Full wwPDB EM Validation Report ⓘ

Dec 15, 2022 – 03:35 pm GMT

PDB ID	:	7P2Q
EMDB ID	:	EMD-13172
Title	:	Human Signal Peptidase Complex Paralog C (SPC-C)
Authors	:	Liaci, A.M.; Foerster, F.
Deposited on	:	2021-07-06
Resolution	:	4.90 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:

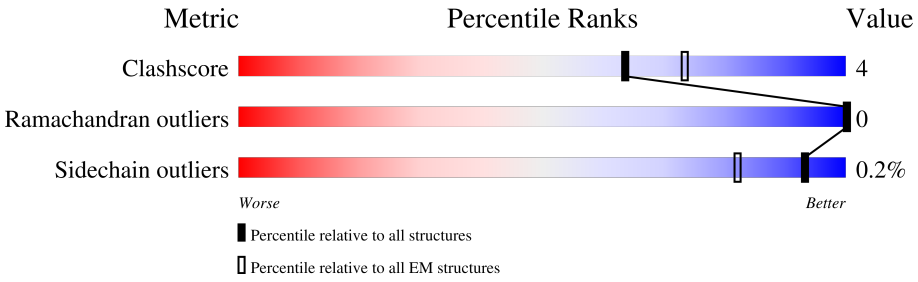
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	211	22% 63% 8% 30%
2	B	201	28% 78% 11% 11%
3	C	248	25% 62% 8% 30%
4	D	191	20% 42% · 55%
5	E	5	100% 20% 40% 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4780 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 Signal peptidase complex catalytic subunit SEC11C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	148	1186	764	204	212	6	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP Q9BY50
A	193	GLY	-	expression tag	UNP Q9BY50
A	194	GLY	-	expression tag	UNP Q9BY50
A	195	SER	-	expression tag	UNP Q9BY50
A	196	PRO	-	expression tag	UNP Q9BY50
A	197	GLY	-	expression tag	UNP Q9BY50
A	198	GLY	-	expression tag	UNP Q9BY50
A	199	SER	-	expression tag	UNP Q9BY50
A	200	GLY	-	expression tag	UNP Q9BY50
A	201	GLY	-	expression tag	UNP Q9BY50
A	202	GLY	-	expression tag	UNP Q9BY50
A	203	SER	-	expression tag	UNP Q9BY50
A	204	ALA	-	expression tag	UNP Q9BY50
A	205	GLU	-	expression tag	UNP Q9BY50
A	206	ASN	-	expression tag	UNP Q9BY50
A	207	LEU	-	expression tag	UNP Q9BY50
A	208	TYR	-	expression tag	UNP Q9BY50
A	209	PHE	-	expression tag	UNP Q9BY50
A	210	GLN	-	expression tag	UNP Q9BY50

- Molecule 2 is a protein called Signal peptidase complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	179	1426	924	237	261	4	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PRO	-	expression tag	UNP P61009
B	181	GLY	-	expression tag	UNP P61009
B	182	SER	-	expression tag	UNP P61009
B	183	GLY	-	expression tag	UNP P61009
B	184	GLU	-	expression tag	UNP P61009
B	185	GLY	-	expression tag	UNP P61009
B	186	ARG	-	expression tag	UNP P61009
B	187	GLY	-	expression tag	UNP P61009
B	188	SER	-	expression tag	UNP P61009
B	189	LEU	-	expression tag	UNP P61009
B	190	LEU	-	expression tag	UNP P61009
B	191	THR	-	expression tag	UNP P61009
B	192	CYS	-	expression tag	UNP P61009
B	193	GLY	-	expression tag	UNP P61009
B	194	ASP	-	expression tag	UNP P61009
B	195	VAL	-	expression tag	UNP P61009
B	196	GLU	-	expression tag	UNP P61009
B	197	GLU	-	expression tag	UNP P61009
B	198	ASN	-	expression tag	UNP P61009
B	199	PRO	-	expression tag	UNP P61009
B	200	GLY	-	expression tag	UNP P61009

- Molecule 3 is a protein called Signal peptidase complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	174	Total	C	N	O	S	0	0
			1411	917	227	259	8		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	227	GLY	-	expression tag	UNP Q15005
C	228	SER	-	expression tag	UNP Q15005
C	229	GLY	-	expression tag	UNP Q15005
C	230	GLN	-	expression tag	UNP Q15005
C	231	CYS	-	expression tag	UNP Q15005
C	232	THR	-	expression tag	UNP Q15005
C	233	ASN	-	expression tag	UNP Q15005
C	234	TYR	-	expression tag	UNP Q15005
C	235	ALA	-	expression tag	UNP Q15005
C	236	LEU	-	expression tag	UNP Q15005
C	237	LEU	-	expression tag	UNP Q15005
C	238	LYS	-	expression tag	UNP Q15005

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Chain	Residue	Modelled	Actual	Comment	Reference
C	239	LEU	-	expression tag	UNP Q15005
C	240	ALA	-	expression tag	UNP Q15005
C	241	GLY	-	expression tag	UNP Q15005
C	242	ASP	-	expression tag	UNP Q15005
C	243	VAL	-	expression tag	UNP Q15005
C	244	GLU	-	expression tag	UNP Q15005
C	245	SER	-	expression tag	UNP Q15005
C	246	ASN	-	expression tag	UNP Q15005
C	247	PRO	-	expression tag	UNP Q15005
C	248	GLY	-	expression tag	UNP Q15005

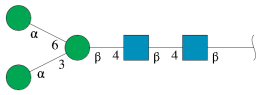
- Molecule 4 is a protein called Signal peptidase complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	86	Total	C	N	O	S	0	0
			696	467	108	116	5		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP Q9Y6A9
D	170	GLY	-	expression tag	UNP Q9Y6A9
D	171	SER	-	expression tag	UNP Q9Y6A9
D	172	GLY	-	expression tag	UNP Q9Y6A9
D	173	ALA	-	expression tag	UNP Q9Y6A9
D	174	THR	-	expression tag	UNP Q9Y6A9
D	175	ASN	-	expression tag	UNP Q9Y6A9
D	176	PHE	-	expression tag	UNP Q9Y6A9
D	177	SER	-	expression tag	UNP Q9Y6A9
D	178	LEU	-	expression tag	UNP Q9Y6A9
D	179	LEU	-	expression tag	UNP Q9Y6A9
D	180	LYS	-	expression tag	UNP Q9Y6A9
D	181	GLN	-	expression tag	UNP Q9Y6A9
D	182	ALA	-	expression tag	UNP Q9Y6A9
D	183	GLY	-	expression tag	UNP Q9Y6A9
D	184	ASP	-	expression tag	UNP Q9Y6A9
D	185	VAL	-	expression tag	UNP Q9Y6A9
D	186	GLU	-	expression tag	UNP Q9Y6A9
D	187	GLU	-	expression tag	UNP Q9Y6A9
D	188	ASN	-	expression tag	UNP Q9Y6A9
D	189	PRO	-	expression tag	UNP Q9Y6A9
D	190	GLY	-	expression tag	UNP Q9Y6A9

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

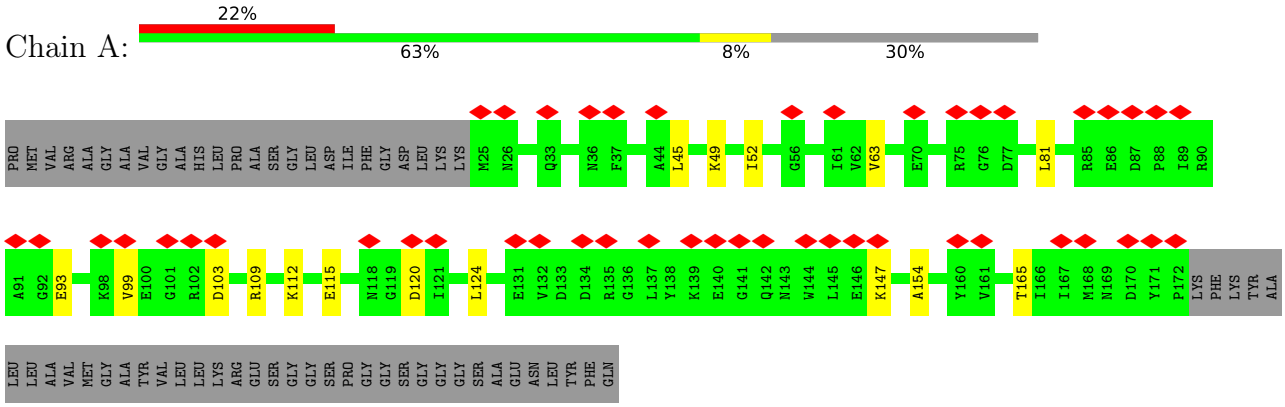


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	5	61	34	2	25	0	0

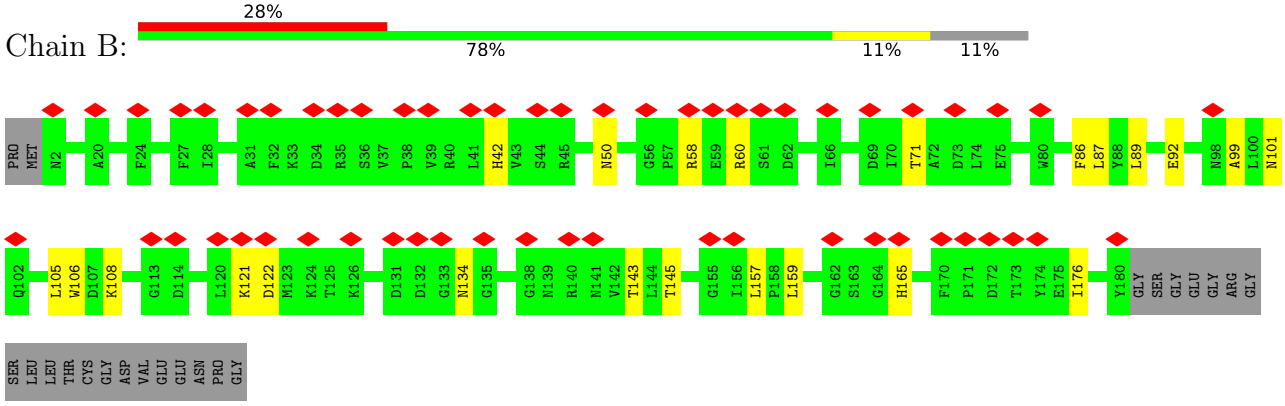
3 Residue-property plots (i)

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

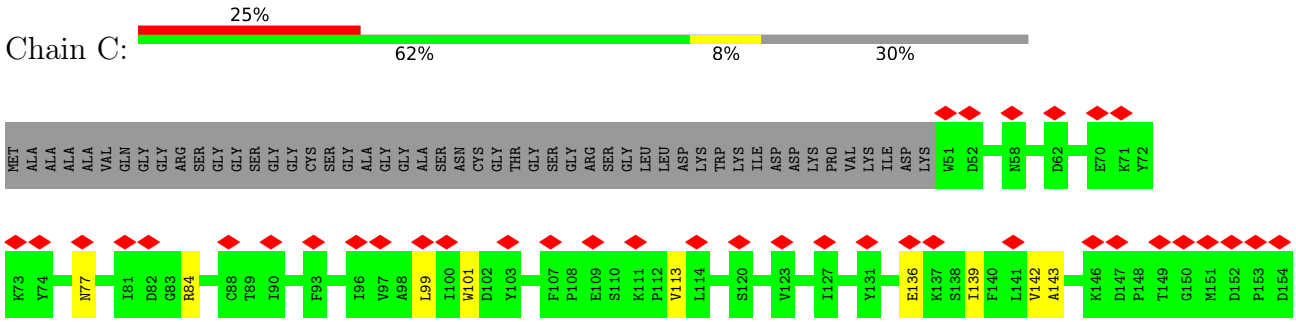
• Molecule 1: Signal peptidase complex catalytic subunit SEC11C

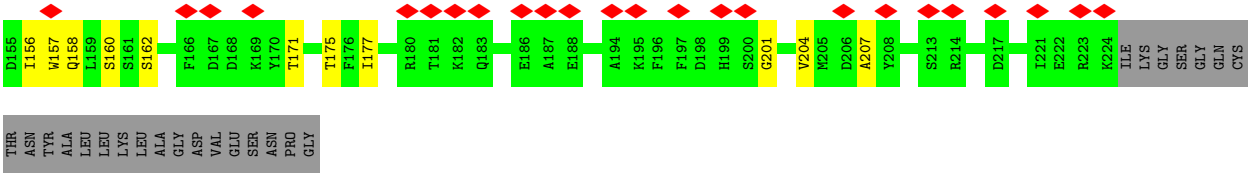


• Molecule 2: Signal peptidase complex subunit 3

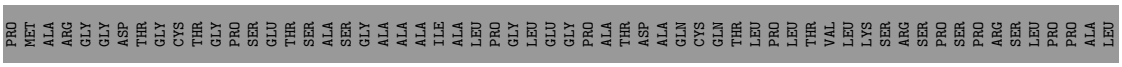


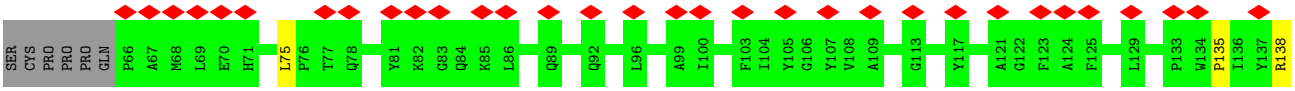
• Molecule 3: Signal peptidase complex subunit 2

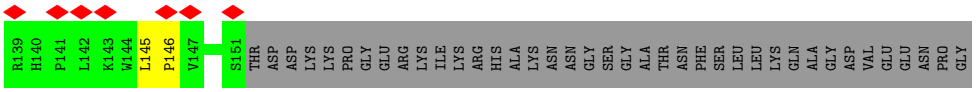




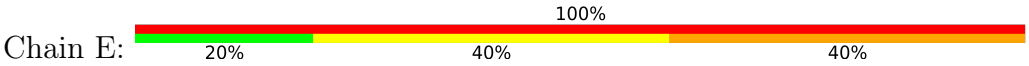
• Molecule 4: Signal peptidase complex subunit 1

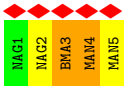






• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60598	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	61, 61	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	162.0, 162.0, 162.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/1210	0.51	0/1633
2	B	0.27	0/1459	0.53	0/1982
3	C	0.27	0/1445	0.48	0/1950
4	D	0.26	0/721	0.45	0/981
All	All	0.27	0/4835	0.50	0/6546

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1186	0	1207	15	0
2	B	1426	0	1431	19	0
3	C	1411	0	1418	11	0
4	D	696	0	694	3	0
5	E	61	0	52	1	0
All	All	4780	0	4802	41	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 (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:LEU:O	2:B:157:LEU:HD12	1.57	1.05
1:A:109:ARG:NH1	2:B:86:PHE:CE1	2.26	1.03
1:A:109:ARG:HH12	2:B:86:PHE:HE1	1.36	0.71
3:C:162:SER:HB3	3:C:171:THR:HB	1.81	0.61
3:C:201:GLY:HA2	4:D:75:LEU:HB3	1.83	0.61
3:C:156:ILE:HB	3:C:177:ILE:HB	1.84	0.60
1:A:112:LYS:HB2	1:A:124:LEU:HB2	1.86	0.58
3:C:84:ARG:NH1	3:C:136:GLU:OE2	2.35	0.58
2:B:92:GLU:HB3	2:B:143:THR:HB	1.86	0.56
2:B:157:LEU:O	2:B:157:LEU:CD1	2.46	0.56
3:C:77:ASN:HD22	3:C:142:VAL:HG12	1.69	0.55
1:A:120:ASP:OD1	1:A:147:LYS:NZ	2.40	0.55
1:A:115:GLU:HB3	2:B:99:ALA:HA	1.88	0.54
1:A:63:VAL:HG21	1:A:165:THR:HG21	1.90	0.54
2:B:87:LEU:HB2	2:B:108:LYS:HB3	1.89	0.53
2:B:89:LEU:HD23	2:B:105:LEU:HD12	1.90	0.53
2:B:50:ASN:H	2:B:176:ILE:HG22	1.73	0.53
3:C:139:ILE:HD13	3:C:160:SER:HB3	1.90	0.52
2:B:121:LYS:O	2:B:122:ASP:OD1	2.29	0.51
1:A:99:VAL:O	1:A:103:ASP:N	2.44	0.50
1:A:45:LEU:HD13	3:C:99:LEU:HD11	1.93	0.50
2:B:42:HIS:HB2	2:B:71:THR:HB	1.94	0.49
2:B:60:ARG:O	2:B:134:ASN:ND2	2.45	0.49
2:B:145:THR:OG1	2:B:165:HIS:ND1	2.44	0.49
1:A:49:LYS:HA	1:A:52:ILE:HG12	1.95	0.48
1:A:109:ARG:NH1	2:B:86:PHE:CD1	2.81	0.48
3:C:158:GLN:HB3	3:C:175:THR:HB	1.96	0.47
1:A:93:GLU:OE2	2:B:159:LEU:HD23	2.14	0.47
2:B:121:LYS:C	2:B:122:ASP:OD1	2.52	0.47
3:C:143:ALA:HB3	3:C:157:TRP:HE3	1.80	0.46
2:B:106:TRP:HZ3	2:B:108:LYS:HB2	1.81	0.46
1:A:99:VAL:O	1:A:103:ASP:HA	2.17	0.45
1:A:81:LEU:HD12	1:A:154:ALA:HA	1.99	0.44
2:B:157:LEU:HD12	2:B:157:LEU:C	2.34	0.43
1:A:99:VAL:O	1:A:103:ASP:CA	2.67	0.42
1:A:115:GLU:HB2	2:B:101:ASN:HD21	1.85	0.41
5:E:3:BMA:H3	5:E:4:MAN:H2	1.85	0.41
4:D:135:PRO:HA	4:D:138:ARG:HG2	2.03	0.41
4:D:145:LEU:HA	4:D:146:PRO:HD3	1.96	0.40
3:C:101:TRP:CH2	3:C:113:VAL:HB	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:VAL:HG12	3:C:207:ALA:H	1.87	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	146/211 (69%)	142 (97%)	4 (3%)	0	100	100
2	B	177/201 (88%)	167 (94%)	10 (6%)	0	100	100
3	C	172/248 (69%)	158 (92%)	14 (8%)	0	100	100
4	D	84/191 (44%)	83 (99%)	1 (1%)	0	100	100
All	All	579/851 (68%)	550 (95%)	29 (5%)	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	130/173 (75%)	130 (100%)	0	100	100
2	B	160/176 (91%)	159 (99%)	1 (1%)	86	92
3	C	157/206 (76%)	157 (100%)	0	100	100
4	D	74/155 (48%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	521/710 (73%)	520 (100%)	1 (0%)	93 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	58	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	84	GLN
3	C	77	ASN
3	C	144	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 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	2,5	14,14,15	0.28	0	17,19,21	0.58	0
5	NAG	E	2	5	14,14,15	0.49	0	17,19,21	1.03	1 (5%)
5	BMA	E	3	5	11,11,12	0.99	1 (9%)	15,15,17	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	E	4	5	11,11,12	0.89	1 (9%)	15,15,17	1.05	2 (13%)
5	MAN	E	5	5	11,11,12	0.84	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	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3	BMA	C1-C2	2.17	1.57	1.52
5	E	4	MAN	C1-C2	2.00	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C2-N2-C7	3.00	127.18	122.90
5	E	5	MAN	C1-O5-C5	2.55	115.64	112.19
5	E	4	MAN	C1-O5-C5	2.53	115.62	112.19
5	E	5	MAN	O2-C2-C3	-2.18	105.78	110.14
5	E	4	MAN	O2-C2-C3	-2.17	105.79	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

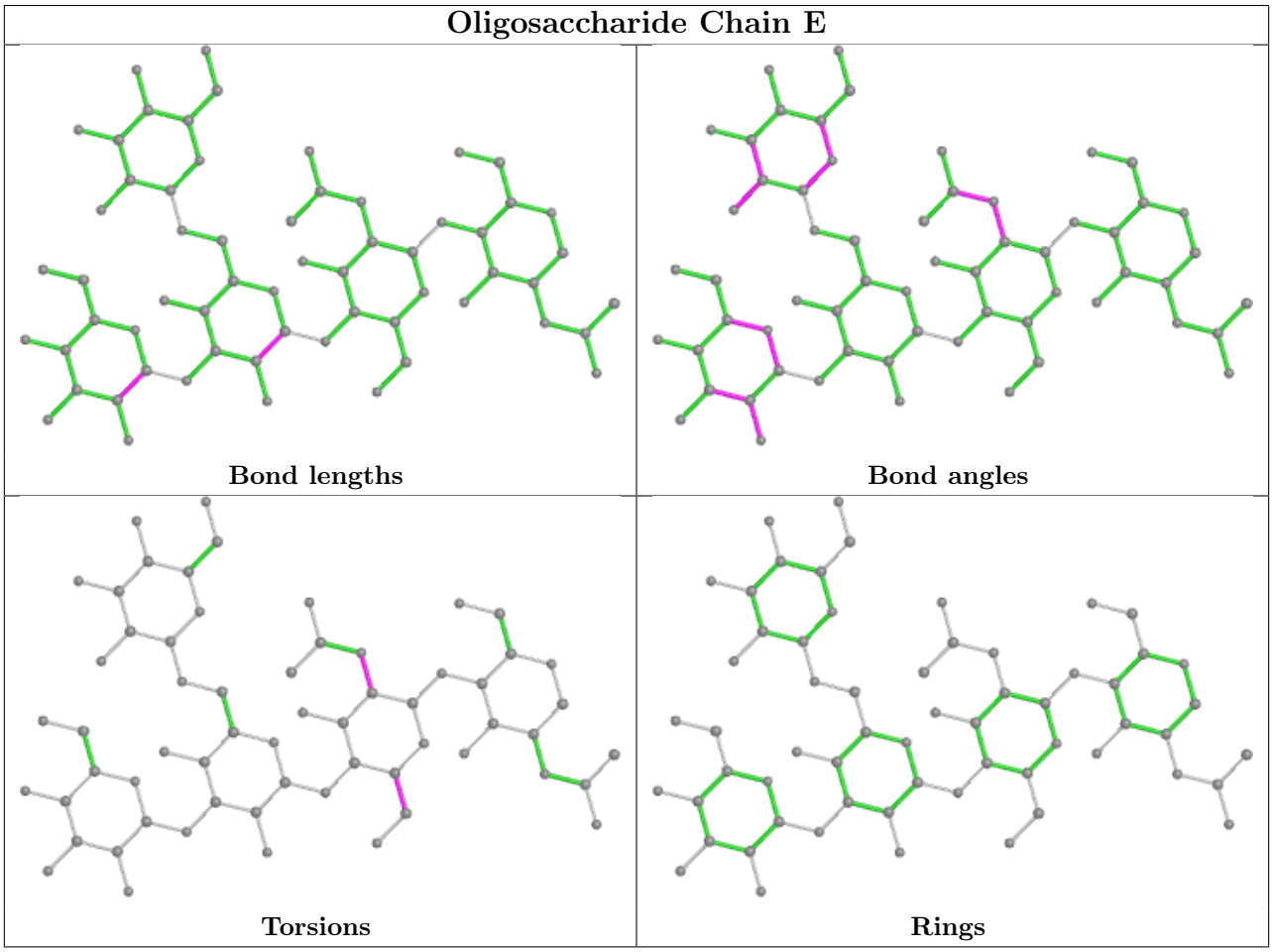
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	4	MAN	1	0
5	E	3	BMA	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

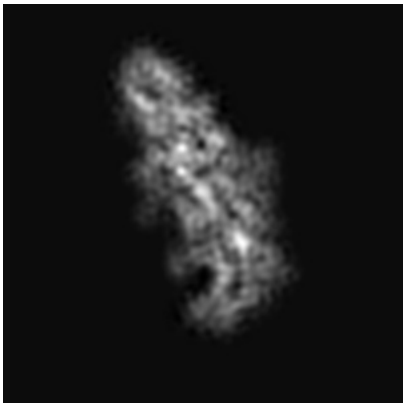
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13172. These allow visual inspection of the internal detail of the map and identification of artifacts.

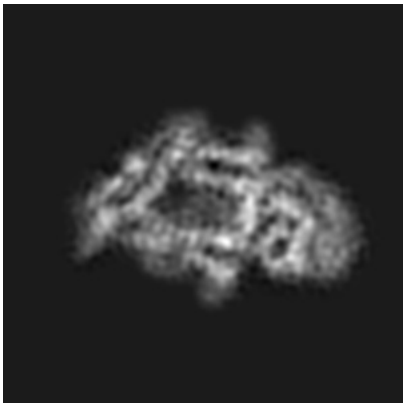
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

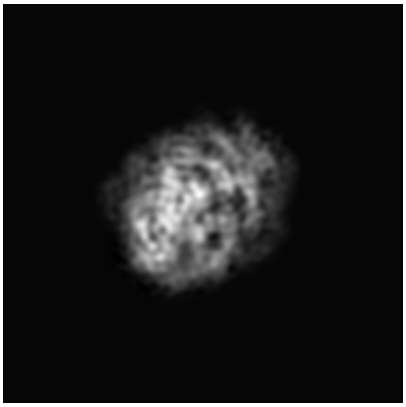
6.1.1 Primary map



X



Y

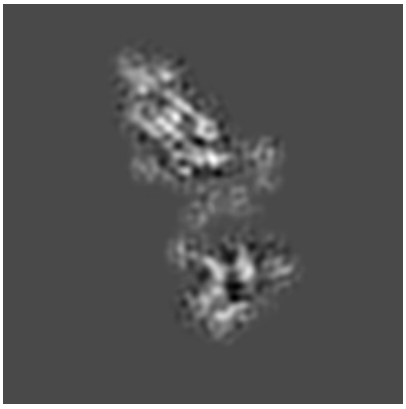


Z

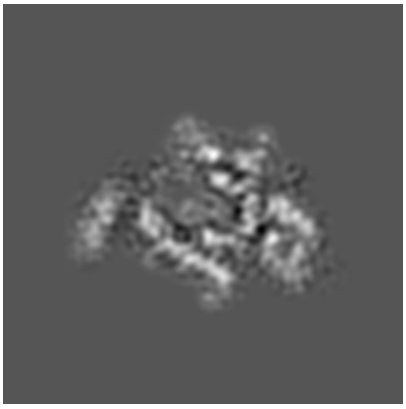
The images above show the map projected in three orthogonal directions.

6.2 Central slices

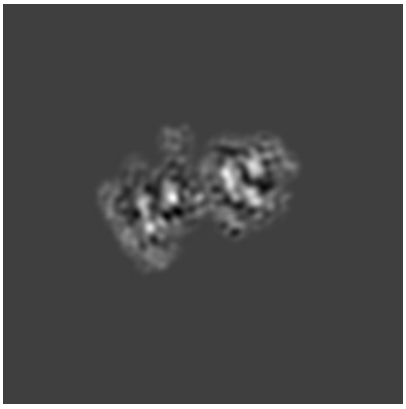
6.2.1 Primary map



X Index: 100



Y Index: 100



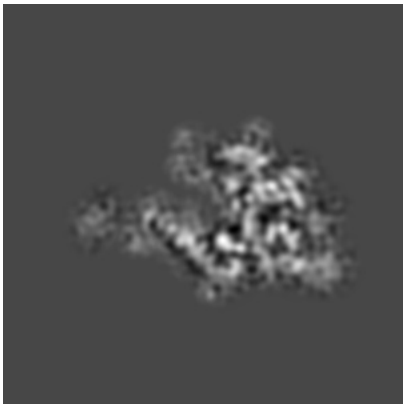
Z Index: 100

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

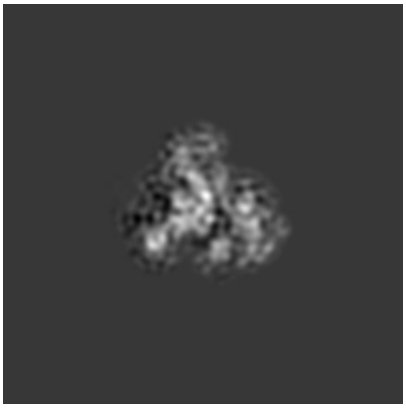
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 83



Y Index: 91



Z Index: 123

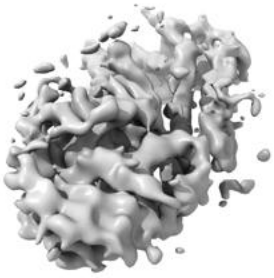
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

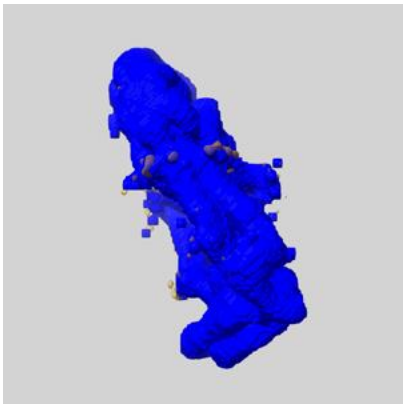
6.5 Mask visualisation (i)

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

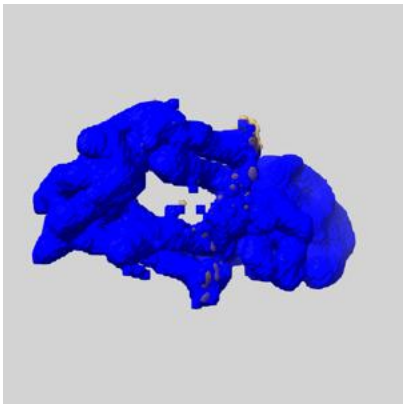
A mask typically either:

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

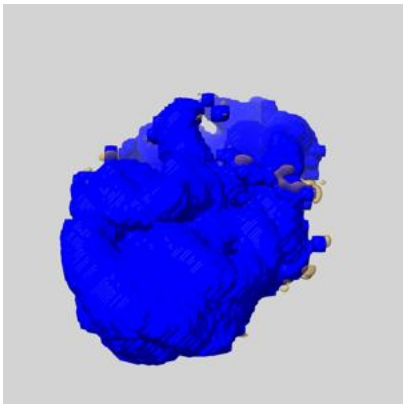
6.5.1 emd_13172_msk_1.map (i)



X



Y

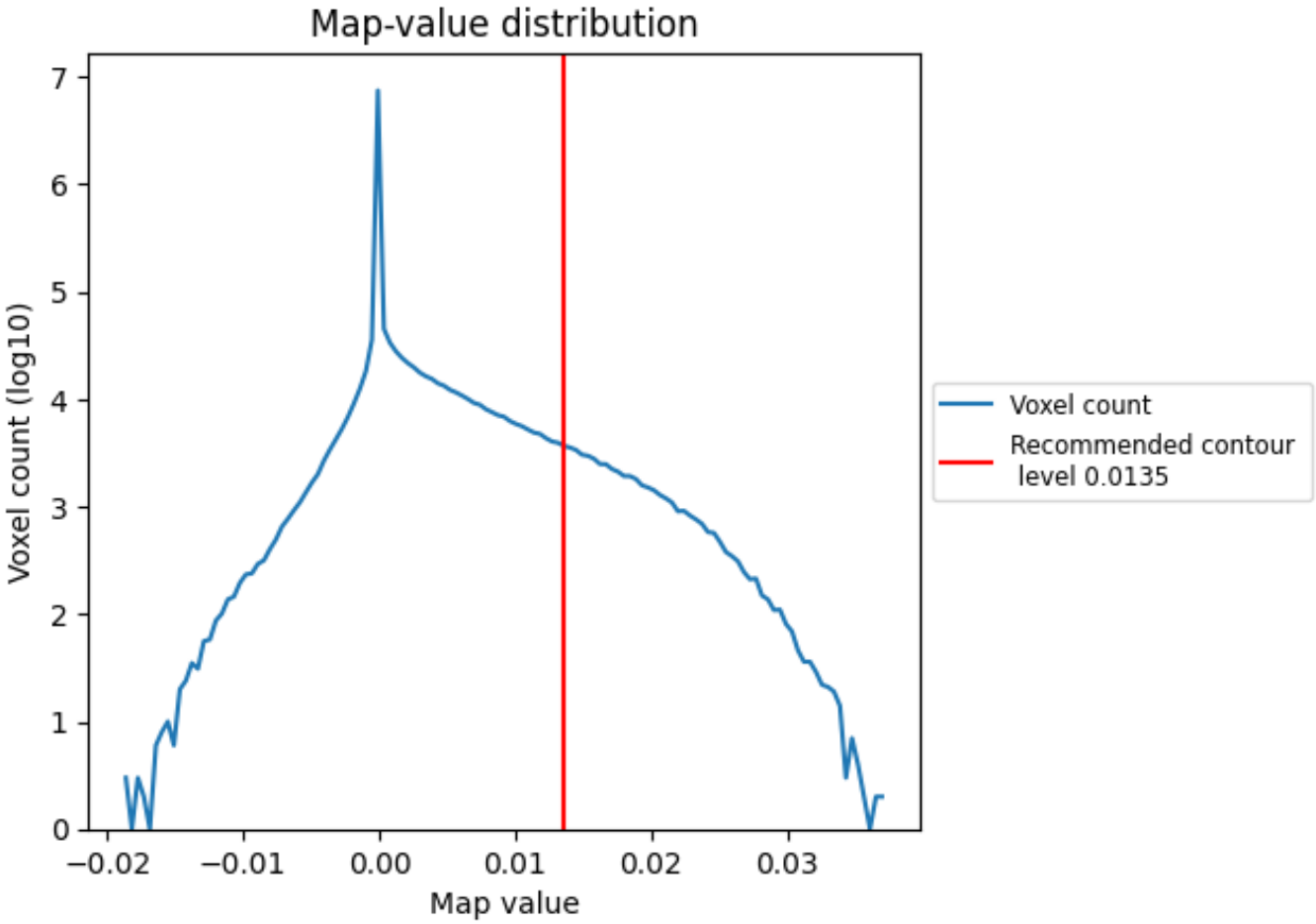


Z

7 Map analysis

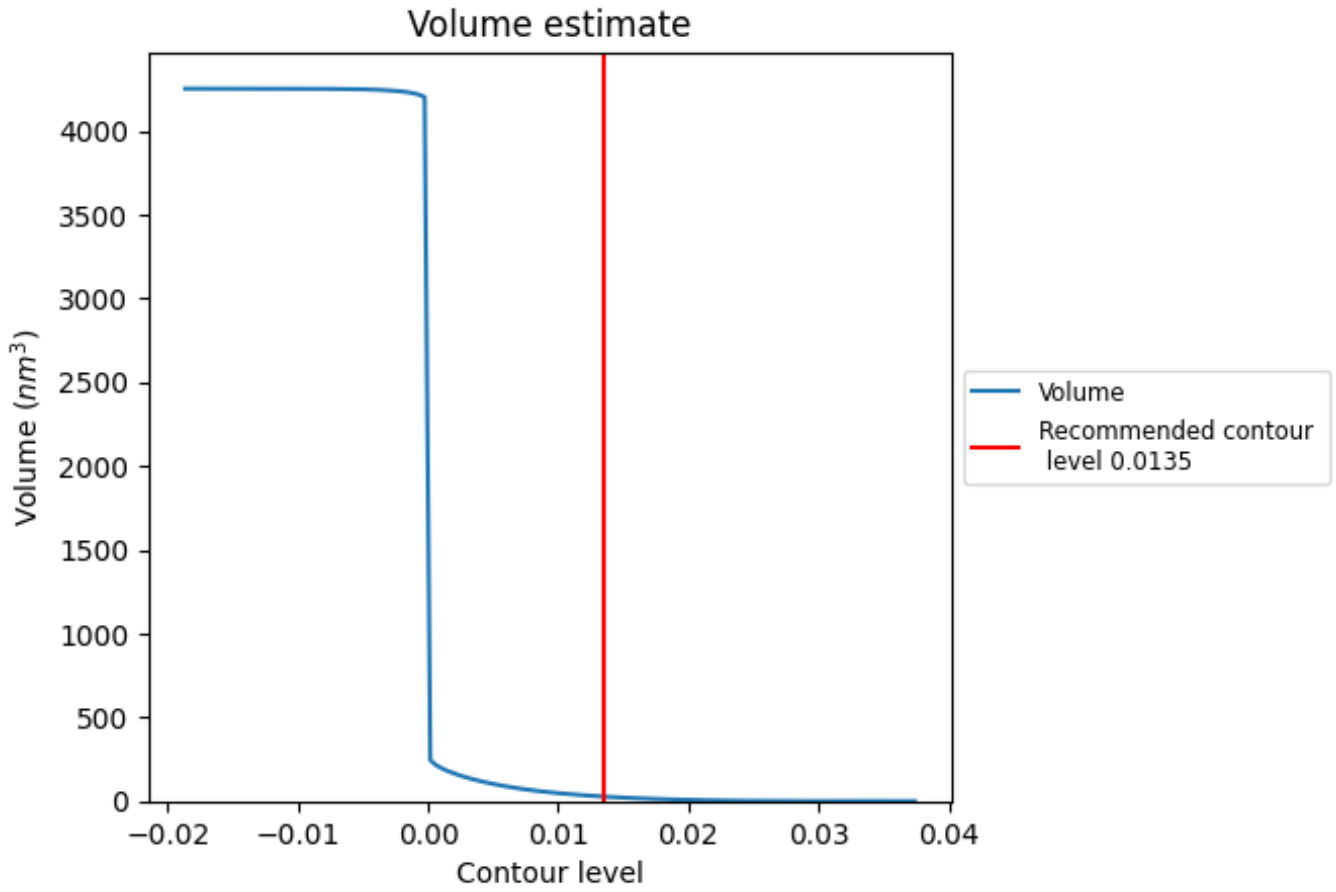
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

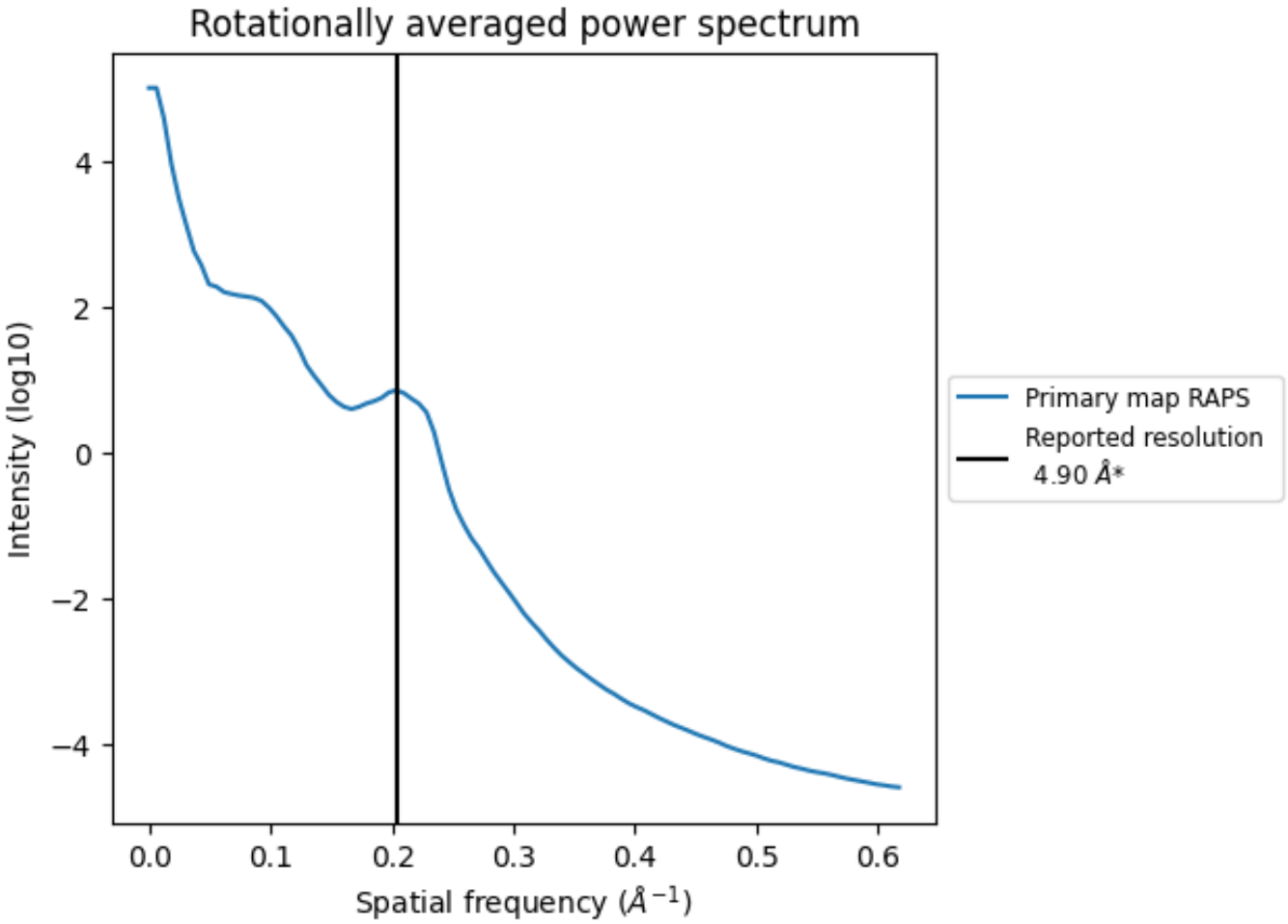
7.2 Volume estimate



The volume at the recommended contour level is 27 nm^3; this corresponds to an approximate mass of 25 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)

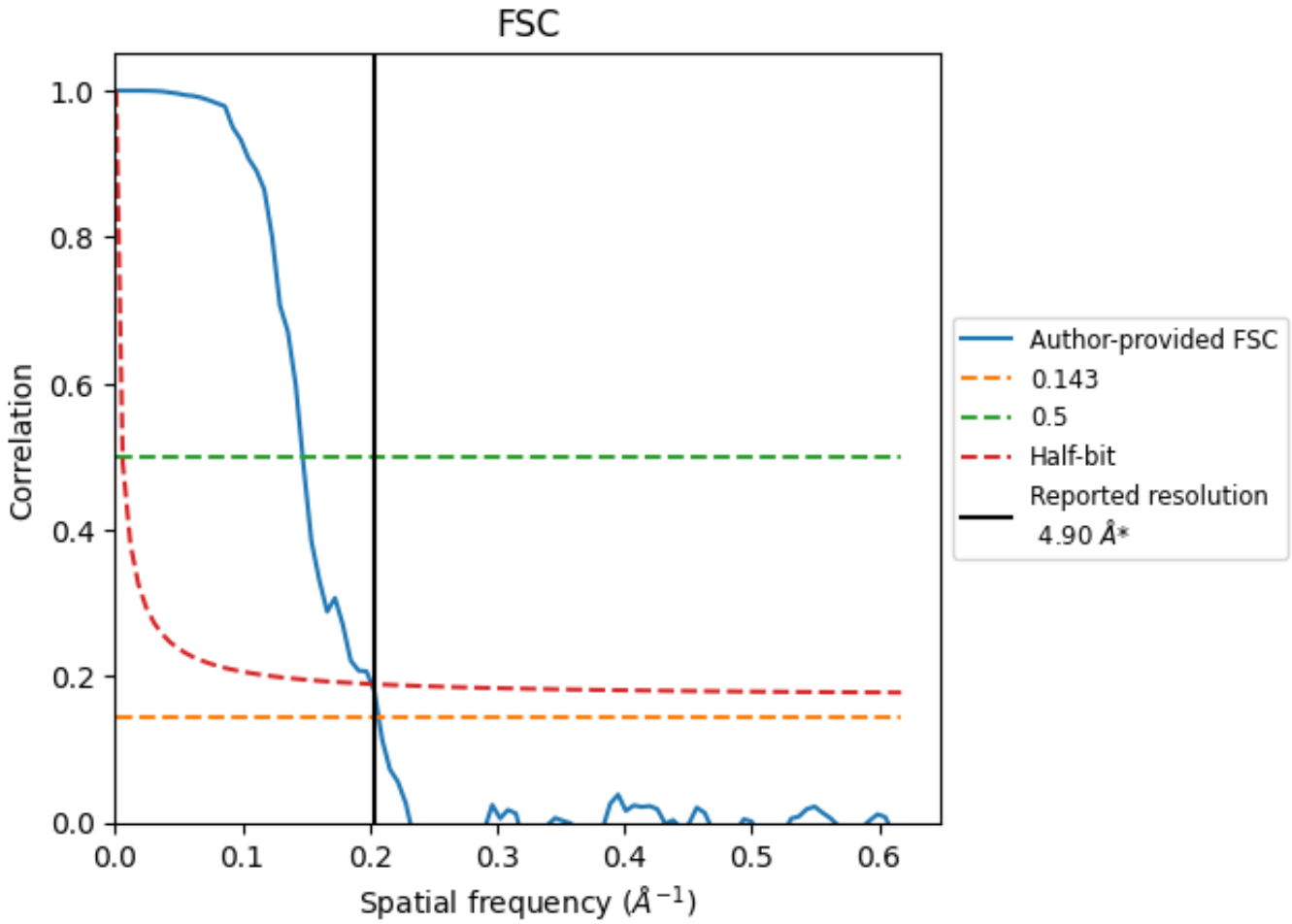


*Reported resolution corresponds to spatial frequency of 0.204 Å^{-1}

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 0.204 Å^{-1}

8.2 Resolution estimates (i)

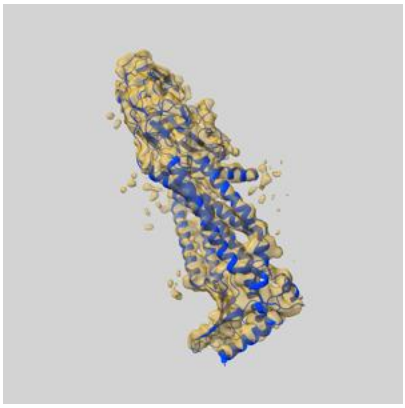
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.83	6.78	4.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

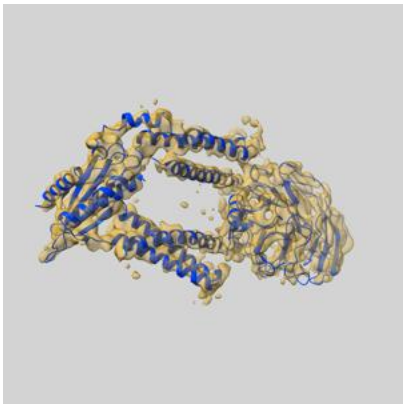
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13172 and PDB model 7P2Q. Per-residue inclusion information can be found in section 3 on page 7.

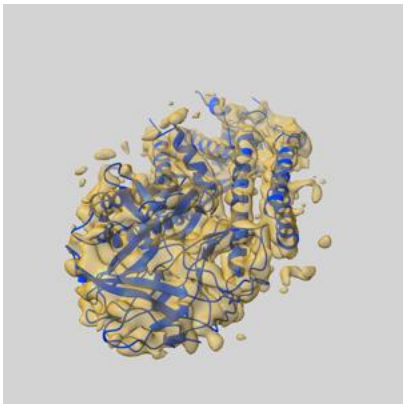
9.1 Map-model overlay



X



Y



Z

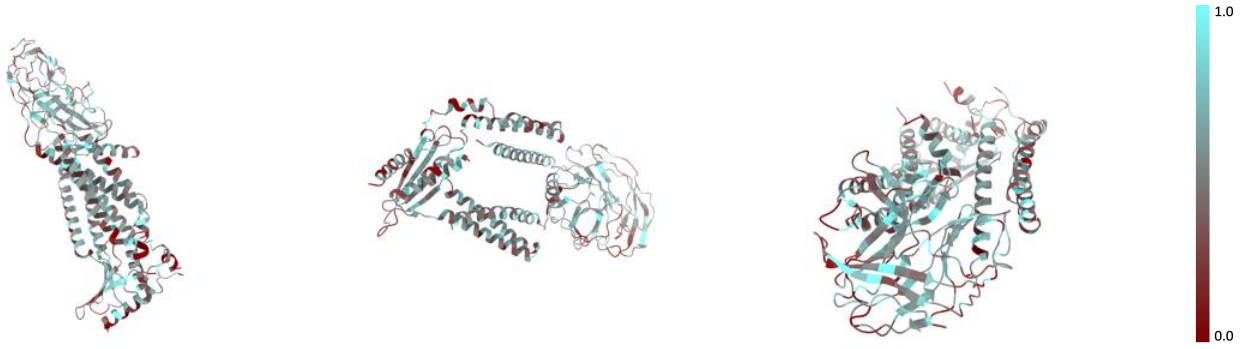
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

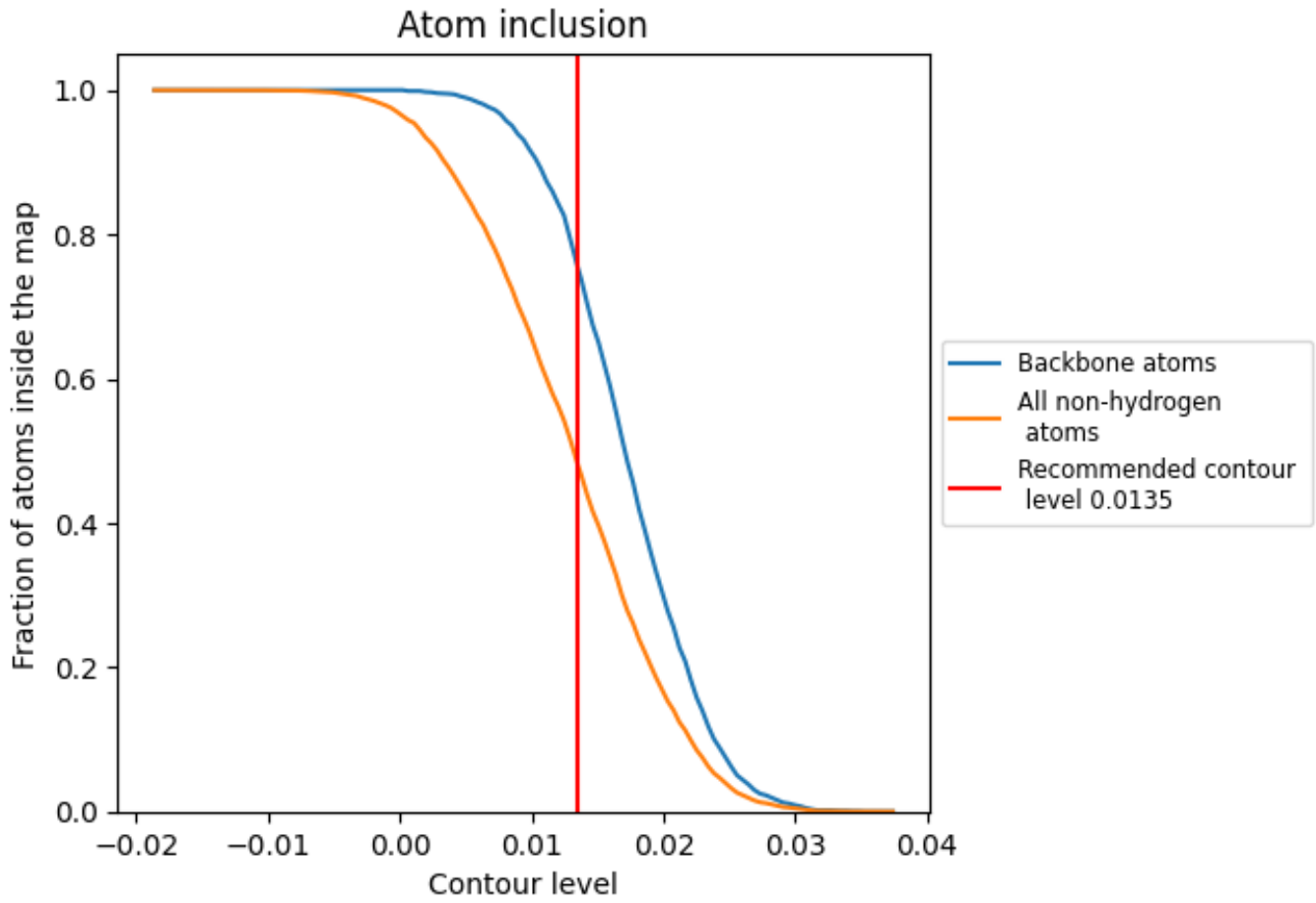
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0135).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 48% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4806	0.2370
A	0.5073	0.2500
B	0.4957	0.2510
C	0.4798	0.2240
D	0.4488	0.2160
E	0.0000	0.2210