



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2025 – 10:33 AM EDT

PDB ID : 9P95 / pdb_00009p95
EMDB ID : EMD-71399
Title : CryoEM structure of integrin alpha4beta7 bound to MAdCAM-1
Authors : Hollis, J.A.; Campbell, M.G.
Deposited on : 2025-06-24
Resolution : 3.05 Å(reported)

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

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

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<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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

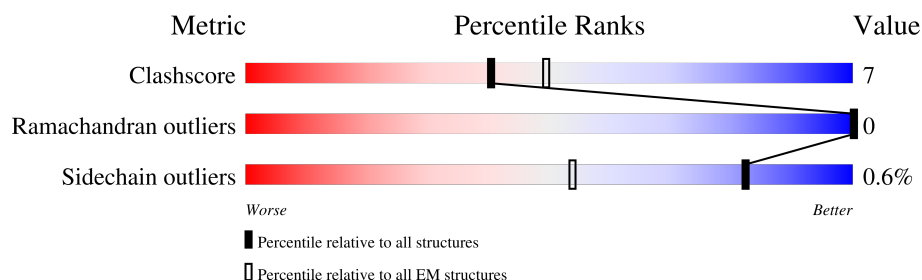
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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 $\leq 5\%$. 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	1023	<div> <div>8%</div> <div>47%</div> <div>9%</div> <div>43%</div> </div>
2	B	776	<div> <div>16%</div> <div>43%</div> <div>6%</div> <div>51%</div> </div>
3	C	370	<div> <div>11%</div> <div>48%</div> <div>7%</div> <div>46%</div> </div>
4	D	4	<div> <div>50%</div> <div>100%</div> </div>
5	E	3	<div> <div>33%</div> <div>33%</div> <div>67%</div> </div>
5	F	3	<div> <div>33%</div> <div>67%</div> </div>
5	G	3	<div> <div>67%</div> <div>33%</div> <div>67%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18066 atoms, of which 8919 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 Integrin alpha-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	582	Total	C	H	N	O	S	0	0
			8858	2835	4362	774	865	22		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	938	GLY	-	expression tag	UNP P13612
A	939	THR	-	expression tag	UNP P13612
A	940	GLY	-	expression tag	UNP P13612
A	941	GLY	-	expression tag	UNP P13612
A	942	LEU	-	expression tag	UNP P13612
A	943	GLU	-	expression tag	UNP P13612
A	944	VAL	-	expression tag	UNP P13612
A	945	LEU	-	expression tag	UNP P13612
A	946	PHE	-	expression tag	UNP P13612
A	947	GLN	-	expression tag	UNP P13612
A	948	GLY	-	expression tag	UNP P13612
A	949	PRO	-	expression tag	UNP P13612
A	950	GLY	-	expression tag	UNP P13612
A	951	GLU	-	expression tag	UNP P13612
A	952	ASN	-	expression tag	UNP P13612
A	953	ALA	-	expression tag	UNP P13612
A	954	GLN	-	expression tag	UNP P13612
A	955	CYS	-	expression tag	UNP P13612
A	956	GLU	-	expression tag	UNP P13612
A	957	LYS	-	expression tag	UNP P13612
A	958	GLU	-	expression tag	UNP P13612
A	959	LEU	-	expression tag	UNP P13612
A	960	GLN	-	expression tag	UNP P13612
A	961	ALA	-	expression tag	UNP P13612
A	962	LEU	-	expression tag	UNP P13612
A	963	GLU	-	expression tag	UNP P13612
A	964	LYS	-	expression tag	UNP P13612
A	965	GLU	-	expression tag	UNP P13612

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Chain	Residue	Modelled	Actual	Comment	Reference
A	966	ASN	-	expression tag	UNP P13612
A	967	ALA	-	expression tag	UNP P13612
A	968	GLN	-	expression tag	UNP P13612
A	969	LEU	-	expression tag	UNP P13612
A	970	GLU	-	expression tag	UNP P13612
A	971	TRP	-	expression tag	UNP P13612
A	972	GLU	-	expression tag	UNP P13612
A	973	LEU	-	expression tag	UNP P13612
A	974	GLN	-	expression tag	UNP P13612
A	975	ALA	-	expression tag	UNP P13612
A	976	LEU	-	expression tag	UNP P13612
A	977	GLU	-	expression tag	UNP P13612
A	978	LYS	-	expression tag	UNP P13612
A	979	GLU	-	expression tag	UNP P13612
A	980	LEU	-	expression tag	UNP P13612
A	981	ALA	-	expression tag	UNP P13612
A	982	GLN	-	expression tag	UNP P13612
A	983	TRP	-	expression tag	UNP P13612
A	984	SER	-	expression tag	UNP P13612
A	985	HIS	-	expression tag	UNP P13612
A	986	PRO	-	expression tag	UNP P13612
A	987	GLN	-	expression tag	UNP P13612
A	988	PHE	-	expression tag	UNP P13612
A	989	GLU	-	expression tag	UNP P13612
A	990	LYS	-	expression tag	UNP P13612

- Molecule 2 is a protein called Integrin beta-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	379	Total	C	H	N	O	S	0	0
			5819	1839	2876	525	566	13		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	705	ASP	-	expression tag	UNP P26010
B	706	THR	-	expression tag	UNP P26010
B	707	SER	-	expression tag	UNP P26010
B	708	GLY	-	expression tag	UNP P26010
B	709	LEU	-	expression tag	UNP P26010
B	710	GLU	-	expression tag	UNP P26010
B	711	VAL	-	expression tag	UNP P26010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	712	LEU	-	expression tag	UNP P26010
B	713	PHE	-	expression tag	UNP P26010
B	714	GLN	-	expression tag	UNP P26010
B	715	GLY	-	expression tag	UNP P26010
B	716	PRO	-	expression tag	UNP P26010
B	717	GLY	-	expression tag	UNP P26010
B	718	LYS	-	expression tag	UNP P26010
B	719	ASN	-	expression tag	UNP P26010
B	720	ALA	-	expression tag	UNP P26010
B	721	GLN	-	expression tag	UNP P26010
B	722	CYS	-	expression tag	UNP P26010
B	723	LYS	-	expression tag	UNP P26010
B	724	LYS	-	expression tag	UNP P26010
B	725	LYS	-	expression tag	UNP P26010
B	726	LEU	-	expression tag	UNP P26010
B	727	GLN	-	expression tag	UNP P26010
B	728	ALA	-	expression tag	UNP P26010
B	729	LEU	-	expression tag	UNP P26010
B	730	LYS	-	expression tag	UNP P26010
B	731	LYS	-	expression tag	UNP P26010
B	732	LYS	-	expression tag	UNP P26010
B	733	ASN	-	expression tag	UNP P26010
B	734	ALA	-	expression tag	UNP P26010
B	735	GLN	-	expression tag	UNP P26010
B	736	LEU	-	expression tag	UNP P26010
B	737	LYS	-	expression tag	UNP P26010
B	738	TRP	-	expression tag	UNP P26010
B	739	LYS	-	expression tag	UNP P26010
B	740	LEU	-	expression tag	UNP P26010
B	741	GLN	-	expression tag	UNP P26010
B	742	ALA	-	expression tag	UNP P26010
B	743	LEU	-	expression tag	UNP P26010
B	744	LYS	-	expression tag	UNP P26010
B	745	LYS	-	expression tag	UNP P26010
B	746	LYS	-	expression tag	UNP P26010
B	747	LEU	-	expression tag	UNP P26010
B	748	ALA	-	expression tag	UNP P26010
B	749	GLN	-	expression tag	UNP P26010
B	750	GLY	-	expression tag	UNP P26010
B	751	GLY	-	expression tag	UNP P26010
B	752	HIS	-	expression tag	UNP P26010
B	753	HIS	-	expression tag	UNP P26010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	HIS	-	expression tag	UNP P26010
B	755	HIS	-	expression tag	UNP P26010
B	756	HIS	-	expression tag	UNP P26010
B	757	HIS	-	expression tag	UNP P26010

- Molecule 3 is a protein called Mucosal addressin cell adhesion molecule 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	201	Total	C	H	N	O	S	0	0
			2974	933	1481	266	287	7		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	296	ASP	-	expression tag	UNP Q13477
C	297	THR	-	expression tag	UNP Q13477
C	298	SER	-	expression tag	UNP Q13477
C	299	GLY	-	expression tag	UNP Q13477
C	300	LEU	-	expression tag	UNP Q13477
C	301	GLU	-	expression tag	UNP Q13477
C	302	VAL	-	expression tag	UNP Q13477
C	303	LEU	-	expression tag	UNP Q13477
C	304	PHE	-	expression tag	UNP Q13477
C	305	GLN	-	expression tag	UNP Q13477
C	306	GLY	-	expression tag	UNP Q13477
C	307	PRO	-	expression tag	UNP Q13477
C	308	GLY	-	expression tag	UNP Q13477
C	309	LYS	-	expression tag	UNP Q13477
C	310	ASN	-	expression tag	UNP Q13477
C	311	ALA	-	expression tag	UNP Q13477
C	312	GLN	-	expression tag	UNP Q13477
C	313	CYS	-	expression tag	UNP Q13477
C	314	LYS	-	expression tag	UNP Q13477
C	315	LYS	-	expression tag	UNP Q13477
C	316	LYS	-	expression tag	UNP Q13477
C	317	LEU	-	expression tag	UNP Q13477
C	318	GLN	-	expression tag	UNP Q13477
C	319	ALA	-	expression tag	UNP Q13477
C	320	LEU	-	expression tag	UNP Q13477
C	321	LYS	-	expression tag	UNP Q13477
C	322	LYS	-	expression tag	UNP Q13477
C	323	LYS	-	expression tag	UNP Q13477

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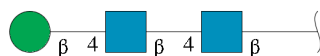
Chain	Residue	Modelled	Actual	Comment	Reference
C	324	ASN	-	expression tag	UNP Q13477
C	325	ALA	-	expression tag	UNP Q13477
C	326	GLN	-	expression tag	UNP Q13477
C	327	LEU	-	expression tag	UNP Q13477
C	328	LYS	-	expression tag	UNP Q13477
C	329	TRP	-	expression tag	UNP Q13477
C	330	LYS	-	expression tag	UNP Q13477
C	331	LEU	-	expression tag	UNP Q13477
C	332	GLN	-	expression tag	UNP Q13477
C	333	ALA	-	expression tag	UNP Q13477
C	334	LEU	-	expression tag	UNP Q13477
C	335	LYS	-	expression tag	UNP Q13477
C	336	LYS	-	expression tag	UNP Q13477
C	337	LYS	-	expression tag	UNP Q13477
C	338	LEU	-	expression tag	UNP Q13477
C	339	ALA	-	expression tag	UNP Q13477
C	340	GLN	-	expression tag	UNP Q13477
C	341	GLY	-	expression tag	UNP Q13477
C	342	GLY	-	expression tag	UNP Q13477
C	343	HIS	-	expression tag	UNP Q13477
C	344	HIS	-	expression tag	UNP Q13477
C	345	HIS	-	expression tag	UNP Q13477
C	346	HIS	-	expression tag	UNP Q13477
C	347	HIS	-	expression tag	UNP Q13477
C	348	HIS	-	expression tag	UNP Q13477

- Molecule 4 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.



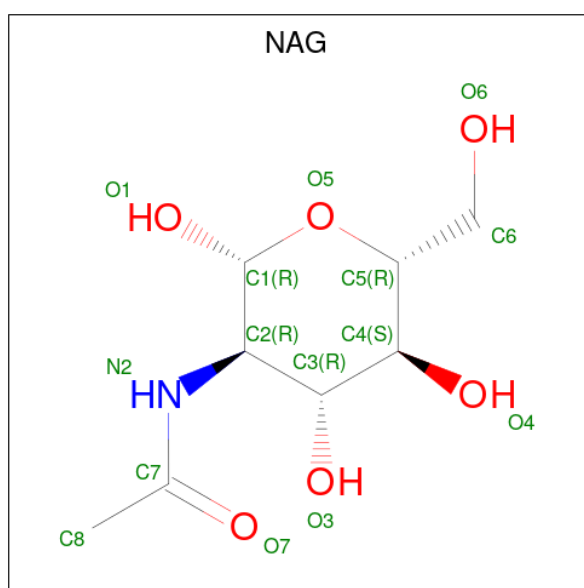
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	4	Total	C	H	N	O	0	0
			97	28	47	2	20		

- Molecule 5 is an oligosaccharide called 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
5	E	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	F	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	G	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

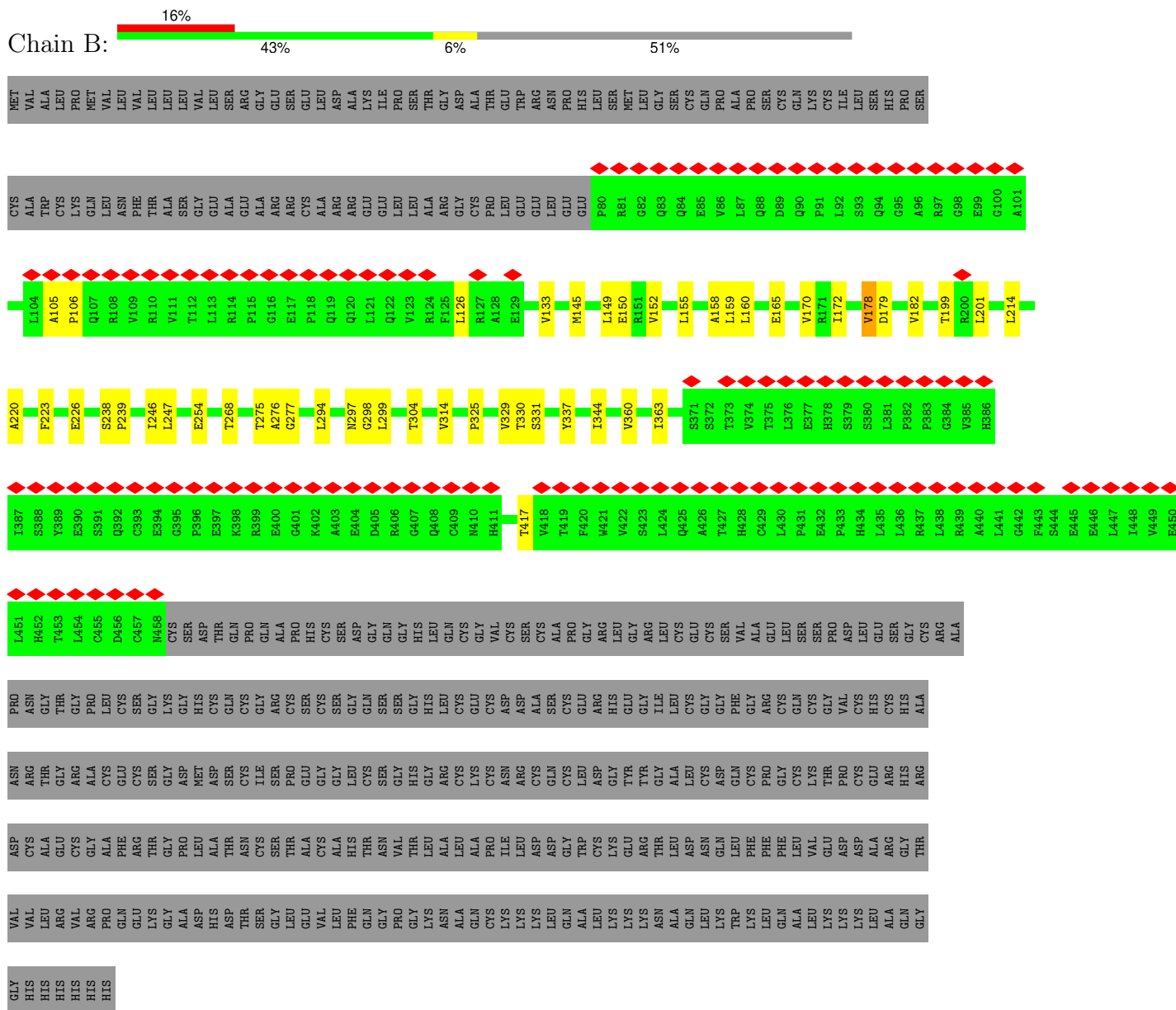
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total	Ca	0
			3	3	

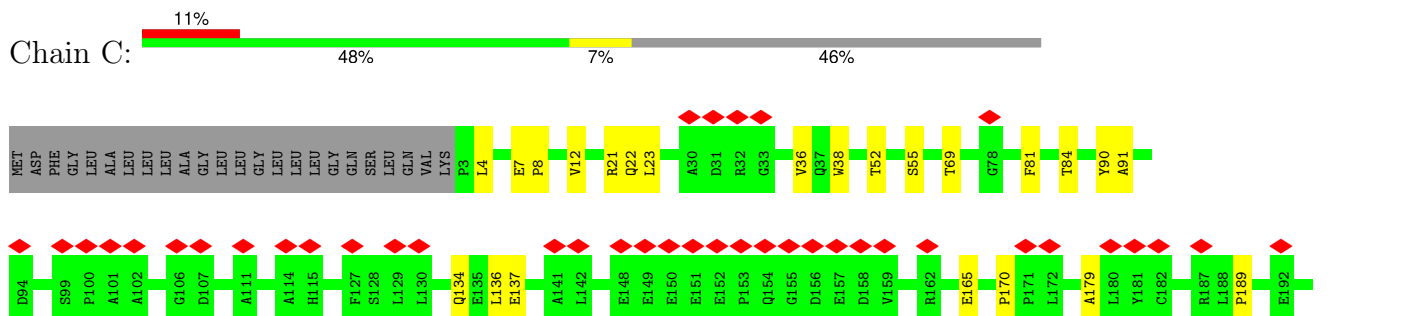
- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
8	B	3	Total 3	Mn 3	0

Chain B:



Chain C:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.957	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (\AA)	408.408, 408.408, 408.408	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.122, 1.122, 1.122	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: MN, CA, MAN, NAG, BMA

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	0.35	0/4596	0.45	1/6225 (0.0%)
2	B	0.29	0/3006	0.40	0/4081
3	C	0.24	0/1525	0.43	0/2089
All	All	0.31	0/9127	0.43	1/12395 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	VAL	N-CA-C	5.54	116.23	109.30

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	4496	4362	4362	64	0
2	B	2943	2876	2874	40	0
3	C	1493	1481	1481	20	0
4	D	50	47	43	0	0
5	E	39	37	34	0	0
5	F	39	37	34	1	0
5	G	39	37	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	14	14	13	1	0
6	B	14	14	13	0	0
6	C	14	14	13	0	0
7	A	3	0	0	0	0
8	B	3	0	0	0	0
All	All	9147	8919	8901	122	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 7.

The worst 5 of 122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ALA:HB1	6:A:1001:NAG:H82	1.69	0.74
2:B:159:LEU:HD22	2:B:363:ILE:CD1	2.23	0.68
2:B:159:LEU:HD22	2:B:363:ILE:HD13	1.75	0.68
1:A:461:VAL:HG12	1:A:531:MET:HE3	1.76	0.68
2:B:160:LEU:HD21	2:B:172:ILE:HD13	1.78	0.66

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	578/1023 (56%)	538 (93%)	40 (7%)	0	100	100
2	B	377/776 (49%)	362 (96%)	15 (4%)	0	100	100
3	C	199/370 (54%)	185 (93%)	14 (7%)	0	100	100
All	All	1154/2169 (53%)	1085 (94%)	69 (6%)	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	487/879 (55%)	483 (99%)	4 (1%)	79	88
2	B	328/651 (50%)	326 (99%)	2 (1%)	84	90
3	C	163/307 (53%)	163 (100%)	0	100	100
All	All	978/1837 (53%)	972 (99%)	6 (1%)	82	90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	ASP
2	B	165	GLU
2	B	178	VAL
1	A	75	SER
1	A	70	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	157	HIS
2	B	248	GLN
3	C	82	GLN
2	B	338	GLN
2	B	84	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 ⓘ

13 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
4	NAG	D	1	4	14,14,15	0.84	1 (7%)	17,19,21	1.39	2 (11%)
4	NAG	D	2	4	14,14,15	0.82	1 (7%)	17,19,21	0.95	1 (5%)
4	BMA	D	3	4	11,11,12	0.85	0	15,15,17	2.57	6 (40%)
4	MAN	D	4	4	11,11,12	0.65	0	15,15,17	1.23	1 (6%)
5	NAG	E	1	5,1	14,14,15	0.81	0	17,19,21	1.33	2 (11%)
5	NAG	E	2	5	14,14,15	0.82	0	17,19,21	0.80	0
5	BMA	E	3	5	11,11,12	0.87	0	15,15,17	2.54	6 (40%)
5	NAG	F	1	5,1	14,14,15	0.88	1 (7%)	17,19,21	1.13	2 (11%)
5	NAG	F	2	5	14,14,15	0.71	0	17,19,21	1.43	3 (17%)
5	BMA	F	3	5	11,11,12	0.91	0	15,15,17	2.58	6 (40%)
5	NAG	G	1	5,1	14,14,15	0.72	0	17,19,21	0.91	0
5	NAG	G	2	5	14,14,15	0.69	0	17,19,21	1.28	3 (17%)
5	BMA	G	3	5	11,11,12	1.31	2 (18%)	15,15,17	3.03	6 (40%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	C1-C2	2.49	1.58	1.52
5	F	1	NAG	O5-C1	-2.41	1.39	1.43
5	G	3	BMA	O5-C1	2.38	1.47	1.43
4	D	1	NAG	O5-C1	-2.22	1.40	1.43
4	D	2	NAG	C1-C2	2.07	1.55	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C1-O5-C5	8.61	123.73	112.19
4	D	3	BMA	C1-O5-C5	7.10	121.70	112.19
5	E	3	BMA	C1-O5-C5	6.92	121.46	112.19
5	F	3	BMA	C1-O5-C5	6.59	121.02	112.19
5	G	3	BMA	C3-C4-C5	4.70	118.75	110.23

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C1-C2-N2-C7
5	G	2	NAG	C1-C2-N2-C7
4	D	4	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7

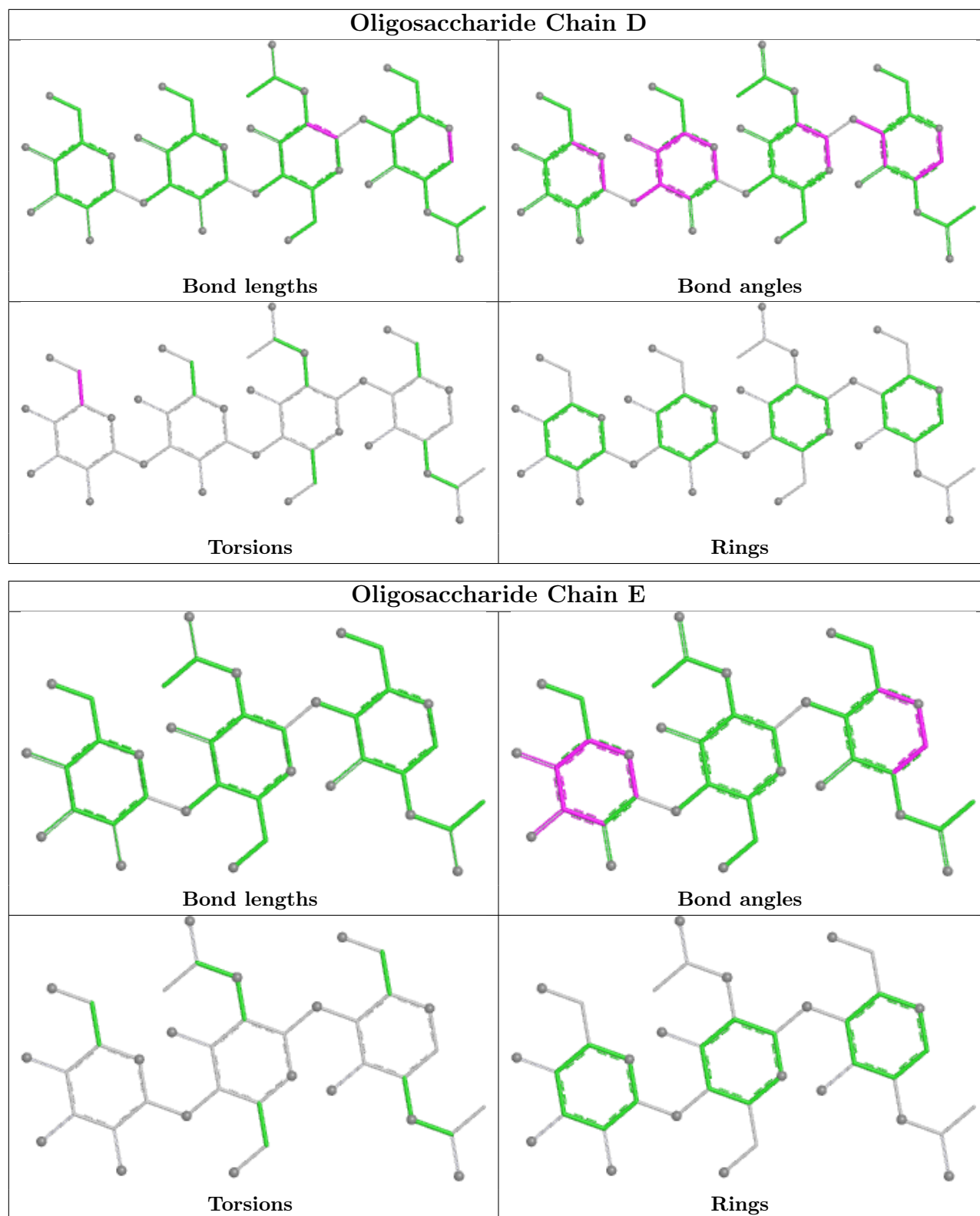
There are no ring outliers.

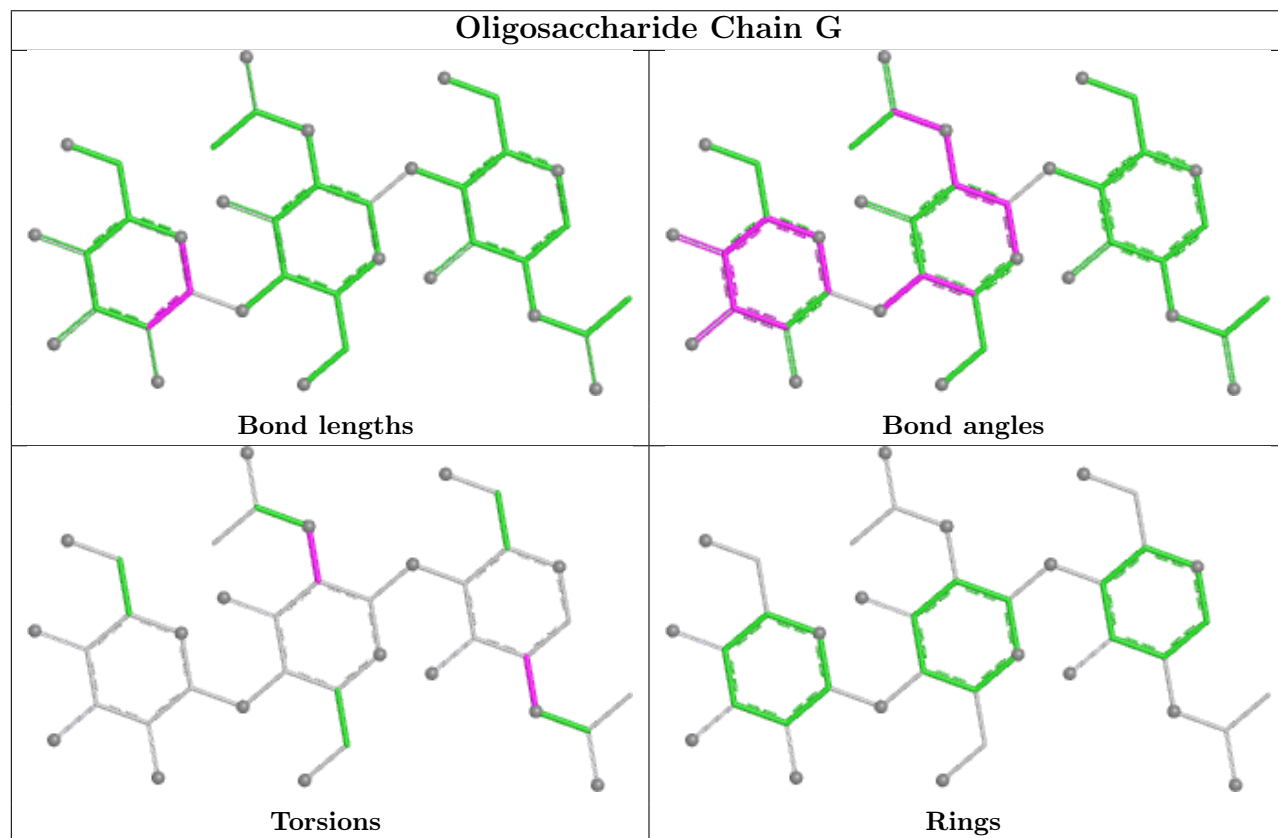
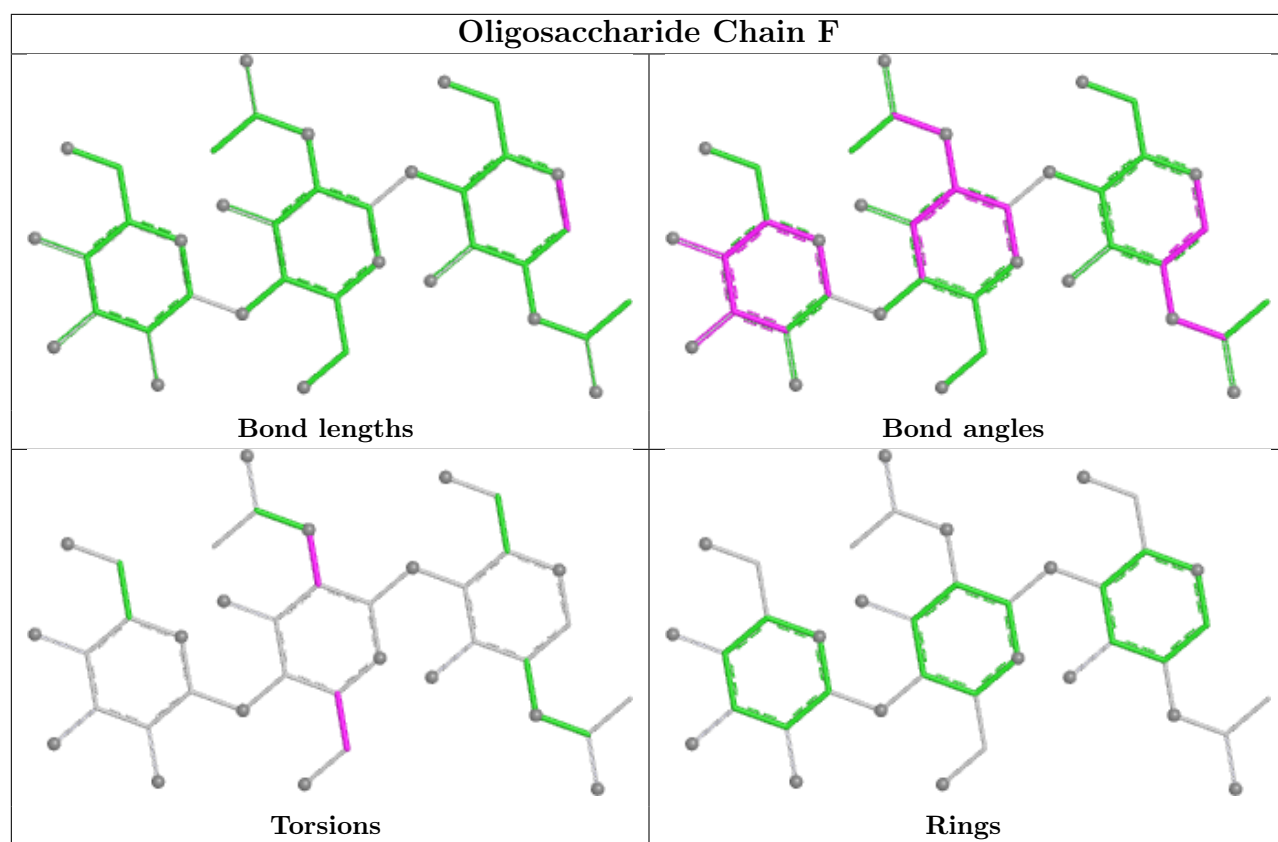
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3	BMA	1	0
5	F	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

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
6	NAG	B	804	2	14,14,15	0.67	0	17,19,21	0.96	0
6	NAG	C	401	3	14,14,15	0.80	0	17,19,21	0.89	0
6	NAG	A	1001	1	14,14,15	0.70	0	17,19,21	0.94	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
6	NAG	B	804	2	-	3/6/23/26	0/1/1/1
6	NAG	C	401	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1001	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	NAG	O5-C1-C2	-2.18	107.91	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	804	NAG	C1-C2-N2-C7
6	B	804	NAG	O5-C5-C6-O6
6	A	1001	NAG	O5-C5-C6-O6
6	B	804	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
6	A	1001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

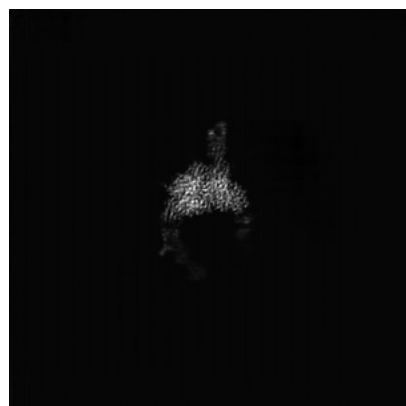
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71399. These allow visual inspection of the internal detail of the map and identification of artifacts.

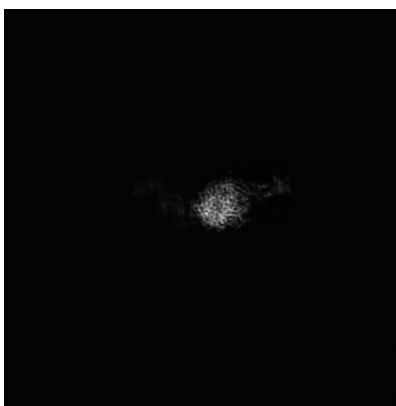
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

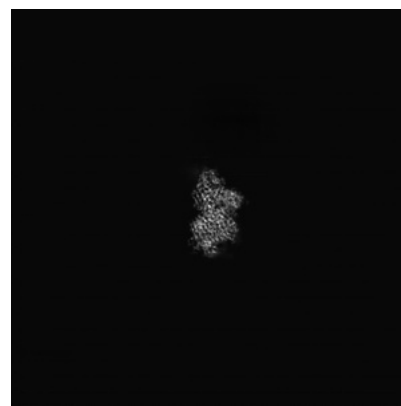
6.1.1 Primary map



X

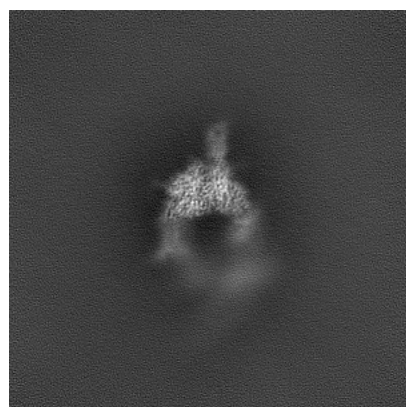


Y

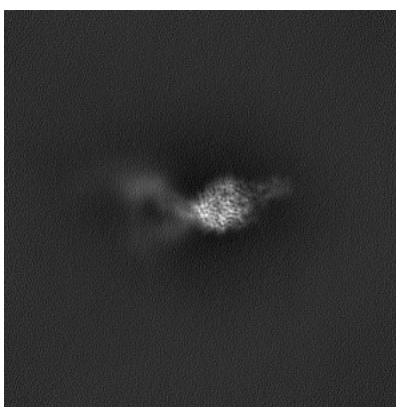


Z

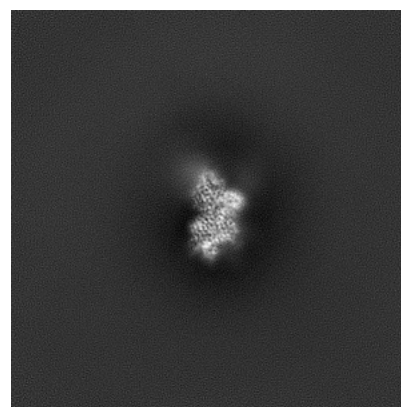
6.1.2 Raw map



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: 182

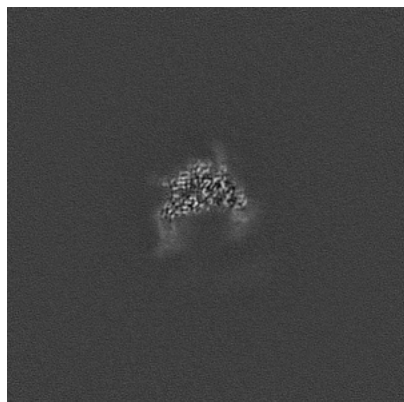


Y Index: 182

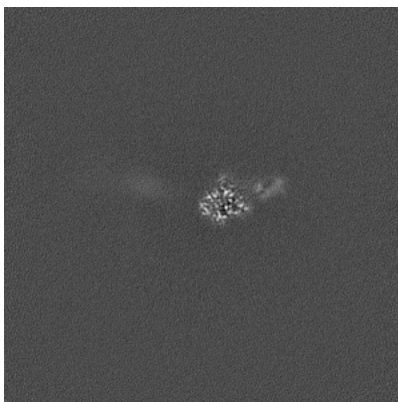


Z Index: 182

6.2.2 Raw map



X Index: 182



Y Index: 182

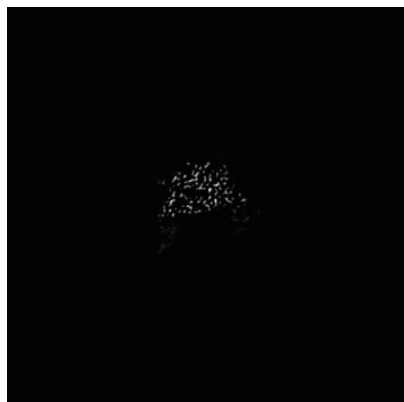


Z Index: 182

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

6.3 Largest variance slices [i](#)

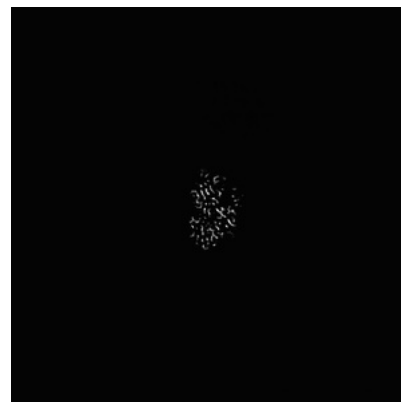
6.3.1 Primary map



X Index: 180

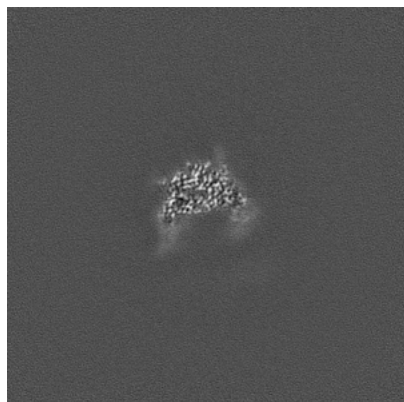


Y Index: 167

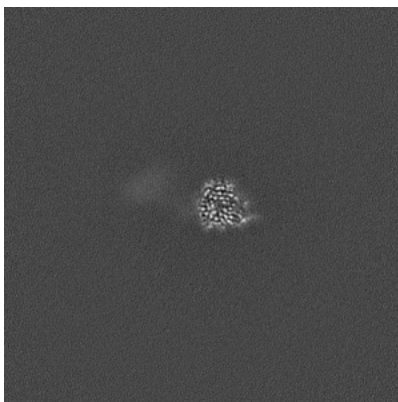


Z Index: 199

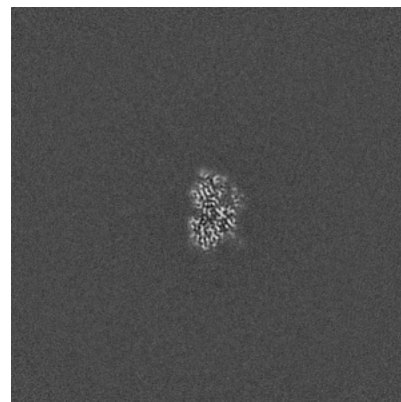
6.3.2 Raw map



X Index: 180



Y Index: 167

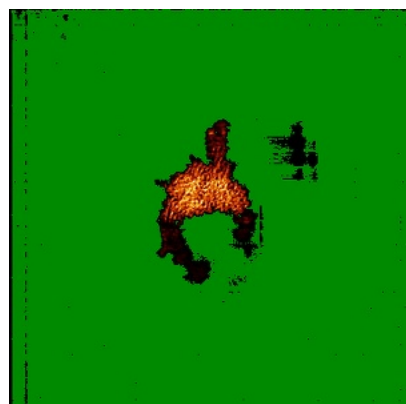


Z Index: 199

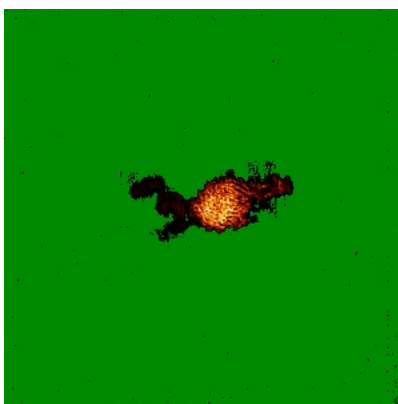
The images above show the largest variance slices of the map in three orthogonal directions.

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

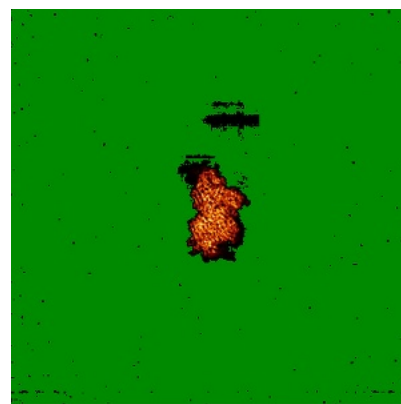
6.4.1 Primary map



X

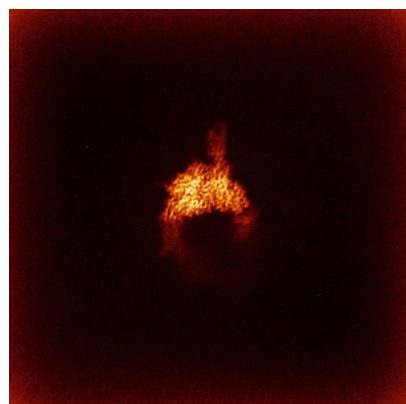


Y



Z

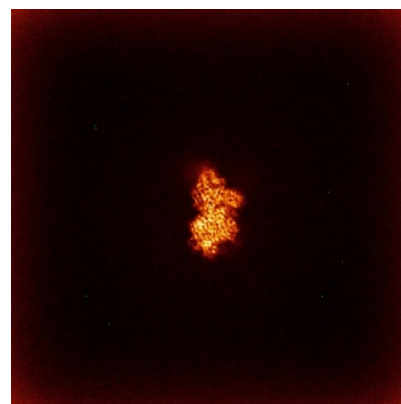
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

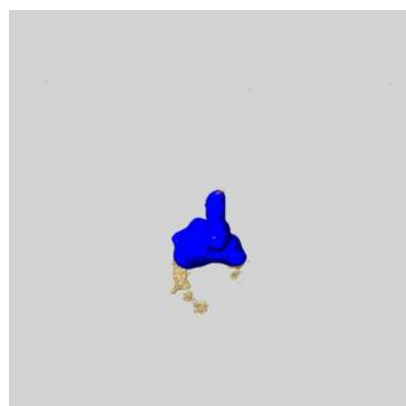
6.6 Mask visualisation [i](#)

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

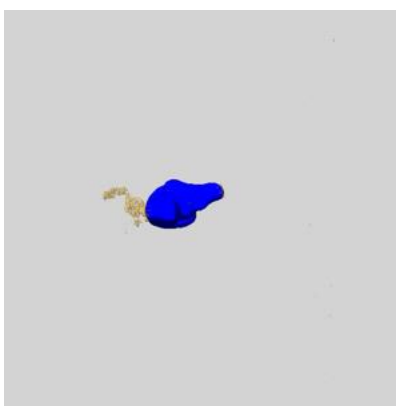
A mask typically either:

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

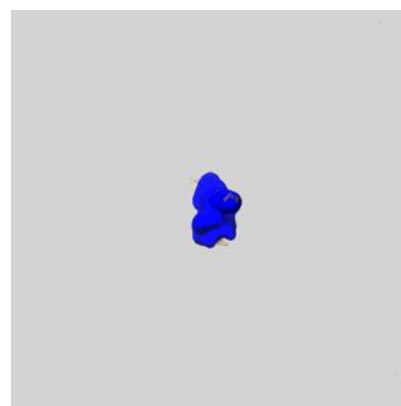
6.6.1 emd_71399_msk_1.map [i](#)



X



Y

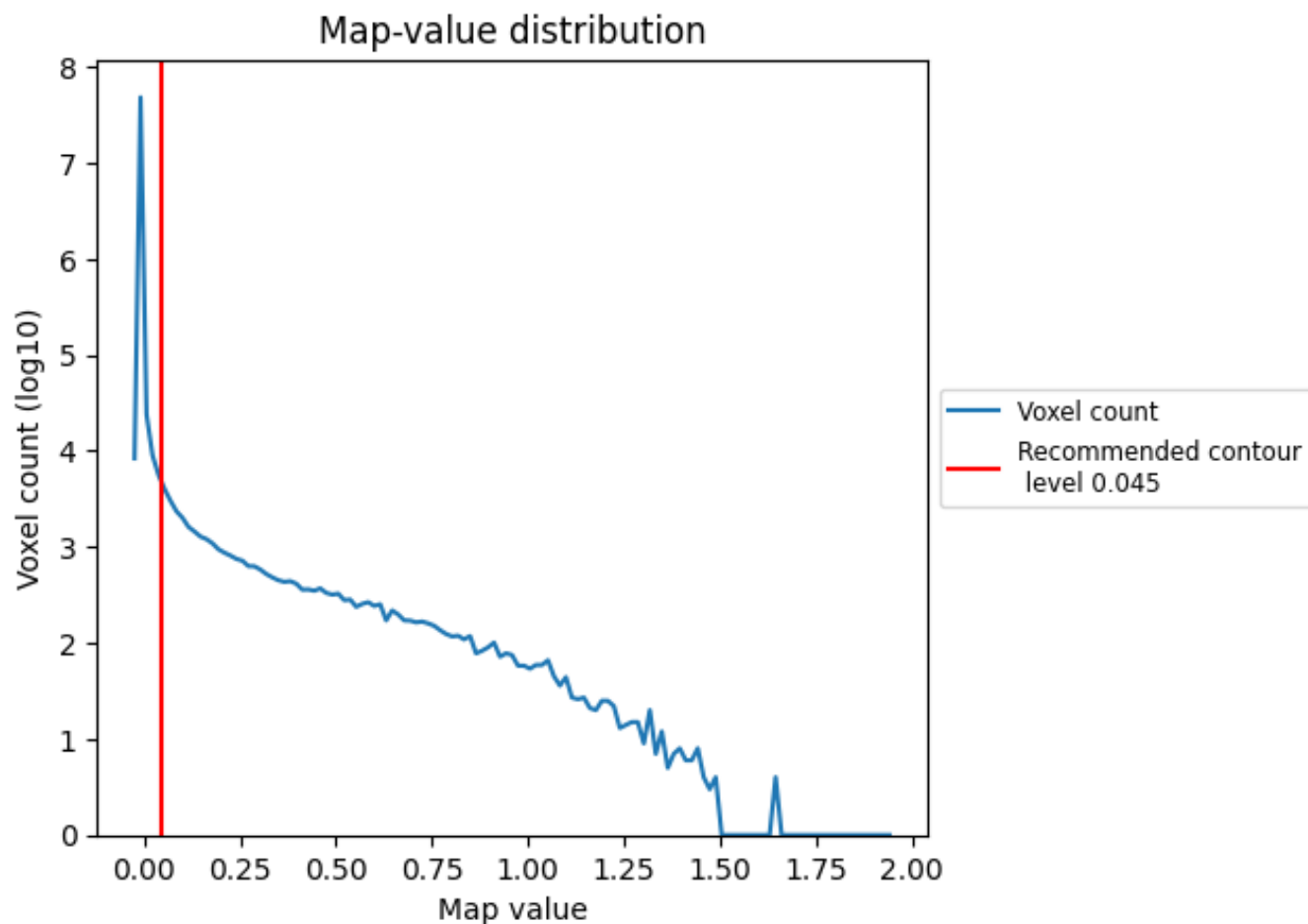


Z

7 Map analysis [i](#)

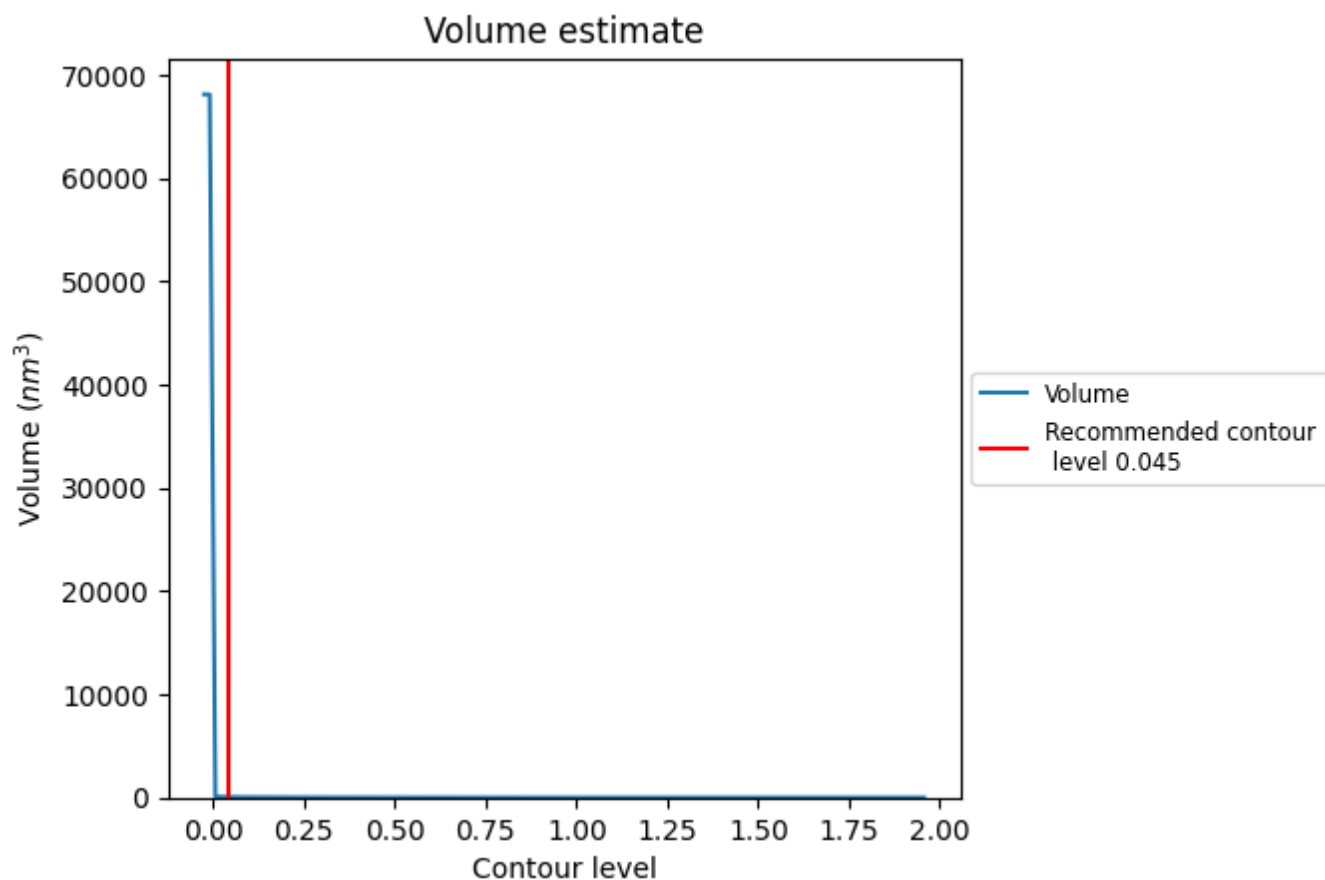
This section contains the results of statistical analysis of the map.

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.

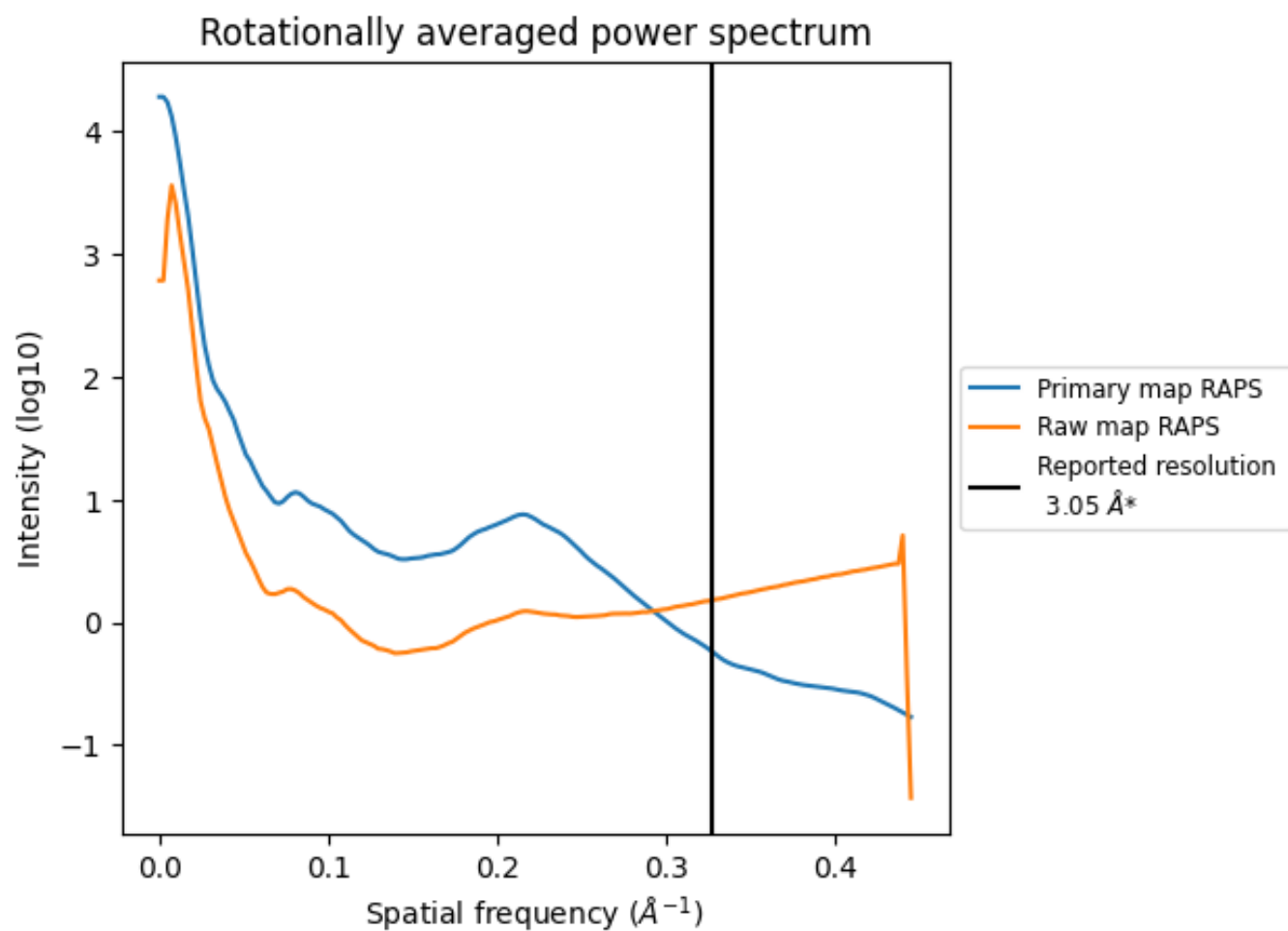
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm^3 ; this corresponds to an approximate mass of 48 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 ⓘ

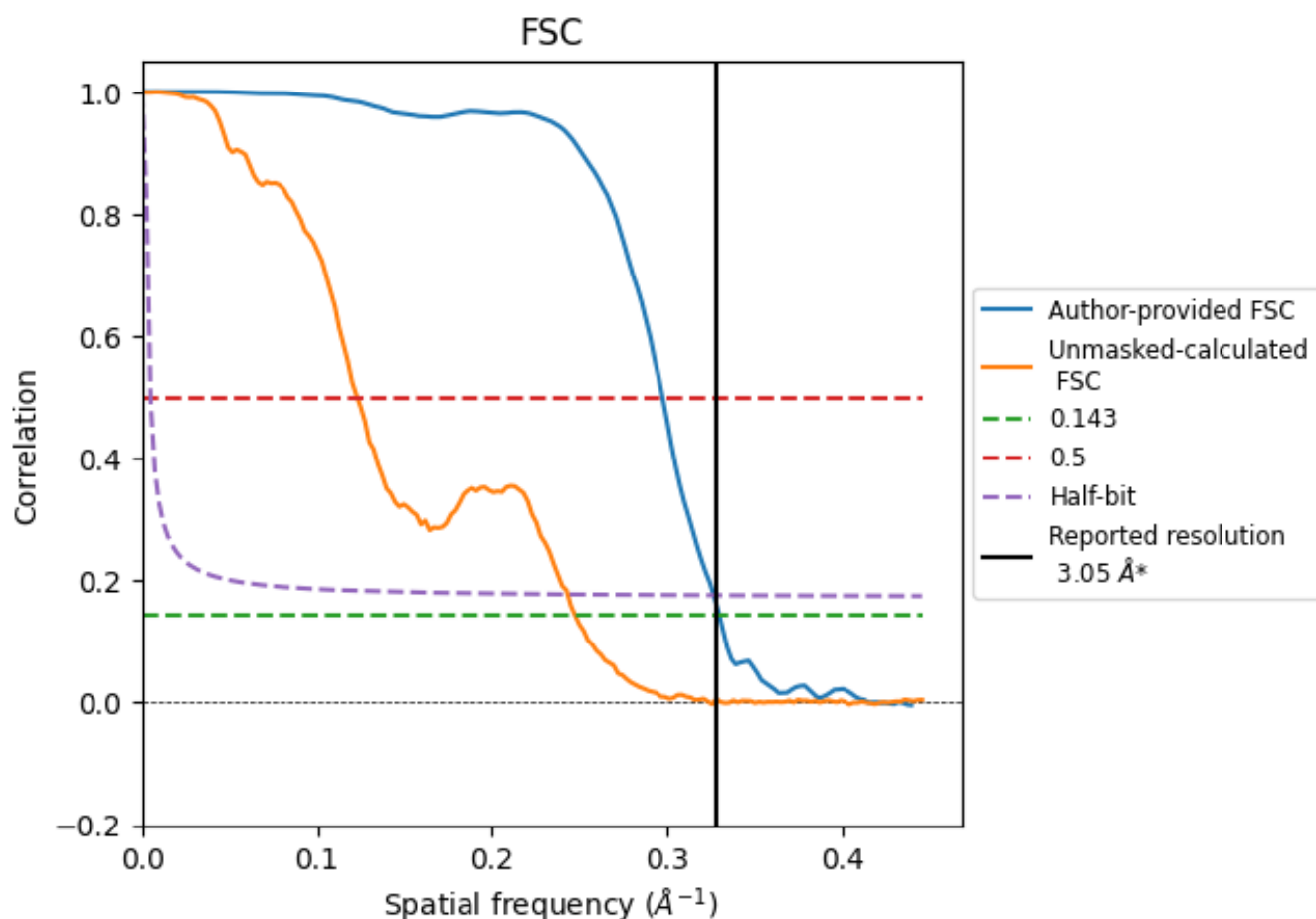


*Reported resolution corresponds to spatial frequency of 0.328 \AA^{-1}

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 0.328\AA^{-1}

8.2 Resolution estimates [i](#)

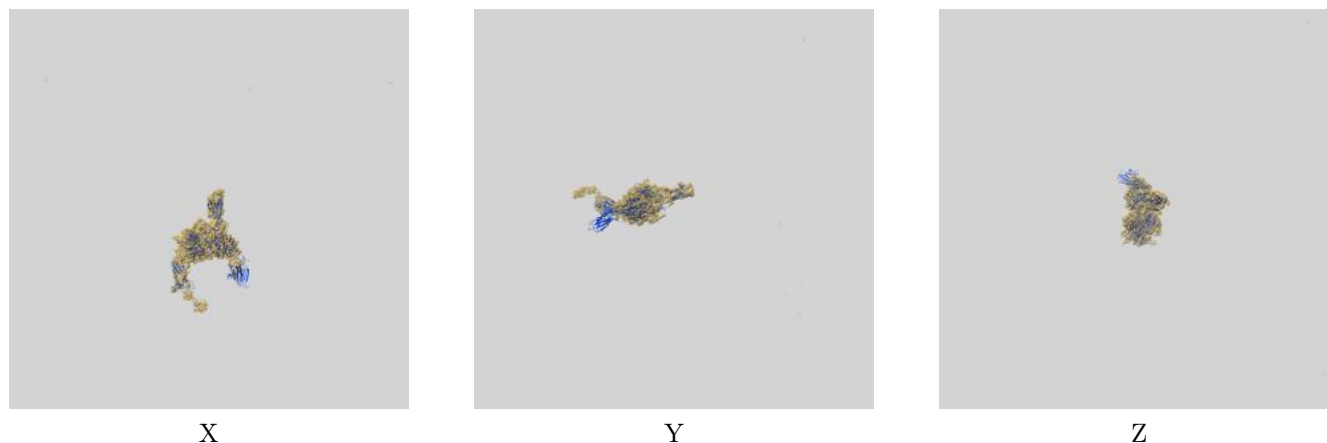
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.03	3.36	3.06
Unmasked-calculated*	4.04	8.14	4.11

*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 4.04 differs from the reported value 3.05 by more than 10 %

9 Map-model fit [i](#)

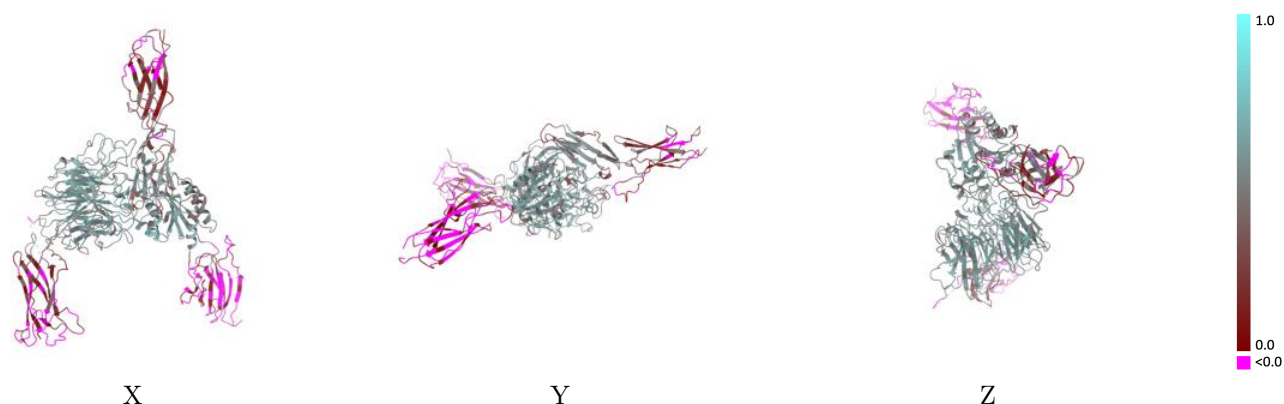
This section contains information regarding the fit between EMDB map EMD-71399 and PDB model 9P95. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



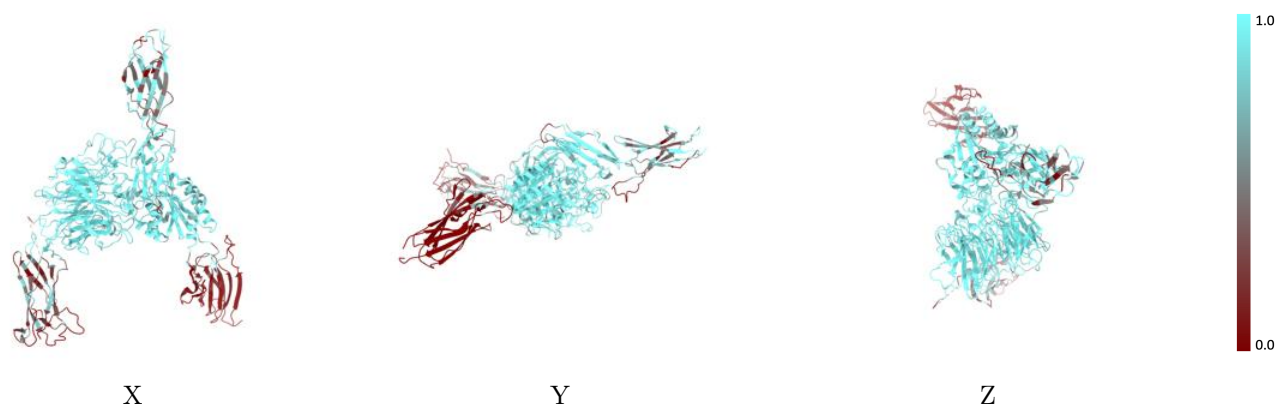
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



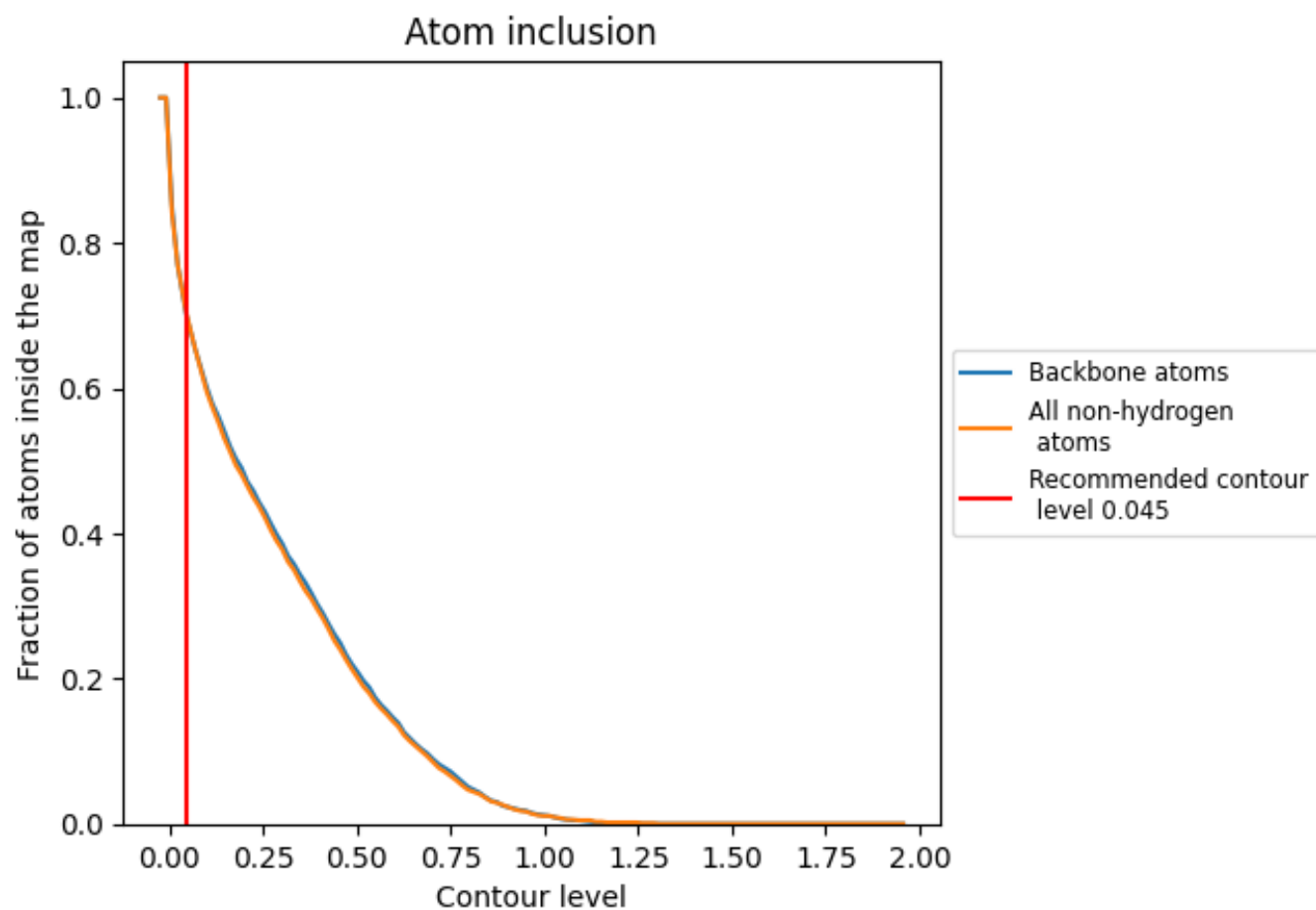
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.3730
A	<div></div> 0.7880	<div></div> 0.4340
B	<div></div> 0.6180	<div></div> 0.3320
C	<div></div> 0.6520	<div></div> 0.2790
D	<div></div> 0.4000	<div></div> 0.3440
E	<div></div> 0.5900	<div></div> 0.4510
F	<div></div> 0.7180	<div></div> 0.3150
G	<div></div> 0.2050	<div></div> 0.1140

1.0

0.0

<0.0