wwPDB EM Validation Summary Report

Oct 28, 2024 – 01:55 am GMT

PDB ID	:	8CI2
EMDB ID	:	EMD-16666
Title	:	human alpha7 nicotinic receptor in complex with the C4 nanobody under sub-saturating conditions
Authors	:	Prevost, M.S.; Barilone, N.; Dejean de la Batie, G.; Pons, S.; Ayme, G.; England, P.; Gielen, M.; Bontems, F.; Pehau-Arnaudet, G.; Maskos, U.; Lafaye, P.; Corringer, P.-J.
Deposited on	:	2023-02-08
Resolution	:	4.40 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*
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:

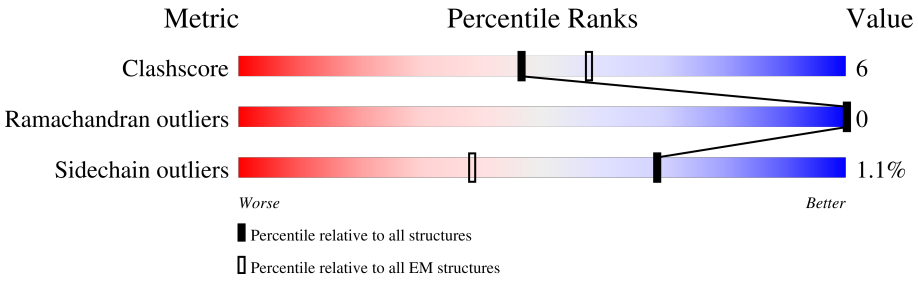
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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 <=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	388	45% 8% 47%
1	B	388	45% 7% 47%
1	C	388	5% 44% 9% 47%
1	D	388	5% 48% 5% 47%
1	E	388	47% 6% 47%
2	F	147	77% 5% 18%
2	G	147	71% 10% 18%
2	I	147	73% 10% 18%

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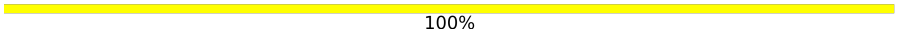
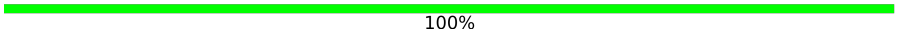
Mol	Chain	Length	Quality of chain
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21802 atoms, of which 10553 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 Neuronal acetylcholine receptor subunit alpha-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	206	Total	C	H	N	O	S	0	0
			3169	1053	1528	276	305	7		
1	B	206	Total	C	H	N	O	S	0	0
			3155	1047	1521	276	304	7		
1	C	206	Total	C	H	N	O	S	0	0
			3172	1050	1532	279	304	7		
1	D	206	Total	C	H	N	O	S	0	0
			3169	1053	1528	276	305	7		
1	E	206	Total	C	H	N	O	S	0	0
			3199	1062	1546	279	305	7		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASP	-	linker	UNP P36544
A	326	GLY	-	linker	UNP P36544
A	327	VAL	-	linker	UNP P36544
A	376	SER	-	expression tag	UNP P36544
A	377	ALA	-	expression tag	UNP P36544
A	378	GLY	-	expression tag	UNP P36544
A	379	LEU	-	expression tag	UNP P36544
A	380	THR	-	expression tag	UNP P36544
A	381	GLU	-	expression tag	UNP P36544
A	382	THR	-	expression tag	UNP P36544
A	383	SER	-	expression tag	UNP P36544
A	384	GLN	-	expression tag	UNP P36544
A	385	VAL	-	expression tag	UNP P36544
A	386	ALA	-	expression tag	UNP P36544
A	387	PRO	-	expression tag	UNP P36544
A	388	ALA	-	expression tag	UNP P36544
B	325	ASP	-	linker	UNP P36544
B	326	GLY	-	linker	UNP P36544
B	327	VAL	-	linker	UNP P36544
B	376	SER	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
B	377	ALA	-	expression tag	UNP P36544
B	378	GLY	-	expression tag	UNP P36544
B	379	LEU	-	expression tag	UNP P36544
B	380	THR	-	expression tag	UNP P36544
B	381	GLU	-	expression tag	UNP P36544
B	382	THR	-	expression tag	UNP P36544
B	383	SER	-	expression tag	UNP P36544
B	384	GLN	-	expression tag	UNP P36544
B	385	VAL	-	expression tag	UNP P36544
B	386	ALA	-	expression tag	UNP P36544
B	387	PRO	-	expression tag	UNP P36544
B	388	ALA	-	expression tag	UNP P36544
C	325	ASP	-	linker	UNP P36544
C	326	GLY	-	linker	UNP P36544
C	327	VAL	-	linker	UNP P36544
C	376	SER	-	expression tag	UNP P36544
C	377	ALA	-	expression tag	UNP P36544
C	378	GLY	-	expression tag	UNP P36544
C	379	LEU	-	expression tag	UNP P36544
C	380	THR	-	expression tag	UNP P36544
C	381	GLU	-	expression tag	UNP P36544
C	382	THR	-	expression tag	UNP P36544
C	383	SER	-	expression tag	UNP P36544
C	384	GLN	-	expression tag	UNP P36544
C	385	VAL	-	expression tag	UNP P36544
C	386	ALA	-	expression tag	UNP P36544
C	387	PRO	-	expression tag	UNP P36544
C	388	ALA	-	expression tag	UNP P36544
D	325	ASP	-	linker	UNP P36544
D	326	GLY	-	linker	UNP P36544
D	327	VAL	-	linker	UNP P36544
D	376	SER	-	expression tag	UNP P36544
D	377	ALA	-	expression tag	UNP P36544
D	378	GLY	-	expression tag	UNP P36544
D	379	LEU	-	expression tag	UNP P36544
D	380	THR	-	expression tag	UNP P36544
D	381	GLU	-	expression tag	UNP P36544
D	382	THR	-	expression tag	UNP P36544
D	383	SER	-	expression tag	UNP P36544
D	384	GLN	-	expression tag	UNP P36544
D	385	VAL	-	expression tag	UNP P36544
D	386	ALA	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
D	387	PRO	-	expression tag	UNP P36544
D	388	ALA	-	expression tag	UNP P36544
E	325	ASP	-	linker	UNP P36544
E	326	GLY	-	linker	UNP P36544
E	327	VAL	-	linker	UNP P36544
E	376	SER	-	expression tag	UNP P36544
E	377	ALA	-	expression tag	UNP P36544
E	378	GLY	-	expression tag	UNP P36544
E	379	LEU	-	expression tag	UNP P36544
E	380	THR	-	expression tag	UNP P36544
E	381	GLU	-	expression tag	UNP P36544
E	382	THR	-	expression tag	UNP P36544
E	383	SER	-	expression tag	UNP P36544
E	384	GLN	-	expression tag	UNP P36544
E	385	VAL	-	expression tag	UNP P36544
E	386	ALA	-	expression tag	UNP P36544
E	387	PRO	-	expression tag	UNP P36544
E	388	ALA	-	expression tag	UNP P36544

- Molecule 2 is a protein called Nanobody C4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	121	Total	C	H	N	O	S	0	0
			1801	585	881	156	176	3		
2	G	121	Total	C	H	N	O	S	0	0
			1801	585	881	156	176	3		
2	I	121	Total	C	H	N	O	S	0	0
			1801	585	881	156	176	3		

- Molecule 3 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
3	P	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

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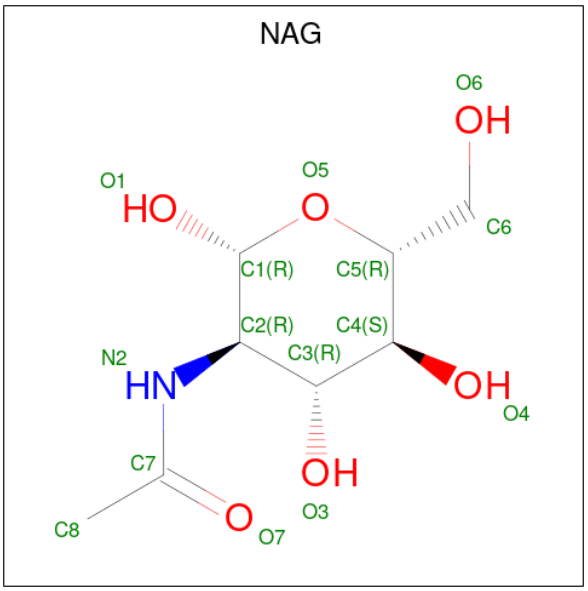
Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	S	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	T	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	D	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	D	1	Total	C	H	N	O	0
			27	8	13	1	5	

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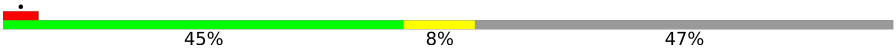
Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	E	1	Total	C	H	N	O	0
			27	8	13	1	5	

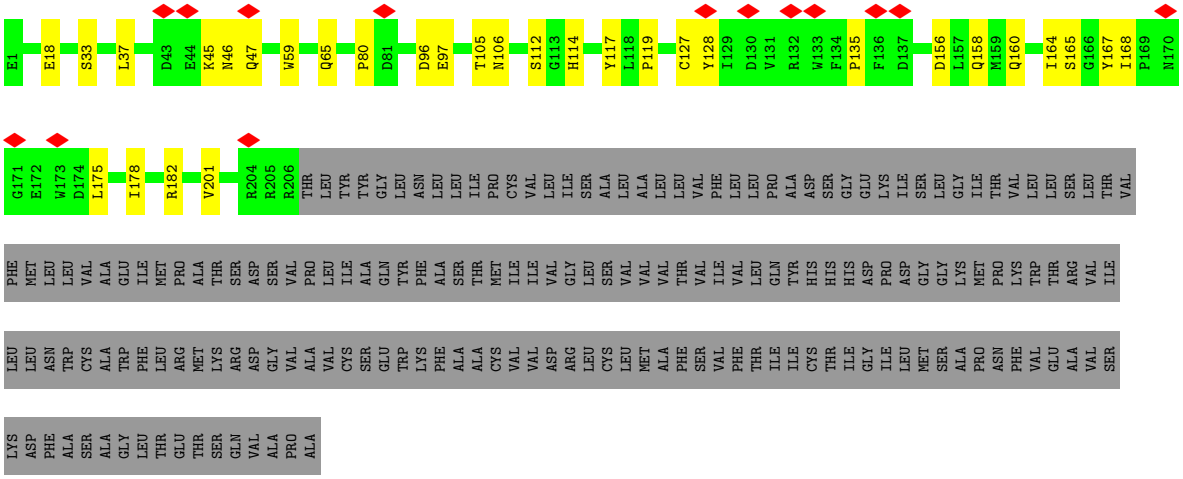
3 Residue-property plots (i)

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: Neuronal acetylcholine receptor subunit alpha-7

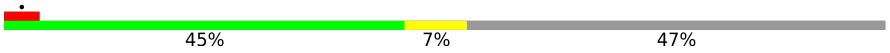
Chain A:

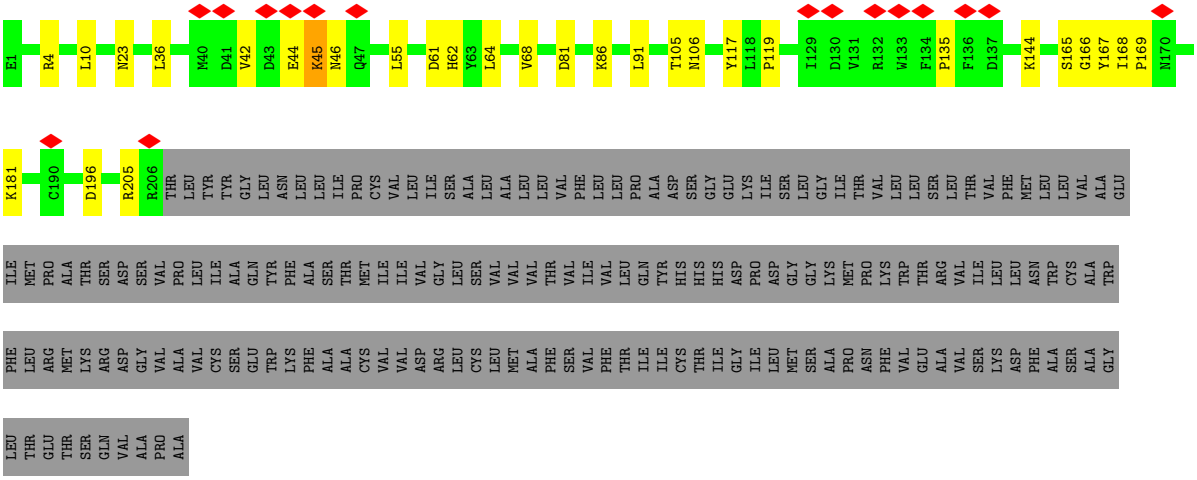




• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

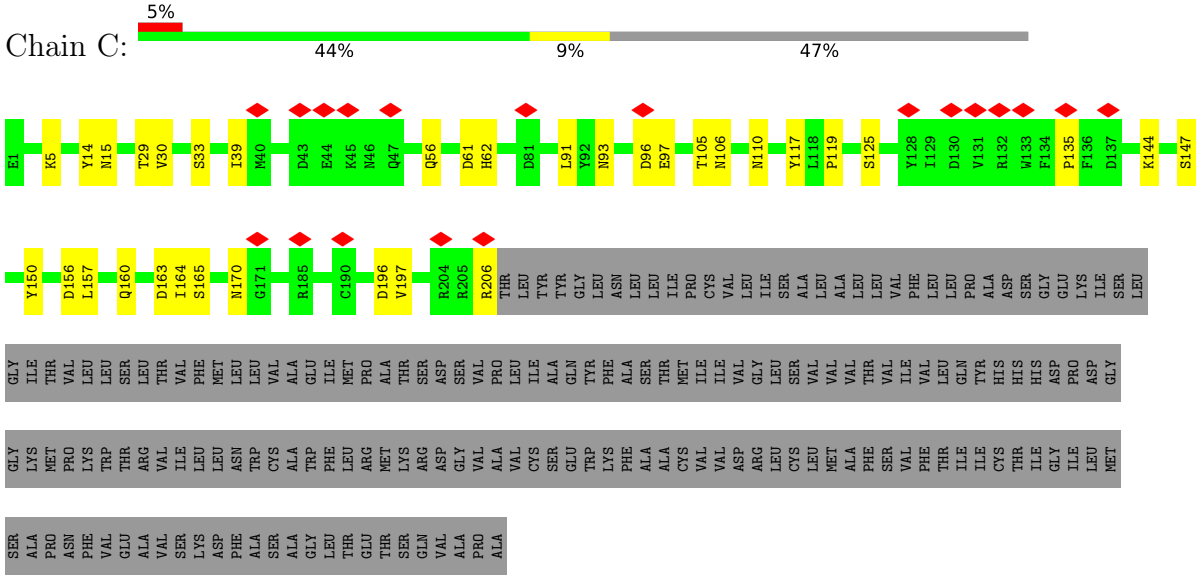
Chain B:





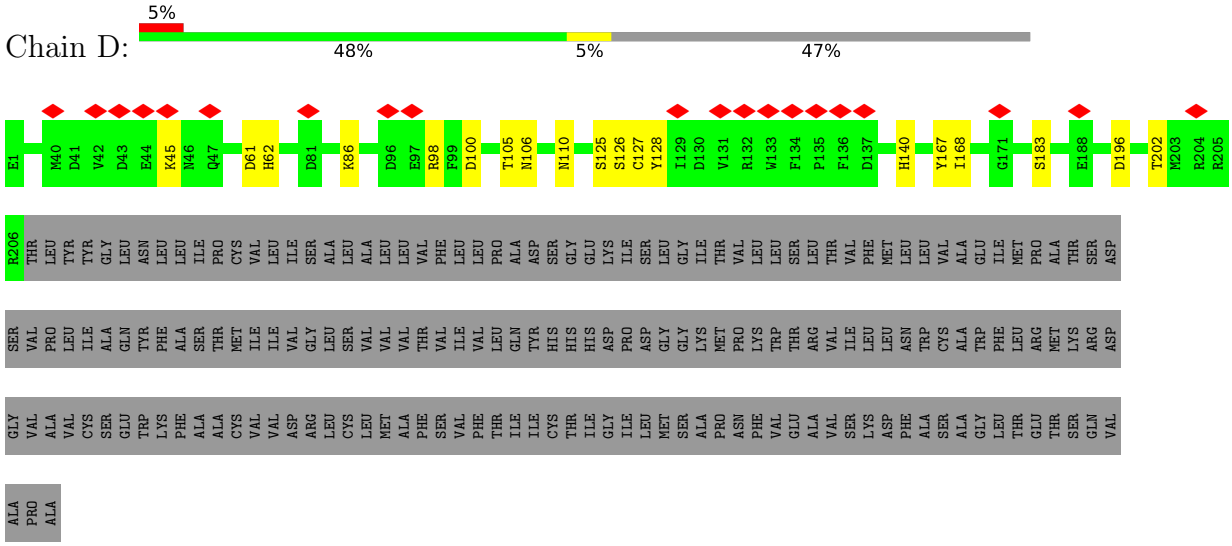
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain C:



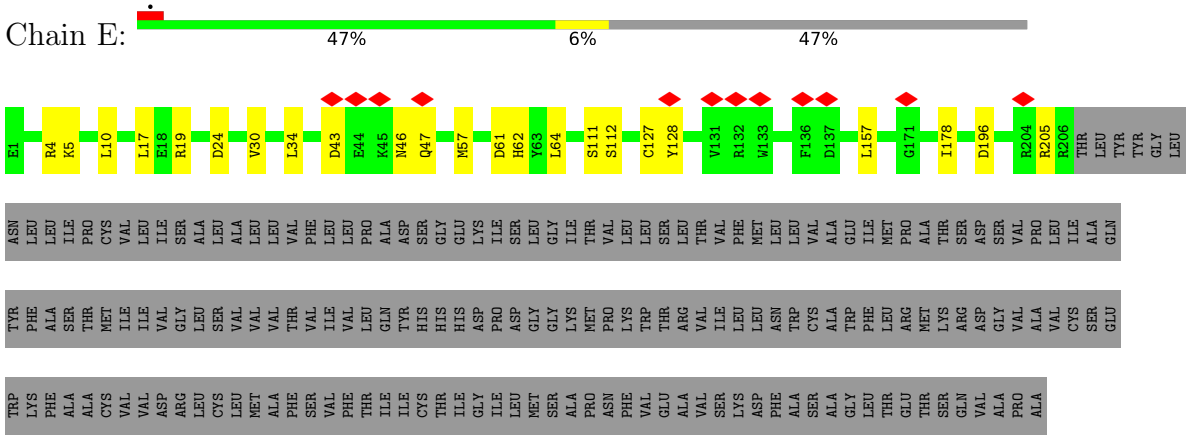
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain D:



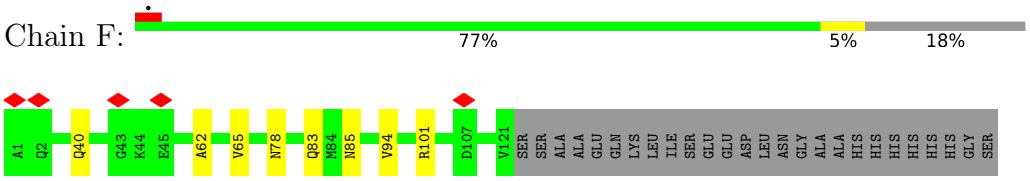
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain E:



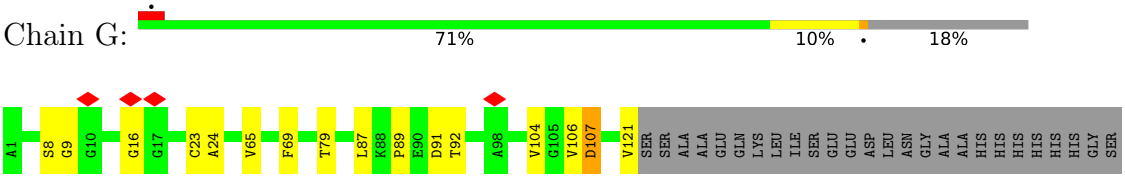
• Molecule 2: Nanobody C4

Chain F:



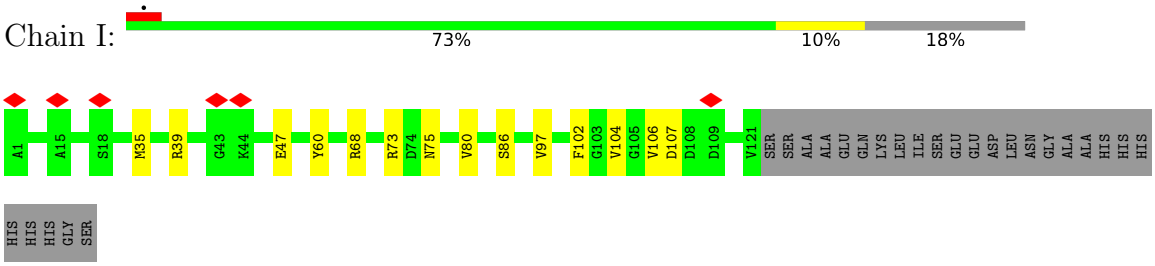
• Molecule 2: Nanobody C4

Chain G:



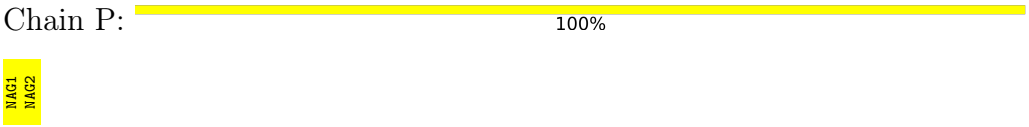
• Molecule 2: Nanobody C4

Chain I:



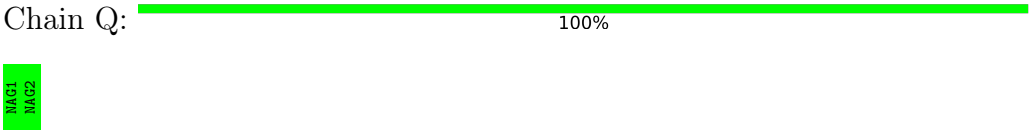
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:



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

Chain R:

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

Chain S:

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

Chain T:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29644	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.015	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00467	Depositor
Map size (Å)	211.2, 211.2, 211.2	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	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

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	0.31	0/1690	0.54	1/2306 (0.0%)
1	B	0.30	0/1682	0.51	0/2295
1	C	0.30	0/1688	0.51	0/2302
1	D	0.30	0/1690	0.49	0/2306
1	E	0.31	0/1703	0.50	0/2322
2	F	0.31	0/942	0.51	0/1277
2	G	0.30	0/942	0.52	0/1277
2	I	0.32	0/942	0.52	0/1277
All	All	0.31	0/11279	0.51	1/15362 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	PRO	CA-N-CD	-7.34	101.23	111.50

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	1641	1528	1528	25	0
1	B	1634	1521	1521	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1640	1532	1532	21	0
1	D	1641	1528	1528	12	0
1	E	1653	1546	1546	15	0
2	F	920	881	881	4	0
2	G	920	881	881	11	0
2	I	920	881	881	11	0
3	P	28	25	25	2	0
3	Q	28	25	25	0	0
3	R	28	25	25	2	0
3	S	28	25	25	1	0
3	T	28	25	25	1	0
4	A	28	26	26	2	0
4	B	28	26	26	3	0
4	C	28	26	26	2	0
4	D	28	26	26	3	0
4	E	28	26	26	3	0
All	All	11249	10553	10553	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 129 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:158:GLN:OE1	1:A:182:ARG:NH1	2.14	0.81
1:E:46:ASN:OD1	1:E:47:GLN:N	2.16	0.78
3:P:1:NAG:O6	3:P:2:NAG:O5	2.01	0.77
1:A:65:GLN:OE1	1:A:112:SER:OG	2.03	0.75
1:C:147:SER:OG	1:C:150:TYR:O	2.03	0.75

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	204/388 (53%)	168 (82%)	36 (18%)	0	100	100
1	B	204/388 (53%)	170 (83%)	34 (17%)	0	100	100
1	C	204/388 (53%)	170 (83%)	34 (17%)	0	100	100
1	D	204/388 (53%)	177 (87%)	27 (13%)	0	100	100
1	E	204/388 (53%)	177 (87%)	27 (13%)	0	100	100
2	F	119/147 (81%)	101 (85%)	18 (15%)	0	100	100
2	G	119/147 (81%)	106 (89%)	13 (11%)	0	100	100
2	I	119/147 (81%)	103 (87%)	16 (13%)	0	100	100
All	All	1377/2381 (58%)	1172 (85%)	205 (15%)	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	174/346 (50%)	172 (99%)	2 (1%)	70	80
1	B	173/346 (50%)	170 (98%)	3 (2%)	56	72
1	C	174/346 (50%)	173 (99%)	1 (1%)	84	88
1	D	174/346 (50%)	173 (99%)	1 (1%)	84	88
1	E	176/346 (51%)	173 (98%)	3 (2%)	56	72
2	F	92/112 (82%)	91 (99%)	1 (1%)	70	80
2	G	92/112 (82%)	91 (99%)	1 (1%)	70	80
2	I	92/112 (82%)	91 (99%)	1 (1%)	70	80
All	All	1147/2066 (56%)	1134 (99%)	13 (1%)	69	80

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	34	LEU
1	E	57	MET
2	I	68	ARG
2	F	101	ARG
2	G	107	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

10 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	$\#\|Z\| > 2$
3	NAG	P	1	3	14,14,15	0.34	0	17,19,21	0.40	0
3	NAG	P	2	3	14,14,15	0.23	0	17,19,21	0.51	0
3	NAG	Q	1	3	14,14,15	0.45	0	17,19,21	0.40	0
3	NAG	Q	2	3	14,14,15	0.30	0	17,19,21	0.44	0
3	NAG	R	1	3	14,14,15	0.58	1 (7%)	17,19,21	0.57	0
3	NAG	R	2	3	14,14,15	0.60	0	17,19,21	0.60	0
3	NAG	S	1	3	14,14,15	0.20	0	17,19,21	0.83	1 (5%)
3	NAG	S	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	T	1	3	14,14,15	0.37	0	17,19,21	0.52	0
3	NAG	T	2	3	14,14,15	0.54	0	17,19,21	0.46	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
3	NAG	P	1	3	-	3/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	NAG	T	1	3	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.07	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	1	NAG	C1-O5-C5	3.12	116.41	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

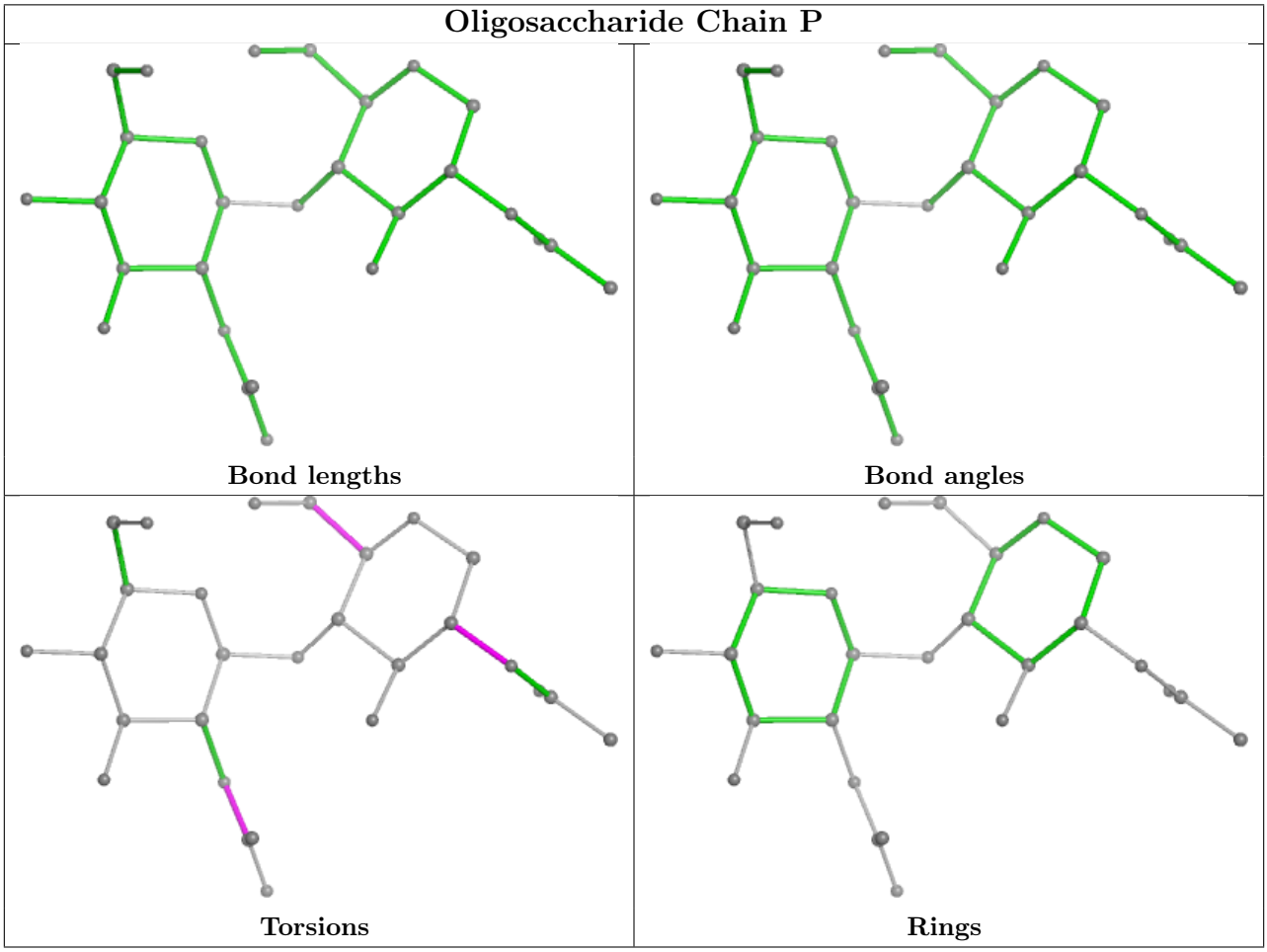
Mol	Chain	Res	Type	Atoms
3	R	1	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2

There are no ring outliers.

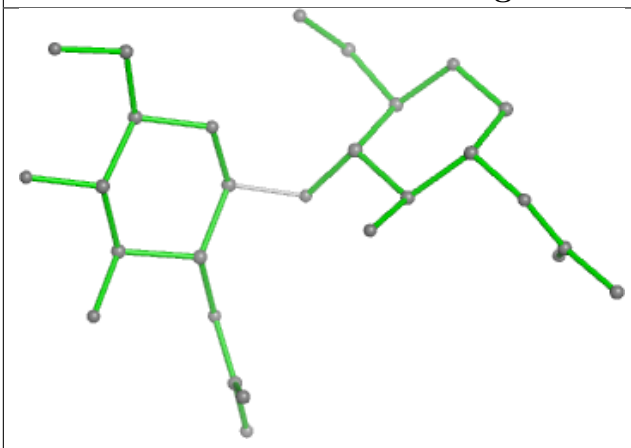
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	NAG	1	0
3	S	1	NAG	1	0
3	T	1	NAG	1	0
3	P	1	NAG	2	0
3	P	2	NAG	2	0
3	R	1	NAG	2	0

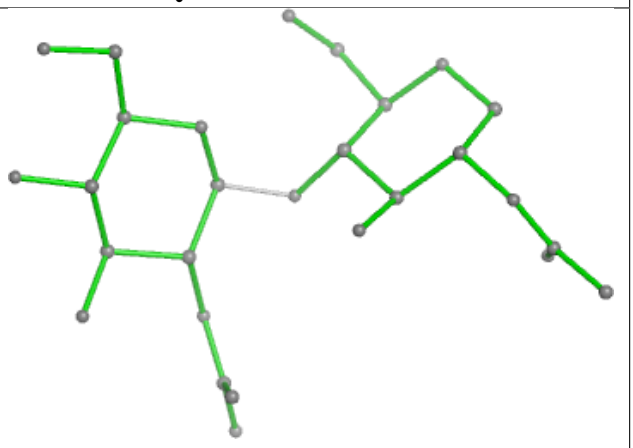
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



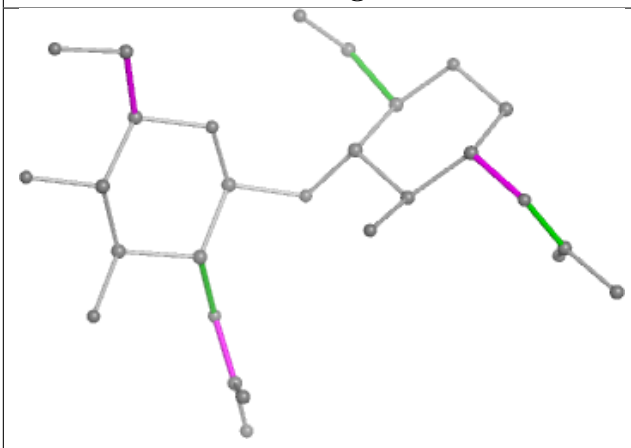
Oligosaccharide Chain Q



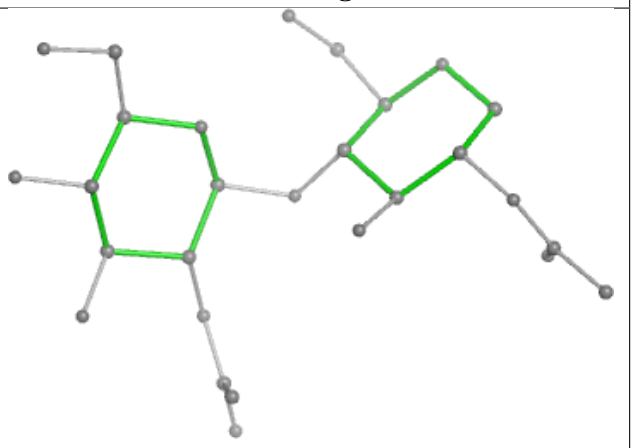
Bond lengths



Bond angles

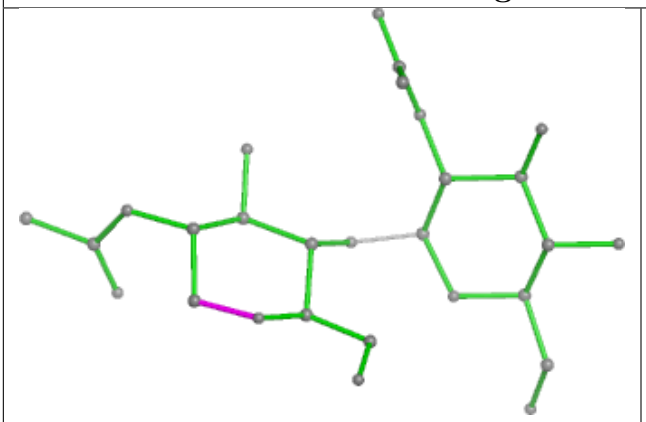


Torsions

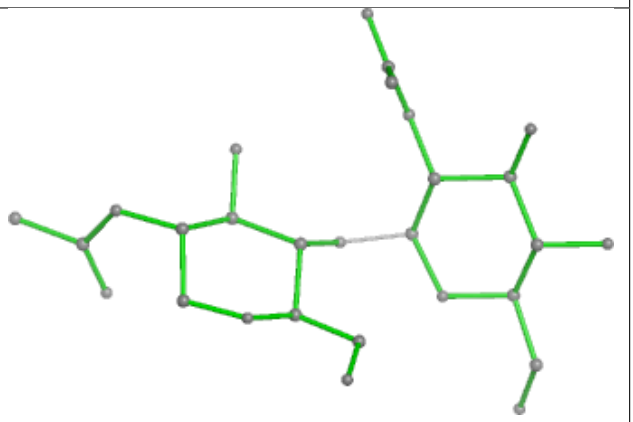


Rings

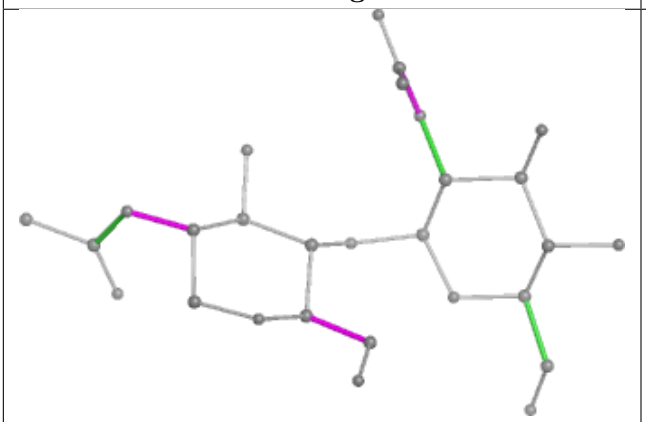
Oligosaccharide Chain R



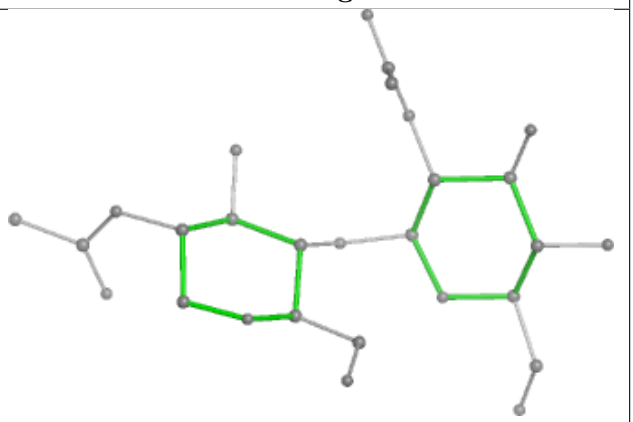
Bond lengths



Bond angles

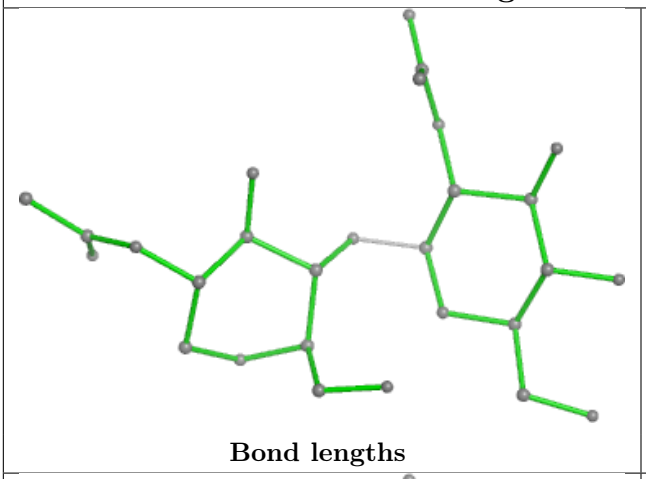


Torsions

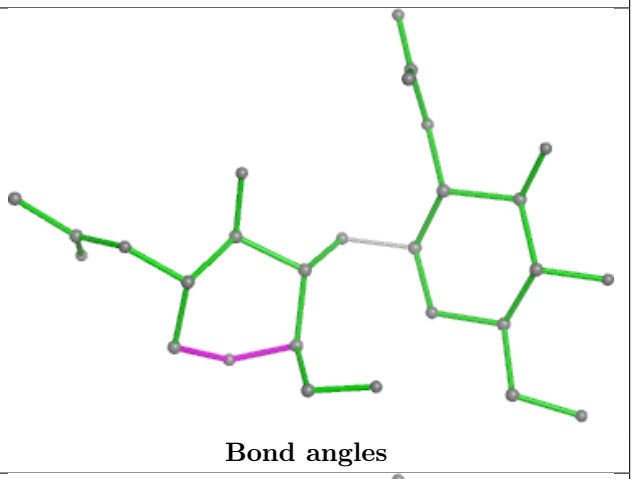


Rings

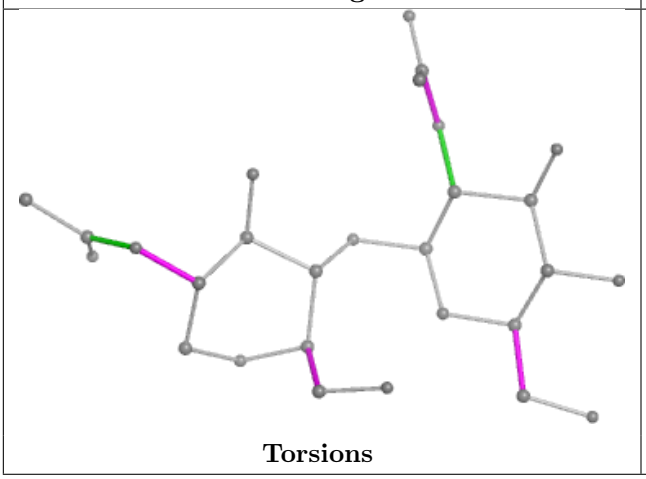
Oligosaccharide Chain S



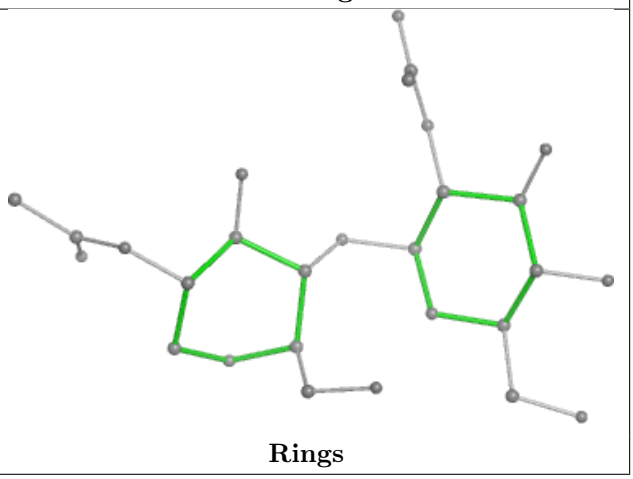
Bond lengths



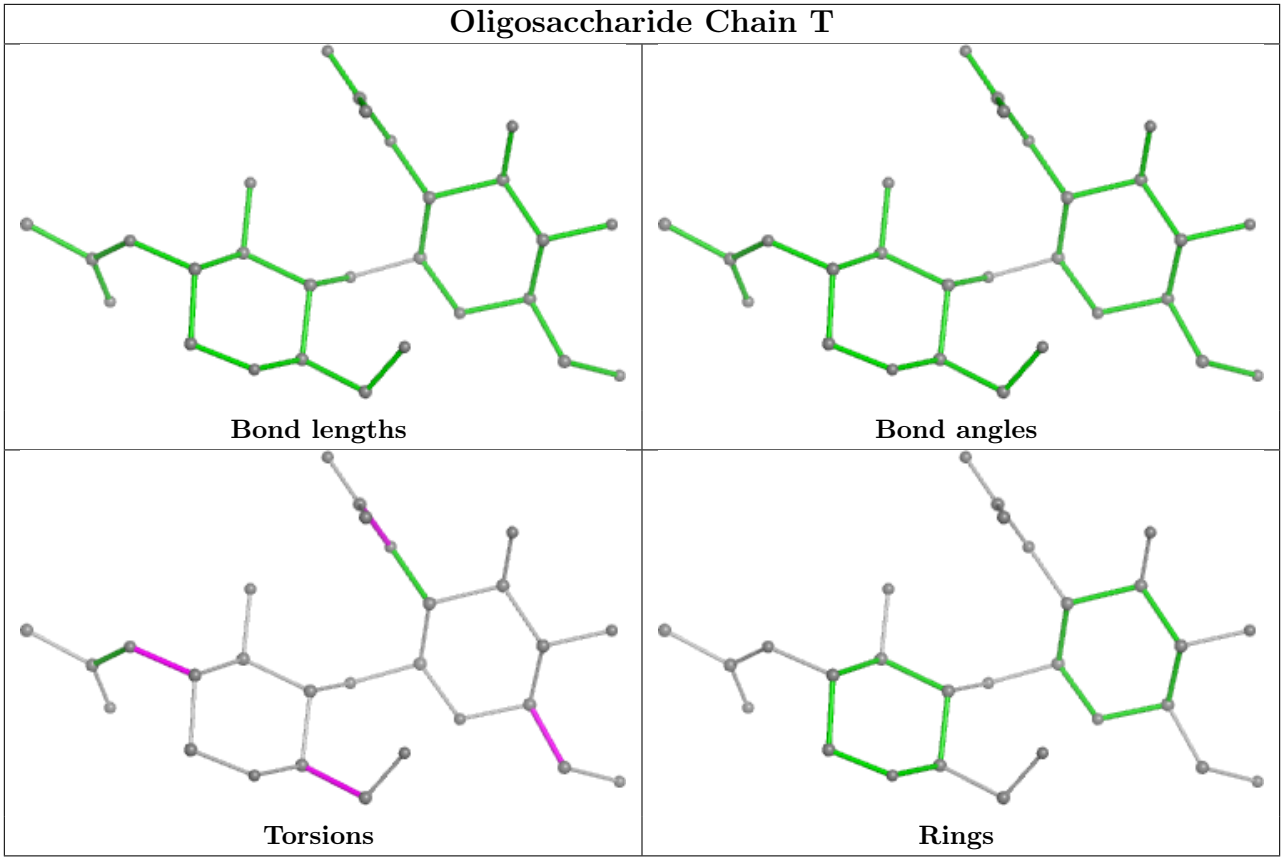
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	NAG	A	401	1	14,14,15	0.24	0	17,19,21	0.88	1 (5%)
4	NAG	A	402	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	C	402	1	14,14,15	0.15	0	17,19,21	0.47	0
4	NAG	B	401	1	14,14,15	0.18	0	17,19,21	0.88	1 (5%)
4	NAG	C	401	1	14,14,15	0.19	0	17,19,21	0.88	1 (5%)
4	NAG	B	402	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	D	401	1	14,14,15	0.19	0	17,19,21	0.90	1 (5%)
4	NAG	D	402	1	14,14,15	0.21	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	401	1	14,14,15	0.21	0	17,19,21	0.91	1 (5%)
4	NAG	E	402	1	14,14,15	0.20	0	17,19,21	0.43	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
4	NAG	A	401	1	-	5/6/23/26	0/1/1/1
4	NAG	A	402	1	-	1/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	401	1	-	5/6/23/26	0/1/1/1
4	NAG	C	401	1	-	3/6/23/26	0/1/1/1
4	NAG	B	402	1	-	2/6/23/26	0/1/1/1
4	NAG	D	401	1	-	5/6/23/26	0/1/1/1
4	NAG	D	402	1	-	0/6/23/26	0/1/1/1
4	NAG	E	401	1	-	5/6/23/26	0/1/1/1
4	NAG	E	402	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	NAG	C2-N2-C7	2.76	126.83	122.90
4	B	401	NAG	C2-N2-C7	2.75	126.82	122.90
4	D	401	NAG	C2-N2-C7	2.69	126.73	122.90
4	A	401	NAG	C2-N2-C7	2.67	126.71	122.90
4	E	401	NAG	C2-N2-C7	2.66	126.70	122.90

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	NAG	O5-C5-C6-O6
4	D	401	NAG	C4-C5-C6-O6
4	A	401	NAG	O5-C5-C6-O6
4	D	401	NAG	O5-C5-C6-O6
4	A	401	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	NAG	2	0
4	B	401	NAG	3	0
4	C	401	NAG	2	0
4	D	401	NAG	3	0
4	E	401	NAG	3	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.

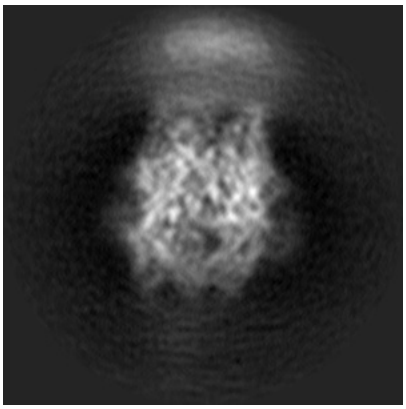
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16666. These allow visual inspection of the internal detail of the map and identification of artifacts.

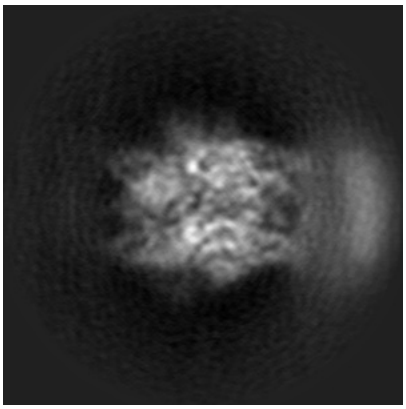
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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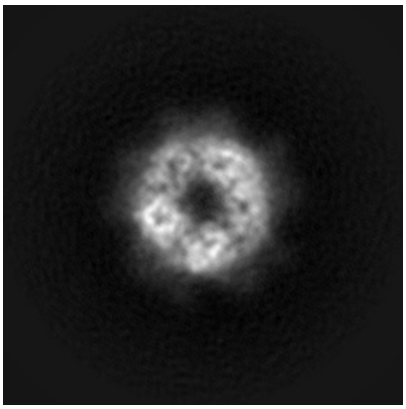
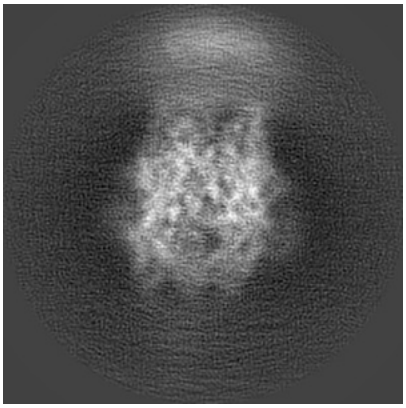


Z

6.1.2 Raw map



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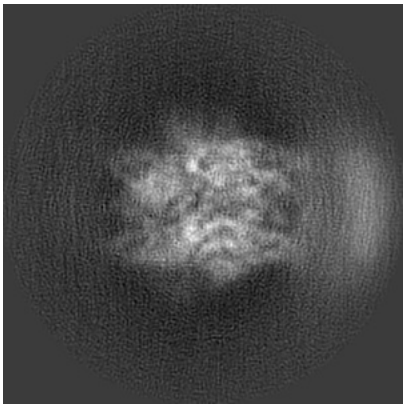

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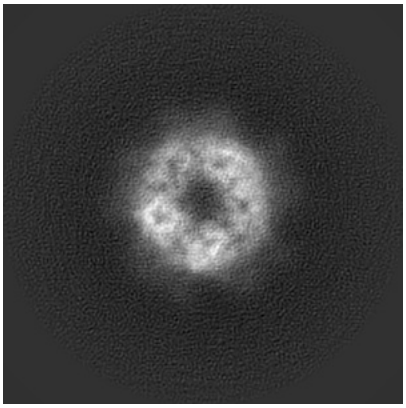
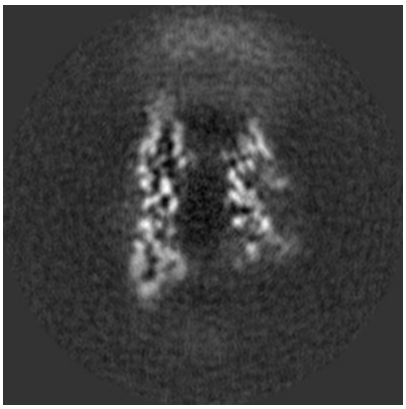


Z

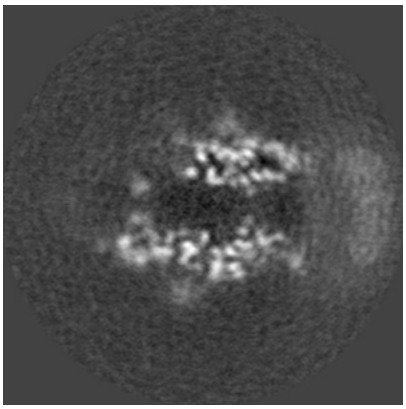
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

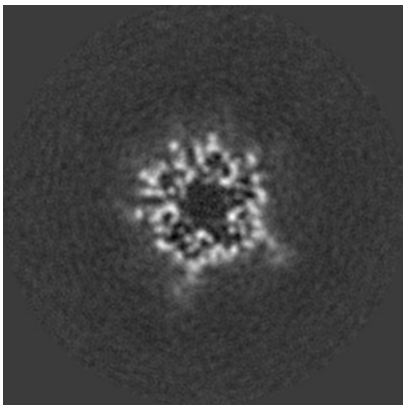
6.2.1 Primary map



X Index: 110

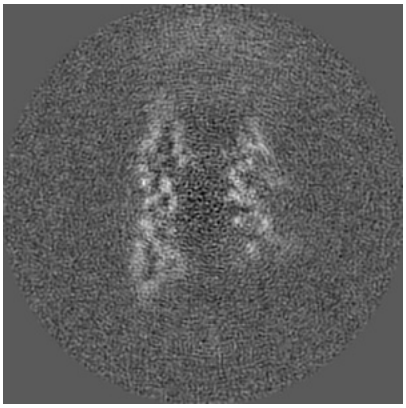


Y Index: 110

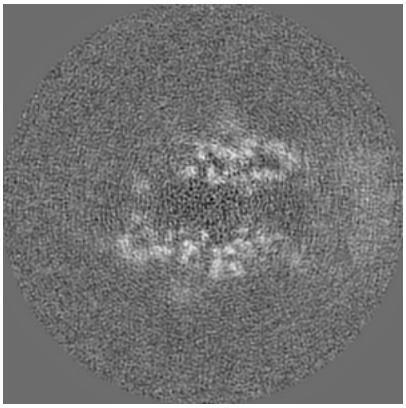


Z Index: 110

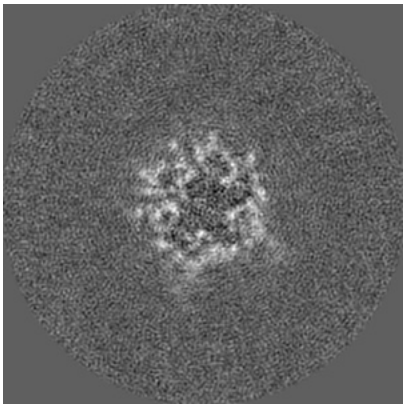
6.2.2 Raw map



X Index: 110



Y Index: 110

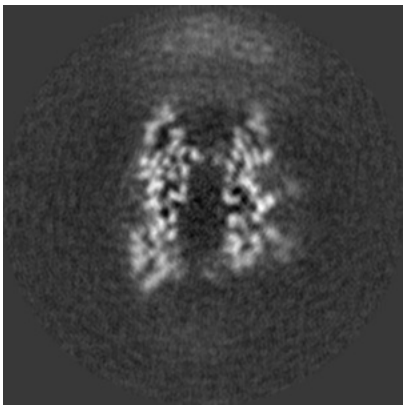


Z Index: 110

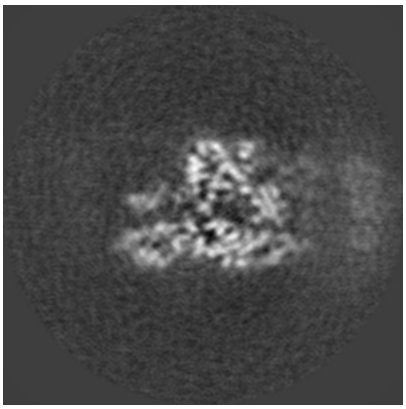
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

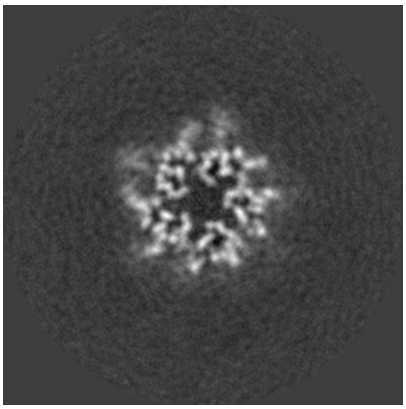
6.3.1 Primary map



X Index: 115

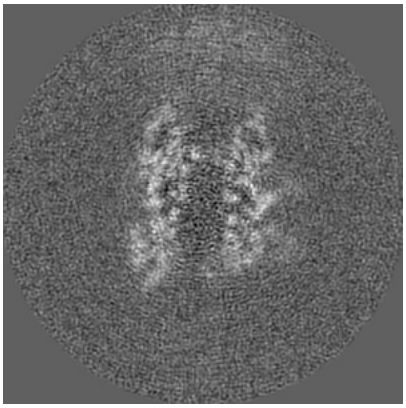


Y Index: 95

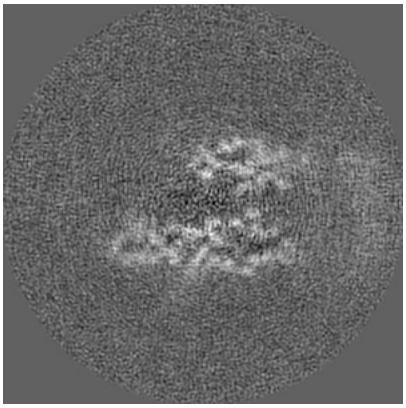


Z Index: 117

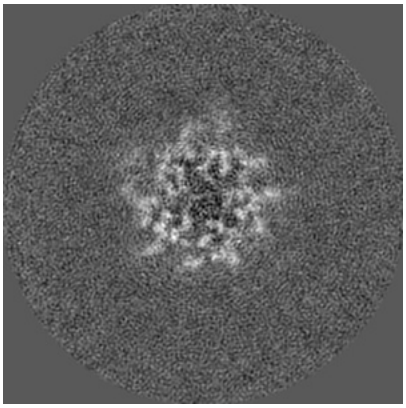
6.3.2 Raw map



X Index: 116



Y Index: 102

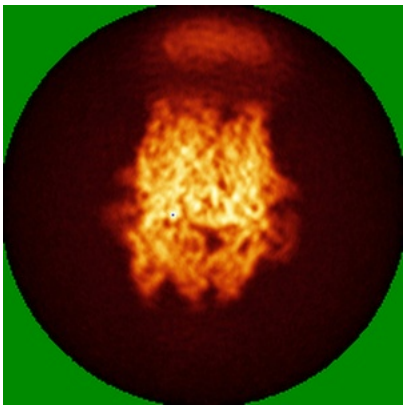


Z Index: 118

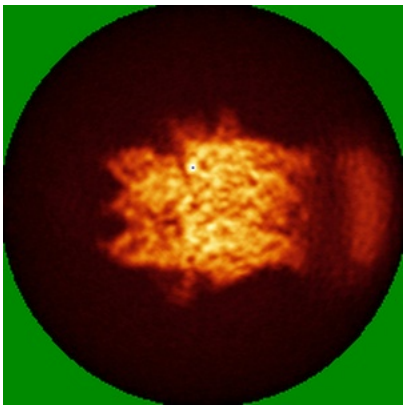
The images above show the largest variance slices of the map in three orthogonal directions.

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

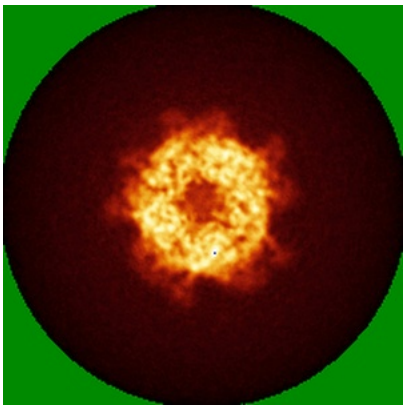
6.4.1 Primary map



X

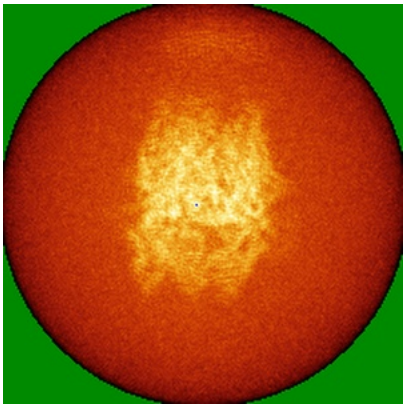


Y

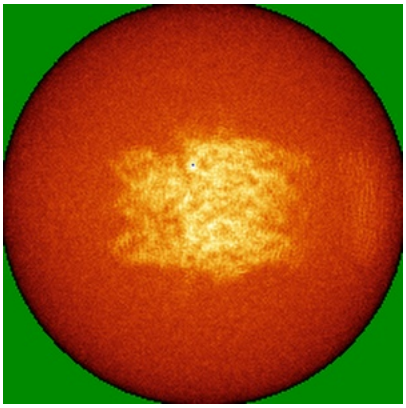


Z

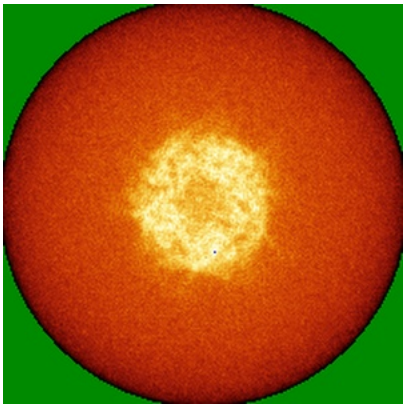
6.4.2 Raw map



X



Y

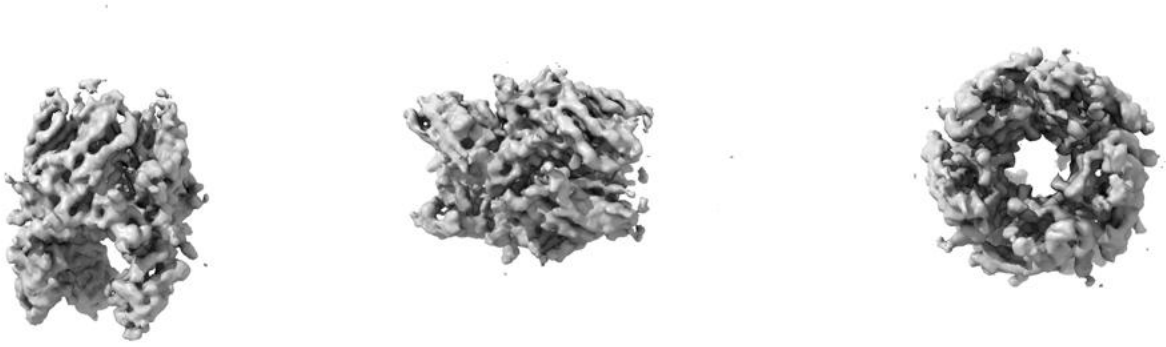


Z

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 0.00467. 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.

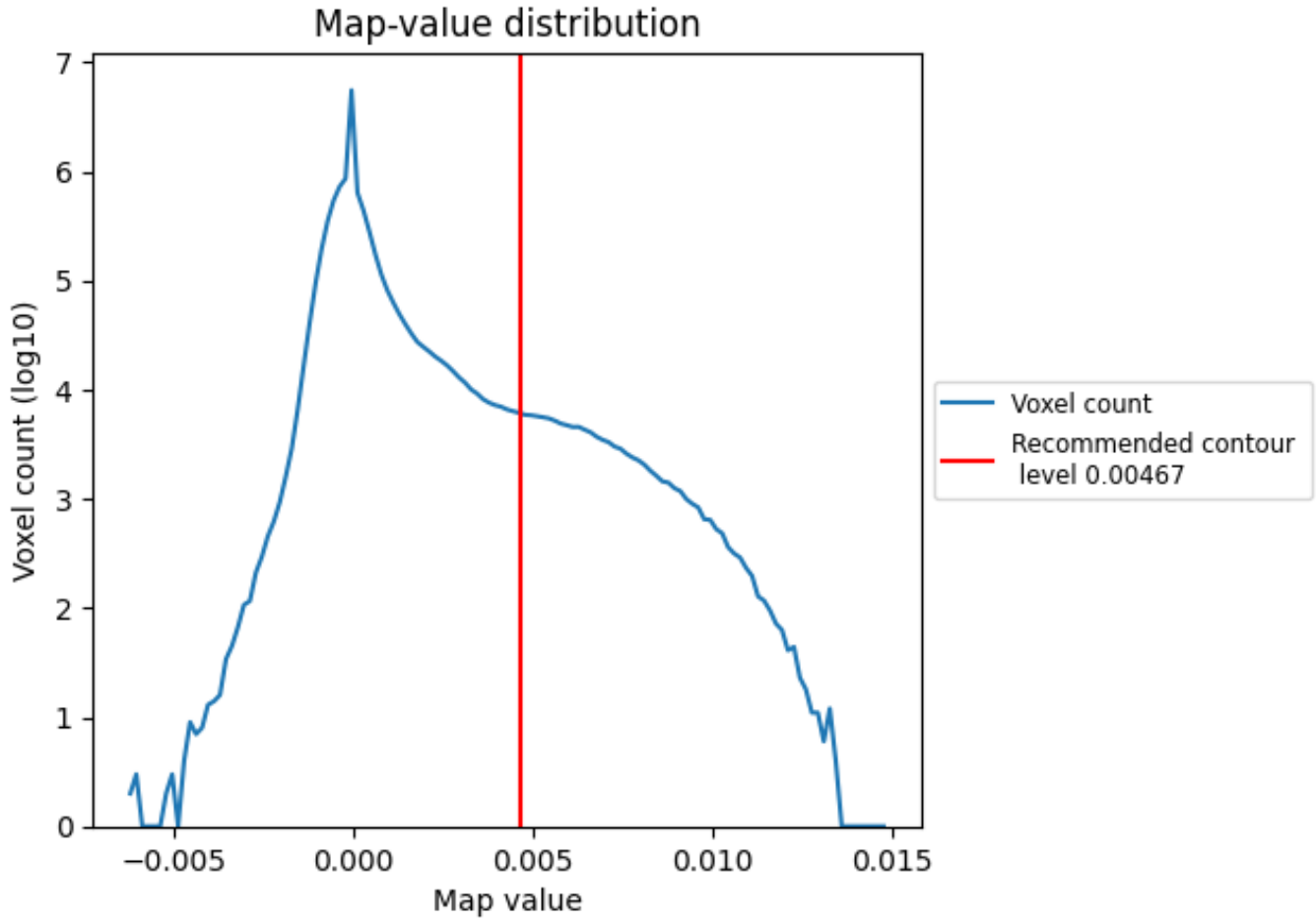
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

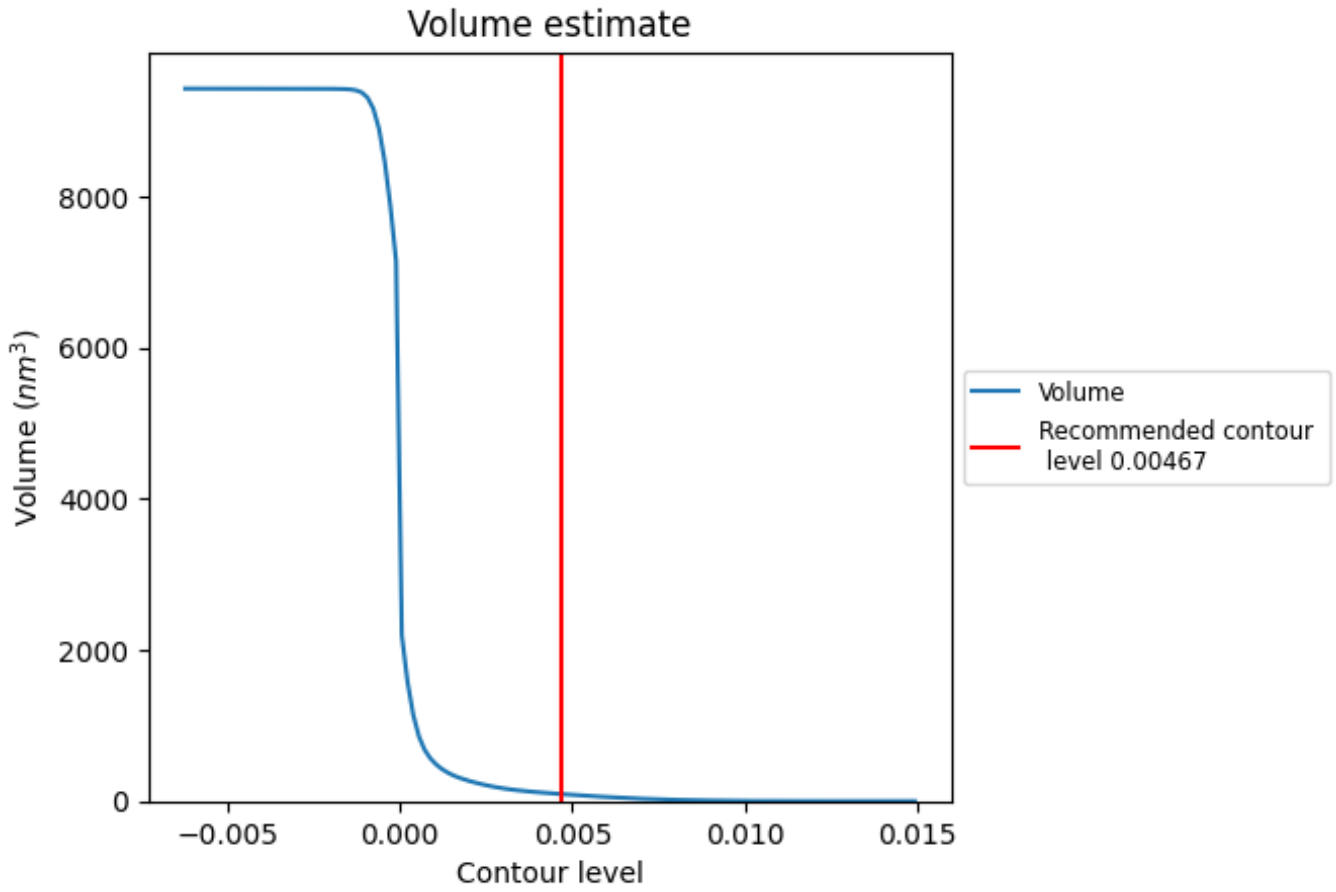
This section contains the results of statistical analysis of the map.

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.

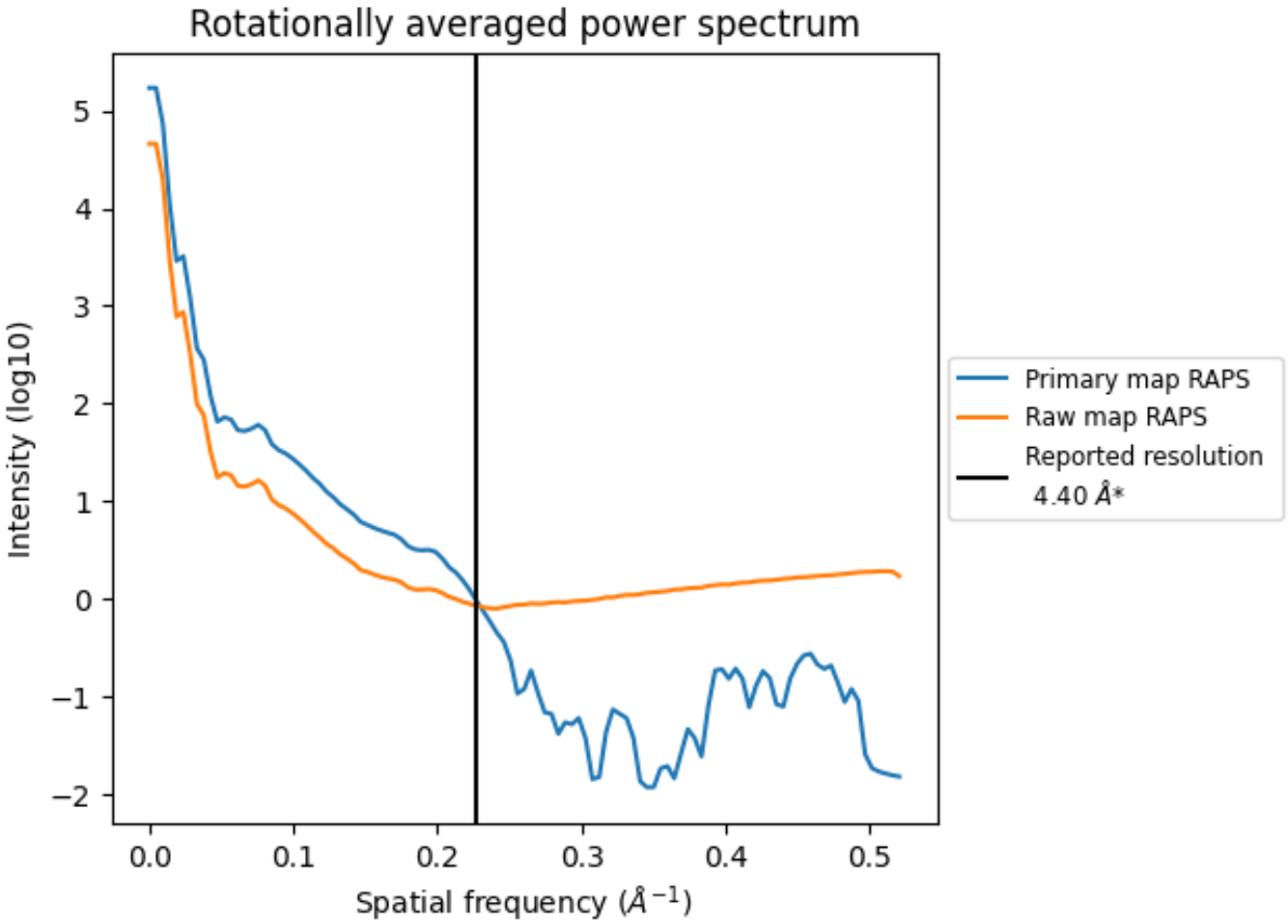
7.2 Volume estimate (i)



The volume at the recommended contour level is 94 nm^3; this corresponds to an approximate mass of 85 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)

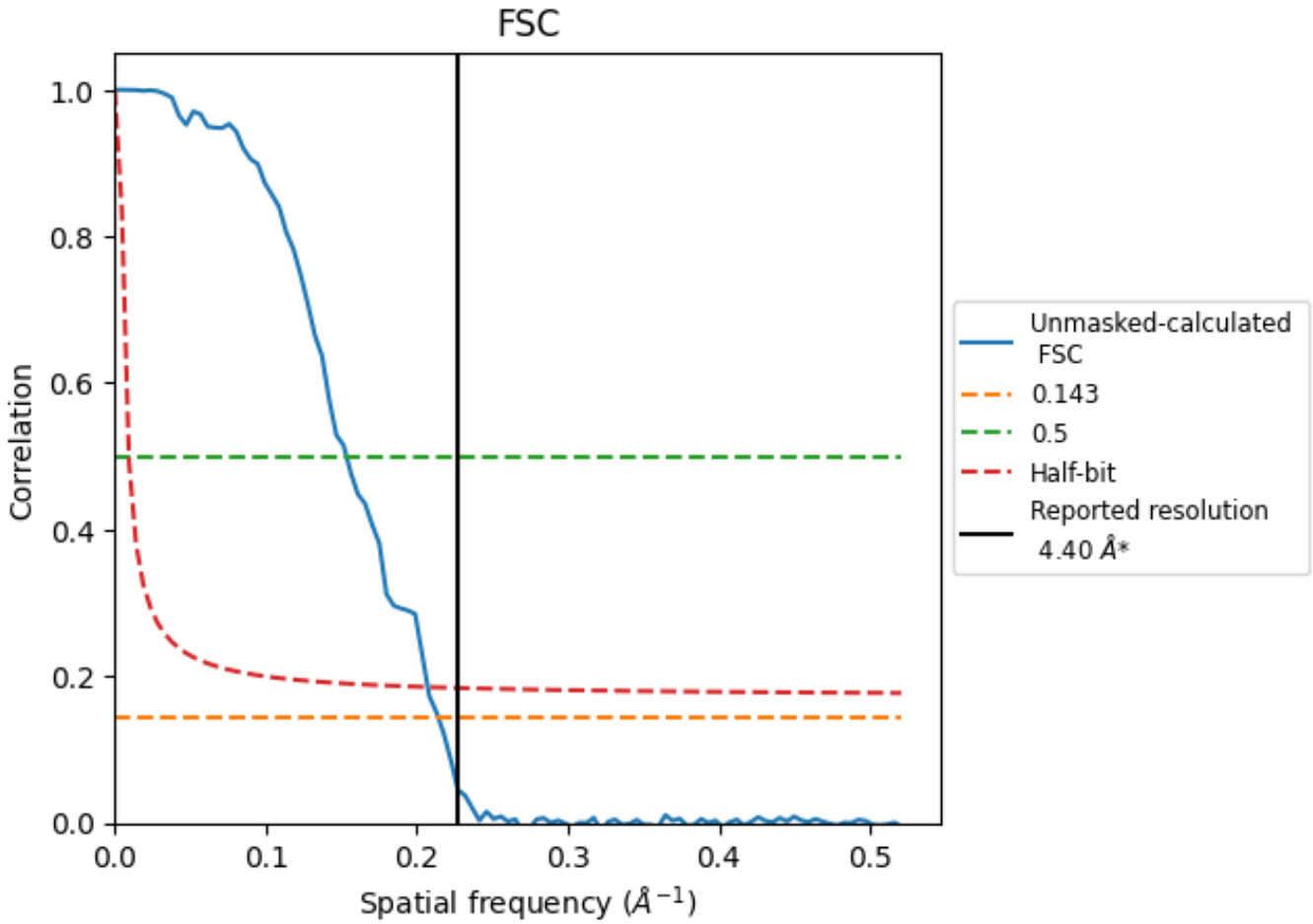


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

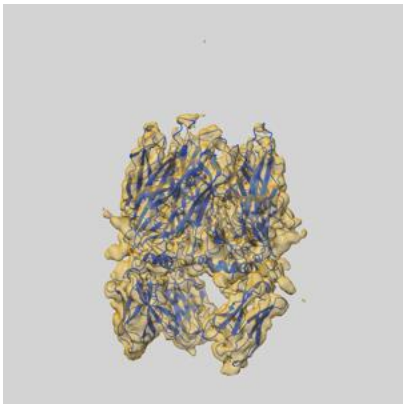
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.67	6.52	4.82

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

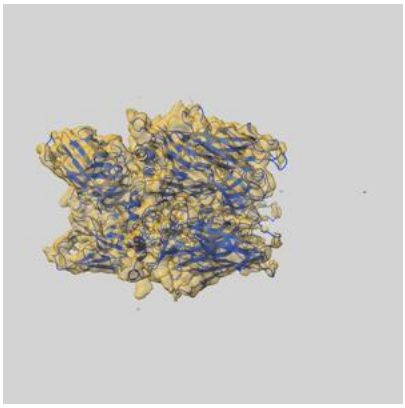
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16666 and PDB model 8CI2. Per-residue inclusion information can be found in section 3 on page 9.

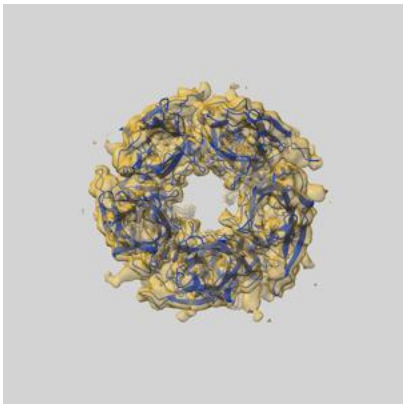
9.1 Map-model overlay



X



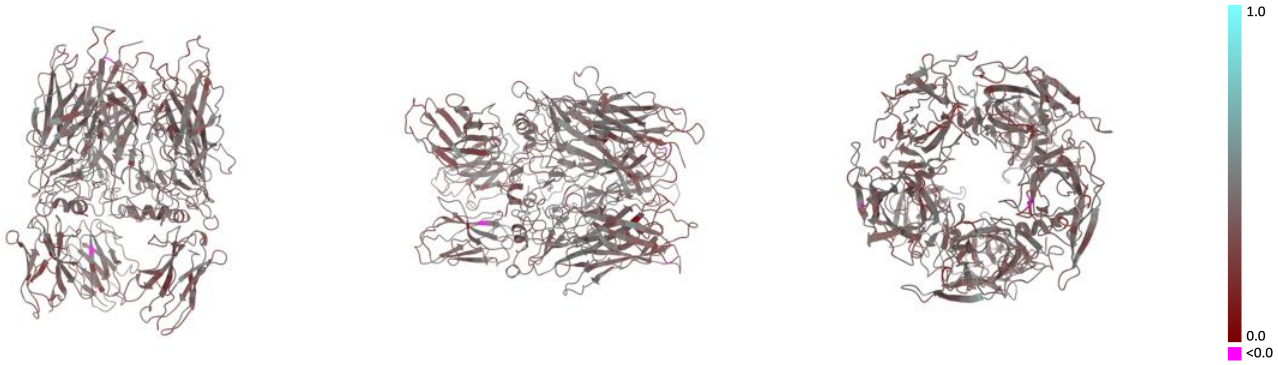
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00467 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.

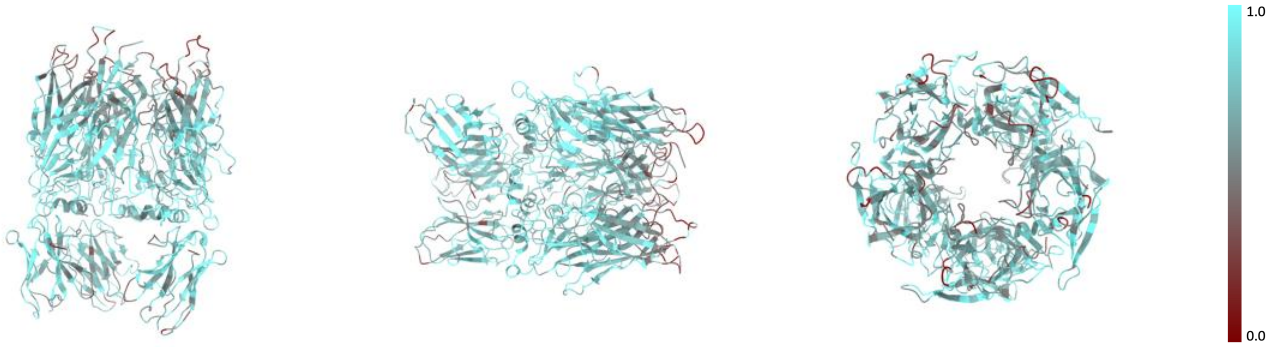
9.2 Q-score mapped to coordinate model (i)



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.

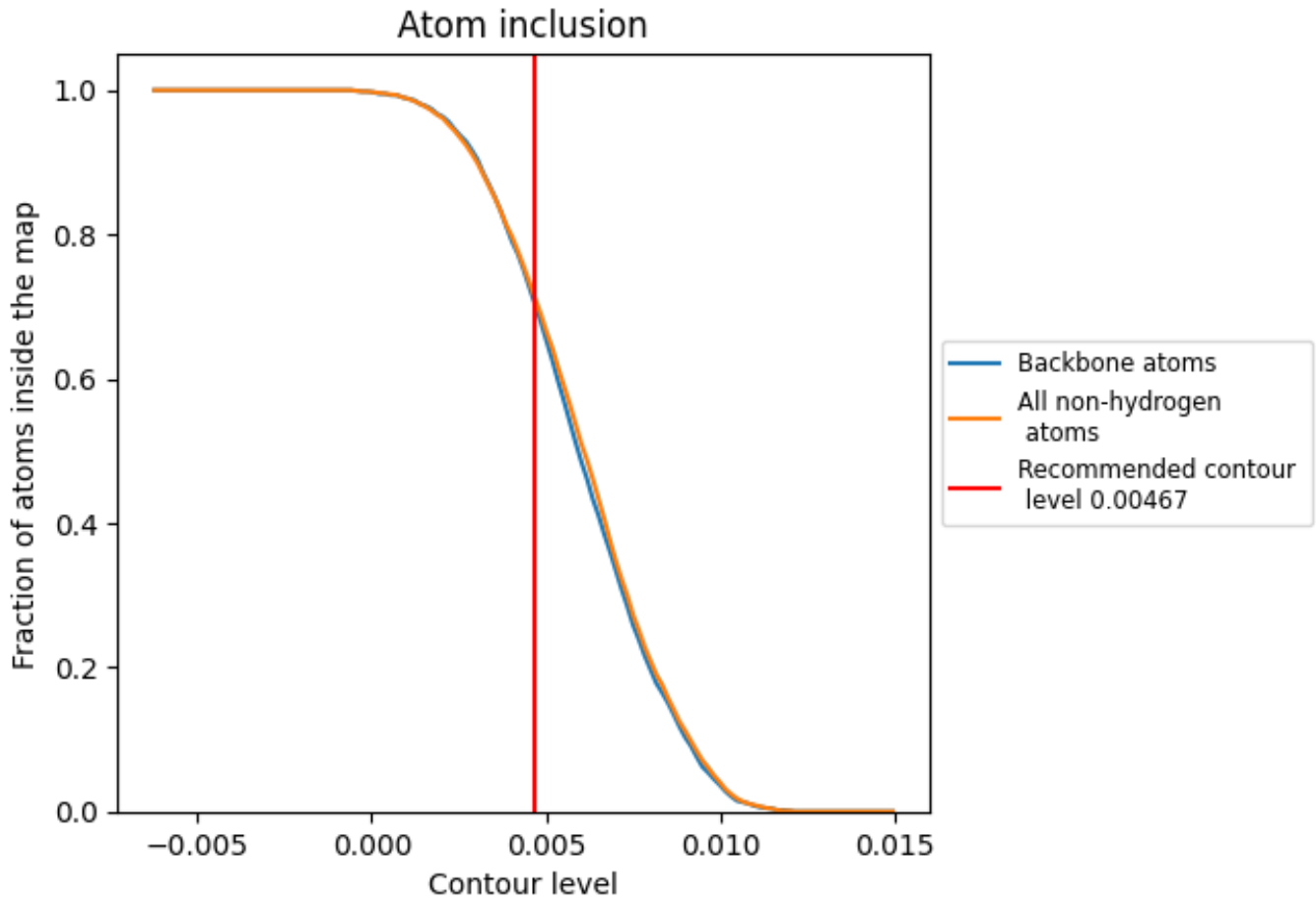
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00467).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 71% 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 (0.00467) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.3810
A	0.7160	0.3930
B	0.7070	0.3870
C	0.7100	0.3850
D	0.7100	0.3810
E	0.7340	0.3850
F	0.7450	0.3650
G	0.7330	0.3670
I	0.7280	0.3680
P	0.6790	0.3520
Q	0.7860	0.2960
R	0.6790	0.3160
S	0.8570	0.4420
T	0.7860	0.4140