wwPDB EM Validation Summary Report (i)

Apr 24, 2025 – 04:19 PM JST

PDB ID	:	8ZRN / pdb_00008zrn
EMDB ID	:	EMD-60400
Title	:	Structure of abt
Authors	:	Su, J.; Yu, Z.; Zhao, Y.
Deposited on	:	2024-06-04
Resolution	:	3.25 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 (i) 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 (i)) were used in the production of this report:

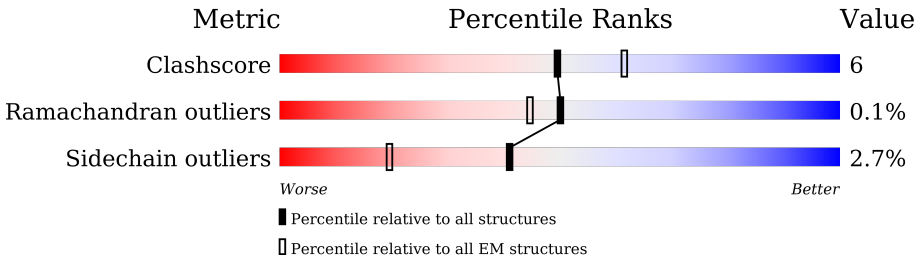
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.25 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	501	62% 15% 24%
1	C	501	5% 65% 11% 24%
2	B	633	52% 9% 40%
2	D	633	5% 51% 10% 39%
2	E	633	6% 49% 11% 39%
3	F	3	33% 67% 33%
3	G	3	67% 33% 67%
3	H	3	33% 33% 67%

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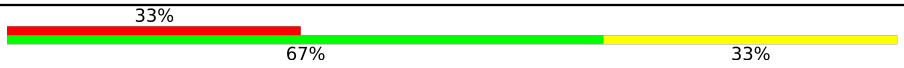
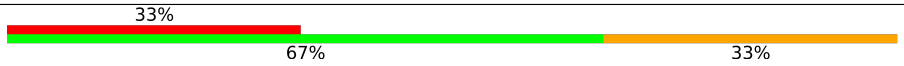
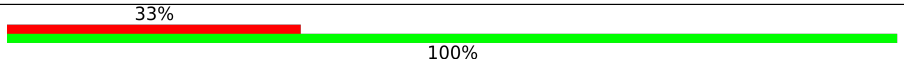
Mol	Chain	Length	Quality of chain
3	I	3	
3	J	3	
3	K	3	
3	L	3	
3	M	3	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15997 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 Neuronal acetylcholine receptor subunit alpha-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total	C	N	O	S	0	0
			3160	2086	493	563	18		
1	C	381	Total	C	N	O	S	0	0
			3150	2079	492	561	18		

There are 118 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	609	GLY	-	linker	UNP Q15825
A	610	SER	-	linker	UNP Q15825
A	611	GLY	-	linker	UNP Q15825
A	612	SER	-	linker	UNP Q15825
A	613	LEU	-	linker	UNP Q15825
A	614	GLU	-	linker	UNP Q15825
A	615	VAL	-	linker	UNP Q15825
A	616	LEU	-	linker	UNP Q15825
A	617	PHE	-	linker	UNP Q15825
A	618	GLN	-	linker	UNP Q15825
A	619	GLY	-	linker	UNP Q15825
A	620	PRO	-	linker	UNP Q15825
A	621	GLY	-	linker	UNP Q15825
A	622	GLY	-	linker	UNP Q15825
A	623	SER	-	linker	UNP Q15825
A	624	GLY	-	linker	UNP Q15825
A	625	SER	-	linker	UNP Q15825
A	626	GLY	-	linker	UNP Q15825
A	627	SER	-	linker	UNP Q15825
A	628	LEU	-	linker	UNP Q15825
A	629	GLU	-	linker	UNP Q15825
A	630	VAL	-	linker	UNP Q15825
A	631	LEU	-	linker	UNP Q15825
A	632	PHE	-	linker	UNP Q15825
A	633	GLN	-	linker	UNP Q15825
A	634	GLY	-	linker	UNP Q15825

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Chain	Residue	Modelled	Actual	Comment	Reference
A	635	PRO	-	linker	UNP Q15825
A	636	GLY	-	linker	UNP Q15825
A	637	GLY	-	linker	UNP Q15825
A	638	SER	-	linker	UNP Q15825
A	652	LEU	VAL	conflict	UNP Q15825
A	653	ALA	GLU	conflict	UNP Q15825
A	655	ILE	VAL	conflict	UNP Q15825
A	656	LEU	ILE	conflict	UNP Q15825
A	658	GLU	SER	conflict	UNP Q15825
A	661	TYR	PHE	conflict	UNP Q15825
A	664	ASN	GLU	conflict	UNP Q15825
A	665	ARG	ASN	conflict	UNP Q15825
A	666	PHE	MET	conflict	UNP Q15825
A	667	ARG	LYS	conflict	UNP Q15825
A	669	GLN	HIS	conflict	UNP Q15825
A	718	SER	-	expression tag	UNP Q15825
A	719	ALA	-	expression tag	UNP Q15825
A	720	SER	-	expression tag	UNP Q15825
A	721	ALA	-	expression tag	UNP Q15825
A	722	SER	-	expression tag	UNP Q15825
A	723	ALA	-	expression tag	UNP Q15825
A	724	SER	-	expression tag	UNP Q15825
A	725	ALA	-	expression tag	UNP Q15825
A	726	SER	-	expression tag	UNP Q15825
A	727	ALA	-	expression tag	UNP Q15825
A	728	HIS	-	expression tag	UNP Q15825
A	729	HIS	-	expression tag	UNP Q15825
A	730	HIS	-	expression tag	UNP Q15825
A	731	HIS	-	expression tag	UNP Q15825
A	732	HIS	-	expression tag	UNP Q15825
A	733	HIS	-	expression tag	UNP Q15825
A	734	HIS	-	expression tag	UNP Q15825
A	735	HIS	-	expression tag	UNP Q15825
C	609	GLY	-	linker	UNP Q15825
C	610	SER	-	linker	UNP Q15825
C	611	GLY	-	linker	UNP Q15825
C	612	SER	-	linker	UNP Q15825
C	613	LEU	-	linker	UNP Q15825
C	614	GLU	-	linker	UNP Q15825
C	615	VAL	-	linker	UNP Q15825
C	616	LEU	-	linker	UNP Q15825
C	617	PHE	-	linker	UNP Q15825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	GLN	-	linker	UNP Q15825
C	619	GLY	-	linker	UNP Q15825
C	620	PRO	-	linker	UNP Q15825
C	621	GLY	-	linker	UNP Q15825
C	622	GLY	-	linker	UNP Q15825
C	623	SER	-	linker	UNP Q15825
C	624	GLY	-	linker	UNP Q15825
C	625	SER	-	linker	UNP Q15825
C	626	GLY	-	linker	UNP Q15825
C	627	SER	-	linker	UNP Q15825
C	628	LEU	-	linker	UNP Q15825
C	629	GLU	-	linker	UNP Q15825
C	630	VAL	-	linker	UNP Q15825
C	631	LEU	-	linker	UNP Q15825
C	632	PHE	-	linker	UNP Q15825
C	633	GLN	-	linker	UNP Q15825
C	634	GLY	-	linker	UNP Q15825
C	635	PRO	-	linker	UNP Q15825
C	636	GLY	-	linker	UNP Q15825
C	637	GLY	-	linker	UNP Q15825
C	638	SER	-	linker	UNP Q15825
C	652	LEU	VAL	conflict	UNP Q15825
C	653	ALA	GLU	conflict	UNP Q15825
C	655	ILE	VAL	conflict	UNP Q15825
C	656	LEU	ILE	conflict	UNP Q15825
C	658	GLU	SER	conflict	UNP Q15825
C	661	TYR	PHE	conflict	UNP Q15825
C	664	ASN	GLU	conflict	UNP Q15825
C	665	ARG	ASN	conflict	UNP Q15825
C	666	PHE	MET	conflict	UNP Q15825
C	667	ARG	LYS	conflict	UNP Q15825
C	669	GLN	HIS	conflict	UNP Q15825
C	718	SER	-	expression tag	UNP Q15825
C	719	ALA	-	expression tag	UNP Q15825
C	720	SER	-	expression tag	UNP Q15825
C	721	ALA	-	expression tag	UNP Q15825
C	722	SER	-	expression tag	UNP Q15825
C	723	ALA	-	expression tag	UNP Q15825
C	724	SER	-	expression tag	UNP Q15825
C	725	ALA	-	expression tag	UNP Q15825
C	726	SER	-	expression tag	UNP Q15825
C	727	ALA	-	expression tag	UNP Q15825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	728	HIS	-	expression tag	UNP Q15825
C	729	HIS	-	expression tag	UNP Q15825
C	730	HIS	-	expression tag	UNP Q15825
C	731	HIS	-	expression tag	UNP Q15825
C	732	HIS	-	expression tag	UNP Q15825
C	733	HIS	-	expression tag	UNP Q15825
C	734	HIS	-	expression tag	UNP Q15825
C	735	HIS	-	expression tag	UNP Q15825

- Molecule 2 is a protein called Neuronal acetylcholine receptor subunit beta-4,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	382	Total	C	N	O	S	0	0
			3104	2027	502	555	20		
2	D	383	Total	C	N	O	S	0	0
			3115	2036	503	556	20		
2	E	384	Total	C	N	O	S	0	0
			3125	2044	504	557	20		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	361	GLY	-	linker	UNP P30926
B	362	SER	-	linker	UNP P30926
B	363	GLY	-	linker	UNP P30926
B	364	SER	-	linker	UNP P30926
B	365	LEU	-	linker	UNP P30926
B	366	GLU	-	linker	UNP P30926
B	367	VAL	-	linker	UNP P30926
B	368	LEU	-	linker	UNP P30926
B	369	PHE	-	linker	UNP P30926
B	370	GLN	-	linker	UNP P30926
B	371	GLY	-	linker	UNP P30926
B	372	PRO	-	linker	UNP P30926
B	373	GLY	-	linker	UNP P30926
B	374	GLY	-	linker	UNP P30926
B	375	SER	-	linker	UNP P30926
B	382	TRP	MET	conflict	UNP P0ABE7
B	477	ILE	HIS	conflict	UNP P0ABE7
B	481	LEU	-	linker	UNP P0ABE7
B	482	GLY	-	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	483	SER	-	linker	UNP P0ABE7
B	484	GLY	-	linker	UNP P0ABE7
B	485	SER	-	linker	UNP P0ABE7
B	486	LEU	-	linker	UNP P0ABE7
B	487	GLU	-	linker	UNP P0ABE7
B	488	VAL	-	linker	UNP P0ABE7
B	489	LEU	-	linker	UNP P0ABE7
B	490	PHE	-	linker	UNP P0ABE7
B	491	GLN	-	linker	UNP P0ABE7
B	492	GLY	-	linker	UNP P0ABE7
B	493	PRO	-	linker	UNP P0ABE7
B	494	GLY	-	linker	UNP P0ABE7
B	495	GLY	-	linker	UNP P0ABE7
B	519	PRO	GLN	conflict	UNP P30926
B	521	LEU	VAL	conflict	UNP P30926
B	522	ALA	GLN	conflict	UNP P30926
B	524	ILE	ALA	conflict	UNP P30926
B	527	GLU	GLY	conflict	UNP P30926
B	530	TYR	PHE	conflict	UNP P30926
B	533	ASN	GLN	conflict	UNP P30926
B	534	ARG	HIS	conflict	UNP P30926
B	535	PHE	MET	conflict	UNP P30926
B	536	ARG	LYS	conflict	UNP P30926
B	538	GLN	ASP	conflict	UNP P30926
B	596	SER	-	expression tag	UNP P30926
B	597	ALA	-	expression tag	UNP P30926
B	598	SER	-	expression tag	UNP P30926
B	599	ALA	-	expression tag	UNP P30926
B	600	SER	-	expression tag	UNP P30926
B	601	ALA	-	expression tag	UNP P30926
B	602	SER	-	expression tag	UNP P30926
B	603	ALA	-	expression tag	UNP P30926
B	604	SER	-	expression tag	UNP P30926
B	605	ALA	-	expression tag	UNP P30926
B	606	TRP	-	expression tag	UNP P30926
B	607	SER	-	expression tag	UNP P30926
B	608	HIS	-	expression tag	UNP P30926
B	609	PRO	-	expression tag	UNP P30926
B	610	GLN	-	expression tag	UNP P30926
B	611	PHE	-	expression tag	UNP P30926
B	612	GLU	-	expression tag	UNP P30926
B	613	LYS	-	expression tag	UNP P30926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	614	GLY	-	expression tag	UNP P30926
B	615	GLY	-	expression tag	UNP P30926
B	616	GLY	-	expression tag	UNP P30926
B	617	SER	-	expression tag	UNP P30926
B	618	GLY	-	expression tag	UNP P30926
B	619	GLY	-	expression tag	UNP P30926
B	620	GLY	-	expression tag	UNP P30926
B	621	SER	-	expression tag	UNP P30926
B	622	GLY	-	expression tag	UNP P30926
B	623	GLY	-	expression tag	UNP P30926
B	624	SER	-	expression tag	UNP P30926
B	625	ALA	-	expression tag	UNP P30926
B	626	TRP	-	expression tag	UNP P30926
B	627	SER	-	expression tag	UNP P30926
B	628	HIS	-	expression tag	UNP P30926
B	629	PRO	-	expression tag	UNP P30926
B	630	GLN	-	expression tag	UNP P30926
B	631	PHE	-	expression tag	UNP P30926
B	632	GLU	-	expression tag	UNP P30926
B	633	LYS	-	expression tag	UNP P30926
D	361	GLY	-	linker	UNP P30926
D	362	SER	-	linker	UNP P30926
D	363	GLY	-	linker	UNP P30926
D	364	SER	-	linker	UNP P30926
D	365	LEU	-	linker	UNP P30926
D	366	GLU	-	linker	UNP P30926
D	367	VAL	-	linker	UNP P30926
D	368	LEU	-	linker	UNP P30926
D	369	PHE	-	linker	UNP P30926
D	370	GLN	-	linker	UNP P30926
D	371	GLY	-	linker	UNP P30926
D	372	PRO	-	linker	UNP P30926
D	373	GLY	-	linker	UNP P30926
D	374	GLY	-	linker	UNP P30926
D	375	SER	-	linker	UNP P30926
D	382	TRP	MET	conflict	UNP P0ABE7
D	477	ILE	HIS	conflict	UNP P0ABE7
D	481	LEU	-	linker	UNP P0ABE7
D	482	GLY	-	linker	UNP P0ABE7
D	483	SER	-	linker	UNP P0ABE7
D	484	GLY	-	linker	UNP P0ABE7
D	485	SER	-	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	486	LEU	-	linker	UNP P0ABE7
D	487	GLU	-	linker	UNP P0ABE7
D	488	VAL	-	linker	UNP P0ABE7
D	489	LEU	-	linker	UNP P0ABE7
D	490	PHE	-	linker	UNP P0ABE7
D	491	GLN	-	linker	UNP P0ABE7
D	492	GLY	-	linker	UNP P0ABE7
D	493	PRO	-	linker	UNP P0ABE7
D	494	GLY	-	linker	UNP P0ABE7
D	495	GLY	-	linker	UNP P0ABE7
D	519	PRO	GLN	conflict	UNP P30926
D	521	LEU	VAL	conflict	UNP P30926
D	522	ALA	GLN	conflict	UNP P30926
D	524	ILE	ALA	conflict	UNP P30926
D	527	GLU	GLY	conflict	UNP P30926
D	530	TYR	PHE	conflict	UNP P30926
D	533	ASN	GLN	conflict	UNP P30926
D	534	ARG	HIS	conflict	UNP P30926
D	535	PHE	MET	conflict	UNP P30926
D	536	ARG	LYS	conflict	UNP P30926
D	538	GLN	ASP	conflict	UNP P30926
D	596	SER	-	expression tag	UNP P30926
D	597	ALA	-	expression tag	UNP P30926
D	598	SER	-	expression tag	UNP P30926
D	599	ALA	-	expression tag	UNP P30926
D	600	SER	-	expression tag	UNP P30926
D	601	ALA	-	expression tag	UNP P30926
D	602	SER	-	expression tag	UNP P30926
D	603	ALA	-	expression tag	UNP P30926
D	604	SER	-	expression tag	UNP P30926
D	605	ALA	-	expression tag	UNP P30926
D	606	TRP	-	expression tag	UNP P30926
D	607	SER	-	expression tag	UNP P30926
D	608	HIS	-	expression tag	UNP P30926
D	609	PRO	-	expression tag	UNP P30926
D	610	GLN	-	expression tag	UNP P30926
D	611	PHE	-	expression tag	UNP P30926
D	612	GLU	-	expression tag	UNP P30926
D	613	LYS	-	expression tag	UNP P30926
D	614	GLY	-	expression tag	UNP P30926
D	615	GLY	-	expression tag	UNP P30926
D	616	GLY	-	expression tag	UNP P30926

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Chain	Residue	Modelled	Actual	Comment	Reference
D	617	SER	-	expression tag	UNP P30926
D	618	GLY	-	expression tag	UNP P30926
D	619	GLY	-	expression tag	UNP P30926
D	620	GLY	-	expression tag	UNP P30926
D	621	SER	-	expression tag	UNP P30926
D	622	GLY	-	expression tag	UNP P30926
D	623	GLY	-	expression tag	UNP P30926
D	624	SER	-	expression tag	UNP P30926
D	625	ALA	-	expression tag	UNP P30926
D	626	TRP	-	expression tag	UNP P30926
D	627	SER	-	expression tag	UNP P30926
D	628	HIS	-	expression tag	UNP P30926
D	629	PRO	-	expression tag	UNP P30926
D	630	GLN	-	expression tag	UNP P30926
D	631	PHE	-	expression tag	UNP P30926
D	632	GLU	-	expression tag	UNP P30926
D	633	LYS	-	expression tag	UNP P30926
E	361	GLY	-	linker	UNP P30926
E	362	SER	-	linker	UNP P30926
E	363	GLY	-	linker	UNP P30926
E	364	SER	-	linker	UNP P30926
E	365	LEU	-	linker	UNP P30926
E	366	GLU	-	linker	UNP P30926
E	367	VAL	-	linker	UNP P30926
E	368	LEU	-	linker	UNP P30926
E	369	PHE	-	linker	UNP P30926
E	370	GLN	-	linker	UNP P30926
E	371	GLY	-	linker	UNP P30926
E	372	PRO	-	linker	UNP P30926
E	373	GLY	-	linker	UNP P30926
E	374	GLY	-	linker	UNP P30926
E	375	SER	-	linker	UNP P30926
E	382	TRP	MET	conflict	UNP P0ABE7
E	477	ILE	HIS	conflict	UNP P0ABE7
E	481	LEU	-	linker	UNP P0ABE7
E	482	GLY	-	linker	UNP P0ABE7
E	483	SER	-	linker	UNP P0ABE7
E	484	GLY	-	linker	UNP P0ABE7
E	485	SER	-	linker	UNP P0ABE7
E	486	LEU	-	linker	UNP P0ABE7
E	487	GLU	-	linker	UNP P0ABE7
E	488	VAL	-	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	489	LEU	-	linker	UNP P0ABE7
E	490	PHE	-	linker	UNP P0ABE7
E	491	GLN	-	linker	UNP P0ABE7
E	492	GLY	-	linker	UNP P0ABE7
E	493	PRO	-	linker	UNP P0ABE7
E	494	GLY	-	linker	UNP P0ABE7
E	495	GLY	-	linker	UNP P0ABE7
E	519	PRO	GLN	conflict	UNP P30926
E	521	LEU	VAL	conflict	UNP P30926
E	522	ALA	GLN	conflict	UNP P30926
E	524	ILE	ALA	conflict	UNP P30926
E	527	GLU	GLY	conflict	UNP P30926
E	530	TYR	PHE	conflict	UNP P30926
E	533	ASN	GLN	conflict	UNP P30926
E	534	ARG	HIS	conflict	UNP P30926
E	535	PHE	MET	conflict	UNP P30926
E	536	ARG	LYS	conflict	UNP P30926
E	538	GLN	ASP	conflict	UNP P30926
E	596	SER	-	expression tag	UNP P30926
E	597	ALA	-	expression tag	UNP P30926
E	598	SER	-	expression tag	UNP P30926
E	599	ALA	-	expression tag	UNP P30926
E	600	SER	-	expression tag	UNP P30926
E	601	ALA	-	expression tag	UNP P30926
E	602	SER	-	expression tag	UNP P30926
E	603	ALA	-	expression tag	UNP P30926
E	604	SER	-	expression tag	UNP P30926
E	605	ALA	-	expression tag	UNP P30926
E	606	TRP	-	expression tag	UNP P30926
E	607	SER	-	expression tag	UNP P30926
E	608	HIS	-	expression tag	UNP P30926
E	609	PRO	-	expression tag	UNP P30926
E	610	GLN	-	expression tag	UNP P30926
E	611	PHE	-	expression tag	UNP P30926
E	612	GLU	-	expression tag	UNP P30926
E	613	LYS	-	expression tag	UNP P30926
E	614	GLY	-	expression tag	UNP P30926
E	615	GLY	-	expression tag	UNP P30926
E	616	GLY	-	expression tag	UNP P30926
E	617	SER	-	expression tag	UNP P30926
E	618	GLY	-	expression tag	UNP P30926
E	619	GLY	-	expression tag	UNP P30926

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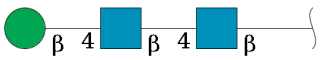
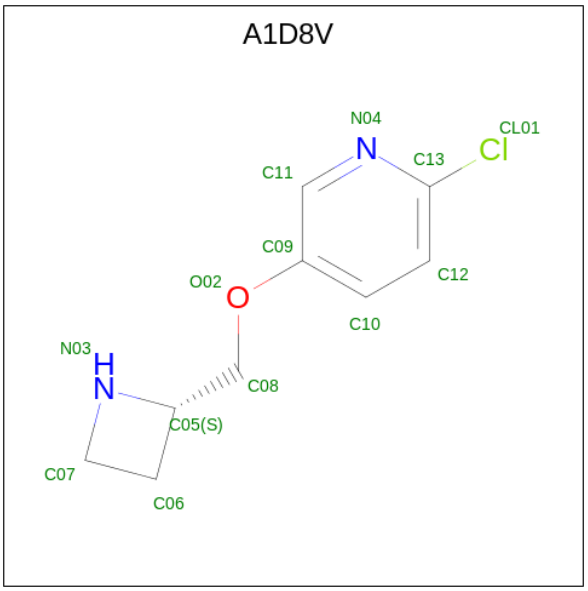
Chain	Residue	Modelled	Actual	Comment	Reference
E	620	GLY	-	expression tag	UNP P30926
E	621	SER	-	expression tag	UNP P30926
E	622	GLY	-	expression tag	UNP P30926
E	623	GLY	-	expression tag	UNP P30926
E	624	SER	-	expression tag	UNP P30926
E	625	ALA	-	expression tag	UNP P30926
E	626	TRP	-	expression tag	UNP P30926
E	627	SER	-	expression tag	UNP P30926
E	628	HIS	-	expression tag	UNP P30926
E	629	PRO	-	expression tag	UNP P30926
E	630	GLN	-	expression tag	UNP P30926
E	631	PHE	-	expression tag	UNP P30926
E	632	GLU	-	expression tag	UNP P30926
E	633	LYS	-	expression tag	UNP P30926

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 5-[[(2 {S})-azetidin-2-yl]methoxy]-2-chloranyl-pyridine (CCD ID: A1D8V) (formula: $C_9H_{11}ClN_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Cl	N	O	0
			13	9	1	2	1	
4	C	1	Total	C	Cl	N	O	0
			13	9	1	2	1	

- Molecule 5 is water.

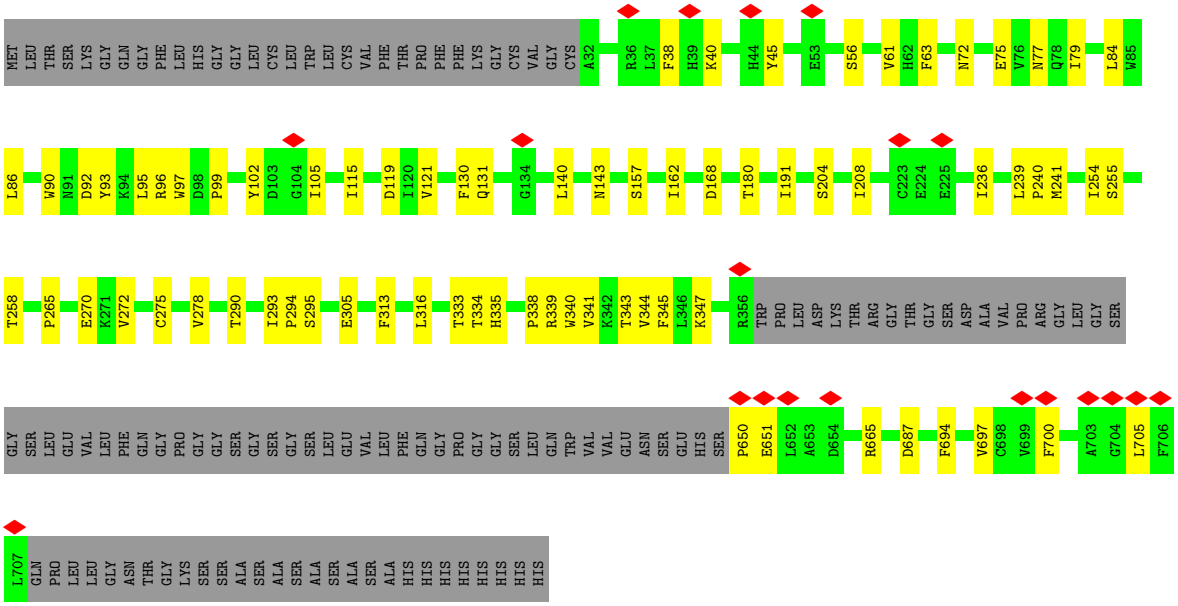
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	O	0
			2	2	
5	C	1	Total	O	0
			1	1	
5	D	2	Total	O	0
			2	2	

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.

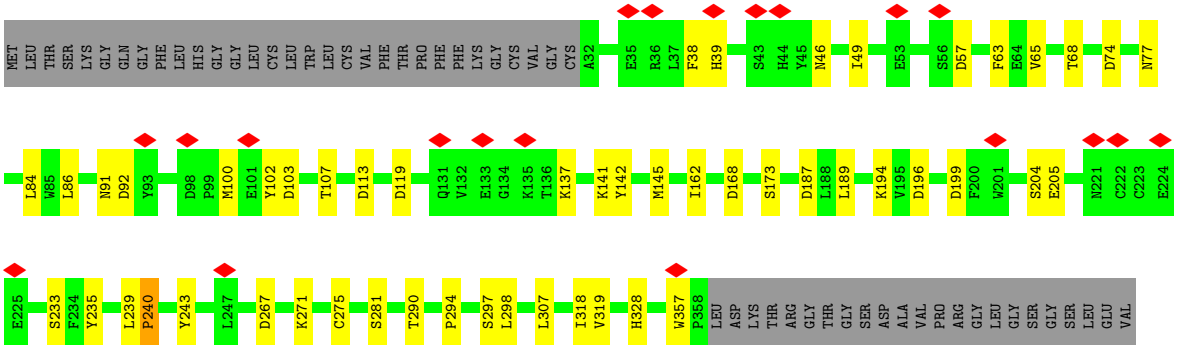
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-6

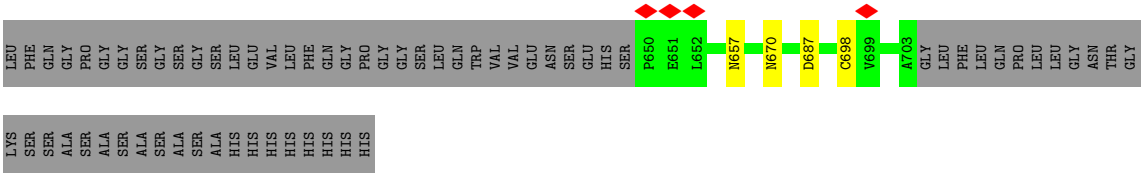
Chain A:



• Molecule 1: Neuronal acetylcholine receptor subunit alpha-6

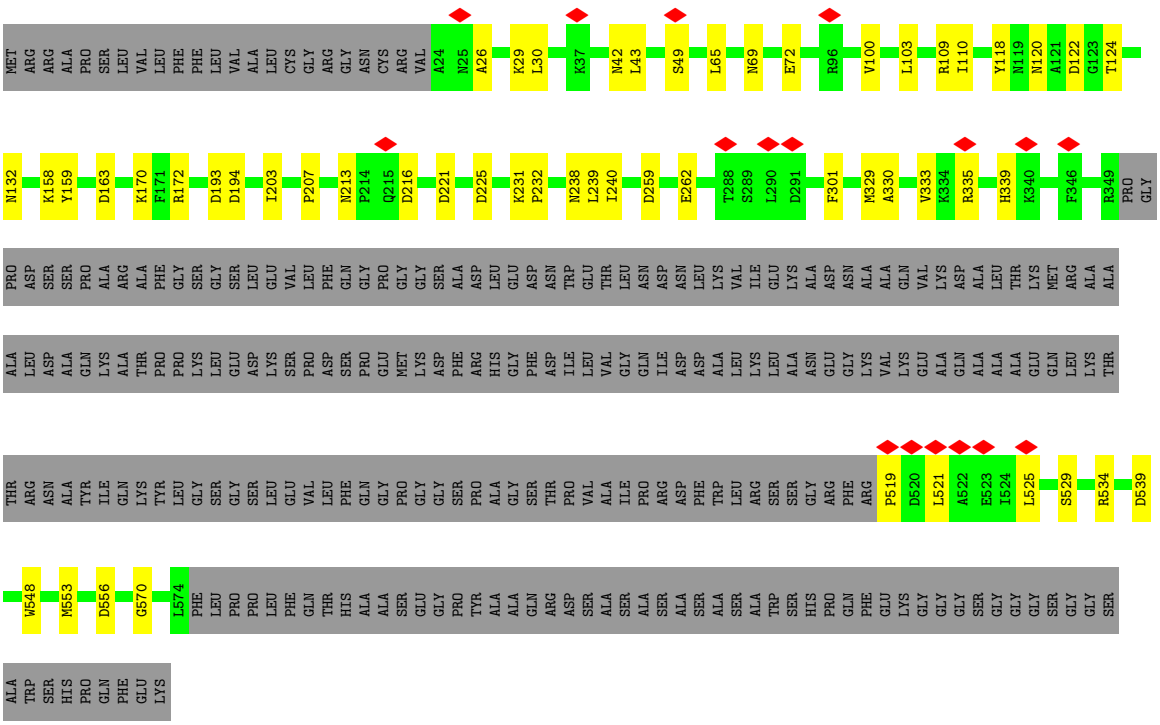
Chain C:





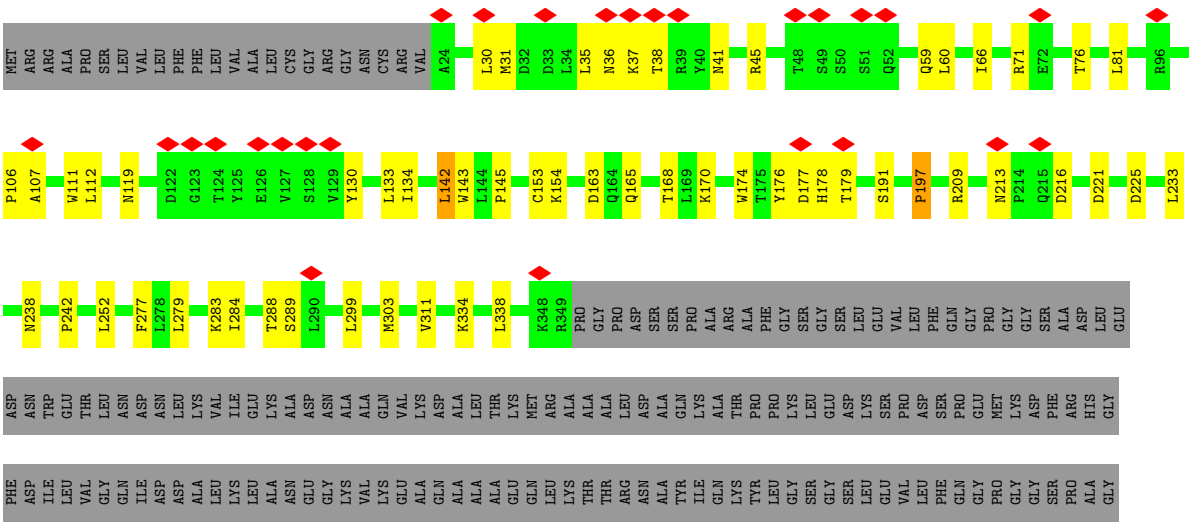
• Molecule 2: Neuronal acetylcholine receptor subunit beta-4,Soluble cytochrome b562

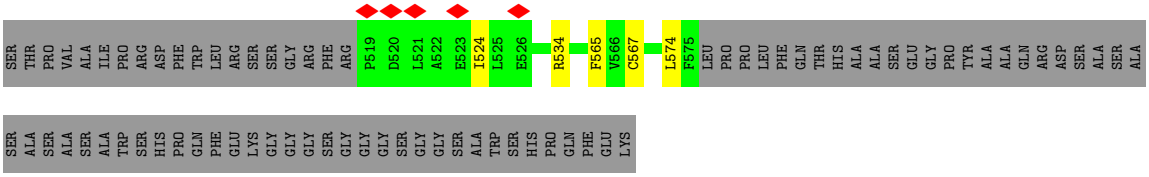
Chain B:



• Molecule 2: Neuronal acetylcholine receptor subunit beta-4,Soluble cytochrome b562

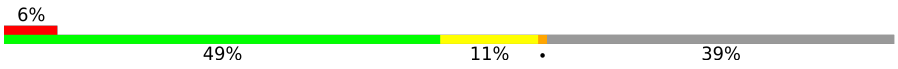
Chain D:

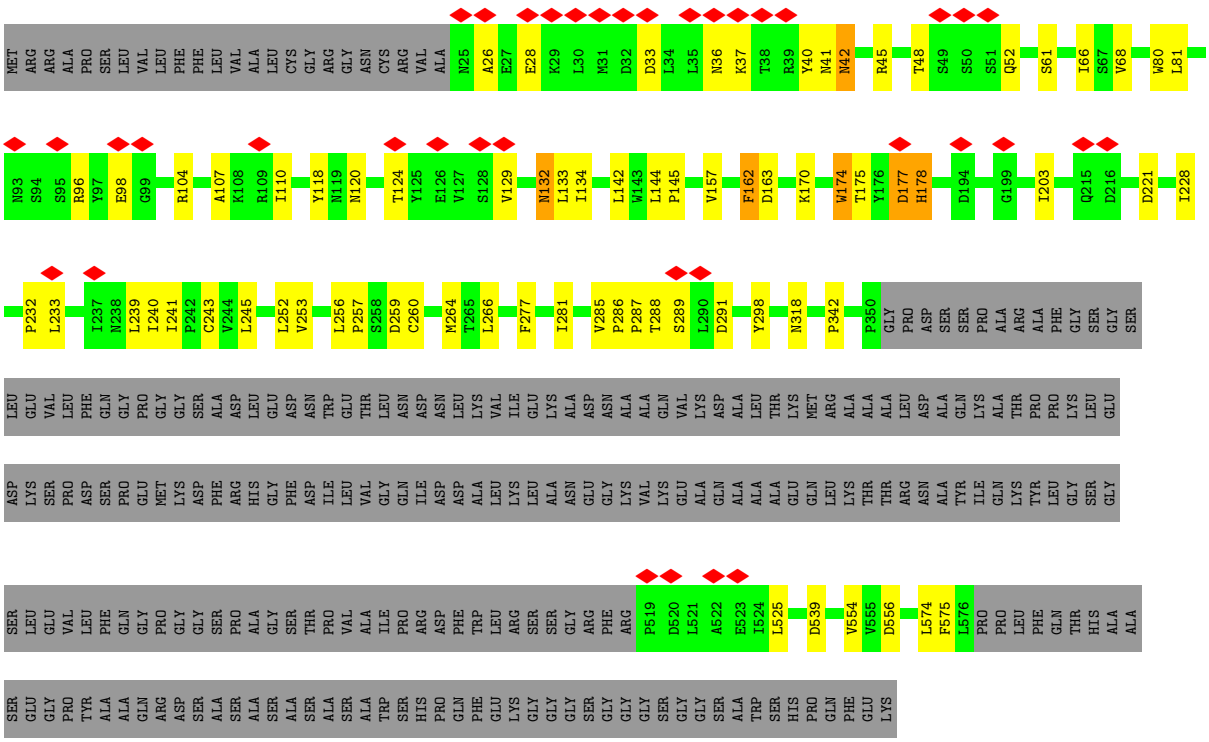




• Molecule 2: Neuronal acetylcholine receptor subunit beta-4,Soluble cytochrome b562

Chain E:





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

Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

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

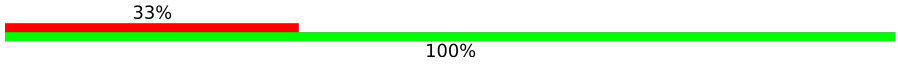
Chain K:

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

Chain L:

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

Chain M:




NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.651	Depositor
Minimum map value	-0.477	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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, BMA, A1D8V

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	0.25	0/3249	0.46	0/4434
1	C	0.24	0/3241	0.45	0/4426
2	B	0.25	0/3182	0.49	0/4341
2	D	0.27	0/3194	0.54	3/4357 (0.1%)
2	E	0.24	0/3205	0.48	0/4373
All	All	0.25	0/16071	0.48	3/21931 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	106	PRO	CA-N-CD	-10.70	96.52	111.50
2	D	197	PRO	CA-N-CD	-9.53	98.16	111.50
2	D	106	PRO	N-CD-CG	-5.41	95.09	103.20

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	3160	0	3153	48	0
1	C	3150	0	3136	30	0
2	B	3104	0	3156	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3115	0	3165	42	0
2	E	3125	0	3178	40	0
3	F	39	0	34	0	0
3	G	39	0	34	2	0
3	H	39	0	34	2	0
3	I	39	0	34	0	0
3	J	39	0	34	1	0
3	K	39	0	34	1	0
3	L	39	0	34	1	0
3	M	39	0	34	0	0
4	A	13	0	0	0	0
4	C	13	0	0	1	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
All	All	15997	0	16060	177	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 177 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:334:THR:HG1	1:A:335:HIS:HD1	1.24	0.84
1:A:97:TRP:HE1	1:A:105:ILE:HG22	1.48	0.76
2:D:311:VAL:HG22	2:E:252:LEU:HD11	1.69	0.75
1:A:95:LEU:HD23	1:A:140:LEU:HD11	1.70	0.72
1:A:290:THR:OG1	2:B:238:ASN:ND2	2.23	0.71

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	379/501 (76%)	350 (92%)	29 (8%)	0	100	100
1	C	377/501 (75%)	361 (96%)	16 (4%)	0	100	100
2	B	378/633 (60%)	341 (90%)	36 (10%)	1 (0%)	37	66
2	D	379/633 (60%)	350 (92%)	29 (8%)	0	100	100
2	E	380/633 (60%)	348 (92%)	31 (8%)	1 (0%)	37	66
All	All	1893/2901 (65%)	1750 (92%)	141 (7%)	2 (0%)	50	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	239	LEU
2	E	66	ILE

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	359/450 (80%)	351 (98%)	8 (2%)	47	68
1	C	358/450 (80%)	346 (97%)	12 (3%)	32	57
2	B	357/548 (65%)	352 (99%)	5 (1%)	62	77
2	D	358/548 (65%)	353 (99%)	5 (1%)	62	77
2	E	360/548 (66%)	342 (95%)	18 (5%)	20	47
All	All	1792/2544 (70%)	1744 (97%)	48 (3%)	41	63

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	565	PHE
2	E	132	ASN
2	D	567	CYS
2	E	42	ASN
2	E	162	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	238	ASN

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)

24 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	F	1	1,3	14,14,15	0.33	0	17,19,21	0.39	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.47	0
3	BMA	F	3	3	11,11,12	1.08	1 (9%)	15,15,17	1.10	1 (6%)
3	NAG	G	1	2,3	14,14,15	0.28	0	17,19,21	0.45	0
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	0.54	0
3	BMA	G	3	3	11,11,12	0.61	0	15,15,17	0.80	0
3	NAG	H	1	2,3	14,14,15	0.51	0	17,19,21	0.41	0
3	NAG	H	2	3	14,14,15	0.32	0	17,19,21	0.36	0
3	BMA	H	3	3	11,11,12	0.65	0	15,15,17	0.73	0
3	NAG	I	1	1,3	14,14,15	0.28	0	17,19,21	0.36	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.37	0
3	BMA	I	3	3	11,11,12	0.93	1 (9%)	15,15,17	1.09	0
3	NAG	J	1	2,3	14,14,15	0.36	0	17,19,21	0.62	0
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	0.36	0
3	BMA	J	3	3	11,11,12	0.57	0	15,15,17	0.71	0
3	NAG	K	1	2,3	14,14,15	0.27	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	K	2	3	14,14,15	0.61	1 (7%)	17,19,21	1.29	1 (5%)
3	BMA	K	3	3	11,11,12	0.60	0	15,15,17	0.74	0
3	NAG	L	1	2,3	14,14,15	0.46	0	17,19,21	0.35	0
3	NAG	L	2	3	14,14,15	0.37	0	17,19,21	0.42	0
3	BMA	L	3	3	11,11,12	0.59	0	15,15,17	0.84	0
3	NAG	M	1	2,3	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.24	0	17,19,21	0.55	0
3	BMA	M	3	3	11,11,12	0.61	0	15,15,17	0.82	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	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	NAG	J	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	1/2/19/22	0/1/1/1
3	NAG	M	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C1-C2	2.24	1.57	1.52
3	I	3	BMA	C1-C2	2.11	1.57	1.52
3	K	2	NAG	O5-C1	2.06	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C1-O5-C5	4.90	118.83	112.19
3	F	3	BMA	C2-C3-C4	2.04	114.42	110.89

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

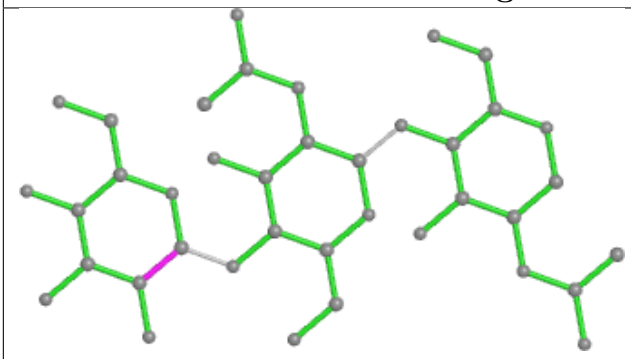
There are no ring outliers.

9 monomers are involved in 7 short contacts:

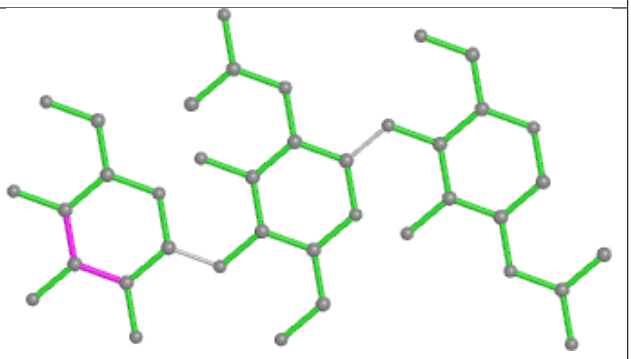
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	1	0
3	H	2	NAG	1	0
3	G	1	NAG	2	0
3	G	2	NAG	2	0
3	K	2	NAG	1	0
3	H	1	NAG	2	0
3	L	2	NAG	1	0
3	J	3	BMA	1	0
3	L	1	NAG	1	0

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

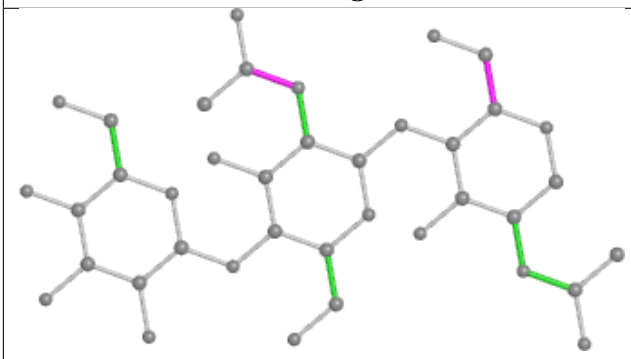
Oligosaccharide Chain F



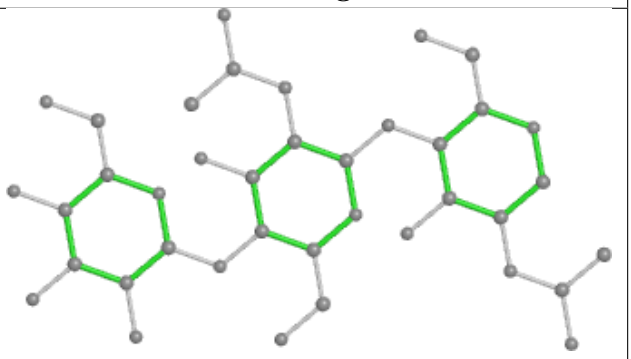
Bond lengths



Bond angles

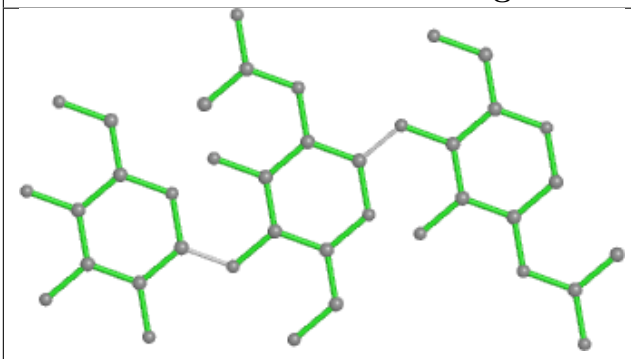


Torsions

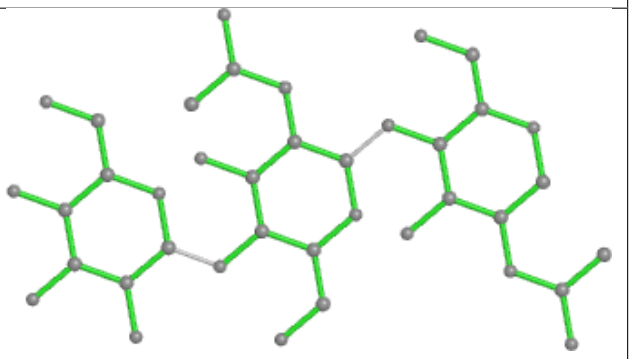


Rings

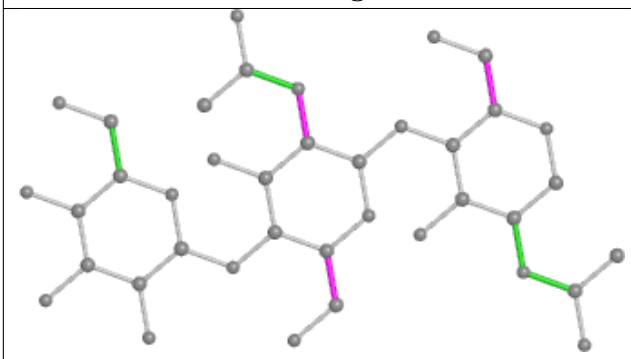
Oligosaccharide Chain G



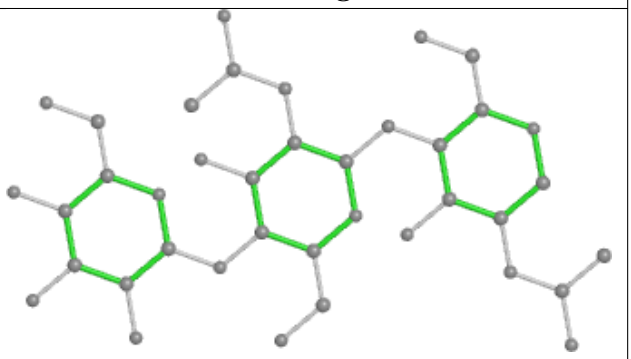
Bond lengths



Bond angles

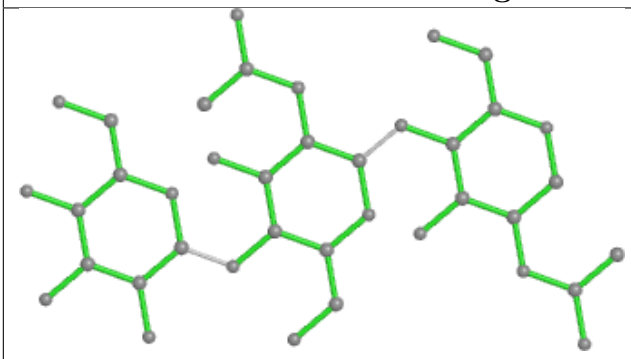


Torsions

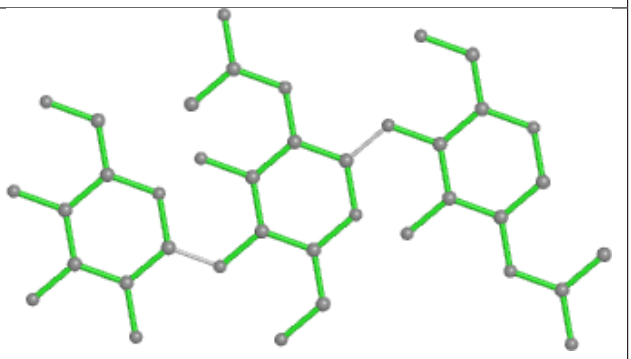


Rings

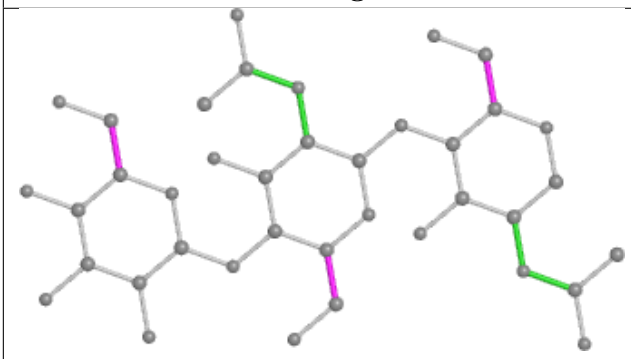
Oligosaccharide Chain H



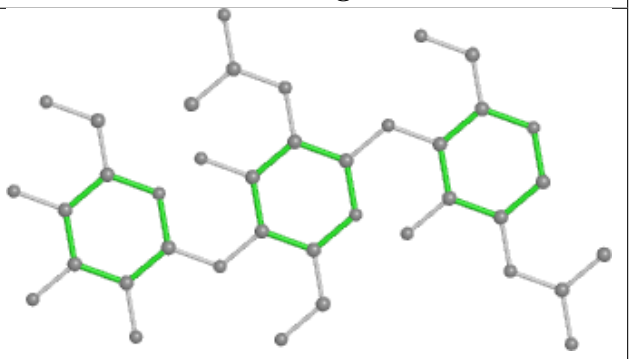
Bond lengths



Bond angles

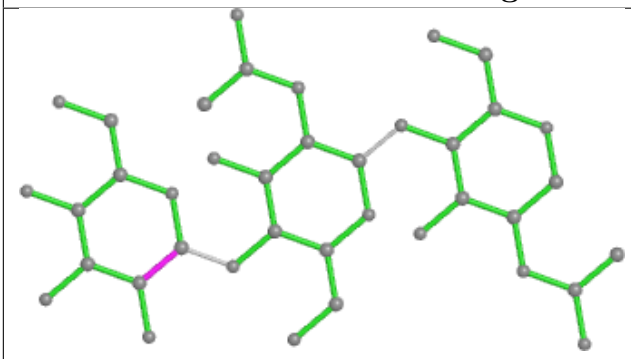


Torsions

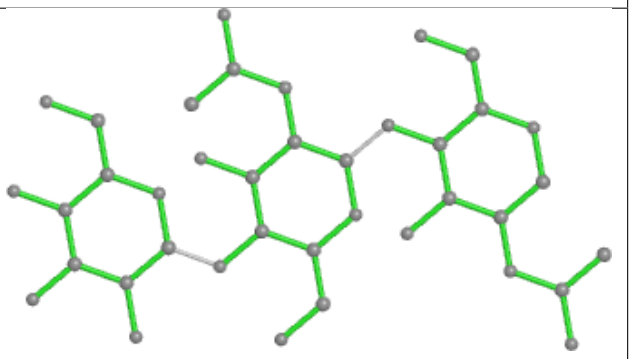


Rings

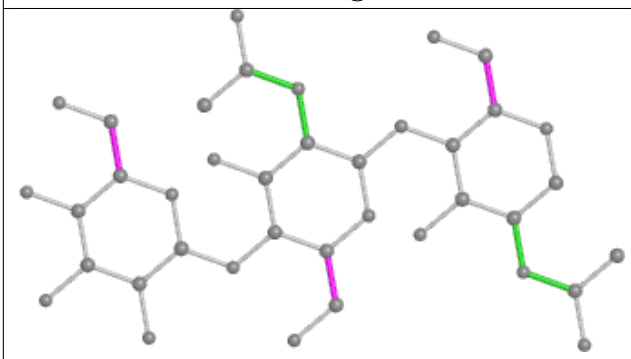
Oligosaccharide Chain I



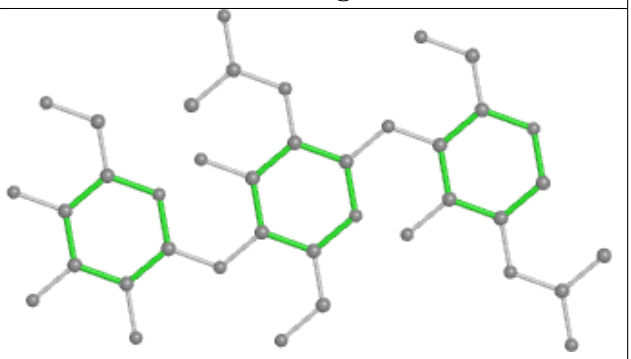
Bond lengths



Bond angles

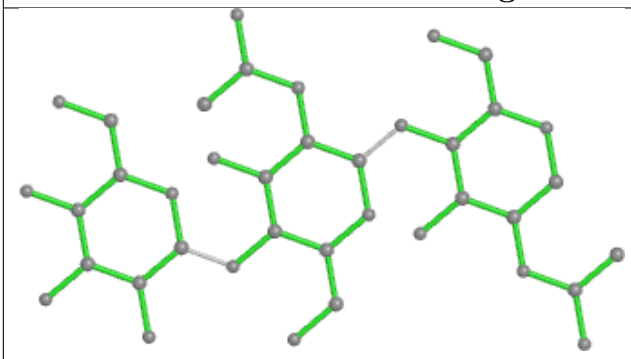


Torsions

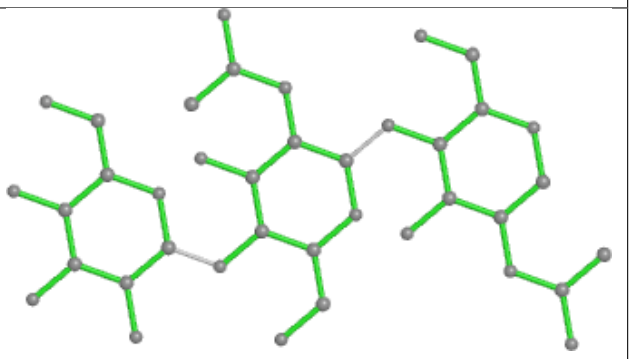


Rings

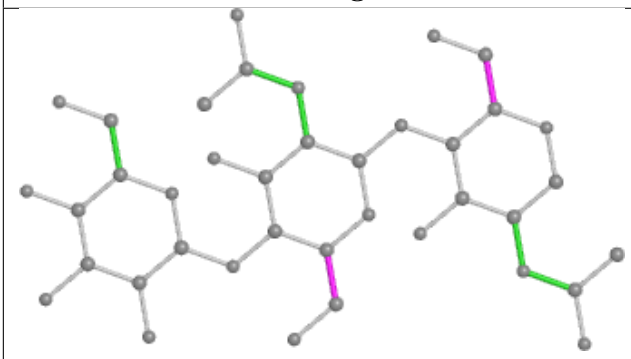
Oligosaccharide Chain J



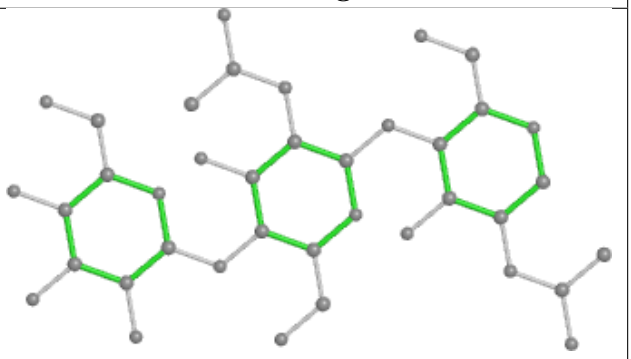
Bond lengths



Bond angles

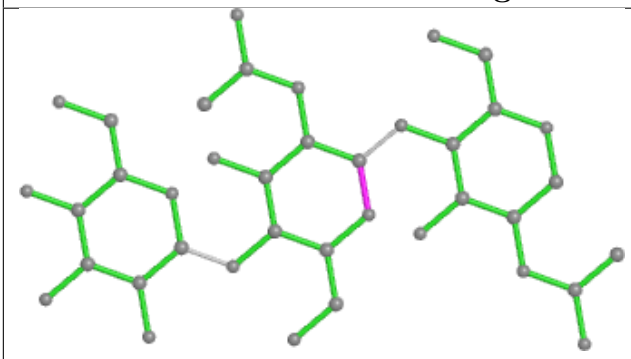


Torsions

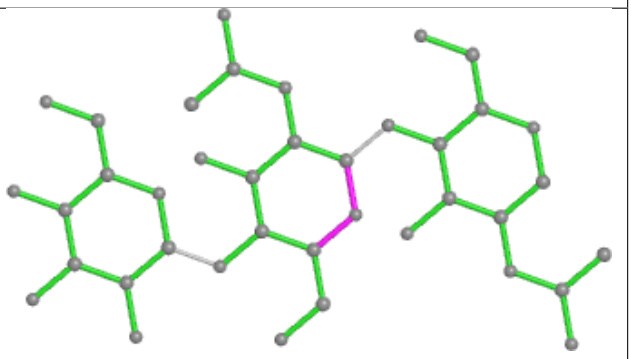


Rings

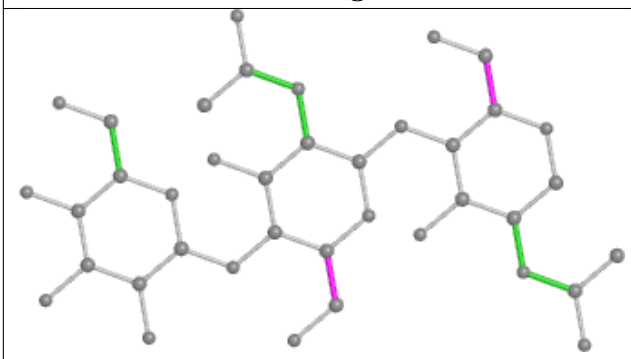
Oligosaccharide Chain K



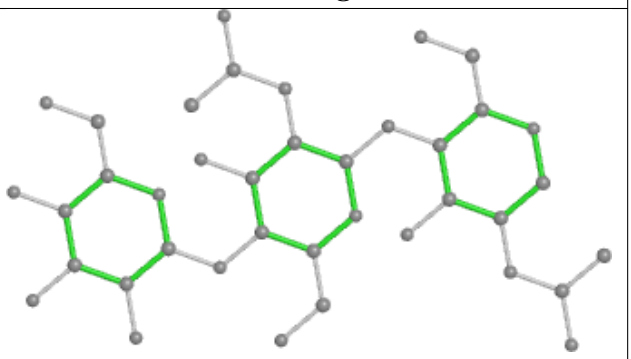
Bond lengths



Bond angles

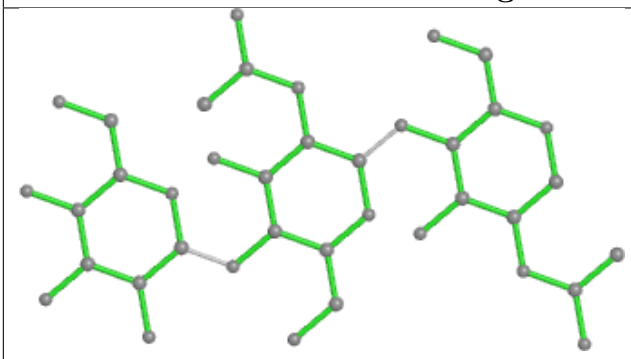


Torsions

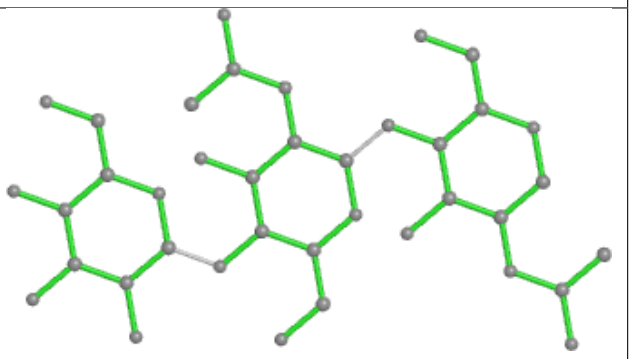


Rings

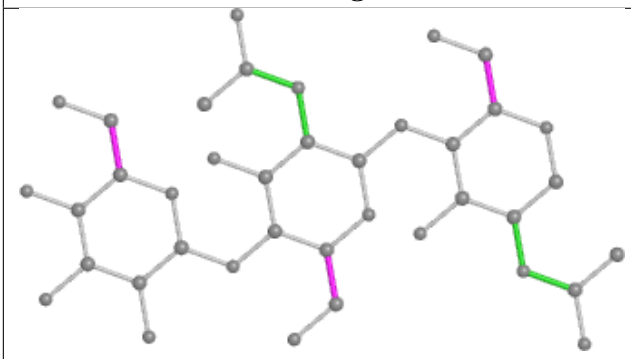
Oligosaccharide Chain L



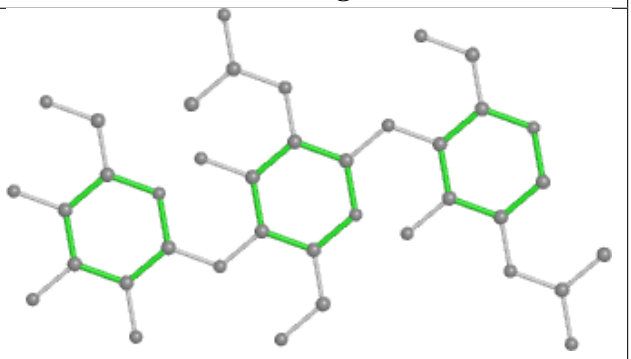
Bond lengths



Bond angles

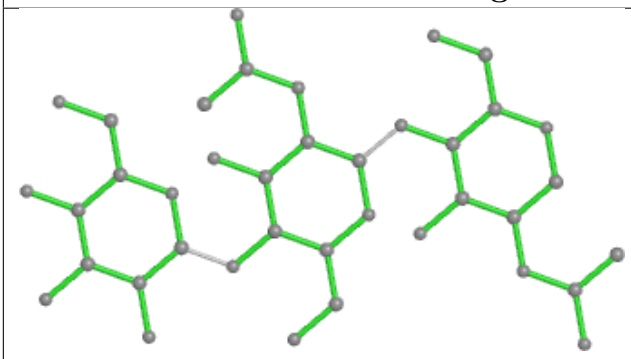


Torsions

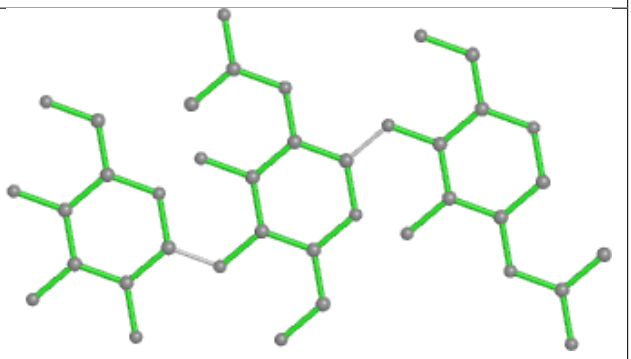


Rings

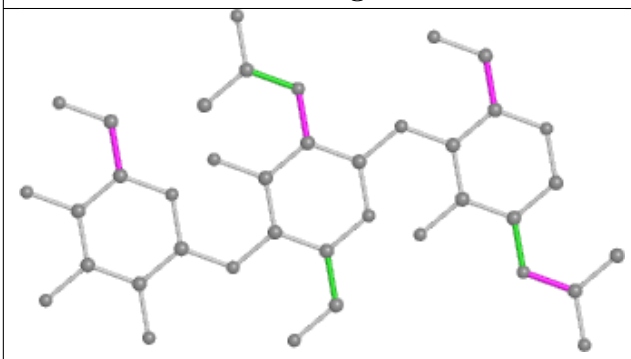
Oligosaccharide Chain M



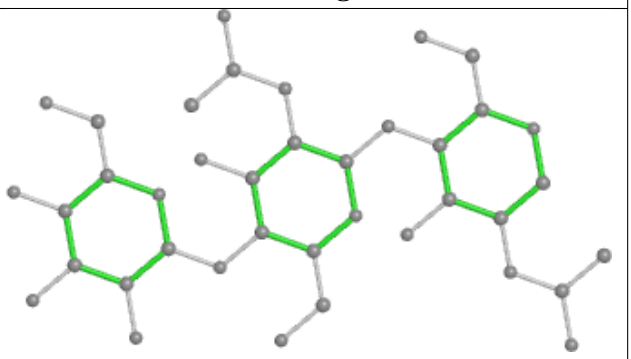
Bond lengths



Bond angles



Torsions



Rings

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	$\#\|Z\| > 2$
4	A1D8V	C	801	-	13,14,14	0.70	0	13,18,18	0.74	0
4	A1D8V	A	801	-	13,14,14	0.68	0	13,18,18	0.68	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	A1D8V	C	801	-	-	1/4/11/11	0/2/2/2
4	A1D8V	A	801	-	-	0/4/11/11	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	801	A1D8V	C06-C05-C08-O02

There are no ring outliers.

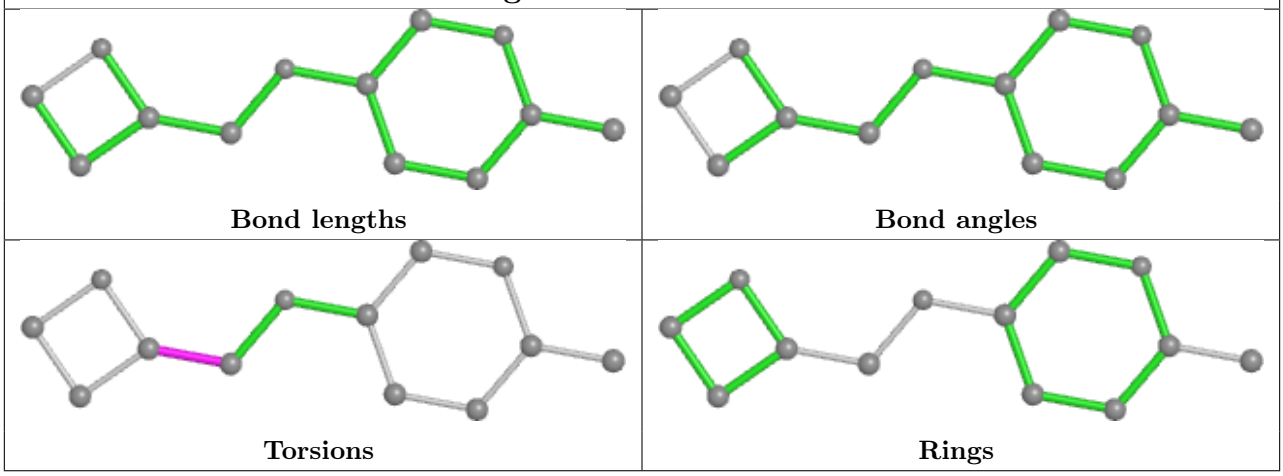
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	801	A1D8V	1	0

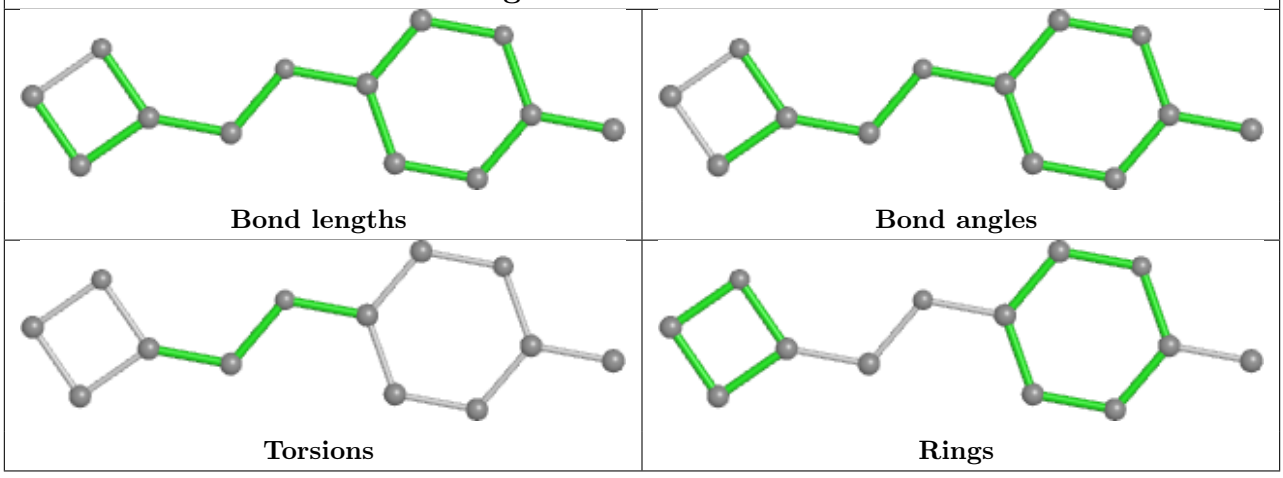
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1D8V C 801



Ligand A1D8V A 801



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.

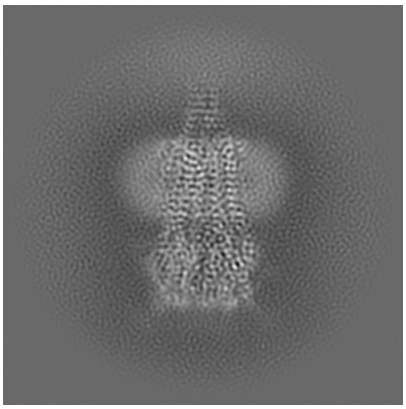
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60400. These allow visual inspection of the internal detail of the map and identification of artifacts.

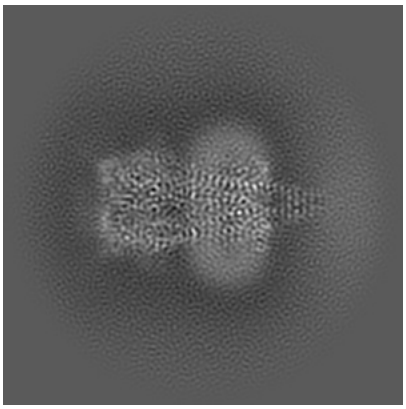
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

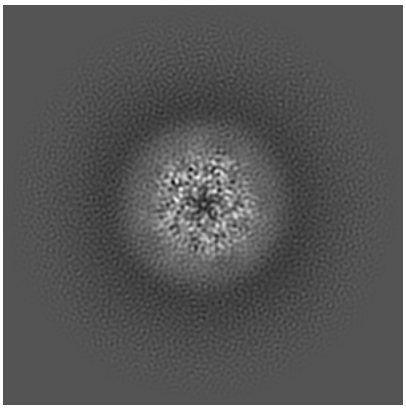
6.1.1 Primary map



X

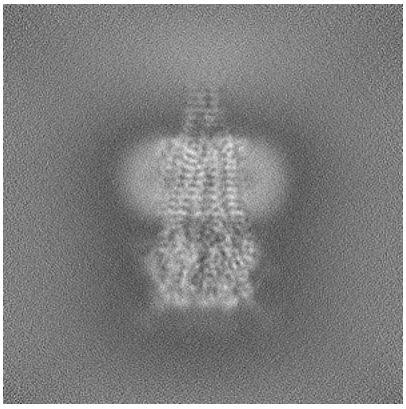


Y

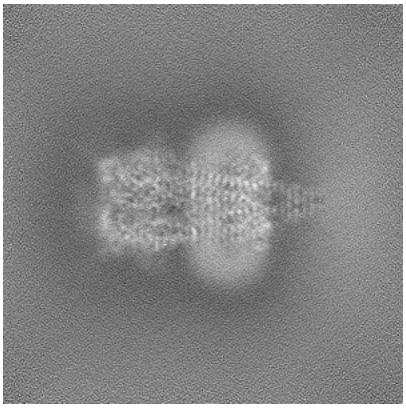


Z

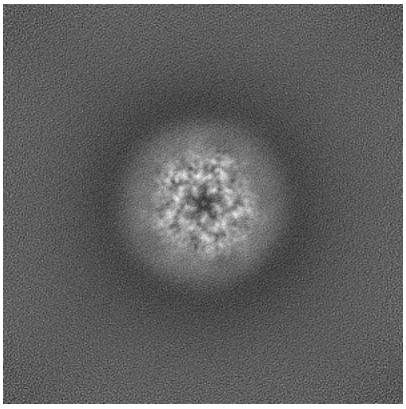
6.1.2 Raw map



X



Y



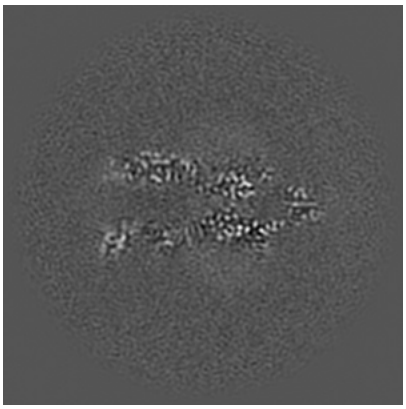
Z

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

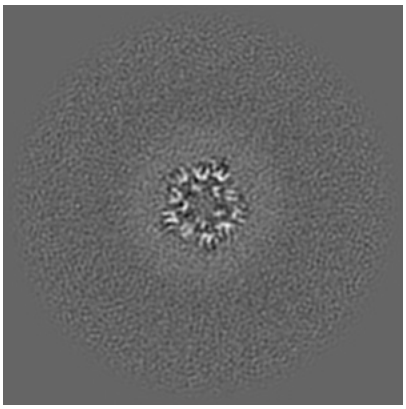
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160

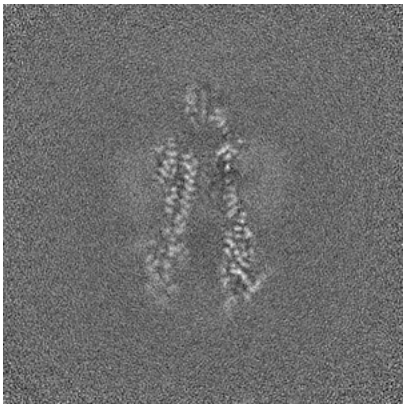


Y Index: 160

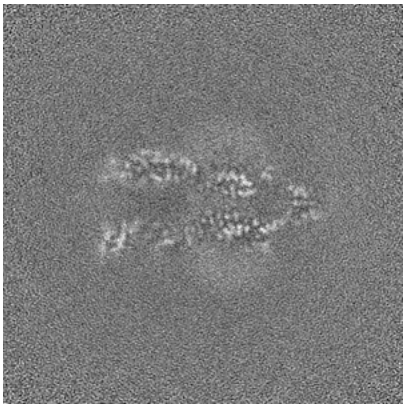


Z Index: 160

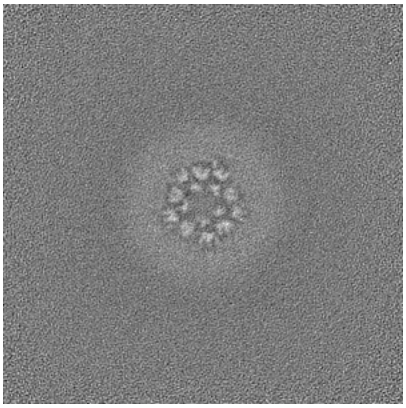
6.2.2 Raw map



X Index: 160



Y Index: 160

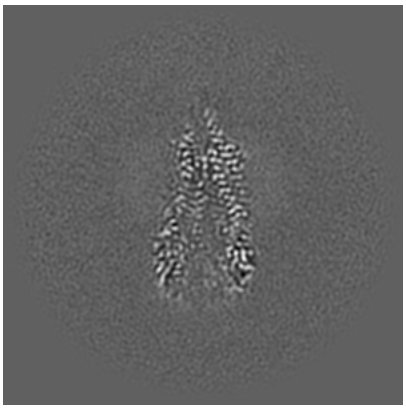


Z Index: 160

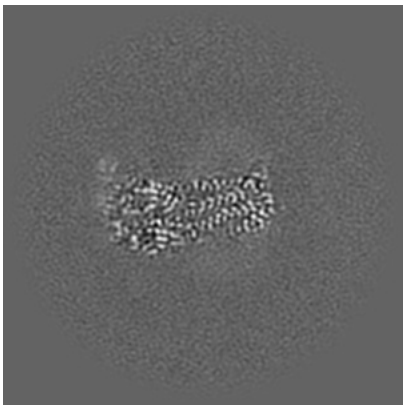
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

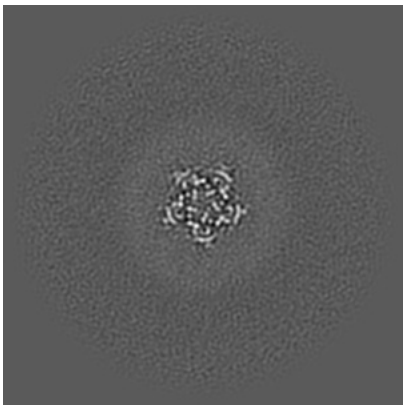
6.3.1 Primary map



X Index: 175

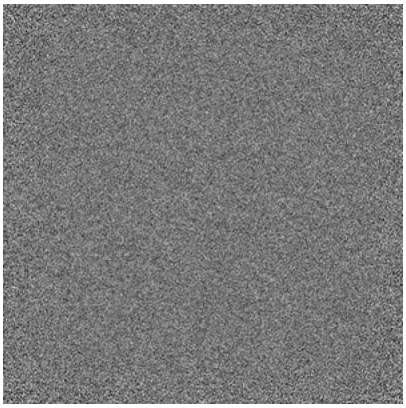


Y Index: 181

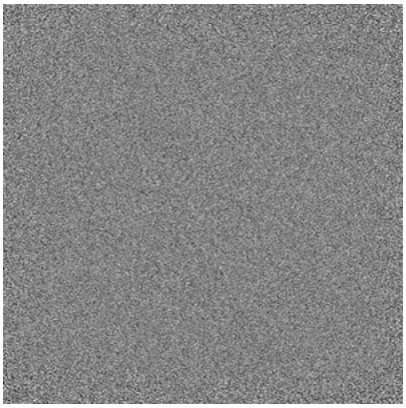


Z Index: 189

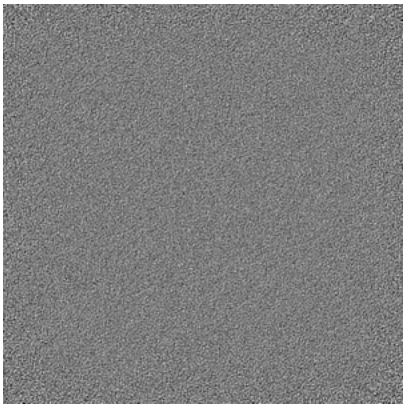
6.3.2 Raw map



X Index: 0



Y Index: 0

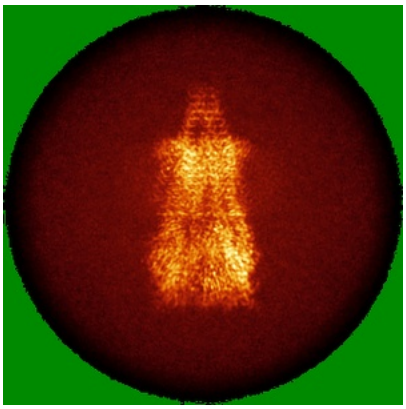


Z Index: 0

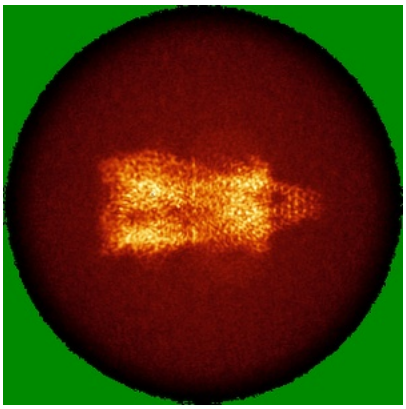
The images above show the largest variance slices of the map in three orthogonal directions.

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

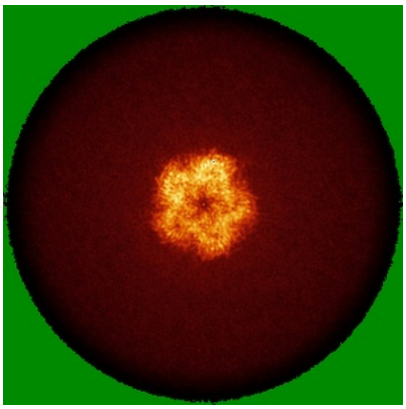
6.4.1 Primary map



X

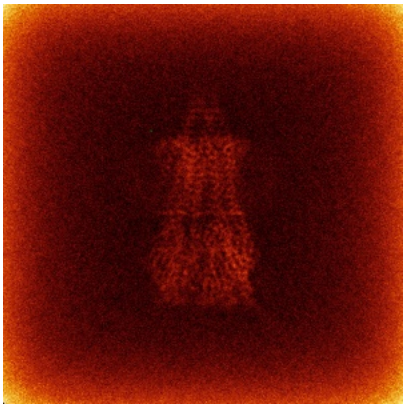


Y

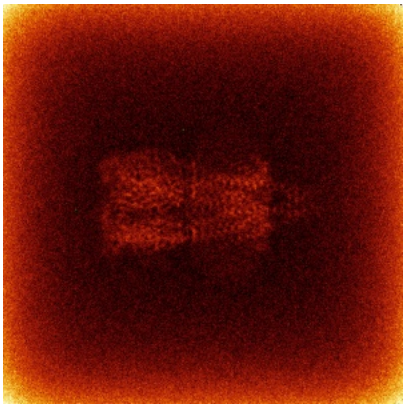


Z

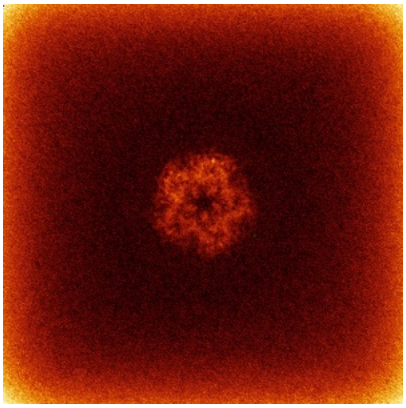
6.4.2 Raw map



X



Y

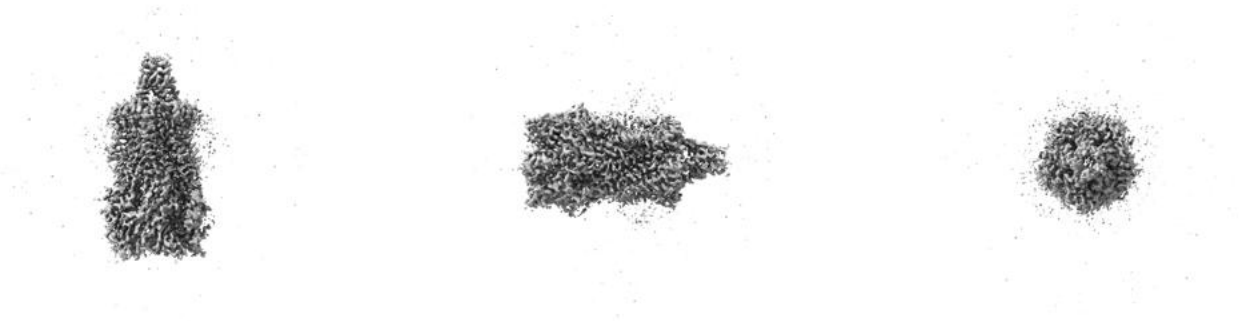


Z

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)

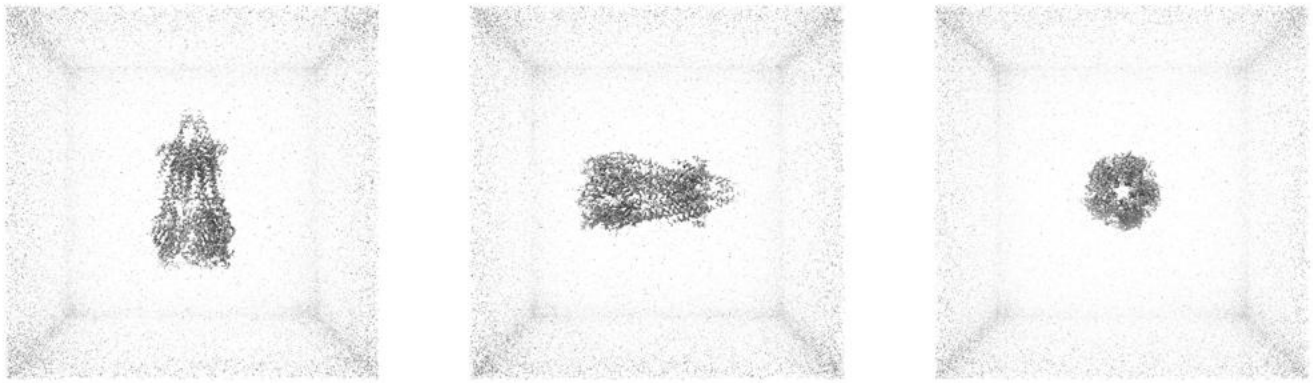
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

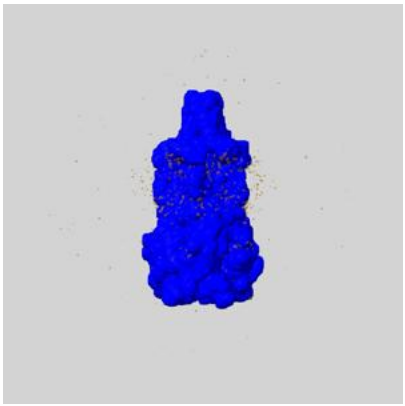
6.6 Mask visualisation (i)

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

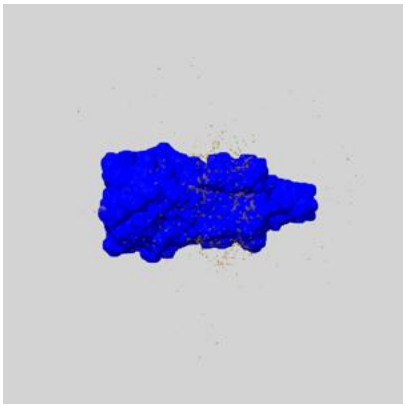
A mask typically either:

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

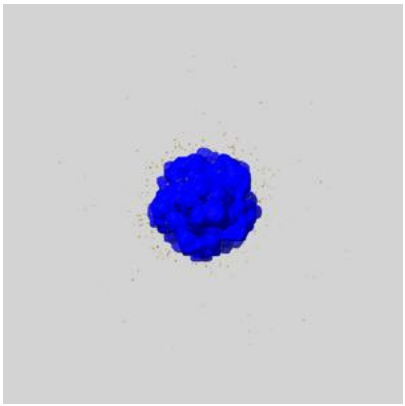
6.6.1 emd_60400_msk_1.map (i)



X



Y

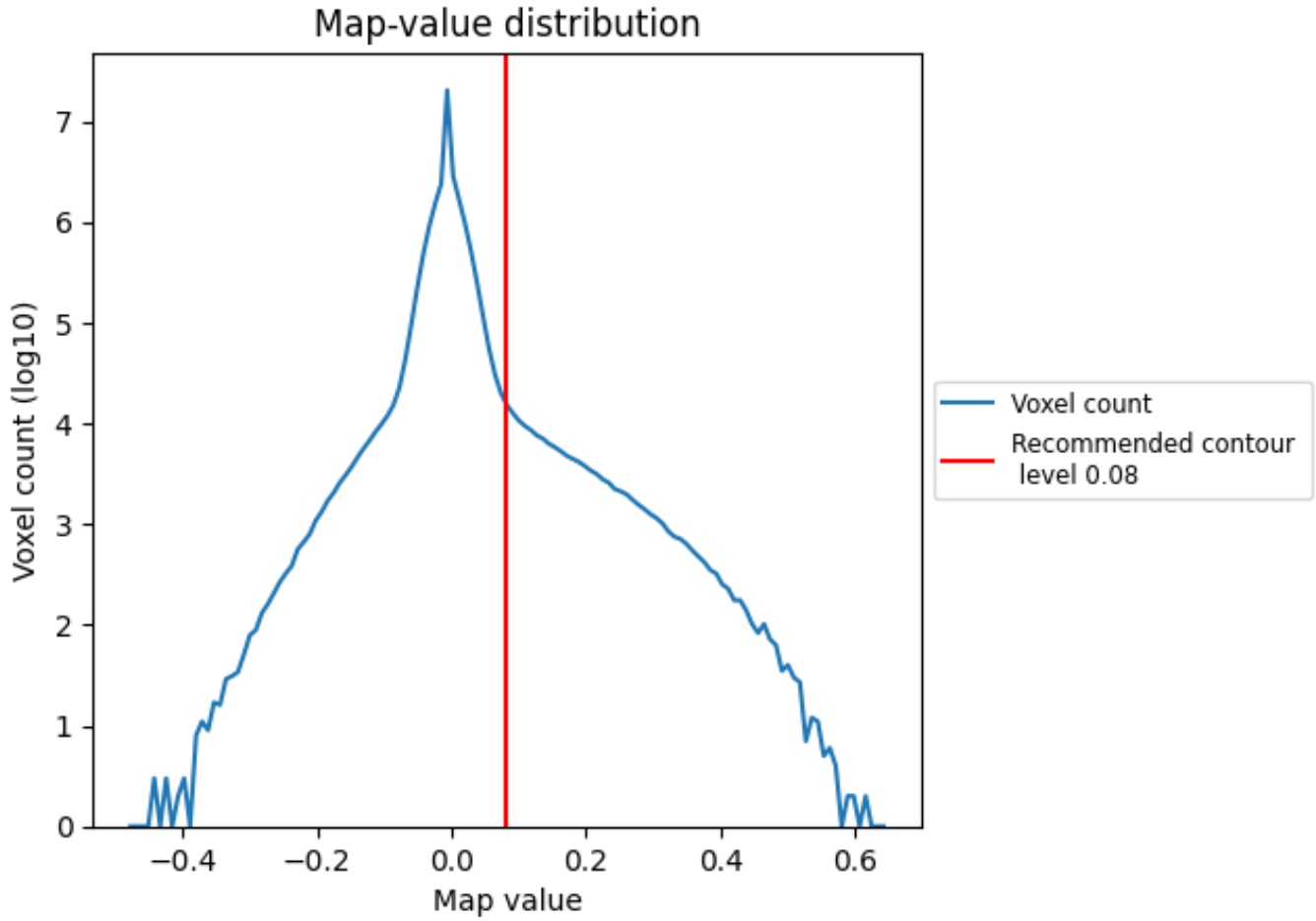


Z

7 Map analysis

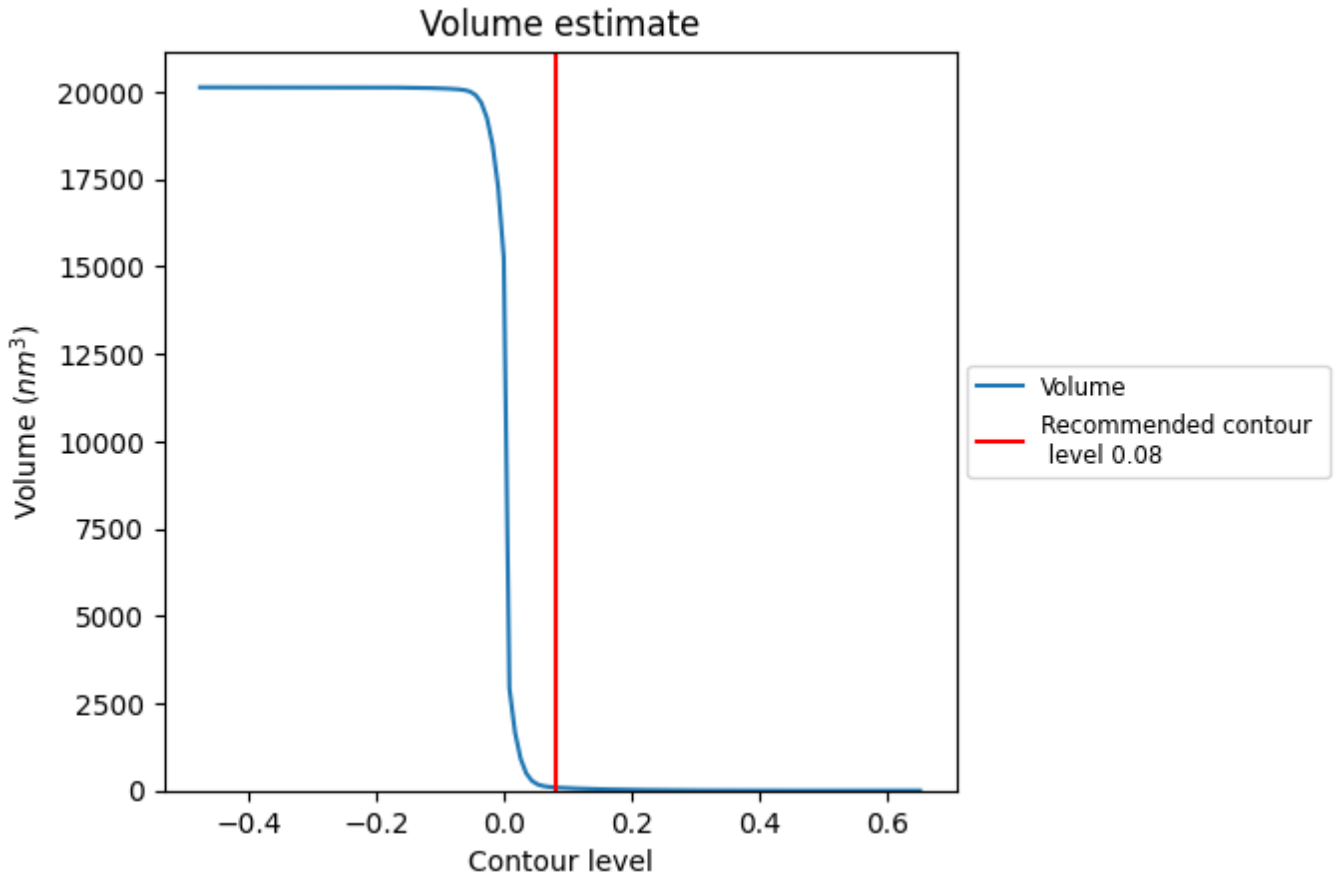
This section contains the results of statistical analysis of the map.

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.

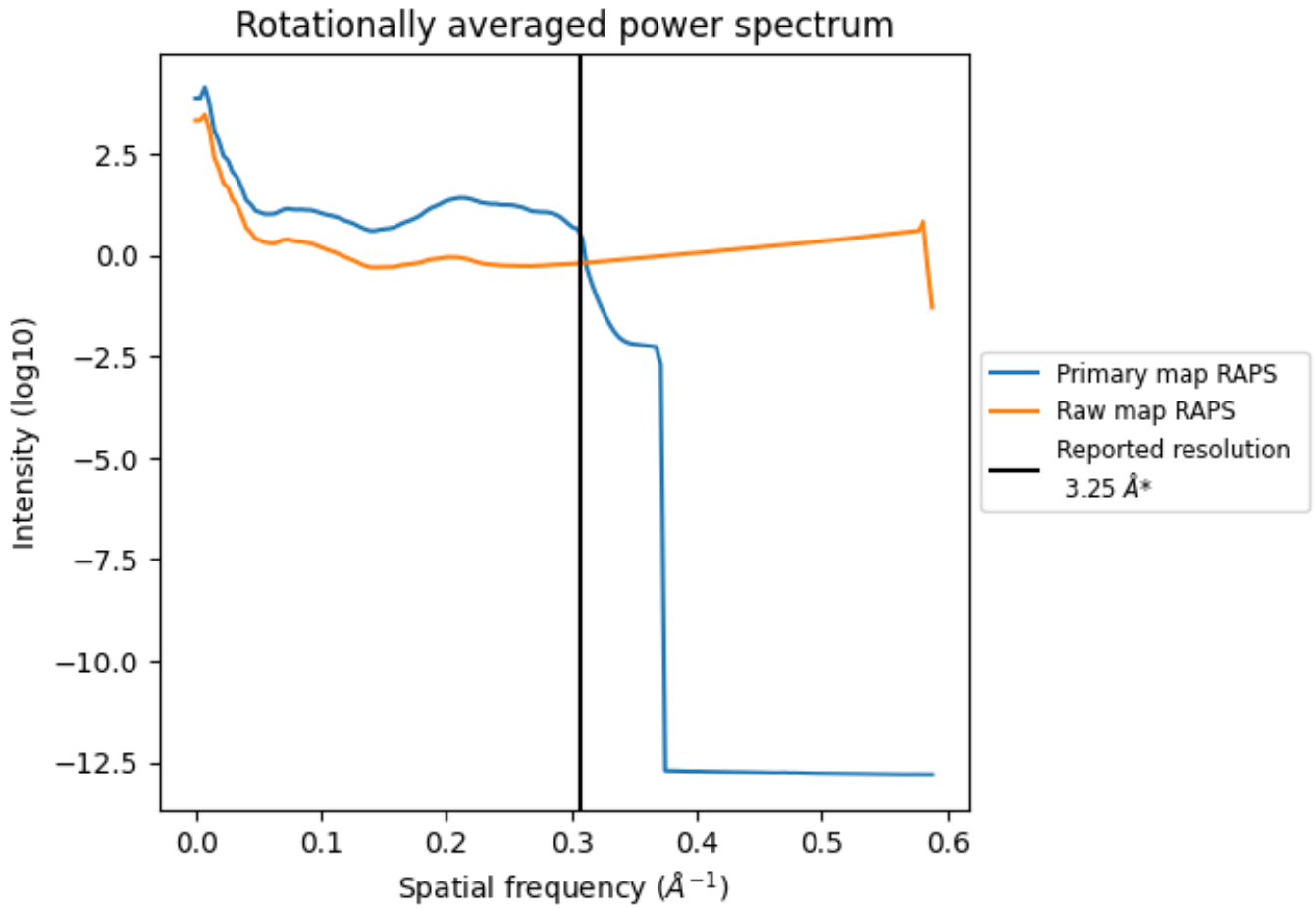
7.2 Volume estimate (i)



The volume at the recommended contour level is 89 nm^3; this corresponds to an approximate mass of 80 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)

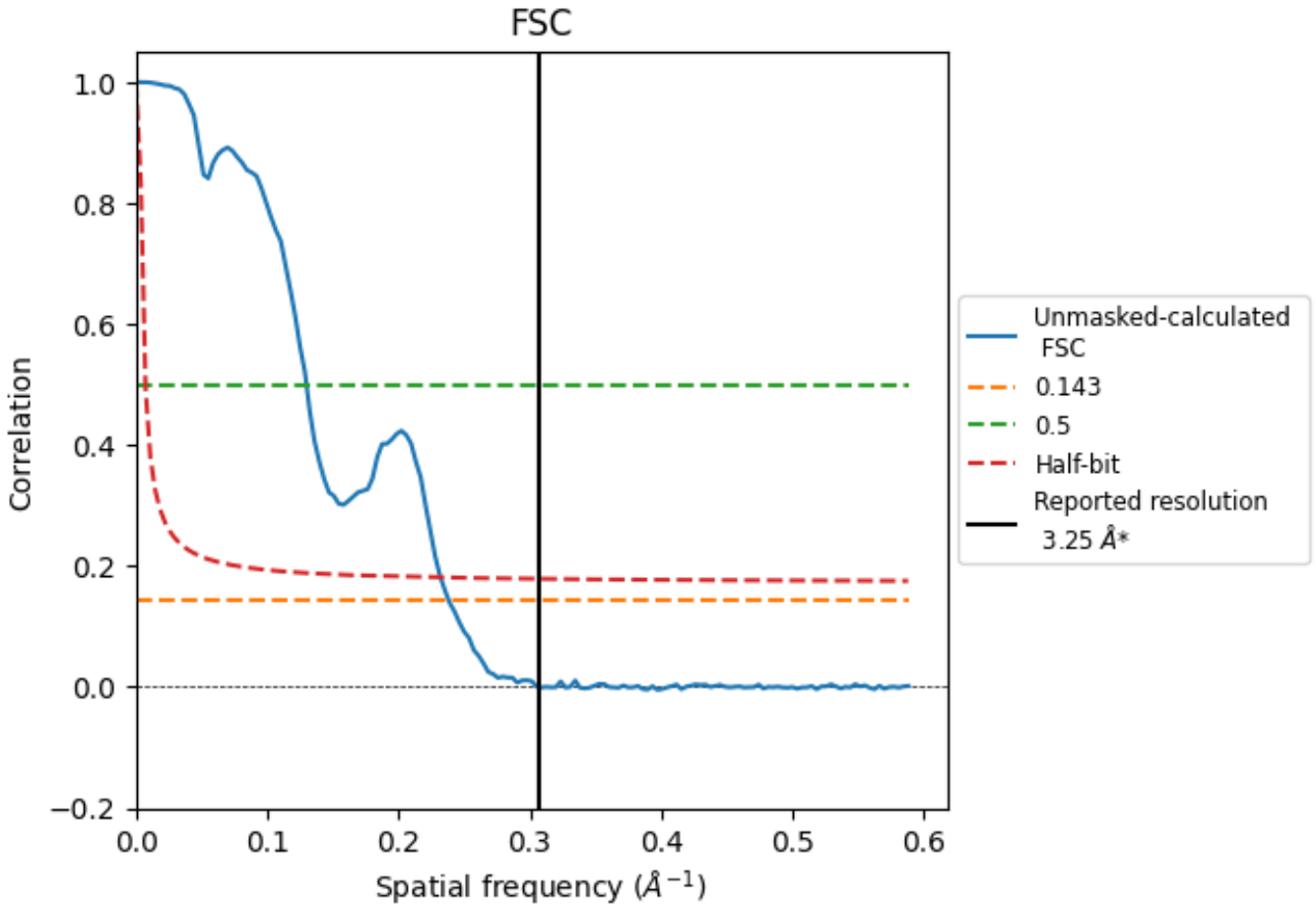


*Reported resolution corresponds to spatial frequency of 0.308 $Å^{-1}$

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 0.308 Å^{-1}

8.2 Resolution estimates (i)

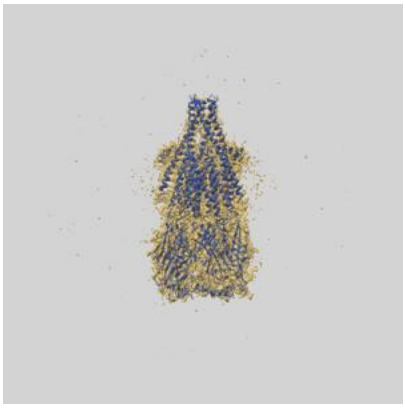
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.70	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.25 by more than 10 %

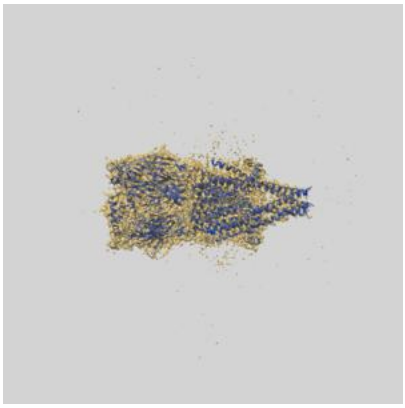
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60400 and PDB model 8ZRN. Per-residue inclusion information can be found in section 3 on page 15.

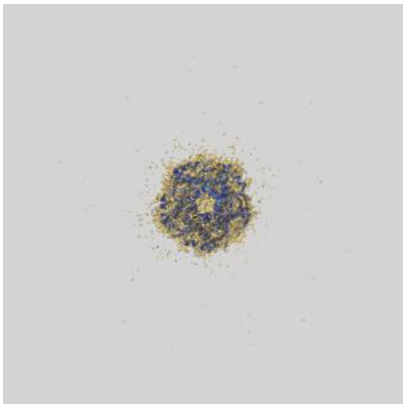
9.1 Map-model overlay



X



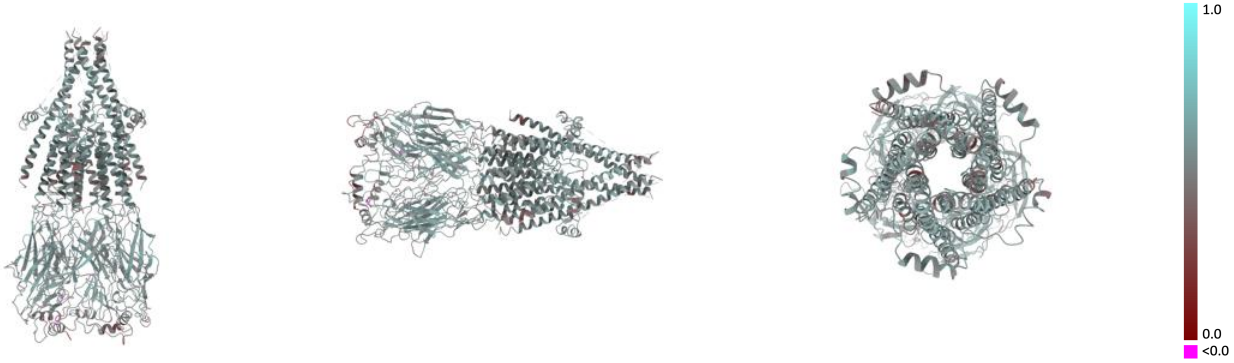
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

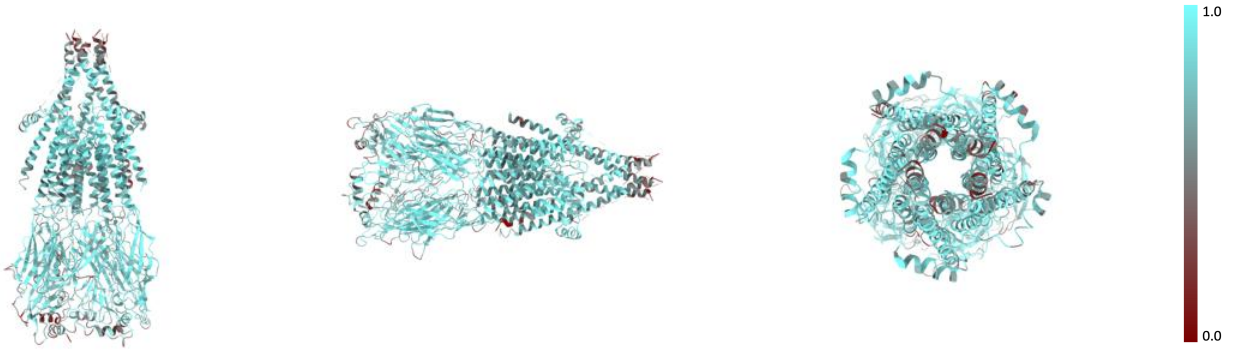
9.2 Q-score mapped to coordinate model (i)



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.

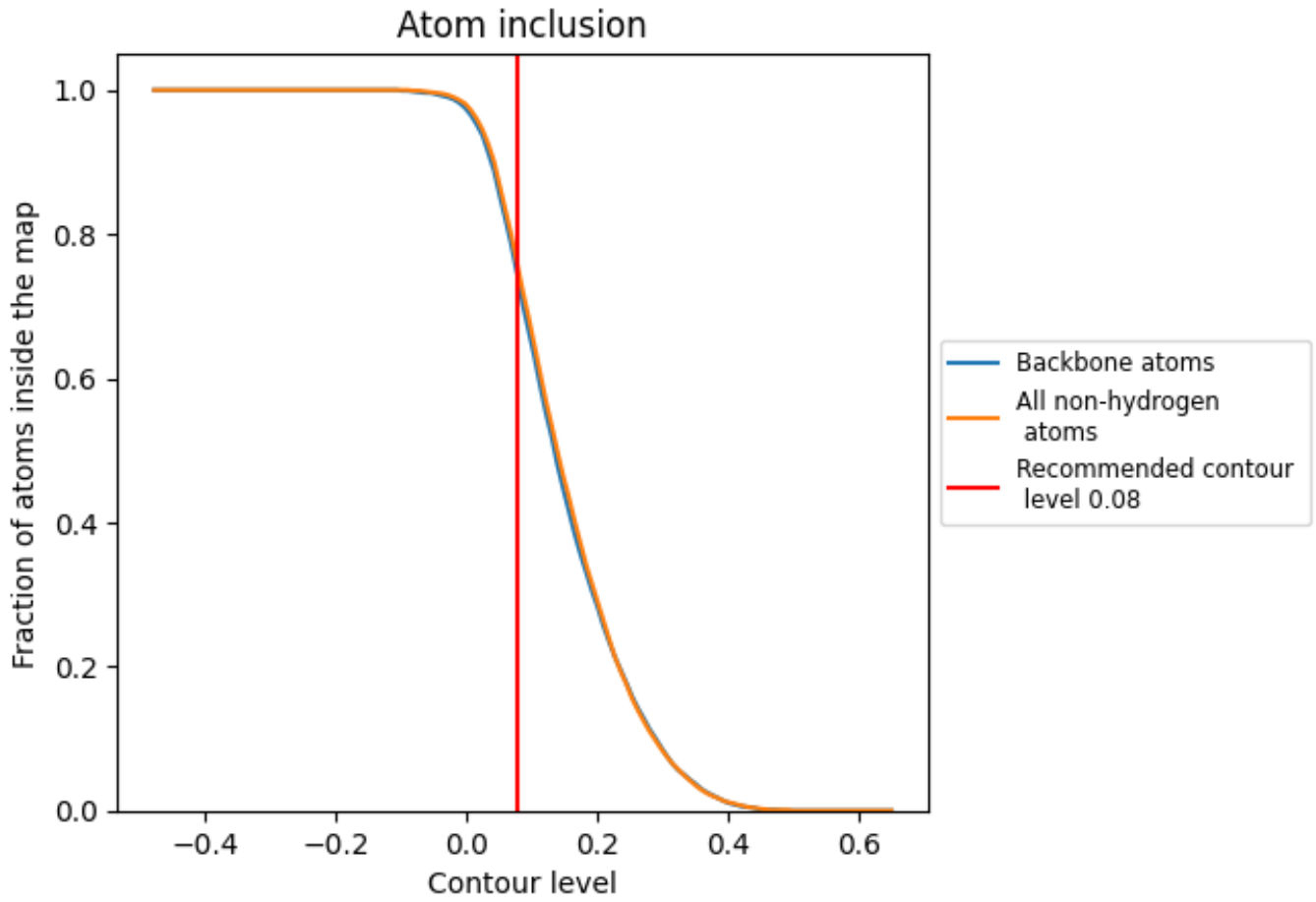
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 75% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.5220
A	0.7840	0.5280
B	0.8030	0.5340
C	0.7340	0.5230
D	0.7590	0.5270
E	0.7320	0.5130
F	0.5130	0.3480
G	0.4100	0.3330
H	0.6410	0.3750
I	0.5900	0.3730
J	0.3080	0.3060
K	0.5640	0.4660
L	0.2560	0.3020
M	0.5900	0.4690