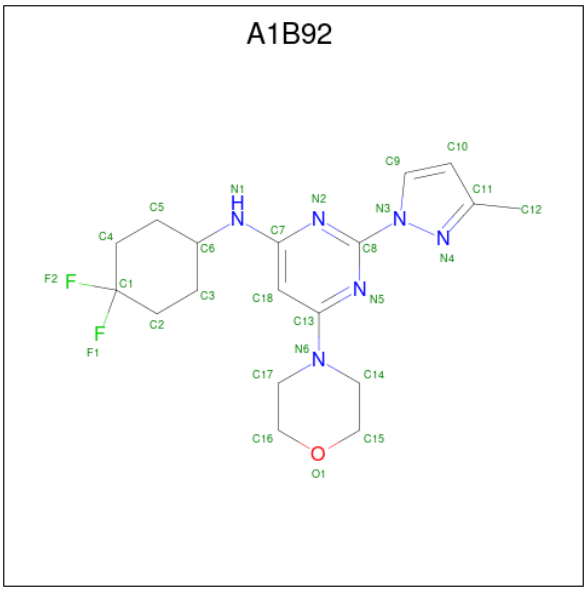

Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C F N O 27 18 2 6 1	0
4	E	1	Total C F N O 27 18 2 6 1	0
4	F	1	Total C F N O 27 18 2 6 1	0
4	H	1	Total C F N O 27 18 2 6 1	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total O 1 1	0
5	B	1	Total O 1 1	0
5	C	1	Total O 1 1	0
5	D	1	Total O 1 1	0

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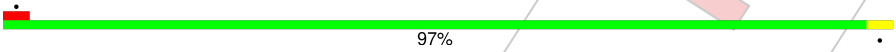
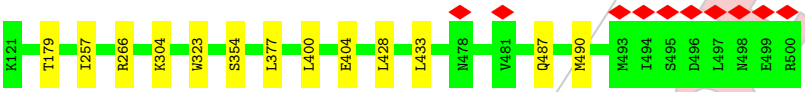
3 Residue-property plots (i)

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: Small conductance calcium-activated potassium channel protein 2

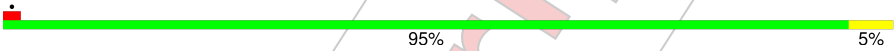
Chain A:

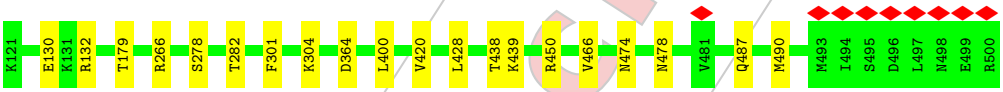




- Molecule 1: Small conductance calcium-activated potassium channel protein 2

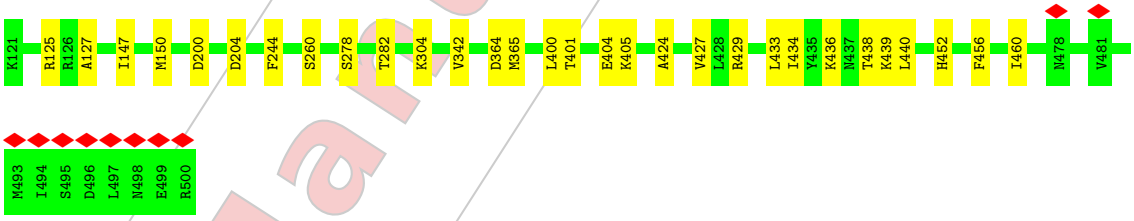
Chain B:





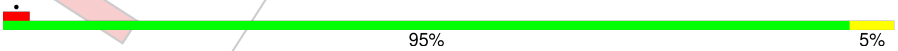
- Molecule 1: Small conductance calcium-activated potassium channel protein 2

Chain C:



- Molecule 1: Small conductance calcium-activated potassium channel protein 2

Chain D:



- Molecule 2: Calmodulin-1

Chain E:

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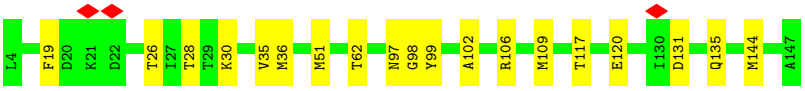
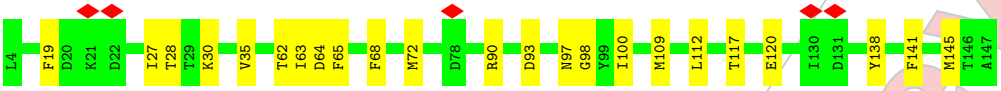


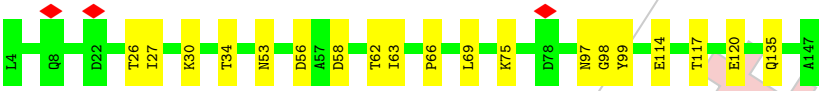
• Molecule 2: Calmodulin-1

Chain F:



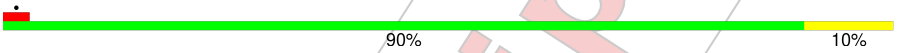
• Molecule 2: Calmodulin-1

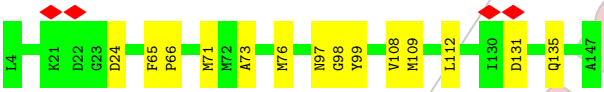
Chain G:



• Molecule 2: Calmodulin-1

Chain H:





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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	74.863	Depositor
Minimum map value	-45.962	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	430.0, 430.0, 430.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

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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: A1B92, K

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	0.19	0/3032	0.32	0/4110
1	B	0.19	0/3032	0.33	0/4110
1	C	0.19	0/3032	0.32	0/4110
1	D	0.19	0/3032	0.34	0/4110
2	E	0.11	0/1024	0.26	0/1388
2	F	0.11	0/1026	0.28	0/1391
2	G	0.10	0/1026	0.28	0/1391
2	H	0.12	0/1023	0.36	0/1387
All	All	0.17	0/16227	0.32	0/21997

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	2973	0	3026	13	0
1	B	2973	0	3026	14	0
1	C	2973	0	3026	19	0
1	D	2973	0	3026	15	0
2	E	1012	0	872	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1014	0	877	13	0
2	G	1014	0	877	12	0
2	H	1011	0	875	9	0
3	A	2	0	0	0	0
4	D	27	0	0	0	0
4	E	27	0	0	0	0
4	F	27	0	0	0	0
4	H	27	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	16057	0	15605	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (91) 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:H:108:VAL:HG13	2:H:112:LEU:HD12	1.63	0.81
2:G:117:THR:OG1	2:G:120:GLU:OE1	2.09	0.68
2:E:19:PHE:HA	2:E:35:VAL:HG21	1.74	0.67
2:E:99:TYR:HD2	2:E:135:GLN:HB3	1.61	0.65
1:C:125:ARG:NH1	1:C:200:ASP:OD1	2.30	0.64
2:F:28:THR:HG22	2:F:30:LYS:H	1.63	0.63
1:A:487:GLN:NE2	1:D:490:MET:SD	2.71	0.63
1:C:438:THR:HG23	1:C:439:LYS:HG2	1.81	0.62
1:C:400:LEU:HB2	1:C:405:LYS:HE3	1.82	0.61
2:F:19:PHE:HA	2:F:35:VAL:HG21	1.83	0.60
2:G:66:PRO:HA	2:G:69:LEU:HD12	1.83	0.60
2:F:117:THR:OG1	2:F:120:GLU:OE1	2.19	0.60
1:A:490:MET:HE1	1:B:490:MET:HE3	1.84	0.59
1:A:490:MET:HE2	1:D:490:MET:HE1	1.86	0.58
1:C:429:ARG:NH1	2:G:114:GLU:OE1	2.37	0.58
1:B:474:ASN:O	1:B:478:ASN:ND2	2.38	0.57
2:F:27:ILE:HG12	2:F:62:THR:HG23	1.88	0.56
1:C:278:SER:O	1:C:282:THR:OG1	2.23	0.56
2:F:90:ARG:HA	2:F:93:ASP:HB3	1.88	0.56
1:B:450:ARG:HD3	1:D:207:ARG:HB2	1.87	0.54
1:A:490:MET:SD	1:B:487:GLN:NE2	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:SER:O	1:D:282:THR:OG1	2.23	0.54
2:F:27:ILE:HD13	2:F:63:ILE:HG12	1.89	0.53
2:E:28:THR:HG22	2:E:30:LYS:H	1.73	0.53
1:C:436:LYS:HD2	1:C:440:LEU:HB2	1.90	0.52
1:B:438:THR:HG23	1:B:439:LYS:HG2	1.90	0.51
1:B:400:LEU:HD23	1:C:304:LYS:HE2	1.93	0.51
2:F:100:ILE:HD12	2:F:138:TYR:HB3	1.92	0.51
2:G:58:ASP:OD1	2:G:58:ASP:N	2.44	0.50
2:G:27:ILE:HB	2:G:63:ILE:HB	1.94	0.50
1:C:125:ARG:C	1:C:127:ALA:H	2.19	0.49
1:C:401:THR:N	1:C:404:GLU:OE1	2.35	0.49
2:G:26:THR:OG1	2:G:62:THR:OG1	2.24	0.49
1:D:428:LEU:HB3	2:H:109:MET:HE1	1.95	0.48
1:A:179:THR:HG22	1:A:266:ARG:HH22	1.77	0.48
2:E:26:THR:HG23	2:E:62:THR:HG23	1.95	0.48
1:A:400:LEU:HD23	1:B:304:LYS:HE2	1.95	0.48
1:C:342:VAL:HG12	1:C:365:MET:HE3	1.96	0.47
1:D:179:THR:HG22	1:D:266:ARG:HH22	1.78	0.47
1:B:278:SER:O	1:B:282:THR:OG1	2.25	0.47
2:H:65:PHE:N	2:H:66:PRO:HD2	2.30	0.47
2:H:97:ASN:OD1	2:H:98:GLY:N	2.48	0.47
1:A:428:LEU:HB3	2:E:109:MET:HE1	1.97	0.46
1:D:436:LYS:HD2	1:D:440:LEU:HB2	1.98	0.46
1:B:179:THR:HG22	1:B:266:ARG:HH22	1.80	0.46
2:G:97:ASN:OD1	2:G:98:GLY:N	2.49	0.46
2:H:73:ALA:HA	2:H:76:MET:HE2	1.97	0.46
1:A:404:GLU:HB3	1:B:301:PHE:HE1	1.81	0.45
1:A:323:TRP:CH2	1:A:354:SER:HB3	2.51	0.45
1:C:150:MET:HE2	1:C:260:SER:OG	2.17	0.45
2:E:97:ASN:OD1	2:E:98:GLY:N	2.49	0.45
1:A:304:LYS:HE2	1:D:400:LEU:HD23	1.99	0.45
2:G:75:LYS:HD3	2:G:75:LYS:HA	1.66	0.44
1:A:257:ILE:HD12	1:A:257:ILE:HA	1.90	0.44
2:F:68:PHE:O	2:F:72:MET:HG2	2.18	0.44
1:B:364:ASP:OD2	1:C:244:PHE:N	2.51	0.44
2:E:36:MET:SD	2:E:51:MET:HE1	2.59	0.43
1:B:428:LEU:HB3	2:F:109:MET:HE1	1.99	0.43
2:H:99:TYR:CD1	2:H:135:GLN:HB3	2.53	0.43
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.90	0.43
2:E:117:THR:HB	2:E:120:GLU:OE1	2.18	0.43
2:G:27:ILE:N	2:G:63:ILE:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:C	1:B:132:ARG:H	2.26	0.43
2:G:99:TYR:HB3	2:G:135:GLN:HB3	2.00	0.43
1:C:147:ILE:O	1:C:150:MET:HG3	2.19	0.43
1:C:456:PHE:O	1:C:460:ILE:HG12	2.18	0.43
1:C:364:ASP:OD2	1:D:244:PHE:N	2.51	0.42
2:E:102:ALA:O	2:E:106:ARG:HG2	2.19	0.42
1:D:400:LEU:HB2	1:D:405:LYS:HE3	2.00	0.42
2:F:97:ASN:OD1	2:F:98:GLY:N	2.52	0.42
1:D:323:TRP:CH2	1:D:354:SER:HB3	2.54	0.42
2:G:30:LYS:O	2:G:34:THR:HG23	2.19	0.42
2:H:131:ASP:OD1	2:H:131:ASP:N	2.51	0.42
1:C:434:ILE:HG13	1:C:452:HIS:HB3	2.01	0.42
2:F:141:PHE:O	2:F:145:MET:HG2	2.19	0.42
1:C:424:ALA:HA	1:C:427:VAL:HG12	2.01	0.42
1:D:299:THR:HA	1:D:302:VAL:HG12	2.01	0.42
1:C:204:ASP:OD1	1:C:204:ASP:N	2.53	0.41
2:H:71:MET:HE3	2:H:71:MET:HB3	1.97	0.41
1:B:420:VAL:HG12	1:B:466:VAL:HG12	2.02	0.41
2:G:53:ASN:HA	2:G:56:ASP:HB2	2.02	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.89	0.41
1:D:334:GLU:OE2	1:D:367:PRO:HA	2.20	0.41
2:E:131:ASP:OD1	2:E:131:ASP:N	2.51	0.41
2:H:24:ASP:OD1	2:H:24:ASP:N	2.54	0.41
1:D:364:ASP:OD1	1:D:364:ASP:N	2.53	0.41
1:D:468:MET:HE2	1:D:468:MET:HB3	1.95	0.41
2:E:144:MET:HE3	2:E:144:MET:HB2	1.93	0.40
2:F:64:ASP:CG	2:F:65:PHE:H	2.28	0.40
2:F:112:LEU:HD23	2:F:112:LEU:HA	1.88	0.40
1:C:433:LEU:HD23	1:C:433:LEU:HA	1.90	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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/380 (100%)	367 (97%)	11 (3%)	0	100	100
1	B	378/380 (100%)	370 (98%)	8 (2%)	0	100	100
1	C	378/380 (100%)	367 (97%)	11 (3%)	0	100	100
1	D	378/380 (100%)	369 (98%)	9 (2%)	0	100	100
2	E	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
2	F	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
2	G	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
2	H	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
All	All	2080/2096 (99%)	1999 (96%)	81 (4%)	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	311/331 (94%)	311 (100%)	0	100	100
1	B	311/331 (94%)	311 (100%)	0	100	100
1	C	311/331 (94%)	311 (100%)	0	100	100
1	D	311/331 (94%)	311 (100%)	0	100	100
2	E	90/123 (73%)	90 (100%)	0	100	100
2	F	91/123 (74%)	91 (100%)	0	100	100
2	G	91/123 (74%)	91 (100%)	0	100	100
2	H	90/123 (73%)	90 (100%)	0	100	100
All	All	1606/1816 (88%)	1606 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

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Mol	Chain	Res	Type
1	A	124	HIS
1	A	487	GLN
1	B	415	GLN
1	B	437	ASN
1	B	453	GLN
1	C	437	ASN
1	D	124	HIS
1	D	437	ASN
2	F	107	HIS
2	G	135	GLN
2	H	137	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	A1B92	F	201	-	30,30,30	0.44	0	36,43,43	0.72	0
4	A1B92	H	201	-	30,30,30	0.45	0	36,43,43	0.67	0
4	A1B92	D	601	-	30,30,30	0.44	0	36,43,43	0.73	1 (2%)
4	A1B92	E	201	-	30,30,30	0.44	0	36,43,43	0.82	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1B92	F	201	-	-	0/12/32/32	1/4/4/4
4	A1B92	H	201	-	-	2/12/32/32	1/4/4/4
4	A1B92	D	601	-	-	2/12/32/32	1/4/4/4
4	A1B92	E	201	-	-	0/12/32/32	1/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	201	A1B92	C5-C4-C1	-2.60	109.31	110.75
4	E	201	A1B92	C3-C2-C1	-2.34	109.45	110.75
4	D	601	A1B92	C5-C4-C1	-2.00	109.64	110.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	601	A1B92	N2-C7-N1-C6
4	D	601	A1B92	C18-C7-N1-C6
4	H	201	A1B92	C18-C7-N1-C6
4	H	201	A1B92	N2-C7-N1-C6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	201	A1B92	C1-C2-C3-C4-C5-C6
4	D	601	A1B92	C1-C2-C3-C4-C5-C6
4	F	201	A1B92	C1-C2-C3-C4-C5-C6
4	E	201	A1B92	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

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

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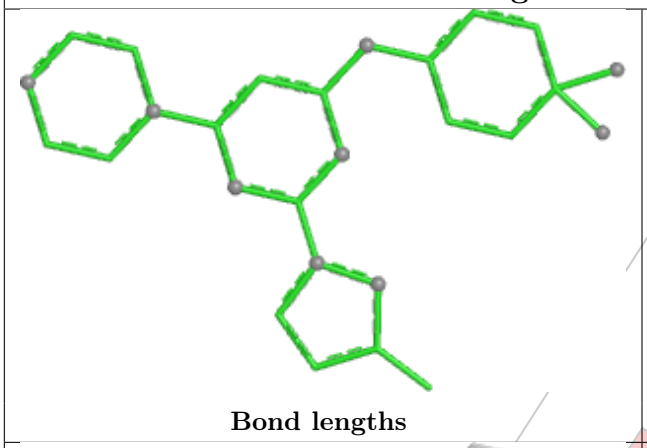
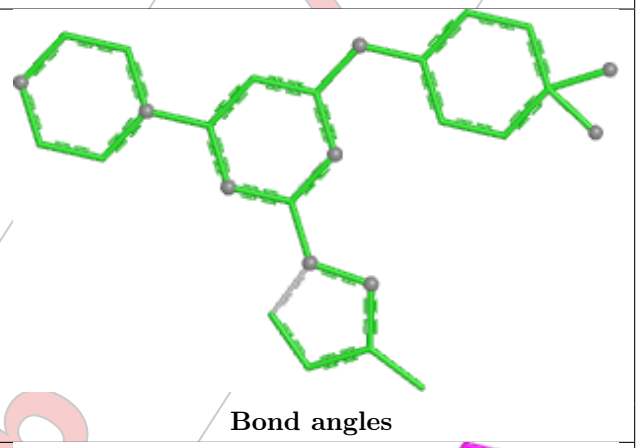
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

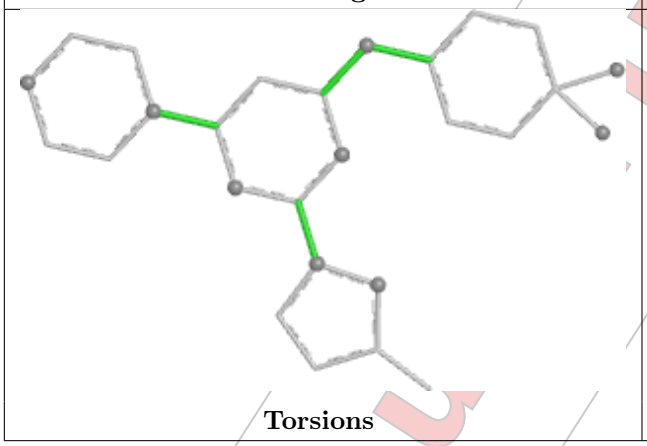
Ligand A1B92 F 201



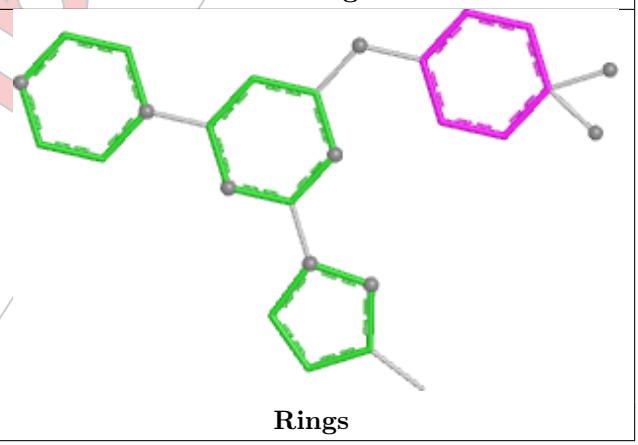
Bond lengths



Bond angles



Torsions



Rings

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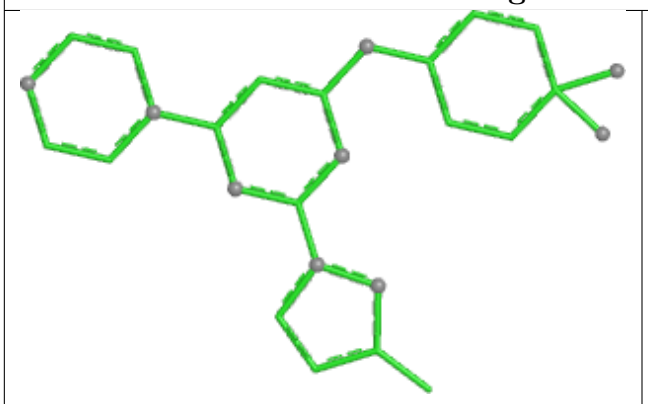
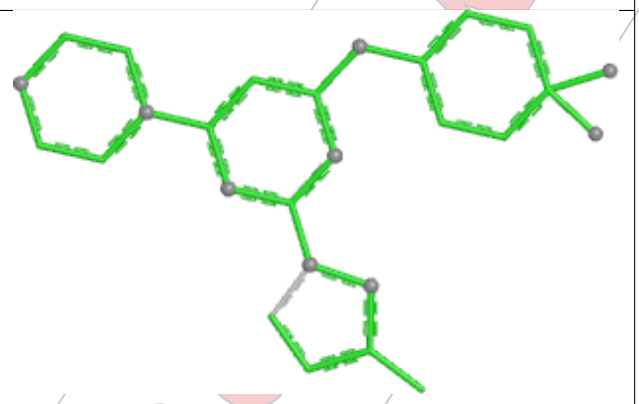
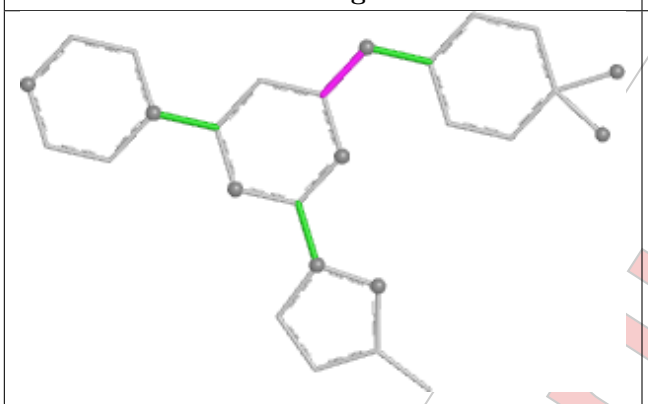
Ligand A1B92 H 201



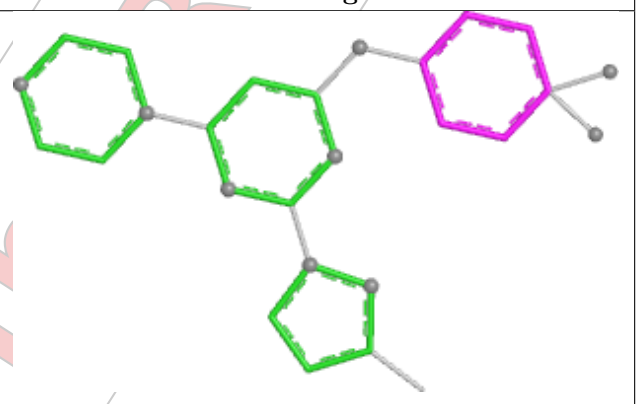
Bond lengths



Bond angles



Torsions



Rings

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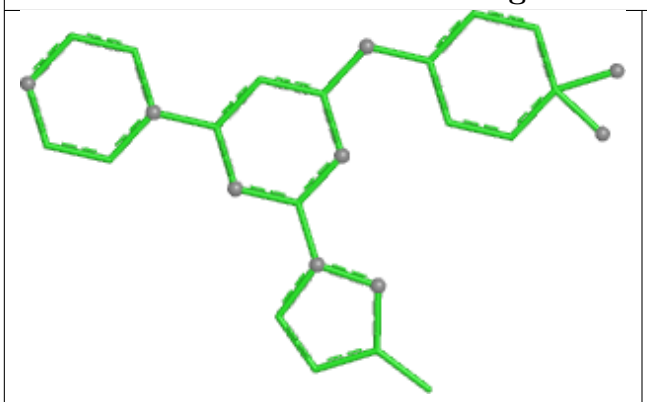
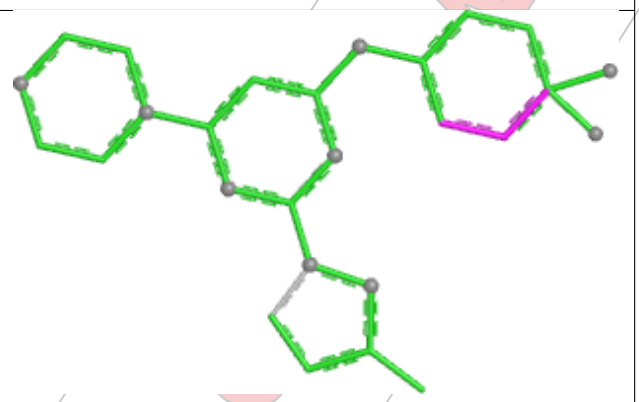
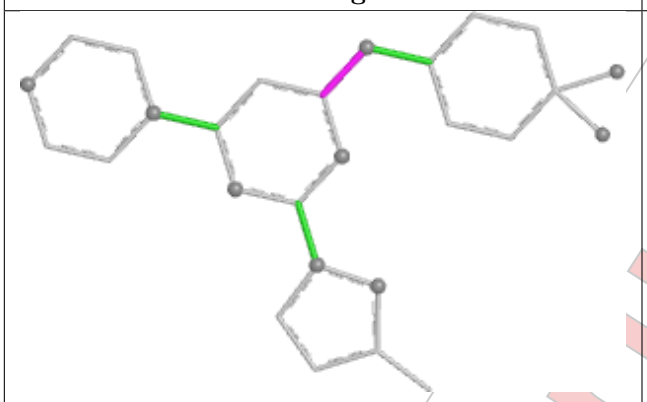
Ligand A1B92 D 601



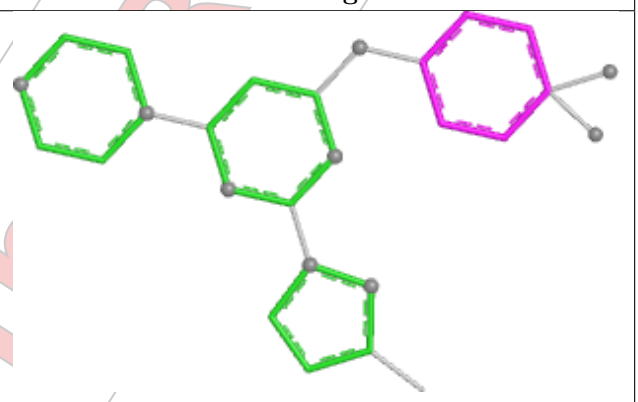
Bond lengths



Bond angles



Torsions



Rings

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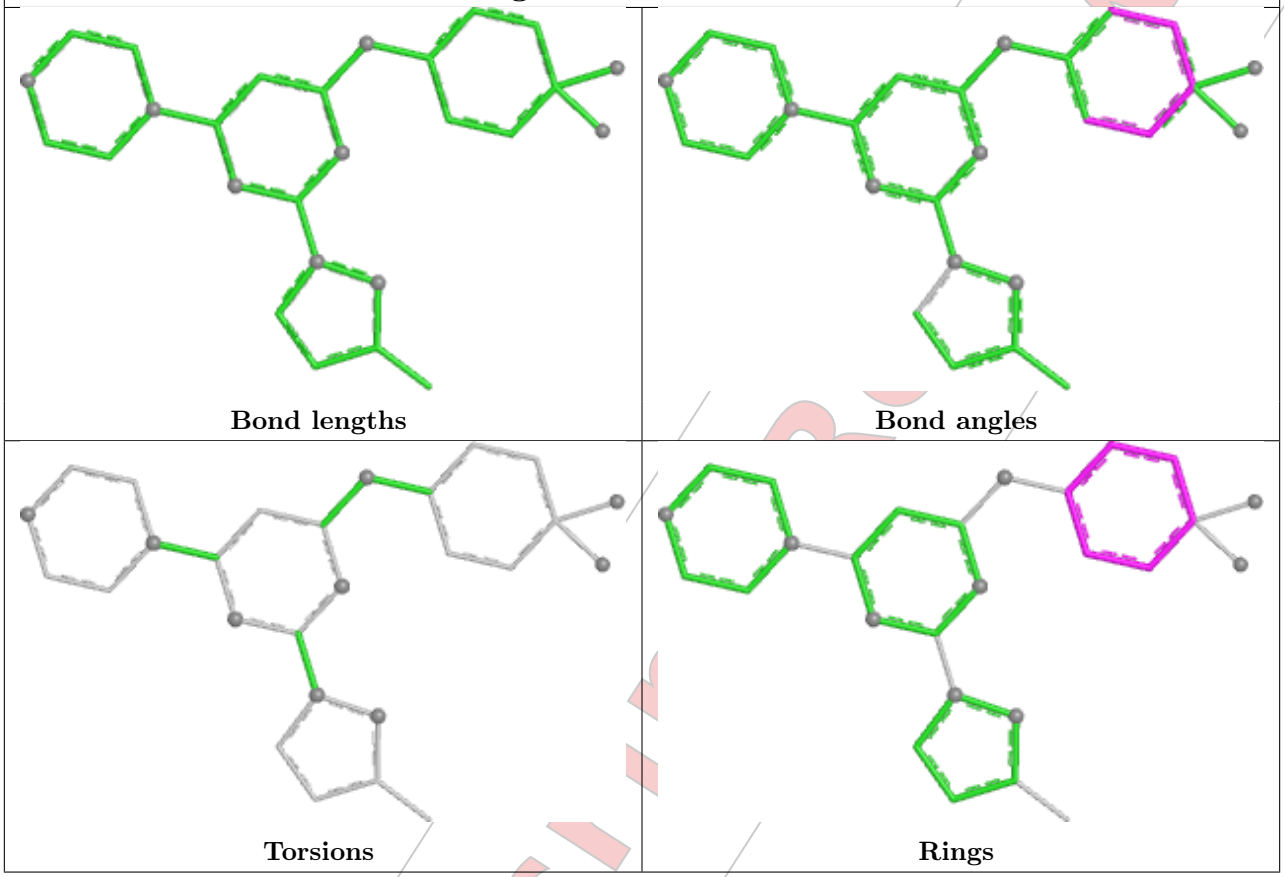
Ligand A1B92 E 201



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.

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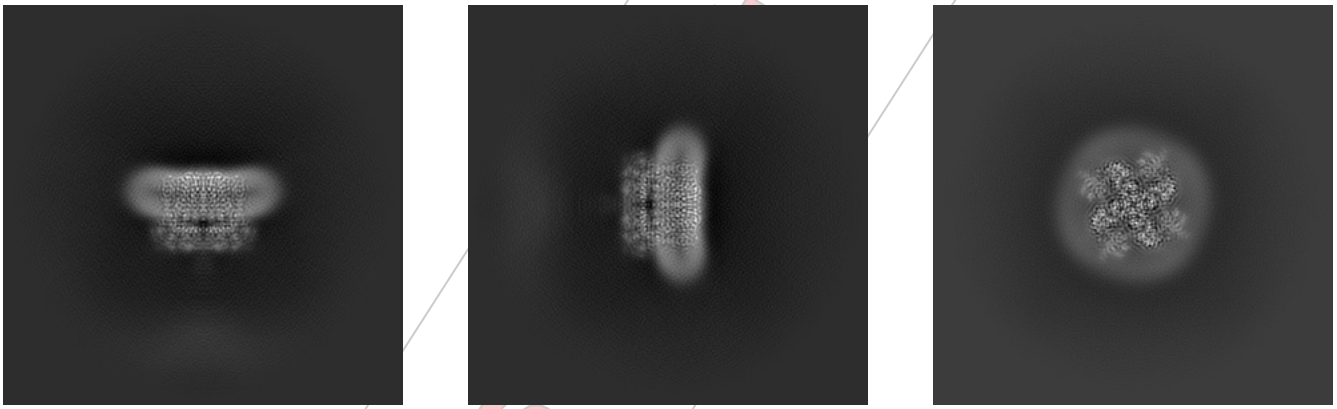
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70240. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

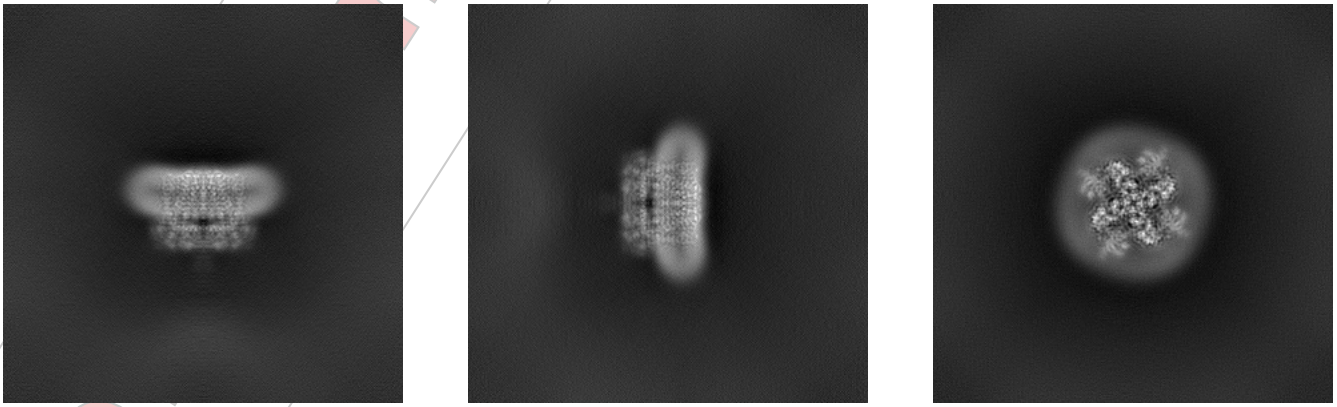
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



X Y Z

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

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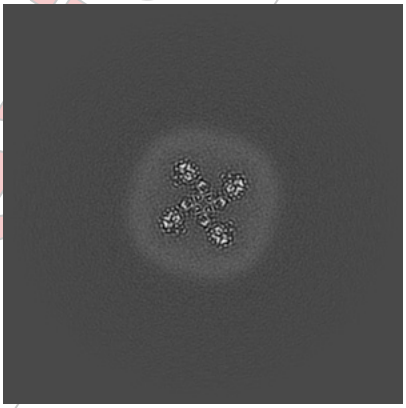
6.2 Central slices (i)

6.2.1 Primary map

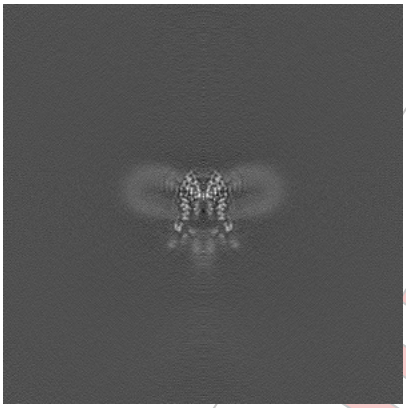
X Index: 250

Y Index: 250

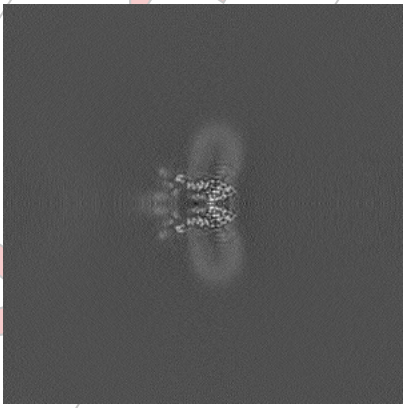


Z Index: 250

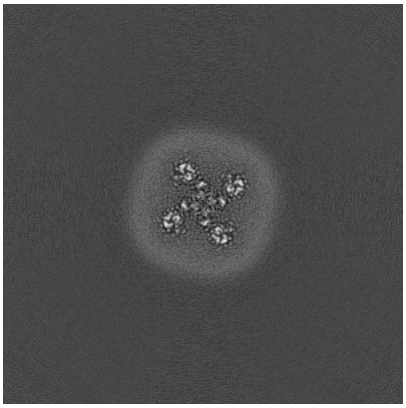
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

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

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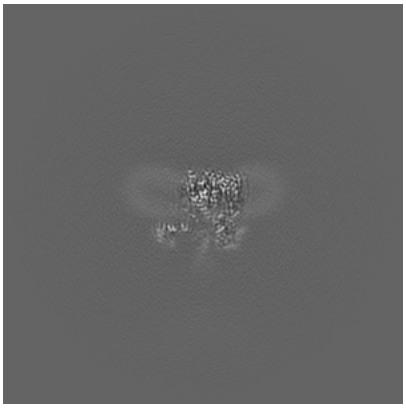
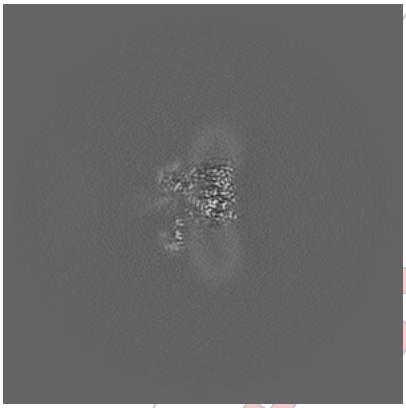
6.3 Largest variance slices (i)

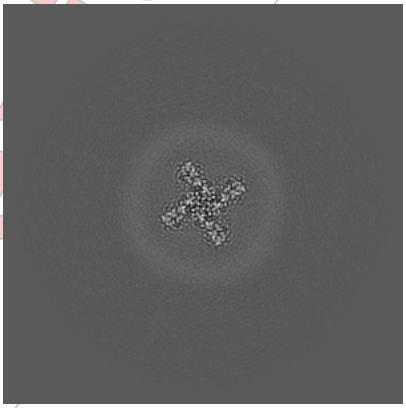
6.3.1 Primary map



X Index: 240

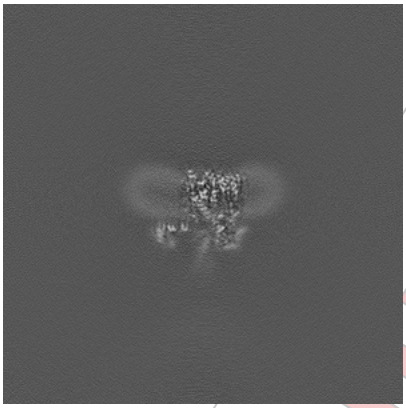


Y Index: 260

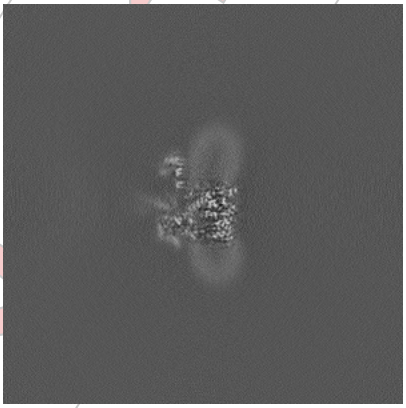


Z Index: 268

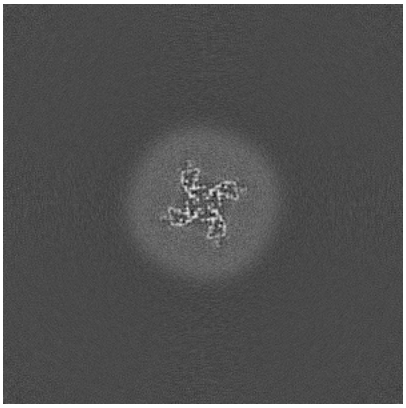
6.3.2 Raw map



X Index: 240



Y Index: 240



Z Index: 284

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

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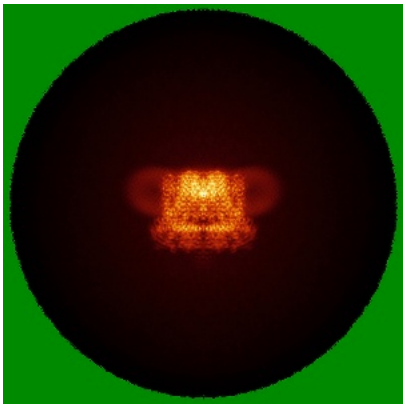
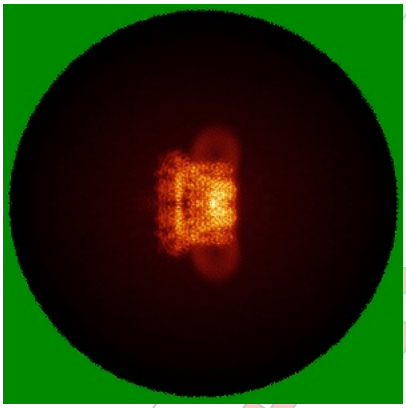
6.4 Orthogonal standard-deviation projections (False-color)

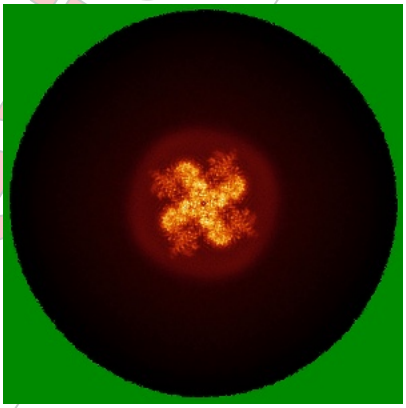
6.4.1 Primary map



X

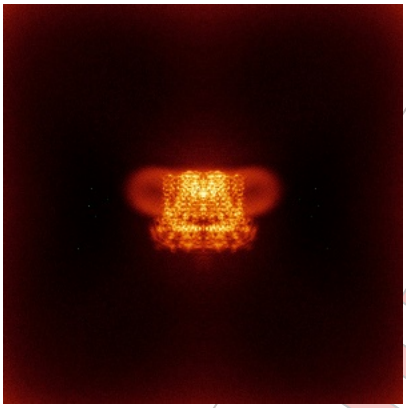


Y

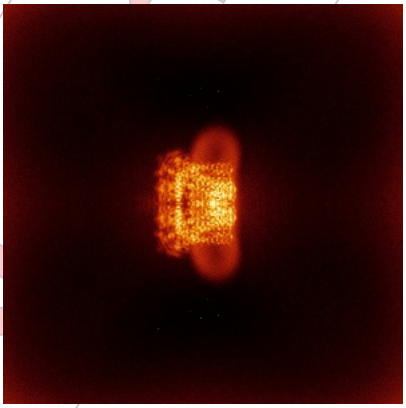


Z

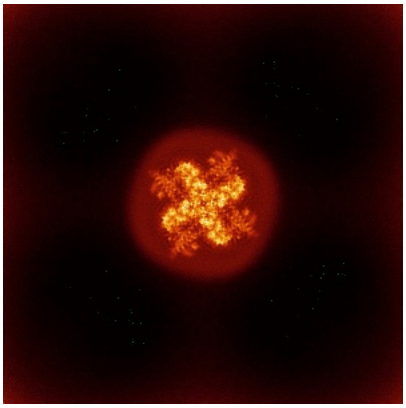
6.4.2 Raw map



X



Y



Z

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

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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

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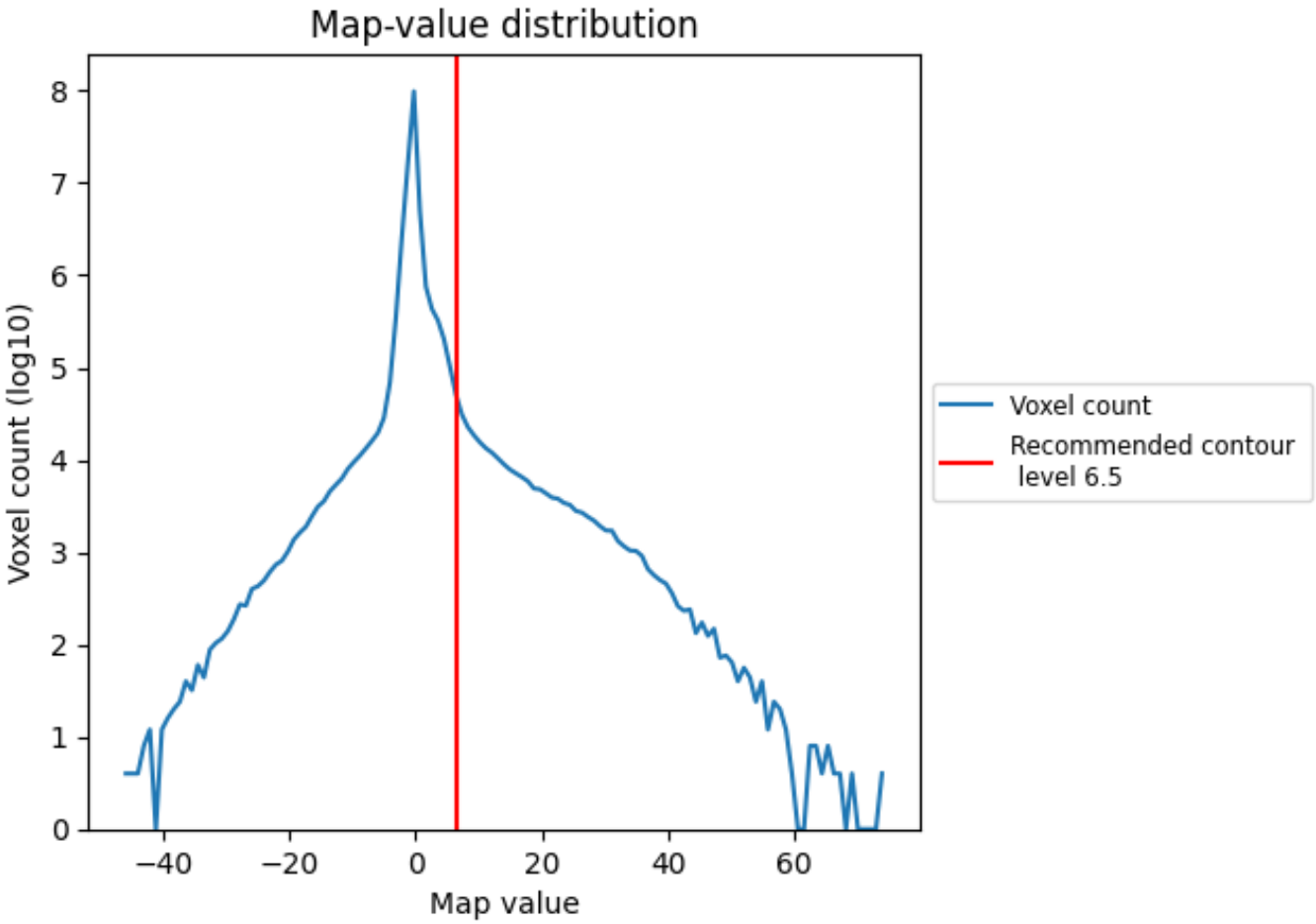
7 Map analysis

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.

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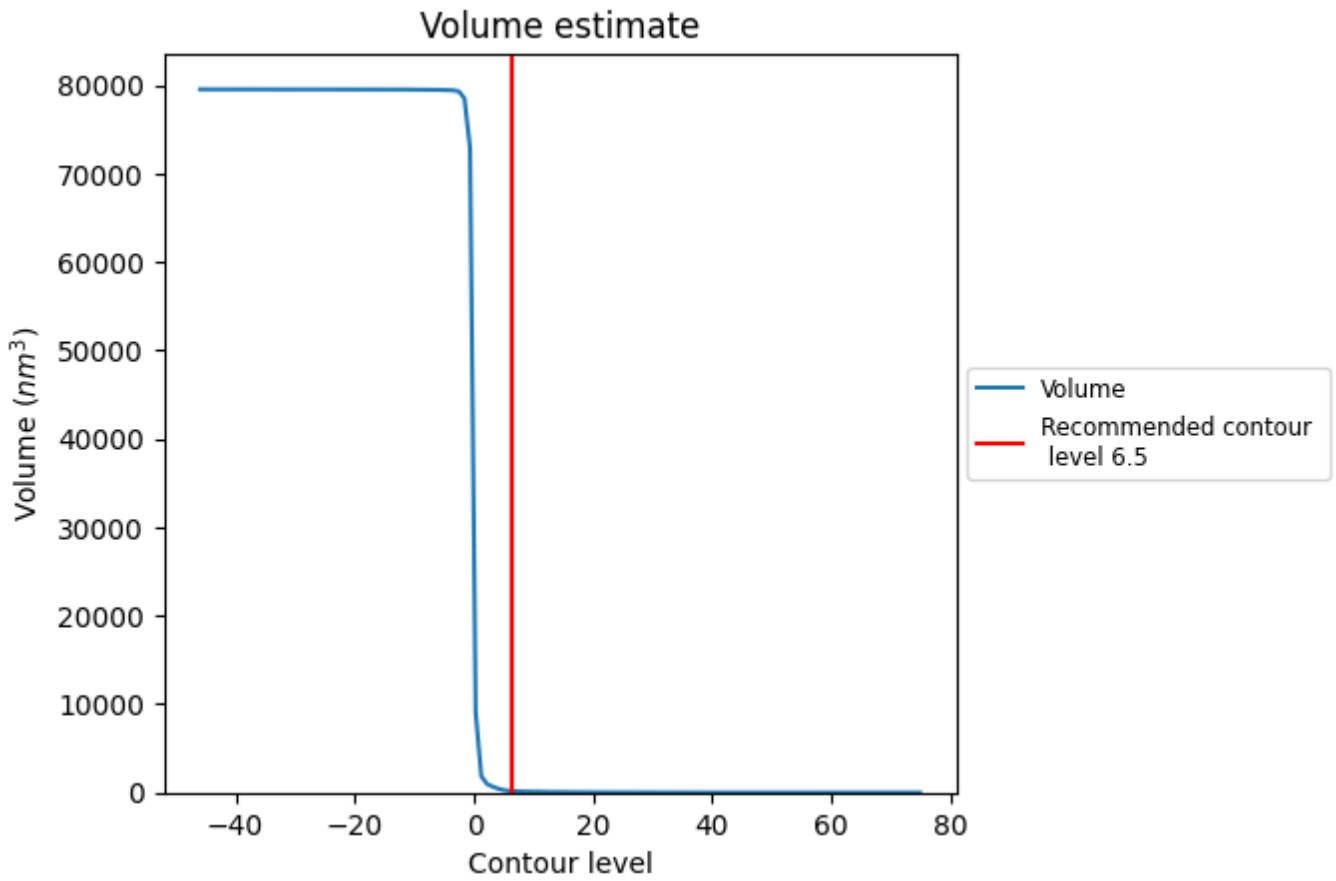
7.2 Volume estimate (i)

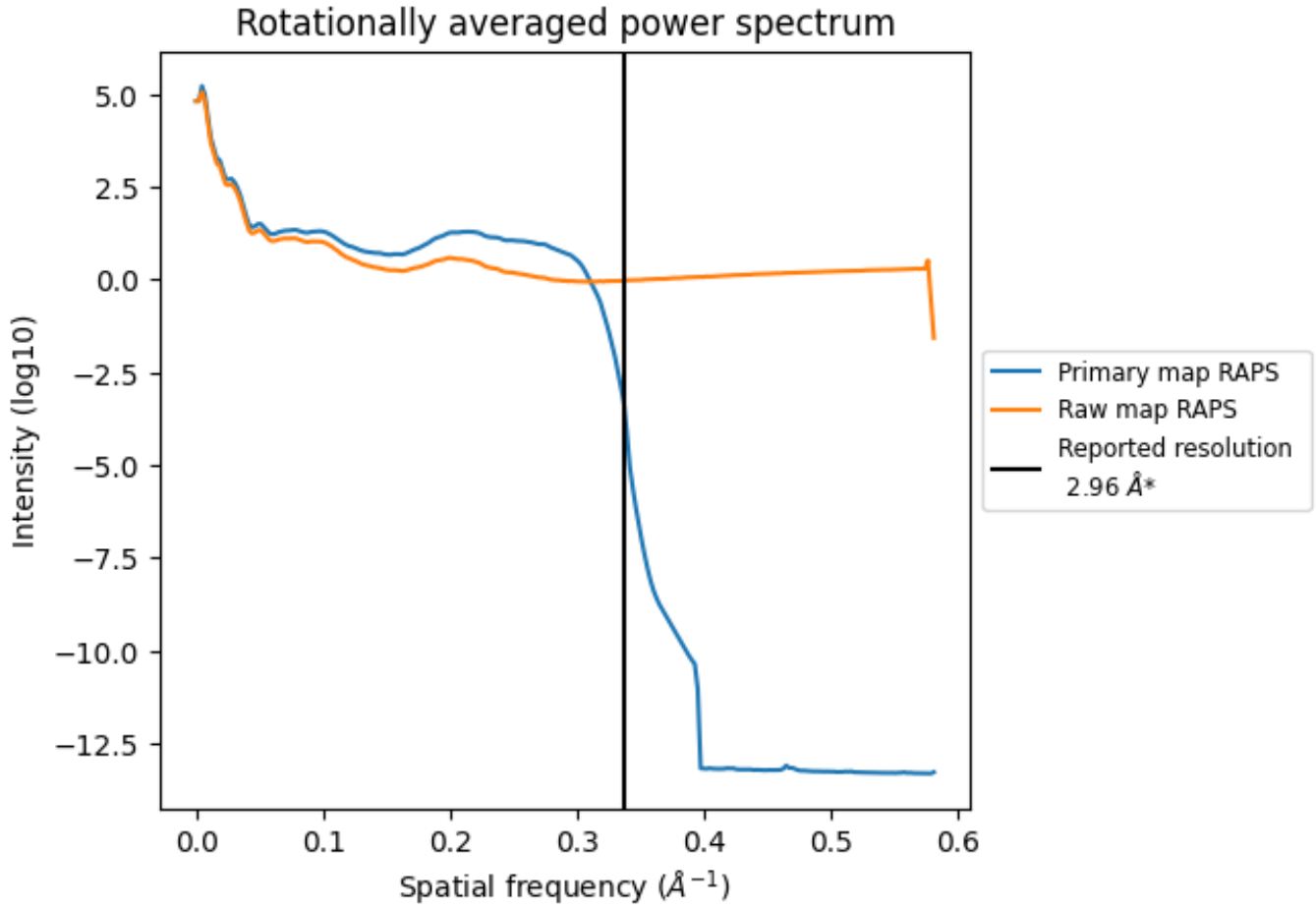


The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 kDa.

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.

For Manus

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

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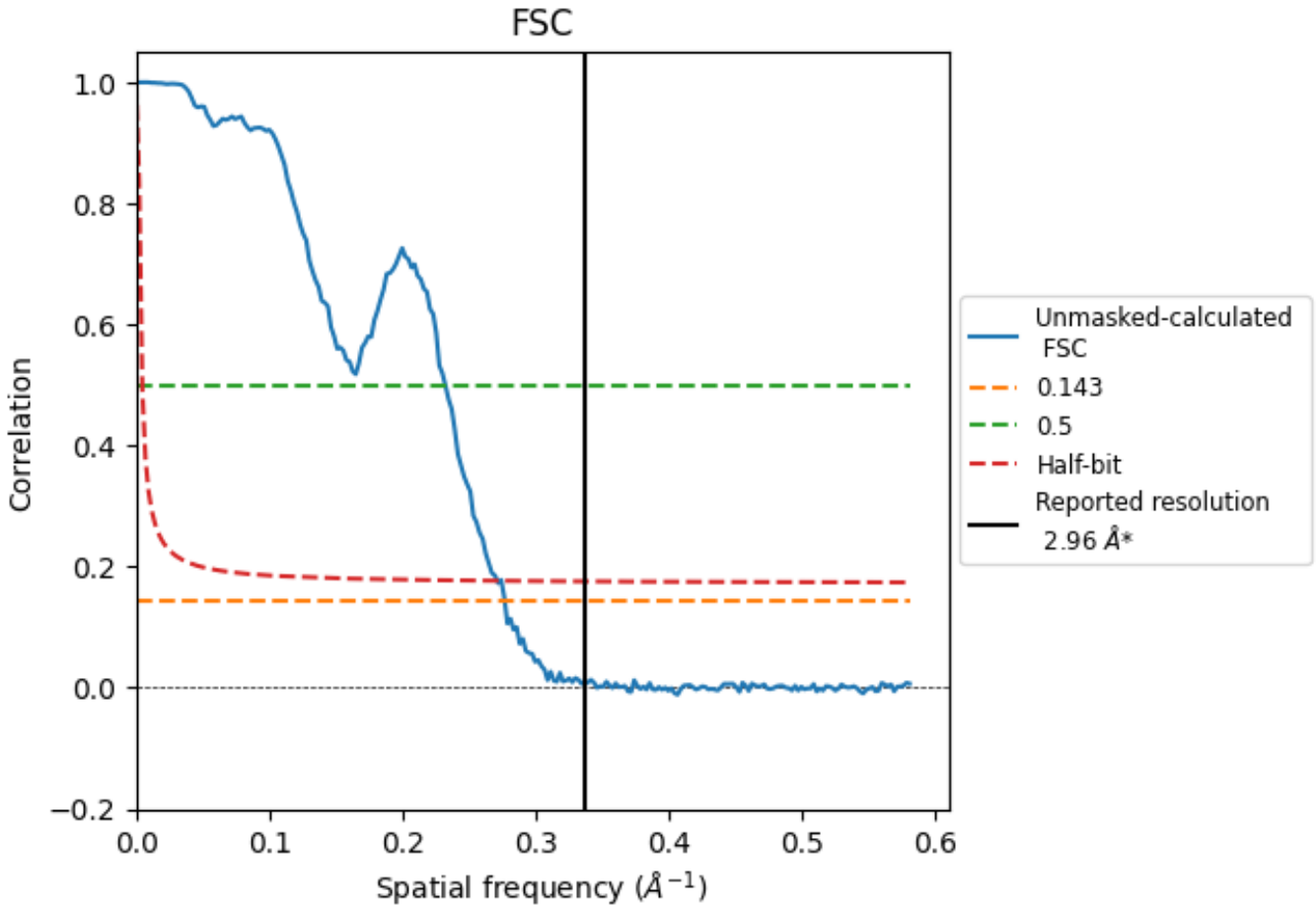
8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.30	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.96 by more than 10 %

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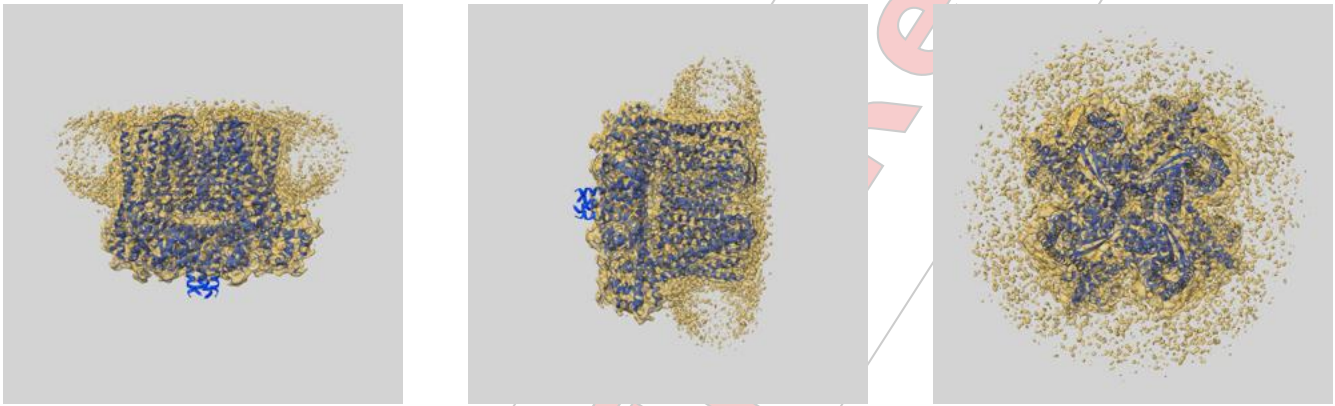
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70240 and PDB model 9O93. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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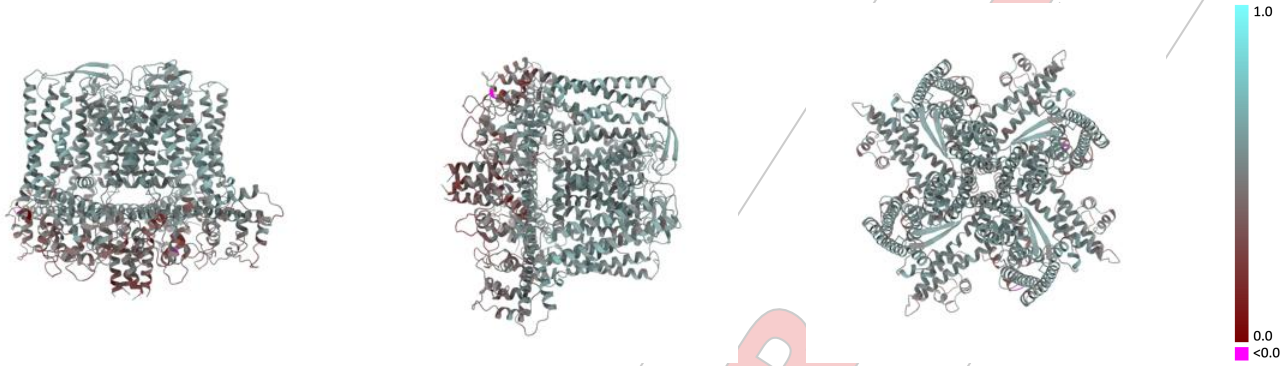
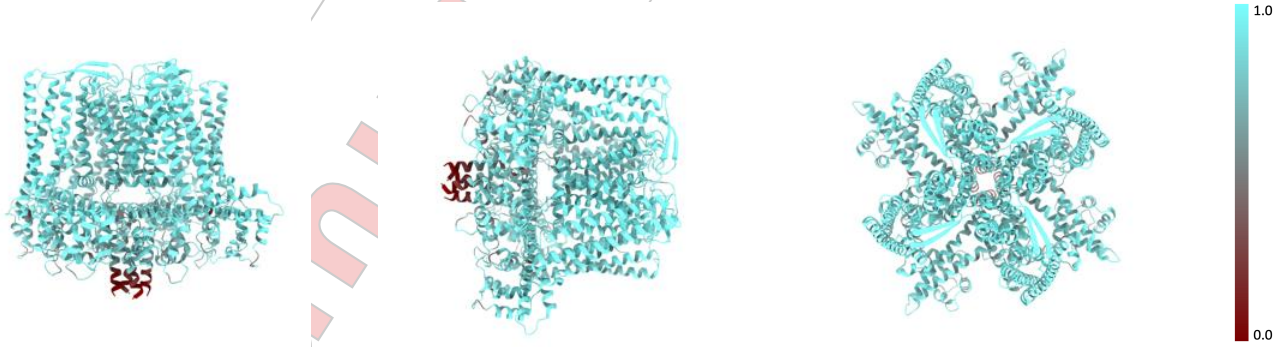
9.2 Q-score mapped to coordinate model (i)



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 (6.5).

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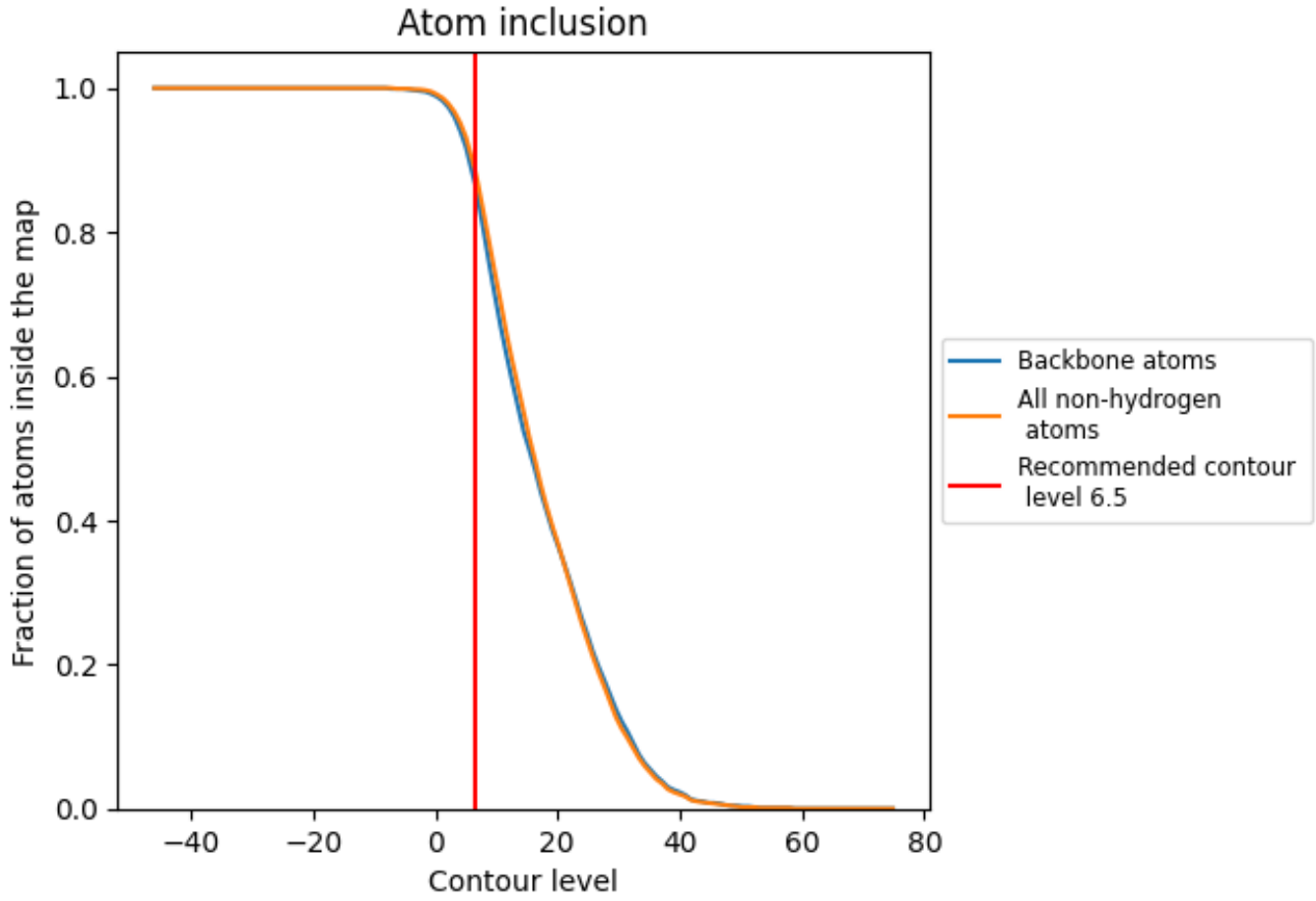
9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8860	0.5170
A	0.9120	0.5460
B	0.9080	0.5450
C	0.9090	0.5440
D	0.9110	0.5460
E	0.8320	0.4380
F	0.8340	0.4360
G	0.8300	0.4340
H	0.8260	0.4370

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Full wwPDB EM Validation Report (i)

May 14, 2025 – 03:23 PM EDT

PDB ID	:	9O85 / pdb_00009o85
EMDB ID	:	EMD-70217
Title	:	Cryo-EM structure of KCa2.2_I/calmodulin channel in complex with rimtuzalcap
Deposited on	:	2025-04-15
Resolution	:	3.13 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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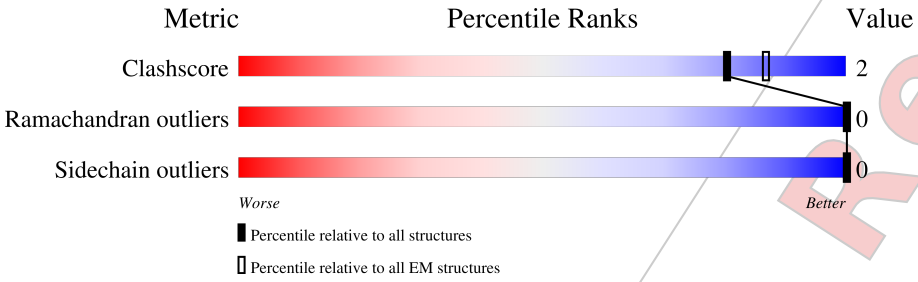
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.13 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	380	94% 6%
1	B	380	93% 7%
1	C	380	94% 6%
1	D	380	94% 6%
2	E	144	89% 10%
2	F	144	94% 6%
2	G	144	92% 8%

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Mol	Chain	Length	Quality of chain
2	H	144	

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2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16403 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 Small conductance calcium-activated potassium channel protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total 2994	C 1939	N 515	O 517	S 23	0	0
1	B	380	Total 2994	C 1939	N 515	O 517	S 23	0	0
1	C	380	Total 2994	C 1939	N 515	O 517	S 23	0	0
1	D	380	Total 2994	C 1939	N 515	O 517	S 23	0	0

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	144	Total 1075	C 668	N 179	O 219	S 9	0	0
2	F	144	Total 1075	C 668	N 179	O 219	S 9	0	0
2	G	144	Total 1075	C 668	N 179	O 219	S 9	0	0
2	H	144	Total 1075	C 668	N 179	O 219	S 9	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total 3	K 3	0

- Molecule 4 is N-(4,4-difluorocyclohexyl)-2-(3-methyl-1H-pyrazol-1-yl)-6-(morpholin-4-yl)pyrimidin-4-amine (CCD ID: A1B92) (formula: $C_{18}H_{24}F_2N_6O$) (labeled as "Ligand of Interest" by depositor).

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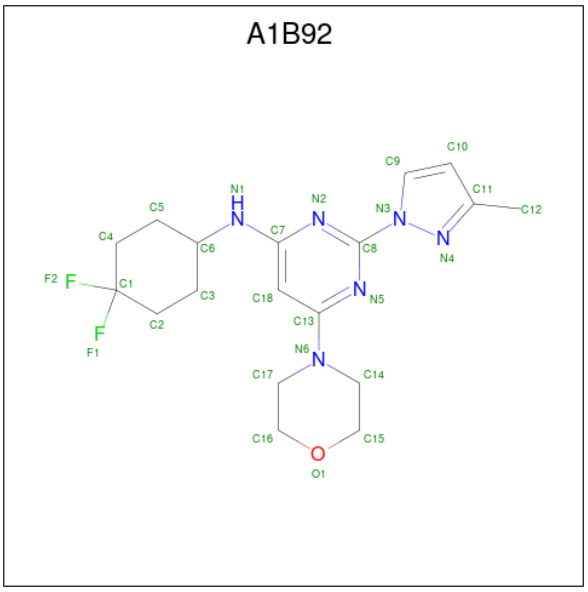

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C F N O 27 18 2 6 1	0
4	C	1	Total C F N O 27 18 2 6 1	0
4	G	1	Total C F N O 27 18 2 6 1	0
4	H	1	Total C F N O 27 18 2 6 1	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	E	2	Total Ca 2 2	0
5	F	2	Total Ca 2 2	0
5	G	2	Total Ca 2 2	0
5	H	2	Total Ca 2 2	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	2	Total O 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
6	B	2	Total O 2 2	0
6	C	2	Total O 2 2	0
6	D	2	Total O 2 2	0

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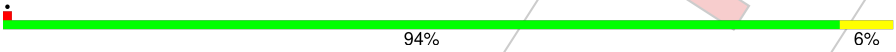
3 Residue-property plots (i)

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.

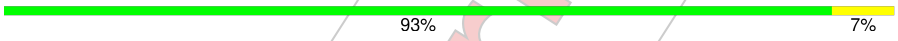
• Molecule 1: Small conductance calcium-activated potassium channel protein 2

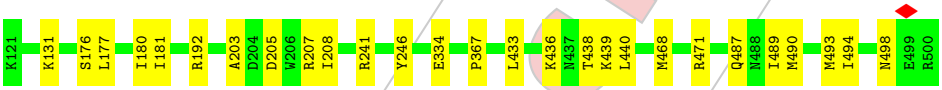
Chain A:



• Molecule 1: Small conductance calcium-activated potassium channel protein 2

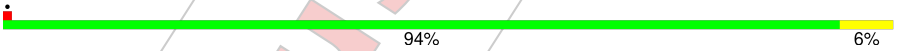
Chain B:





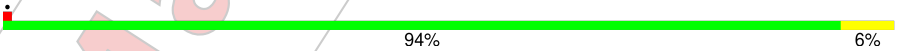
• Molecule 1: Small conductance calcium-activated potassium channel protein 2

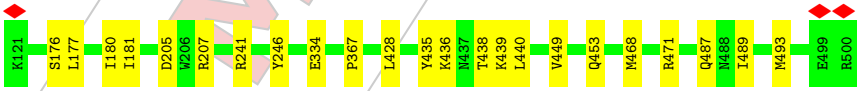
Chain C:



• Molecule 1: Small conductance calcium-activated potassium channel protein 2

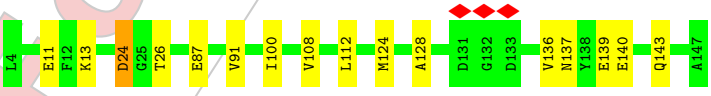
Chain D:





• Molecule 2: Calmodulin-1

Chain E:



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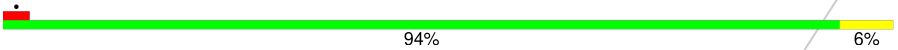
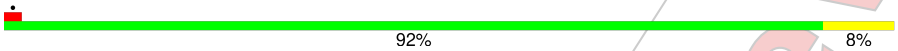
• Molecule 2: Calmodulin-1

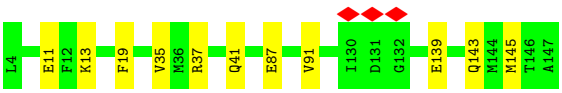
Chain F:



• Molecule 2: Calmodulin-1

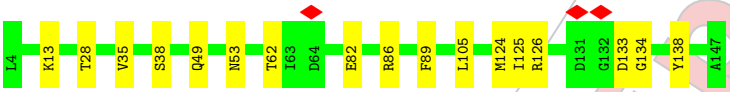
Chain G:





• Molecule 2: Calmodulin-1

Chain H:



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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	59.444	Depositor
Minimum map value	-44.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7.2	Depositor
Map size (Å)	430.0, 430.0, 430.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

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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: CA, A1B92, K

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	0.15	0/3052	0.31	0/4136
1	B	0.14	0/3052	0.29	0/4136
1	C	0.14	0/3052	0.30	0/4136
1	D	0.15	0/3052	0.31	0/4136
2	E	0.15	0/1087	0.38	1/1464 (0.1%)
2	F	0.14	0/1087	0.46	1/1464 (0.1%)
2	G	0.10	0/1087	0.28	0/1464
2	H	0.16	0/1087	0.50	0/1464
All	All	0.14	0/16556	0.34	2/22400 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	20	ASP	CA-CB-CG	9.29	121.89	112.60
2	E	24	ASP	CA-CB-CG	6.47	119.07	112.60

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	2994	0	3080	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2994	0	3080	17	0
1	C	2994	0	3080	13	0
1	D	2994	0	3080	13	0
2	E	1075	0	995	8	0
2	F	1075	0	995	6	0
2	G	1075	0	994	6	0
2	H	1075	0	994	10	0
3	A	3	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	G	27	0	0	0	0
4	H	27	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	16403	0	16298	80	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 2.

All (80) 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:B:490:MET:SD	1:C:487:GLN:NE2	2.65	0.69
1:A:490:MET:SD	1:B:487:GLN:NE2	2.66	0.68
2:E:108:VAL:HG23	2:E:112:LEU:HD12	1.75	0.68
2:F:108:VAL:HG23	2:F:112:LEU:HD12	1.79	0.65
1:A:468:MET:SD	1:A:471:ARG:NH1	2.73	0.61
1:A:242:LEU:HD22	1:A:368:ASN:HD21	1.64	0.61
2:E:137:ASN:ND2	2:E:140:GLU:OE1	2.36	0.58
1:D:468:MET:SD	1:D:471:ARG:NH2	2.77	0.58
1:B:468:MET:SD	1:B:471:ARG:NH2	2.78	0.57
1:C:468:MET:SD	1:C:471:ARG:NH2	2.78	0.57
1:D:438:THR:HG23	1:D:439:LYS:HG3	1.88	0.56
1:D:449:VAL:O	1:D:453:GLN:HG3	2.06	0.56
2:H:89:PHE:CD2	2:H:138:TYR:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:THR:HG23	1:B:439:LYS:HG3	1.88	0.54
2:F:139:GLU:OE2	2:F:143:GLN:NE2	2.34	0.54
2:H:82:GLU:O	2:H:86:ARG:NE	2.34	0.54
2:G:19:PHE:HA	2:G:35:VAL:HG21	1.90	0.52
2:G:139:GLU:OE2	2:G:143:GLN:NE2	2.42	0.52
2:F:19:PHE:HD1	2:F:35:VAL:HG21	1.76	0.51
1:B:436:LYS:HG3	1:B:440:LEU:HD12	1.93	0.50
1:C:203:ALA:HB1	1:C:208:ILE:HD12	1.92	0.50
1:C:483:LEU:HD22	1:D:487:GLN:HE21	1.77	0.50
2:G:11:GLU:C	2:G:13:LYS:H	2.20	0.49
2:H:105:LEU:HD22	2:H:125:ILE:HD11	1.93	0.49
1:C:435:TYR:HA	1:C:438:THR:HG22	1.95	0.48
1:A:497:LEU:HD21	1:B:498:ASN:HA	1.96	0.48
1:B:176:SER:O	1:B:180:ILE:HG12	2.14	0.48
2:E:124:MET:O	2:E:128:ALA:HB2	2.13	0.48
1:D:176:SER:O	1:D:180:ILE:HG12	2.14	0.48
2:E:139:GLU:OE2	2:E:143:GLN:NE2	2.47	0.48
1:C:176:SER:O	1:C:180:ILE:HG12	2.14	0.47
1:B:177:LEU:O	1:B:181:ILE:HD12	2.14	0.47
1:A:176:SER:O	1:A:180:ILE:HG12	2.14	0.47
2:H:35:VAL:O	2:H:38:SER:OG	2.27	0.47
1:A:241:ARG:HH11	1:A:246:TYR:HD1	1.63	0.47
2:F:86:ARG:HH21	2:F:143:GLN:HE21	1.62	0.46
1:B:241:ARG:HH11	1:B:246:TYR:HD1	1.64	0.46
1:C:241:ARG:HH11	1:C:246:TYR:HD1	1.64	0.46
2:H:49:GLN:NE2	2:H:53:ASN:OD1	2.49	0.46
1:D:241:ARG:HH11	1:D:246:TYR:HD1	1.64	0.46
1:A:162:ASP:OD1	1:A:162:ASP:N	2.44	0.45
1:D:177:LEU:O	1:D:181:ILE:HD12	2.16	0.45
1:B:490:MET:O	1:B:494:ILE:HG12	2.17	0.45
1:C:432:TRP:HA	2:G:145:MET:HE1	1.98	0.45
1:C:177:LEU:O	1:C:181:ILE:HD12	2.16	0.45
2:E:11:GLU:C	2:E:13:LYS:H	2.26	0.44
2:E:100:ILE:HG23	2:E:136:VAL:HB	1.99	0.44
1:A:364:ASP:OD1	1:A:364:ASP:N	2.49	0.44
2:H:28:THR:HG22	2:H:62:THR:HG22	1.98	0.44
1:B:205:ASP:OD2	1:B:207:ARG:NE	2.48	0.44
1:B:131:LYS:HD3	1:B:192:ARG:HE	1.83	0.44
1:A:177:LEU:O	1:A:181:ILE:HD12	2.17	0.44
2:F:133:ASP:OD1	2:F:133:ASP:N	2.50	0.43
1:C:436:LYS:O	1:C:440:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ASP:OD1	1:D:207:ARG:NH2	2.44	0.43
1:A:205:ASP:OD1	1:A:207:ARG:NE	2.47	0.43
2:F:86:ARG:HH21	2:F:143:GLN:NE2	2.17	0.43
1:B:205:ASP:OD1	1:B:207:ARG:NH2	2.49	0.43
1:B:203:ALA:HB1	1:B:208:ILE:HD12	2.01	0.42
1:B:334:GLU:OE2	1:B:367:PRO:HB3	2.20	0.42
1:D:334:GLU:OE2	1:D:367:PRO:HB3	2.20	0.42
2:G:87:GLU:O	2:G:91:VAL:HG23	2.20	0.42
2:H:13:LYS:HA	2:H:13:LYS:HD3	1.89	0.42
1:C:334:GLU:OE2	1:C:367:PRO:HB3	2.20	0.42
1:A:426:ASN:O	1:A:430:GLU:HG2	2.20	0.42
1:C:205:ASP:OD1	1:C:207:ARG:NH2	2.41	0.42
1:D:436:LYS:HG3	1:D:440:LEU:HD12	2.01	0.42
2:H:124:MET:O	2:H:126:ARG:N	2.51	0.41
2:E:87:GLU:O	2:E:91:VAL:HG23	2.21	0.41
1:B:489:ILE:O	1:B:493:MET:HG3	2.21	0.41
2:E:24:ASP:OD1	2:E:26:THR:OG1	2.36	0.41
1:A:489:ILE:O	1:A:493:MET:HG3	2.20	0.41
2:G:37:ARG:HA	2:G:41:GLN:O	2.20	0.41
1:D:489:ILE:O	1:D:493:MET:HG3	2.21	0.41
2:H:133:ASP:OD1	2:H:134:GLY:N	2.55	0.40
1:A:126:ARG:HD2	1:A:126:ARG:HA	1.81	0.40
1:D:428:LEU:HD22	2:H:89:PHE:CE1	2.57	0.40
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.87	0.40
1:C:438:THR:HG23	1:C:439:LYS:HG3	2.03	0.40
1:D:435:TYR:HA	1:D:438:THR:HG22	2.04	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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/380 (100%)	367 (97%)	11 (3%)	0	100	100
1	B	378/380 (100%)	361 (96%)	17 (4%)	0	100	100
1	C	378/380 (100%)	365 (97%)	13 (3%)	0	100	100
1	D	378/380 (100%)	366 (97%)	12 (3%)	0	100	100
2	E	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
2	F	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
2	G	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
2	H	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
All	All	2080/2096 (99%)	1990 (96%)	90 (4%)	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	320/331 (97%)	320 (100%)	0	100	100
1	B	320/331 (97%)	320 (100%)	0	100	100
1	C	320/331 (97%)	320 (100%)	0	100	100
1	D	320/331 (97%)	320 (100%)	0	100	100
2	E	106/123 (86%)	106 (100%)	0	100	100
2	F	106/123 (86%)	106 (100%)	0	100	100
2	G	106/123 (86%)	106 (100%)	0	100	100
2	H	106/123 (86%)	106 (100%)	0	100	100
All	All	1704/1816 (94%)	1704 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

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Mol	Chain	Res	Type
1	A	340	GLN
1	C	124	HIS
1	C	277	HIS
1	D	277	HIS
1	D	453	GLN
2	E	135	GLN
2	G	111	ASN
2	H	111	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	A1B92	H	201	-	30,30,30	0.44	0	36,43,43	0.89	2 (5%)
4	A1B92	G	201	-	30,30,30	0.44	0	36,43,43	0.98	2 (5%)
4	A1B92	C	601	-	30,30,30	0.44	0	36,43,43	0.99	2 (5%)
4	A1B92	B	601	-	30,30,30	0.44	0	36,43,43	1.30	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1B92	H	201	-	-	0/12/32/32	1/4/4/4
4	A1B92	G	201	-	-	2/12/32/32	1/4/4/4
4	A1B92	C	601	-	-	2/12/32/32	1/4/4/4
4	A1B92	B	601	-	-	2/12/32/32	0/4/4/4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	A1B92	C5-C4-C1	-5.05	107.95	110.75
4	B	601	A1B92	C3-C2-C1	-4.73	108.13	110.75
4	C	601	A1B92	C5-C4-C1	-3.94	108.57	110.75
4	G	201	A1B92	C5-C4-C1	-3.93	108.57	110.75
4	H	201	A1B92	C3-C2-C1	-3.28	108.93	110.75
4	C	601	A1B92	C3-C2-C1	-2.76	109.22	110.75
4	G	201	A1B92	C3-C2-C1	-2.72	109.25	110.75
4	H	201	A1B92	C5-C4-C1	-2.37	109.44	110.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	A1B92	N5-C8-N3-N4
4	C	601	A1B92	N5-C8-N3-N4
4	G	201	A1B92	N5-C8-N3-N4
4	B	601	A1B92	N2-C8-N3-C9
4	C	601	A1B92	N2-C8-N3-C9
4	G	201	A1B92	N2-C8-N3-C9

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	201	A1B92	C1-C2-C3-C4-C5-C6
4	C	601	A1B92	C1-C2-C3-C4-C5-C6
4	H	201	A1B92	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

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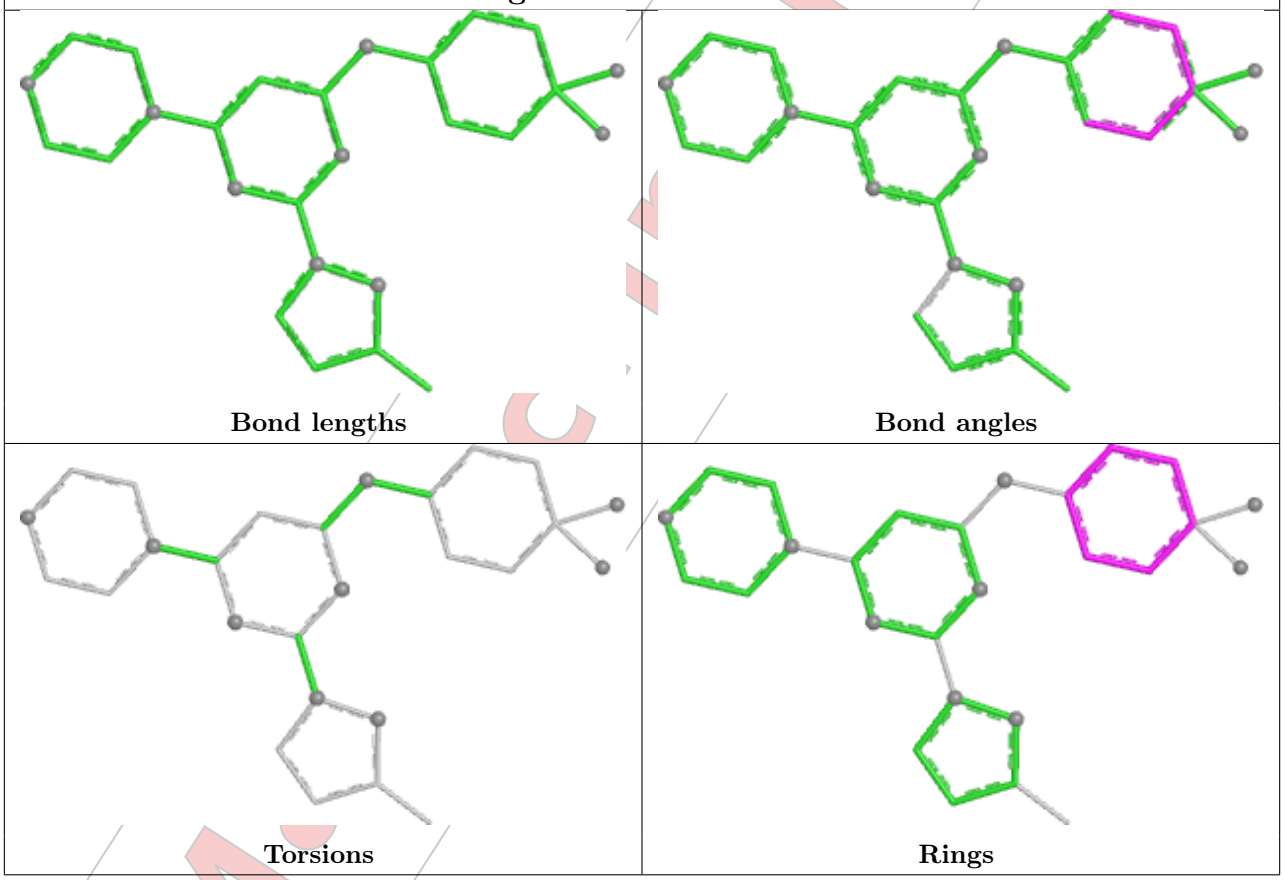
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1B92 H 201



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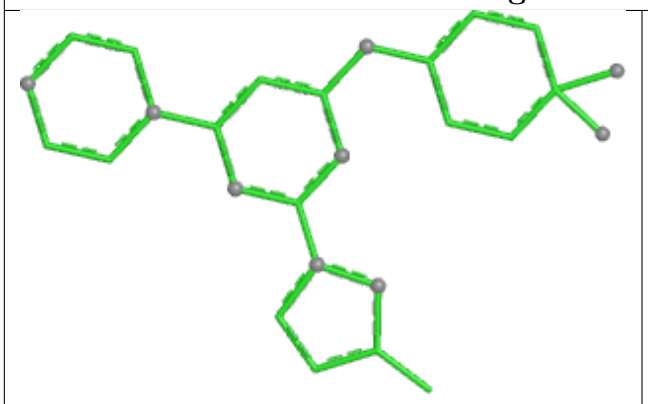
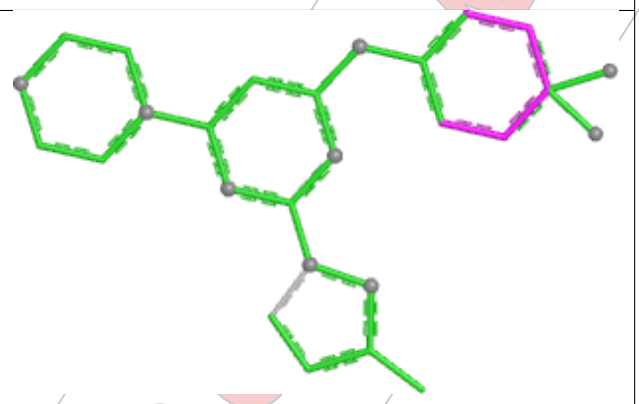
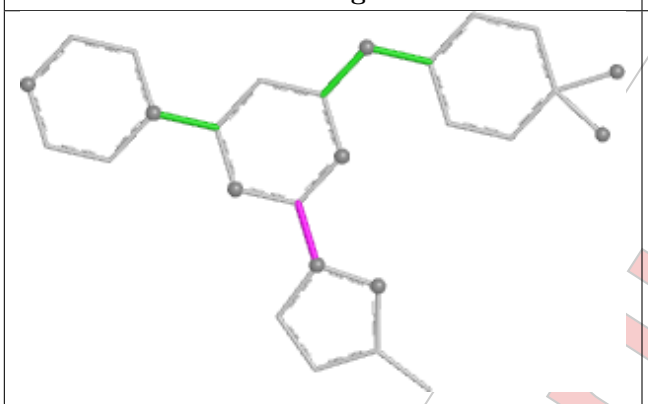
Ligand A1B92 G 201



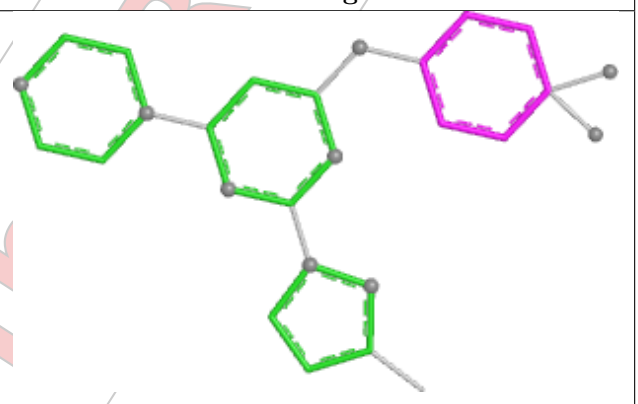
Bond lengths



Bond angles



Torsions



Rings

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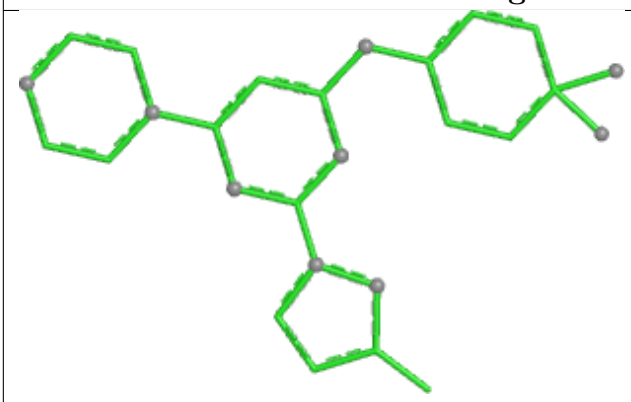
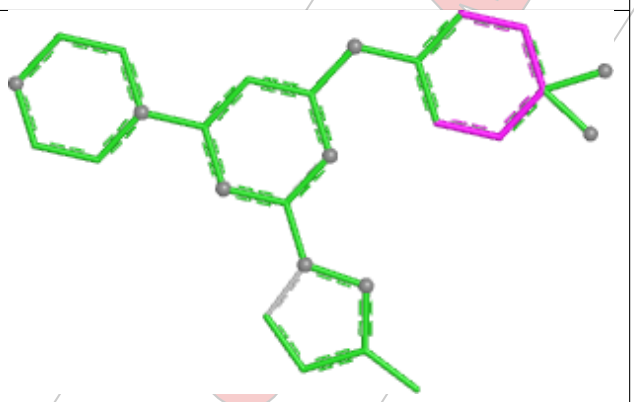
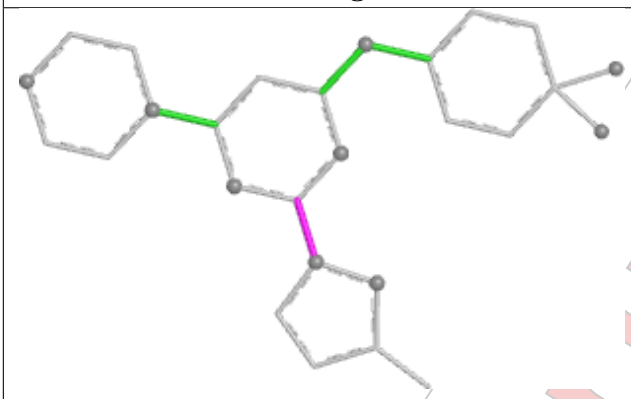
Ligand A1B92 C 601



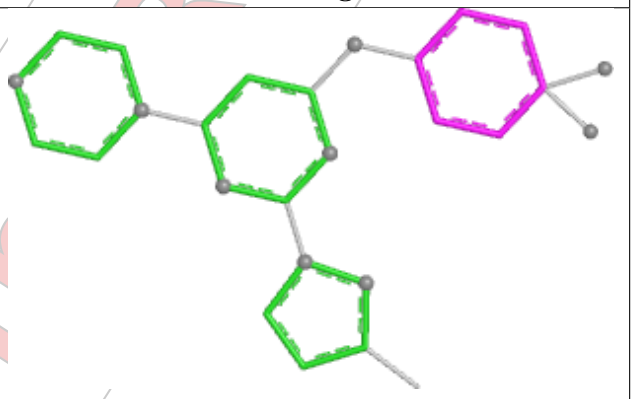
Bond lengths



Bond angles



Torsions



Rings

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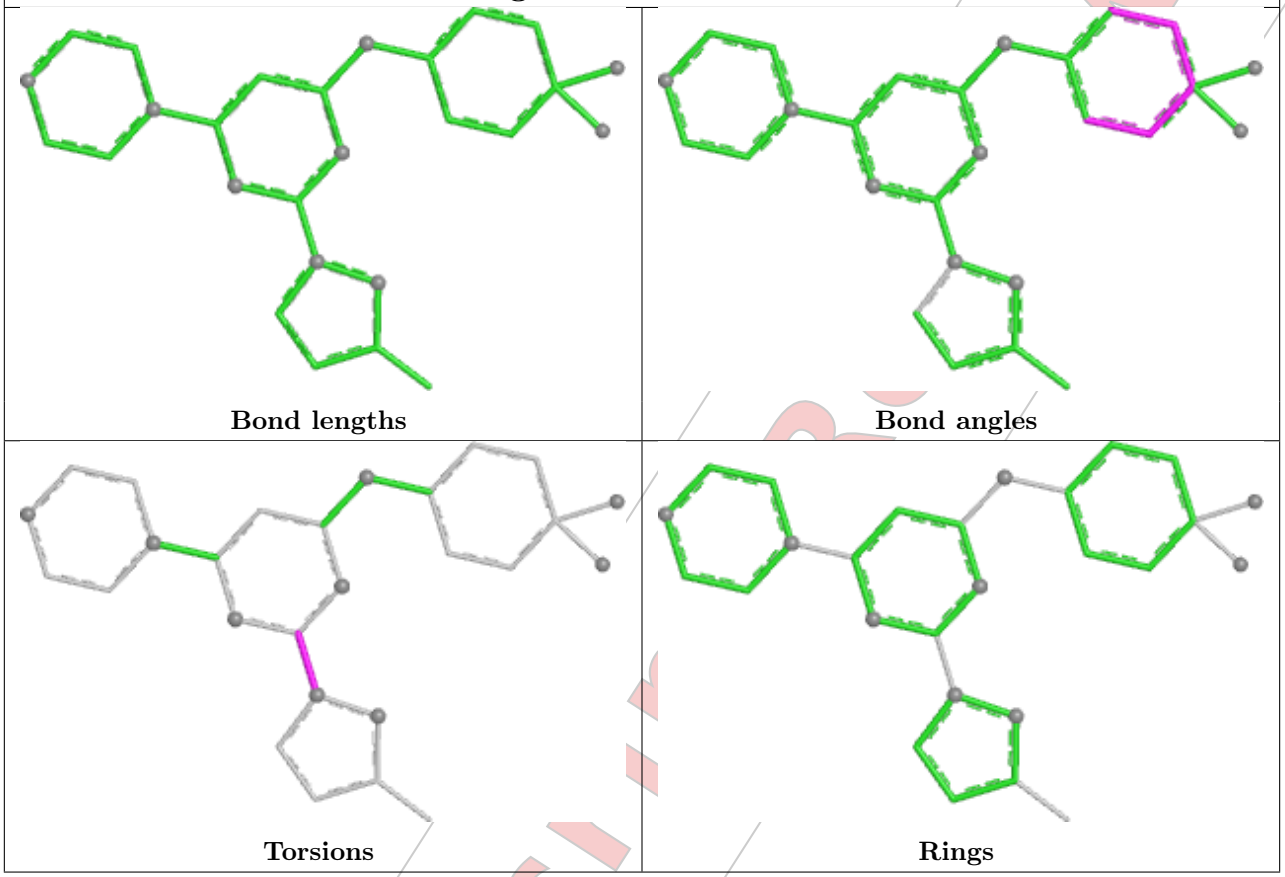
Ligand A1B92 B 601



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.

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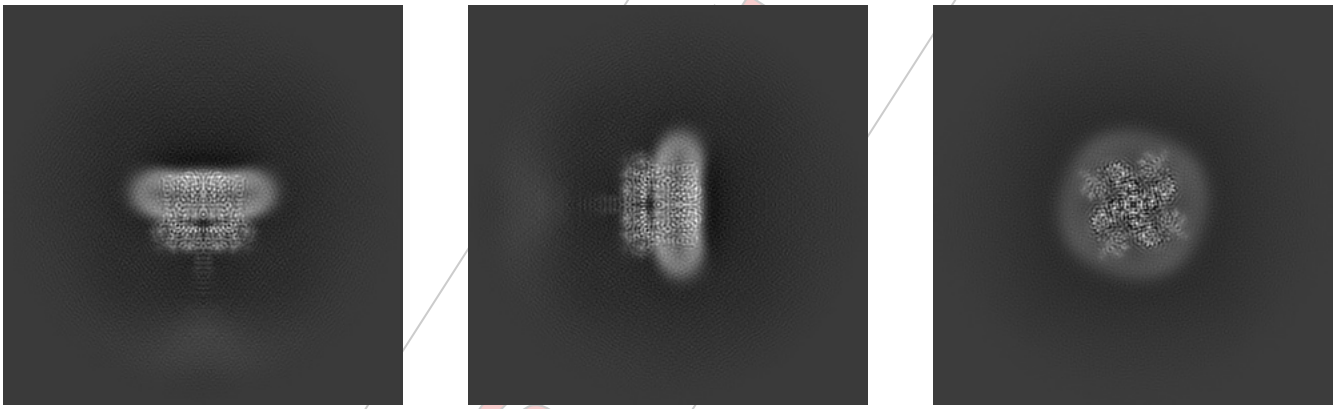
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70217. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

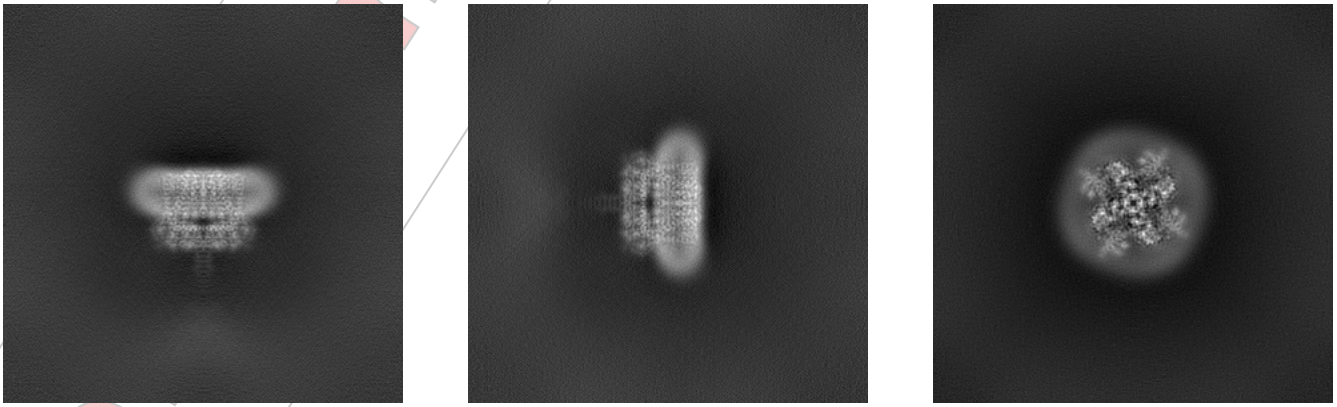
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



X Y Z

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

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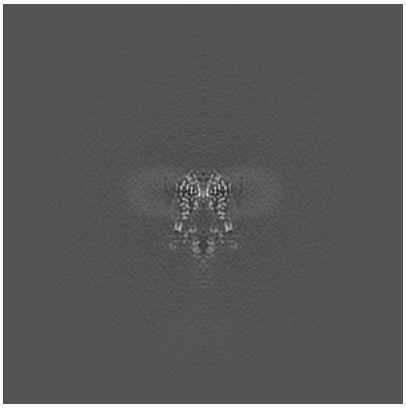
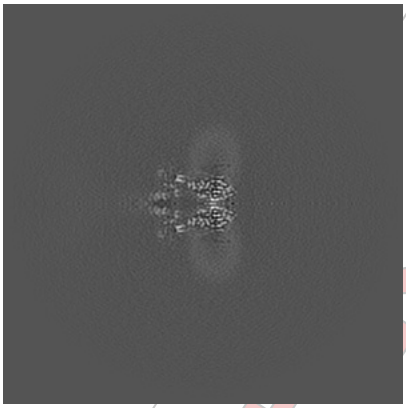
6.2 Central slices (i)

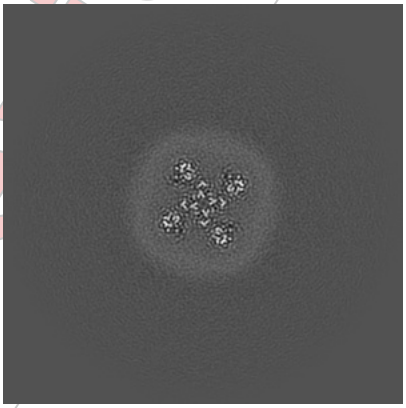
6.2.1 Primary map



X Index: 250

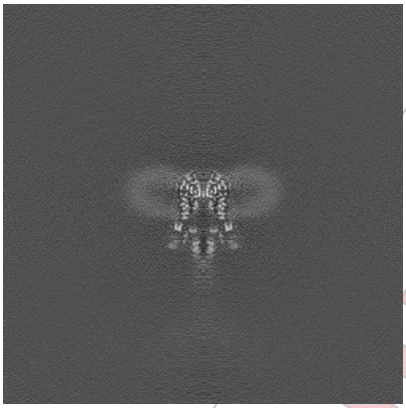


Y Index: 250

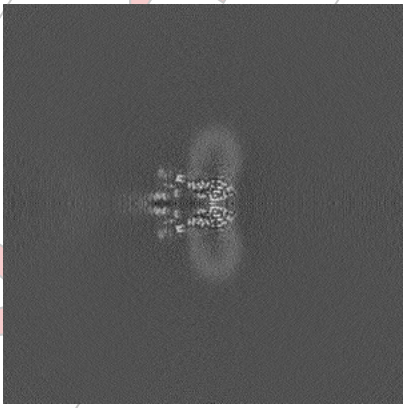


Z Index: 250

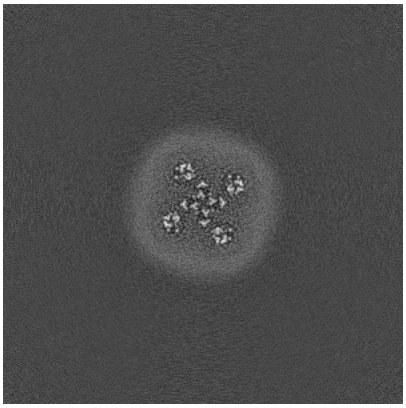
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

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

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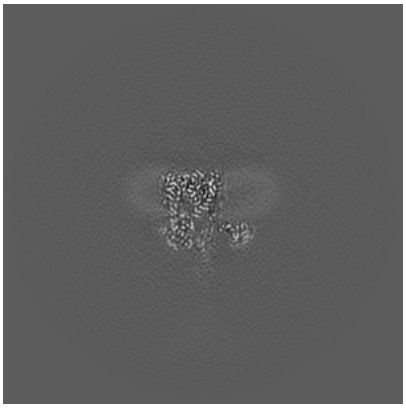
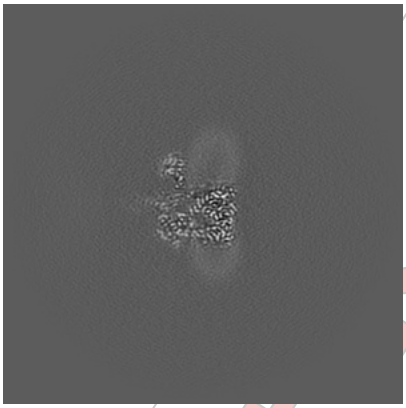
6.3 Largest variance slices (i)

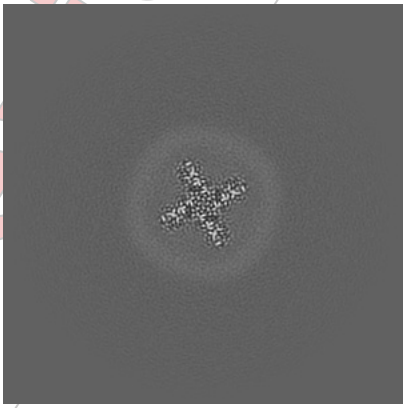
6.3.1 Primary map



X Index: 262

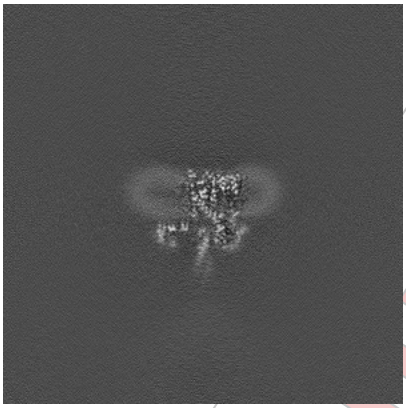


Y Index: 238

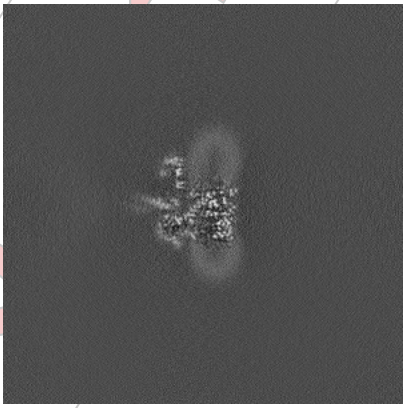


Z Index: 269

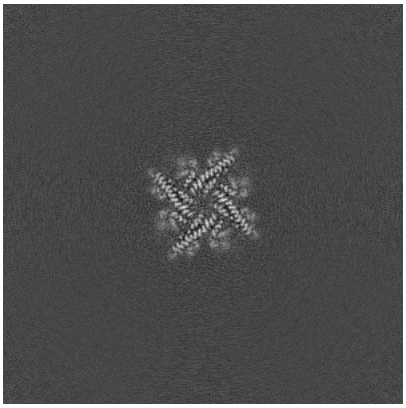
6.3.2 Raw map



X Index: 240



Y Index: 240



Z Index: 219

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

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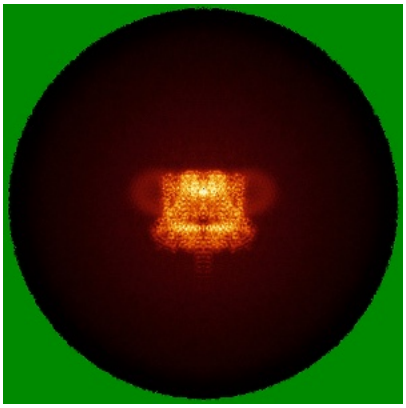
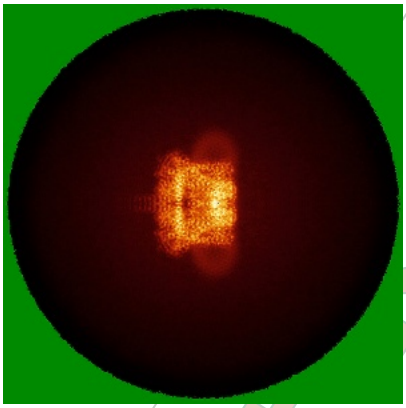
6.4 Orthogonal standard-deviation projections (False-color)

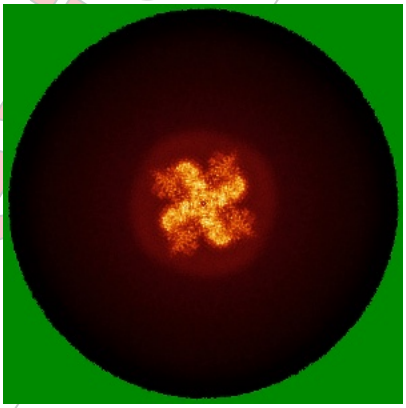
6.4.1 Primary map



X

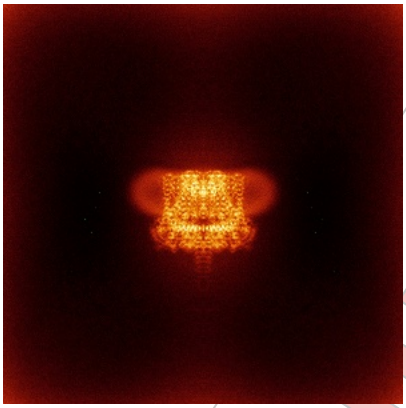


Y

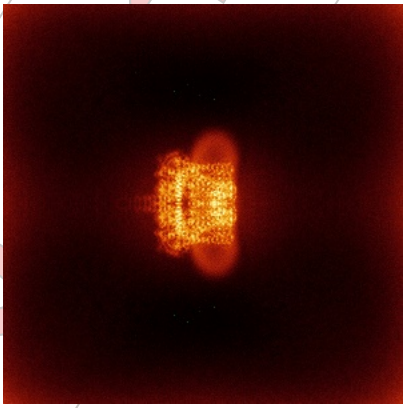


Z

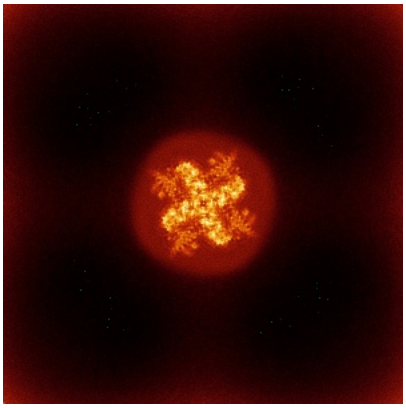
6.4.2 Raw map



X



Y



Z

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

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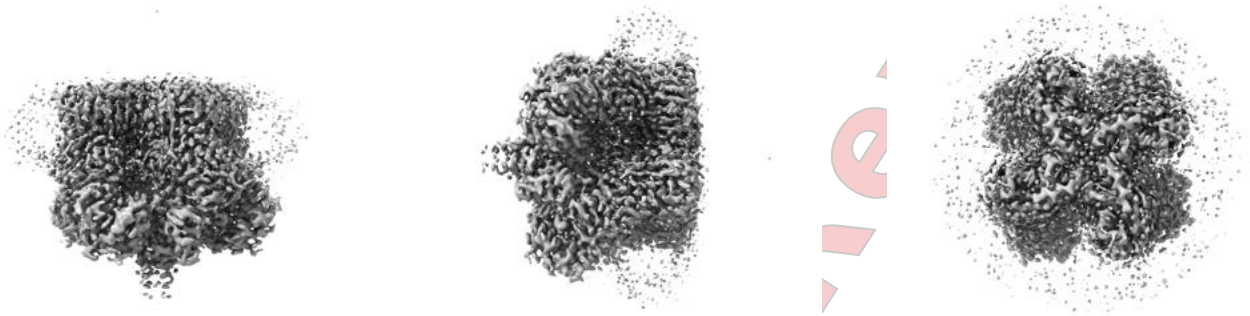
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

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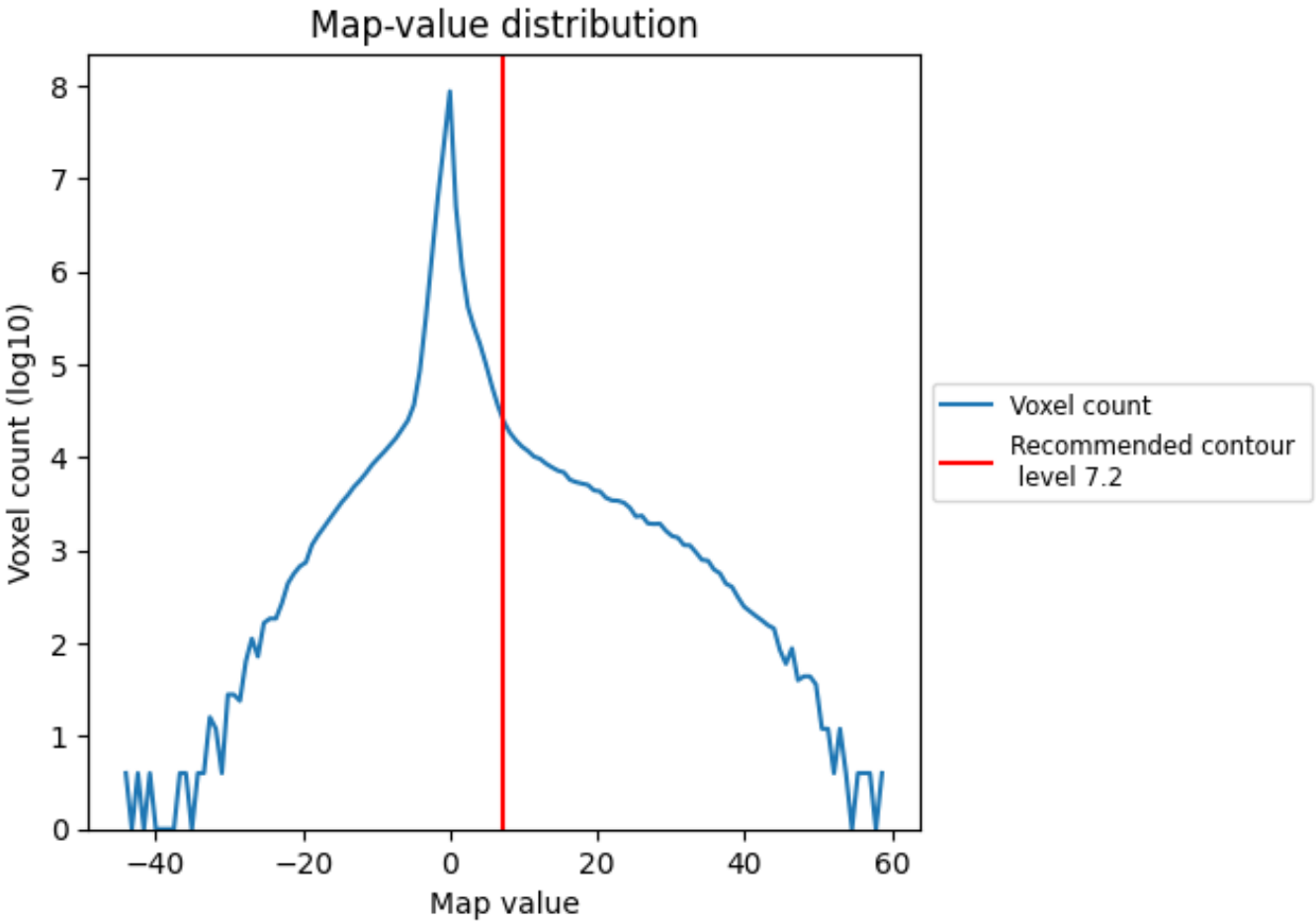
7 Map analysis

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.

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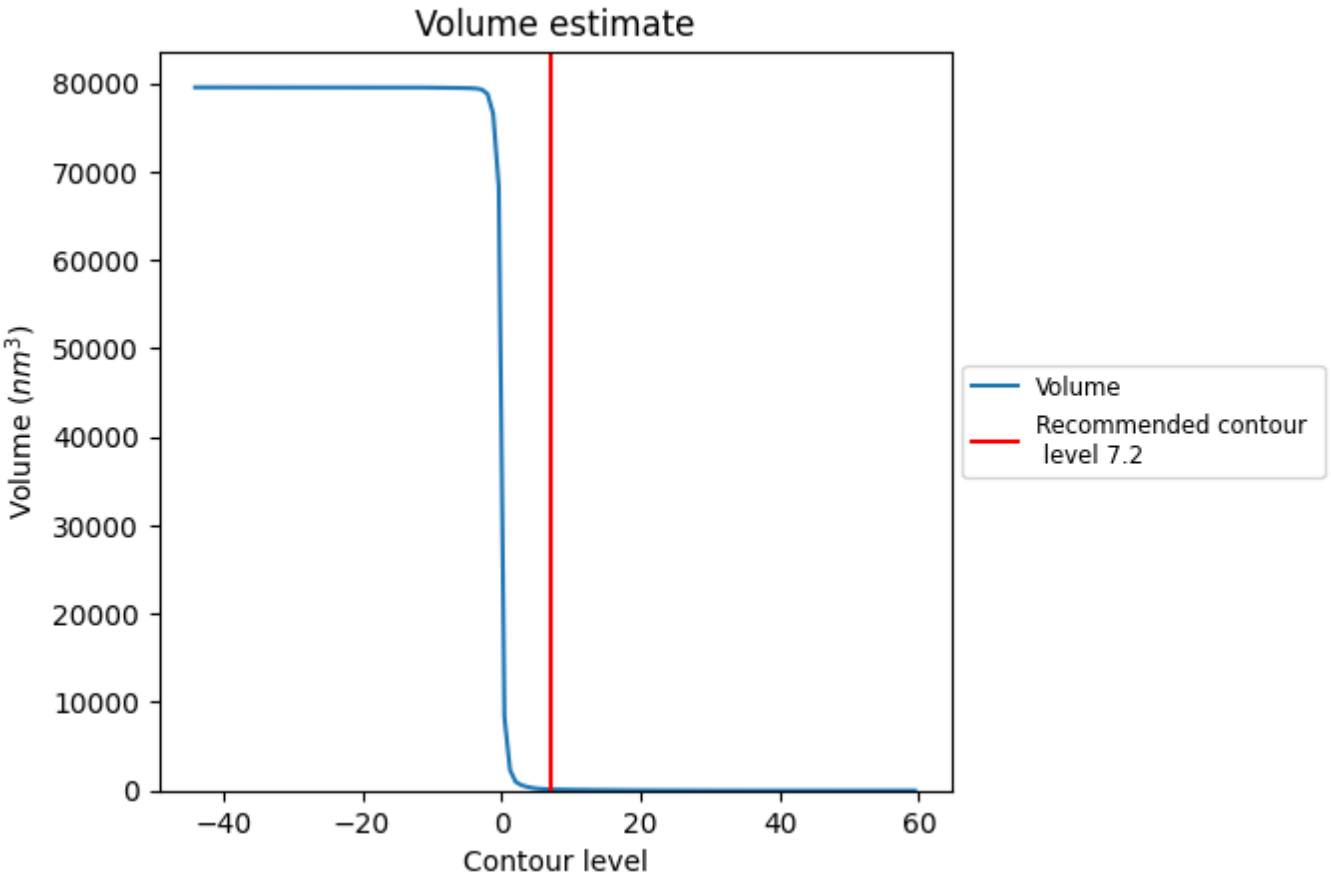
7.2 Volume estimate (i)



The volume at the recommended contour level is 132 nm^3; this corresponds to an approximate mass of 119 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.

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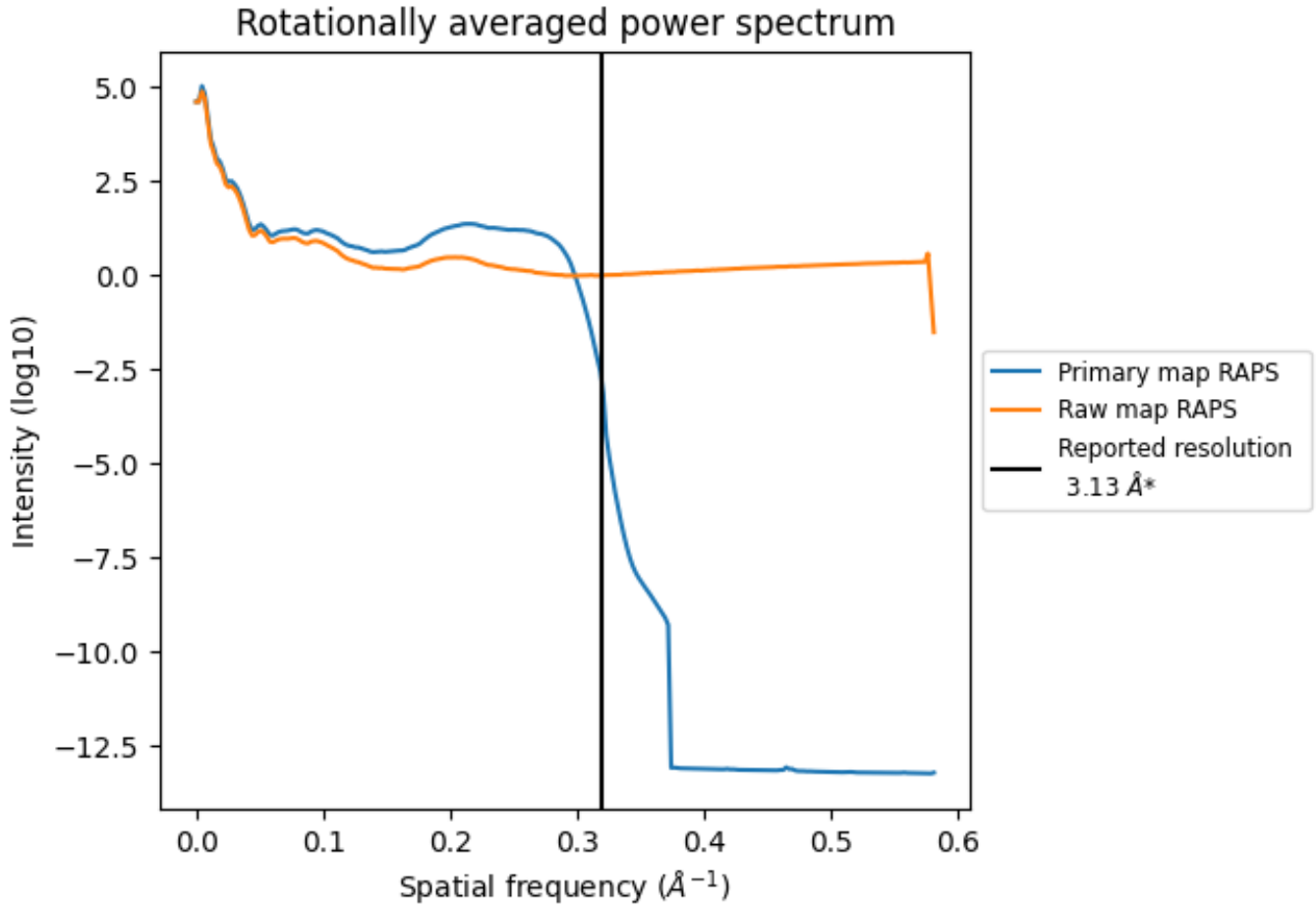
7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

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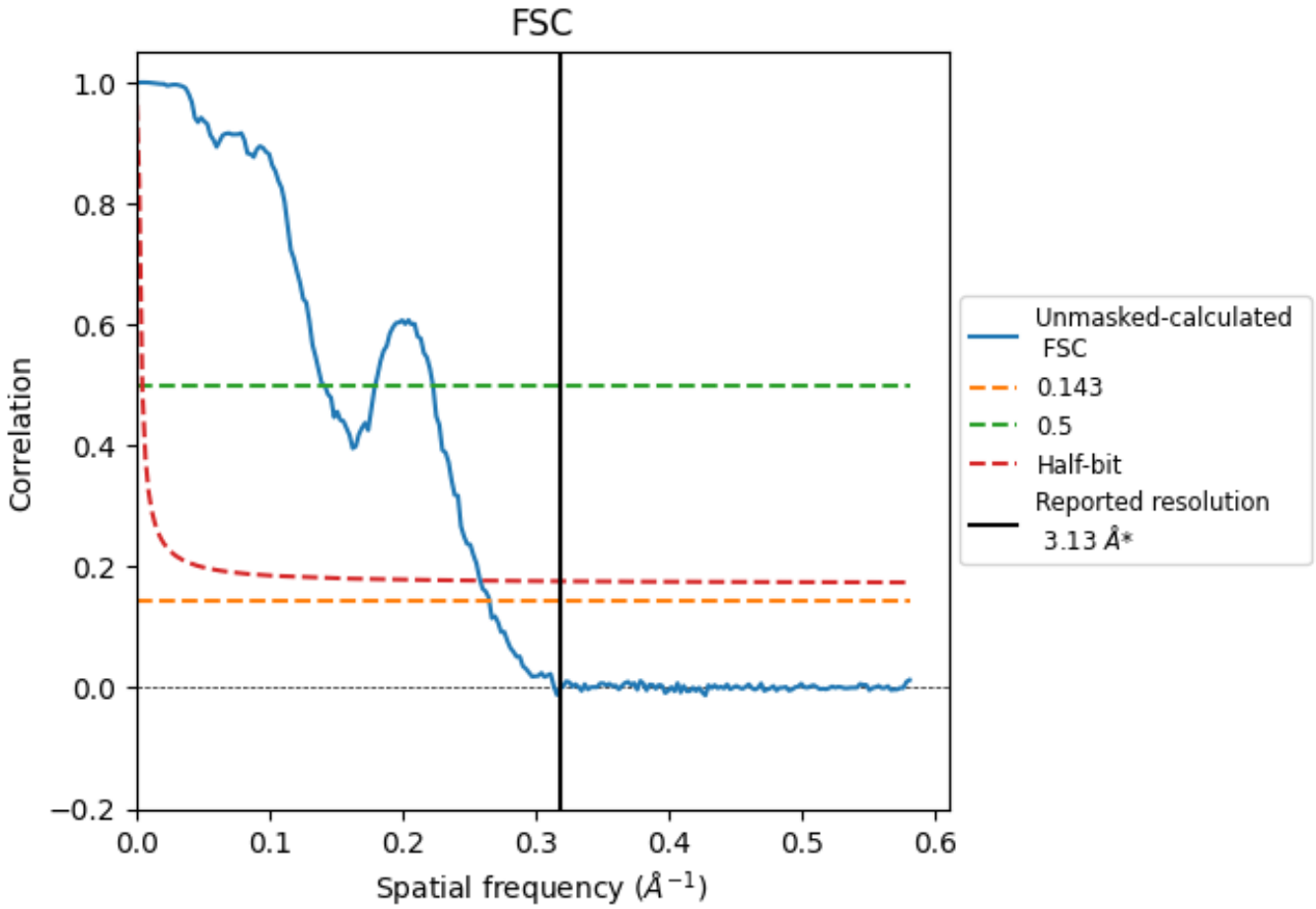
8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.77	7.09	3.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 3.13 by more than 10 %

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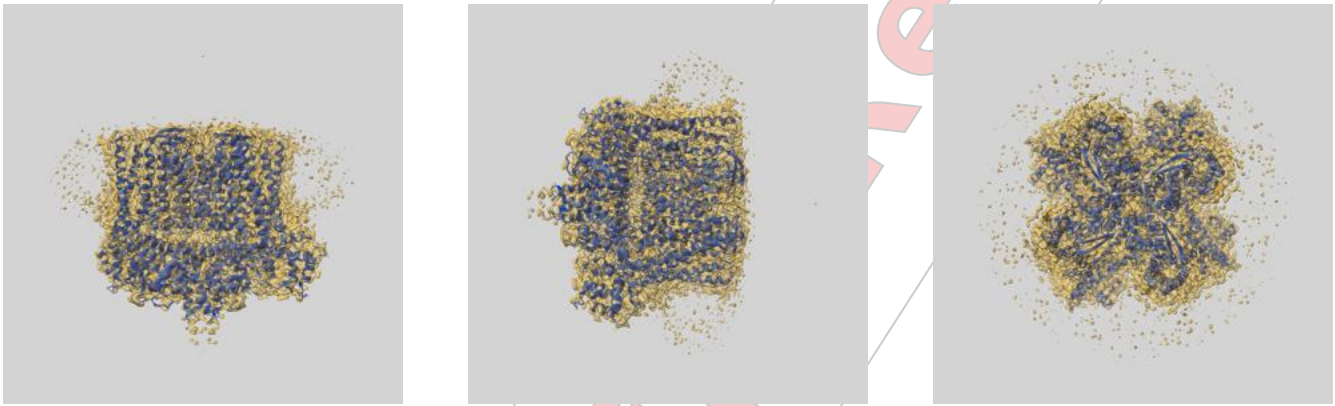
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70217 and PDB model 9O85. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.2 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.

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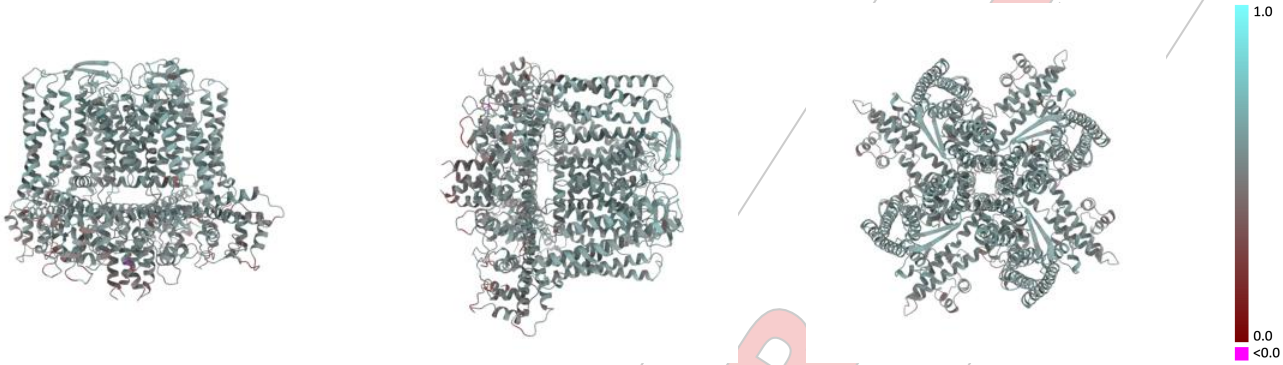
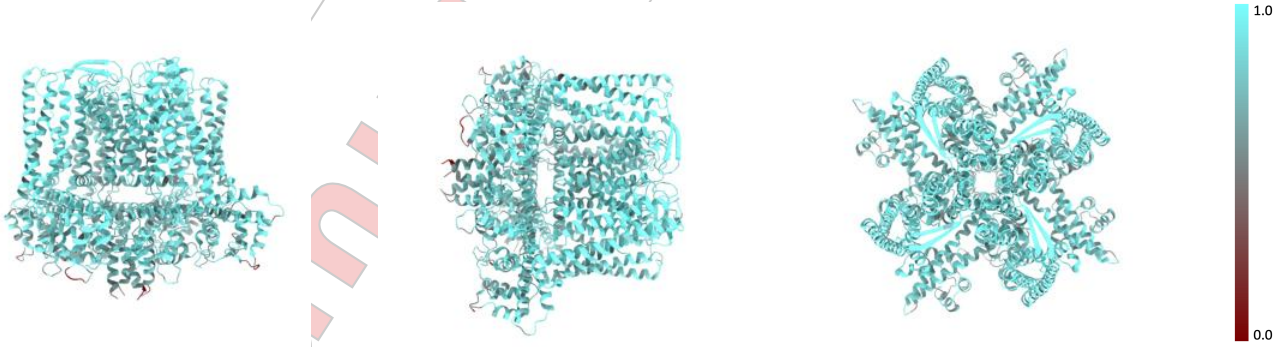
9.2 Q-score mapped to coordinate model (i)



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 (7.2).

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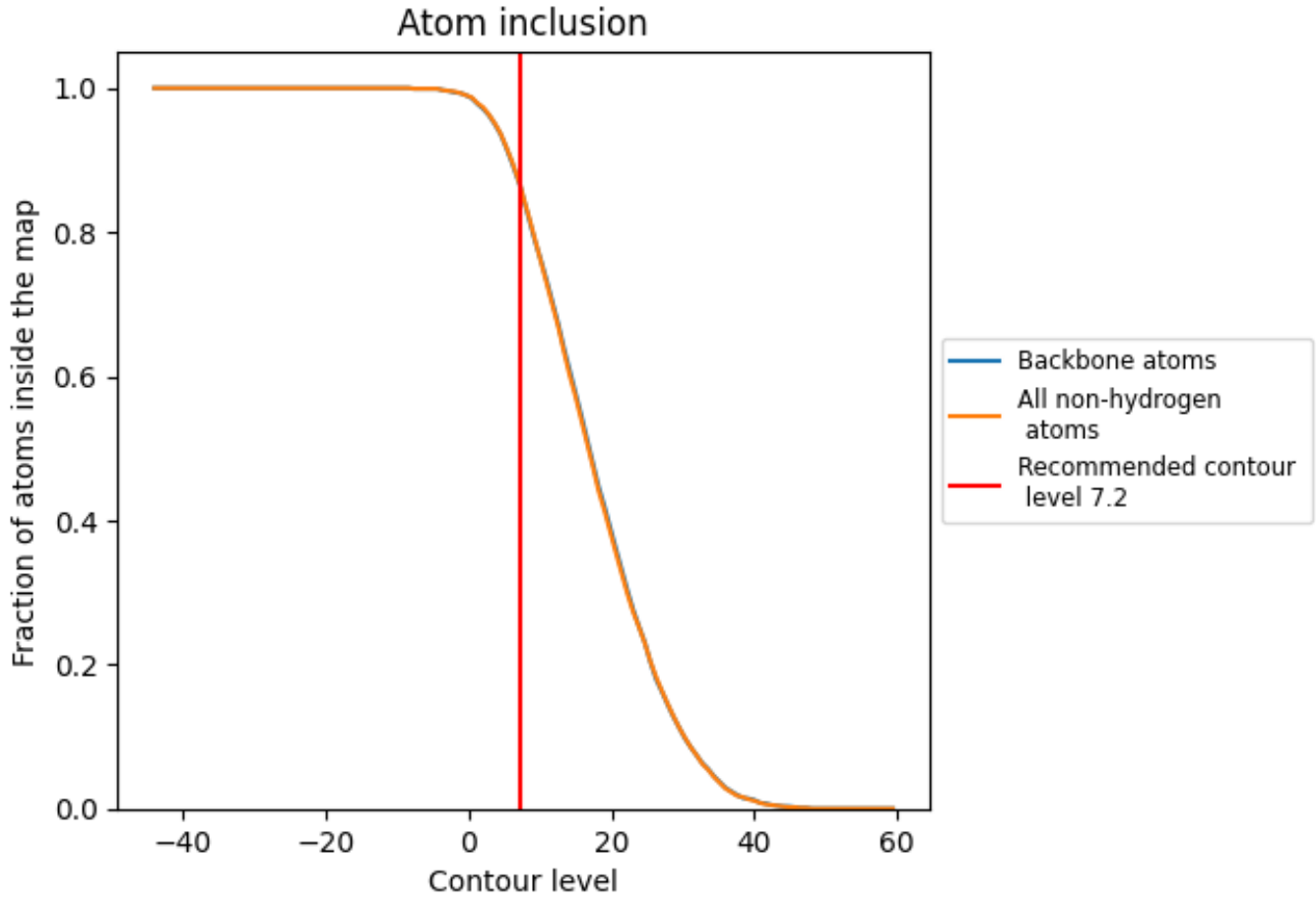
9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (7.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8660	0.5390
A	0.8940	0.5540
B	0.8950	0.5560
C	0.8940	0.5560
D	0.8930	0.5530
E	0.7940	0.4920
F	0.7930	0.4960
G	0.8050	0.5010
H	0.8040	0.4960

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