



Full wwPDB EM Validation Report ⓘ

Aug 18, 2025 – 04:13 pm BST

PDB ID : 9GTU / pdb_00009gtu
EMDB ID : EMD-51567
Title : Collagen VI alpha 1, 2, 3 heterotrimer recombinant C terminal region. Local refinement.
Authors : Godwin, A.; Snee, M.; Dajani, R.; Becker, M.; Roseman, A.; Baldock, C.
Deposited on : 2024-09-18
Resolution : 3.14 Å(reported)
Based on initial model : .

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.dev126
Mogul : 1.8.4, CSD as541be (2020)
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

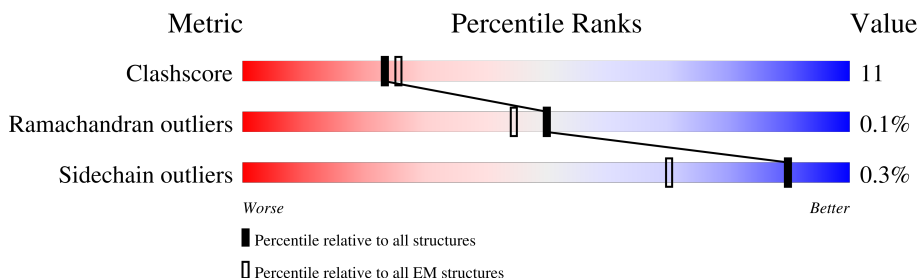
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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	C	492	
2	B	476	
3	A	479	
4	D	3	
4	E	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11077 atoms, of which 5464 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 Collagen alpha-3(VI) chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	454	Total	C	H	N	O	S	2	0
			7088	2240	3550	609	670	19		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2329	ASP	-	expression tag	UNP P12111
C	2330	TYR	-	expression tag	UNP P12111
C	2331	LYS	-	expression tag	UNP P12111
C	2332	ASP	-	expression tag	UNP P12111
C	2333	ASP	-	expression tag	UNP P12111
C	2334	ASP	-	expression tag	UNP P12111
C	2335	ASP	-	expression tag	UNP P12111
C	2336	LYS	-	expression tag	UNP P12111
C	2337	GLY	-	expression tag	UNP P12111
C	2338	GLY	-	expression tag	UNP P12111
C	2339	GLY	-	expression tag	UNP P12111
C	2340	GLY	-	expression tag	UNP P12111
C	2341	SER	-	expression tag	UNP P12111
C	2342	GLY	-	expression tag	UNP P12111
C	2343	GLY	-	expression tag	UNP P12111
C	2345	GLY	ASN	conflict	UNP P12111
C	2357	ARG	ASP	conflict	UNP P12111
C	2367	ARG	LYS	conflict	UNP P12111
C	2431	VAL	ASP	variant	UNP P12111
C	2441	THR	ARG	conflict	UNP P12111
C	2609	ALA	ARG	conflict	UNP P12111
C	2610	ALA	ARG	conflict	UNP P12111

- Molecule 2 is a protein called Collagen alpha-2(VI) chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	227	Total	C	H	N	O	S	0	0
			3455	1094	1693	320	338	10		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	SER	-	expression tag	UNP P12110
B	545	ALA	-	expression tag	UNP P12110
B	546	TRP	-	expression tag	UNP P12110
B	547	SER	-	expression tag	UNP P12110
B	548	HIS	-	expression tag	UNP P12110
B	549	PRO	-	expression tag	UNP P12110
B	550	GLN	-	expression tag	UNP P12110
B	551	PHE	-	expression tag	UNP P12110
B	552	GLU	-	expression tag	UNP P12110
B	553	LYS	-	expression tag	UNP P12110
B	554	GLY	-	expression tag	UNP P12110
B	555	GLY	-	expression tag	UNP P12110
B	556	GLY	-	expression tag	UNP P12110
B	557	GLY	-	expression tag	UNP P12110
B	558	SER	-	expression tag	UNP P12110
B	559	GLY	-	expression tag	UNP P12110
B	560	GLY	-	expression tag	UNP P12110
B	561	GLY	-	expression tag	UNP P12110
B	562	GLY	-	expression tag	UNP P12110
B	563	SER	-	expression tag	UNP P12110
B	680	HIS	ARG	conflict	UNP P12110
B	966	ASN	LYS	conflict	UNP P12110
B	967	GLU	GLN	conflict	UNP P12110

- Molecule 3 is a protein called Collagen alpha-1(VI) chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	25	Total	C	H	N	O	S	0	0
			311	101	145	29	31	5		

There are 16 discrepancies between the modelled and reference sequences:

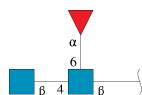
Chain	Residue	Modelled	Actual	Comment	Reference
A	550	HIS	-	expression tag	UNP P12109
A	551	HIS	-	expression tag	UNP P12109
A	552	HIS	-	expression tag	UNP P12109
A	553	HIS	-	expression tag	UNP P12109

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	-	expression tag	UNP P12109
A	555	HIS	-	expression tag	UNP P12109
A	556	GLY	-	expression tag	UNP P12109
A	557	GLY	-	expression tag	UNP P12109
A	558	GLY	-	expression tag	UNP P12109
A	559	GLY	-	expression tag	UNP P12109
A	560	SER	-	expression tag	UNP P12109
A	561	GLY	-	expression tag	UNP P12109
A	562	GLY	-	expression tag	UNP P12109
A	563	GLY	-	expression tag	UNP P12109
A	564	GLY	-	expression tag	UNP P12109
A	565	SER	-	expression tag	UNP P12109

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



Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	3	Total	C	H	N	O	0	0
			64	22	26	2	14		
4	E	3	Total	C	H	N	O	0	0
			64	22	26	2	14		

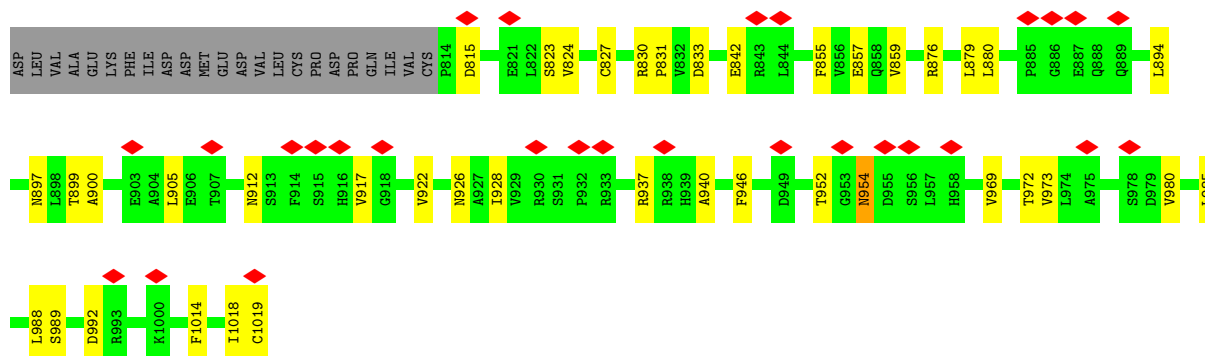
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	H	N	O	0
			26	8	12	1	5	
5	B	1	Total	C	H	N	O	0
			26	8	12	1	5	

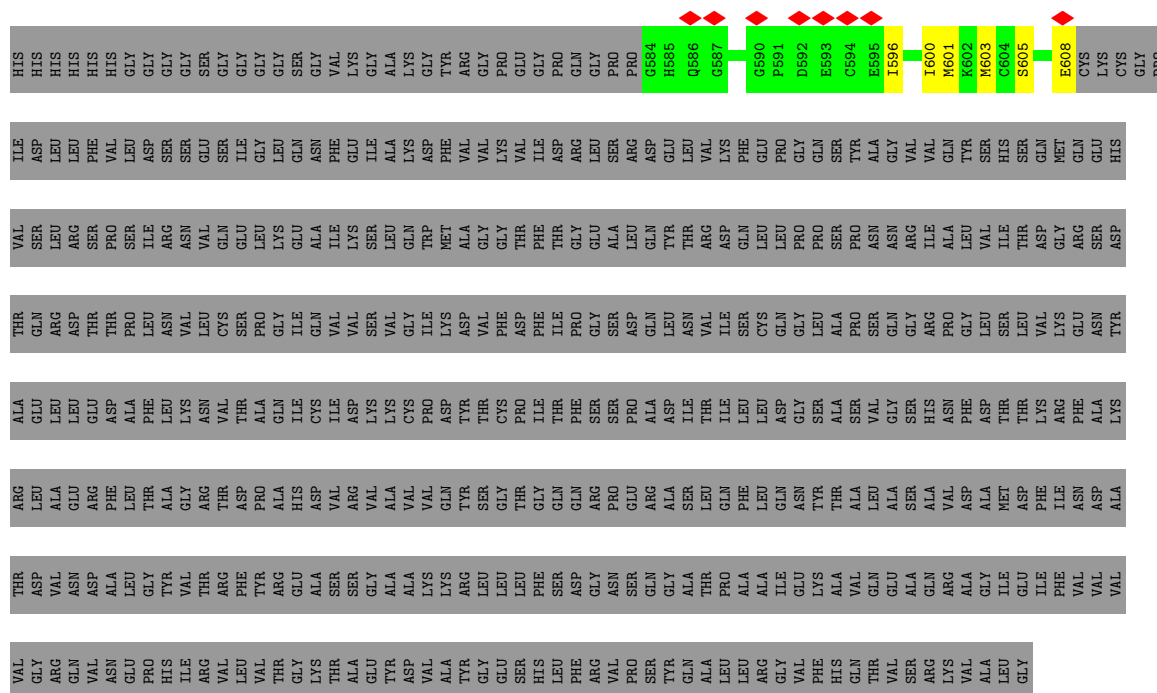
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	C	29	Total	O	0
			29	29	
6	B	14	Total	O	0
			14	14	



• Molecule 3: Collagen alpha-1(VI) chain

Chain A: 95%



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	246984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.11	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.939	Depositor
Minimum map value	-1.097	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.242	Depositor
Map size (\AA)	260.40002, 260.40002, 260.40002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3020002, 1.3020002, 1.3020002	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.12	0/3606	0.29	0/4886
2	B	0.11	0/1796	0.28	0/2436
3	A	0.18	0/169	0.46	0/228
All	All	0.12	0/5571	0.30	0/7550

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	C	3538	3550	3550	88	0
2	B	1762	1693	1693	38	0
3	A	166	145	145	7	0
4	D	38	26	34	1	0
4	E	38	26	34	3	0
5	B	14	12	13	1	0
5	C	14	12	13	0	0
6	B	14	0	0	0	0
6	C	29	0	0	0	0
All	All	5613	5464	5482	119	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 11.

All (119) 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:880:LEU:HD23	2:B:928:ILE:HD11	1.57	0.86
1:C:2626:SER:O	1:C:2630:THR:OG1	1.95	0.83
1:C:2504:ASN:OD1	2:B:823:SER:N	2.17	0.78
1:C:2588:LEU:O	1:C:2590:ILE:HG22	1.84	0.77
1:C:2512:ALA:HB2	1:C:2538:ILE:HD11	1.66	0.77
1:C:2628:GLU:O	1:C:2713:ARG:NH2	2.20	0.74
1:C:2629:THR:OG1	1:C:2713:ARG:NH2	2.22	0.73
3:A:601:MET:O	3:A:605:SER:OG	2.07	0.73
1:C:2738:ILE:HD11	1:C:2820:VAL:HG21	1.77	0.67
1:C:2557:ILE:O	1:C:2557:ILE:HD12	1.93	0.67
1:C:2628:GLU:O	1:C:2629:THR:OG1	2.16	0.64
2:B:857:GLU:HB3	2:B:905:LEU:HD23	1.80	0.64
1:C:2630:THR:O	1:C:2708:GLN:NE2	2.31	0.63
1:C:2414:ASN:N	1:C:2417:THR:OG1	2.32	0.62
1:C:2557:ILE:HA	4:D:3:FUC:H4	1.82	0.61
2:B:946:PHE:CD2	2:B:973:VAL:HG12	2.34	0.61
1:C:2559:ASN:HD22	1:C:2815:LEU:HD22	1.65	0.60
1:C:2604:PRO:O	1:C:2607:ARG:NH1	2.34	0.60
1:C:2459:ARG:NH2	2:B:969:VAL:O	2.34	0.59
1:C:2374:ILE:HD11	1:C:2379:LEU:HD22	1.82	0.59
2:B:922:VAL:O	2:B:926:ASN:ND2	2.36	0.59
1:C:2486:SER:HG	1:C:2489:THR:HG1	1.51	0.58
1:C:2629:THR:O	1:C:2744:THR:OG1	2.16	0.58
1:C:2646:VAL:HG11	1:C:2698:LEU:HD22	1.85	0.58
2:B:897:ASN:HB3	2:B:900:ALA:HB3	1.86	0.58
1:C:2512:ALA:CB	1:C:2538:ILE:HD11	2.33	0.57
1:C:2520:THR:O	1:C:2550:GLN:NE2	2.37	0.56
1:C:2622:PHE:HZ	1:C:2645:LEU:HD23	1.70	0.56
1:C:2680:MET:SD	1:C:2680:MET:N	2.76	0.56
1:C:2637:GLU:OE1	1:C:2805:ASN:ND2	2.34	0.55
1:C:2414:ASN:OD1	1:C:2416:ASP:N	2.40	0.54
1:C:2509:ARG:NH2	1:C:2589:ASP:OD2	2.40	0.54
2:B:946:PHE:HD2	2:B:973:VAL:HG12	1.72	0.54
1:C:2383:ILE:HG21	2:B:601:THR:CG2	2.38	0.54
1:C:2669:HIS:O	1:C:2709:LEU:HD11	2.07	0.54
2:B:833:ASP:OD1	2:B:937:ARG:NH1	2.41	0.54
2:B:954:ASN:HB3	5:B:1101:NAG:H2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2544:THR:OG1	1:C:2566:LEU:O	2.23	0.53
2:B:989:SER:OG	2:B:992:ASP:O	2.26	0.53
1:C:2425:VAL:O	1:C:2429:VAL:HG13	2.09	0.53
1:C:2578:LEU:HA	1:C:2581:VAL:HG12	1.91	0.52
1:C:2622:PHE:CZ	1:C:2645:LEU:HD23	2.45	0.52
2:B:876:ARG:NH1	2:B:894:LEU:O	2.43	0.52
2:B:594:VAL:HG11	3:A:596:ILE:HD12	1.91	0.51
1:C:2507:LEU:H	1:C:2507:LEU:HD23	1.77	0.50
1:C:2414:ASN:OD1	1:C:2414:ASN:C	2.54	0.50
2:B:880:LEU:CD2	2:B:928:ILE:HD11	2.34	0.50
2:B:899:THR:OG1	4:E:1:NAG:O5	2.30	0.49
1:C:2371:GLY:N	2:B:586:ASP:O	2.45	0.49
1:C:2629:THR:HG1	1:C:2713:ARG:HH21	1.60	0.49
1:C:2798:VAL:CG1	1:C:2809:LEU:HD11	2.42	0.49
2:B:590:THR:OG1	2:B:591:GLU:N	2.45	0.49
1:C:2689:LEU:HD11	1:C:2727:PHE:HD1	1.77	0.49
1:C:2688:SER:OG	1:C:2689:LEU:N	2.46	0.49
1:C:2500:LYS:NZ	2:B:1019:CYS:O	2.41	0.49
1:C:2649:LEU:O	1:C:2695:LYS:NZ	2.40	0.48
2:B:879:LEU:O	2:B:880:LEU:HD22	2.13	0.48
1:C:2516:SER:HB3	1:C:2544:THR:HG22	1.95	0.48
1:C:2735:ASP:OD1	1:C:2736:LEU:N	2.47	0.48
1:C:2590:ILE:HD11	1:C:2605:SER:N	2.29	0.48
1:C:2698:LEU:C	1:C:2698:LEU:HD23	2.38	0.48
1:C:2611:ALA:O	1:C:2614:SER:OG	2.32	0.48
1:C:2403:LEU:HD11	1:C:2513:VAL:HG23	1.95	0.48
1:C:2383:ILE:HA	3:A:600:ILE:HD11	1.95	0.47
2:B:900:ALA:HB2	4:E:1:NAG:C7	2.44	0.47
1:C:2388:PRO:O	3:A:608:GLU:N	2.47	0.47
2:B:900:ALA:HB2	4:E:1:NAG:N2	2.28	0.47
2:B:972:THR:O	2:B:972:THR:HG23	2.15	0.47
1:C:2379:LEU:HD11	3:A:596:ILE:HD11	1.95	0.47
1:C:2668:GLN:NE2	1:C:2707:THR:O	2.48	0.47
2:B:1014:PHE:O	2:B:1018:ILE:HG12	2.15	0.46
1:C:2534:SER:O	1:C:2811:ARG:NH2	2.40	0.46
1:C:2465:ARG:HB3	1:C:2468:VAL:HG12	1.98	0.46
1:C:2418:PHE:HD1	1:C:2418:PHE:O	1.98	0.46
1:C:2557:ILE:O	1:C:2557:ILE:CD1	2.62	0.46
1:C:2383:ILE:HG21	2:B:601:THR:HG21	1.97	0.45
1:C:2551:LEU:O	1:C:2555:LEU:HD12	2.16	0.45
2:B:855:PHE:O	2:B:859:VAL:HG22	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:GLU:OE2	2:B:912:ASN:ND2	2.49	0.45
1:C:2422:ARG:NH1	1:C:2476:LEU:O	2.49	0.45
1:C:2549[A]:ARG:NH2	1:C:2553:ASN:OD1	2.50	0.44
2:B:917:VAL:HG11	2:B:988:LEU:HD11	2.00	0.44
1:C:2383:ILE:O	1:C:2387:CYS:HB2	2.17	0.44
1:C:2651:MET:HA	1:C:2651:MET:HE2	2.00	0.44
1:C:2426:LEU:HD11	1:C:2474:LYS:HG3	2.00	0.44
1:C:2644:TYR:OH	1:C:2814:ARG:NH1	2.47	0.43
2:B:595:MET:SD	3:A:603:MET:CE	3.07	0.43
1:C:2667:VAL:HG13	1:C:2683:VAL:HB	1.99	0.43
1:C:2719:ILE:HD13	1:C:2759:ILE:HD11	2.00	0.43
1:C:2561:ALA:HB2	1:C:2607:ARG:HE	1.83	0.43
1:C:2594:ASP:O	1:C:2595:PRO:C	2.61	0.43
2:B:594:VAL:CG1	3:A:596:ILE:HD12	2.48	0.43
1:C:2379:LEU:HD23	2:B:597:TYR:CE1	2.53	0.43
1:C:2728:GLU:OE2	1:C:2765:LYS:NZ	2.25	0.43
1:C:2619:ASP:OD1	1:C:2689:LEU:HD22	2.19	0.43
1:C:2407:LEU:HD21	1:C:2425:VAL:HG21	2.01	0.42
1:C:2590:ILE:HG12	1:C:2591:CYS:HB2	2.01	0.42
1:C:2399:PHE:O	1:C:2400:PRO:C	2.62	0.42
1:C:2559:ASN:N	1:C:2559:ASN:OD1	2.52	0.42
2:B:831:PRO:HB2	2:B:940:ALA:HB2	2.02	0.42
1:C:2370:ARG:NH1	1:C:2805:ASN:O	2.50	0.42
1:C:2594:ASP:O	1:C:2596:SER:N	2.52	0.41
2:B:980:VAL:HG21	2:B:985:LEU:HD21	2.01	0.41
1:C:2807:GLU:N	1:C:2808:PRO:HD2	2.35	0.41
1:C:2517:ASN:O	1:C:2545:ARG:NH2	2.54	0.41
1:C:2621:ALA:HB2	1:C:2727:PHE:CE1	2.56	0.41
1:C:2618:ILE:HD11	1:C:2738:ILE:HD13	2.03	0.41
2:B:827:CYS:HB3	2:B:1019:CYS:C	2.46	0.41
1:C:2663:ARG:NH1	1:C:2731:PRO:O	2.43	0.41
1:C:2497:ASN:OD1	2:B:830:ARG:NH1	2.54	0.41
1:C:2798:VAL:O	1:C:2798:VAL:HG23	2.20	0.41
2:B:917:VAL:HG23	2:B:952:THR:CG2	2.50	0.41
2:B:596:THR:OG1	2:B:600:GLU:OE1	2.37	0.41
1:C:2557:ILE:O	1:C:2557:ILE:CG1	2.69	0.40
1:C:2429:VAL:HG23	1:C:2470:LEU:HD21	2.03	0.40
1:C:2683:VAL:HG22	1:C:2721:TYR:CD2	2.56	0.40
1:C:2756:GLN:HG3	1:C:2757:ARG:N	2.37	0.40
2:B:815:ASP:N	2:B:815:ASP:OD1	2.53	0.40
1:C:2405:PHE:HB2	1:C:2447:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	454/492 (92%)	409 (90%)	45 (10%)	0	100	100
2	B	223/476 (47%)	211 (95%)	11 (5%)	1 (0%)	30	60
3	A	23/479 (5%)	19 (83%)	4 (17%)	0	100	100
All	All	700/1447 (48%)	639 (91%)	60 (9%)	1 (0%)	50	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	824	VAL

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	C	393/418 (94%)	391 (100%)	2 (0%)	86	92
2	B	192/400 (48%)	191 (100%)	1 (0%)	86	92
3	A	17/395 (4%)	17 (100%)	0	100	100
All	All	602/1213 (50%)	599 (100%)	3 (0%)	90	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2521[A]	ARG
1	C	2521[B]	ARG
2	B	954	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2564	HIS
1	C	2669	HIS
1	C	2725	ASN
2	B	998	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	1,4	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	D	2	4	14,14,15	0.17	0	17,19,21	0.43	0
4	FUC	D	3	4	10,10,11	0.74	0	14,14,16	0.66	0
4	NAG	E	1	2,4	14,14,15	0.45	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.25	0	17,19,21	0.44	0
4	FUC	E	3	4	10,10,11	0.66	0	14,14,16	1.07	2 (14%)

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	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1
4	NAG	E	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	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(°)
4	E	3	FUC	C1-O5-C5	2.49	118.41	112.78
4	E	3	FUC	O5-C5-C4	2.09	113.26	109.52

There are no chirality outliers.

All (13) torsion outliers are listed below:

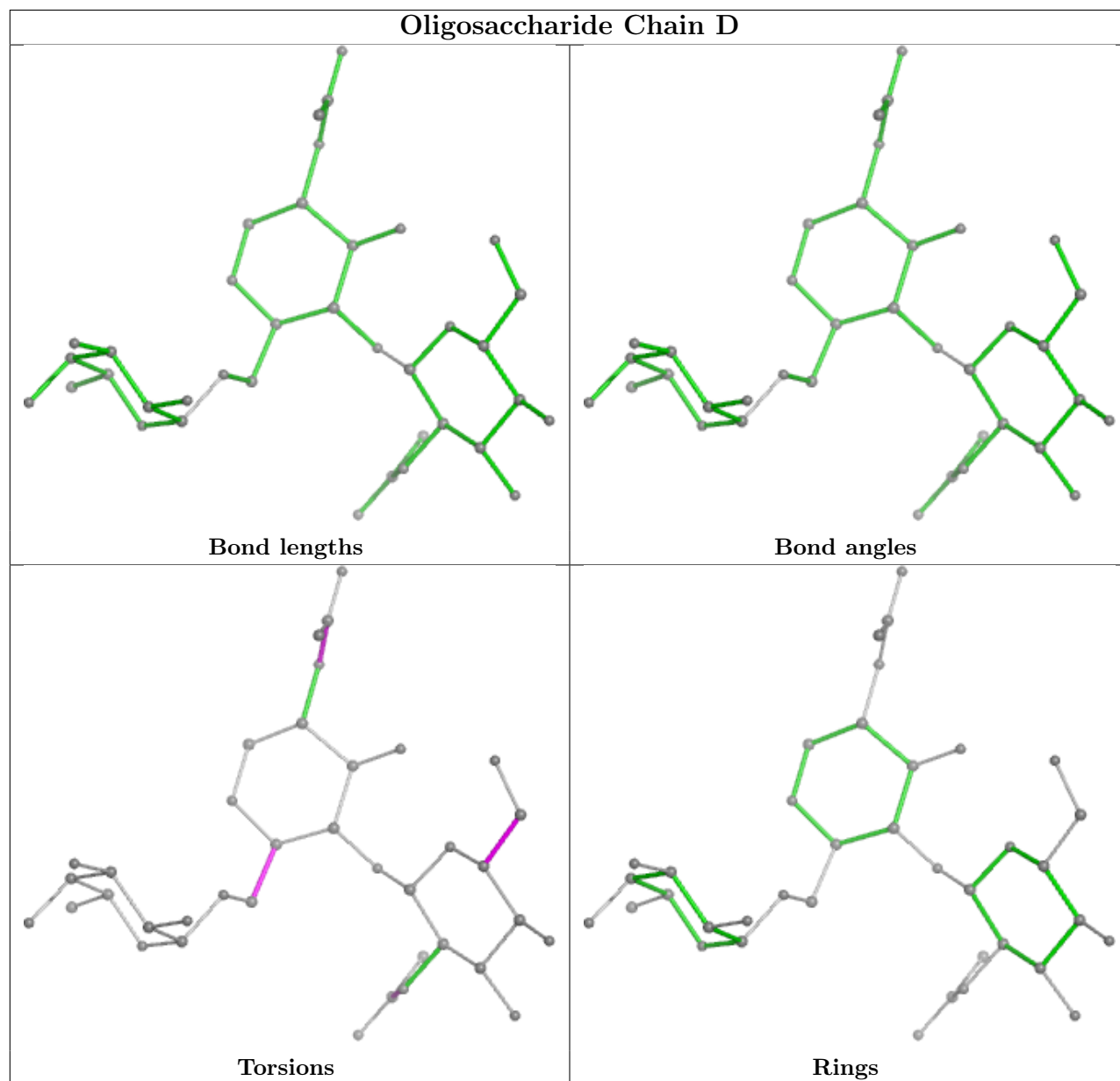
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

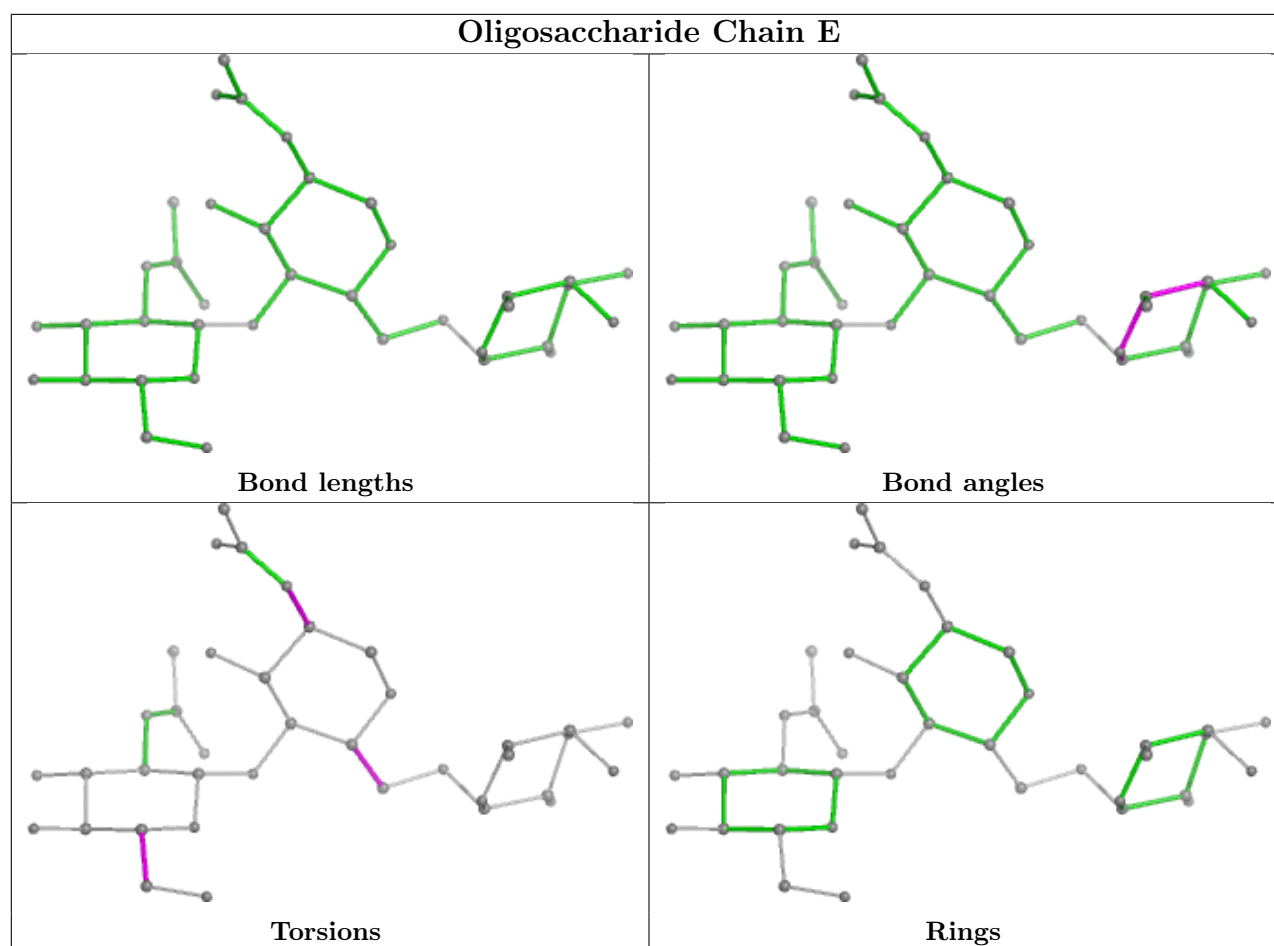
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	3	0
4	D	3	FUC	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](#)

2 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	$\# Z > 2$
5	NAG	B	1101	2	14,14,15	0.19	0	17,19,21	0.33	0
5	NAG	C	2901	1	14,14,15	0.26	0	17,19,21	0.39	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
5	NAG	B	1101	2	-	3/6/23/26	0/1/1/1
5	NAG	C	2901	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	NAG	C4-C5-C6-O6
5	C	2901	NAG	O5-C5-C6-O6
5	B	1101	NAG	O5-C5-C6-O6
5	C	2901	NAG	C4-C5-C6-O6
5	C	2901	NAG	C8-C7-N2-C2
5	C	2901	NAG	O7-C7-N2-C2
5	B	1101	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	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.

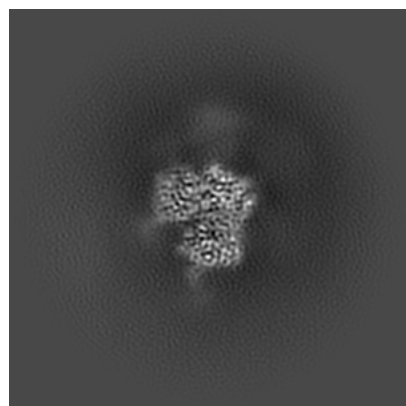
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51567. These allow visual inspection of the internal detail of the map and identification of artifacts.

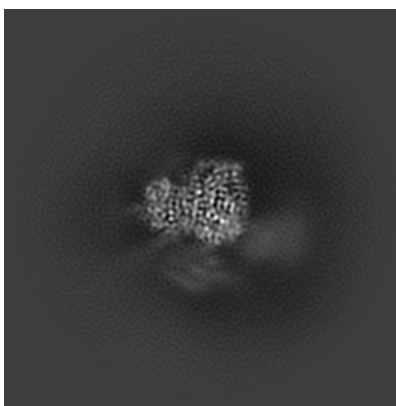
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

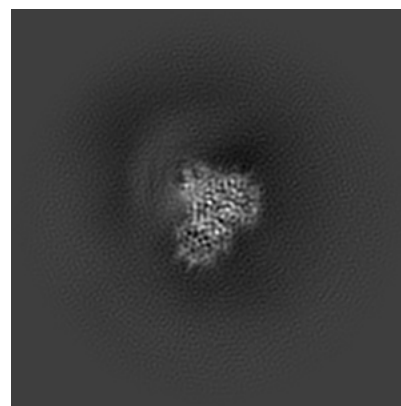
6.1.1 Primary map



X

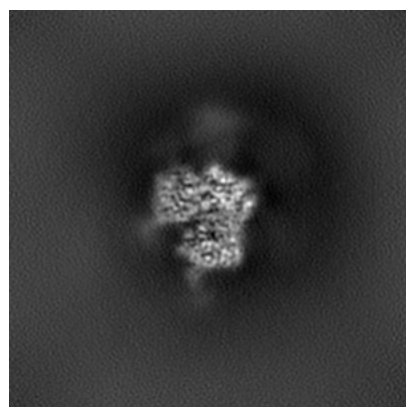


Y

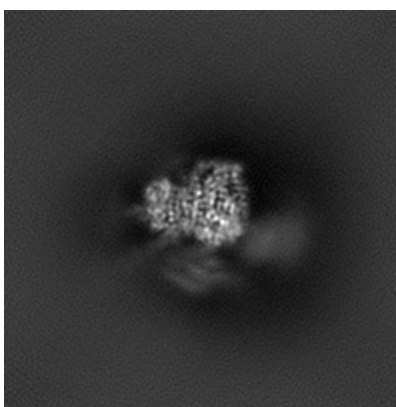


Z

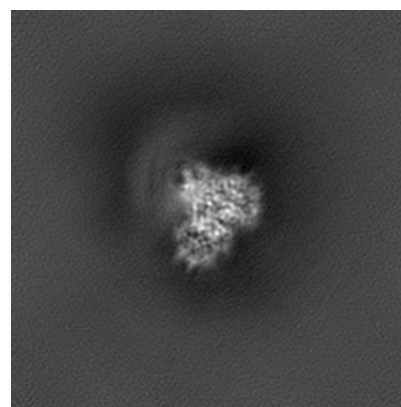
6.1.2 Raw map



X



Y

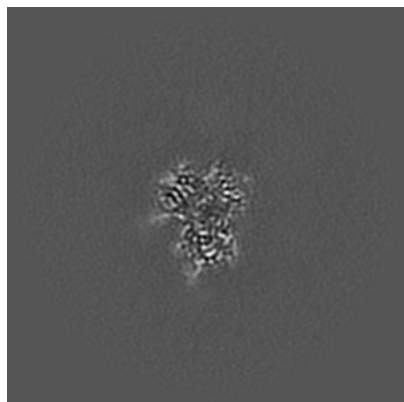


Z

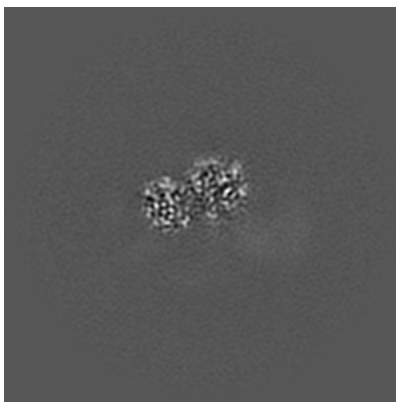
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

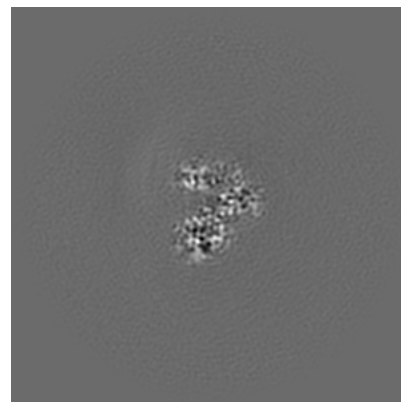
6.2.1 Primary map



X Index: 100

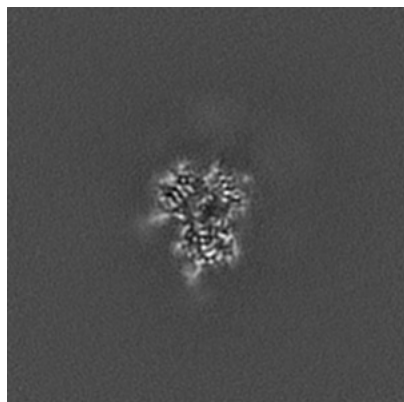


Y Index: 100

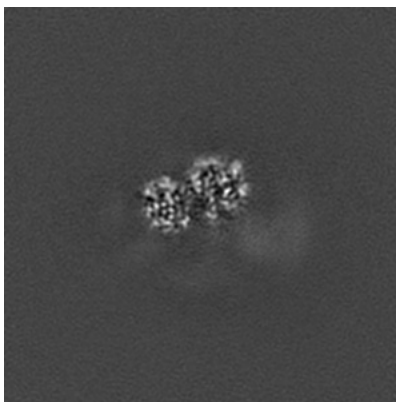


Z Index: 100

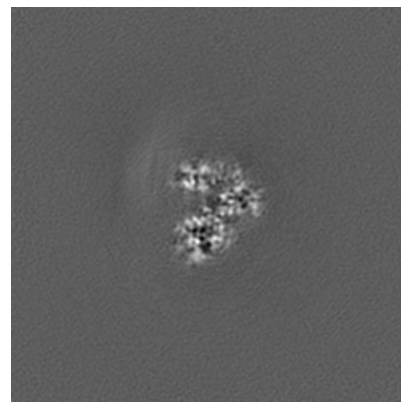
6.2.2 Raw map



X Index: 100



Y Index: 100

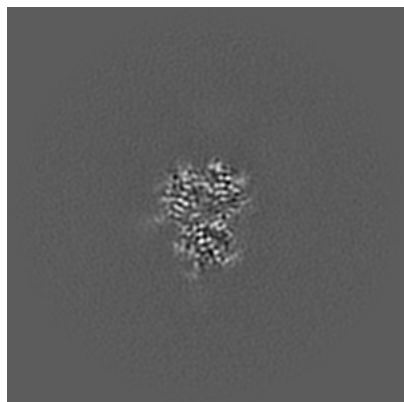


Z Index: 100

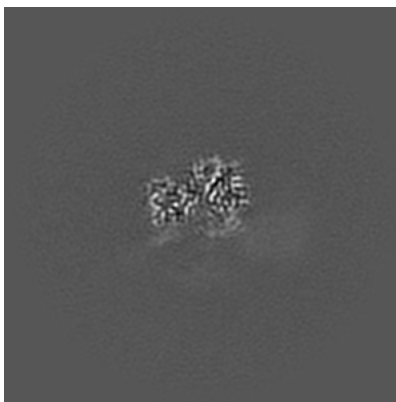
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

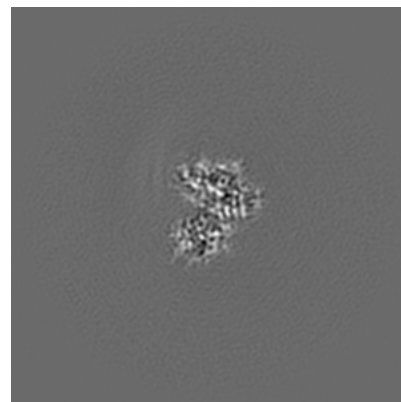
6.3.1 Primary map



X Index: 102

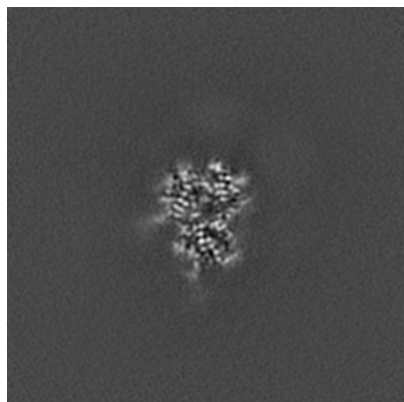


Y Index: 106

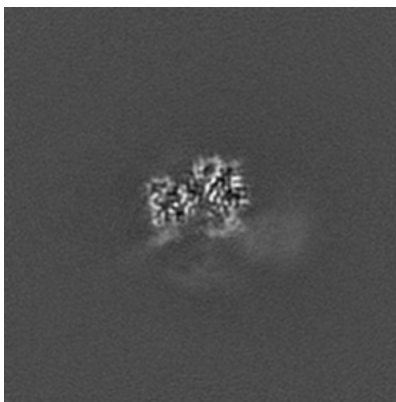


Z Index: 103

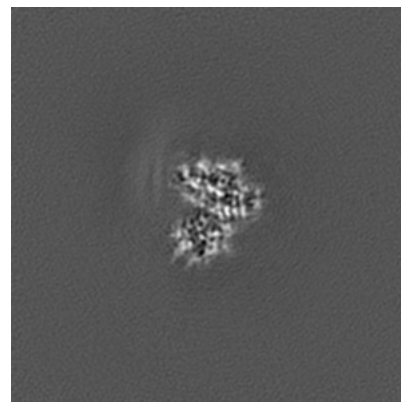
6.3.2 Raw map



X Index: 102



Y Index: 106

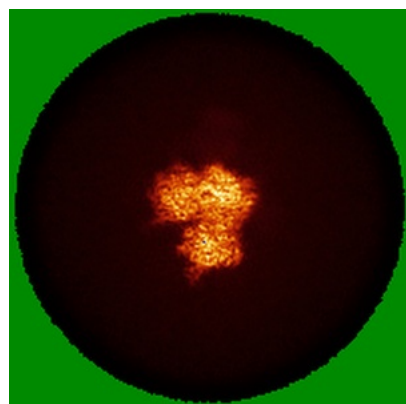


Z Index: 103

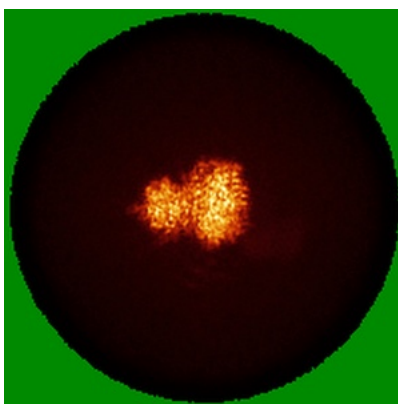
The images above show the largest variance slices of the map in three orthogonal directions.

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

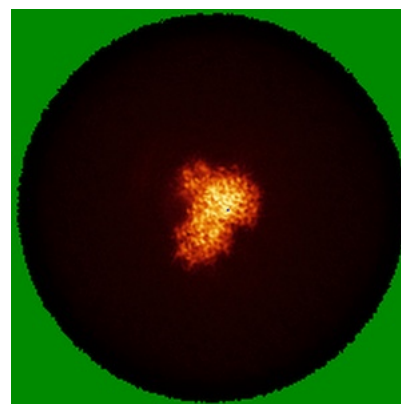
6.4.1 Primary map



X

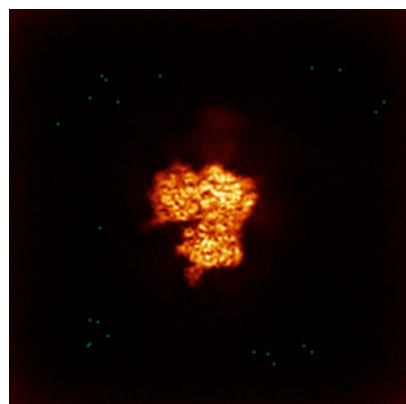


Y

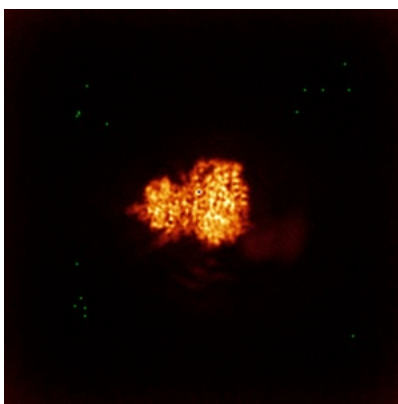


Z

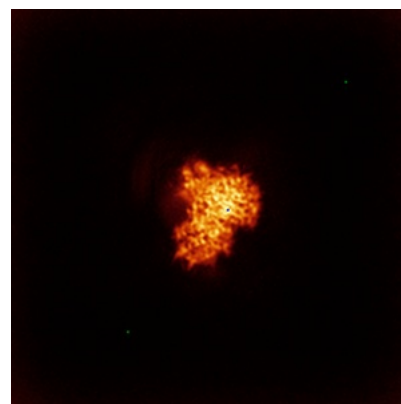
6.4.2 Raw map



X



Y

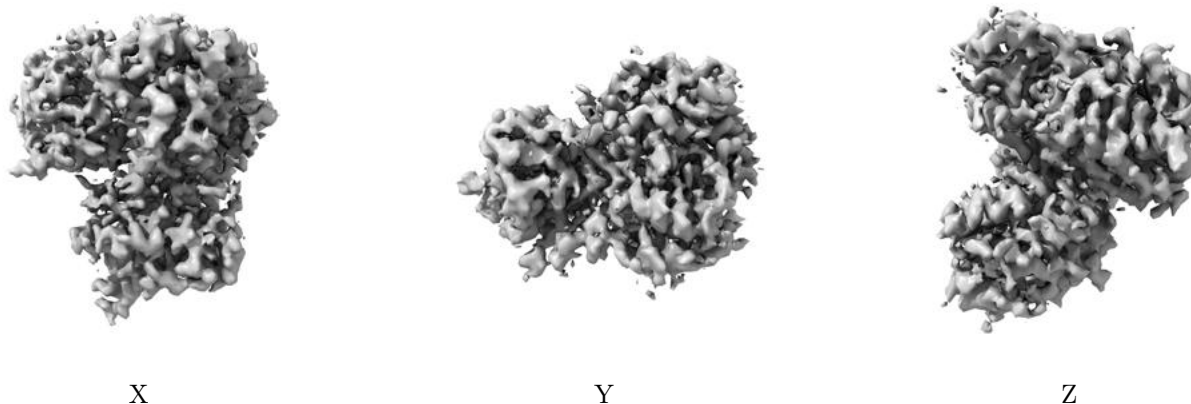


Z

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

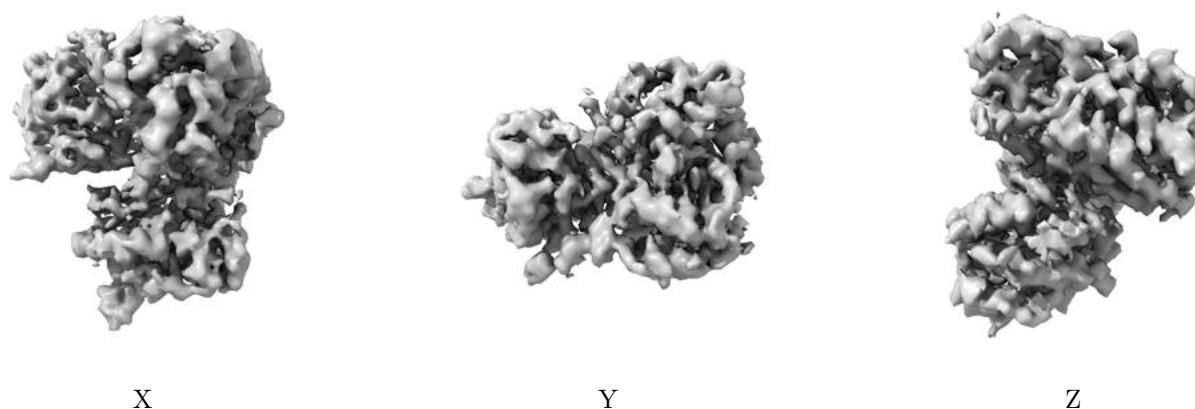
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.242. 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.

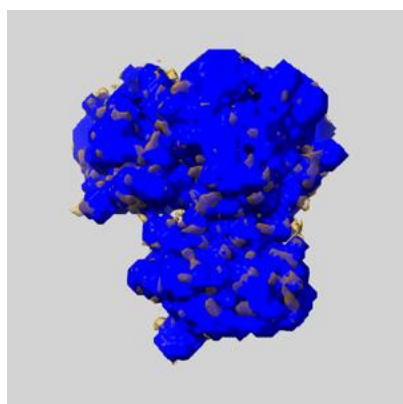
6.6 Mask visualisation [i](#)

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

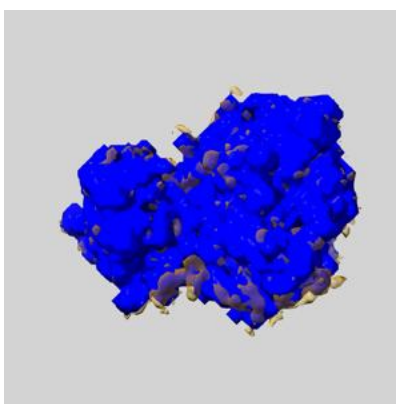
A mask typically either:

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

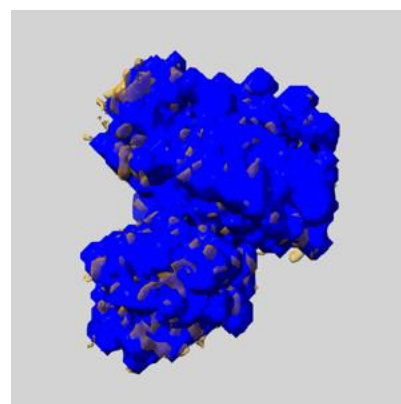
6.6.1 emd_51567_msk_1.map [i](#)



X



Y

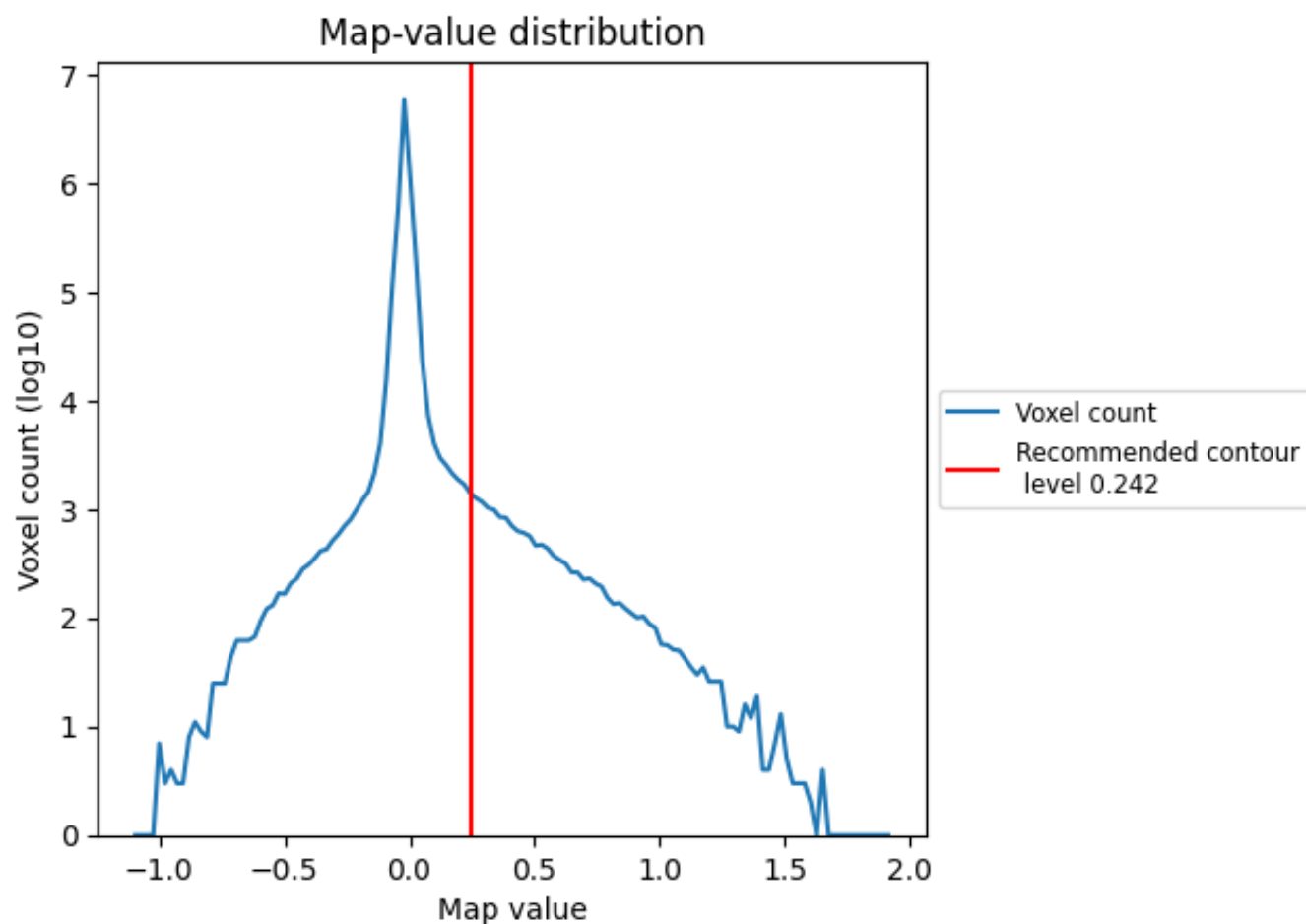


Z

7 Map analysis [i](#)

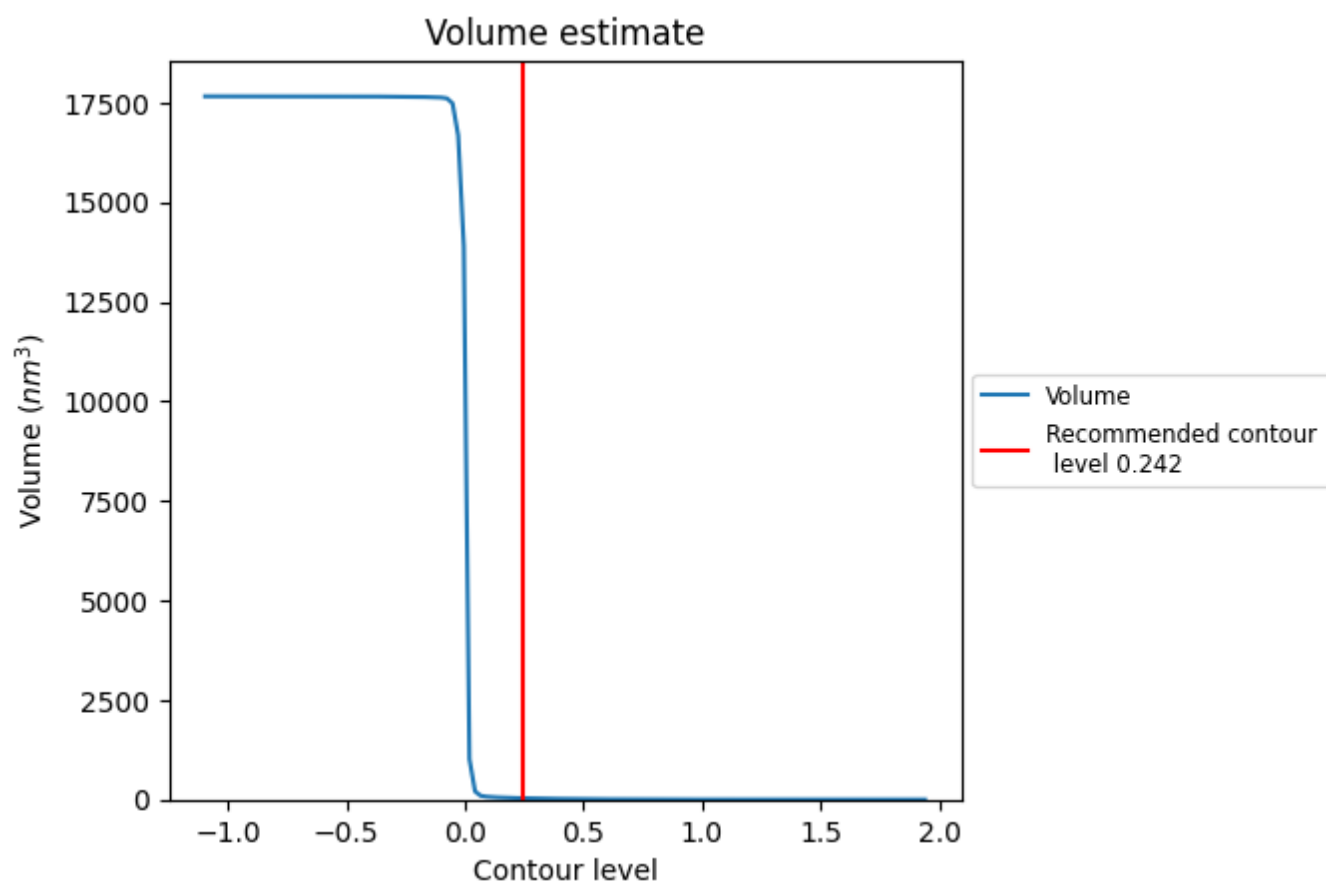
This section contains the results of statistical analysis of the map.

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.

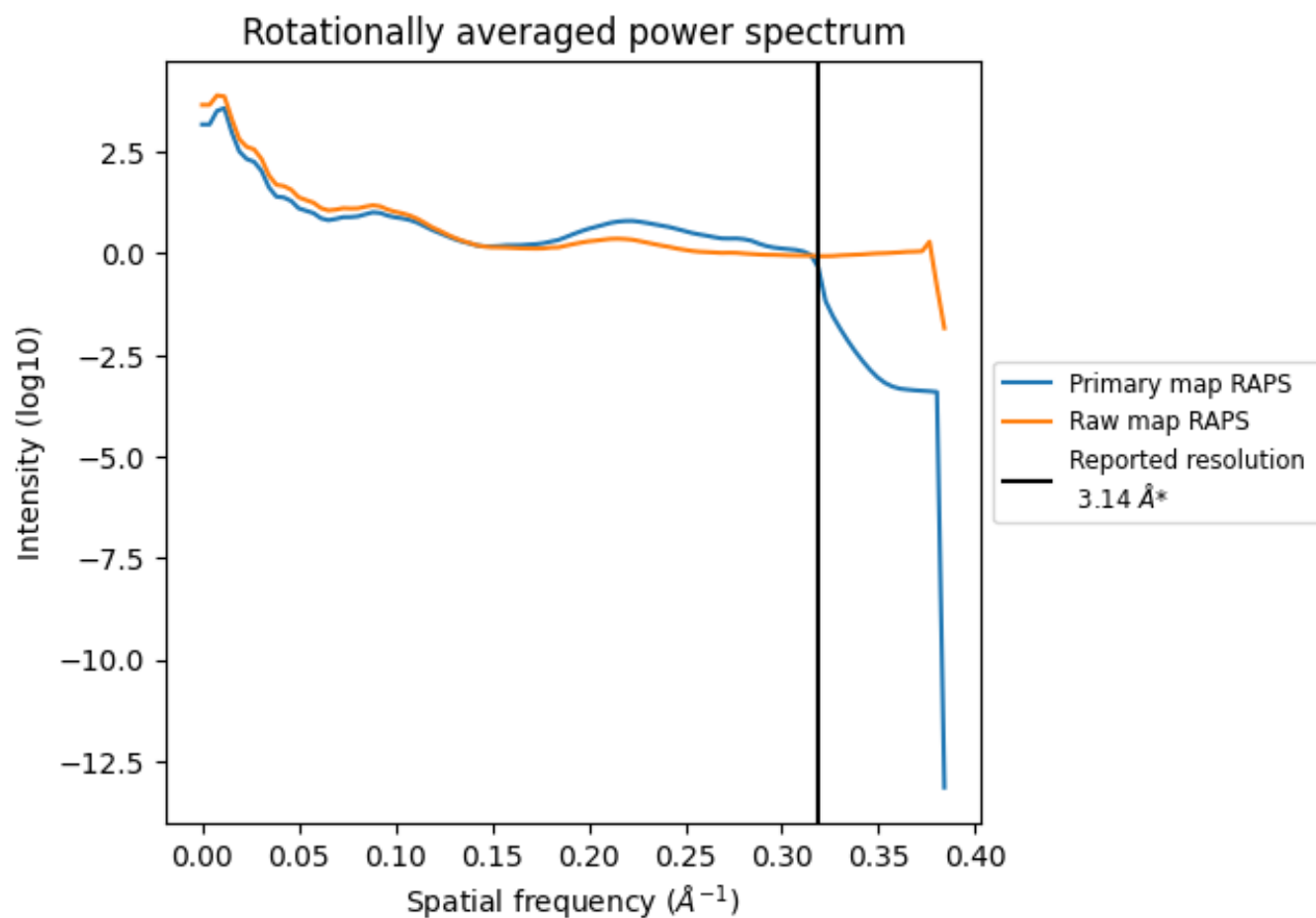
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm³; this corresponds to an approximate mass of 31 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 ⓘ

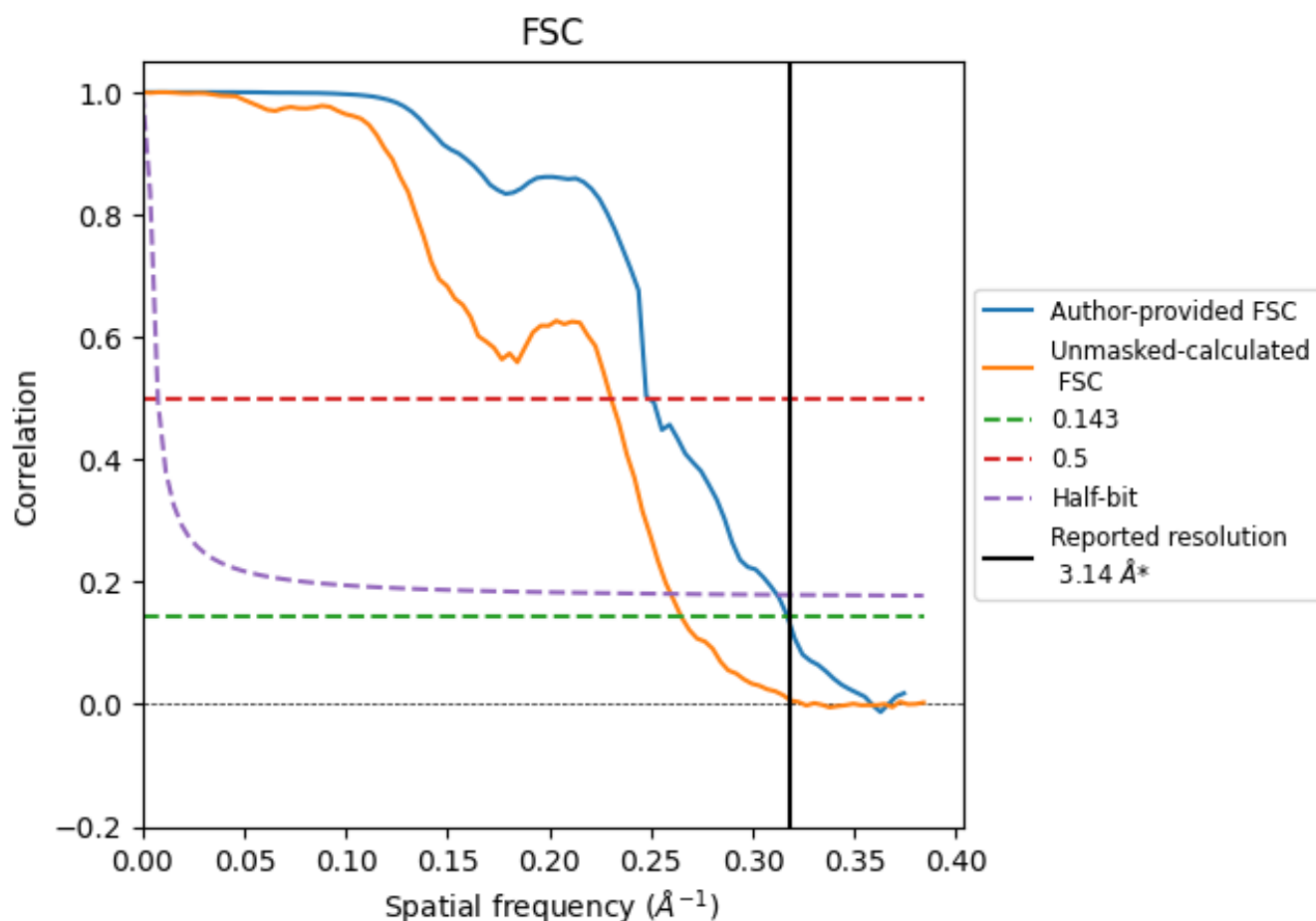


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 0.318 \AA^{-1}

8.2 Resolution estimates [i](#)

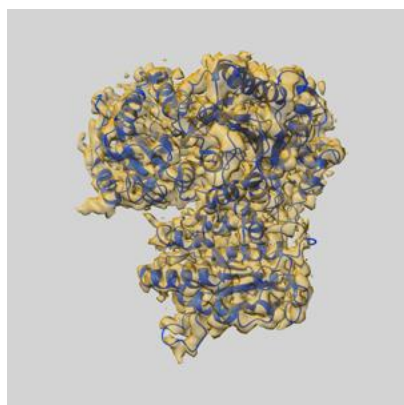
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.15	4.02	3.21
Unmasked-calculated*	3.78	4.34	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.14 by more than 10 %

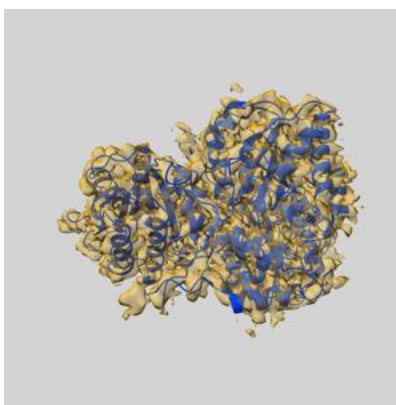
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51567 and PDB model 9GTU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

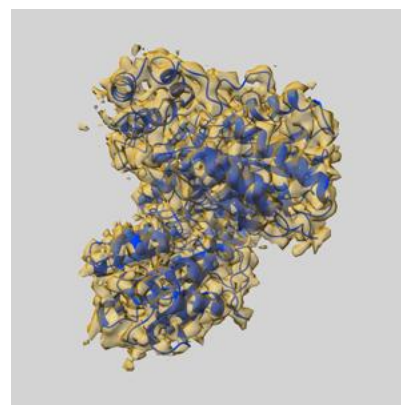
9.1 Map-model overlay [i](#)



X



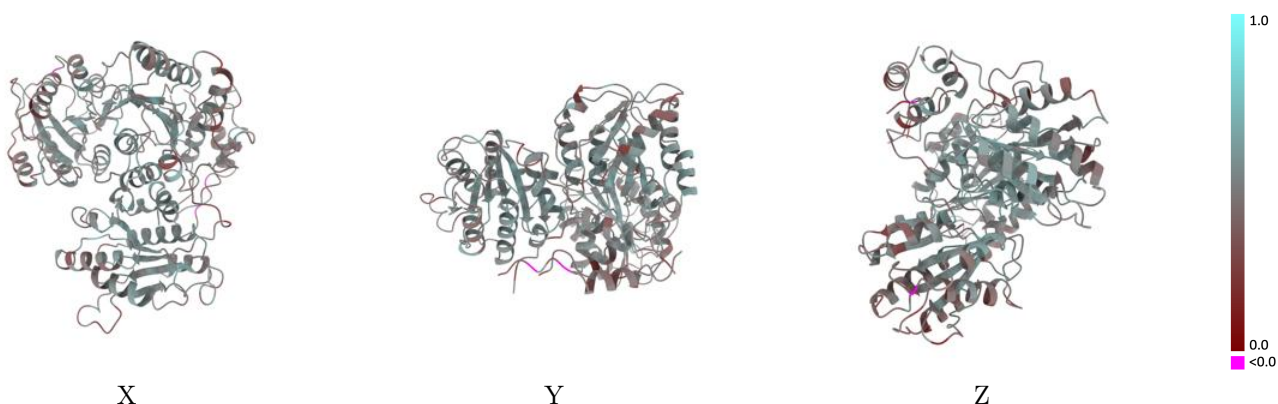
Y



Z

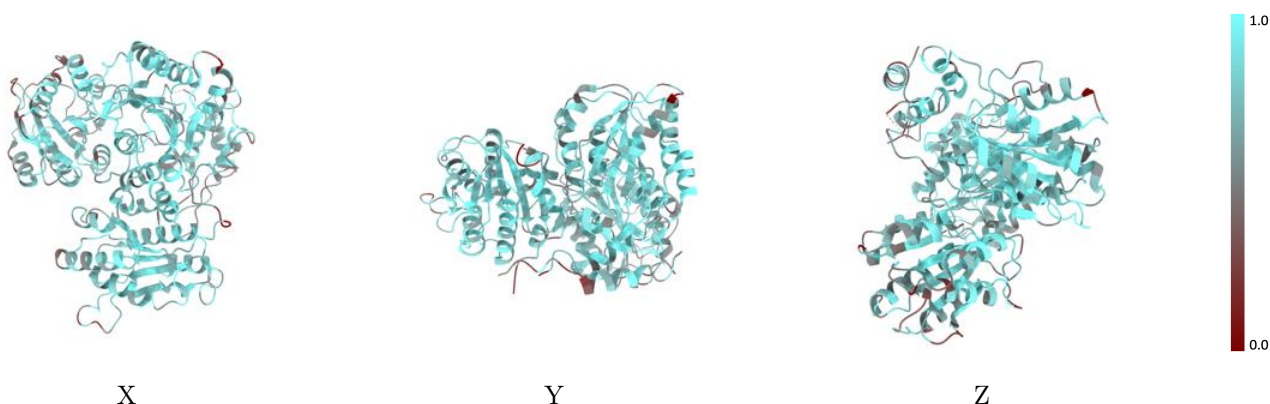
The images above show the 3D surface view of the map at the recommended contour level 0.242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



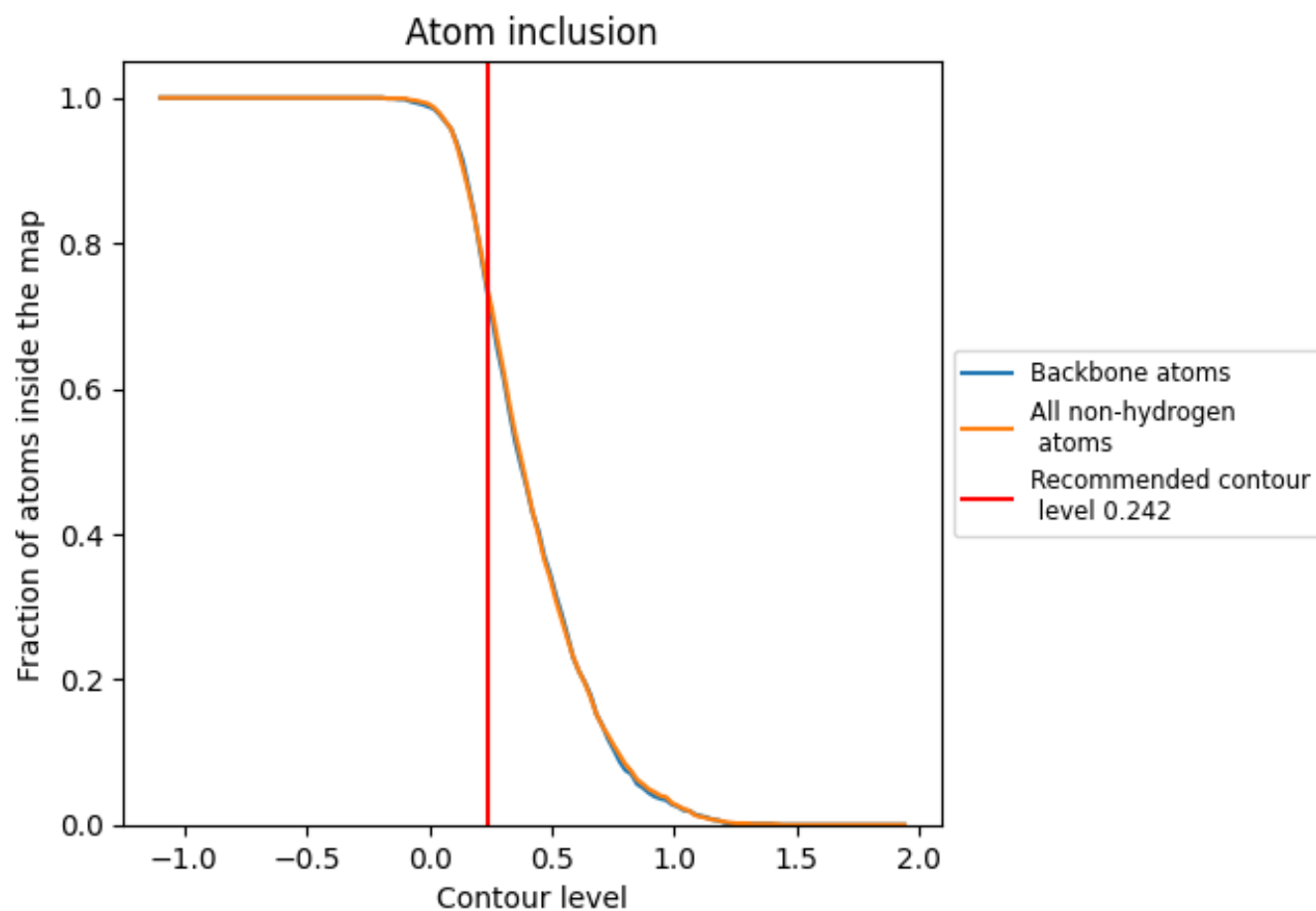
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.242).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 73% 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 (0.242) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7300	<div></div> 0.4770
A	<div></div> 0.5780	<div></div> 0.3790
B	<div></div> 0.7050	<div></div> 0.4520
C	<div></div> 0.7820	<div></div> 0.4970
D	<div></div> 0.2100	<div></div> 0.4040
E	<div></div> 0.2100	<div></div> 0.2780

