Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:19 AM EST

PDB ID	:	7MN5
EMDB ID	:	EMD-23916
Title	:	Structure of the HER2/HER3/NRG1b Heterodimer Extracellular Domain
Authors	:	Diwanji, D.; Trenker, R.; Verba, K.A.; Jura, N.
Deposited on	:	2021-04-30
Resolution	:	2.93 Å(reported)
Based on initial models	:	1N8Z, 3U7U, 1M6B

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:

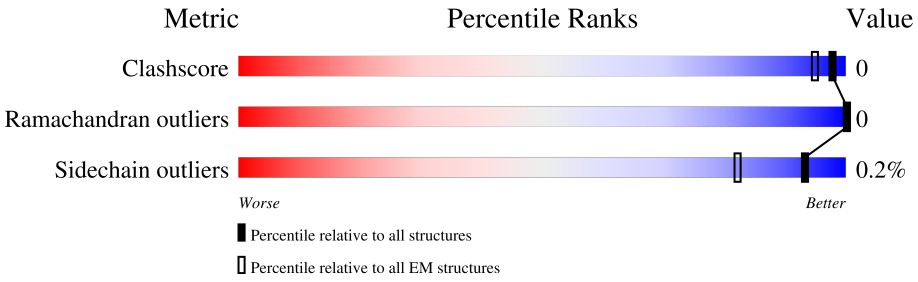
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.93 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	1066	7%, 54%, 45%
2	H	87	53%, 44%
3	B	1455	39%, 60%
4	C	4	50%, 100%
5	D	2	50%, 100%
5	E	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9526 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	585	4496	2776	814	848	58	0	0

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	809	ARG	GLN	conflict	UNP P21860
A	928	GLY	GLU	conflict	UNP P21860
A	1022	GLY	-	expression tag	UNP P21860
A	1023	GLY	-	expression tag	UNP P21860
A	1024	SER	-	expression tag	UNP P21860
A	1025	LEU	-	expression tag	UNP P21860
A	1026	GLU	-	expression tag	UNP P21860
A	1027	VAL	-	expression tag	UNP P21860
A	1028	LEU	-	expression tag	UNP P21860
A	1029	PHE	-	expression tag	UNP P21860
A	1030	GLN	-	expression tag	UNP P21860
A	1031	GLY	-	expression tag	UNP P21860
A	1032	PRO	-	expression tag	UNP P21860
A	1033	SER	-	expression tag	UNP P21860
A	1034	SER	-	expression tag	UNP P21860
A	1035	PRO	-	expression tag	UNP P21860
A	1036	SER	-	expression tag	UNP P21860
A	1037	ALA	-	expression tag	UNP P21860
A	1038	TRP	-	expression tag	UNP P21860
A	1039	SER	-	expression tag	UNP P21860
A	1040	HIS	-	expression tag	UNP P21860
A	1041	PRO	-	expression tag	UNP P21860
A	1042	GLN	-	expression tag	UNP P21860
A	1043	PHE	-	expression tag	UNP P21860
A	1044	GLU	-	expression tag	UNP P21860
A	1045	LYS	-	expression tag	UNP P21860
A	1046	GLY	-	expression tag	UNP P21860
A	1047	GLY	-	expression tag	UNP P21860

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1048	GLY	-	expression tag	UNP P21860
A	1049	SER	-	expression tag	UNP P21860
A	1050	GLY	-	expression tag	UNP P21860
A	1051	GLY	-	expression tag	UNP P21860
A	1052	GLY	-	expression tag	UNP P21860
A	1053	SER	-	expression tag	UNP P21860
A	1054	GLY	-	expression tag	UNP P21860
A	1055	GLY	-	expression tag	UNP P21860
A	1056	SER	-	expression tag	UNP P21860
A	1057	SER	-	expression tag	UNP P21860
A	1058	ALA	-	expression tag	UNP P21860
A	1059	TRP	-	expression tag	UNP P21860
A	1060	SER	-	expression tag	UNP P21860
A	1061	HIS	-	expression tag	UNP P21860
A	1062	PRO	-	expression tag	UNP P21860
A	1063	GLN	-	expression tag	UNP P21860
A	1064	PHE	-	expression tag	UNP P21860
A	1065	GLU	-	expression tag	UNP P21860
A	1066	LYS	-	expression tag	UNP P21860

- Molecule 2 is a protein called Isoform 6 of Pro-neuregulin-1, membrane-bound isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	49	Total	C	N	O	S	0	0
			383	237	67	71	8		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	175	GLY	-	cloning artifact	UNP Q02297-6
H	176	PRO	-	cloning artifact	UNP Q02297-6
H	237	GLY	-	expression tag	UNP Q02297-6
H	238	SER	-	expression tag	UNP Q02297-6
H	239	GLY	-	expression tag	UNP Q02297-6
H	240	SER	-	expression tag	UNP Q02297-6
H	241	GLY	-	expression tag	UNP Q02297-6
H	242	SER	-	expression tag	UNP Q02297-6
H	243	ASP	-	expression tag	UNP Q02297-6
H	244	TYR	-	expression tag	UNP Q02297-6
H	245	LYS	-	expression tag	UNP Q02297-6
H	246	ASP	-	expression tag	UNP Q02297-6
H	247	ASP	-	expression tag	UNP Q02297-6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	248	ASP	-	expression tag	UNP Q02297-6
H	249	ASP	-	expression tag	UNP Q02297-6
H	250	LYS	-	expression tag	UNP Q02297-6
H	251	ALA	-	expression tag	UNP Q02297-6
H	252	ALA	-	expression tag	UNP Q02297-6
H	253	ALA	-	expression tag	UNP Q02297-6
H	254	LEU	-	expression tag	UNP Q02297-6
H	255	GLU	-	expression tag	UNP Q02297-6
H	256	HIS	-	expression tag	UNP Q02297-6
H	257	HIS	-	expression tag	UNP Q02297-6
H	258	HIS	-	expression tag	UNP Q02297-6
H	259	HIS	-	expression tag	UNP Q02297-6
H	260	HIS	-	expression tag	UNP Q02297-6
H	261	HIS	-	expression tag	UNP Q02297-6

- Molecule 3 is a protein called Receptor tyrosine-protein kinase erbB-2,Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	579	Total	C	N	O	S	0	0
			4471	2783	803	833	52		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	778	ASP	GLY	conflict	UNP P04626
B	1030	GLY	-	linker	UNP P04626
B	1031	GLY	-	linker	UNP P04626
B	1032	SER	-	linker	UNP P04626
B	1033	LEU	-	linker	UNP P04626
B	1034	GLU	-	linker	UNP P04626
B	1035	VAL	-	linker	UNP P04626
B	1036	LEU	-	linker	UNP P04626
B	1037	PHE	-	linker	UNP P04626
B	1038	GLN	-	linker	UNP P04626
B	1039	GLY	-	linker	UNP P04626
B	1040	PRO	-	linker	UNP P04626
B	1041	SER	-	linker	UNP P04626
B	1042	SER	-	linker	UNP P04626
B	1043	PRO	-	linker	UNP P04626
B	1044	SER	-	linker	UNP P04626
B	1045	GLY	-	linker	UNP P04626

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1046	SER	-	linker	UNP P04626
B	1047	SER	-	linker	UNP P04626
B	1048	MET	-	linker	UNP P04626
B	1415	ASN	-	expression tag	UNP P0AEX9
B	1416	SER	-	expression tag	UNP P0AEX9
B	1417	SER	-	expression tag	UNP P0AEX9
B	1418	SER	-	expression tag	UNP P0AEX9
B	1419	SER	-	expression tag	UNP P0AEX9
B	1420	GLY	-	expression tag	UNP P0AEX9
B	1421	PRO	-	expression tag	UNP P0AEX9
B	1422	SER	-	expression tag	UNP P0AEX9
B	1423	SER	-	expression tag	UNP P0AEX9
B	1424	PRO	-	expression tag	UNP P0AEX9
B	1425	SER	-	expression tag	UNP P0AEX9
B	1426	ALA	-	expression tag	UNP P0AEX9
B	1427	TRP	-	expression tag	UNP P0AEX9
B	1428	SER	-	expression tag	UNP P0AEX9
B	1429	HIS	-	expression tag	UNP P0AEX9
B	1430	PRO	-	expression tag	UNP P0AEX9
B	1431	GLN	-	expression tag	UNP P0AEX9
B	1432	PHE	-	expression tag	UNP P0AEX9
B	1433	GLU	-	expression tag	UNP P0AEX9
B	1434	LYS	-	expression tag	UNP P0AEX9
B	1435	GLY	-	expression tag	UNP P0AEX9
B	1436	GLY	-	expression tag	UNP P0AEX9
B	1437	GLY	-	expression tag	UNP P0AEX9
B	1438	SER	-	expression tag	UNP P0AEX9
B	1439	GLY	-	expression tag	UNP P0AEX9
B	1440	GLY	-	expression tag	UNP P0AEX9
B	1441	GLY	-	expression tag	UNP P0AEX9
B	1442	SER	-	expression tag	UNP P0AEX9
B	1443	GLY	-	expression tag	UNP P0AEX9
B	1444	GLY	-	expression tag	UNP P0AEX9
B	1445	SER	-	expression tag	UNP P0AEX9
B	1446	SER	-	expression tag	UNP P0AEX9
B	1447	ALA	-	expression tag	UNP P0AEX9
B	1448	TRP	-	expression tag	UNP P0AEX9
B	1449	SER	-	expression tag	UNP P0AEX9
B	1450	HIS	-	expression tag	UNP P0AEX9
B	1451	PRO	-	expression tag	UNP P0AEX9
B	1452	GLN	-	expression tag	UNP P0AEX9
B	1453	PHE	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1454	GLU	-	expression tag	UNP P0AEX9
B	1455	LYS	-	expression tag	UNP P0AEX9

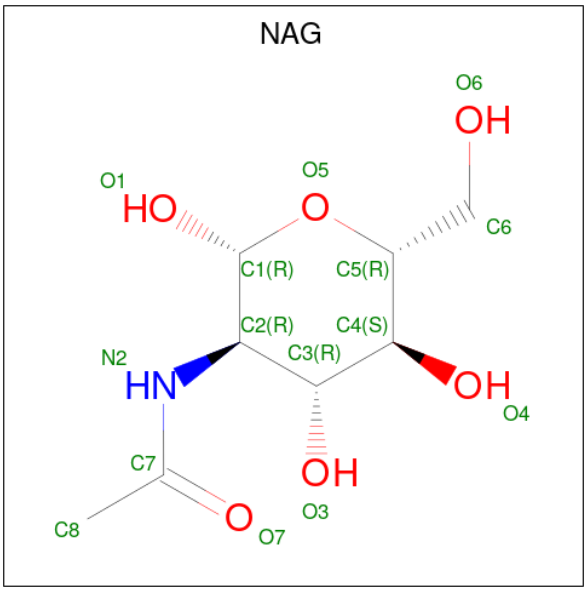
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		

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



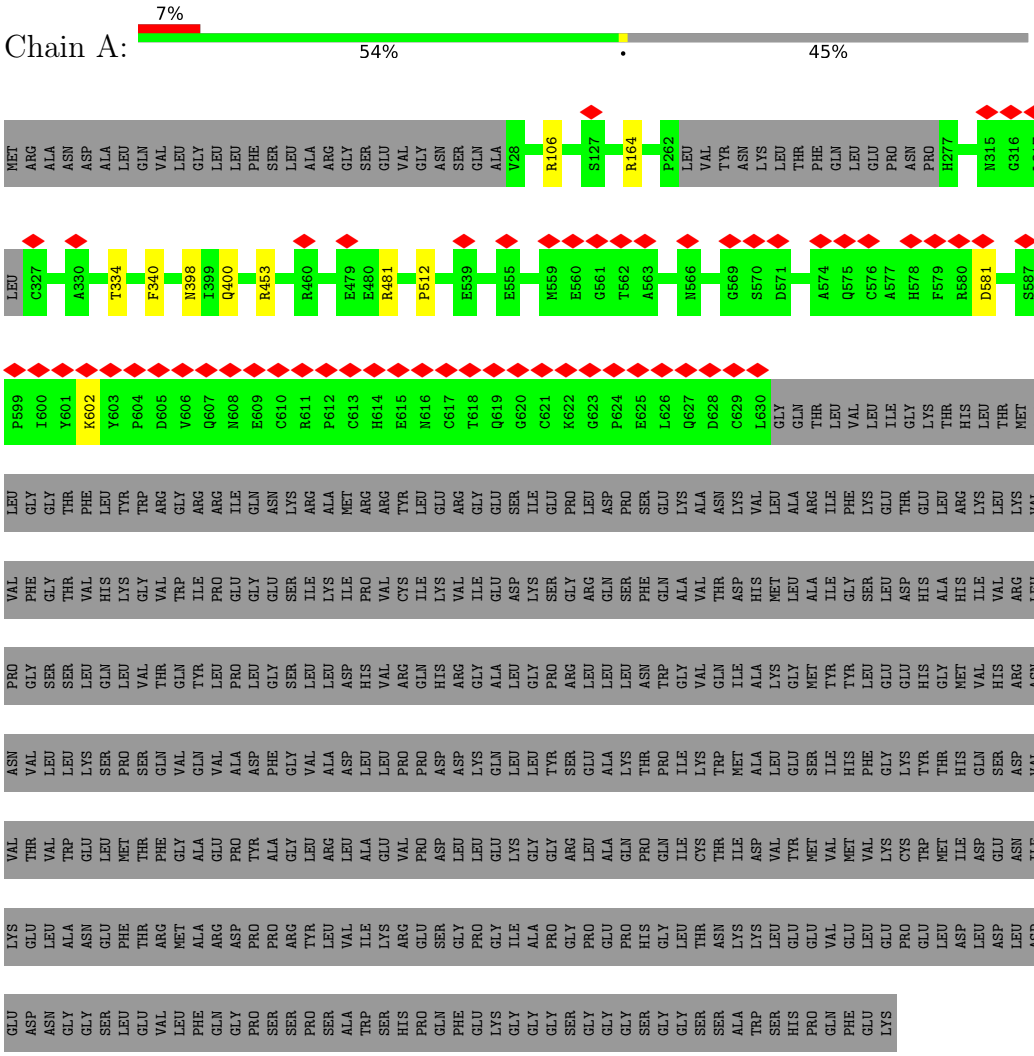
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	B	1	Total	C	N	O	0
			28	16	2	10	

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.

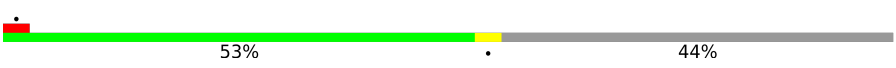
• Molecule 1: Receptor tyrosine-protein kinase erbB-3

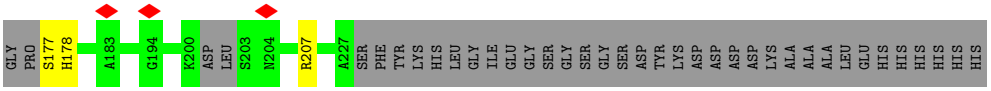
Chain A:



• Molecule 2: Isoform 6 of Pro-neuregulin-1, membrane-bound isoform

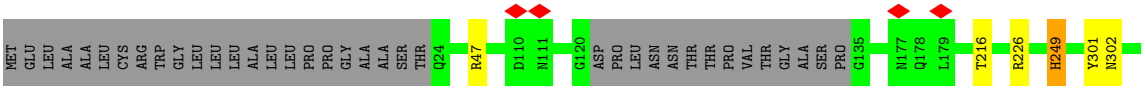
Chain H:

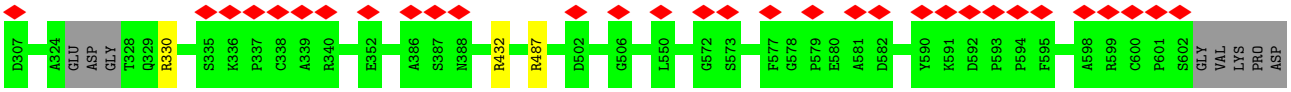


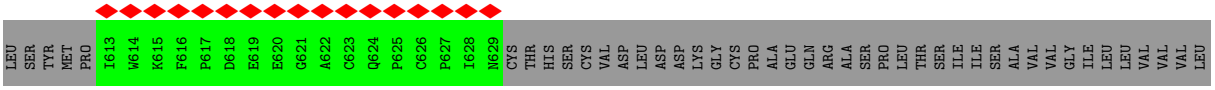


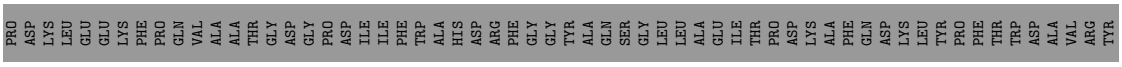
• Molecule 3: Receptor tyrosine-protein kinase erbB-2,Maltose/maltodextrin-binding periplasmic protein

Chain B:









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

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 5: 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, C1	Depositor
Number of particles used	123173	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 ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.471	Depositor
Minimum map value	-1.313	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	300.6, 300.6, 300.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83500004, 0.83500004, 0.83500004	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.70	1/4602 (0.0%)	0.78	4/6241 (0.1%)
2	H	0.77	0/389	0.87	1/518 (0.2%)
3	B	0.71	0/4576	0.73	3/6223 (0.0%)
All	All	0.71	1/9567 (0.0%)	0.76	8/12982 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	PRO	N-CD	-5.35	1.40	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	ARG	NE-CZ-NH1	7.88	124.24	120.30
3	B	47	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	106	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	H	207	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	164	ARG	NE-CZ-NH1	5.40	123.00	120.30
3	B	432	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	B	487	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	453	ARG	NE-CZ-NH1	5.15	122.88	120.30

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	4496	0	4254	3	0
2	H	383	0	363	1	0
3	B	4471	0	4277	3	0
4	C	50	0	43	0	0
5	D	28	0	25	0	0
5	E	28	0	25	0	0
6	A	42	0	39	0	0
6	B	28	0	26	0	0
All	All	9526	0	9052	7	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 0.

All (7) 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:581:ASP:OD1	1:A:602:LYS:NZ	2.39	0.53
3:B:216:THR:OG1	3:B:226:ARG:NH1	2.46	0.48
1:A:398:ASN:HD21	1:A:400:GLN:HE21	1.61	0.48
3:B:249:HIS:ND1	3:B:249:HIS:N	2.61	0.43
2:H:177:SER:OG	2:H:178:HIS:N	2.51	0.43
3:B:301:TYR:O	3:B:302:ASN:HB2	2.19	0.42
1:A:334:THR:OG1	1:A:340:PHE:O	2.31	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	579/1066 (54%)	561 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	45/87 (52%)	43 (96%)	2 (4%)	0	100	100
3	B	571/1455 (39%)	551 (96%)	20 (4%)	0	100	100
All	All	1195/2608 (46%)	1155 (97%)	40 (3%)	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	507/909 (56%)	507 (100%)	0	100	100
2	H	44/74 (60%)	44 (100%)	0	100	100
3	B	499/1229 (41%)	497 (100%)	2 (0%)	91	97
All	All	1050/2212 (48%)	1048 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	249	HIS
3	B	330	ARG

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

Mol	Chain	Res	Type
1	A	398	ASN
3	B	24	GLN
3	B	239	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 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	C	1	4,3	14,14,15	1.09	1 (7%)	17,19,21	0.77	0
4	NAG	C	2	4	14,14,15	1.49	2 (14%)	17,19,21	1.00	1 (5%)
4	BMA	C	3	4	11,11,12	0.77	0	15,15,17	0.97	1 (6%)
4	MAN	C	4	4	11,11,12	1.52	3 (27%)	15,15,17	0.67	0
5	NAG	D	1	1,5	14,14,15	1.25	2 (14%)	17,19,21	0.99	1 (5%)
5	NAG	D	2	5	14,14,15	1.51	2 (14%)	17,19,21	1.01	1 (5%)
5	NAG	E	1	1,5	14,14,15	1.11	1 (7%)	17,19,21	1.11	2 (11%)
5	NAG	E	2	5	14,14,15	1.38	2 (14%)	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
4	NAG	C	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	1/2/19/22	0/1/1/1
4	MAN	C	4	4	-	1/2/19/22	0/1/1/1
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	1/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2	NAG	C1-C2	3.44	1.57	1.52
4	C	2	NAG	C1-C2	3.38	1.57	1.52
5	E	1	NAG	C1-C2	3.17	1.57	1.52
5	E	2	NAG	C1-C2	3.09	1.57	1.52
5	E	2	NAG	O5-C5	2.60	1.48	1.43
4	C	2	NAG	O5-C5	2.60	1.48	1.43
4	C	4	MAN	O5-C5	2.59	1.48	1.43
5	D	2	NAG	O5-C5	2.58	1.48	1.43
5	D	1	NAG	O4-C4	2.57	1.49	1.43
5	D	1	NAG	O5-C5	2.20	1.47	1.43
4	C	1	NAG	O5-C5	2.18	1.47	1.43
4	C	4	MAN	C2-C3	2.15	1.55	1.52
4	C	4	MAN	C1-C2	2.10	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1	NAG	C1-O5-C5	2.77	115.94	112.19
5	D	2	NAG	C8-C7-N2	2.64	120.56	116.10
5	E	1	NAG	C8-C7-N2	2.55	120.41	116.10
4	C	2	NAG	C8-C7-N2	2.52	120.36	116.10
5	E	2	NAG	C8-C7-N2	2.29	119.97	116.10
5	E	1	NAG	C2-N2-C7	-2.27	119.67	122.90
4	C	3	BMA	C2-C3-C4	-2.08	107.30	110.89

There are no chirality outliers.

All (7) torsion outliers are listed below:

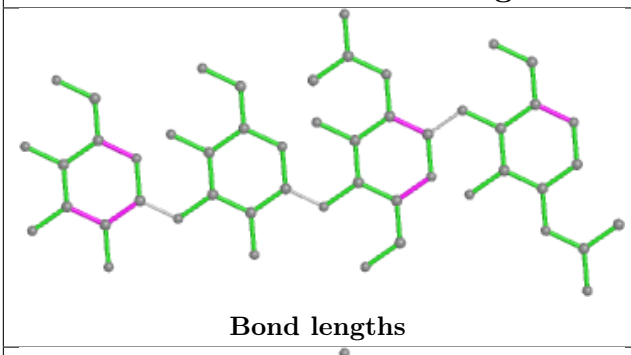
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
4	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

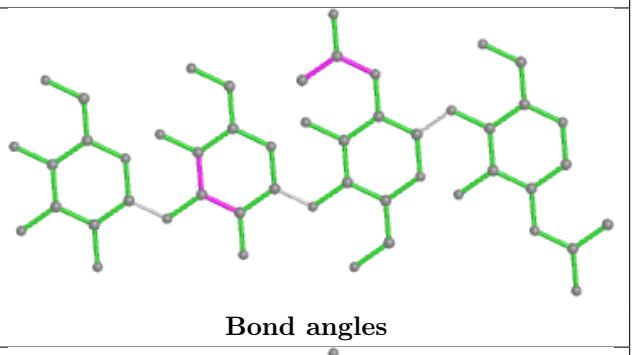
No monomer is involved in short contacts.

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

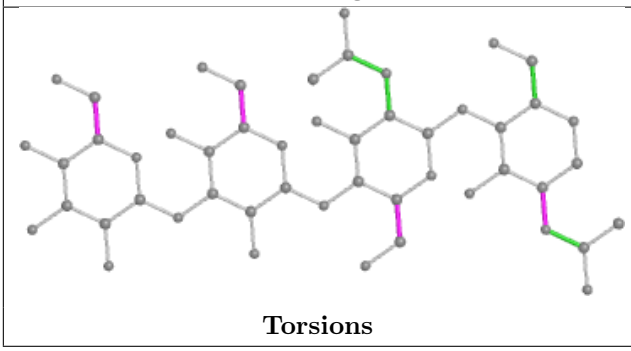
Oligosaccharide Chain C



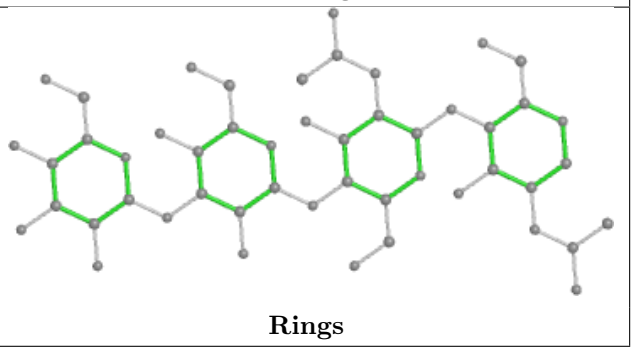
Bond lengths



Bond angles

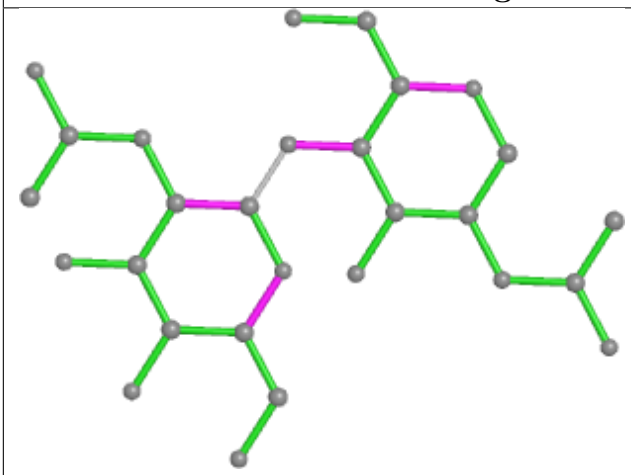


Torsions

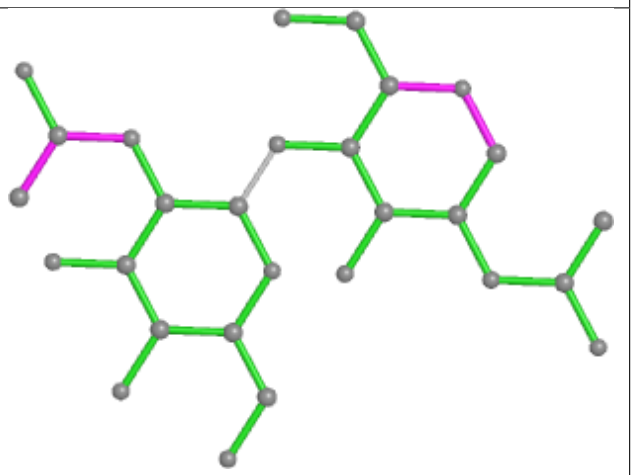


Rings

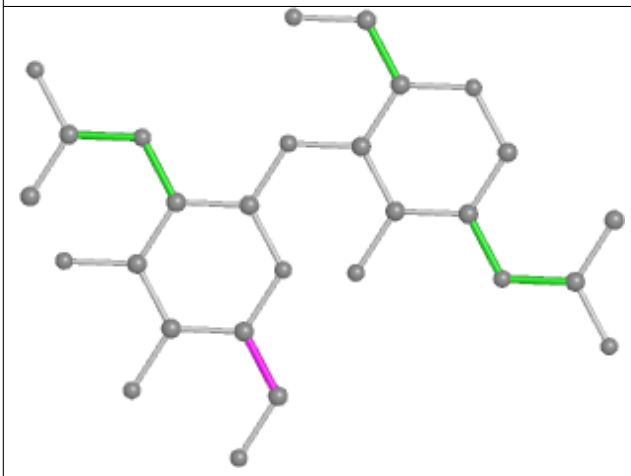
Oligosaccharide Chain D



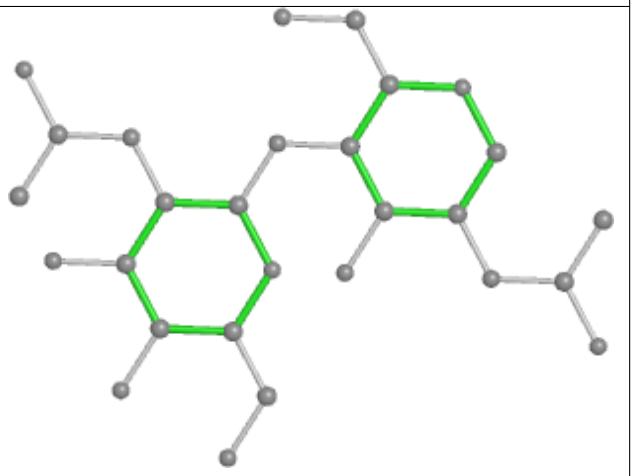
Bond lengths



Bond angles

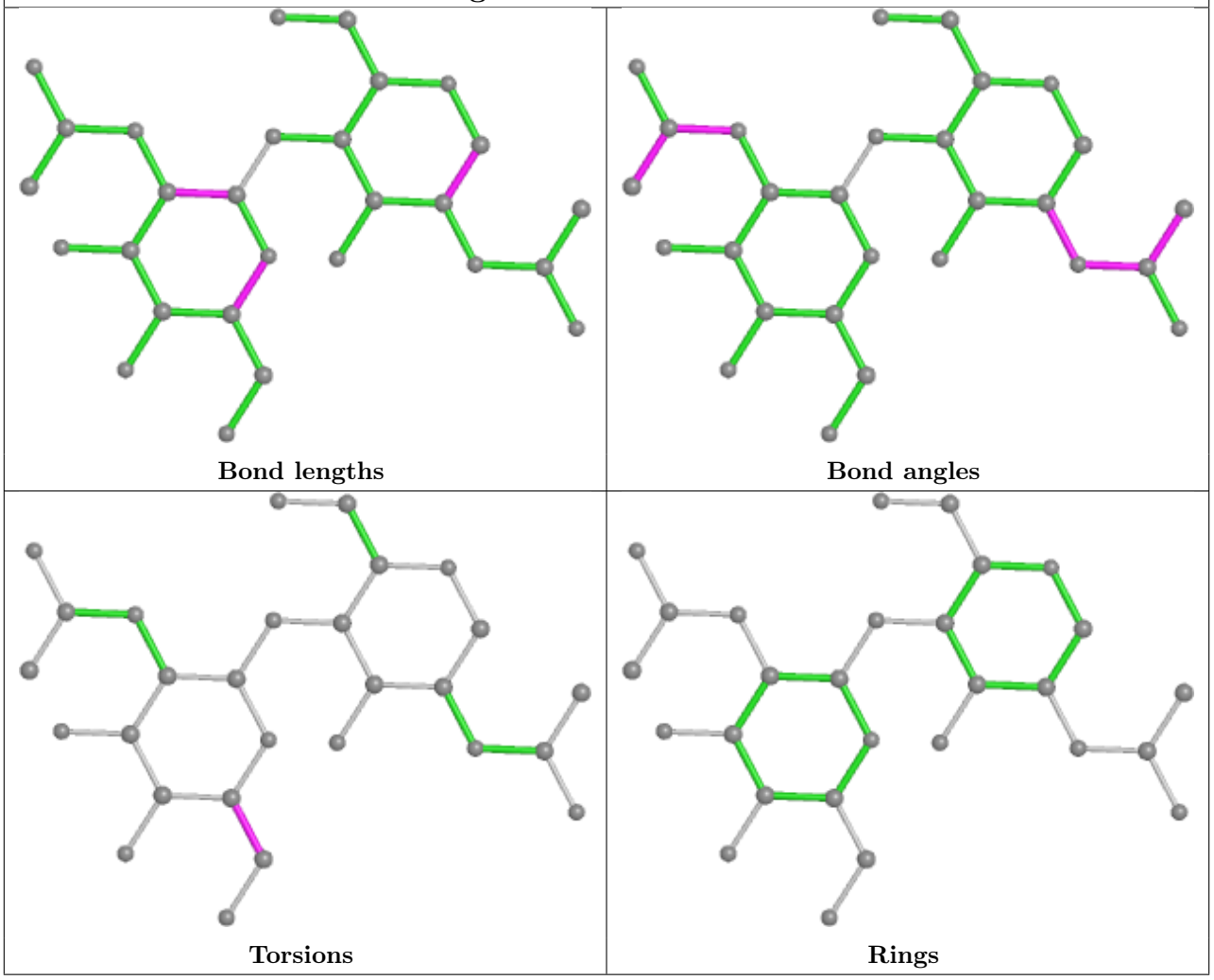


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	1102	1	14,14,15	1.33	2 (14%)	17,19,21	1.00	1 (5%)
6	NAG	B	1501	3	14,14,15	1.18	1 (7%)	17,19,21	0.87	1 (5%)
6	NAG	A	1103	1	14,14,15	1.45	4 (28%)	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	1502	3	14,14,15	1.52	2 (14%)	17,19,21	1.10	1 (5%)
6	NAG	A	1101	1	14,14,15	1.26	2 (14%)	17,19,21	1.78	4 (23%)

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	A	1102	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1501	3	-	1/6/23/26	0/1/1/1
6	NAG	A	1103	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1502	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1101	1	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1502	NAG	C1-C2	3.51	1.57	1.52
6	A	1102	NAG	O5-C5	3.33	1.50	1.43
6	A	1103	NAG	C1-C2	2.75	1.56	1.52
6	A	1101	NAG	O5-C1	2.62	1.47	1.43
6	B	1501	NAG	O5-C5	2.56	1.48	1.43
6	B	1502	NAG	O5-C5	2.51	1.48	1.43
6	A	1103	NAG	O5-C5	2.38	1.48	1.43
6	A	1101	NAG	C1-C2	2.37	1.55	1.52
6	A	1103	NAG	C8-C7	2.10	1.54	1.50
6	A	1102	NAG	C1-C2	2.08	1.55	1.52
6	A	1103	NAG	O5-C1	2.04	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1101	NAG	C1-O5-C5	4.56	118.37	112.19
6	A	1103	NAG	C1-O5-C5	4.23	117.93	112.19
6	A	1101	NAG	C4-C3-C2	3.60	116.30	111.02
6	B	1502	NAG	C8-C7-N2	2.61	120.52	116.10
6	A	1101	NAG	O3-C3-C4	-2.35	104.92	110.35
6	A	1102	NAG	C1-O5-C5	2.14	115.09	112.19
6	B	1501	NAG	C1-O5-C5	2.08	115.00	112.19
6	A	1101	NAG	O5-C5-C4	-2.02	105.91	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1103	NAG	O5-C5-C6-O6
6	B	1502	NAG	O5-C5-C6-O6
6	A	1101	NAG	O5-C5-C6-O6
6	A	1103	NAG	C4-C5-C6-O6
6	A	1102	NAG	O5-C5-C6-O6
6	B	1502	NAG	C4-C5-C6-O6
6	B	1501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

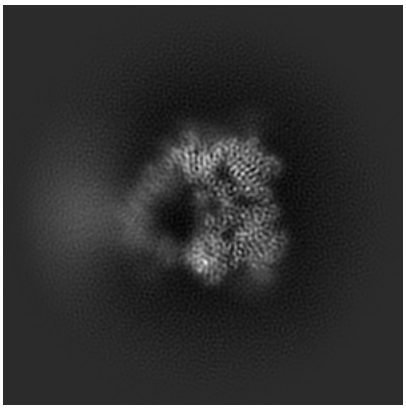
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23916. These allow visual inspection of the internal detail of the map and identification of artifacts.

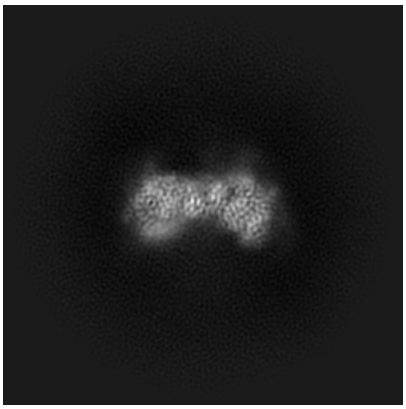
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

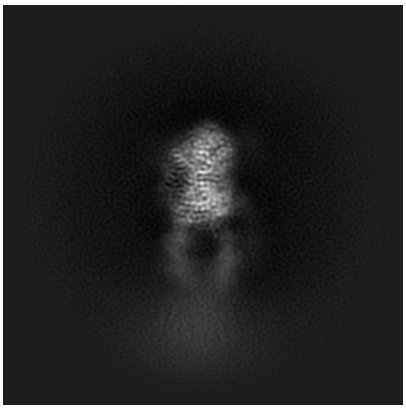
6.1.1 Primary map



X

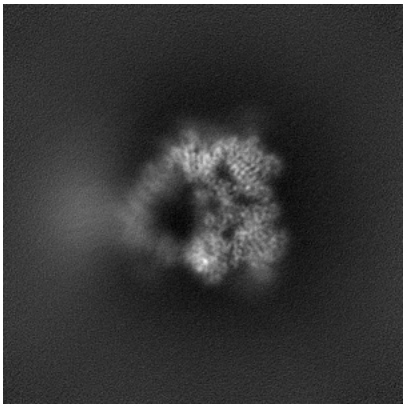


Y

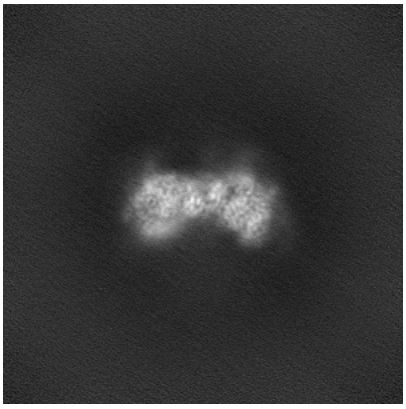


Z

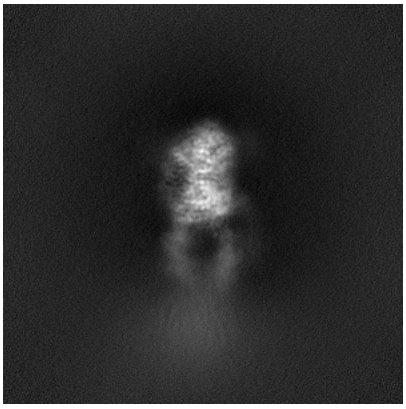
6.1.2 Raw map



X



Y

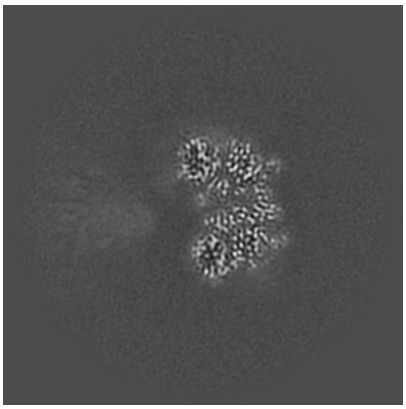


Z

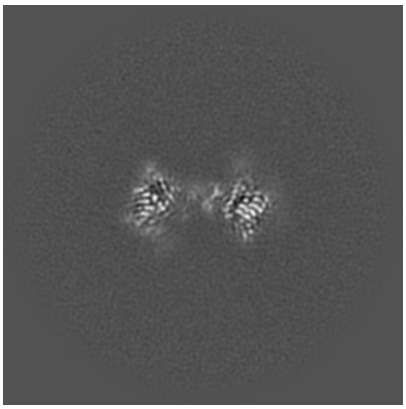
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



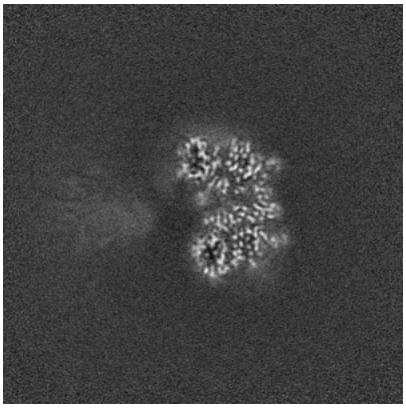
X Index: 180



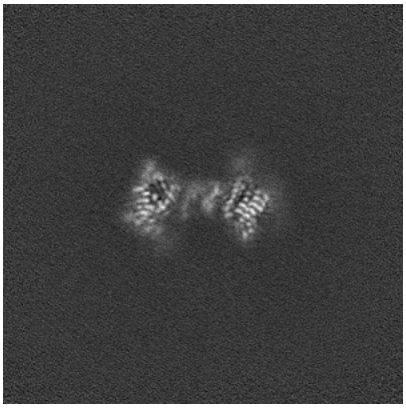
Y Index: 180

Z Index: 180

6.2.2 Raw map



X Index: 180



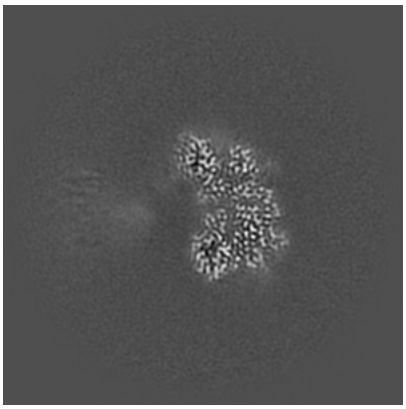
Y Index: 180

Z Index: 180

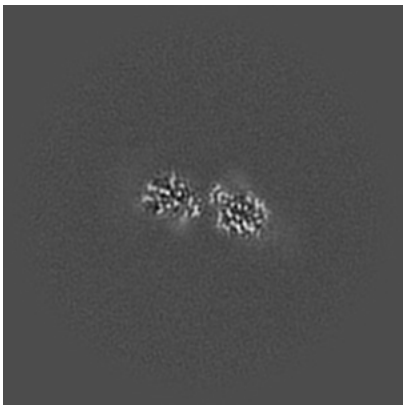
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

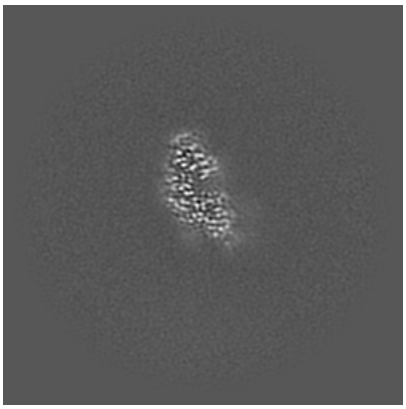
6.3.1 Primary map



X Index: 184

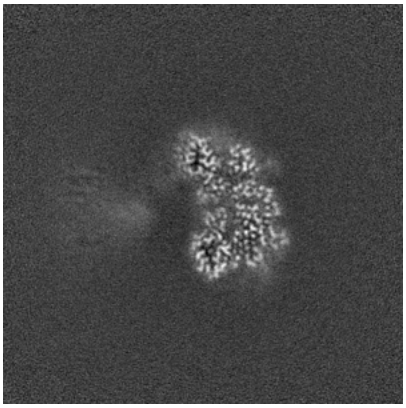


Y Index: 220

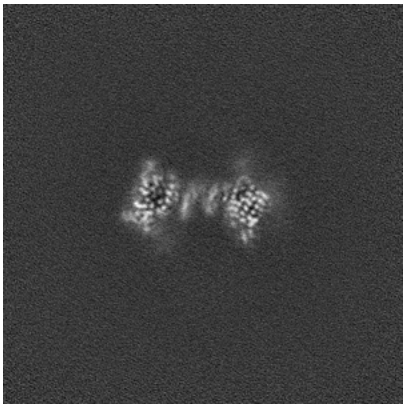


Z Index: 223

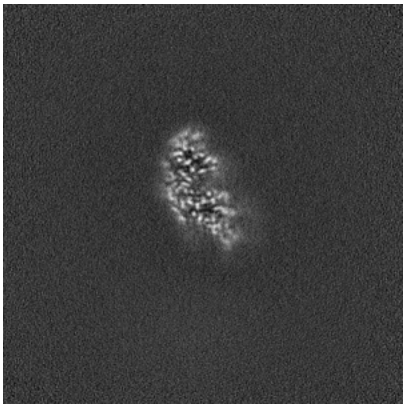
6.3.2 Raw map



X Index: 184



Y Index: 182



Z Index: 221

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

6.4.2 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.

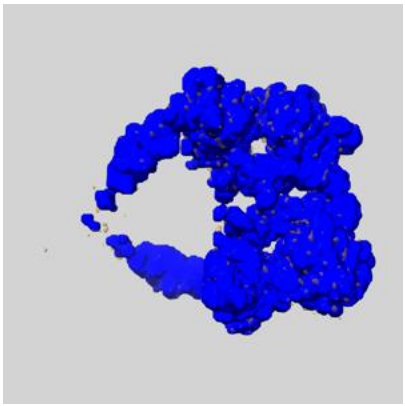
6.5 Mask visualisation (i)

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

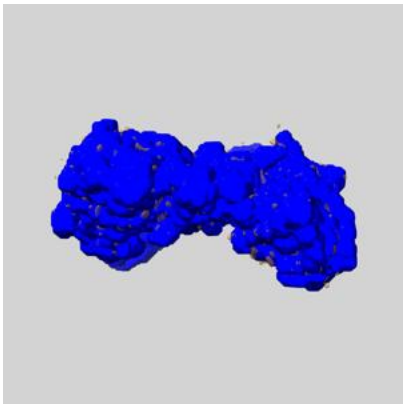
A mask typically either:

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

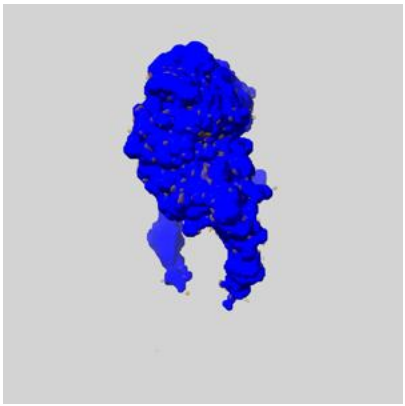
6.5.1 emd_23916_msk_1.map (i)



X



Y

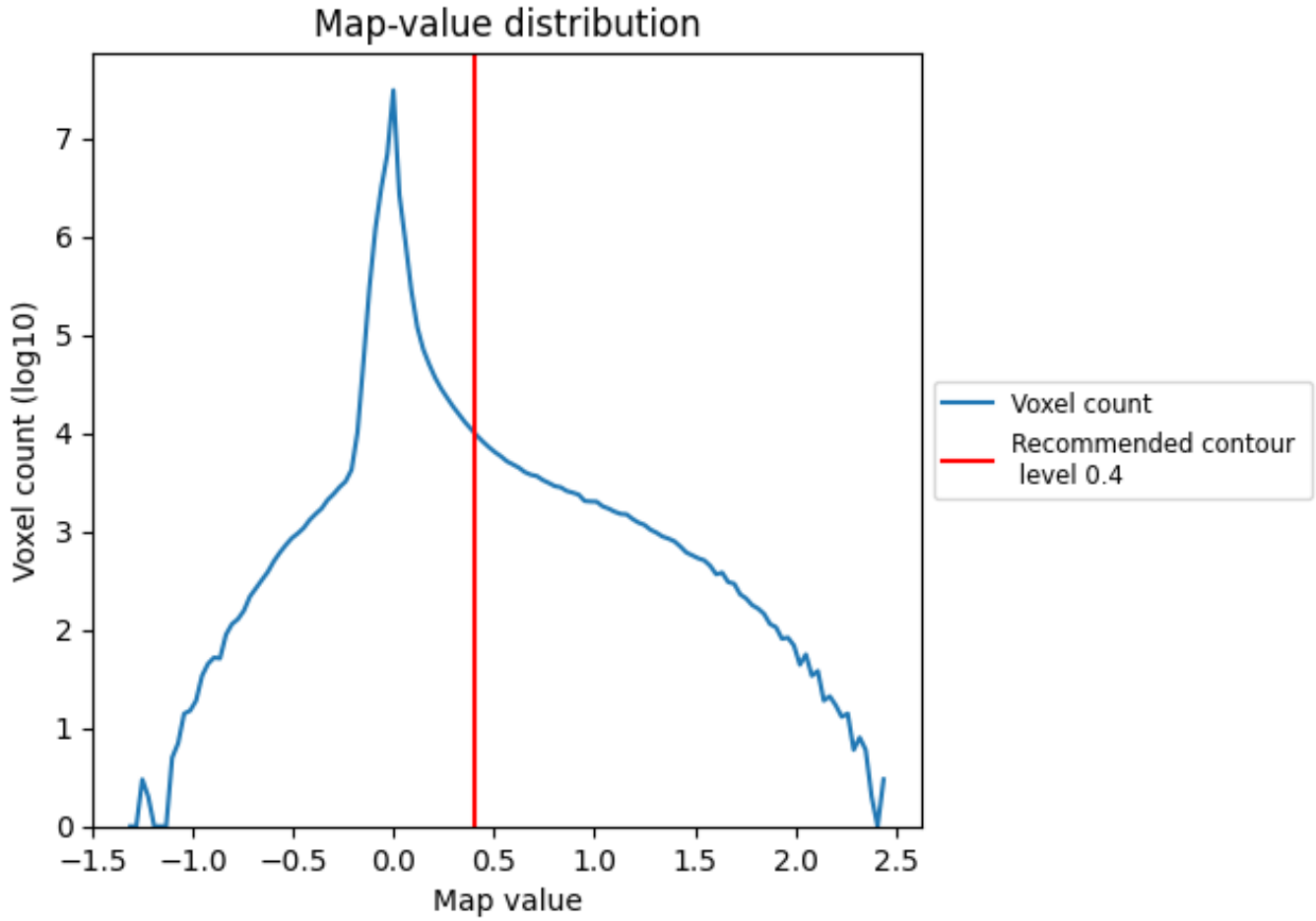


Z

7 Map analysis

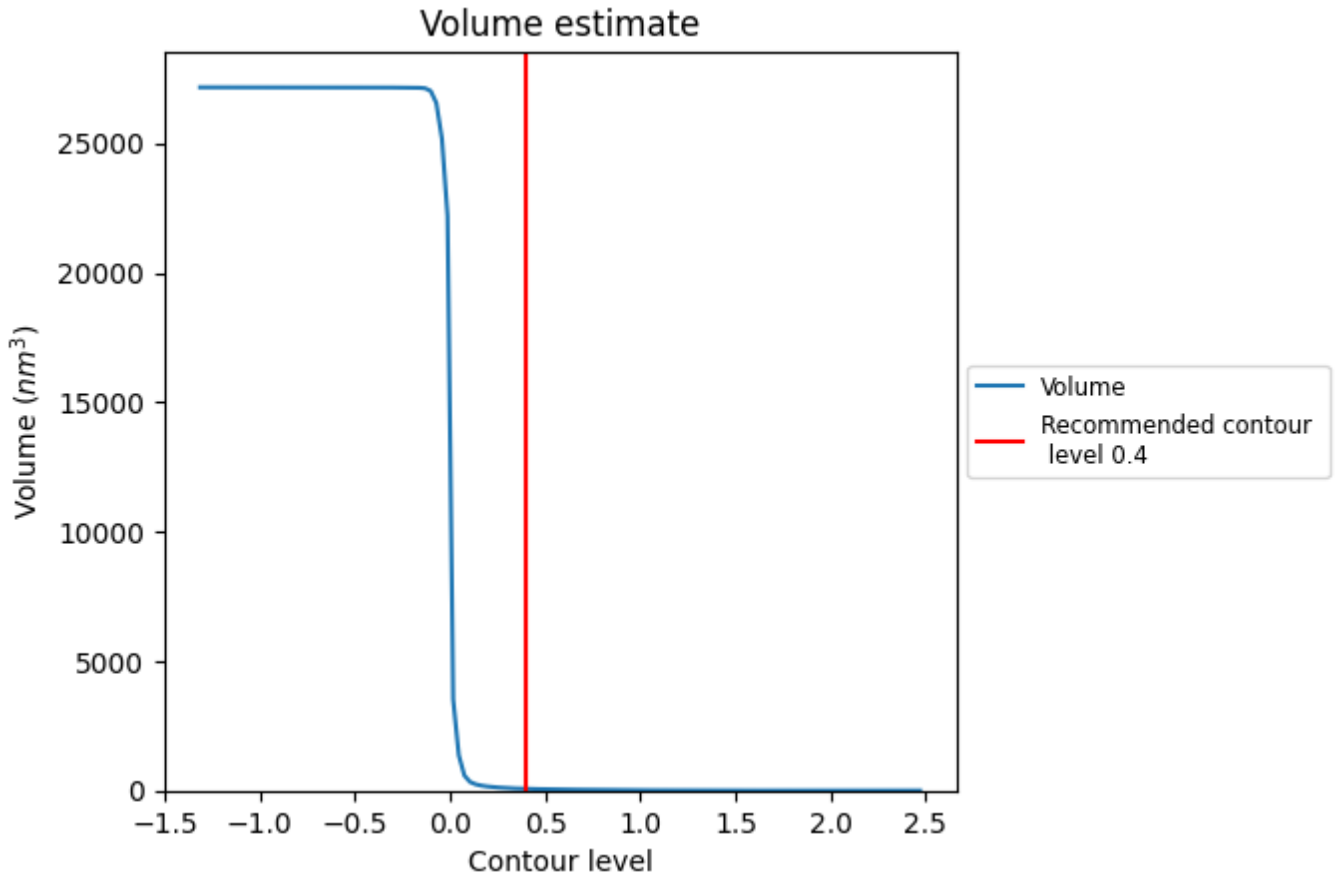
This section contains the results of statistical analysis of the map.

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.

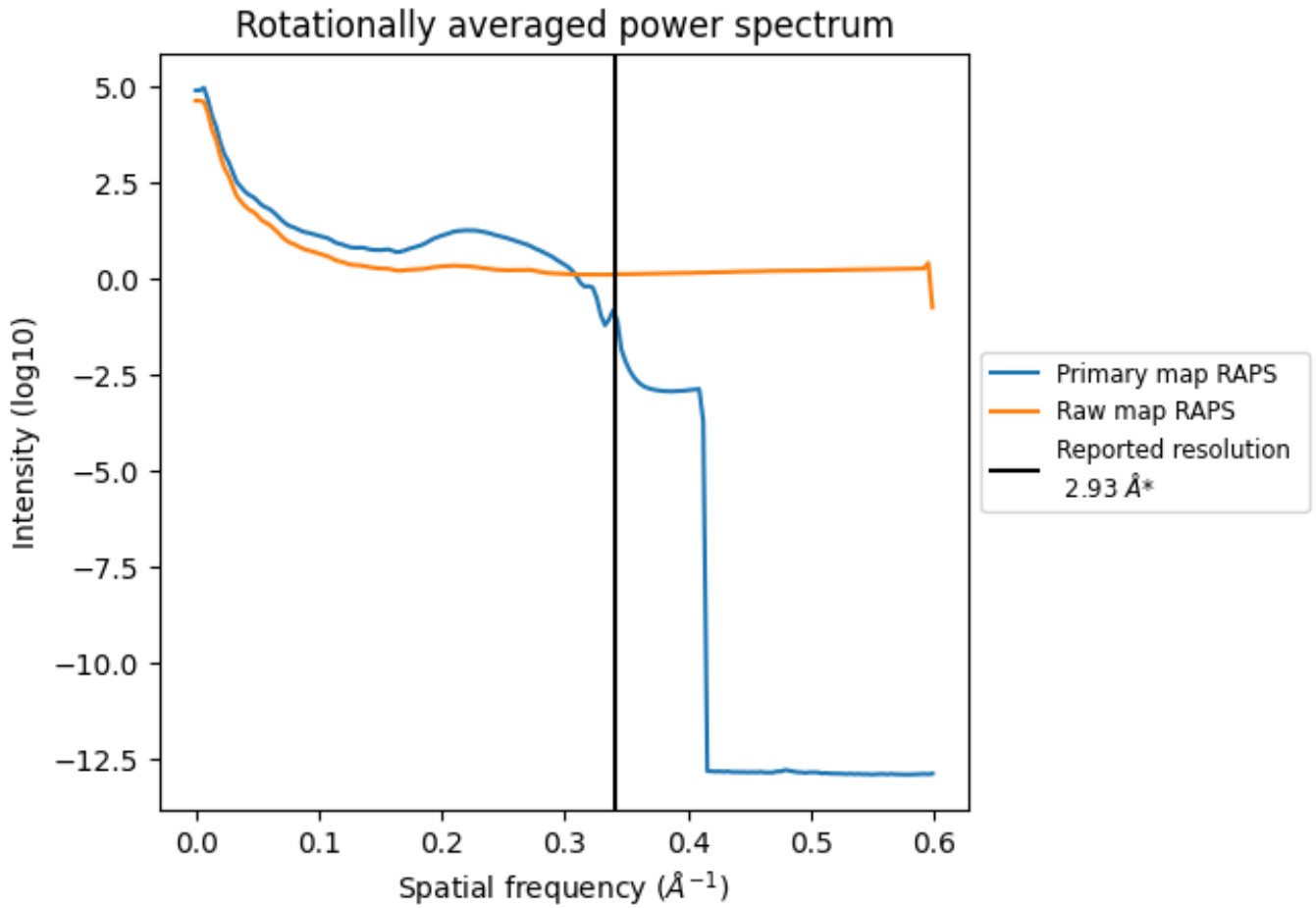
7.2 Volume estimate



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 61 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)

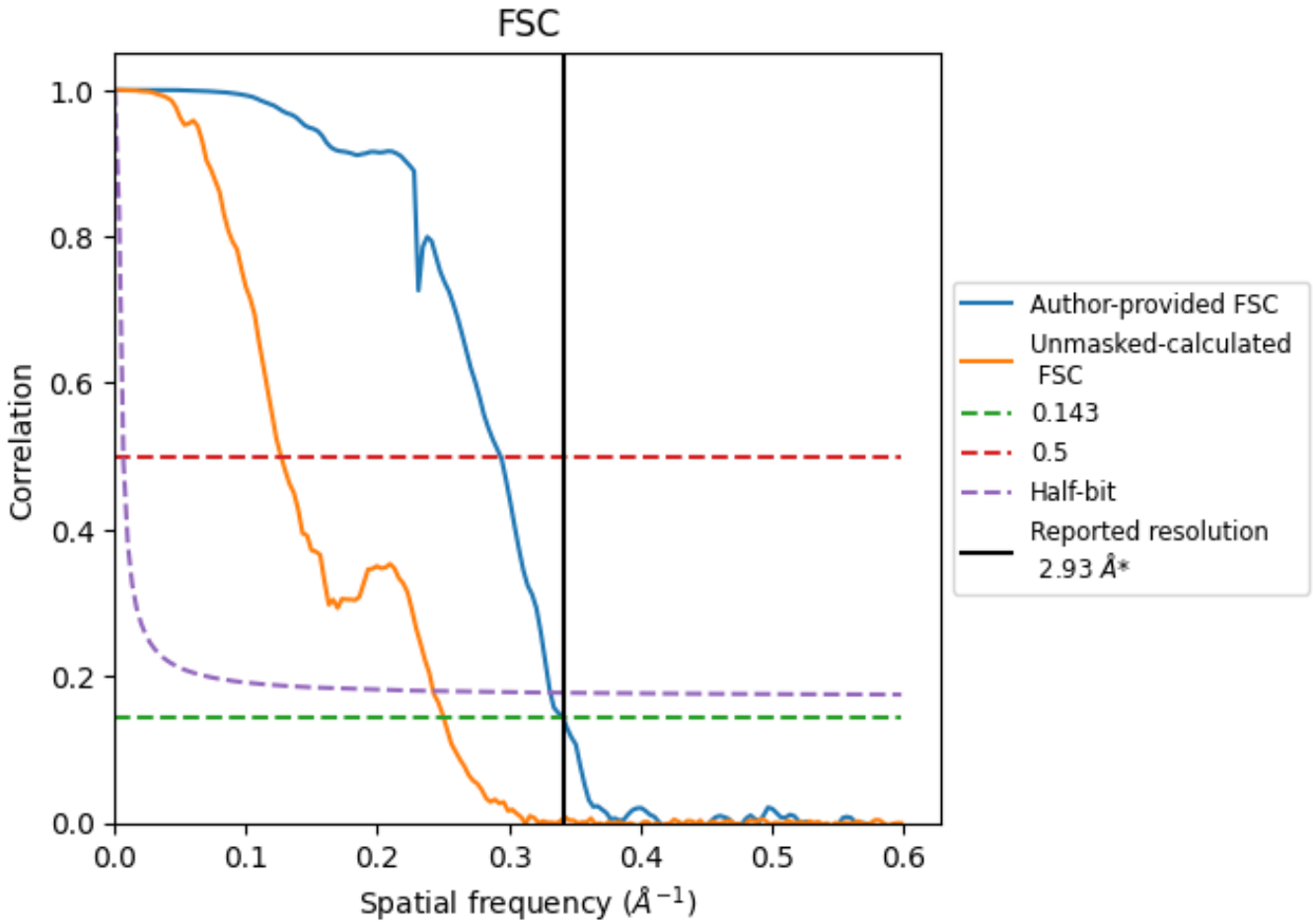


*Reported resolution corresponds to spatial frequency of 0.341 $Å^{-1}$

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 0.341 Å^{-1}

8.2 Resolution estimates (i)

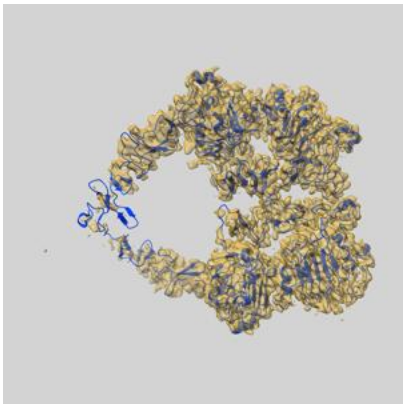
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.93	3.40	3.02
Unmasked-calculated*	3.99	7.90	4.13

*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 3.99 differs from the reported value 2.93 by more than 10 %

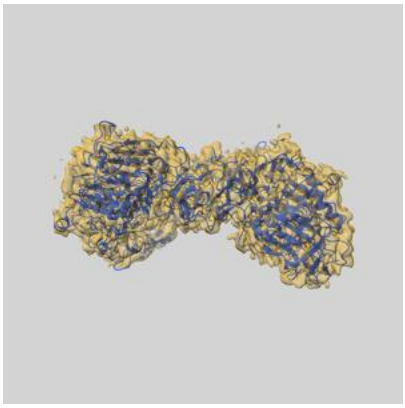
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23916 and PDB model 7MN5. Per-residue inclusion information can be found in section 3 on page 9.

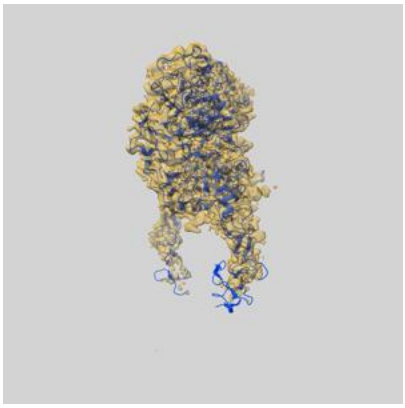
9.1 Map-model overlay



X



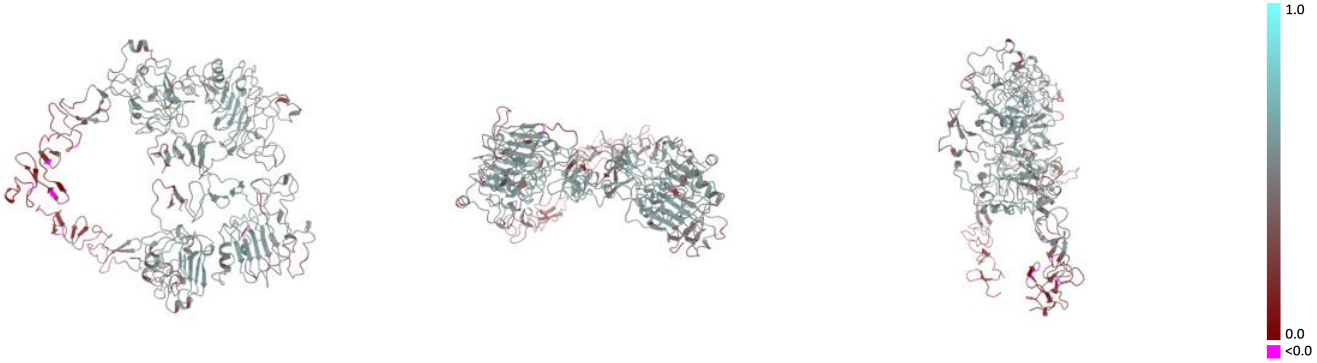
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

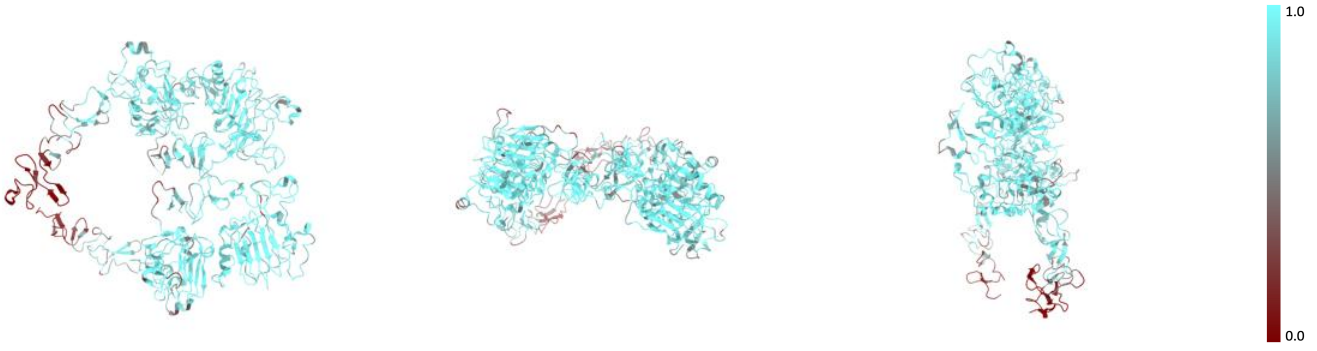
9.2 Q-score mapped to coordinate model (i)



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.

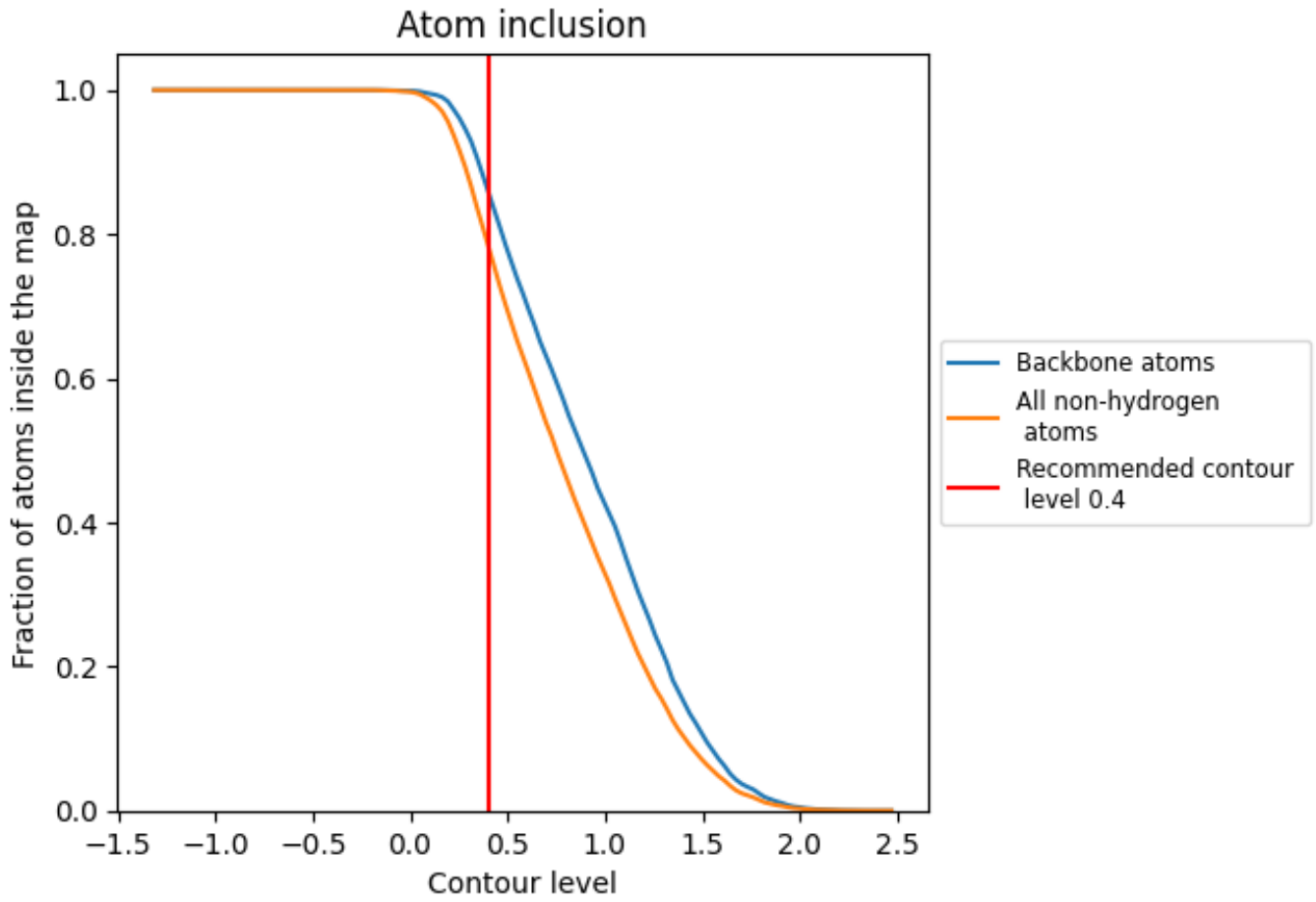
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.4540
A	0.7684	0.4510
B	0.8045	0.4580
C	0.5000	0.3180
D	0.4286	0.1640
E	0.7500	0.5110
H	0.8196	0.4710