



Full wwPDB EM Validation Report ⓘ

Apr 20, 2024 – 12:12 pm BST

PDB ID : 8PB1
EMDB ID : EMD-17580
Title : Cryo-EM structure of a pre-dimerized murine IL-12 complete extracellular signaling complex (Class 1), obtained after local refinement.
Authors : Felix, J.; Bloch, Y.; Savvides, S.N.
Deposited on : 2023-06-08
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

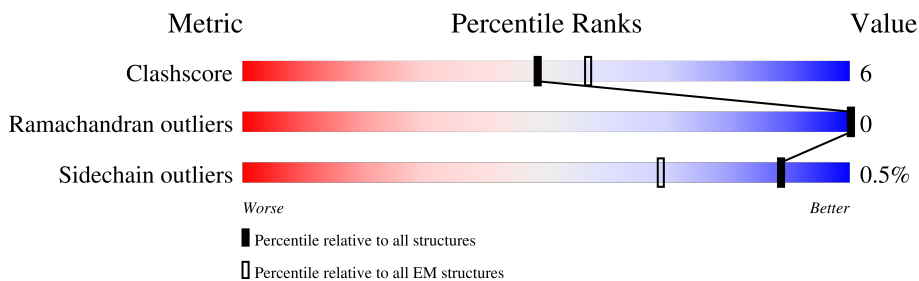
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	231	
2	B	313	
3	C	572	
4	D	769	
5	E	4	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6652 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 Interleukin-12 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	157	1247	775	221	236	15	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	GLY	-	expression tag	UNP P43431
A	217	THR	-	expression tag	UNP P43431
A	218	SER	-	expression tag	UNP P43431
A	219	ASP	-	expression tag	UNP P43431
A	220	GLU	-	expression tag	UNP P43431
A	221	VAL	-	expression tag	UNP P43431
A	222	ASP	-	expression tag	UNP P43431
A	223	GLY	-	expression tag	UNP P43431
A	224	GLY	-	expression tag	UNP P43431
A	225	SER	-	expression tag	UNP P43431
A	226	GLY	-	expression tag	UNP P43431
A	227	GLY	-	expression tag	UNP P43431
A	228	SER	-	expression tag	UNP P43431
A	229	GLY	-	expression tag	UNP P43431
A	230	LEU	-	expression tag	UNP P43431
A	231	ASN	-	expression tag	UNP P43431
A	232	ASP	-	expression tag	UNP P43431
A	233	ILE	-	expression tag	UNP P43431
A	234	PHE	-	expression tag	UNP P43431
A	235	GLU	-	expression tag	UNP P43431
A	236	ALA	-	expression tag	UNP P43431
A	237	GLN	-	expression tag	UNP P43431
A	238	LYS	-	expression tag	UNP P43431
A	239	ILE	-	expression tag	UNP P43431
A	240	GLU	-	expression tag	UNP P43431
A	241	TRP	-	expression tag	UNP P43431
A	242	HIS	-	expression tag	UNP P43431
A	243	GLU	-	expression tag	UNP P43431

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Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP P43431
A	245	ARG	-	expression tag	UNP P43431
A	246	THR	-	expression tag	UNP P43431
A	247	LYS	-	expression tag	UNP P43431
A	248	HIS	-	expression tag	UNP P43431
A	249	HIS	-	expression tag	UNP P43431
A	250	HIS	-	expression tag	UNP P43431
A	251	HIS	-	expression tag	UNP P43431
A	252	HIS	-	expression tag	UNP P43431
A	253	HIS	-	expression tag	UNP P43431

- Molecule 2 is a protein called Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	293	2336	1470	388	462	16	0	0

- Molecule 3 is a protein called Interleukin-12 receptor subunit beta-1,Death-associated protein kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	190	1542	962	282	283	15	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	562	GLY	-	linker	UNP Q60837
C	563	THR	-	linker	UNP Q60837
C	564	GLY	-	linker	UNP Q60837
C	565	GLY	-	linker	UNP Q60837
C	566	SER	-	linker	UNP Q60837
C	567	GLY	-	linker	UNP Q60837
C	568	GLY	-	linker	UNP Q60837
C	569	SER	-	linker	UNP Q60837
C	570	GLY	-	linker	UNP Q60837
C	571	GLY	-	linker	UNP Q60837

- Molecule 4 is a protein called Interleukin-12 receptor subunit beta-2,Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	189	1420	893	240	277	10	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	638	GLY	-	linker	UNP P97378
D	639	THR	-	linker	UNP P97378
D	640	GLY	-	linker	UNP P97378
D	641	GLY	-	linker	UNP P97378
D	642	SER	-	linker	UNP P97378
D	643	GLY	-	linker	UNP P97378
D	644	GLY	-	linker	UNP P97378
D	645	SER	-	linker	UNP P97378
D	646	GLY	-	linker	UNP P97378
D	647	GLY	-	linker	UNP P97378

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	4	50	28	2	20	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
6	C	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	D	1	14	8	1	5	0
6	D	1	14	8	1	5	0

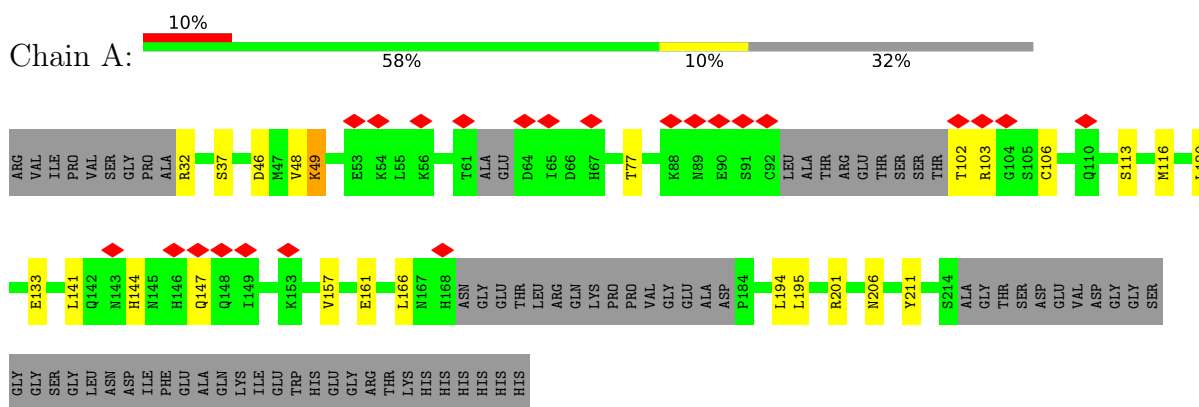
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
7	B	1	1	1	0

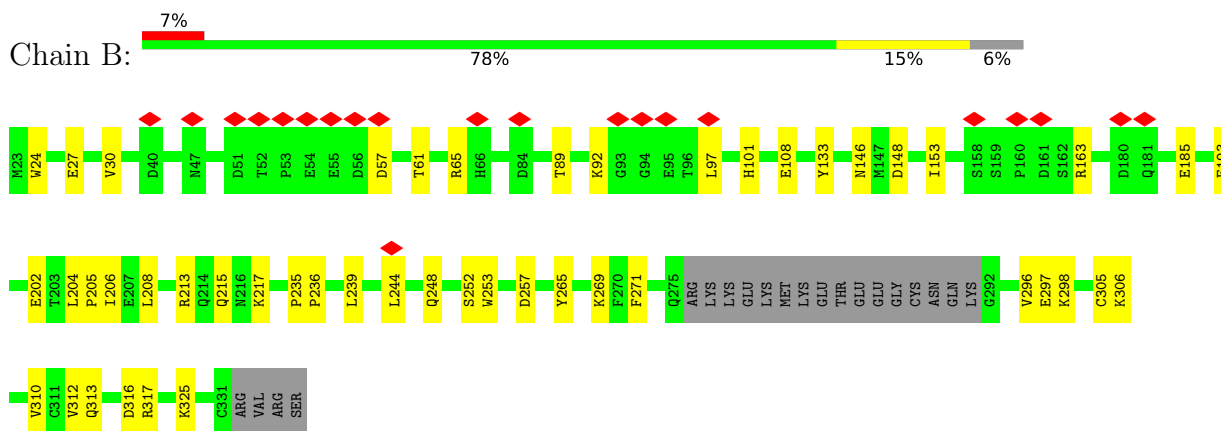
3 Residue-property plots

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.

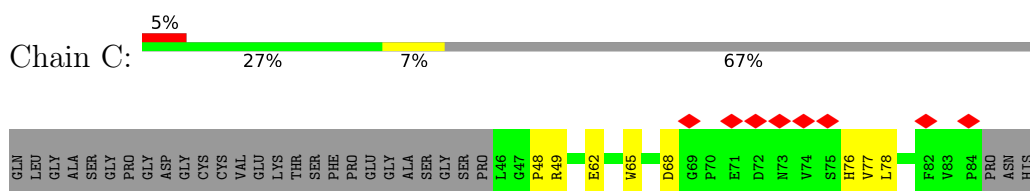
- Molecule 1: Interleukin-12 subunit alpha

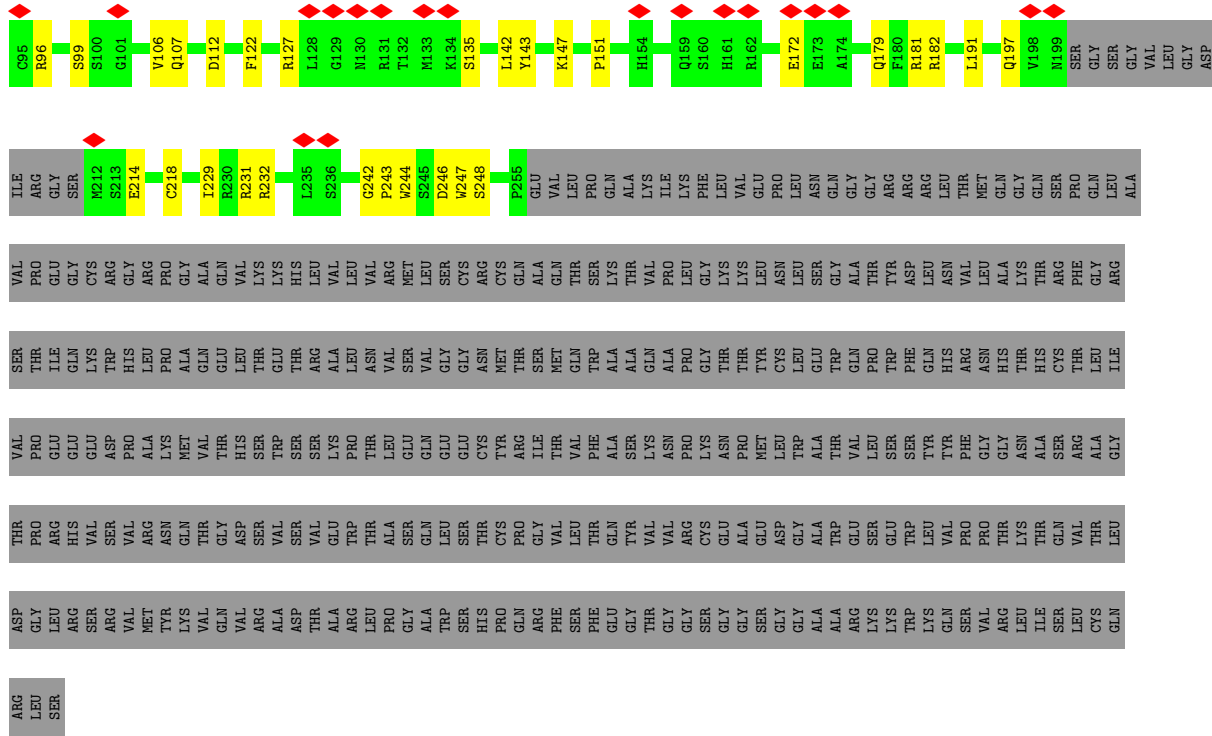


- Molecule 2: Interleukin-12 subunit beta

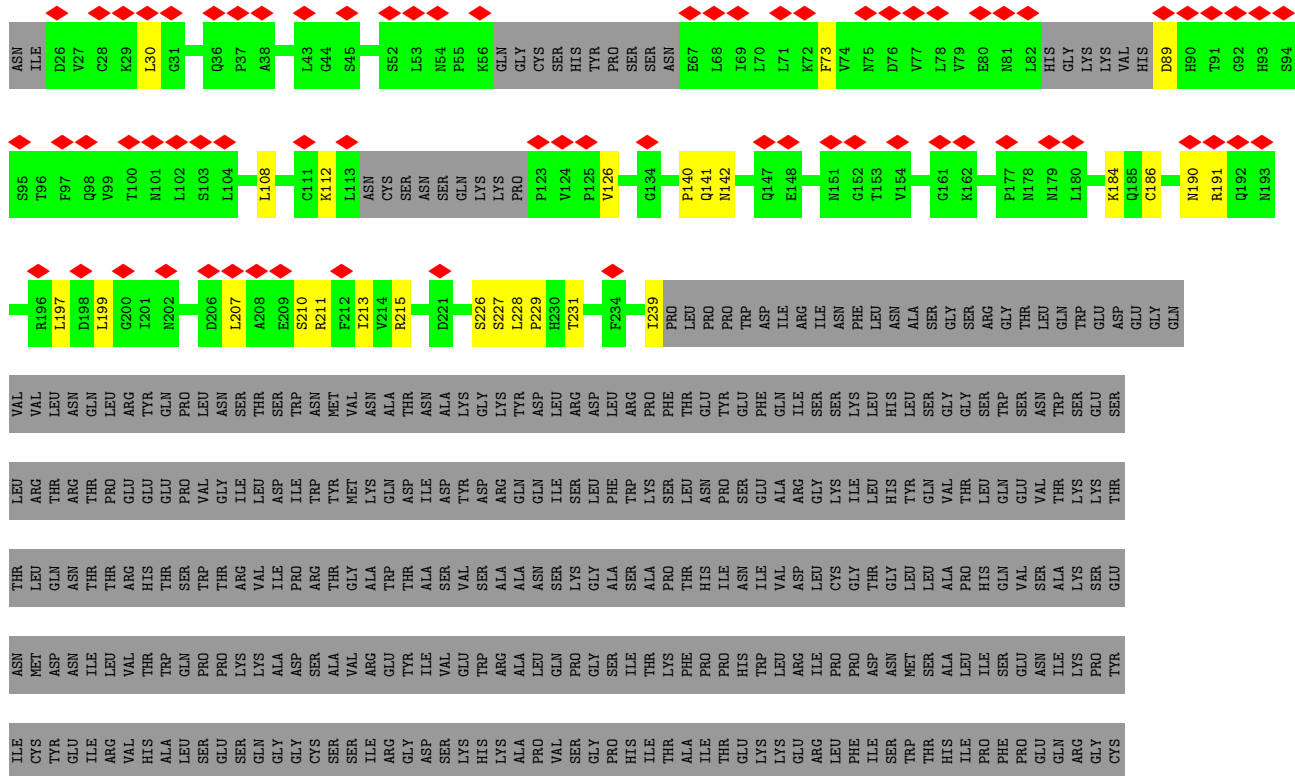


- Molecule 3: Interleukin-12 receptor subunit beta-1,Death-associated protein kinase 1





● Molecule 4: Interleukin-12 receptor subunit beta-2, Calmodulin-1



ILE
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- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  25% 75%


MAC1
MAC2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	268498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.462	Depositor
Minimum map value	-0.216	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	332.2, 332.2, 332.2	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75500005, 0.75500005, 0.75500005	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/1261	0.57	0/1694
2	B	0.30	0/2392	0.54	0/3246
3	C	0.28	0/1586	0.56	0/2152
4	D	0.30	0/1442	0.57	0/1965
All	All	0.29	0/6681	0.56	0/9057

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	1247	0	1260	14	0
2	B	2336	0	2230	31	0
3	C	1542	0	1463	24	0
4	D	1420	0	1417	16	0
5	E	50	0	43	1	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
7	B	1	0	0	0	0
All	All	6652	0	6465	81	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 6.

All (81) 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)
3:C:179:GLN:HE21	3:C:191:LEU:HD21	1.50	0.75
2:B:65:ARG:HG2	3:C:94:ARG:HH12	1.60	0.66
3:C:62:GLU:HG3	3:C:107:GLN:HG3	1.80	0.63
2:B:236:PRO:HG2	2:B:312:VAL:HG23	1.80	0.63
4:D:140:PRO:HD2	4:D:227:SER:HB3	1.81	0.63
2:B:146:ASN:ND2	2:B:185:GLU:OE1	2.34	0.61
2:B:253:TRP:CE3	2:B:312:VAL:HG11	2.36	0.61
4:D:30:LEU:HB3	4:D:126:VAL:HG23	1.81	0.61
1:A:141:LEU:HD23	1:A:144:HIS:HE2	1.66	0.60
3:C:182:ARG:NH1	3:C:218:CYS:SG	2.76	0.59
1:A:77:THR:OG1	1:A:201:ARG:NH1	2.37	0.58
1:A:147:GLN:HE22	4:D:190:ASN:HB2	1.68	0.58
2:B:204:LEU:HD12	2:B:205:PRO:HD2	1.86	0.57
2:B:163:ARG:NH2	2:B:202:GLU:OE2	2.37	0.56
4:D:226:SER:OG	4:D:227:SER:N	2.39	0.56
2:B:297:GLU:OE1	2:B:317:ARG:NH1	2.39	0.56
3:C:48:PRO:HG2	3:C:135:SER:HB3	1.87	0.55
2:B:153:ILE:HD11	2:B:208:LEU:HD13	1.90	0.54
2:B:61:THR:OG1	2:B:89:THR:OG1	2.26	0.54
1:A:102:THR:OG1	1:A:103:ARG:N	2.41	0.54
3:C:172:GLU:OE1	3:C:231:ARG:NH2	2.42	0.53
3:C:214:GLU:OE2	3:C:231:ARG:NH1	2.43	0.52
2:B:305:CYS:SG	2:B:306:LYS:N	2.82	0.52
3:C:151:PRO:HD2	3:C:248:SER:HB2	1.92	0.51
2:B:163:ARG:HH21	2:B:206:ILE:HG12	1.76	0.50
2:B:236:PRO:HG2	2:B:312:VAL:CG2	2.41	0.50
1:A:157:VAL:O	1:A:161:GLU:HG3	2.12	0.50
1:A:32:ARG:NH2	1:A:106:CYS:O	2.45	0.49
3:C:127:ARG:HA	3:C:127:ARG:NH1	2.27	0.49
4:D:210:SER:OG	4:D:211:ARG:N	2.45	0.49
2:B:148:ASP:HB3	2:B:215:GLN:HB2	1.95	0.49
3:C:96:ARG:NH1	3:C:112:ASP:O	2.44	0.49
3:C:122:PHE:HE2	3:C:142:LEU:HD21	1.77	0.49
3:C:197:GLN:HG3	3:C:214:GLU:HG2	1.95	0.48
3:C:232:ARG:NH2	3:C:242:GLY:O	2.46	0.48
1:A:46:ASP:O	1:A:49:LYS:HG3	2.14	0.48
3:C:77:VAL:HG12	3:C:99:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:GLU:OE2	3:C:143:TYR:OH	2.29	0.47
2:B:269:LYS:HG2	2:B:317:ARG:HA	1.96	0.47
2:B:271:PHE:HB2	2:B:313:GLN:HG2	1.96	0.47
3:C:65:TRP:HZ2	3:C:76:HIS:HB3	1.79	0.47
4:D:213:ILE:HG13	4:D:231:THR:HG22	1.96	0.47
1:A:113:SER:HB2	1:A:116:MET:HG2	1.96	0.46
1:A:48:VAL:HG23	1:A:195:LEU:HD13	1.98	0.46
3:C:49:ARG:NE	3:C:68:ASP:OD1	2.47	0.46
2:B:133:TYR:OH	2:B:316:ASP:OD2	2.32	0.46
3:C:151:PRO:HG2	3:C:229:ILE:HG23	1.97	0.45
2:B:213:ARG:HA	2:B:217:LYS:O	2.16	0.45
3:C:78:LEU:HD22	3:C:106:VAL:HG21	1.97	0.45
2:B:30:VAL:HG22	2:B:101:HIS:HB2	1.98	0.45
3:C:172:GLU:HB2	3:C:231:ARG:HH22	1.81	0.45
2:B:163:ARG:NH1	2:B:193:GLU:OE2	2.49	0.45
2:B:244:LEU:HD23	2:B:244:LEU:HA	1.79	0.45
4:D:112:LYS:HE2	4:D:112:LYS:HB2	1.78	0.44
4:D:186:CYS:HB2	4:D:197:LEU:HD12	1.99	0.44
2:B:296:VAL:HG12	2:B:298:LYS:H	1.82	0.43
2:B:257:ASP:N	2:B:257:ASP:OD1	2.52	0.43
3:C:246:ASP:N	3:C:246:ASP:OD1	2.49	0.43
4:D:215:ARG:HG2	4:D:229:PRO:HA	2.01	0.43
3:C:147:LYS:HB2	3:C:243:PRO:HG2	2.01	0.43
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.81	0.43
2:B:24:TRP:CG	5:E:2:NAG:H5	2.54	0.43
2:B:92:LYS:HE3	2:B:92:LYS:HB3	1.92	0.42
4:D:184:LYS:NZ	4:D:199:LEU:O	2.45	0.42
1:A:120:LEU:HD12	1:A:166:LEU:HD21	2.01	0.42
2:B:27:GLU:HG2	2:B:30:VAL:HB	2.01	0.42
2:B:235:PRO:HG3	2:B:325:LYS:O	2.20	0.42
4:D:141:GLN:OE1	4:D:142:ASN:N	2.51	0.42
4:D:89:ASP:OD1	4:D:89:ASP:N	2.52	0.42
4:D:207:LEU:HD11	4:D:210:SER:HB3	2.02	0.41
4:D:228:LEU:HD12	4:D:229:PRO:HD2	2.03	0.41
2:B:92:LYS:HE3	2:B:97:LEU:HD21	2.01	0.41
4:D:73:PHE:HB2	4:D:108:LEU:HB2	2.03	0.41
2:B:57:ASP:N	2:B:57:ASP:OD1	2.54	0.41
3:C:181:ARG:HG2	3:C:247:TRP:CZ3	2.56	0.41
1:A:37:SER:HB3	1:A:206:ASN:ND2	2.36	0.40
1:A:211:TYR:HB2	2:B:265:TYR:HB2	2.02	0.40
1:A:133:GLU:HG2	1:A:194:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:ARG:HD2	3:C:244:TRP:CE2	2.56	0.40
4:D:239:ILE:HD12	4:D:239:ILE:HA	1.93	0.40
2:B:239:LEU:HD12	2:B:252:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/231 (64%)	141 (95%)	8 (5%)	0	100	100
2	B	289/313 (92%)	280 (97%)	9 (3%)	0	100	100
3	C	184/572 (32%)	179 (97%)	5 (3%)	0	100	100
4	D	181/769 (24%)	173 (96%)	8 (4%)	0	100	100
All	All	803/1885 (43%)	773 (96%)	30 (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	146/205 (71%)	145 (99%)	1 (1%)	84	93
2	B	267/287 (93%)	265 (99%)	2 (1%)	84	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	174/492 (35%)	174 (100%)	0	100	100
4	D	170/675 (25%)	169 (99%)	1 (1%)	86	94
All	All	757/1659 (46%)	753 (100%)	4 (0%)	89	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
2	B	248	GLN
2	B	310	VAL
4	D	191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	179	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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1	5,2	14,14,15	0.22	0	17,19,21	0.73	1 (5%)
5	NAG	E	2	5	14,14,15	0.22	0	17,19,21	0.49	0
5	BMA	E	3	5	11,11,12	0.57	0	15,15,17	0.74	0
5	MAN	E	4	5	11,11,12	0.69	0	15,15,17	1.04	2 (13%)

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
5	NAG	E	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	4	MAN	C1-O5-C5	2.45	115.51	112.19
5	E	4	MAN	O2-C2-C3	-2.22	105.69	110.14
5	E	1	NAG	C2-N2-C7	2.04	125.81	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

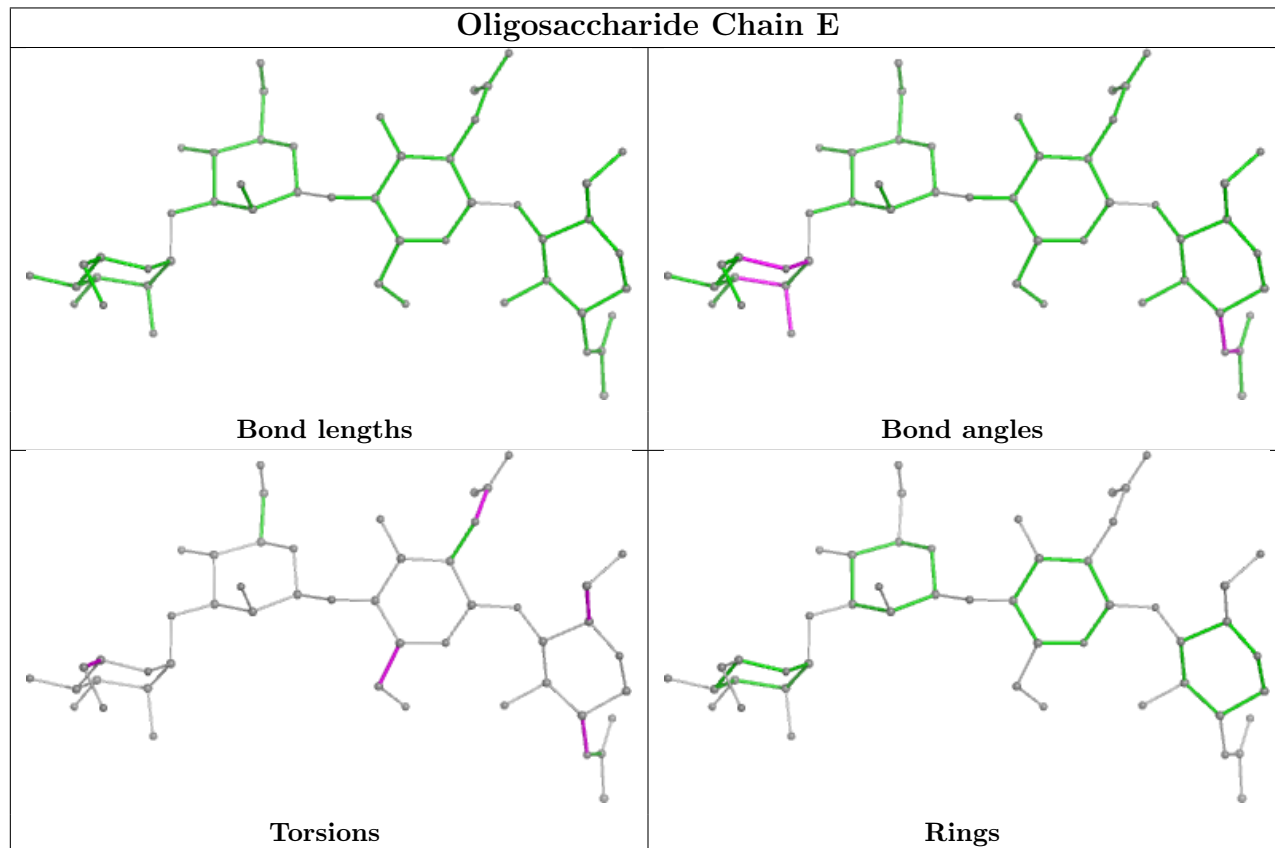
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
5	E	4	MAN	C4-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	601	3	14,14,15	0.59	0	17,19,21	1.74	2 (11%)
6	NAG	D	801	4	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	C	602	3	14,14,15	0.29	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	802	4	14,14,15	0.23	0	17,19,21	0.47	0

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
6	NAG	C	601	3	-	5/6/23/26	0/1/1/1
6	NAG	D	801	4	-	2/6/23/26	0/1/1/1
6	NAG	C	602	3	-	3/6/23/26	0/1/1/1
6	NAG	D	802	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C2-N2-C7	6.10	131.58	122.90
6	C	601	NAG	C1-C2-N2	2.74	115.17	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	602	NAG	C4-C5-C6-O6
6	D	802	NAG	O5-C5-C6-O6
6	D	801	NAG	O5-C5-C6-O6
6	C	601	NAG	O5-C5-C6-O6
6	C	602	NAG	O5-C5-C6-O6
6	D	802	NAG	C4-C5-C6-O6
6	C	601	NAG	C8-C7-N2-C2
6	C	601	NAG	O7-C7-N2-C2
6	D	801	NAG	C4-C5-C6-O6
6	C	601	NAG	C4-C5-C6-O6
6	C	601	NAG	C3-C2-N2-C7
6	C	602	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

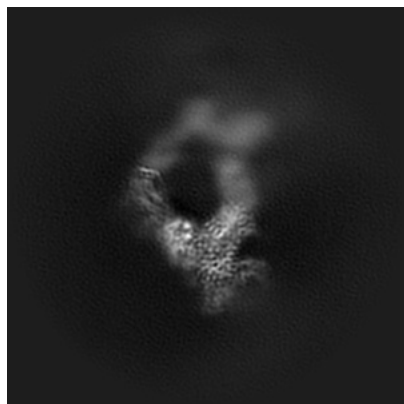
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17580. These allow visual inspection of the internal detail of the map and identification of artifacts.

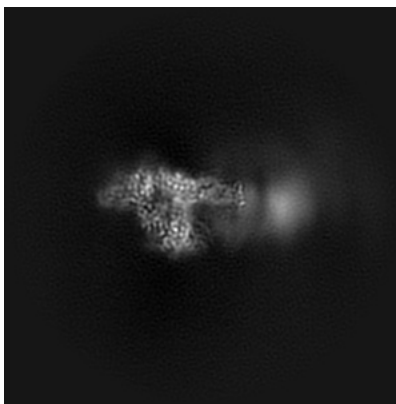
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

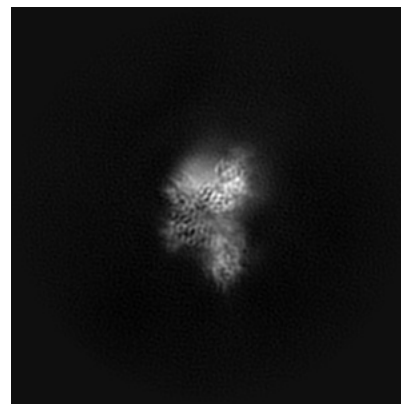
6.1.1 Primary map



X

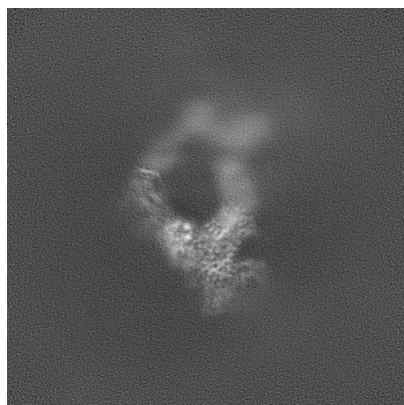


Y

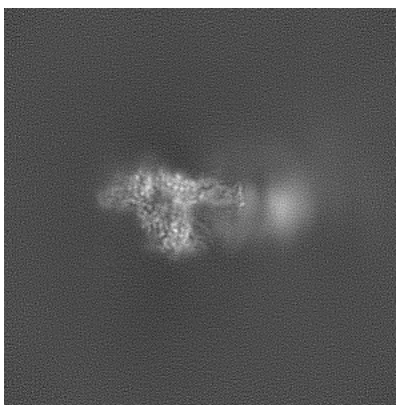


Z

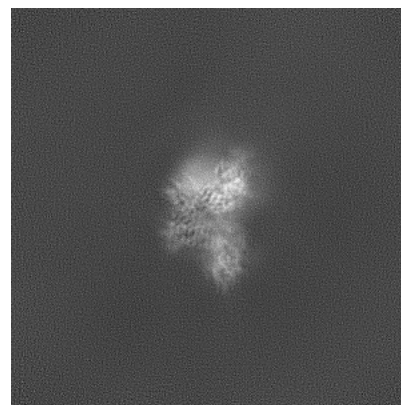
6.1.2 Raw map



X



Y

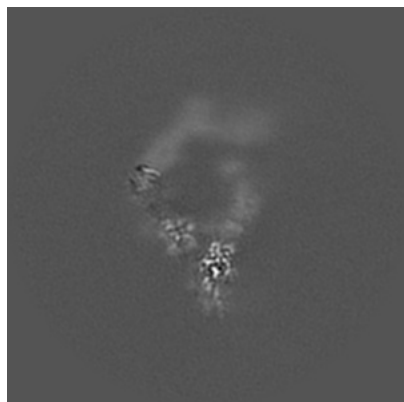


Z

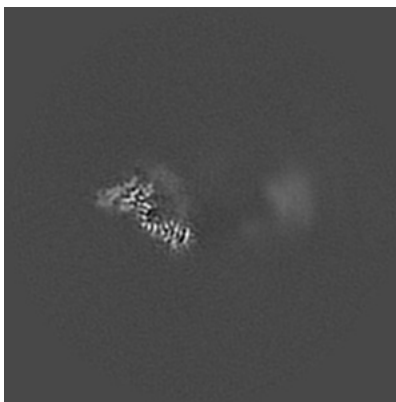
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

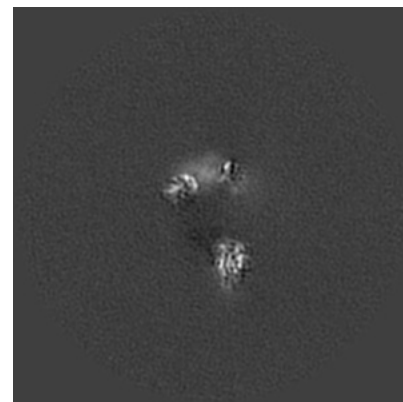
6.2.1 Primary map



X Index: 220

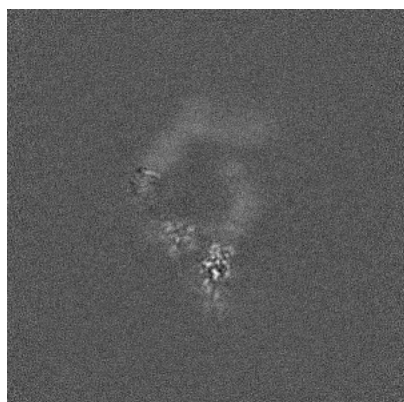


Y Index: 220

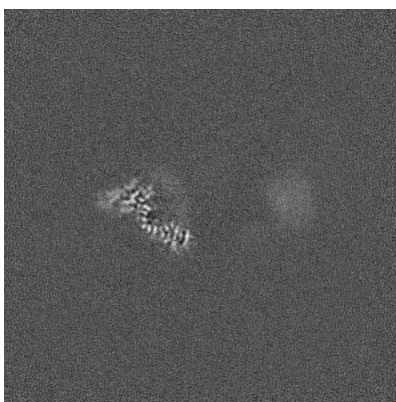


Z Index: 220

6.2.2 Raw map



X Index: 220



Y Index: 220

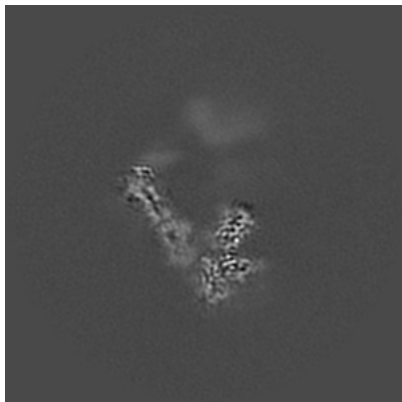


Z Index: 220

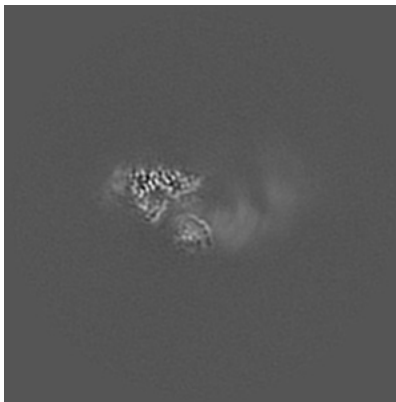
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

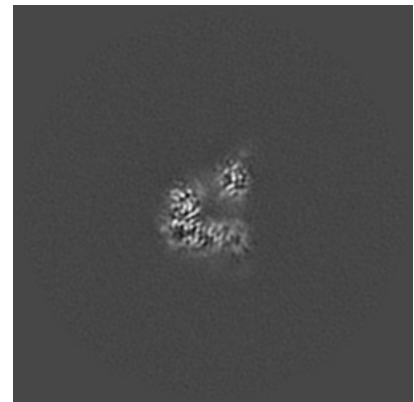
6.3.1 Primary map



X Index: 241

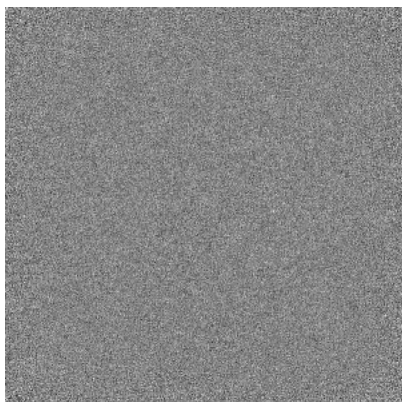


Y Index: 244

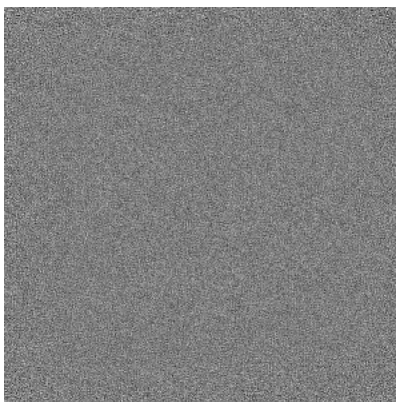


Z Index: 188

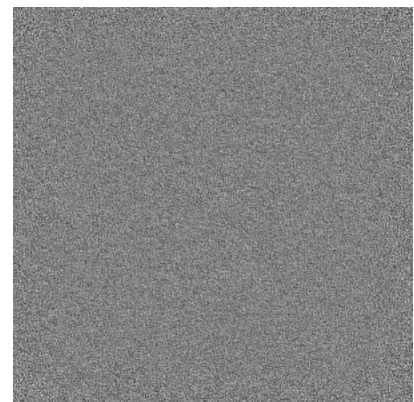
6.3.2 Raw map



X Index: 0



Y Index: 0

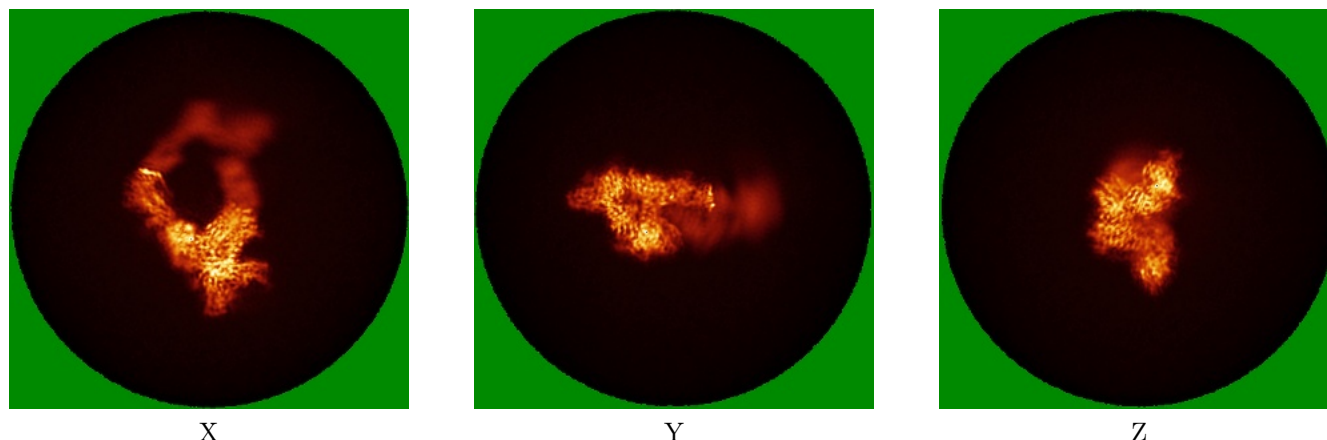


Z Index: 439

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

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

6.4.1 Primary map

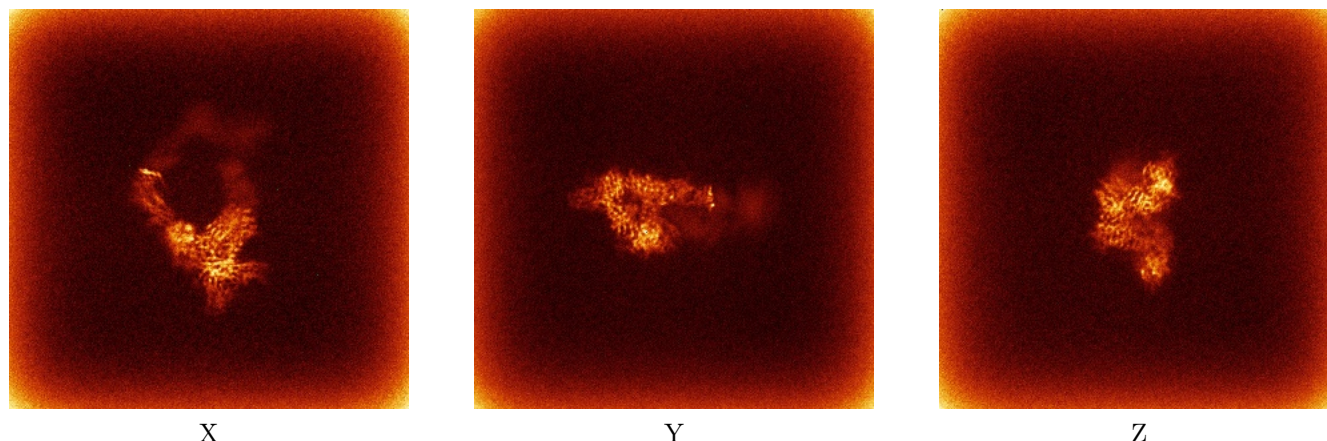


X

Y

Z

6.4.2 Raw map



X

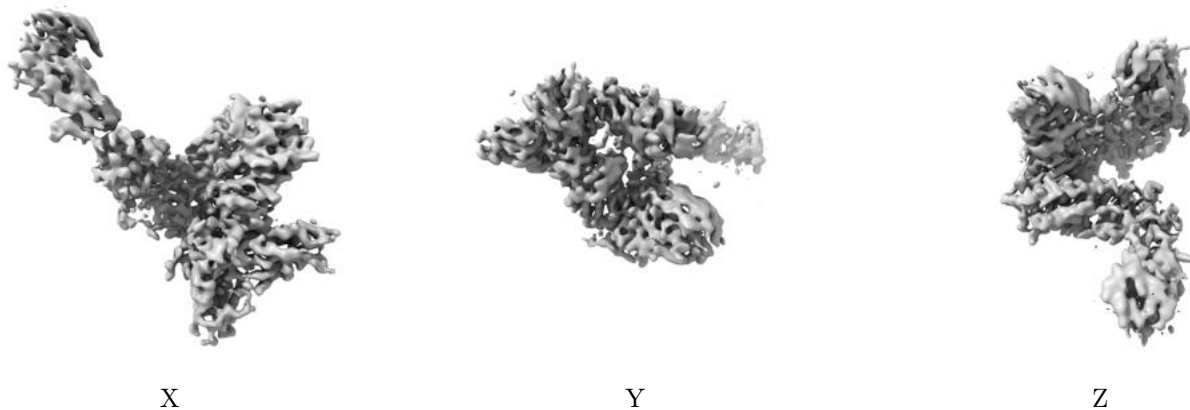
Y

Z

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

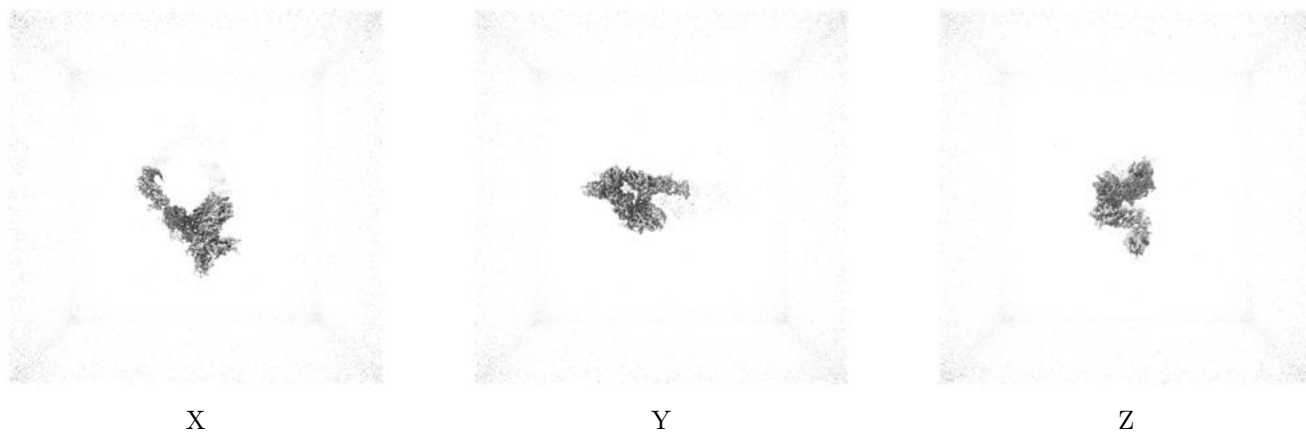
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

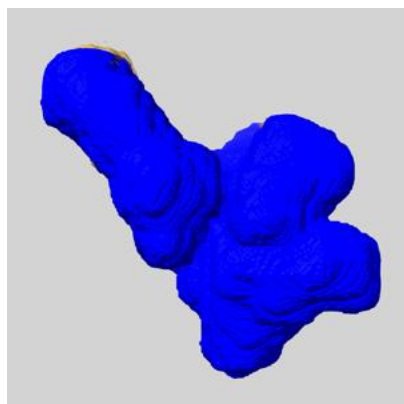
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

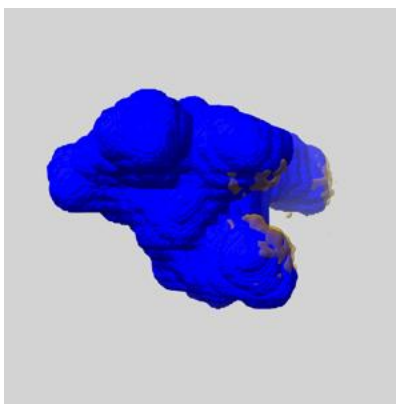
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

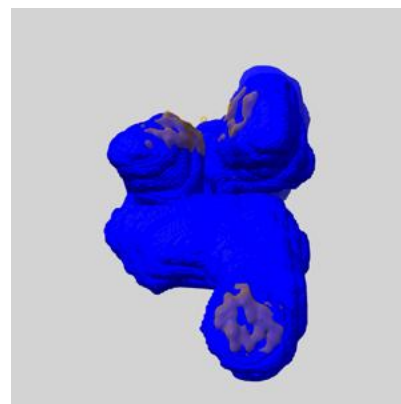
6.6.1 emd_17580_msk_1.map [i](#)



X

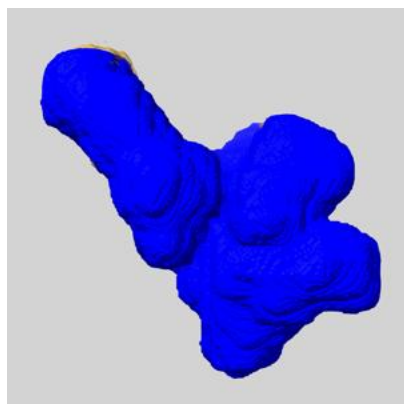


Y

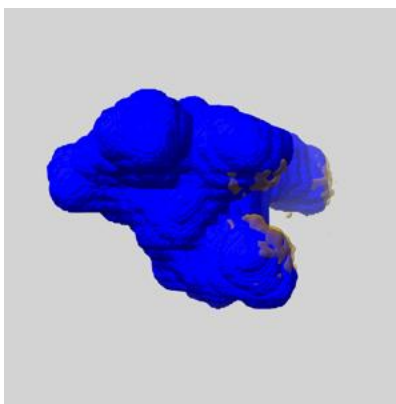


Z

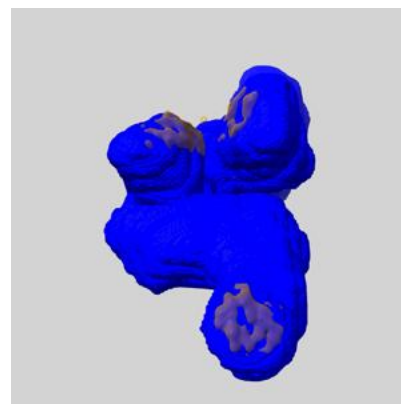
6.6.2 emd_17580_msk_2.map [i](#)



X



Y

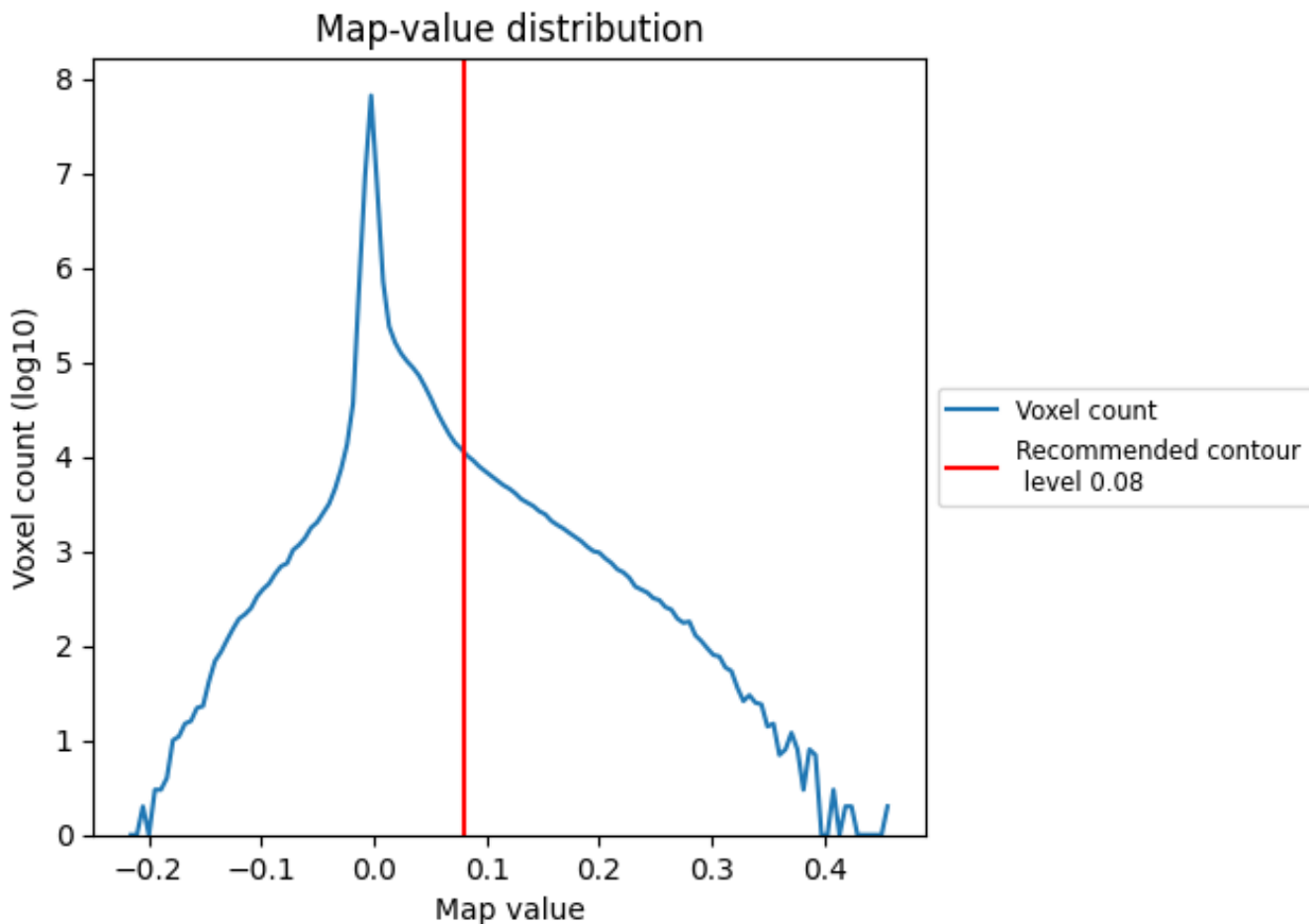


Z

7 Map analysis [i](#)

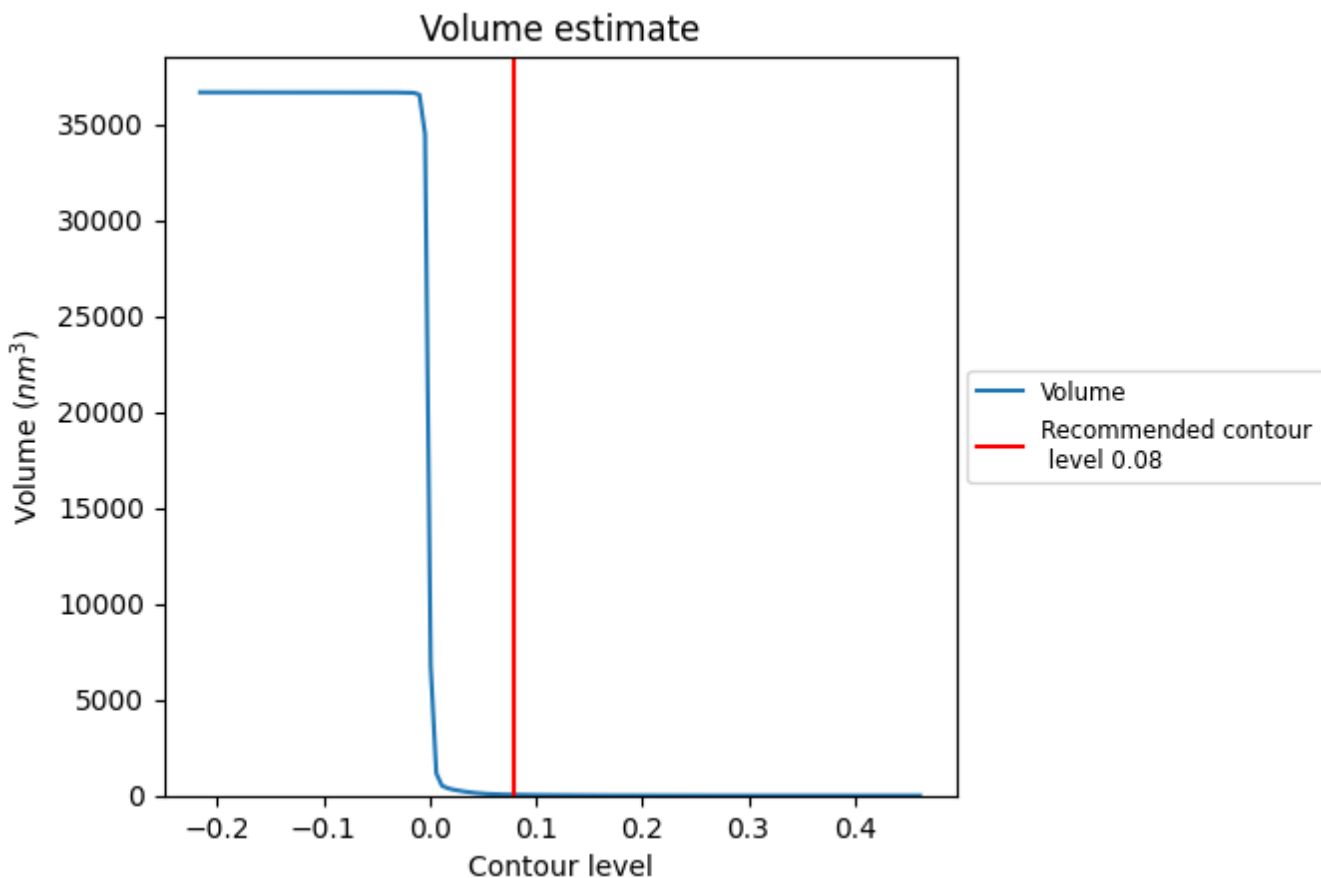
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

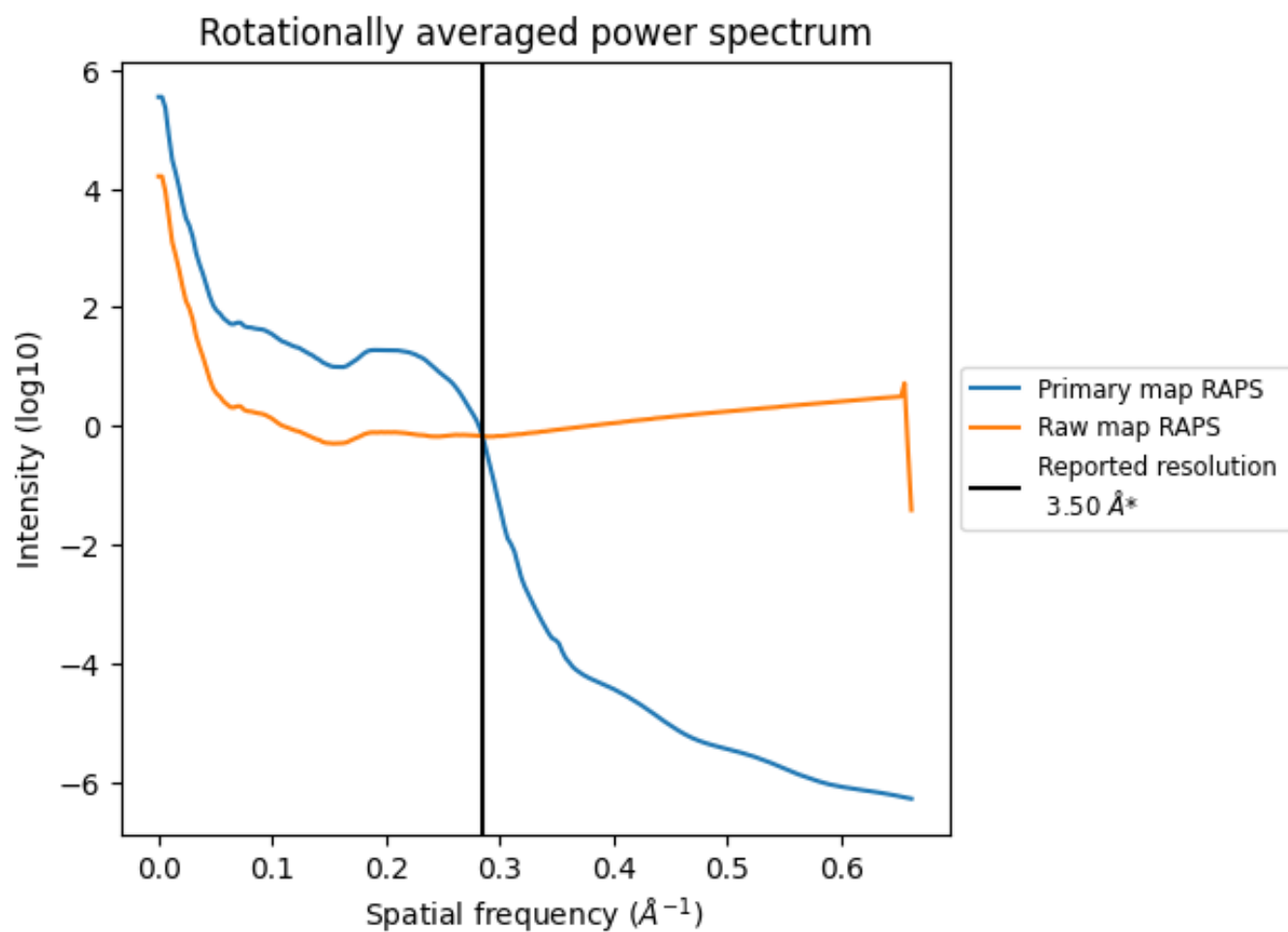
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm³; this corresponds to an approximate mass of 39 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)

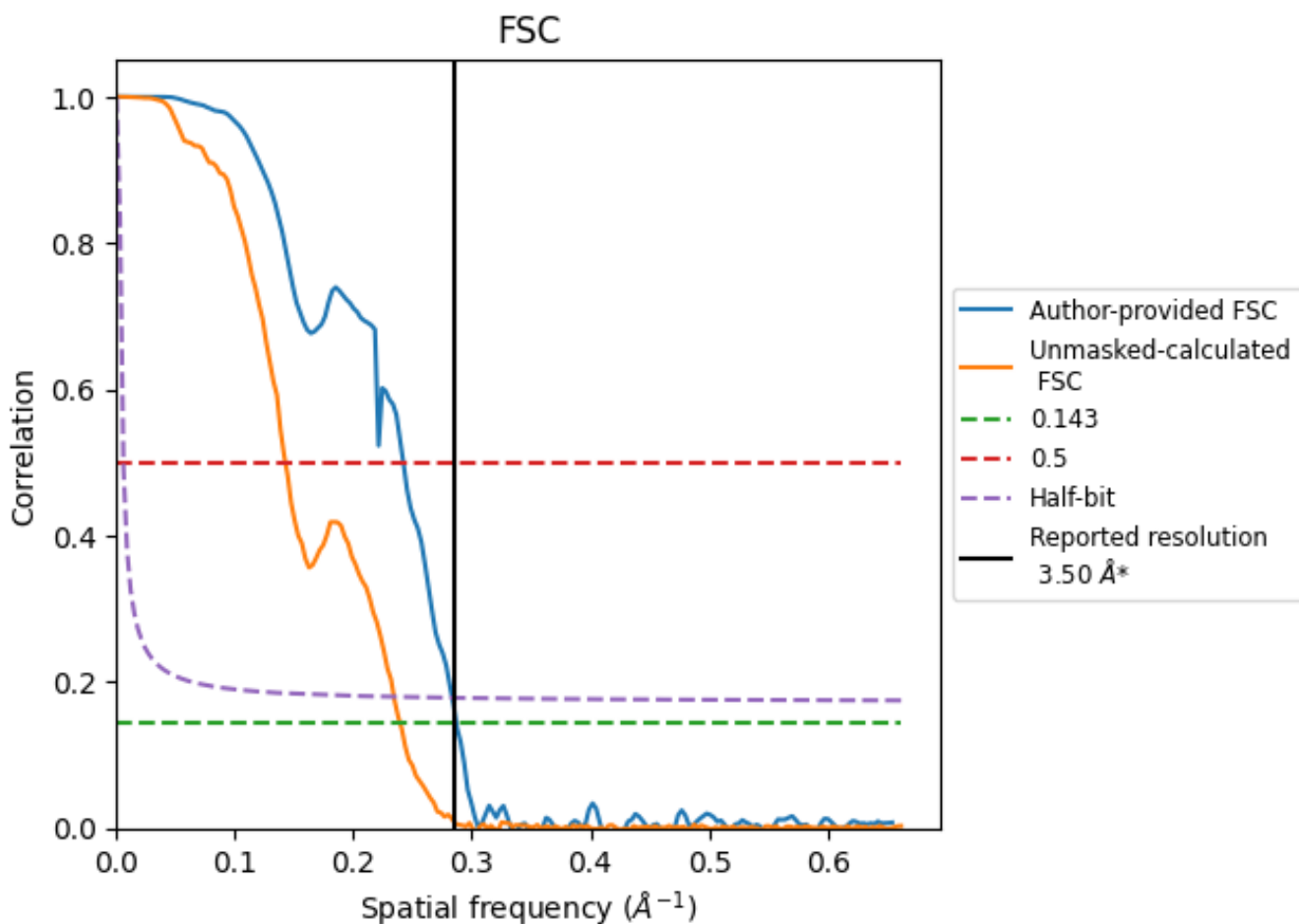


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

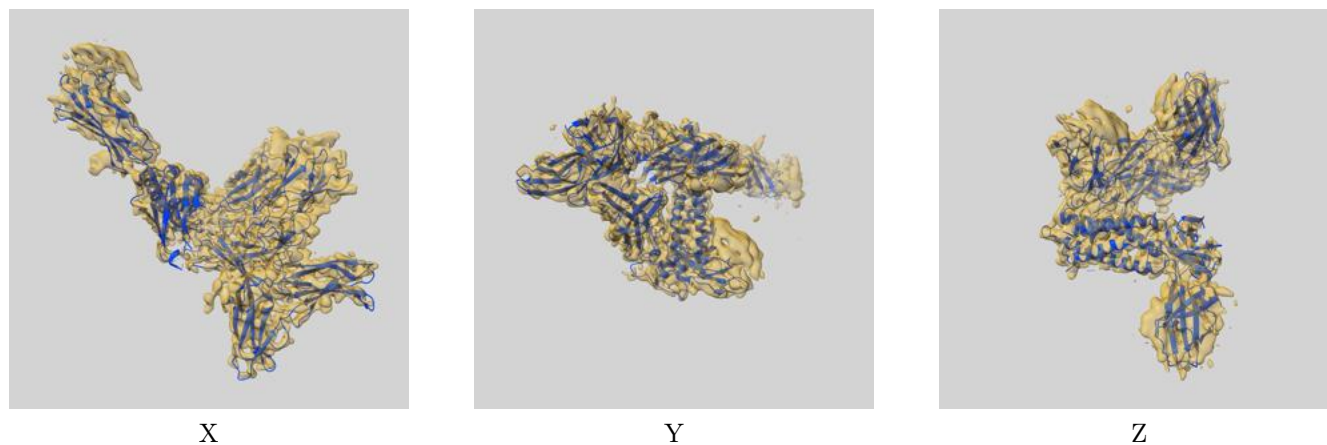
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.13	3.53
Unmasked-calculated*	4.18	7.01	4.27

*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 4.18 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

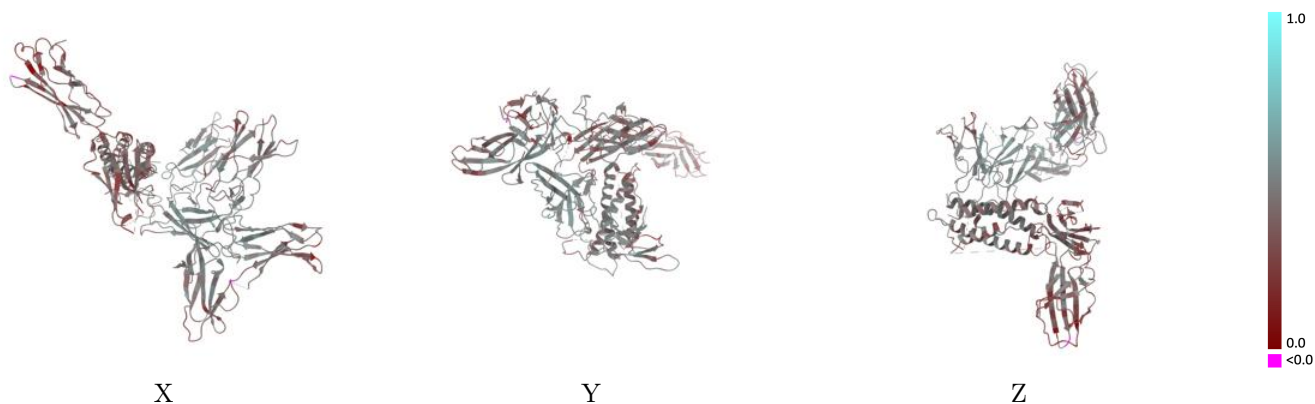
This section contains information regarding the fit between EMDB map EMD-17580 and PDB model 8PB1. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



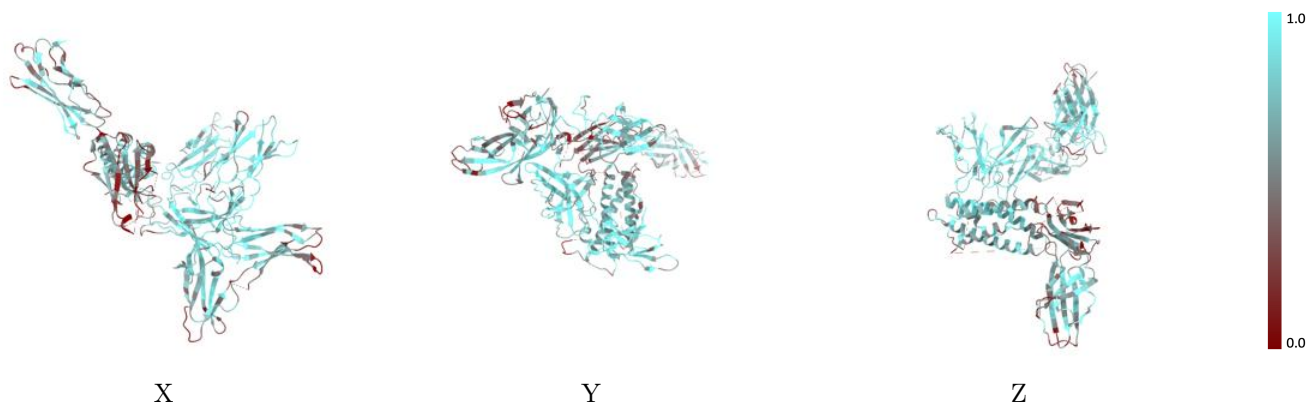
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



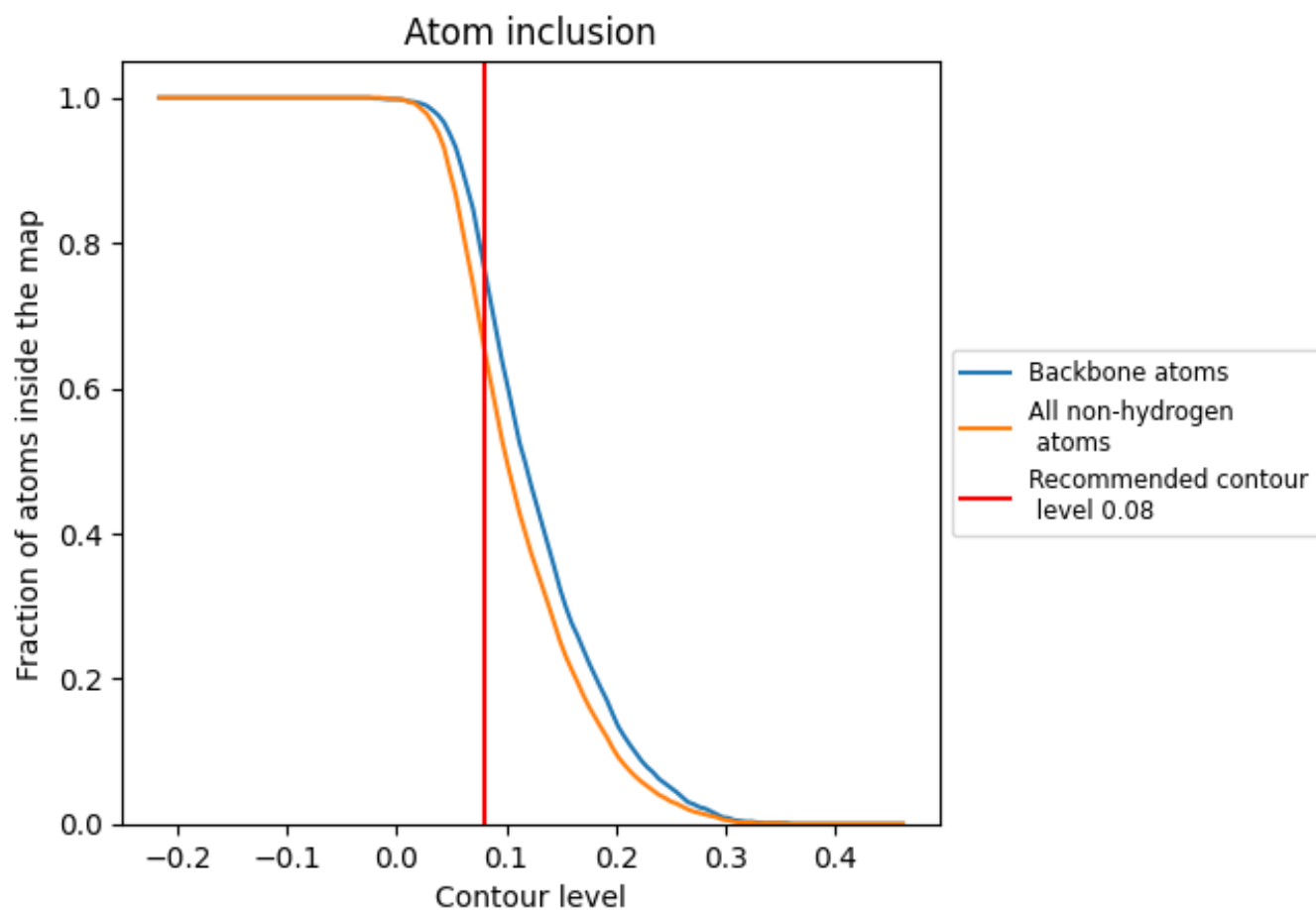
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).













9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.4240
A	 0.6520	 0.4200
B	 0.7590	 0.4740
C	 0.6920	 0.4350
D	 0.4740	 0.3330
E	 0.6200	 0.4440

