Full wwPDB EM Validation Report ⓘ

May 24, 2025 – 04:15 pm BST

PDB ID	:	9FFL / pdb_00009ffl
EMDB ID	:	EMD-50365
Title	:	Cryo-EM structure of the alpha1beta3 GABA(A) receptor in complex with GABA and Mb25 in the short-lived symmetric pre-active state
Authors	:	Mihaylov, D.B.; Malinauskas, T.; Aricescu, A.R.
Deposited on	:	2024-05-23
Resolution	:	2.80 Å(reported)
Based on initial model	:	6HUK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

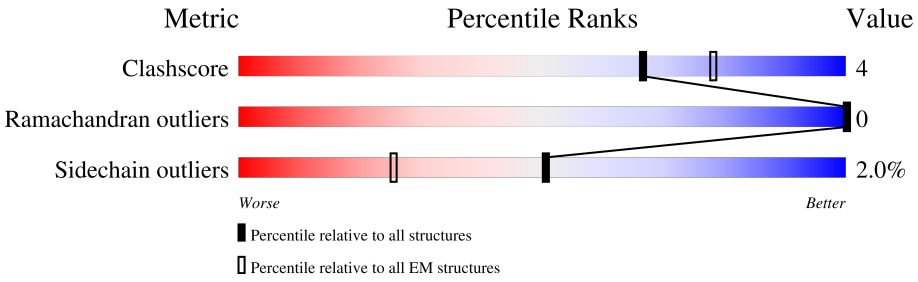
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	411	73% 8% • 18%
1	D	411	73% 8% • 18%
2	B	395	74% 10% 16%
2	C	395	76% 8% 16%
2	E	395	72% 12% 16%
3	F	522	20% • 78%
4	a	5	100%
4	b	5	80% 20%

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Mol	Chain	Length	Quality of chain
4	c	5	80% 20%
4	d	5	80% 20%
4	e	5	100%
5	G	2	100%
5	H	2	100%
5	I	2	100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15223 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	336	Total	C	N	O	S	2	0
			2727	1763	462	486	16		
1	A	336	Total	C	N	O	S	2	0
			2727	1763	462	486	16		

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	MET	-	initiating methionine	UNP P14867
D	-51	ASP	-	expression tag	UNP P14867
D	-50	GLU	-	expression tag	UNP P14867
D	-49	LYS	-	expression tag	UNP P14867
D	-48	THR	-	expression tag	UNP P14867
D	-47	THR	-	expression tag	UNP P14867
D	-46	GLY	-	expression tag	UNP P14867
D	-45	TRP	-	expression tag	UNP P14867
D	-44	ARG	-	expression tag	UNP P14867
D	-43	GLY	-	expression tag	UNP P14867
D	-42	GLY	-	expression tag	UNP P14867
D	-41	HIS	-	expression tag	UNP P14867
D	-40	VAL	-	expression tag	UNP P14867
D	-39	VAL	-	expression tag	UNP P14867
D	-38	GLU	-	expression tag	UNP P14867
D	-37	GLY	-	expression tag	UNP P14867
D	-36	LEU	-	expression tag	UNP P14867
D	-35	ALA	-	expression tag	UNP P14867
D	-34	GLY	-	expression tag	UNP P14867
D	-33	GLU	-	expression tag	UNP P14867
D	-32	LEU	-	expression tag	UNP P14867
D	-31	GLU	-	expression tag	UNP P14867
D	-30	GLN	-	expression tag	UNP P14867
D	-29	LEU	-	expression tag	UNP P14867
D	-28	ARG	-	expression tag	UNP P14867
D	-27	ALA	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-26	ARG	-	expression tag	UNP P14867
D	-25	LEU	-	expression tag	UNP P14867
D	-24	GLU	-	expression tag	UNP P14867
D	-23	HIS	-	expression tag	UNP P14867
D	-22	HIS	-	expression tag	UNP P14867
D	-21	PRO	-	expression tag	UNP P14867
D	-20	GLN	-	expression tag	UNP P14867
D	-19	GLY	-	expression tag	UNP P14867
D	-18	GLN	-	expression tag	UNP P14867
D	-17	ARG	-	expression tag	UNP P14867
D	-16	GLU	-	expression tag	UNP P14867
D	-15	PRO	-	expression tag	UNP P14867
D	-14	ASP	-	expression tag	UNP P14867
D	-13	TYR	-	expression tag	UNP P14867
D	-12	ASP	-	expression tag	UNP P14867
D	-11	ILE	-	expression tag	UNP P14867
D	-10	PRO	-	expression tag	UNP P14867
D	-9	THR	-	expression tag	UNP P14867
D	-8	THR	-	expression tag	UNP P14867
D	-7	GLU	-	expression tag	UNP P14867
D	-6	ASN	-	expression tag	UNP P14867
D	-5	LEU	-	expression tag	UNP P14867
D	-4	TYR	-	expression tag	UNP P14867
D	-3	PHE	-	expression tag	UNP P14867
D	-2	GLN	-	expression tag	UNP P14867
D	-1	GLY	-	expression tag	UNP P14867
D	0	THR	-	expression tag	UNP P14867
D	1	GLY	-	expression tag	UNP P14867
D	2	GLN	-	expression tag	UNP P14867
D	3	PRO	-	expression tag	UNP P14867
D	4	SER	-	expression tag	UNP P14867
D	313	SER	-	linker	UNP P14867
D	385	GLN	-	linker	UNP P14867
D	386	PRO	-	linker	UNP P14867
D	387	ALA	-	linker	UNP P14867
D	388	ARG	-	linker	UNP P14867
D	389	ALA	-	linker	UNP P14867
D	390	ALA	-	linker	UNP P14867
A	-52	MET	-	initiating methionine	UNP P14867
A	-51	ASP	-	expression tag	UNP P14867
A	-50	GLU	-	expression tag	UNP P14867
A	-49	LYS	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-48	THR	-	expression tag	UNP P14867
A	-47	THR	-	expression tag	UNP P14867
A	-46	GLY	-	expression tag	UNP P14867
A	-45	TRP	-	expression tag	UNP P14867
A	-44	ARG	-	expression tag	UNP P14867
A	-43	GLY	-	expression tag	UNP P14867
A	-42	GLY	-	expression tag	UNP P14867
A	-41	HIS	-	expression tag	UNP P14867
A	-40	VAL	-	expression tag	UNP P14867
A	-39	VAL	-	expression tag	UNP P14867
A	-38	GLU	-	expression tag	UNP P14867
A	-37	GLY	-	expression tag	UNP P14867
A	-36	LEU	-	expression tag	UNP P14867
A	-35	ALA	-	expression tag	UNP P14867
A	-34	GLY	-	expression tag	UNP P14867
A	-33	GLU	-	expression tag	UNP P14867
A	-32	LEU	-	expression tag	UNP P14867
A	-31	GLU	-	expression tag	UNP P14867
A	-30	GLN	-	expression tag	UNP P14867
A	-29	LEU	-	expression tag	UNP P14867
A	-28	ARG	-	expression tag	UNP P14867
A	-27	ALA	-	expression tag	UNP P14867
A	-26	ARG	-	expression tag	UNP P14867
A	-25	LEU	-	expression tag	UNP P14867
A	-24	GLU	-	expression tag	UNP P14867
A	-23	HIS	-	expression tag	UNP P14867
A	-22	HIS	-	expression tag	UNP P14867
A	-21	PRO	-	expression tag	UNP P14867
A	-20	GLN	-	expression tag	UNP P14867
A	-19	GLY	-	expression tag	UNP P14867
A	-18	GLN	-	expression tag	UNP P14867
A	-17	ARG	-	expression tag	UNP P14867
A	-16	GLU	-	expression tag	UNP P14867
A	-15	PRO	-	expression tag	UNP P14867
A	-14	ASP	-	expression tag	UNP P14867
A	-13	TYR	-	expression tag	UNP P14867
A	-12	ASP	-	expression tag	UNP P14867
A	-11	ILE	-	expression tag	UNP P14867
A	-10	PRO	-	expression tag	UNP P14867
A	-9	THR	-	expression tag	UNP P14867
A	-8	THR	-	expression tag	UNP P14867
A	-7	GLU	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP P14867
A	-5	LEU	-	expression tag	UNP P14867
A	-4	TYR	-	expression tag	UNP P14867
A	-3	PHE	-	expression tag	UNP P14867
A	-2	GLN	-	expression tag	UNP P14867
A	-1	GLY	-	expression tag	UNP P14867
A	0	THR	-	expression tag	UNP P14867
A	1	GLY	-	expression tag	UNP P14867
A	2	GLN	-	expression tag	UNP P14867
A	3	PRO	-	expression tag	UNP P14867
A	4	SER	-	expression tag	UNP P14867
A	313	SER	-	linker	UNP P14867
A	385	GLN	-	linker	UNP P14867
A	386	PRO	-	linker	UNP P14867
A	387	ALA	-	linker	UNP P14867
A	388	ARG	-	linker	UNP P14867
A	389	ALA	-	linker	UNP P14867
A	390	ALA	-	linker	UNP P14867

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	333	Total	C	N	O	S	1	0
			2739	1796	446	481	16		
2	B	333	Total	C	N	O	S	4	0
			2754	1808	447	482	17		
2	C	333	Total	C	N	O	S	2	0
			2744	1799	447	482	16		

There are 183 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-53	MET	-	initiating methionine	UNP P28472
E	-52	ASP	-	expression tag	UNP P28472
E	-51	GLU	-	expression tag	UNP P28472
E	-50	LYS	-	expression tag	UNP P28472
E	-49	THR	-	expression tag	UNP P28472
E	-48	THR	-	expression tag	UNP P28472
E	-47	GLY	-	expression tag	UNP P28472
E	-46	TRP	-	expression tag	UNP P28472
E	-45	ARG	-	expression tag	UNP P28472
E	-44	GLY	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-43	GLY	-	expression tag	UNP P28472
E	-42	HIS	-	expression tag	UNP P28472
E	-41	VAL	-	expression tag	UNP P28472
E	-40	VAL	-	expression tag	UNP P28472
E	-39	GLU	-	expression tag	UNP P28472
E	-38	GLY	-	expression tag	UNP P28472
E	-37	LEU	-	expression tag	UNP P28472
E	-36	ALA	-	expression tag	UNP P28472
E	-35	GLY	-	expression tag	UNP P28472
E	-34	GLU	-	expression tag	UNP P28472
E	-33	LEU	-	expression tag	UNP P28472
E	-32	GLU	-	expression tag	UNP P28472
E	-31	GLN	-	expression tag	UNP P28472
E	-30	LEU	-	expression tag	UNP P28472
E	-29	ARG	-	expression tag	UNP P28472
E	-28	ALA	-	expression tag	UNP P28472
E	-27	ARG	-	expression tag	UNP P28472
E	-26	LEU	-	expression tag	UNP P28472
E	-25	GLU	-	expression tag	UNP P28472
E	-24	HIS	-	expression tag	UNP P28472
E	-23	HIS	-	expression tag	UNP P28472
E	-22	PRO	-	expression tag	UNP P28472
E	-21	GLN	-	expression tag	UNP P28472
E	-20	GLY	-	expression tag	UNP P28472
E	-19	GLN	-	expression tag	UNP P28472
E	-18	ARG	-	expression tag	UNP P28472
E	-17	GLU	-	expression tag	UNP P28472
E	-16	PRO	-	expression tag	UNP P28472
E	-15	ASP	-	expression tag	UNP P28472
E	-14	TYR	-	expression tag	UNP P28472
E	-13	ASP	-	expression tag	UNP P28472
E	-12	ILE	-	expression tag	UNP P28472
E	-11	PRO	-	expression tag	UNP P28472
E	-10	THR	-	expression tag	UNP P28472
E	-9	THR	-	expression tag	UNP P28472
E	-8	GLU	-	expression tag	UNP P28472
E	-7	ASN	-	expression tag	UNP P28472
E	-6	LEU	-	expression tag	UNP P28472
E	-5	TYR	-	expression tag	UNP P28472
E	-4	PHE	-	expression tag	UNP P28472
E	-3	GLN	-	expression tag	UNP P28472
E	-2	GLY	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	THR	-	expression tag	UNP P28472
E	0	GLY	-	expression tag	UNP P28472
E	308	SER	-	linker	UNP P28472
E	309	GLN	-	linker	UNP P28472
E	310	PRO	-	linker	UNP P28472
E	311	ALA	-	linker	UNP P28472
E	312	ARG	-	linker	UNP P28472
E	313	ALA	-	linker	UNP P28472
E	314	ALA	-	linker	UNP P28472
B	-53	MET	-	initiating methionine	UNP P28472
B	-52	ASP	-	expression tag	UNP P28472
B	-51	GLU	-	expression tag	UNP P28472
B	-50	LYS	-	expression tag	UNP P28472
B	-49	THR	-	expression tag	UNP P28472
B	-48	THR	-	expression tag	UNP P28472
B	-47	GLY	-	expression tag	UNP P28472
B	-46	TRP	-	expression tag	UNP P28472
B	-45	ARG	-	expression tag	UNP P28472
B	-44	GLY	-	expression tag	UNP P28472
B	-43	GLY	-	expression tag	UNP P28472
B	-42	HIS	-	expression tag	UNP P28472
B	-41	VAL	-	expression tag	UNP P28472
B	-40	VAL	-	expression tag	UNP P28472
B	-39	GLU	-	expression tag	UNP P28472
B	-38	GLY	-	expression tag	UNP P28472
B	-37	LEU	-	expression tag	UNP P28472
B	-36	ALA	-	expression tag	UNP P28472
B	-35	GLY	-	expression tag	UNP P28472
B	-34	GLU	-	expression tag	UNP P28472
B	-33	LEU	-	expression tag	UNP P28472
B	-32	GLU	-	expression tag	UNP P28472
B	-31	GLN	-	expression tag	UNP P28472
B	-30	LEU	-	expression tag	UNP P28472
B	-29	ARG	-	expression tag	UNP P28472
B	-28	ALA	-	expression tag	UNP P28472
B	-27	ARG	-	expression tag	UNP P28472
B	-26	LEU	-	expression tag	UNP P28472
B	-25	GLU	-	expression tag	UNP P28472
B	-24	HIS	-	expression tag	UNP P28472
B	-23	HIS	-	expression tag	UNP P28472
B	-22	PRO	-	expression tag	UNP P28472
B	-21	GLN	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	GLY	-	expression tag	UNP P28472
B	-19	GLN	-	expression tag	UNP P28472
B	-18	ARG	-	expression tag	UNP P28472
B	-17	GLU	-	expression tag	UNP P28472
B	-16	PRO	-	expression tag	UNP P28472
B	-15	ASP	-	expression tag	UNP P28472
B	-14	TYR	-	expression tag	UNP P28472
B	-13	ASP	-	expression tag	UNP P28472
B	-12	ILE	-	expression tag	UNP P28472
B	-11	PRO	-	expression tag	UNP P28472
B	-10	THR	-	expression tag	UNP P28472
B	-9	THR	-	expression tag	UNP P28472
B	-8	GLU	-	expression tag	UNP P28472
B	-7	ASN	-	expression tag	UNP P28472
B	-6	LEU	-	expression tag	UNP P28472
B	-5	TYR	-	expression tag	UNP P28472
B	-4	PHE	-	expression tag	UNP P28472
B	-3	GLN	-	expression tag	UNP P28472
B	-2	GLY	-	expression tag	UNP P28472
B	-1	THR	-	expression tag	UNP P28472
B	0	GLY	-	expression tag	UNP P28472
B	308	SER	-	linker	UNP P28472
B	309	GLN	-	linker	UNP P28472
B	310	PRO	-	linker	UNP P28472
B	311	ALA	-	linker	UNP P28472
B	312	ARG	-	linker	UNP P28472
B	313	ALA	-	linker	UNP P28472
B	314	ALA	-	linker	UNP P28472
C	-53	MET	-	initiating methionine	UNP P28472
C	-52	ASP	-	expression tag	UNP P28472
C	-51	GLU	-	expression tag	UNP P28472
C	-50	LYS	-	expression tag	UNP P28472
C	-49	THR	-	expression tag	UNP P28472
C	-48	THR	-	expression tag	UNP P28472
C	-47	GLY	-	expression tag	UNP P28472
C	-46	TRP	-	expression tag	UNP P28472
C	-45	ARG	-	expression tag	UNP P28472
C	-44	GLY	-	expression tag	UNP P28472
C	-43	GLY	-	expression tag	UNP P28472
C	-42	HIS	-	expression tag	UNP P28472
C	-41	VAL	-	expression tag	UNP P28472
C	-40	VAL	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-39	GLU	-	expression tag	UNP P28472
C	-38	GLY	-	expression tag	UNP P28472
C	-37	LEU	-	expression tag	UNP P28472
C	-36	ALA	-	expression tag	UNP P28472
C	-35	GLY	-	expression tag	UNP P28472
C	-34	GLU	-	expression tag	UNP P28472
C	-33	LEU	-	expression tag	UNP P28472
C	-32	GLU	-	expression tag	UNP P28472
C	-31	GLN	-	expression tag	UNP P28472
C	-30	LEU	-	expression tag	UNP P28472
C	-29	ARG	-	expression tag	UNP P28472
C	-28	ALA	-	expression tag	UNP P28472
C	-27	ARG	-	expression tag	UNP P28472
C	-26	LEU	-	expression tag	UNP P28472
C	-25	GLU	-	expression tag	UNP P28472
C	-24	HIS	-	expression tag	UNP P28472
C	-23	HIS	-	expression tag	UNP P28472
C	-22	PRO	-	expression tag	UNP P28472
C	-21	GLN	-	expression tag	UNP P28472
C	-20	GLY	-	expression tag	UNP P28472
C	-19	GLN	-	expression tag	UNP P28472
C	-18	ARG	-	expression tag	UNP P28472
C	-17	GLU	-	expression tag	UNP P28472
C	-16	PRO	-	expression tag	UNP P28472
C	-15	ASP	-	expression tag	UNP P28472
C	-14	TYR	-	expression tag	UNP P28472
C	-13	ASP	-	expression tag	UNP P28472
C	-12	ILE	-	expression tag	UNP P28472
C	-11	PRO	-	expression tag	UNP P28472
C	-10	THR	-	expression tag	UNP P28472
C	-9	THR	-	expression tag	UNP P28472
C	-8	GLU	-	expression tag	UNP P28472
C	-7	ASN	-	expression tag	UNP P28472
C	-6	LEU	-	expression tag	UNP P28472
C	-5	TYR	-	expression tag	UNP P28472
C	-4	PHE	-	expression tag	UNP P28472
C	-3	GLN	-	expression tag	UNP P28472
C	-2	GLY	-	expression tag	UNP P28472
C	-1	THR	-	expression tag	UNP P28472
C	0	GLY	-	expression tag	UNP P28472
C	308	SER	-	linker	UNP P28472
C	309	GLN	-	linker	UNP P28472

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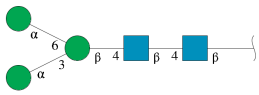
Chain	Residue	Modelled	Actual	Comment	Reference
C	310	PRO	-	linker	UNP P28472
C	311	ALA	-	linker	UNP P28472
C	312	ARG	-	linker	UNP P28472
C	313	ALA	-	linker	UNP P28472
C	314	ALA	-	linker	UNP P28472

- Molecule 3 is a protein called Megabody25,Outer membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	113	Total	C	N	O	S	0	0
			891	563	152	172	4		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

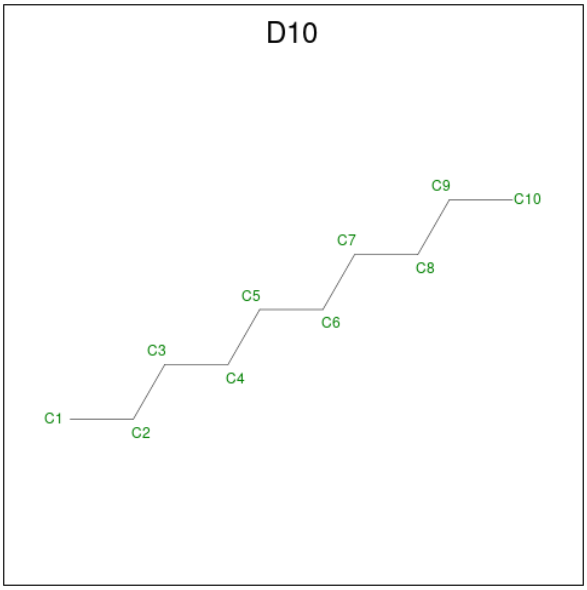


Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	5	Total	C	N	O	0	0
			61	34	2	25		
4	b	5	Total	C	N	O	0	0
			61	34	2	25		
4	c	5	Total	C	N	O	0	0
			61	34	2	25		
4	d	5	Total	C	N	O	0	0
			61	34	2	25		
4	e	5	Total	C	N	O	0	0
			61	34	2	25		

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

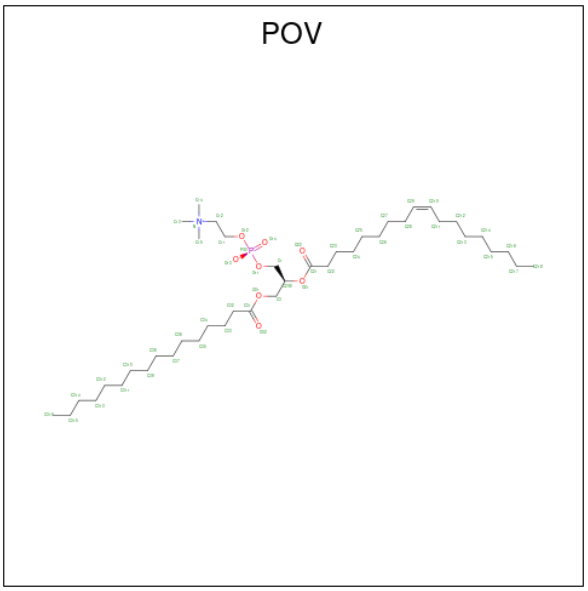
Mol	Chain	Residues	Atoms	AltConf	Trace
5	G	2	Total C N O 28 16 2 10	0	0
5	H	2	Total C N O 28 16 2 10	0	0
5	I	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total C 10 10	0
6	E	1	Total C 10 10	0
6	B	1	Total C 10 10	0
6	B	1	Total C 10 10	0
6	B	1	Total C 10 10	0
6	C	1	Total C 10 10	0

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).

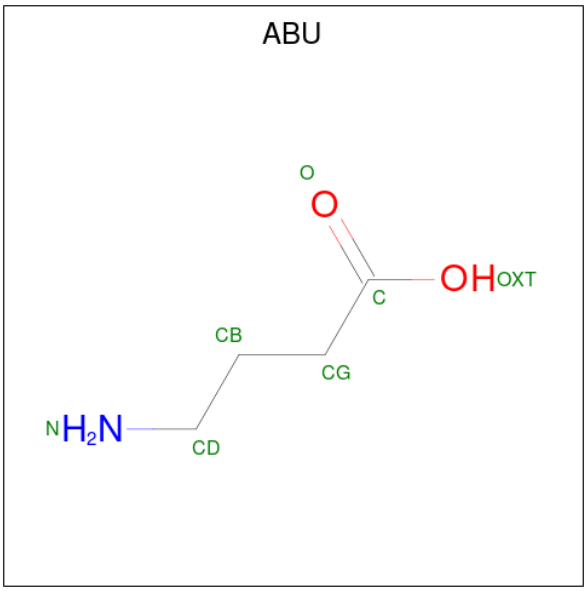


Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

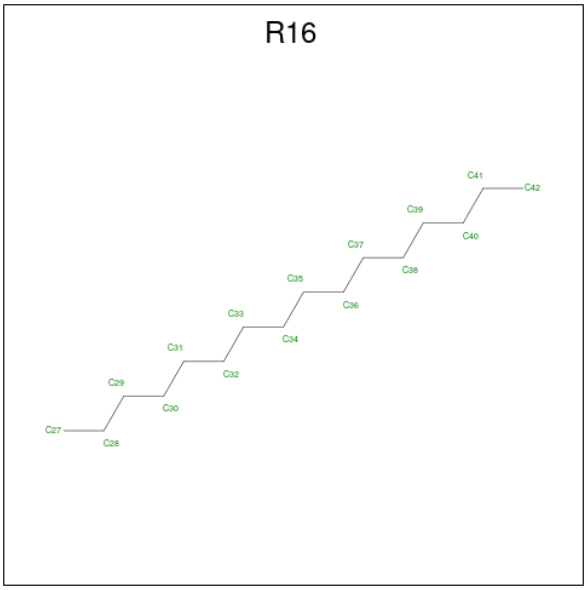
Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Cl	0
			1	1	
8	A	1	Total	Cl	0
			1	1	

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	E	1	Total C N O 7 4 1 2	0
9	B	1	Total C N O 7 4 1 2	0

- Molecule 10 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total C 16 16	0

- Molecule 11 is water.

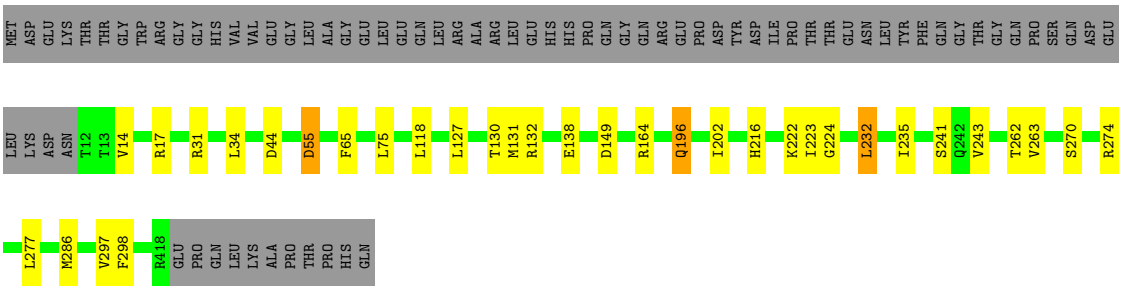
Mol	Chain	Residues	Atoms	AltConf
11	D	13	Total O 13 13	0
11	E	11	Total O 11 11	0
11	B	9	Total O 9 9	0
11	A	9	Total O 9 9	0
11	C	14	Total O 14 14	0

3 Residue-property plots

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.

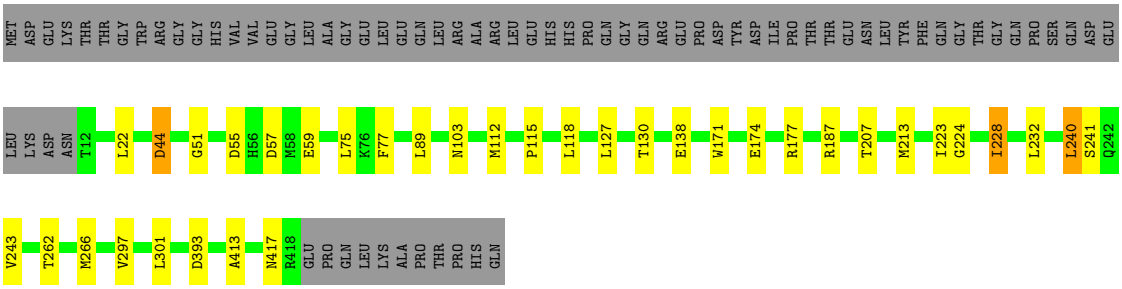
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain D:



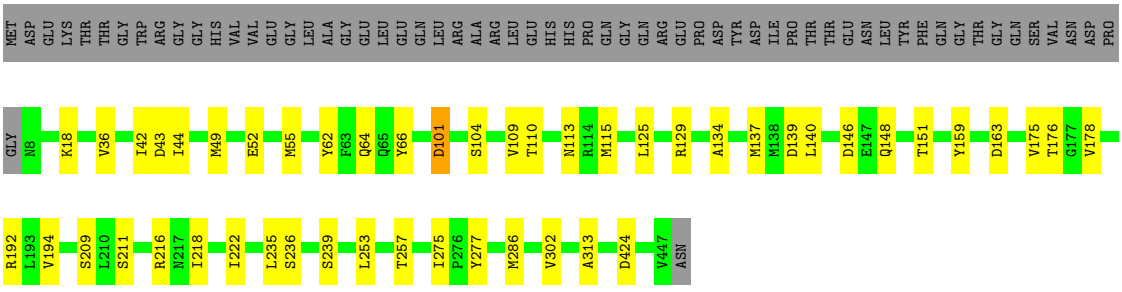
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A:



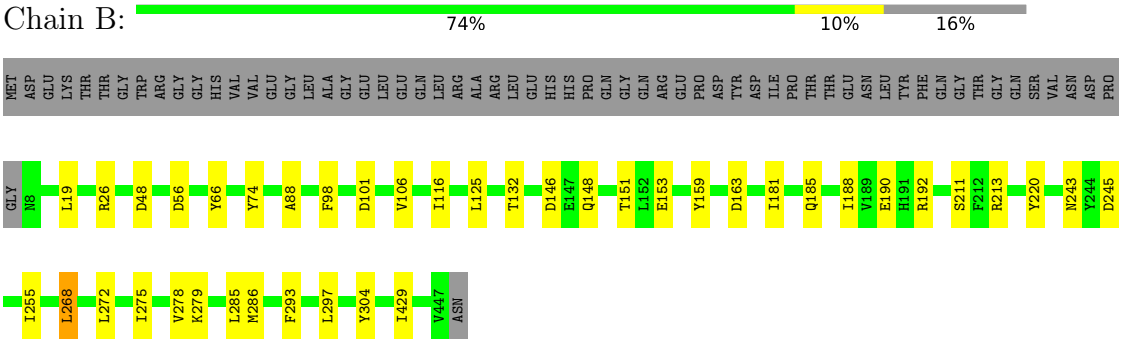
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain E:



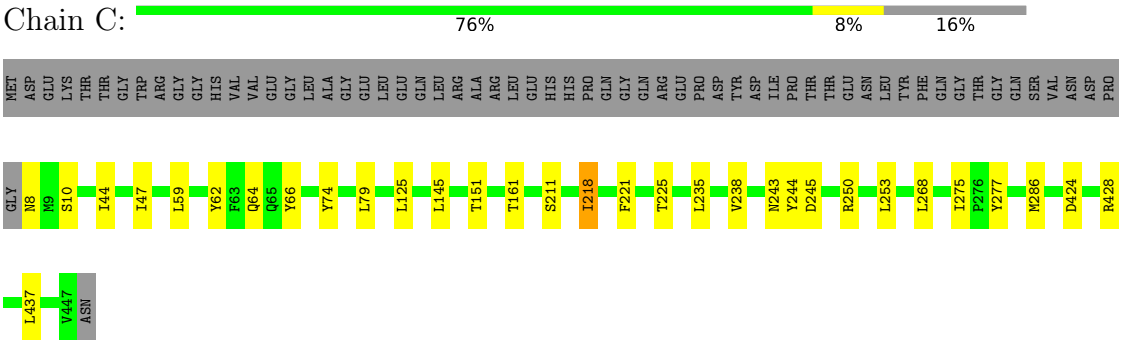
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain B:



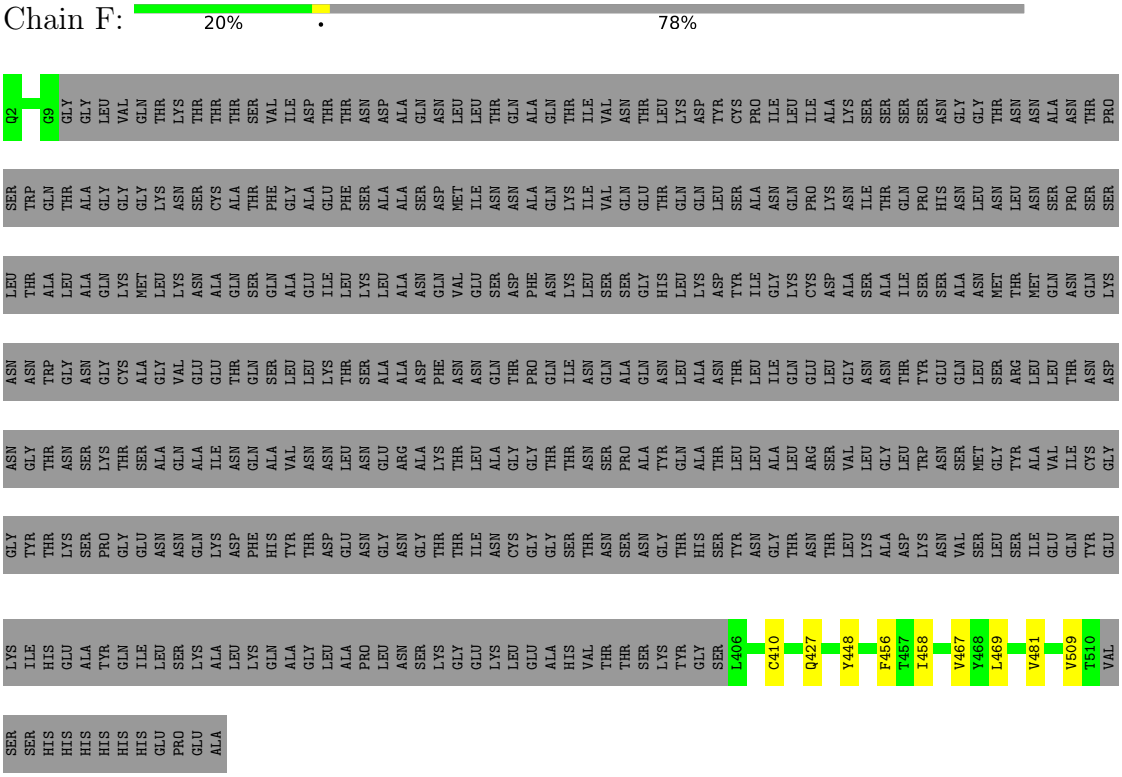
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain C:



• Molecule 3: Megabody25,Outer membrane protein

Chain F:



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

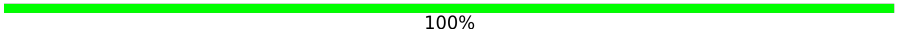
Chain c:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

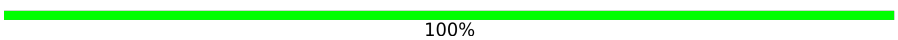
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



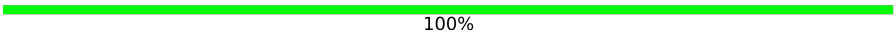
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



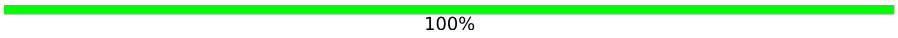
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	176000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.907	Depositor
Minimum map value	-0.664	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	260.3832, 260.3832, 260.3832	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23992, 1.23992, 1.23992	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, R16, POV, MAN, D10, CL, BMA, ABU

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	0.24	0/2802	0.34	0/3808
1	D	0.24	0/2802	0.32	0/3808
2	B	0.23	0/2841	0.35	0/3868
2	C	0.23	0/2825	0.34	0/3846
2	E	0.24	0/2817	0.36	0/3835
3	F	0.15	0/914	0.30	0/1238
All	All	0.23	0/15001	0.34	0/20403

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2727	0	2733	24	0
1	D	2727	0	2733	23	0
2	B	2754	0	2760	23	0
2	C	2744	0	2740	17	0
2	E	2739	0	2734	28	0
3	F	891	0	833	4	0
4	a	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	b	61	0	52	1	0
4	c	61	0	52	1	0
4	d	61	0	52	1	0
4	e	61	0	52	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
6	B	30	0	66	1	0
6	C	10	0	22	1	0
6	D	10	0	22	1	0
6	E	10	0	22	0	0
7	A	52	0	82	1	0
7	D	52	0	82	5	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	7	0	0	1	0
9	E	7	0	0	1	0
10	B	16	0	34	0	0
11	A	9	0	0	0	0
11	B	9	0	0	1	0
11	C	14	0	0	1	0
11	D	13	0	0	1	0
11	E	11	0	0	0	0
All	All	15223	0	15198	111	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 4.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:ASN:HD22	2:E:129:ARG:HE	1.35	0.72
2:B:106:VAL:HG23	1:A:112:MET:HE1	1.71	0.72
2:C:62:TYR:HB3	2:C:64:GLN:HE22	1.58	0.69
1:A:413:ALA:O	1:A:417:ASN:ND2	2.28	0.66
2:C:243[A]:ASN:ND2	2:C:245:ASP:OD2	2.29	0.66
2:E:159:TYR:HB3	2:E:163:ASP:HB2	1.79	0.63
2:B:243[B]:ASN:ND2	2:B:245:ASP:OD1	2.32	0.62
1:A:118:LEU:HG	1:A:130:THR:HB	1.82	0.61
1:D:270:SER:HB3	1:D:274:ARG:HH21	1.67	0.60
1:A:44:ASP:N	1:A:44:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:ARG:NH2	4:b:1:NAG:O7	2.36	0.58
1:A:115:PRO:HD3	4:d:1:NAG:H82	1.85	0.58
2:C:8:ASN:OD1	2:C:10:SER:OG	2.22	0.58
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.34	0.57
1:D:243:VAL:HG22	6:D:501:D10:H72	1.86	0.57
2:C:47:ILE:HG12	2:C:59:LEU:HD12	1.86	0.57
2:C:225:THR:HG22	2:C:268:LEU:HD11	1.85	0.57
2:C:145:LEU:HD23	2:C:218:ILE:HG21	1.87	0.57
2:E:101:ASP:OD2	2:E:104:SER:OG	2.21	0.56
2:B:190:GLU:OE1	2:B:213:ARG:NH1	2.27	0.56
2:B:192:ARG:NH2	4:c:1:NAG:O7	2.38	0.56
1:D:222:LYS:HB3	7:D:502:POV:H14B	1.86	0.56
2:B:151:THR:HG22	2:B:211:SER:HB3	1.86	0.56
2:B:268:LEU:HD22	2:B:285:LEU:HD11	1.89	0.55
2:C:44:ILE:HD12	2:C:59:LEU:HD11	1.89	0.55
2:E:55:MET:HE3	2:E:137:MET:HA	1.87	0.55
1:D:75:LEU:HD12	1:D:127:LEU:HD21	1.89	0.54
1:D:118:LEU:HG	1:D:130:THR:HB	1.90	0.54
1:A:174:GLU:OE2	1:A:177:ARG:NH1	2.41	0.54
1:D:277:LEU:HD21	1:D:286:MET:HG2	1.90	0.53
2:E:66[A]:TYR:CZ	2:E:125:LEU:HD13	2.43	0.53
1:D:241:SER:HB3	1:D:262:THR:HG21	1.91	0.53
2:C:64:GLN:NE2	11:C:601:HOH:O	2.24	0.52
2:B:66[A]:TYR:CZ	2:B:125:LEU:HD13	2.43	0.52
2:E:236:SER:HB2	2:E:257:THR:HG21	1.92	0.51
1:A:241:SER:HB3	1:A:262:THR:HG21	1.91	0.51
2:C:66[A]:TYR:CZ	2:C:125:LEU:HD13	2.46	0.51
2:E:139:ASP:H	2:E:148:GLN:HE22	1.59	0.50
2:B:56:ASP:OD1	11:B:601:HOH:O	2.20	0.50
2:E:235:LEU:HD21	1:A:301:LEU:HD23	1.94	0.50
2:E:42:ILE:HB	2:E:175:VAL:HG22	1.93	0.49
2:B:26:ARG:HG2	1:A:89:LEU:HD21	1.95	0.49
1:D:149:ASP:OD1	1:D:149:ASP:N	2.46	0.49
1:A:22:LEU:HD21	1:A:77:PHE:HB3	1.94	0.48
1:D:65:PHE:HE1	1:D:132:ARG:HD2	1.77	0.48
1:D:44:ASP:N	1:D:44:ASP:OD1	2.47	0.47
2:B:159:TYR:HB3	2:B:163:ASP:HB2	1.96	0.47
2:B:190:GLU:OE2	2:B:192:ARG:NH1	2.47	0.47
2:C:238:VAL:HG22	6:C:501:D10:H91	1.95	0.47
2:E:18:LYS:HE2	2:E:18:LYS:HB3	1.82	0.46
2:C:151:THR:HG22	2:C:211:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:502:POV:H15	2:E:277:TYR:HB2	1.97	0.46
1:D:298:PHE:CE1	2:C:235:LEU:HD13	2.51	0.46
2:B:293:PHE:CE1	1:A:240:LEU:HD13	2.51	0.46
2:E:140:LEU:HD13	2:E:275:ILE:HD13	1.97	0.46
2:E:44:ILE:HD12	2:E:178:VAL:HG22	1.98	0.46
1:D:232:LEU:HD23	2:E:286:MET:HE2	1.97	0.45
2:E:62:TYR:HB3	2:E:64:GLN:HE22	1.81	0.45
1:D:31:ARG:HG2	1:D:34:LEU:HD12	1.98	0.45
1:D:55:ASP:OD1	1:D:55:ASP:N	2.46	0.45
2:B:275:ILE:HB	2:B:279:LYS:HE3	1.97	0.45
2:E:194:VAL:HB	2:E:209:SER:HB2	1.99	0.45
3:F:427:GLN:HB3	3:F:481:VAL:HG13	1.97	0.45
1:A:51:GLY:HA2	1:A:187:ARG:HB2	1.99	0.44
2:C:424:ASP:O	2:C:428:ARG:HG3	2.18	0.44
3:F:410:CYS:HB3	3:F:467:VAL:HG23	1.99	0.44
1:D:138:GLU:OE2	11:D:601:HOH:O	2.21	0.44
2:E:101:ASP:HA	2:E:134:ALA:HA	2.00	0.44
2:B:98:PHE:HA	2:B:153:GLU:O	2.17	0.44
2:E:66[A]:TYR:CE2	2:E:125:LEU:HD13	2.53	0.44
2:E:52:GLU:OE2	2:E:216:ARG:NH2	2.41	0.44
2:E:109:VAL:HA	2:E:110:THR:HA	1.79	0.43
1:D:14:VAL:O	1:D:17:ARG:HG2	2.19	0.43
2:B:220:TYR:HB2	2:C:277:TYR:HA	1.99	0.43
1:A:75:LEU:HD12	1:A:127:LEU:HD21	1.99	0.43
1:D:263:VAL:HG22	1:D:297:VAL:HG12	2.00	0.43
2:B:185:GLN:OE1	2:B:185:GLN:N	2.51	0.43
1:A:57:ASP:HB2	1:A:59:GLU:HG2	2.01	0.43
3:F:448:TYR:HE1	3:F:458:ILE:HG13	1.82	0.43
2:B:181:ILE:HG21	2:B:188:ILE:HD11	2.01	0.42
1:A:171:TRP:CE2	1:A:213:MET:HE3	2.55	0.42
1:D:164:ARG:HD3	1:D:202:ILE:HD12	2.02	0.42
1:D:196:GLN:HA	1:D:216:HIS:O	2.19	0.42
2:E:115:MET:HE1	1:A:207:THR:HG21	2.02	0.42
2:B:19:LEU:HD11	2:B:74:TYR:HB3	2.02	0.42
9:B:501:ABU:OXT	1:A:130:THR:HG21	2.19	0.42
2:E:151:THR:HG22	2:E:211:SER:HB3	2.02	0.42
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.91	0.42
2:E:49:MET:HE2	2:E:49:MET:HB3	1.88	0.41
2:B:88:ALA:HB2	2:B:116:ILE:HG13	2.02	0.41
1:A:112:MET:HE2	1:A:112:MET:HB2	1.73	0.41
1:D:235:ILE:HD13	7:D:502:POV:H310	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLY:HA2	7:A:501:POV:H22A	2.02	0.41
2:C:221:PHE:O	2:C:225:THR:OG1	2.25	0.41
1:A:103:ASN:HB2	1:A:138:GLU:HG2	2.01	0.41
1:A:266:MET:HG3	1:A:297:VAL:HG21	2.01	0.41
1:D:130:THR:HG21	9:E:501:ABU:O	2.21	0.41
2:E:239:SER:HB3	2:E:253:LEU:HD23	2.03	0.41
2:B:255:ILE:HD12	2:B:255:ILE:HA	1.92	0.41
7:D:502:POV:H14A	7:D:502:POV:H11	1.89	0.40
2:B:278:VAL:HG22	1:A:228:ILE:HG21	2.02	0.40
1:D:224:GLY:HA3	7:D:502:POV:H11	2.02	0.40
2:E:43:ASP:OD1	2:E:176:THR:OG1	2.39	0.40
2:C:244:TYR:HA	2:C:250:ARG:HH11	1.86	0.40
3:F:456:PHE:HB3	3:F:469:LEU:HD11	2.02	0.40
2:E:146:ASP:OD1	2:E:146:ASP:N	2.50	0.40
2:B:304:TYR:CE2	6:B:502:D10:H52	2.56	0.40
2:E:302:VAL:HG13	2:E:313:ALA:HB1	2.02	0.40
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.89	0.40
1:D:131:MET:HE2	1:D:131:MET:HB3	1.95	0.40
2:C:74:TYR:OH	2:C:79:LEU:O	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/411 (82%)	329 (98%)	7 (2%)	0	100	100
1	D	336/411 (82%)	330 (98%)	6 (2%)	0	100	100
2	B	335/395 (85%)	335 (100%)	0	0	100	100
2	C	333/395 (84%)	326 (98%)	7 (2%)	0	100	100
2	E	332/395 (84%)	327 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	109/522 (21%)	105 (96%)	4 (4%)	0	100	100
All	All	1781/2529 (70%)	1752 (98%)	29 (2%)	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	300/362 (83%)	293 (98%)	7 (2%)	45	78
1	D	300/362 (83%)	296 (99%)	4 (1%)	65	88
2	B	302/349 (86%)	294 (97%)	8 (3%)	41	75
2	C	300/349 (86%)	294 (98%)	6 (2%)	50	81
2	E	299/349 (86%)	294 (98%)	5 (2%)	56	84
3	F	92/430 (21%)	91 (99%)	1 (1%)	70	90
All	All	1593/2201 (72%)	1562 (98%)	31 (2%)	50	82

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	55	ASP
1	D	196	GLN
1	D	223	ILE
1	D	232	LEU
2	E	36	VAL
2	E	101	ASP
2	E	218	ILE
2	E	222	ILE
2	E	424	ASP
2	B	48	ASP
2	B	101	ASP
2	B	132	THR
2	B	268	LEU

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Mol	Chain	Res	Type
2	B	272	LEU
2	B	286	MET
2	B	297	LEU
2	B	429	ILE
1	A	44	ASP
1	A	55	ASP
1	A	223	ILE
1	A	228	ILE
1	A	240	LEU
1	A	243	VAL
1	A	393	ASP
2	C	161	THR
2	C	218	ILE
2	C	253	LEU
2	C	275	ILE
2	C	286	MET
2	C	437	LEU
3	F	509	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	242	GLN
1	D	408	ASN
2	E	64	GLN
2	E	113	ASN
2	E	148	GLN
2	E	265	ASN
2	E	309	GLN
2	B	85	ASN
2	B	191	HIS
2	B	224	GLN
2	B	265	ASN
2	B	303	ASN
2	B	439	ASN
1	A	102	HIS
1	A	218	HIS
1	A	229	GLN
1	A	242	GLN
2	C	64	GLN
2	C	439	ASN
3	F	473	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)

31 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	$\#\|Z\| > 2$
5	NAG	G	1	2,5	14,14,15	0.22	0	17,19,21	0.53	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	H	1	2,5	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	H	2	5	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	I	1	2,5	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	I	2	5	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	a	1	1,4	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	a	2	4	14,14,15	0.23	0	17,19,21	0.45	0
4	BMA	a	3	4	11,11,12	0.19	0	15,15,17	0.43	0
4	MAN	a	4	4	11,11,12	0.19	0	15,15,17	0.37	0
4	MAN	a	5	4	11,11,12	0.20	0	15,15,17	0.45	0
4	NAG	b	1	2,4	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	b	2	4	14,14,15	0.26	0	17,19,21	0.48	0
4	BMA	b	3	4	11,11,12	0.19	0	15,15,17	0.50	0
4	MAN	b	4	4	11,11,12	0.20	0	15,15,17	0.46	0
4	MAN	b	5	4	11,11,12	0.22	0	15,15,17	0.45	0
4	NAG	c	1	2,4	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	c	2	4	14,14,15	0.24	0	17,19,21	0.61	0
4	BMA	c	3	4	11,11,12	0.18	0	15,15,17	0.39	0
4	MAN	c	4	4	11,11,12	0.21	0	15,15,17	0.39	0
4	MAN	c	5	4	11,11,12	0.18	0	15,15,17	0.37	0
4	NAG	d	1	1,4	14,14,15	0.25	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	d	2	4	14,14,15	0.22	0	17,19,21	0.54	0
4	BMA	d	3	4	11,11,12	0.17	0	15,15,17	0.43	0
4	MAN	d	4	4	11,11,12	0.19	0	15,15,17	0.39	0
4	MAN	d	5	4	11,11,12	0.21	0	15,15,17	0.47	0
4	NAG	e	1	2,4	14,14,15	0.25	0	17,19,21	0.54	0
4	NAG	e	2	4	14,14,15	0.23	0	17,19,21	0.51	0
4	BMA	e	3	4	11,11,12	0.19	0	15,15,17	0.47	0
4	MAN	e	4	4	11,11,12	0.18	0	15,15,17	0.39	0
4	MAN	e	5	4	11,11,12	0.21	0	15,15,17	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	NAG	I	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	BMA	a	3	4	-	0/2/19/22	0/1/1/1
4	MAN	a	4	4	-	0/2/19/22	0/1/1/1
4	MAN	a	5	4	-	0/2/19/22	0/1/1/1
4	NAG	b	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	BMA	b	3	4	-	0/2/19/22	0/1/1/1
4	MAN	b	4	4	-	0/2/19/22	0/1/1/1
4	MAN	b	5	4	-	0/2/19/22	0/1/1/1
4	NAG	c	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	BMA	c	3	4	-	0/2/19/22	0/1/1/1
4	MAN	c	4	4	-	0/2/19/22	0/1/1/1
4	MAN	c	5	4	-	0/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	d	2	4	-	1/6/23/26	0/1/1/1
4	BMA	d	3	4	-	0/2/19/22	0/1/1/1
4	MAN	d	4	4	-	1/2/19/22	0/1/1/1
4	MAN	d	5	4	-	0/2/19/22	0/1/1/1
4	NAG	e	1	2,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	BMA	e	3	4	-	0/2/19/22	0/1/1/1
4	MAN	e	4	4	-	0/2/19/22	0/1/1/1
4	MAN	e	5	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

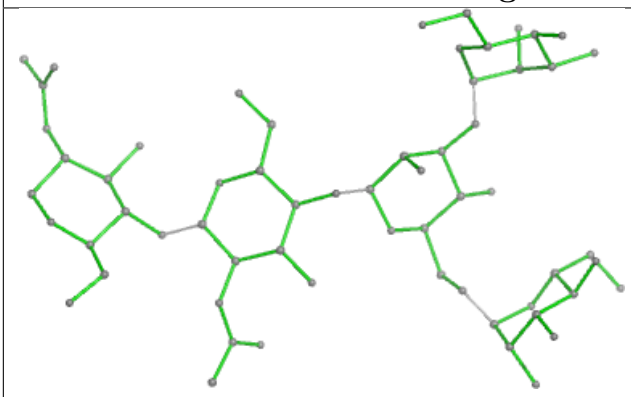
There are no ring outliers.

3 monomers are involved in 3 short contacts:

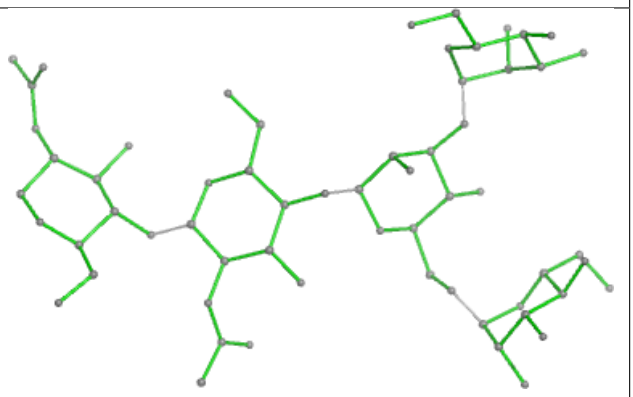
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	d	1	NAG	1	0
4	c	1	NAG	1	0
4	b	1	NAG	1	0

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

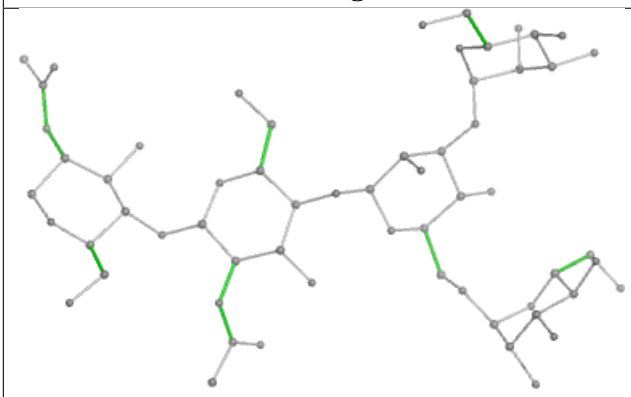
Oligosaccharide Chain a



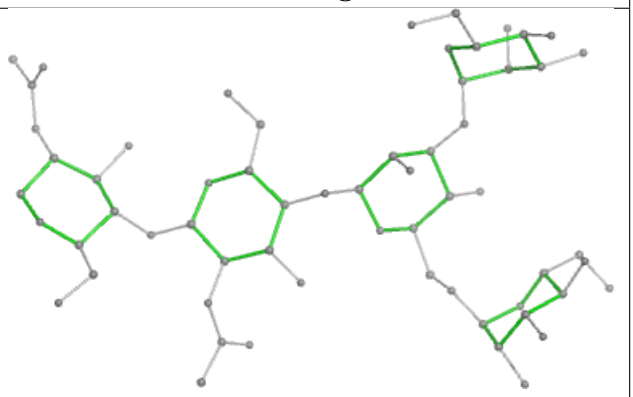
Bond lengths



Bond angles

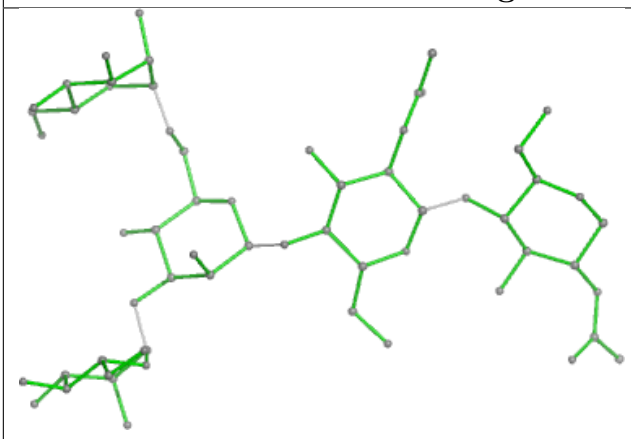


Torsions

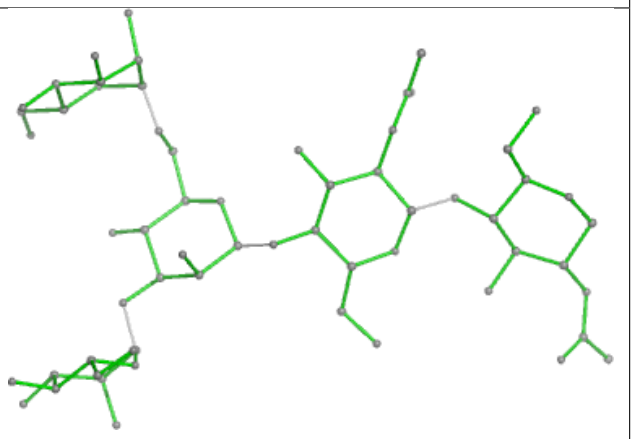


Rings

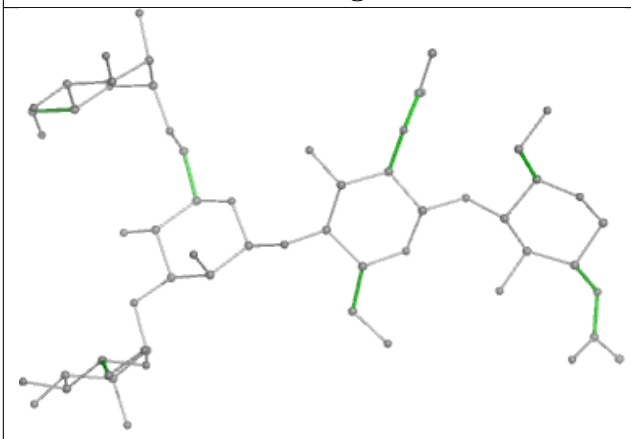
Oligosaccharide Chain b



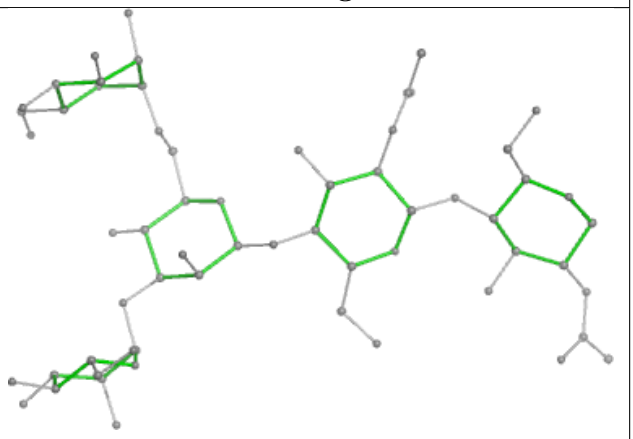
Bond lengths



Bond angles

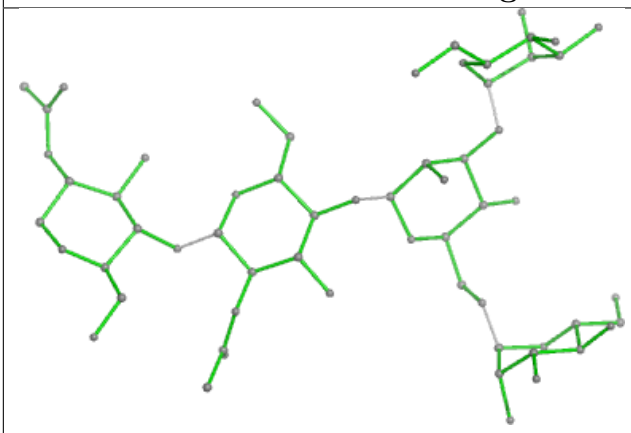


Torsions

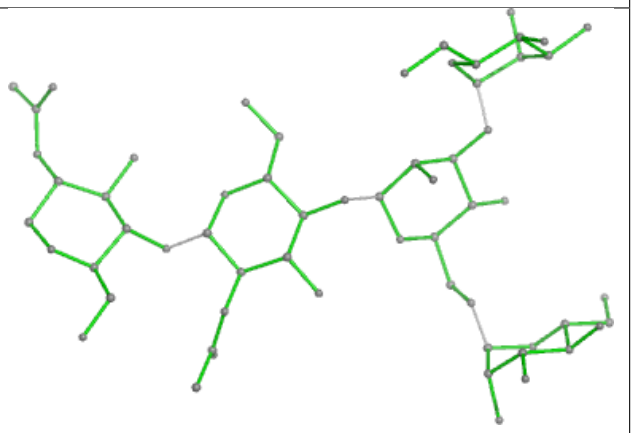


Rings

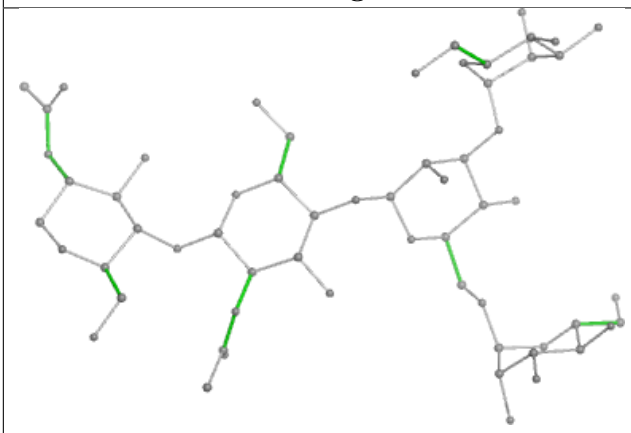
Oligosaccharide Chain c



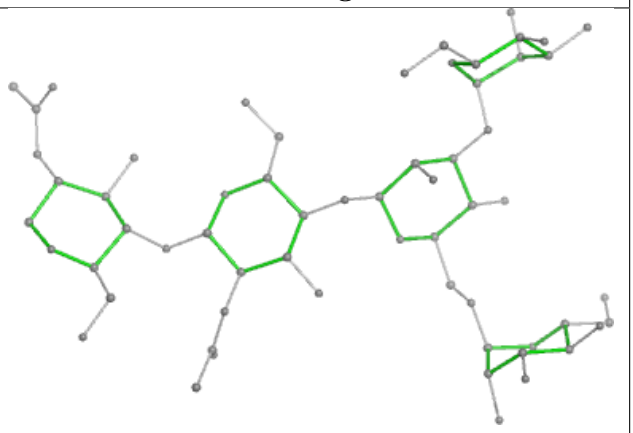
Bond lengths



Bond angles

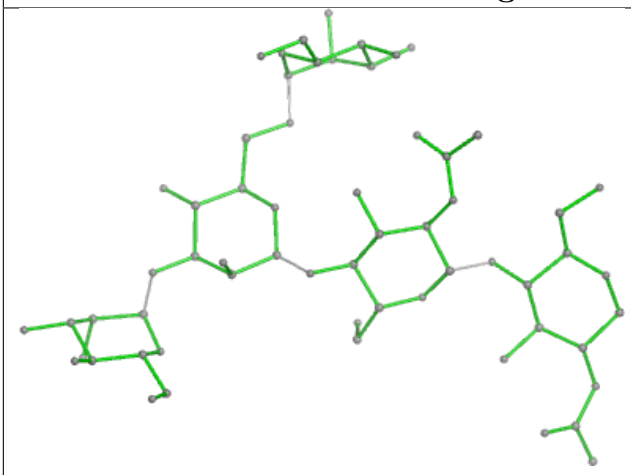


Torsions

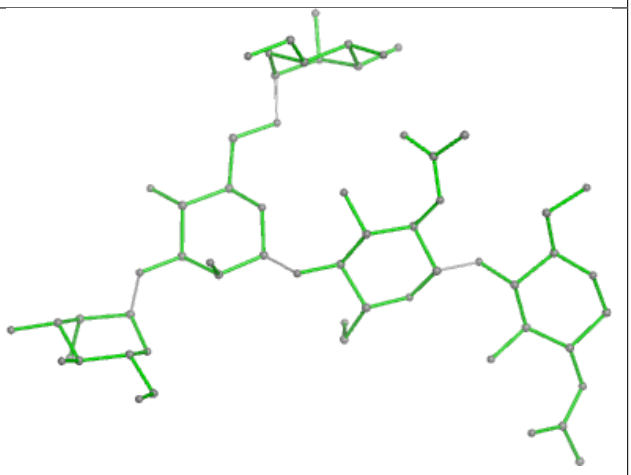


Rings

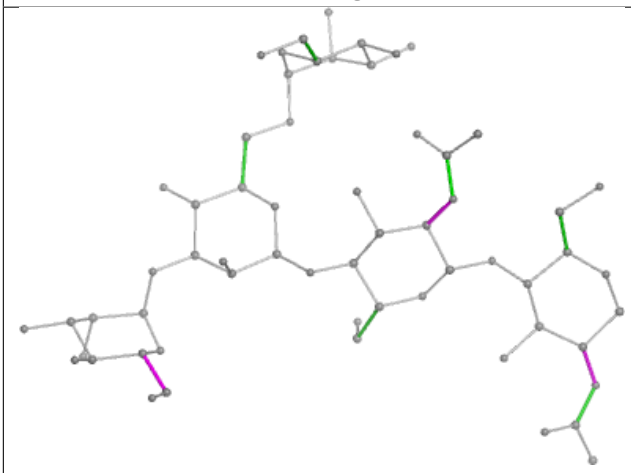
Oligosaccharide Chain d



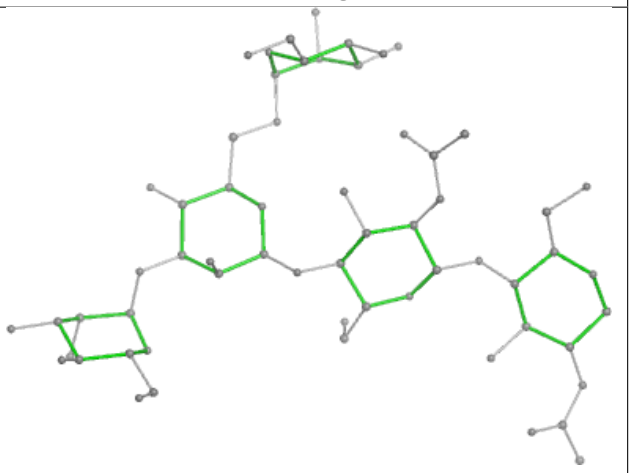
Bond lengths



Bond angles

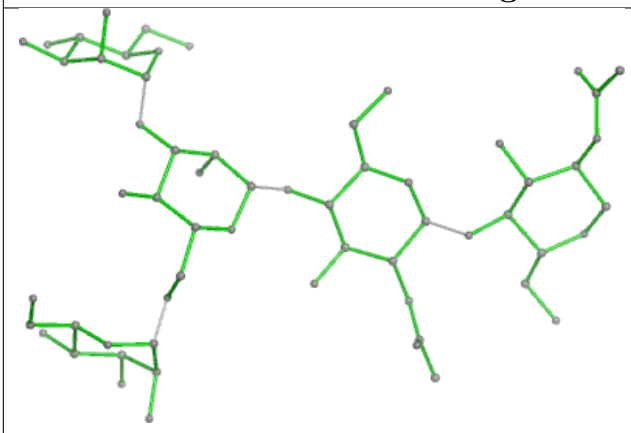


Torsions

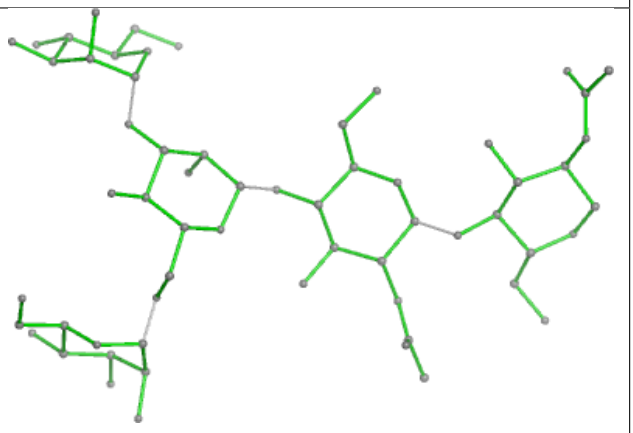


Rings

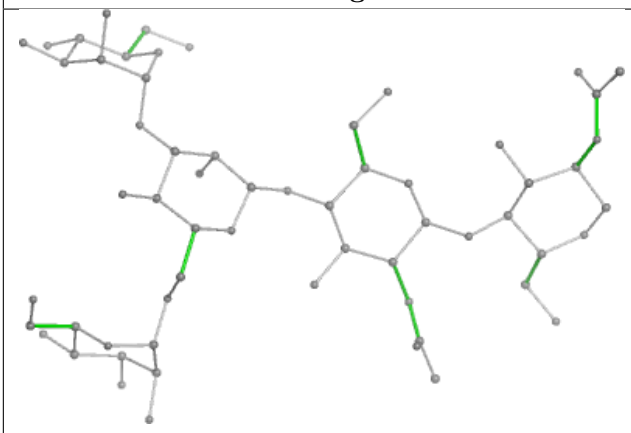
Oligosaccharide Chain e



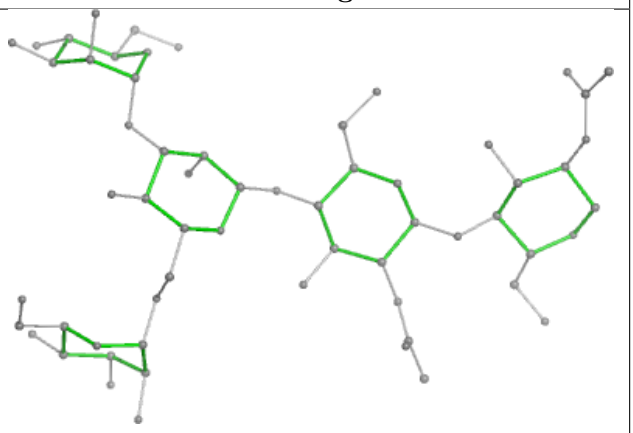
Bond lengths



Bond angles

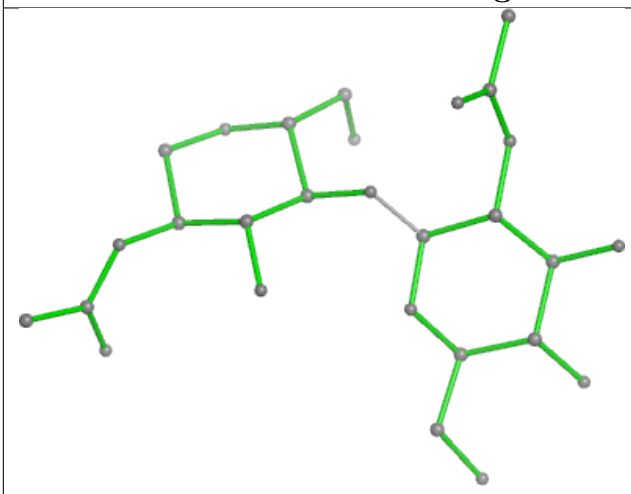


Torsions

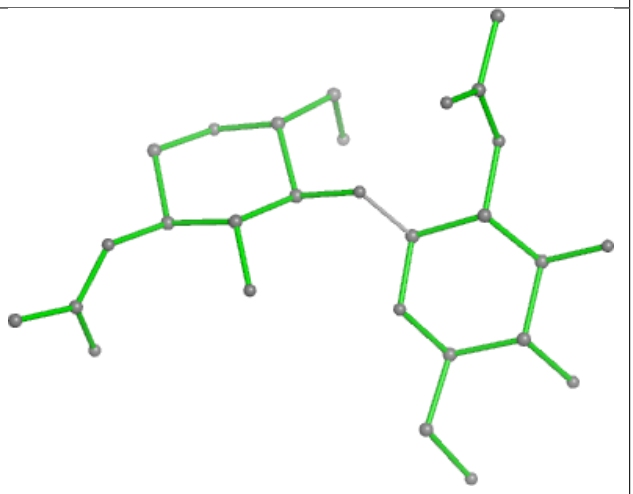


Rings

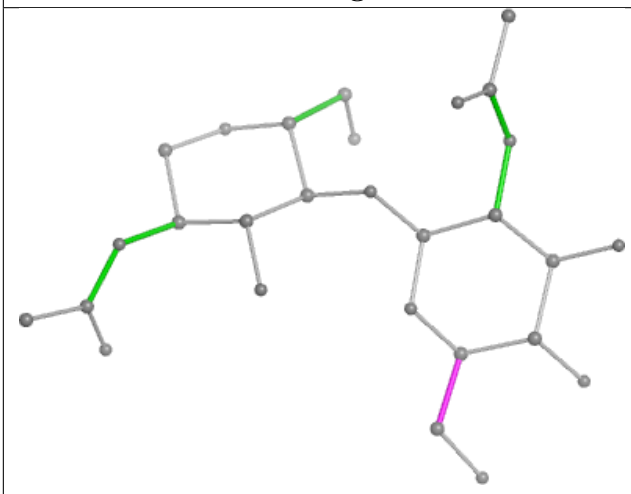
Oligosaccharide Chain G



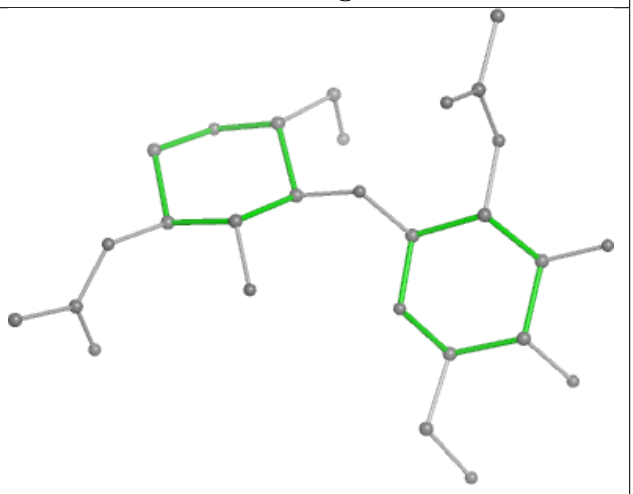
Bond lengths



Bond angles

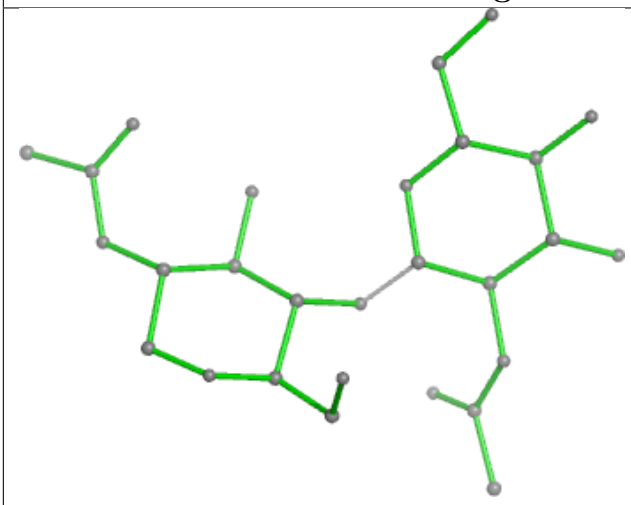


Torsions

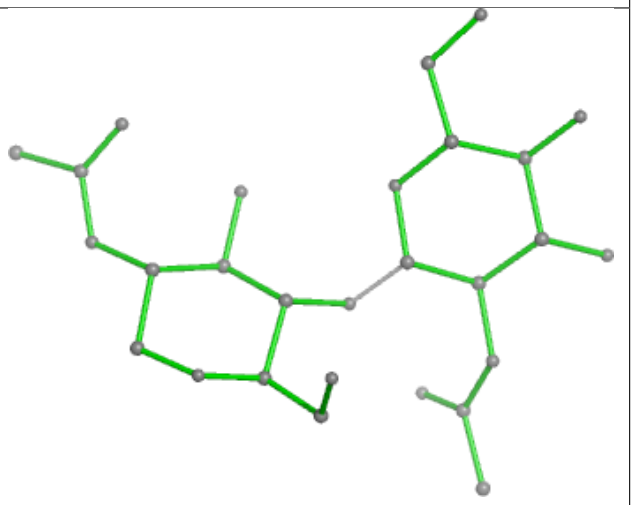


Rings

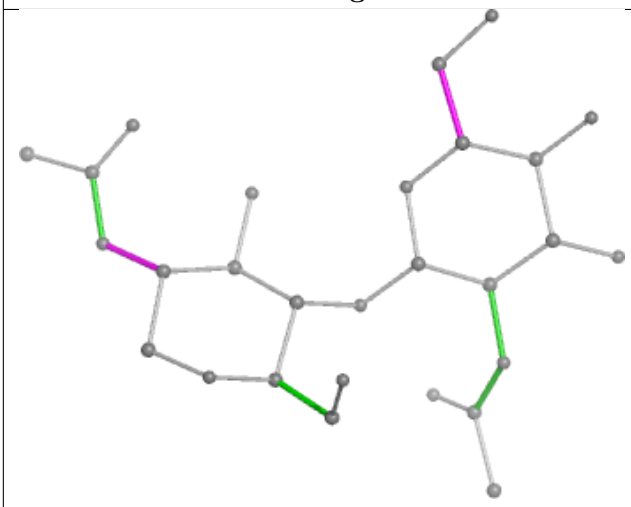
Oligosaccharide Chain H



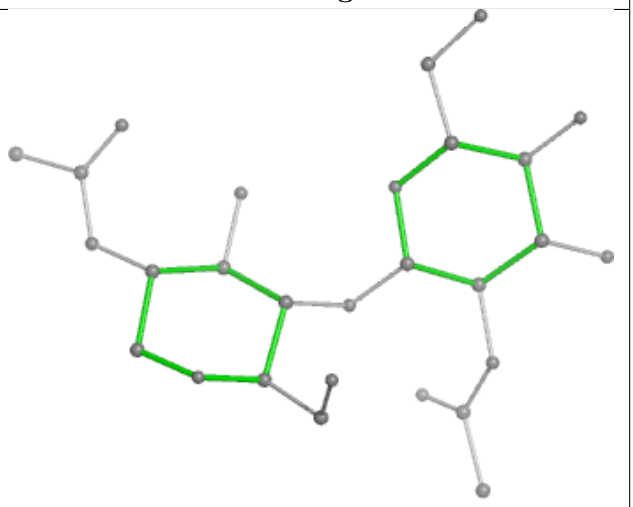
Bond lengths



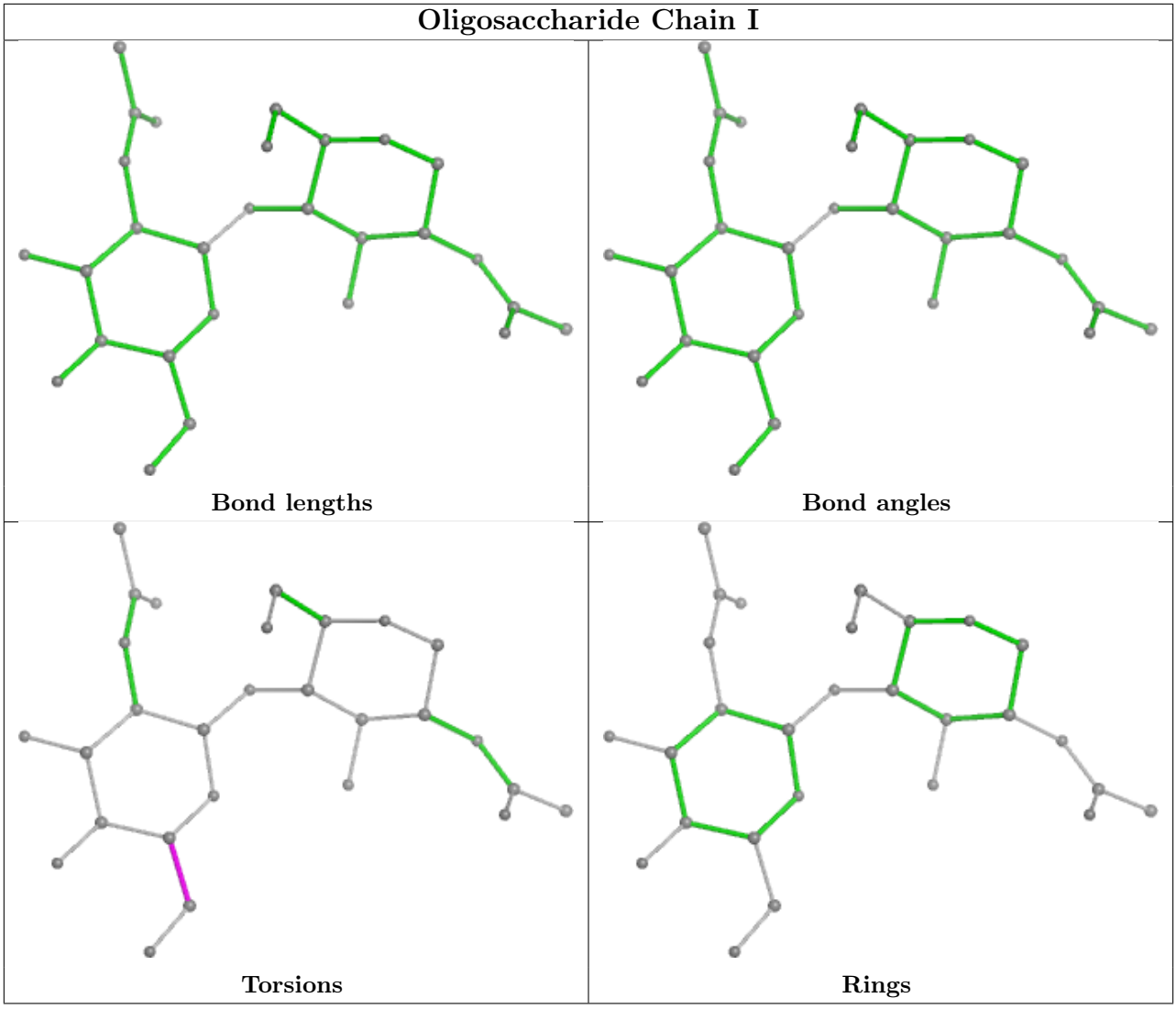
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	POV	D	502	-	51,51,51	0.28	0	57,59,59	0.29	0
10	R16	B	504	-	15,15,15	0.11	0	14,14,14	0.18	0
6	D10	B	505	-	9,9,9	0.11	0	8,8,8	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	D10	B	503	-	9,9,9	0.13	0	8,8,8	0.10	0
9	ABU	B	501	-	6,6,6	0.78	0	6,6,6	0.84	0
6	D10	C	501	-	9,9,9	0.12	0	8,8,8	0.13	0
9	ABU	E	501	-	6,6,6	0.86	0	6,6,6	0.94	0
6	D10	E	502	-	9,9,9	0.12	0	8,8,8	0.13	0
6	D10	D	501	-	9,9,9	0.12	0	8,8,8	0.13	0
6	D10	B	502	-	9,9,9	0.12	0	8,8,8	0.13	0
7	POV	A	501	-	51,51,51	0.28	0	57,59,59	0.30	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
7	POV	D	502	-	-	12/55/55/55	-
10	R16	B	504	-	-	0/13/13/13	-
6	D10	B	505	-	-	0/7/7/7	-
6	D10	B	503	-	-	0/7/7/7	-
9	ABU	B	501	-	-	0/4/4/4	-
6	D10	C	501	-	-	0/7/7/7	-
9	ABU	E	501	-	-	2/4/4/4	-
6	D10	E	502	-	-	0/7/7/7	-
6	D10	D	501	-	-	0/7/7/7	-
6	D10	B	502	-	-	0/7/7/7	-
7	POV	A	501	-	-	16/55/55/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	502	POV	C1-O11-P-O13
7	D	502	POV	C11-O12-P-O13
7	D	502	POV	C11-O12-P-O14
7	A	501	POV	C1-O11-P-O13
7	A	501	POV	O21-C2-C3-O31
7	D	502	POV	C11-C12-N-C14
7	D	502	POV	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	D	502	POV	C11-O12-P-O11
7	A	501	POV	C1-O11-P-O12
7	D	502	POV	C11-C12-N-C13
7	D	502	POV	C11-C12-N-C15
7	D	502	POV	C29-C210-C211-C212
7	D	502	POV	O21-C2-C3-O31
7	A	501	POV	C1-C2-C3-O31
7	A	501	POV	C11-O12-P-O11
7	A	501	POV	C11-O12-P-O14
7	A	501	POV	O12-C11-C12-N
7	A	501	POV	C11-C12-N-C15
7	A	501	POV	C33-C34-C35-C36
7	D	502	POV	C1-C2-C3-O31
9	E	501	ABU	OXT-C-CG-CB
7	A	501	POV	C21-C22-C23-C24
7	D	502	POV	O31-C31-C32-C33
9	E	501	ABU	O-C-CG-CB
7	A	501	POV	C29-C210-C211-C212
7	A	501	POV	C11-C12-N-C13
7	A	501	POV	C11-C12-N-C14
7	A	501	POV	O21-C21-C22-C23
7	A	501	POV	C27-C28-C29-C210
7	A	501	POV	O22-C21-C22-C23

There are no ring outliers.

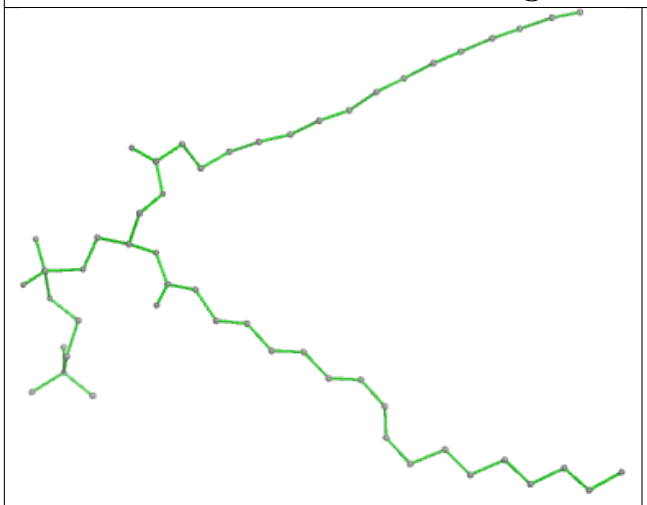
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	502	POV	5	0
9	B	501	ABU	1	0
6	C	501	D10	1	0
9	E	501	ABU	1	0
6	D	501	D10	1	0
6	B	502	D10	1	0
7	A	501	POV	1	0

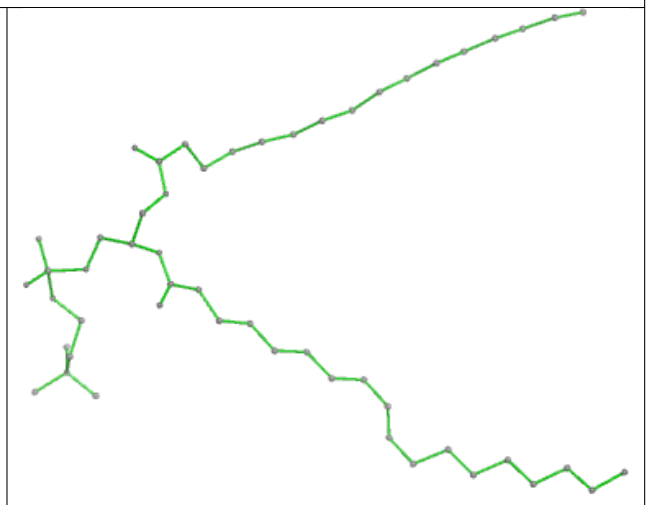
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

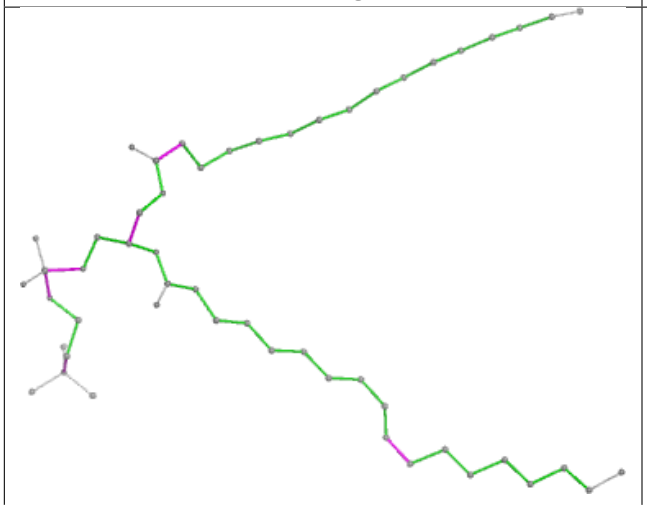
Ligand POV D 502



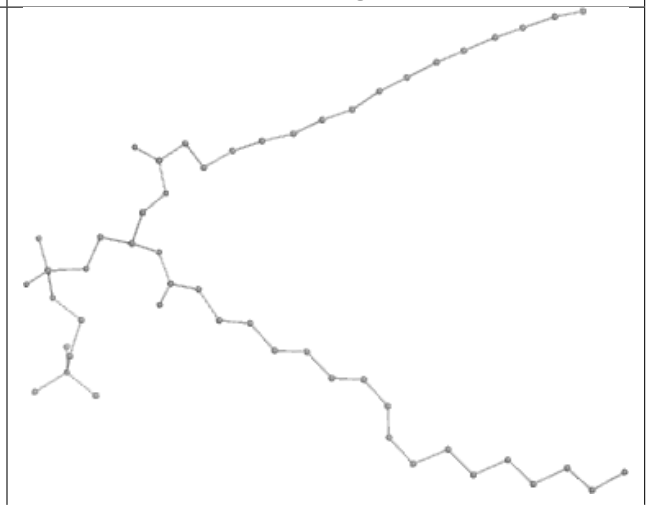
Bond lengths



Bond angles

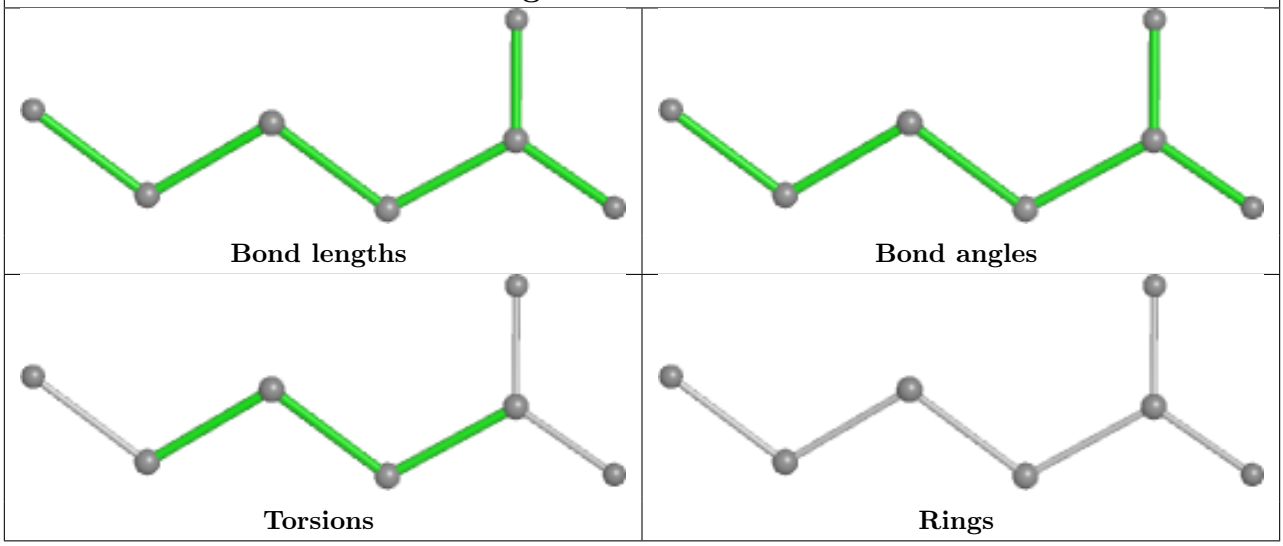


Torsions

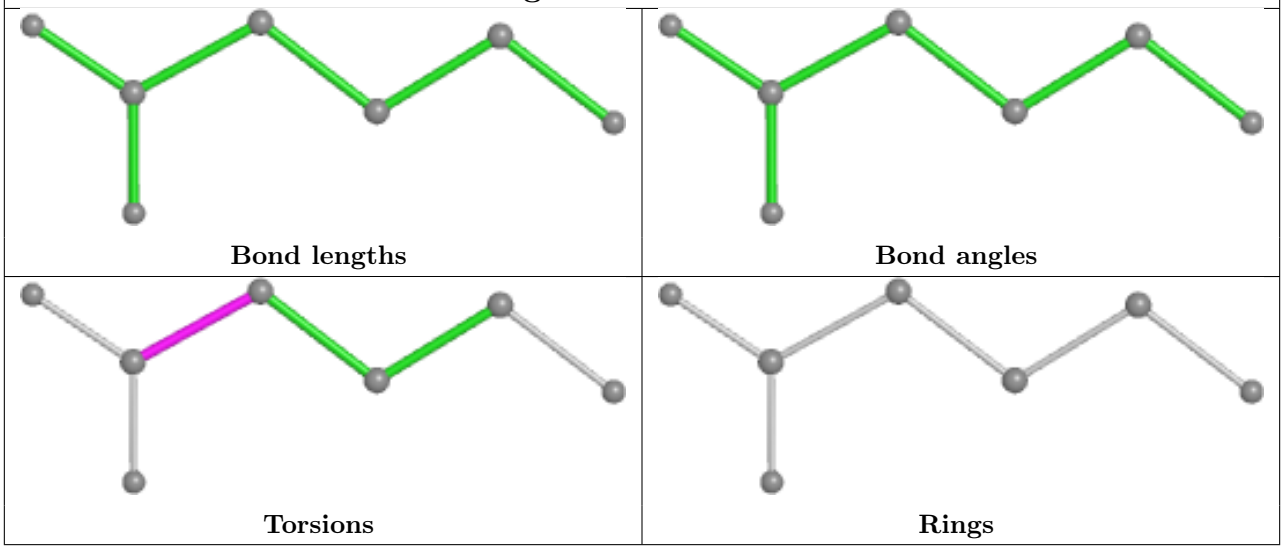


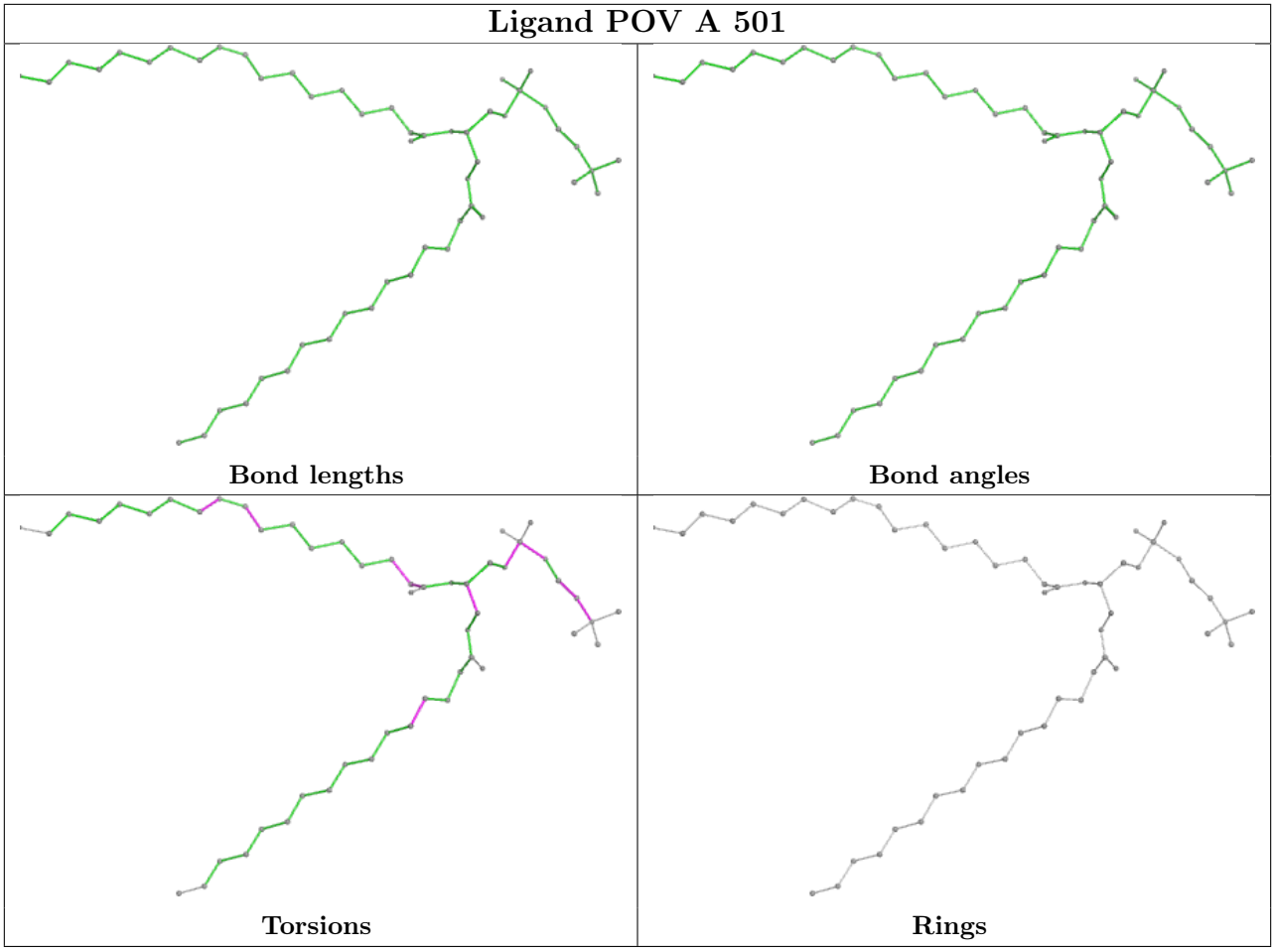
Rings

Ligand ABU B 501



Ligand ABU E 501





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.

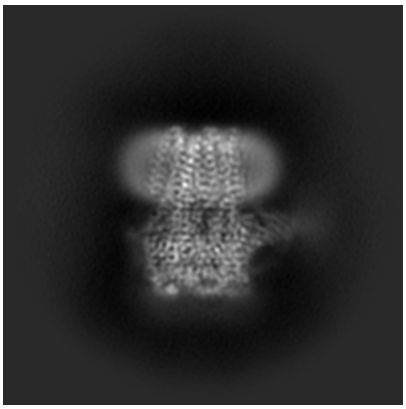
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50365. These allow visual inspection of the internal detail of the map and identification of artifacts.

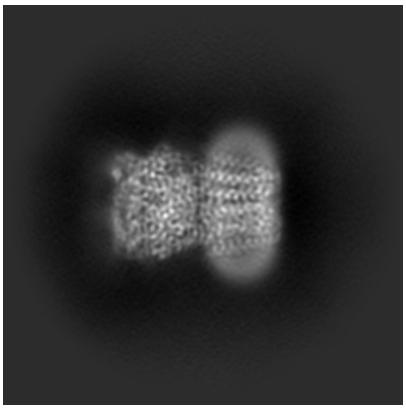
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

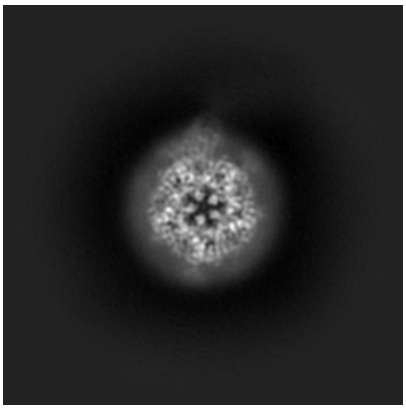
6.1.1 Primary map



X

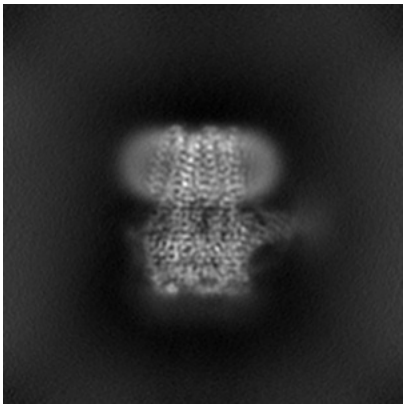


Y

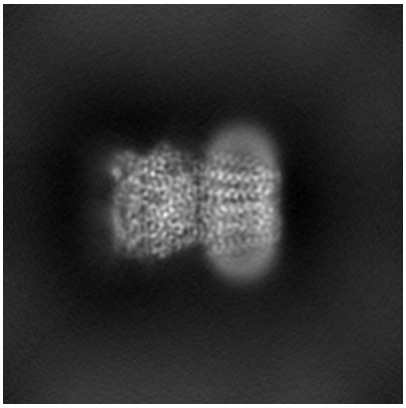


Z

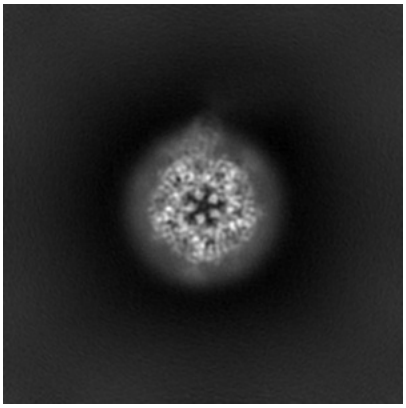
6.1.2 Raw map



X



Y

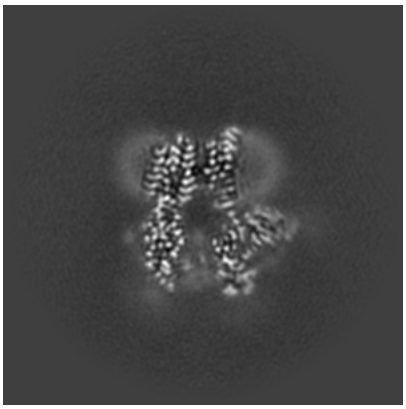


Z

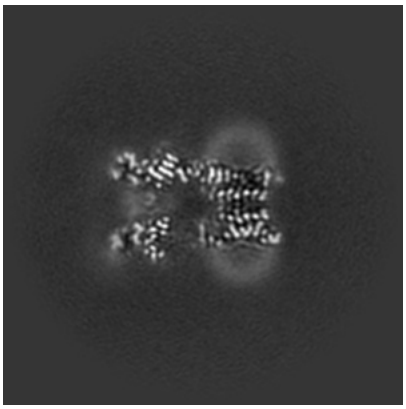
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

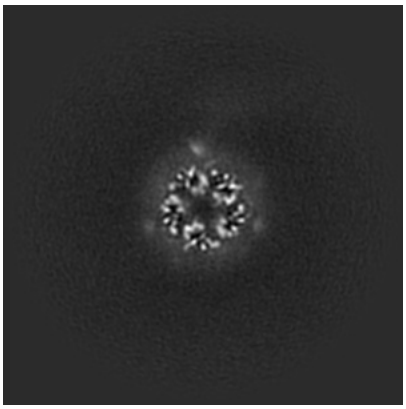
6.2.1 Primary map



X Index: 105

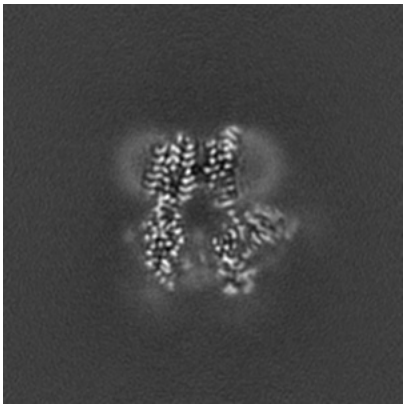


Y Index: 105

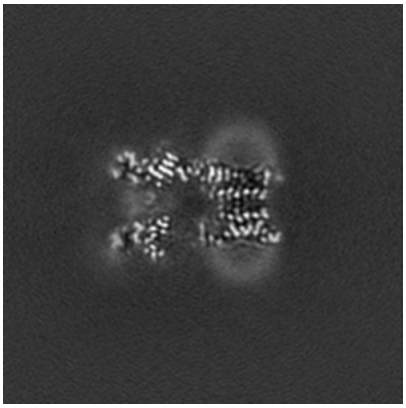


Z Index: 105

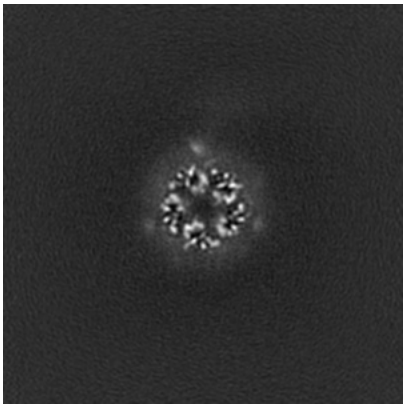
6.2.2 Raw map



X Index: 105



Y Index: 105

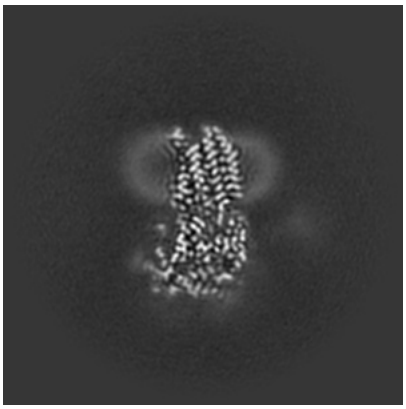


Z Index: 105

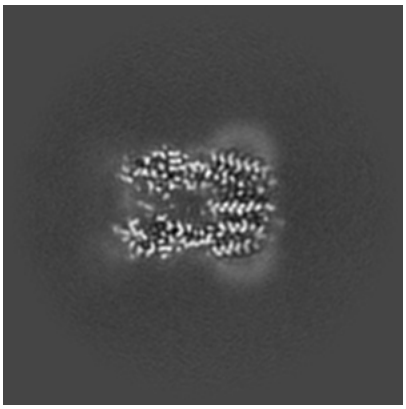
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

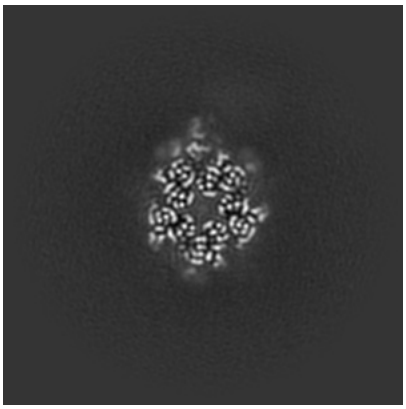
6.3.1 Primary map



X Index: 119

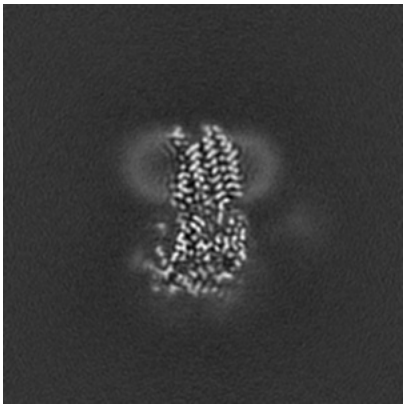


Y Index: 96

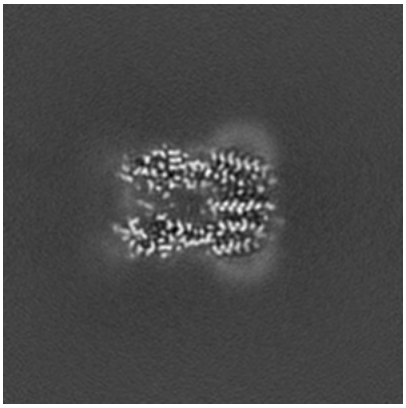


Z Index: 84

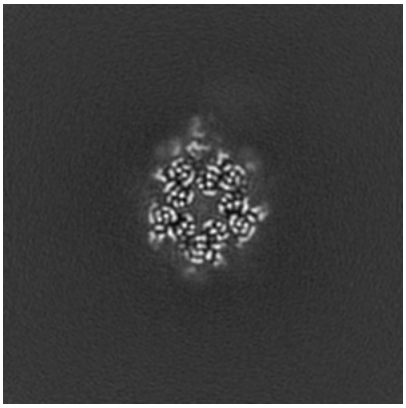
6.3.2 Raw map



X Index: 119



Y Index: 96

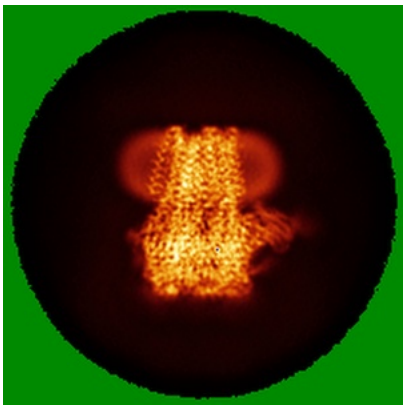


Z Index: 84

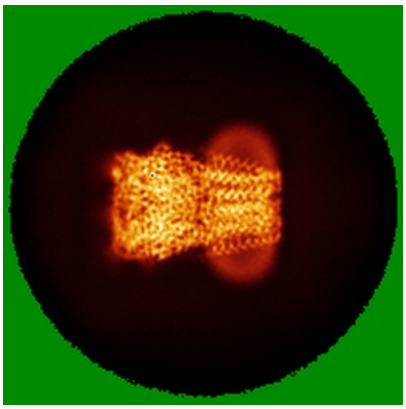
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



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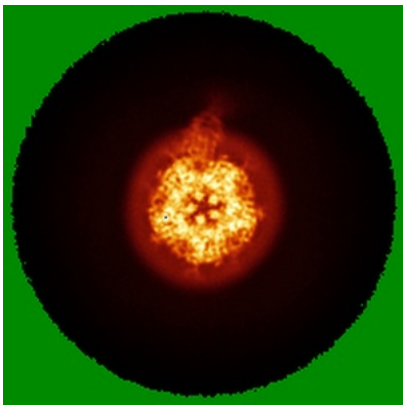
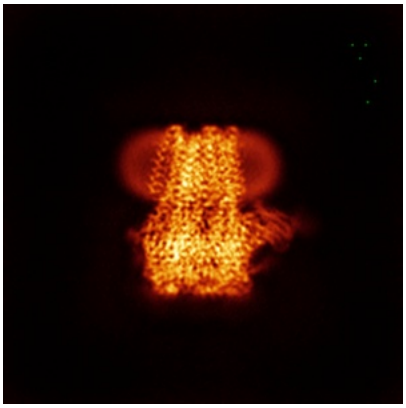
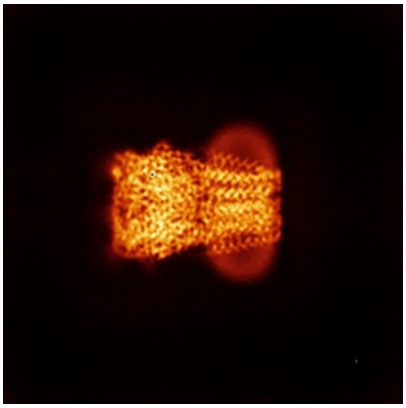


Z

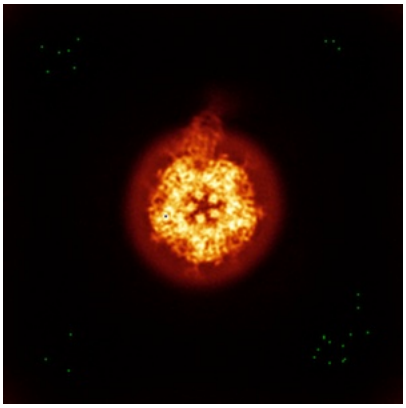
6.4.2 Raw map



X



Y

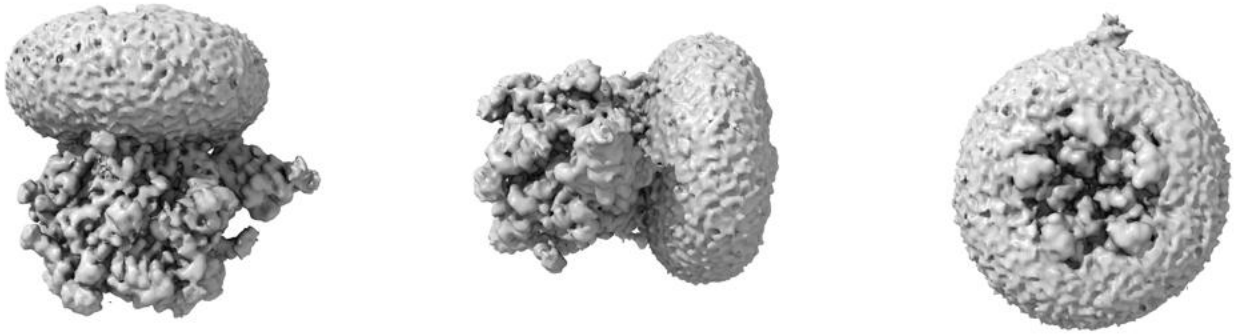


Z

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)

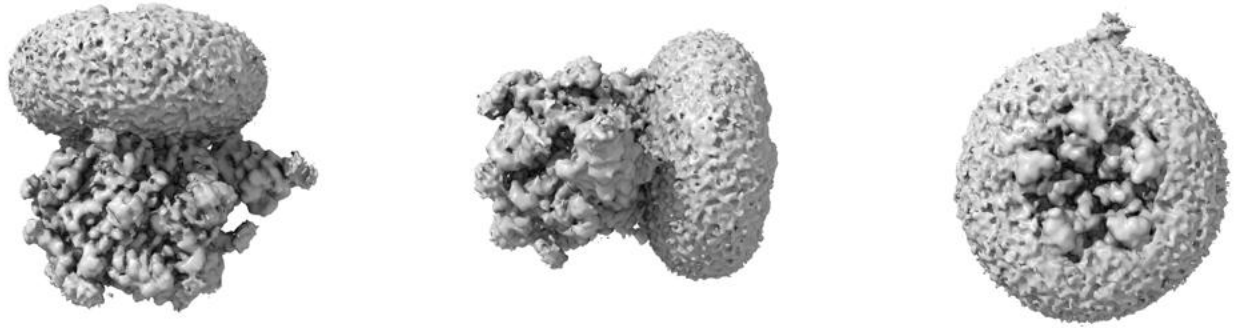
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

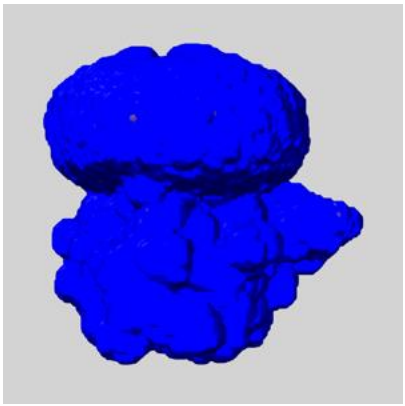
6.6 Mask visualisation (i)

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

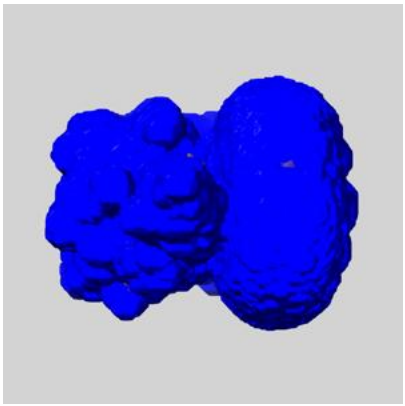
A mask typically either:

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

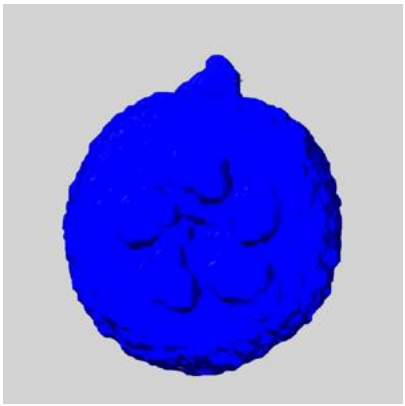
6.6.1 emd_50365_msk_1.map (i)



X



Y

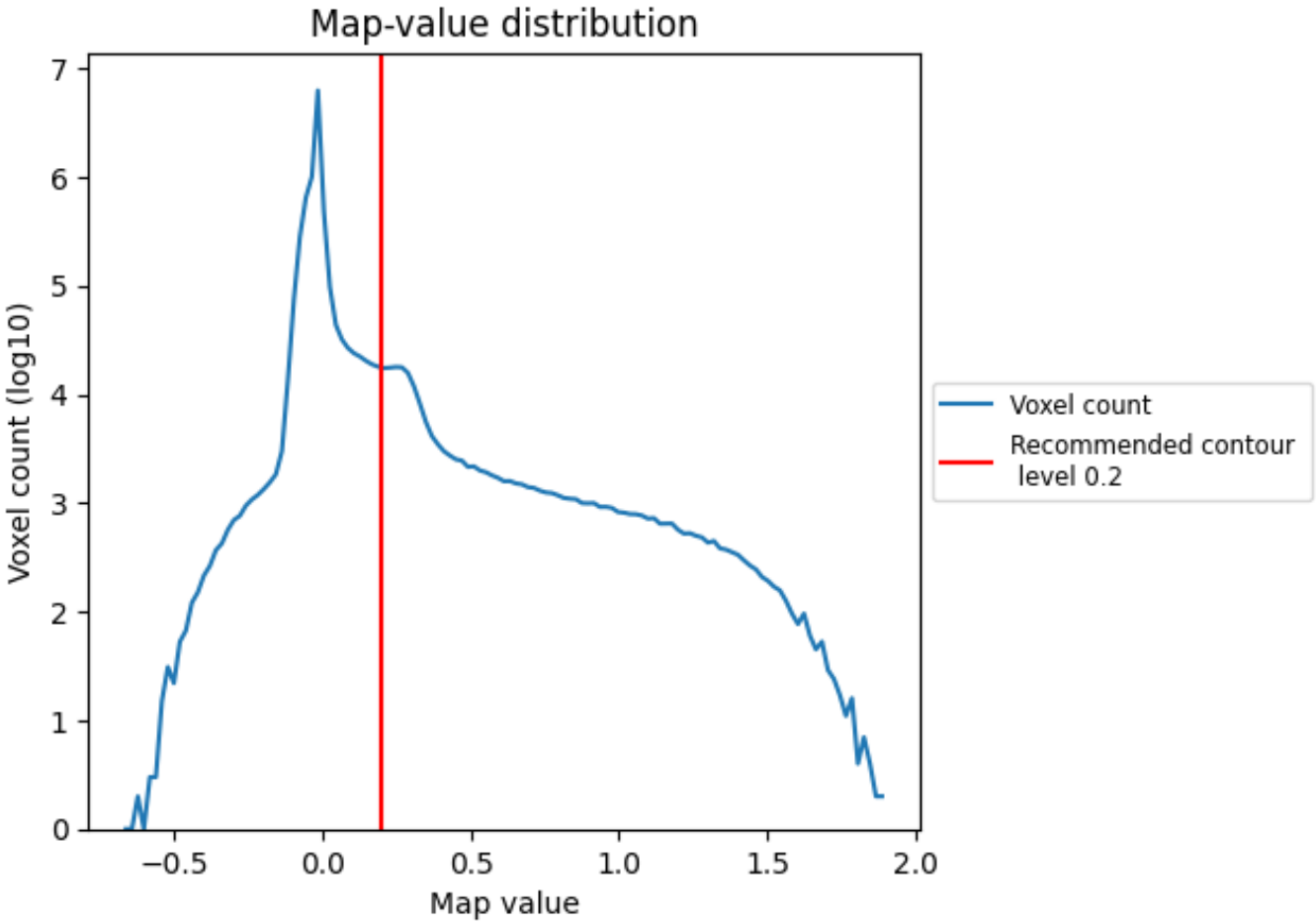


Z

7 Map analysis

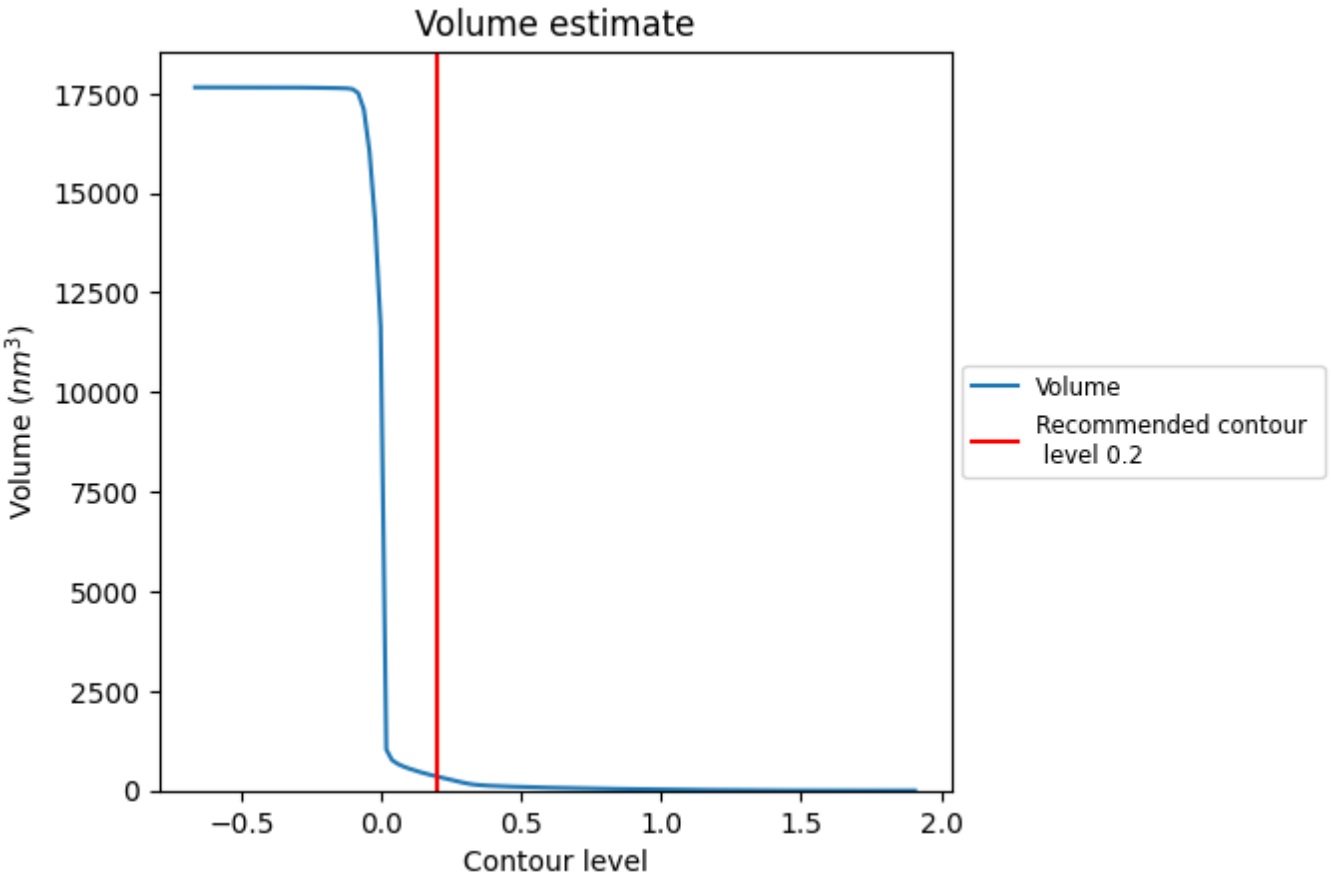
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

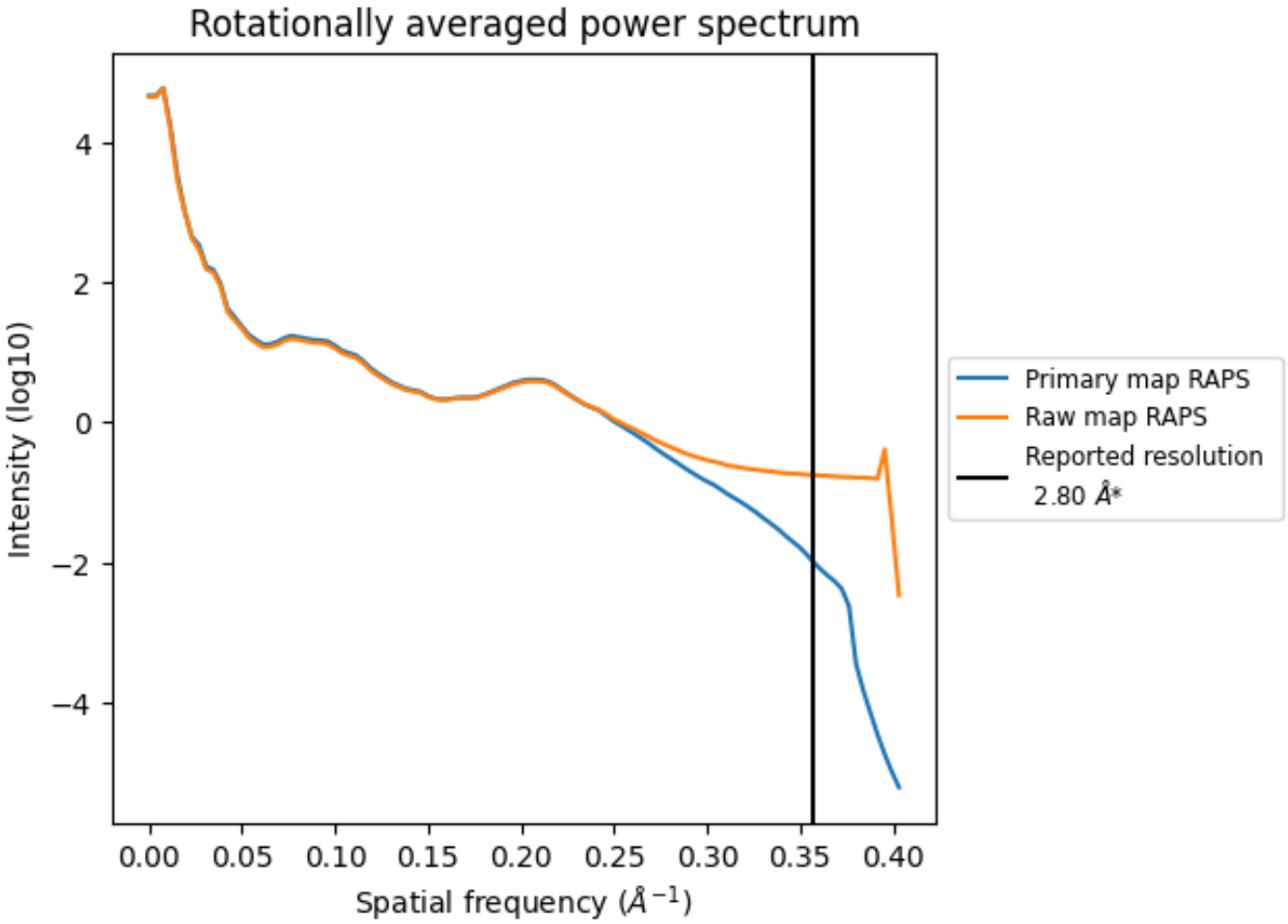
7.2 Volume estimate



The volume at the recommended contour level is 353 nm^3; this corresponds to an approximate mass of 319 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)

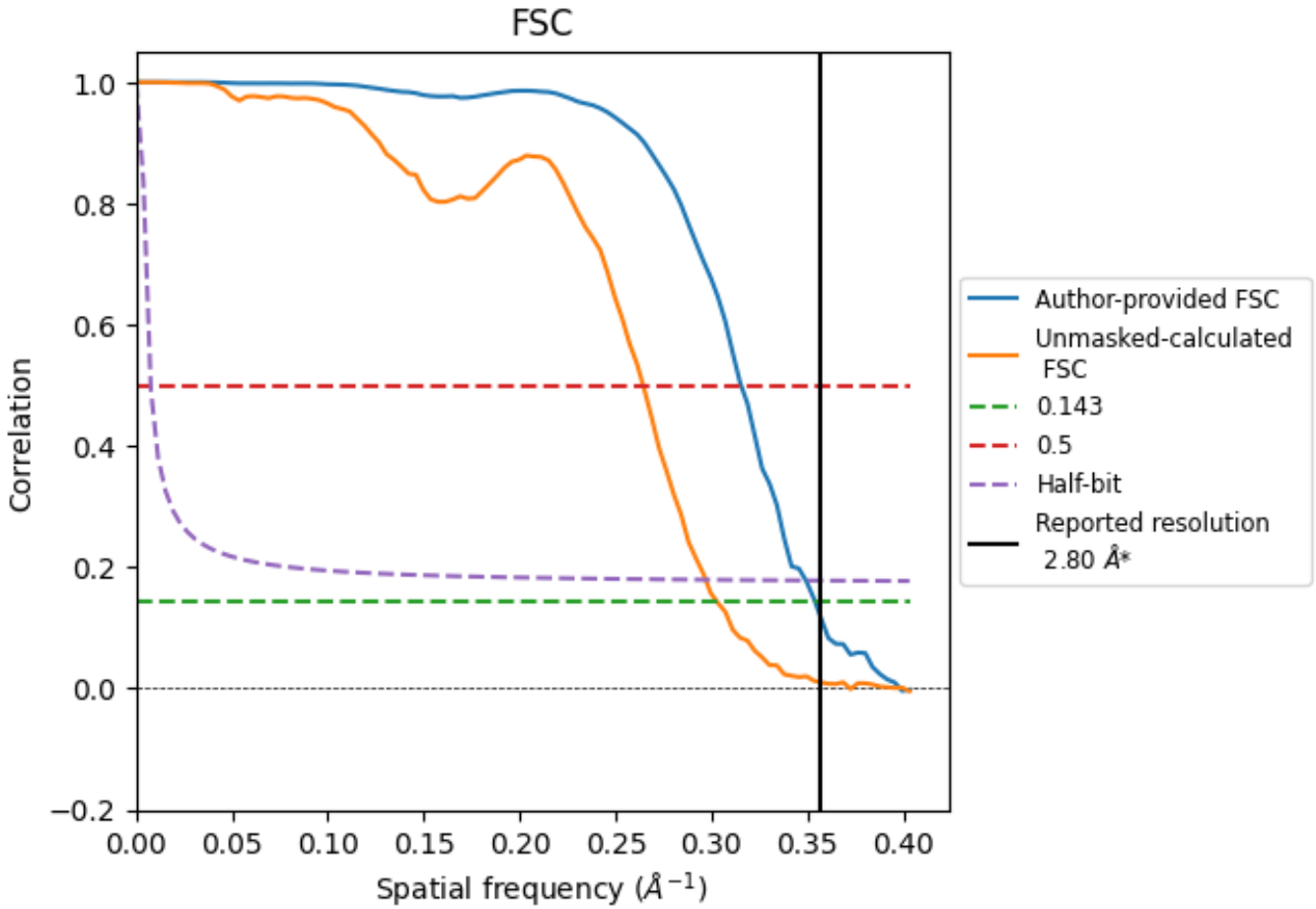


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

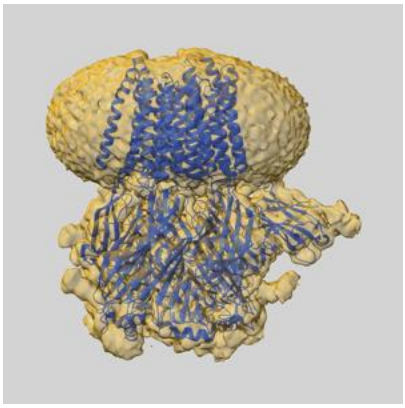
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.17	2.86
Unmasked-calculated*	3.30	3.78	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.8 by more than 10 %

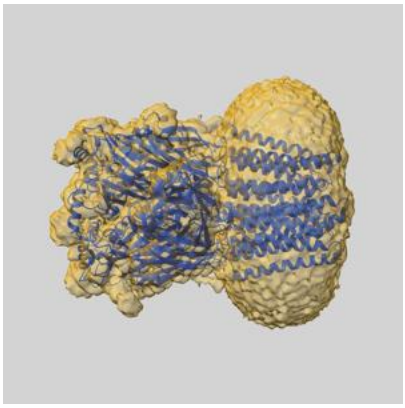
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50365 and PDB model 9FFL. Per-residue inclusion information can be found in section 3 on page 17.

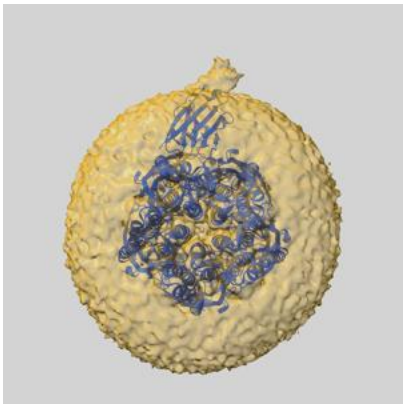
9.1 Map-model overlay



X



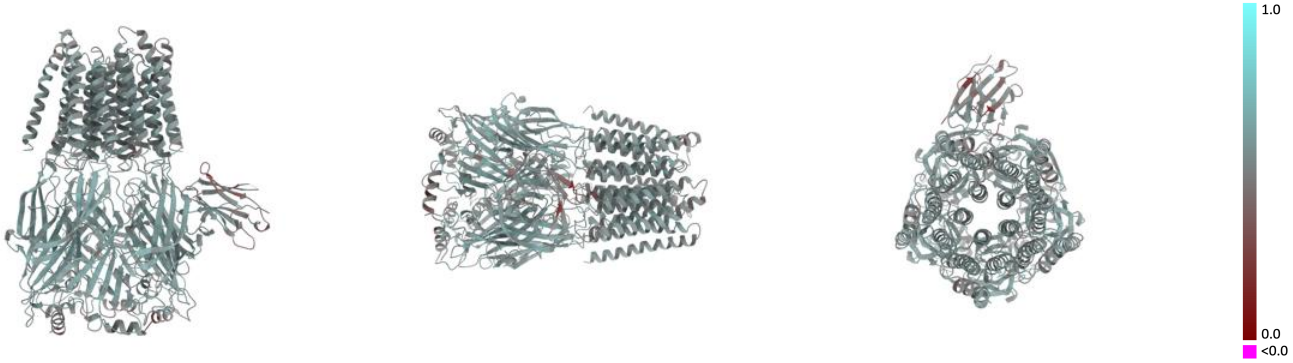
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

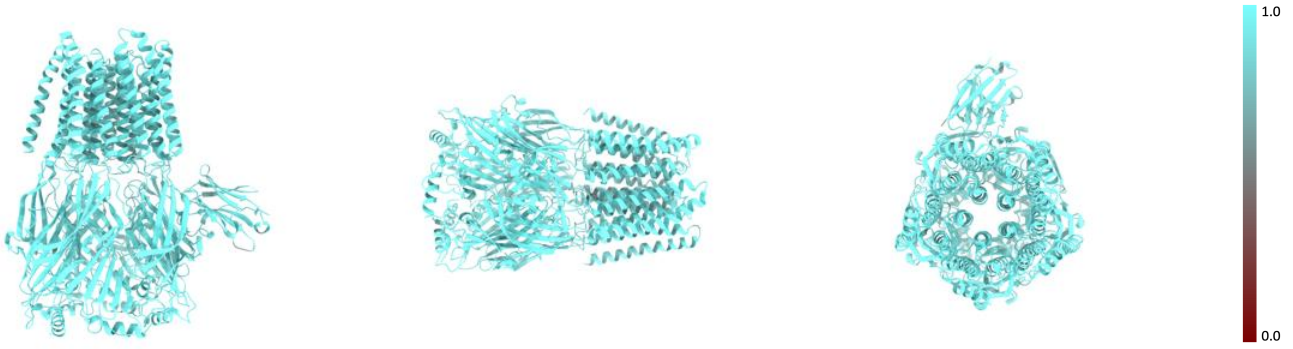
9.2 Q-score mapped to coordinate model (i)



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.

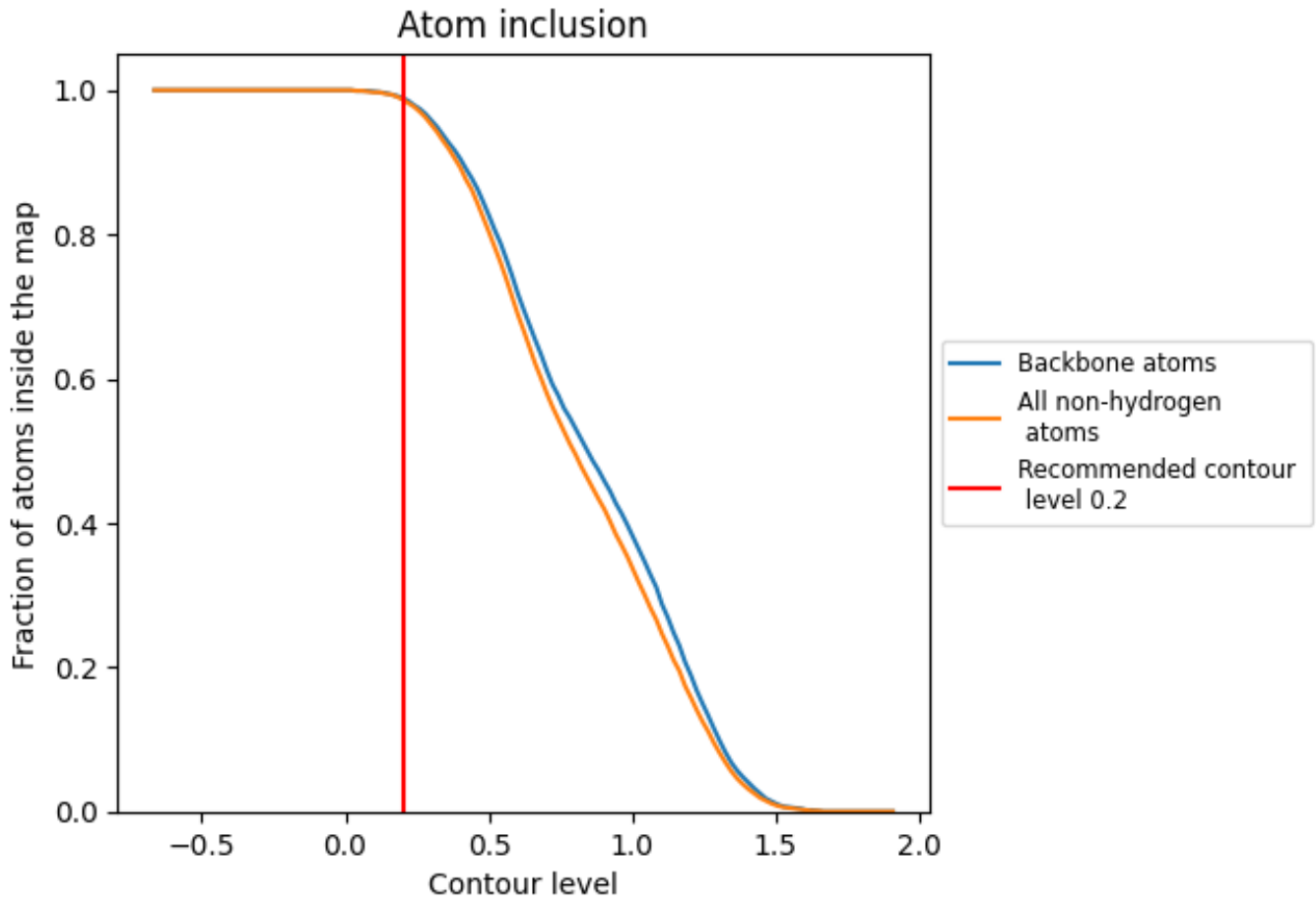
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9870	0.5430
A	0.9900	0.5490
B	0.9900	0.5460
C	0.9910	0.5460
D	0.9890	0.5500
E	0.9900	0.5500
F	0.9500	0.4800
G	1.0000	0.4820
H	1.0000	0.5230
I	1.0000	0.4620
a	1.0000	0.4930
b	1.0000	0.5340
c	1.0000	0.5320
d	0.9670	0.4640
e	1.0000	0.5430