Full wwPDB EM Validation Report

Mar 24, 2026 – 09:05 PM UTC

PDB ID	:	9HLC / pdb_00009hlc
EMDB ID	:	EMD-52250
Title	:	TRPML1 in complex with compound 11
Authors	:	Reeks, J.; Mahajan, P.; Clark, M.; Cowan, S.R.; Di Daniel, E.; Earl, C.P.; Fisher, S.; Holvey, R.S.; Jackson, S.M.; Lloyd-Evans, E.; Morgillo, C.M.; Mortenson, P.N.; O'Reilly, M.; Richardson, C.J.; Schopf, P.; Tams, D.M.; Waller-Evans, H.; Ward, S.E.; Whibley, S.; Williams, P.A.; Johnson, C.N.
Deposited on	:	2024-12-04
Resolution	:	2.10 Å(reported)
Based on initial model	:	.

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

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

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

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

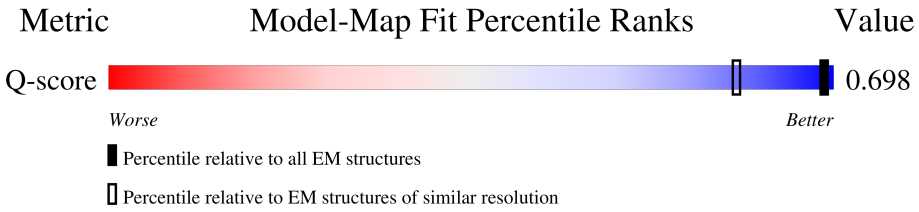
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	2317 (1.60 - 2.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15860 atoms, of which 104 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 Mucolipin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	458	Total	C	N	O	S	2	0
			3707	2431	615	636	25		
1	B	458	Total	C	N	O	S	2	0
			3707	2431	615	636	25		
1	C	458	Total	C	N	O	S	2	0
			3707	2431	615	636	25		
1	D	458	Total	C	N	O	S	2	0
			3707	2431	615	636	25		

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-47	MET	-	initiating methionine	UNP Q9GZU1
A	-46	HIS	-	expression tag	UNP Q9GZU1
A	-45	HIS	-	expression tag	UNP Q9GZU1
A	-44	HIS	-	expression tag	UNP Q9GZU1
A	-43	HIS	-	expression tag	UNP Q9GZU1
A	-42	HIS	-	expression tag	UNP Q9GZU1
A	-41	HIS	-	expression tag	UNP Q9GZU1
A	-40	HIS	-	expression tag	UNP Q9GZU1
A	-39	HIS	-	expression tag	UNP Q9GZU1
A	-38	GLY	-	expression tag	UNP Q9GZU1
A	-37	GLY	-	expression tag	UNP Q9GZU1
A	-36	SER	-	expression tag	UNP Q9GZU1
A	-35	ASP	-	expression tag	UNP Q9GZU1
A	-34	TYR	-	expression tag	UNP Q9GZU1
A	-33	LYS	-	expression tag	UNP Q9GZU1
A	-32	ASP	-	expression tag	UNP Q9GZU1
A	-31	HIS	-	expression tag	UNP Q9GZU1
A	-30	ASP	-	expression tag	UNP Q9GZU1
A	-29	GLY	-	expression tag	UNP Q9GZU1
A	-28	ASP	-	expression tag	UNP Q9GZU1
A	-27	TYR	-	expression tag	UNP Q9GZU1
A	-26	LYS	-	expression tag	UNP Q9GZU1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	ASP	-	expression tag	UNP Q9GZU1
A	-24	HIS	-	expression tag	UNP Q9GZU1
A	-23	ASP	-	expression tag	UNP Q9GZU1
A	-22	ILE	-	expression tag	UNP Q9GZU1
A	-21	ASP	-	expression tag	UNP Q9GZU1
A	-20	TYR	-	expression tag	UNP Q9GZU1
A	-19	LYS	-	expression tag	UNP Q9GZU1
A	-18	ASP	-	expression tag	UNP Q9GZU1
A	-17	ASP	-	expression tag	UNP Q9GZU1
A	-16	ASP	-	expression tag	UNP Q9GZU1
A	-15	ASP	-	expression tag	UNP Q9GZU1
A	-14	LYS	-	expression tag	UNP Q9GZU1
A	-13	GLY	-	expression tag	UNP Q9GZU1
A	-12	GLY	-	expression tag	UNP Q9GZU1
A	-11	SER	-	expression tag	UNP Q9GZU1
A	-10	GLY	-	expression tag	UNP Q9GZU1
A	-9	GLY	-	expression tag	UNP Q9GZU1
A	-8	SER	-	expression tag	UNP Q9GZU1
A	-7	GLU	-	expression tag	UNP Q9GZU1
A	-6	ASN	-	expression tag	UNP Q9GZU1
A	-5	LEU	-	expression tag	UNP Q9GZU1
A	-4	TYR	-	expression tag	UNP Q9GZU1
A	-3	PHE	-	expression tag	UNP Q9GZU1
A	-2	GLN	-	expression tag	UNP Q9GZU1
A	-1	GLY	-	expression tag	UNP Q9GZU1
A	0	PRO	-	expression tag	UNP Q9GZU1
A	1	GLY	-	expression tag	UNP Q9GZU1
B	-47	MET	-	initiating methionine	UNP Q9GZU1
B	-46	HIS	-	expression tag	UNP Q9GZU1
B	-45	HIS	-	expression tag	UNP Q9GZU1
B	-44	HIS	-	expression tag	UNP Q9GZU1
B	-43	HIS	-	expression tag	UNP Q9GZU1
B	-42	HIS	-	expression tag	UNP Q9GZU1
B	-41	HIS	-	expression tag	UNP Q9GZU1
B	-40	HIS	-	expression tag	UNP Q9GZU1
B	-39	HIS	-	expression tag	UNP Q9GZU1
B	-38	GLY	-	expression tag	UNP Q9GZU1
B	-37	GLY	-	expression tag	UNP Q9GZU1
B	-36	SER	-	expression tag	UNP Q9GZU1
B	-35	ASP	-	expression tag	UNP Q9GZU1
B	-34	TYR	-	expression tag	UNP Q9GZU1
B	-33	LYS	-	expression tag	UNP Q9GZU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	ASP	-	expression tag	UNP Q9GZU1
B	-31	HIS	-	expression tag	UNP Q9GZU1
B	-30	ASP	-	expression tag	UNP Q9GZU1
B	-29	GLY	-	expression tag	UNP Q9GZU1
B	-28	ASP	-	expression tag	UNP Q9GZU1
B	-27	TYR	-	expression tag	UNP Q9GZU1
B	-26	LYS	-	expression tag	UNP Q9GZU1
B	-25	ASP	-	expression tag	UNP Q9GZU1
B	-24	HIS	-	expression tag	UNP Q9GZU1
B	-23	ASP	-	expression tag	UNP Q9GZU1
B	-22	ILE	-	expression tag	UNP Q9GZU1
B	-21	ASP	-	expression tag	UNP Q9GZU1
B	-20	TYR	-	expression tag	UNP Q9GZU1
B	-19	LYS	-	expression tag	UNP Q9GZU1
B	-18	ASP	-	expression tag	UNP Q9GZU1
B	-17	ASP	-	expression tag	UNP Q9GZU1
B	-16	ASP	-	expression tag	UNP Q9GZU1
B	-15	ASP	-	expression tag	UNP Q9GZU1
B	-14	LYS	-	expression tag	UNP Q9GZU1
B	-13	GLY	-	expression tag	UNP Q9GZU1
B	-12	GLY	-	expression tag	UNP Q9GZU1
B	-11	SER	-	expression tag	UNP Q9GZU1
B	-10	GLY	-	expression tag	UNP Q9GZU1
B	-9	GLY	-	expression tag	UNP Q9GZU1
B	-8	SER	-	expression tag	UNP Q9GZU1
B	-7	GLU	-	expression tag	UNP Q9GZU1
B	-6	ASN	-	expression tag	UNP Q9GZU1
B	-5	LEU	-	expression tag	UNP Q9GZU1
B	-4	TYR	-	expression tag	UNP Q9GZU1
B	-3	PHE	-	expression tag	UNP Q9GZU1
B	-2	GLN	-	expression tag	UNP Q9GZU1
B	-1	GLY	-	expression tag	UNP Q9GZU1
B	0	PRO	-	expression tag	UNP Q9GZU1
B	1	GLY	-	expression tag	UNP Q9GZU1
C	-47	MET	-	initiating methionine	UNP Q9GZU1
C	-46	HIS	-	expression tag	UNP Q9GZU1
C	-45	HIS	-	expression tag	UNP Q9GZU1
C	-44	HIS	-	expression tag	UNP Q9GZU1
C	-43	HIS	-	expression tag	UNP Q9GZU1
C	-42	HIS	-	expression tag	UNP Q9GZU1
C	-41	HIS	-	expression tag	UNP Q9GZU1
C	-40	HIS	-	expression tag	UNP Q9GZU1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-39	HIS	-	expression tag	UNP Q9GZU1
C	-38	GLY	-	expression tag	UNP Q9GZU1
C	-37	GLY	-	expression tag	UNP Q9GZU1
C	-36	SER	-	expression tag	UNP Q9GZU1
C	-35	ASP	-	expression tag	UNP Q9GZU1
C	-34	TYR	-	expression tag	UNP Q9GZU1
C	-33	LYS	-	expression tag	UNP Q9GZU1
C	-32	ASP	-	expression tag	UNP Q9GZU1
C	-31	HIS	-	expression tag	UNP Q9GZU1
C	-30	ASP	-	expression tag	UNP Q9GZU1
C	-29	GLY	-	expression tag	UNP Q9GZU1
C	-28	ASP	-	expression tag	UNP Q9GZU1
C	-27	TYR	-	expression tag	UNP Q9GZU1
C	-26	LYS	-	expression tag	UNP Q9GZU1
C	-25	ASP	-	expression tag	UNP Q9GZU1
C	-24	HIS	-	expression tag	UNP Q9GZU1
C	-23	ASP	-	expression tag	UNP Q9GZU1
C	-22	ILE	-	expression tag	UNP Q9GZU1
C	-21	ASP	-	expression tag	UNP Q9GZU1
C	-20	TYR	-	expression tag	UNP Q9GZU1
C	-19	LYS	-	expression tag	UNP Q9GZU1
C	-18	ASP	-	expression tag	UNP Q9GZU1
C	-17	ASP	-	expression tag	UNP Q9GZU1
C	-16	ASP	-	expression tag	UNP Q9GZU1
C	-15	ASP	-	expression tag	UNP Q9GZU1
C	-14	LYS	-	expression tag	UNP Q9GZU1
C	-13	GLY	-	expression tag	UNP Q9GZU1
C	-12	GLY	-	expression tag	UNP Q9GZU1
C	-11	SER	-	expression tag	UNP Q9GZU1
C	-10	GLY	-	expression tag	UNP Q9GZU1
C	-9	GLY	-	expression tag	UNP Q9GZU1
C	-8	SER	-	expression tag	UNP Q9GZU1
C	-7	GLU	-	expression tag	UNP Q9GZU1
C	-6	ASN	-	expression tag	UNP Q9GZU1
C	-5	LEU	-	expression tag	UNP Q9GZU1
C	-4	TYR	-	expression tag	UNP Q9GZU1
C	-3	PHE	-	expression tag	UNP Q9GZU1
C	-2	GLN	-	expression tag	UNP Q9GZU1
C	-1	GLY	-	expression tag	UNP Q9GZU1
C	0	PRO	-	expression tag	UNP Q9GZU1
C	1	GLY	-	expression tag	UNP Q9GZU1
D	-47	MET	-	initiating methionine	UNP Q9GZU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-46	HIS	-	expression tag	UNP Q9GZU1
D	-45	HIS	-	expression tag	UNP Q9GZU1
D	-44	HIS	-	expression tag	UNP Q9GZU1
D	-43	HIS	-	expression tag	UNP Q9GZU1
D	-42	HIS	-	expression tag	UNP Q9GZU1
D	-41	HIS	-	expression tag	UNP Q9GZU1
D	-40	HIS	-	expression tag	UNP Q9GZU1
D	-39	HIS	-	expression tag	UNP Q9GZU1
D	-38	GLY	-	expression tag	UNP Q9GZU1
D	-37	GLY	-	expression tag	UNP Q9GZU1
D	-36	SER	-	expression tag	UNP Q9GZU1
D	-35	ASP	-	expression tag	UNP Q9GZU1
D	-34	TYR	-	expression tag	UNP Q9GZU1
D	-33	LYS	-	expression tag	UNP Q9GZU1
D	-32	ASP	-	expression tag	UNP Q9GZU1
D	-31	HIS	-	expression tag	UNP Q9GZU1
D	-30	ASP	-	expression tag	UNP Q9GZU1
D	-29	GLY	-	expression tag	UNP Q9GZU1
D	-28	ASP	-	expression tag	UNP Q9GZU1
D	-27	TYR	-	expression tag	UNP Q9GZU1
D	-26	LYS	-	expression tag	UNP Q9GZU1
D	-25	ASP	-	expression tag	UNP Q9GZU1
D	-24	HIS	-	expression tag	UNP Q9GZU1
D	-23	ASP	-	expression tag	UNP Q9GZU1
D	-22	ILE	-	expression tag	UNP Q9GZU1
D	-21	ASP	-	expression tag	UNP Q9GZU1
D	-20	TYR	-	expression tag	UNP Q9GZU1
D	-19	LYS	-	expression tag	UNP Q9GZU1
D	-18	ASP	-	expression tag	UNP Q9GZU1
D	-17	ASP	-	expression tag	UNP Q9GZU1
D	-16	ASP	-	expression tag	UNP Q9GZU1
D	-15	ASP	-	expression tag	UNP Q9GZU1
D	-14	LYS	-	expression tag	UNP Q9GZU1
D	-13	GLY	-	expression tag	UNP Q9GZU1
D	-12	GLY	-	expression tag	UNP Q9GZU1
D	-11	SER	-	expression tag	UNP Q9GZU1
D	-10	GLY	-	expression tag	UNP Q9GZU1
D	-9	GLY	-	expression tag	UNP Q9GZU1
D	-8	SER	-	expression tag	UNP Q9GZU1
D	-7	GLU	-	expression tag	UNP Q9GZU1
D	-6	ASN	-	expression tag	UNP Q9GZU1
D	-5	LEU	-	expression tag	UNP Q9GZU1

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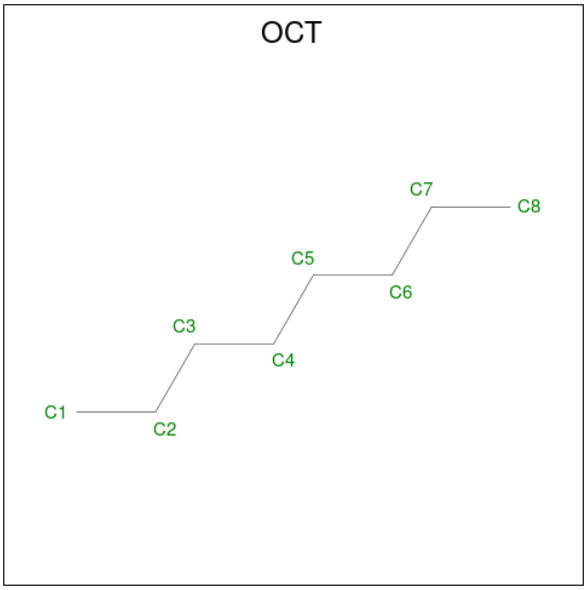
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	TYR	-	expression tag	UNP Q9GZU1
D	-3	PHE	-	expression tag	UNP Q9GZU1
D	-2	GLN	-	expression tag	UNP Q9GZU1
D	-1	GLY	-	expression tag	UNP Q9GZU1
D	0	PRO	-	expression tag	UNP Q9GZU1
D	1	GLY	-	expression tag	UNP Q9GZU1

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



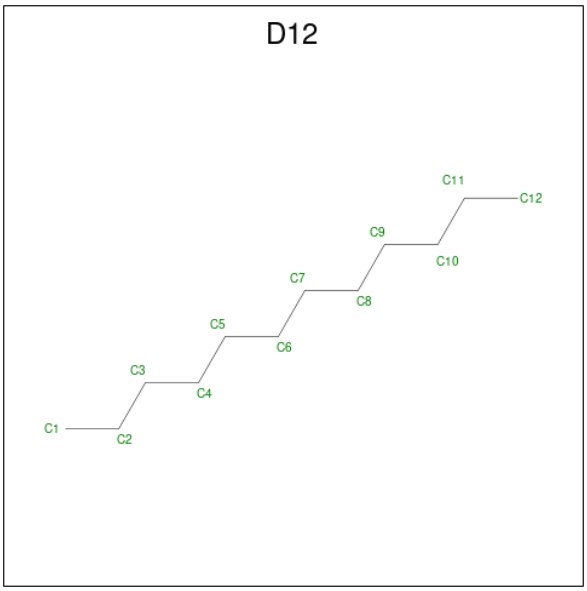
Mol	Chain	Residues	Atoms	AltConf	Trace
2	E	2	Total C N O 28 16 2 10	0	0
2	F	2	Total C N O 28 16 2 10	0	0
2	G	2	Total C N O 28 16 2 10	0	0
2	H	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C 8 8	0
3	A	1	Total C 8 8	0
3	B	1	Total C 8 8	0
3	B	1	Total C 8 8	0
3	C	1	Total C 8 8	0
3	C	1	Total C 8 8	0
3	D	1	Total C 8 8	0
3	D	1	Total C 8 8	0

- Molecule 4 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



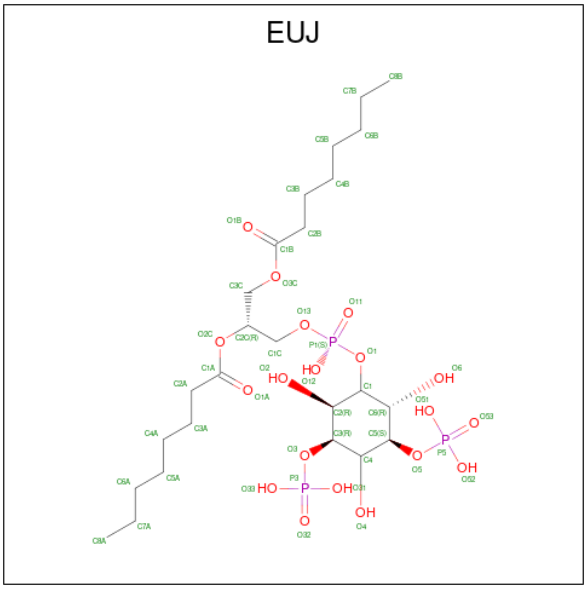
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 12 12	0
4	A	1	Total C 12 12	0
4	B	1	Total C 12 12	0
4	B	1	Total C 12 12	0

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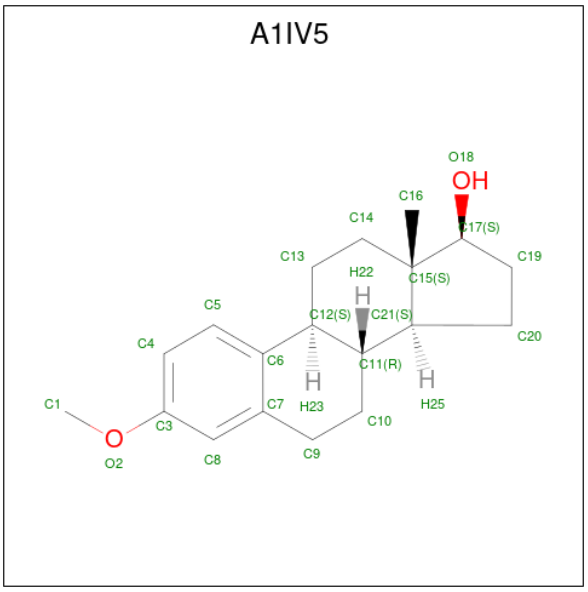
Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total C 12 12	0
4	C	1	Total C 12 12	0
4	D	1	Total C 12 12	0
4	D	1	Total C 12 12	0

- Molecule 5 is (2R)-3-{[(S)-hydroxy{[(1S,2R,3R,4S,5S,6R)-2,4,6-trihydroxy-3,5-bis(phosphonooxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dioctanoate (CCD ID: EUJ) (formula: $C_{25}H_{49}O_{19}P_3$).



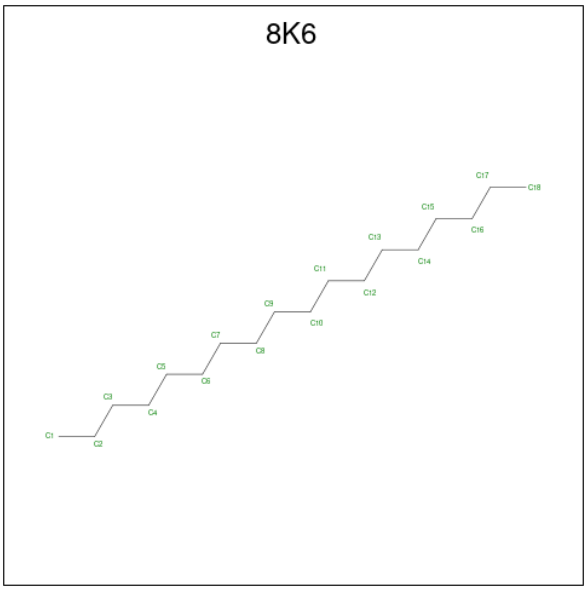
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O P 47 25 19 3	0
5	B	1	Total C O P 47 25 19 3	0
5	C	1	Total C O P 47 25 19 3	0
5	D	1	Total C O P 47 25 19 3	0

- Molecule 6 is (8R,9S,13S,14S,17S)-3-methoxy-13-methyl-6,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-17-ol (CCD ID: A1IV5) (formula: $C_{19}H_{26}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	H	O	0
			47	19	26	2	
6	B	1	Total	C	H	O	0
			47	19	26	2	
6	C	1	Total	C	H	O	0
			47	19	26	2	
6	D	1	Total	C	H	O	0
			47	19	26	2	

- Molecule 7 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 18 18	0
7	B	1	Total C 18 18	0
7	C	1	Total C 18 18	0
7	D	1	Total C 18 18	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	AltConf
8	A	78	Total O 78 78	0
8	B	78	Total O 78 78	0
8	C	78	Total O 78 78	0
8	D	78	Total O 78 78	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	190155	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 ($e^-/Å^2$)	43.81	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.571	Depositor
Minimum map value	-1.434	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.397	Depositor
Map size (Å)	379.42902, 379.42902, 379.42902	wwPDB
Map dimensions	590, 590, 590	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6431, 0.6431, 0.6431	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	1,2	14,14,15	0.78	0	17,19,21	1.68	3 (17%)
2	NAG	E	2	2	14,14,15	0.79	0	17,19,21	1.23	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.79	0	17,19,21	1.70	3 (17%)
2	NAG	F	2	2	14,14,15	0.80	0	17,19,21	1.23	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.79	0	17,19,21	1.68	3 (17%)
2	NAG	G	2	2	14,14,15	0.79	0	17,19,21	1.24	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.80	0	17,19,21	1.69	3 (17%)
2	NAG	H	2	2	14,14,15	0.79	0	17,19,21	1.23	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C1-O5-C5	4.52	118.25	112.19
2	H	1	NAG	C1-O5-C5	4.42	118.11	112.19
2	G	1	NAG	C1-O5-C5	4.41	118.09	112.19
2	E	1	NAG	C1-O5-C5	4.39	118.07	112.19
2	H	1	NAG	C2-N2-C7	3.55	127.65	122.90
2	F	1	NAG	C2-N2-C7	3.53	127.63	122.90
2	F	2	NAG	C2-N2-C7	3.52	127.61	122.90
2	E	1	NAG	C2-N2-C7	3.51	127.61	122.90
2	G	1	NAG	C2-N2-C7	3.48	127.57	122.90
2	H	2	NAG	C2-N2-C7	3.48	127.56	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C2-N2-C7	3.47	127.56	122.90
2	G	2	NAG	C2-N2-C7	3.44	127.51	122.90
2	G	1	NAG	O4-C4-C5	2.42	115.28	109.32
2	E	1	NAG	O4-C4-C5	2.39	115.20	109.32
2	F	1	NAG	O4-C4-C5	2.38	115.19	109.32
2	H	1	NAG	O4-C4-C5	2.38	115.18	109.32
2	G	2	NAG	O5-C1-C2	-2.04	108.13	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

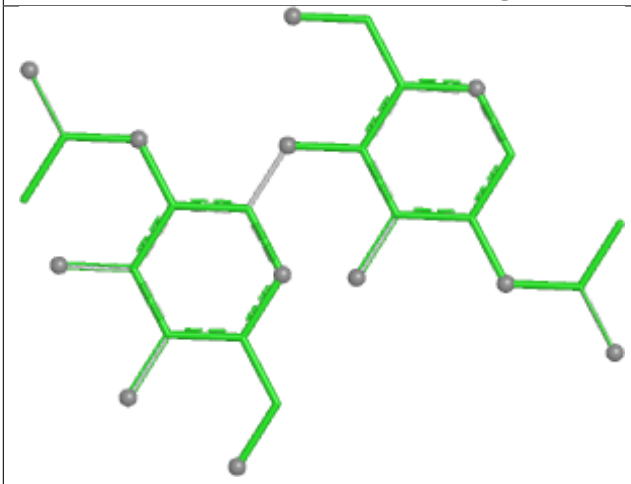
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2

There are no ring outliers.

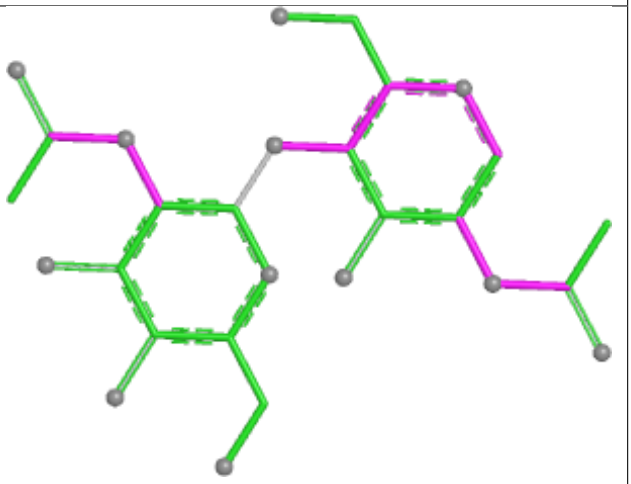
No monomer is involved in short contacts.

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

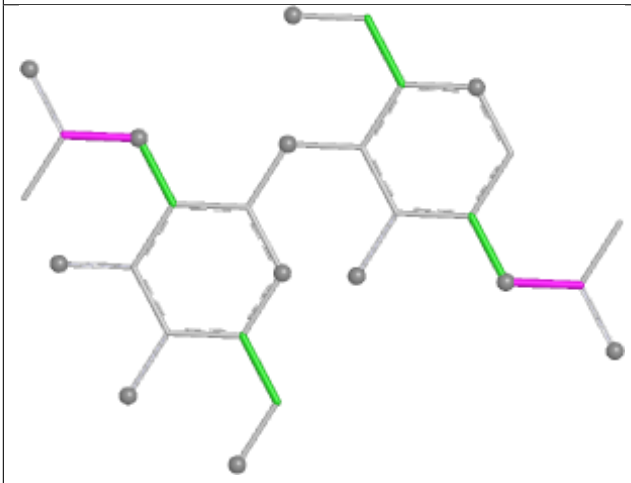
Oligosaccharide Chain E



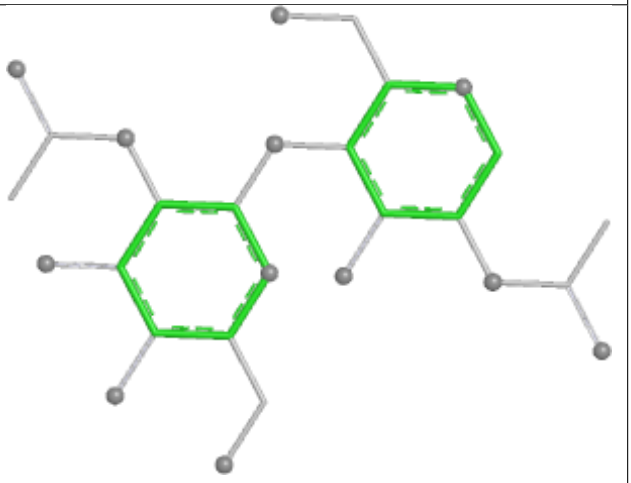
Bond lengths



Bond angles

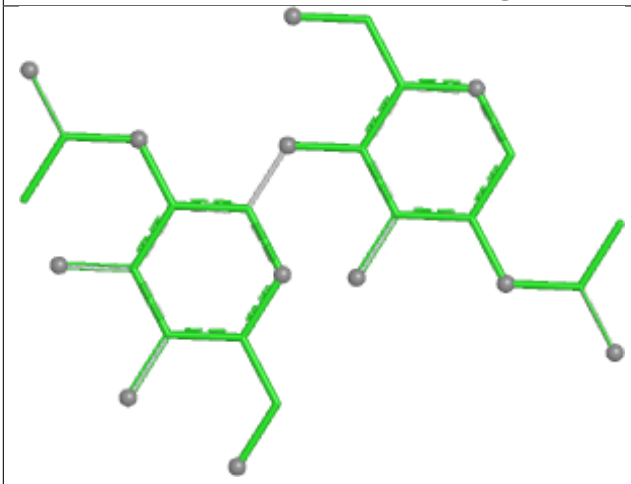


Torsions

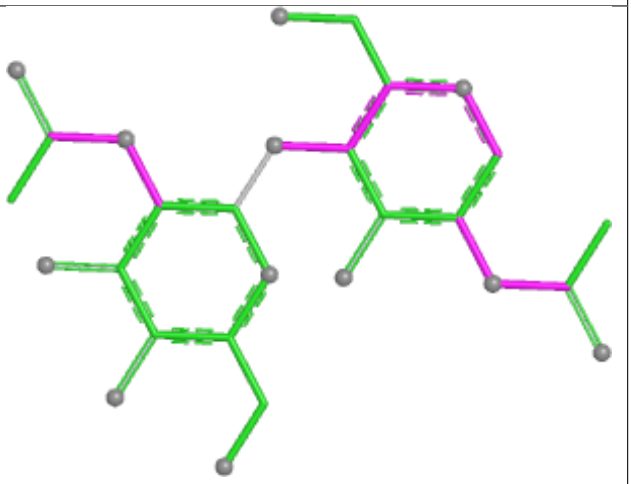


Rings

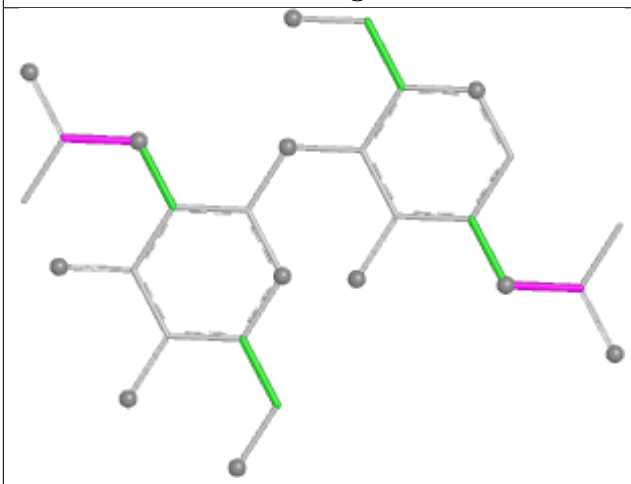
Oligosaccharide Chain F



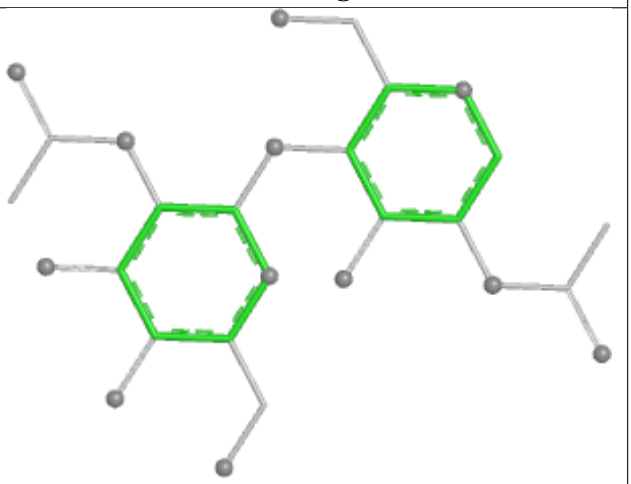
Bond lengths



Bond angles

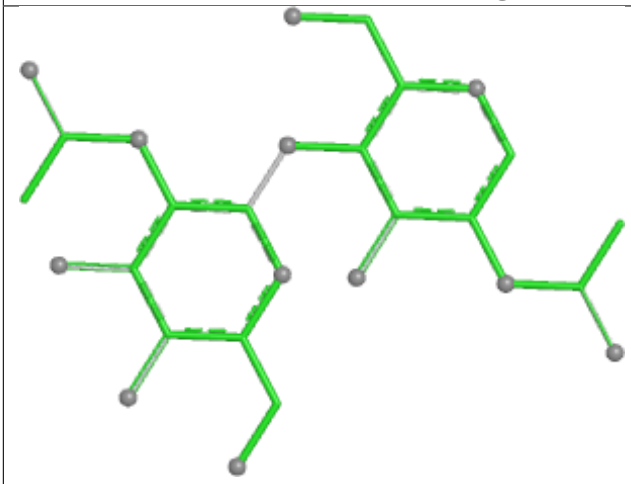


Torsions

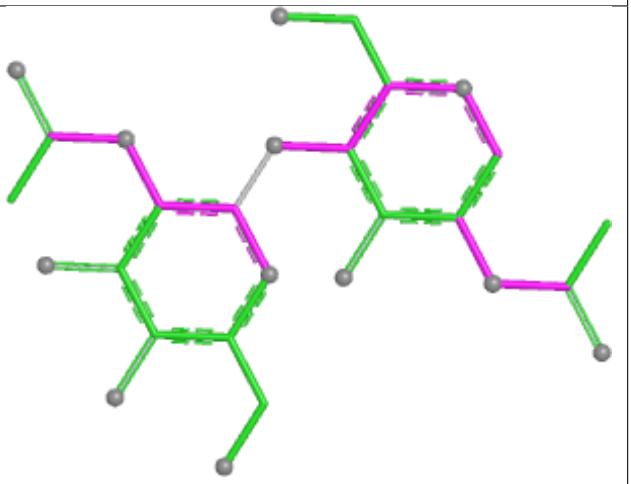


Rings

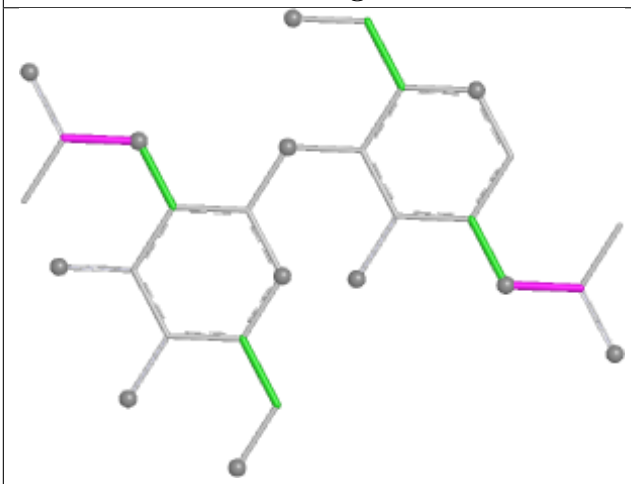
Oligosaccharide Chain G



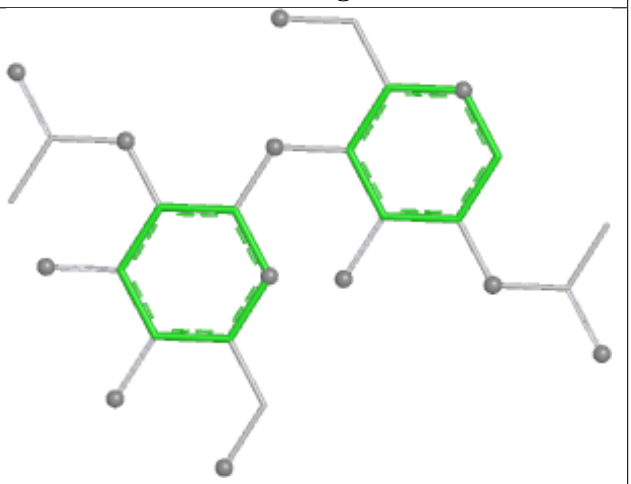
Bond lengths



Bond angles

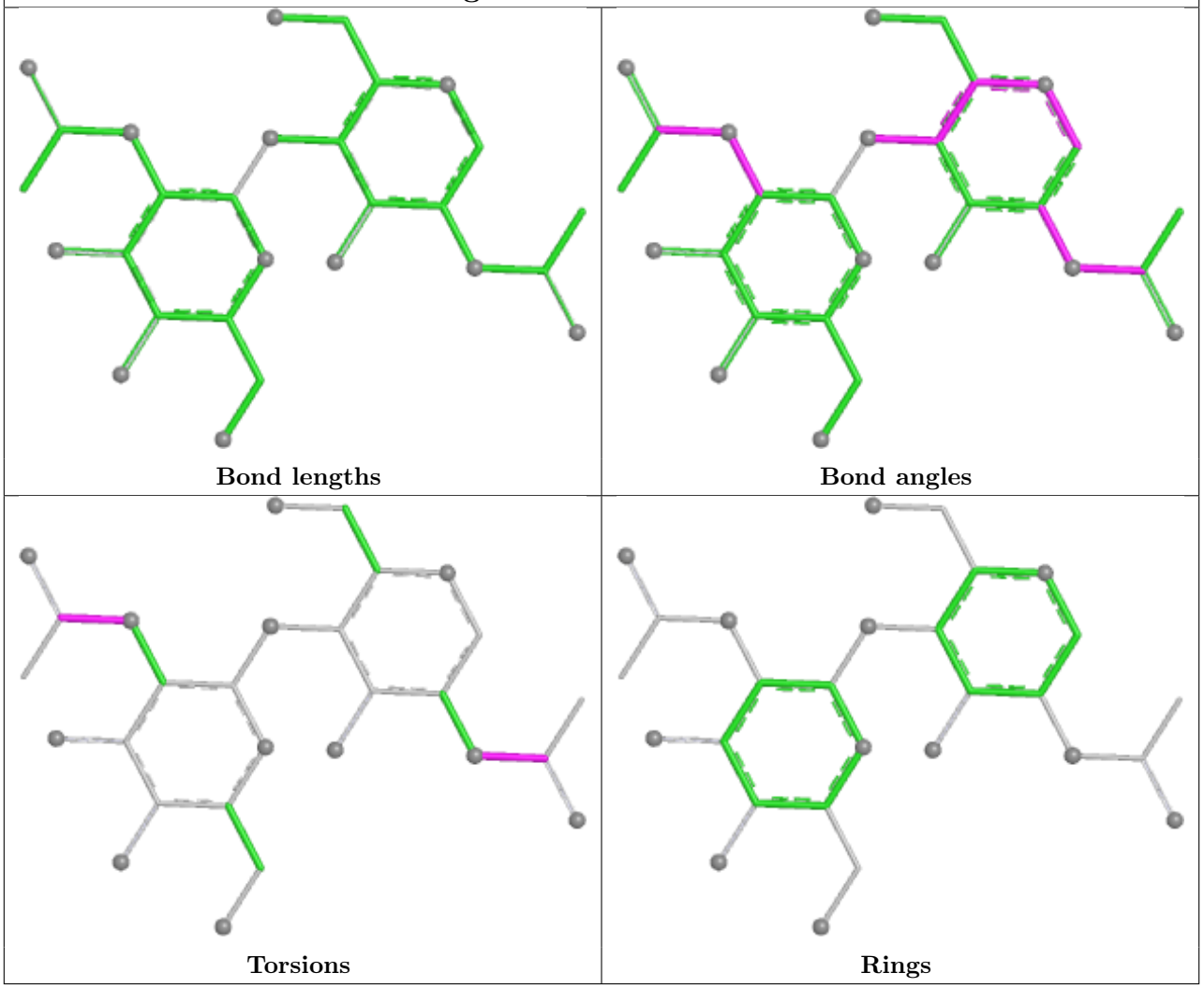


Torsions



Rings

Oligosaccharide Chain H



4.6 Ligand geometry (i)

28 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	D12	C	602	-	11,11,11	0.23	0	10,10,10	0.15	0
5	EUJ	A	604	-	47,47,47	0.49	0	62,65,65	0.40	0
5	EUJ	B	606	-	47,47,47	0.49	0	62,65,65	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	D12	D	603	-	11,11,11	0.23	0	10,10,10	0.15	0
4	D12	D	606	-	11,11,11	0.23	0	10,10,10	0.14	0
6	A1IV5	A	605	-	24,24,24	0.46	0	37,37,37	0.84	0
4	D12	B	602	-	11,11,11	0.23	0	10,10,10	0.15	0
3	OCT	C	603	-	7,7,7	0.23	0	6,6,6	0.16	0
6	A1IV5	D	601	-	24,24,24	0.46	0	37,37,37	0.84	0
3	OCT	B	603	-	7,7,7	0.23	0	6,6,6	0.16	0
7	8K6	B	601	-	17,17,17	0.22	0	16,16,16	0.19	0
7	8K6	C	601	-	17,17,17	0.22	0	16,16,16	0.19	0
3	OCT	B	604	-	7,7,7	0.23	0	6,6,6	0.19	0
4	D12	B	605	-	11,11,11	0.23	0	10,10,10	0.14	0
3	OCT	D	604	-	7,7,7	0.23	0	6,6,6	0.17	0
3	OCT	D	605	-	7,7,7	0.23	0	6,6,6	0.19	0
3	OCT	A	601	-	7,7,7	0.23	0	6,6,6	0.16	0
5	EUJ	C	606	-	47,47,47	0.49	0	62,65,65	0.41	0
3	OCT	A	602	-	7,7,7	0.23	0	6,6,6	0.19	0
4	D12	A	607	-	11,11,11	0.23	0	10,10,10	0.15	0
4	D12	A	603	-	11,11,11	0.23	0	10,10,10	0.14	0
5	EUJ	D	607	-	47,47,47	0.49	0	62,65,65	0.40	0
6	A1IV5	B	607	-	24,24,24	0.46	0	37,37,37	0.84	0
7	8K6	A	606	-	17,17,17	0.22	0	16,16,16	0.19	0
6	A1IV5	C	607	-	24,24,24	0.45	0	37,37,37	0.84	0
3	OCT	C	604	-	7,7,7	0.23	0	6,6,6	0.19	0
7	8K6	D	602	-	17,17,17	0.22	0	16,16,16	0.19	0
4	D12	C	605	-	11,11,11	0.23	0	10,10,10	0.14	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	D12	C	602	-	-	3/9/9/9	-
5	EUJ	A	604	-	-	5/44/68/68	0/1/1/1
5	EUJ	B	606	-	-	5/44/68/68	0/1/1/1
4	D12	D	603	-	-	3/9/9/9	-
4	D12	D	606	-	-	6/9/9/9	-
6	A1IV5	A	605	-	-	0/2/42/42	0/4/4/4
4	D12	B	602	-	-	3/9/9/9	-
3	OCT	C	603	-	-	2/5/5/5	-
6	A1IV5	D	601	-	-	0/2/42/42	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCT	B	603	-	-	1/5/5/5	-
7	8K6	B	601	-	-	6/15/15/15	-
7	8K6	C	601	-	-	6/15/15/15	-
3	OCT	B	604	-	-	2/5/5/5	-
4	D12	B	605	-	-	5/9/9/9	-
3	OCT	D	604	-	-	2/5/5/5	-
3	OCT	D	605	-	-	2/5/5/5	-
3	OCT	A	601	-	-	1/5/5/5	-
5	EUJ	C	606	-	-	6/44/68/68	0/1/1/1
3	OCT	A	602	-	-	2/5/5/5	-
4	D12	A	607	-	-	3/9/9/9	-
4	D12	A	603	-	-	6/9/9/9	-
5	EUJ	D	607	-	-	5/44/68/68	0/1/1/1
6	A1IV5	B	607	-	-	0/2/42/42	0/4/4/4
7	8K6	A	606	-	-	6/15/15/15	-
6	A1IV5	C	607	-	-	0/2/42/42	0/4/4/4
3	OCT	C	604	-	-	2/5/5/5	-
7	8K6	D	602	-	-	6/15/15/15	-
4	D12	C	605	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	606	EUJ	C1-O1-P1-O11
4	B	602	D12	C11-C10-C9-C8
4	A	607	D12	C11-C10-C9-C8
4	C	605	D12	C3-C4-C5-C6
4	C	602	D12	C11-C10-C9-C8
4	D	603	D12	C11-C10-C9-C8
4	A	603	D12	C3-C4-C5-C6
4	D	606	D12	C4-C5-C6-C7
4	A	603	D12	C4-C5-C6-C7
4	D	606	D12	C3-C4-C5-C6
4	B	605	D12	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	B	605	D12	C4-C5-C6-C7
4	C	605	D12	C4-C5-C6-C7
7	A	606	8K6	C13-C14-C15-C16
7	B	601	8K6	C13-C14-C15-C16
7	C	601	8K6	C13-C14-C15-C16
7	D	602	8K6	C13-C14-C15-C16
7	C	601	8K6	C3-C4-C5-C6
7	A	606	8K6	C3-C4-C5-C6
7	D	602	8K6	C3-C4-C5-C6
7	B	601	8K6	C3-C4-C5-C6
4	B	602	D12	C6-C7-C8-C9
4	C	602	D12	C6-C7-C8-C9
4	D	603	D12	C6-C7-C8-C9
4	A	607	D12	C6-C7-C8-C9
5	C	606	EUJ	C1C-C2C-C3C-O3C
4	B	605	D12	C5-C6-C7-C8
4	C	605	D12	C5-C6-C7-C8
4	D	606	D12	C5-C6-C7-C8
4	A	603	D12	C5-C6-C7-C8
5	A	604	EUJ	O2C-C2C-C3C-O3C
5	B	606	EUJ	O2C-C2C-C3C-O3C
5	C	606	EUJ	O2C-C2C-C3C-O3C
5	D	607	EUJ	O2C-C2C-C3C-O3C
7	D	602	8K6	C1-C2-C3-C4
3	A	601	OCT	C2-C3-C4-C5
7	A	606	8K6	C1-C2-C3-C4
7	C	601	8K6	C1-C2-C3-C4
3	B	603	OCT	C2-C3-C4-C5
3	C	604	OCT	C2-C3-C4-C5
3	D	605	OCT	C2-C3-C4-C5
3	A	602	OCT	C2-C3-C4-C5
3	B	604	OCT	C2-C3-C4-C5
7	B	601	8K6	C1-C2-C3-C4
3	C	603	OCT	C2-C3-C4-C5
5	A	604	EUJ	C1C-C2C-C3C-O3C
5	B	606	EUJ	C1C-C2C-C3C-O3C
5	D	607	EUJ	C1C-C2C-C3C-O3C
3	D	604	OCT	C2-C3-C4-C5
7	A	606	8K6	C11-C10-C9-C8
7	B	601	8K6	C11-C10-C9-C8
7	C	601	8K6	C11-C10-C9-C8
7	D	602	8K6	C11-C10-C9-C8

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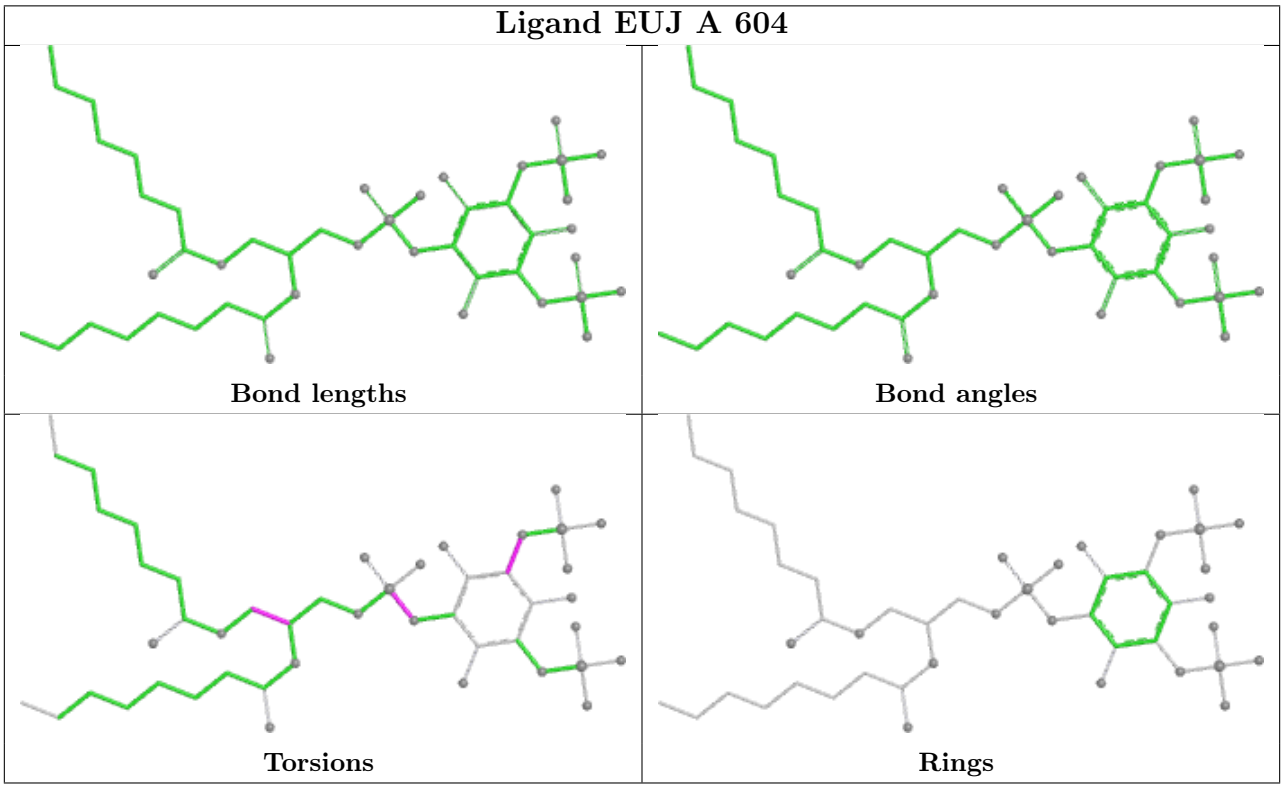
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Mol	Chain	Res	Type	Atoms
4	C	602	D12	C5-C6-C7-C8
4	A	607	D12	C5-C6-C7-C8
4	B	602	D12	C5-C6-C7-C8
4	D	603	D12	C5-C6-C7-C8
7	A	606	8K6	C15-C16-C17-C18
7	B	601	8K6	C15-C16-C17-C18
7	C	601	8K6	C15-C16-C17-C18
7	D	602	8K6	C15-C16-C17-C18
5	C	606	EUJ	C1B-C2B-C3B-C4B
5	A	604	EUJ	C2-C3-O3-P3
5	B	606	EUJ	C2-C3-O3-P3
5	C	606	EUJ	C2-C3-O3-P3
5	D	607	EUJ	C2-C3-O3-P3
4	B	605	D12	C6-C7-C8-C9
4	A	603	D12	C6-C7-C8-C9
4	D	606	D12	C6-C7-C8-C9
4	C	605	D12	C6-C7-C8-C9
5	A	604	EUJ	C4-C3-O3-P3
5	B	606	EUJ	C4-C3-O3-P3
5	C	606	EUJ	C4-C3-O3-P3
5	D	607	EUJ	C4-C3-O3-P3
5	A	604	EUJ	C1-O1-P1-O11
5	B	606	EUJ	C1-O1-P1-O11
5	D	607	EUJ	C1-O1-P1-O11
7	C	601	8K6	C11-C12-C13-C14
7	D	602	8K6	C11-C12-C13-C14
7	B	601	8K6	C11-C12-C13-C14
4	B	605	D12	C1-C2-C3-C4
3	B	604	OCT	C4-C5-C6-C7
3	D	605	OCT	C4-C5-C6-C7
7	A	606	8K6	C11-C12-C13-C14
3	A	602	OCT	C4-C5-C6-C7
3	C	604	OCT	C4-C5-C6-C7
3	D	604	OCT	C4-C5-C6-C7
3	C	603	OCT	C4-C5-C6-C7
4	C	605	D12	C1-C2-C3-C4
4	A	603	D12	C2-C3-C4-C5
4	D	606	D12	C2-C3-C4-C5
4	D	606	D12	C1-C2-C3-C4
4	A	603	D12	C1-C2-C3-C4
4	C	605	D12	C2-C3-C4-C5

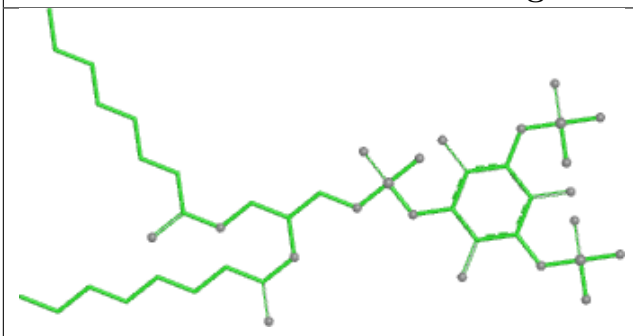
There are no ring outliers.

No monomer is involved in short contacts.

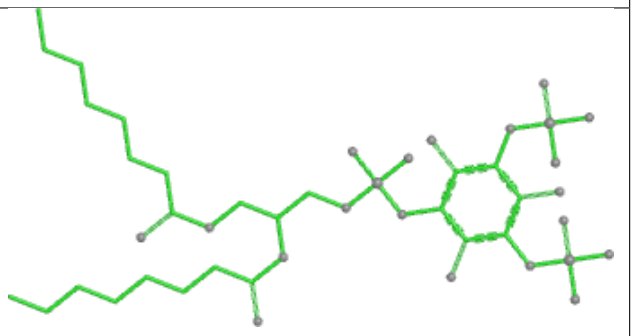
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



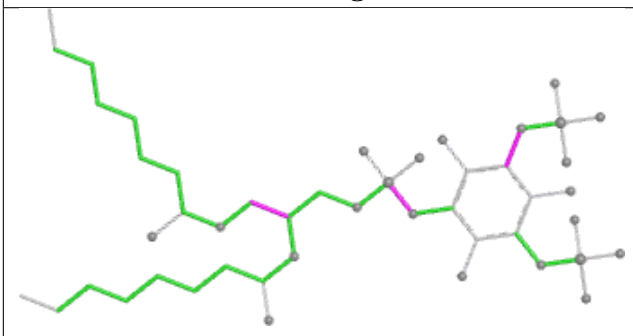
Ligand EUJ B 606



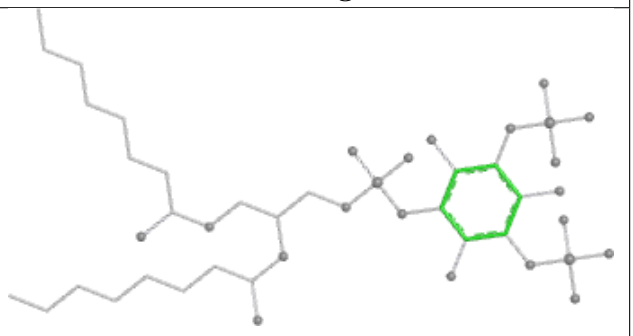
Bond lengths



Bond angles

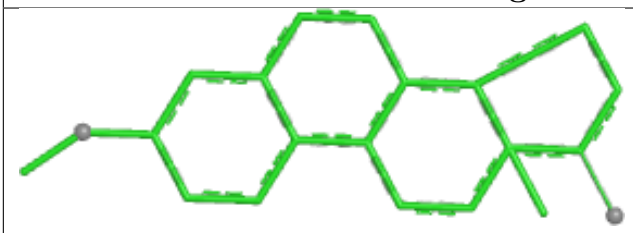


Torsions

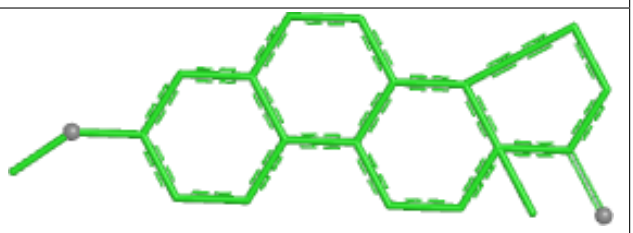


Rings

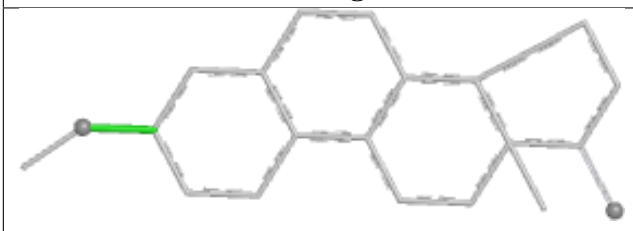
Ligand A1IV5 A 605



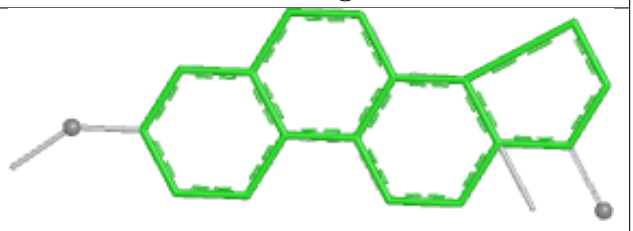
Bond lengths



Bond angles

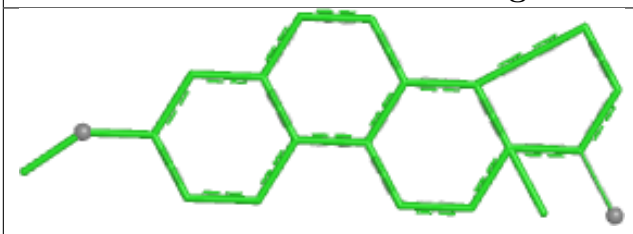


Torsions

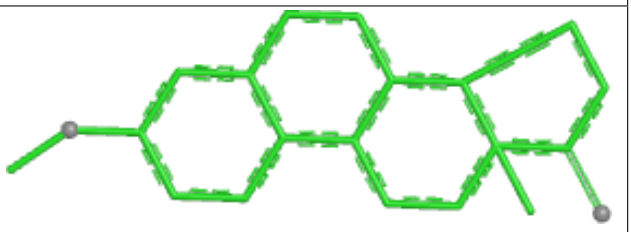


Rings

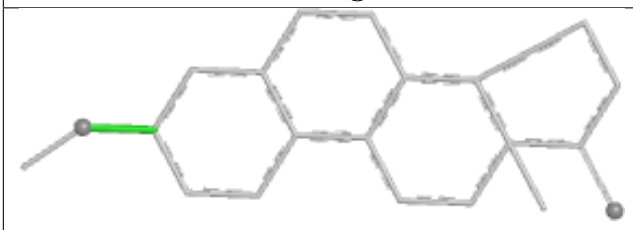
Ligand A1IV5 D 601



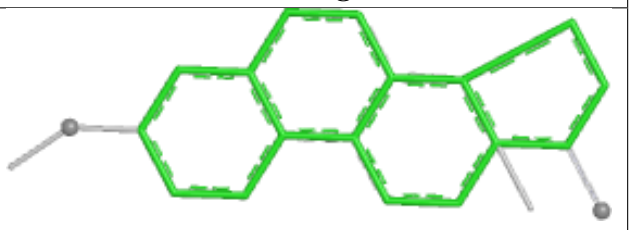
Bond lengths



Bond angles

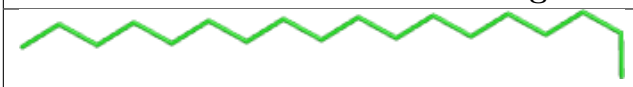


Torsions

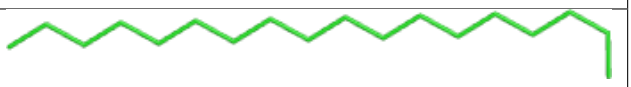


Rings

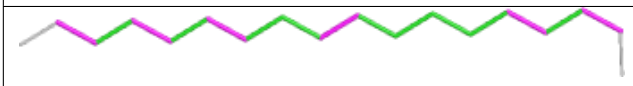
Ligand 8K6 B 601



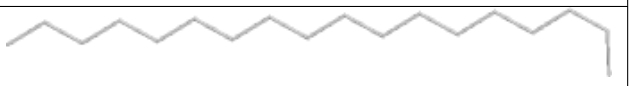
Bond lengths



Bond angles

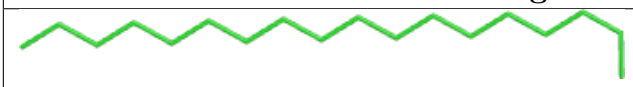


Torsions

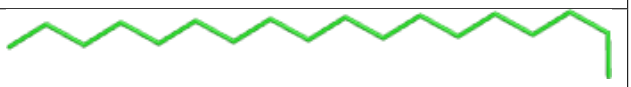


Rings

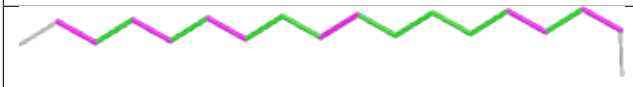
Ligand 8K6 C 601



Bond lengths



Bond angles

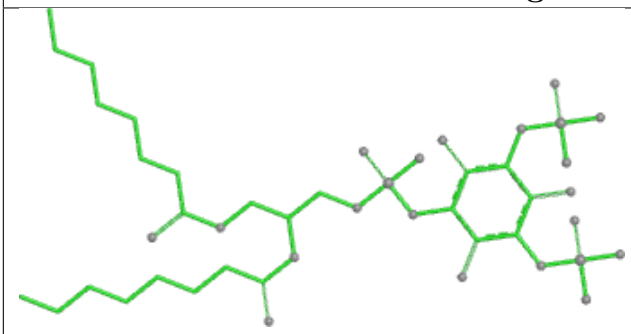


Torsions

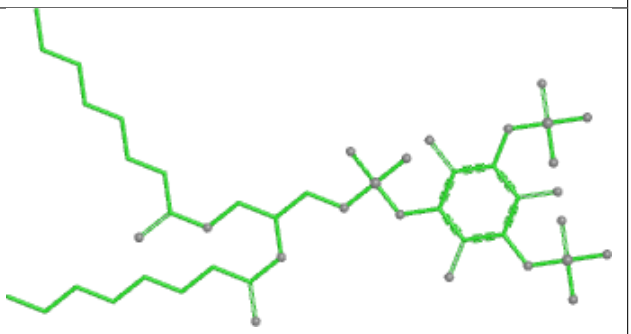


Rings

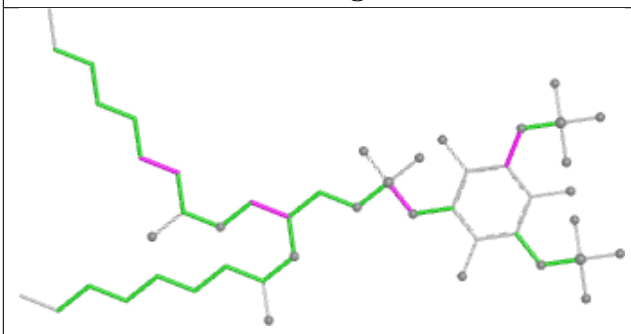
Ligand EUJ C 606



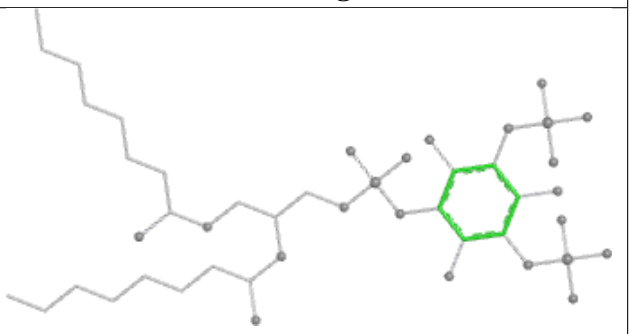
Bond lengths



Bond angles

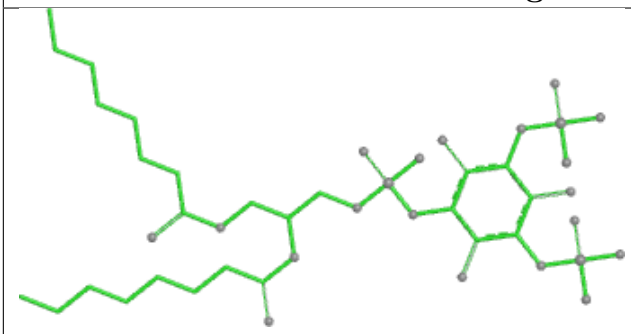


Torsions

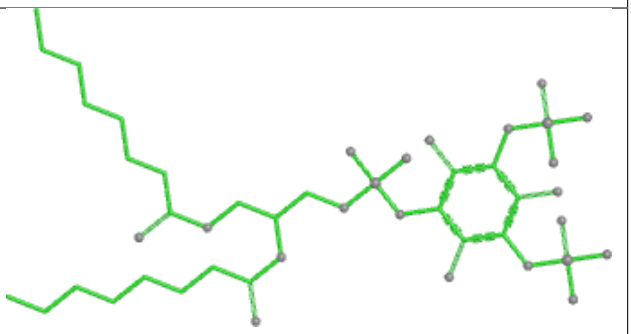


Rings

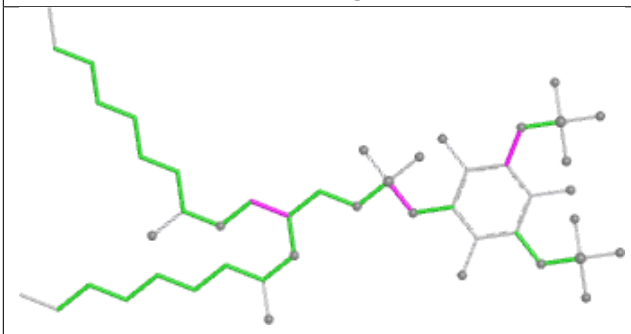
Ligand EUJ D 607



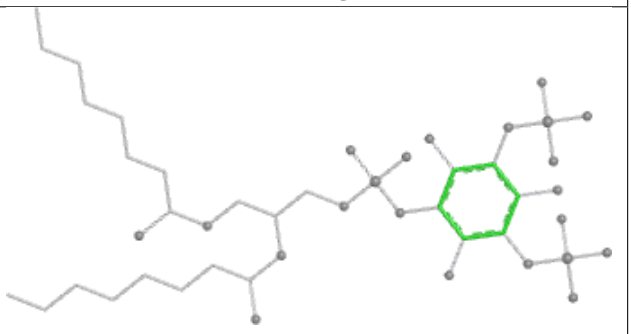
Bond lengths



Bond angles

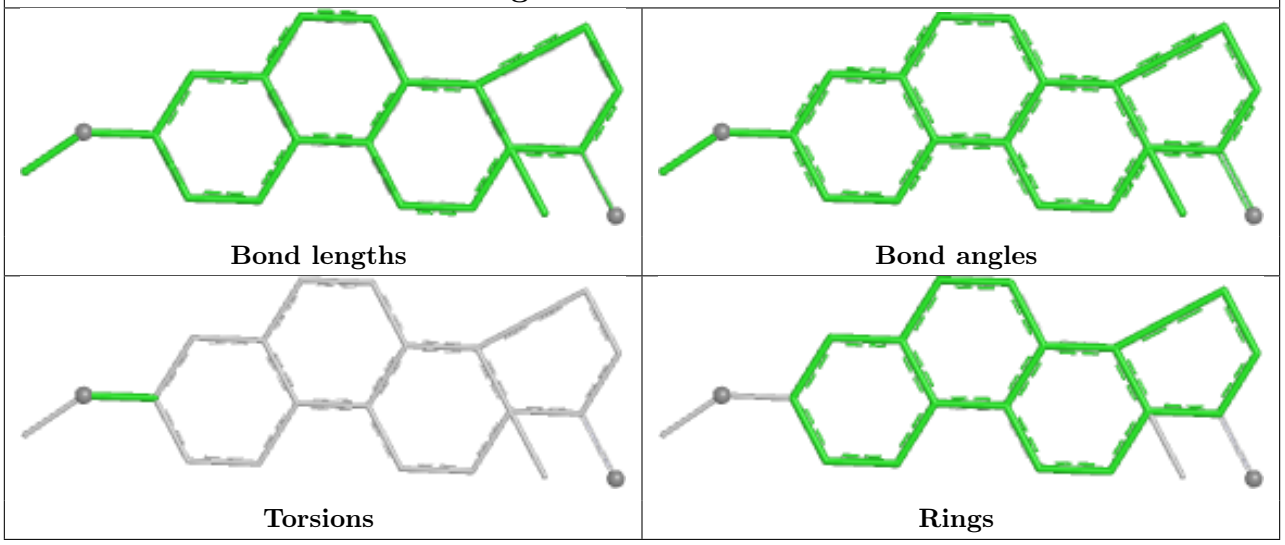


Torsions

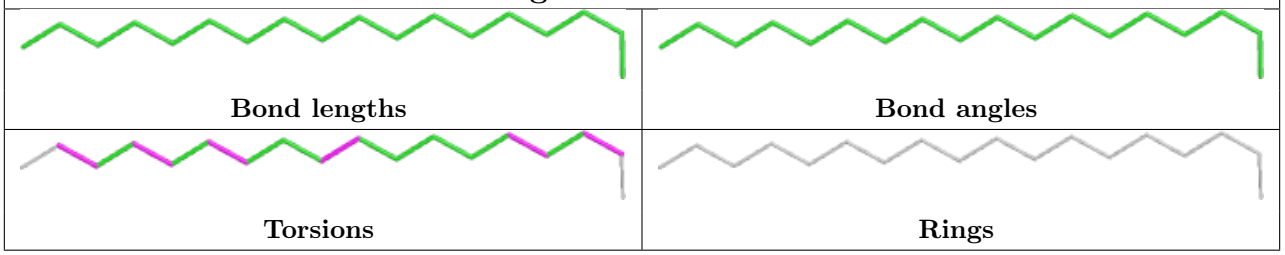


Rings

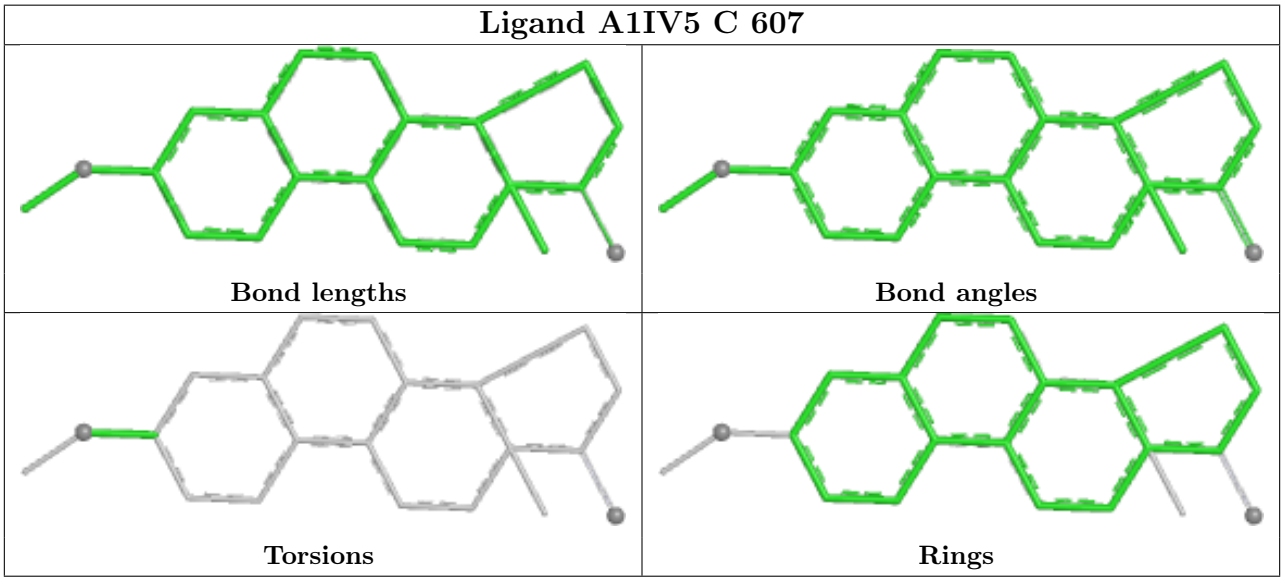
Ligand A1IV5 B 607



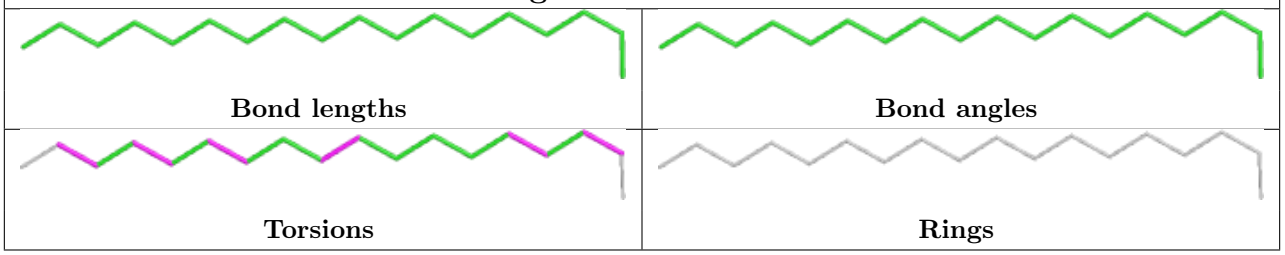
Ligand 8K6 A 606



Ligand A1IV5 C 607



Ligand 8K6 D 602



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

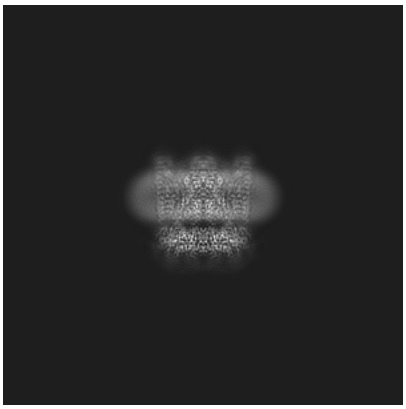
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-52250. These allow visual inspection of the internal detail of the map and identification of artifacts.

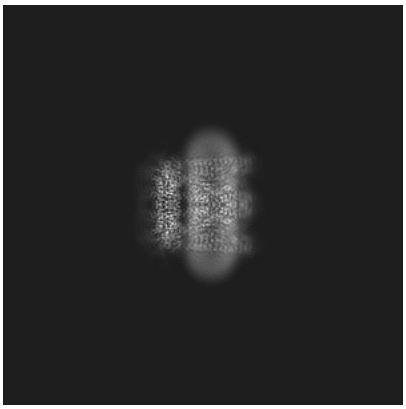
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

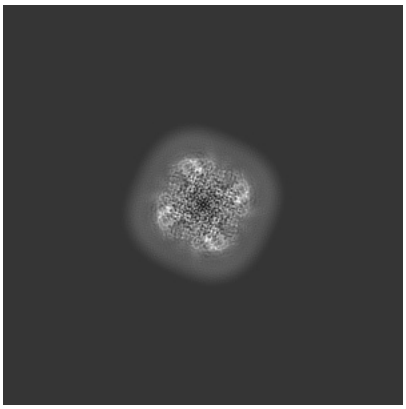
5.1.1 Primary map



X

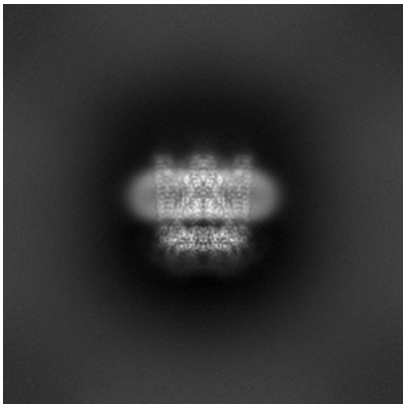


Y

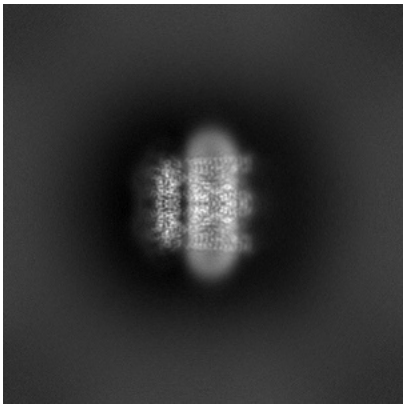


Z

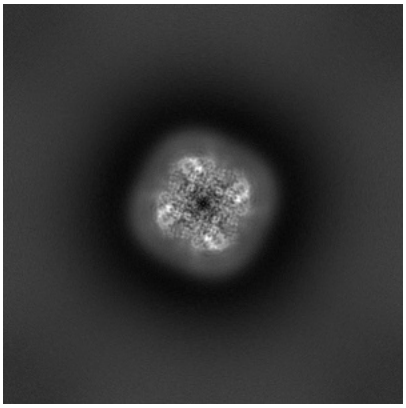
5.1.2 Raw map



X



Y

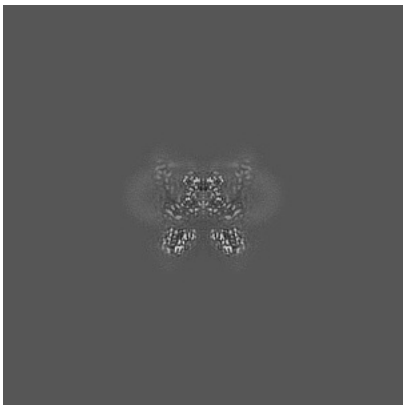


Z

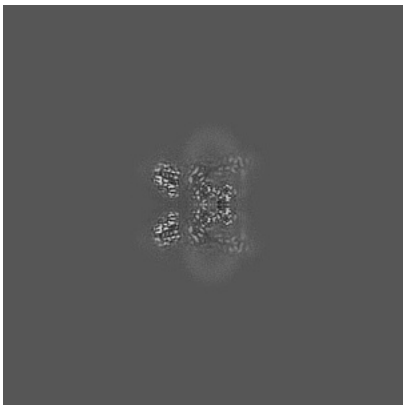
The images above show the map projected in three orthogonal directions.

5.2 Central slices (i)

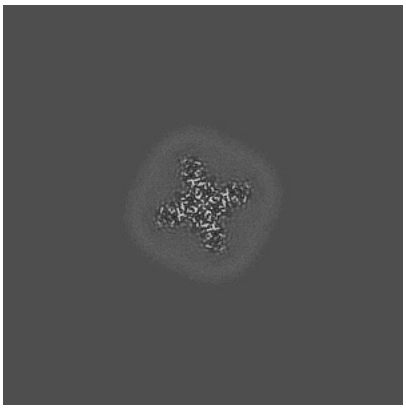
5.2.1 Primary map



X Index: 295

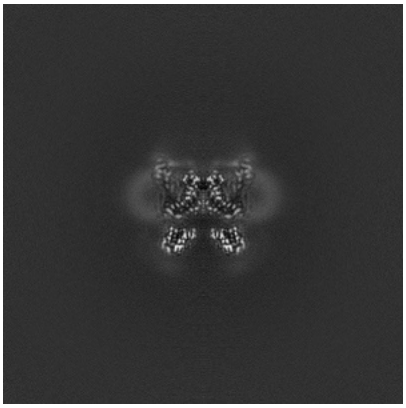


Y Index: 295

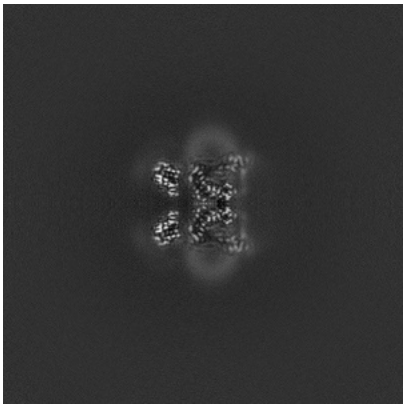


Z Index: 295

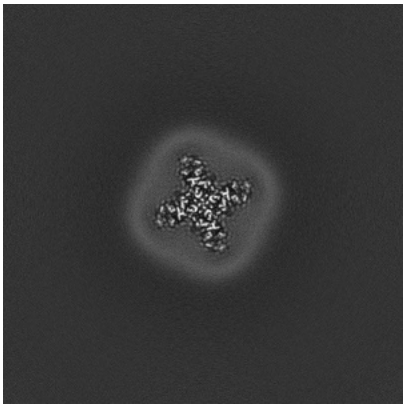
5.2.2 Raw map



X Index: 295



Y Index: 295

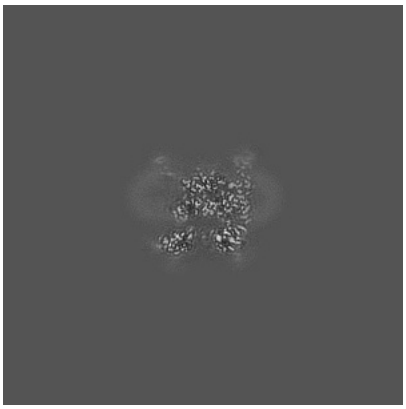


Z Index: 295

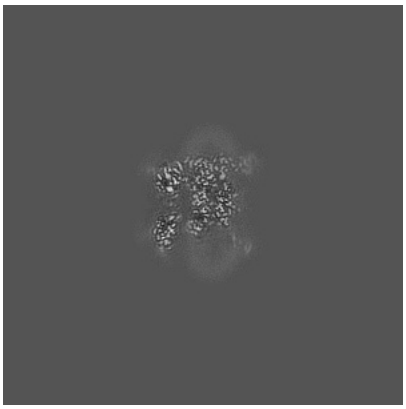
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

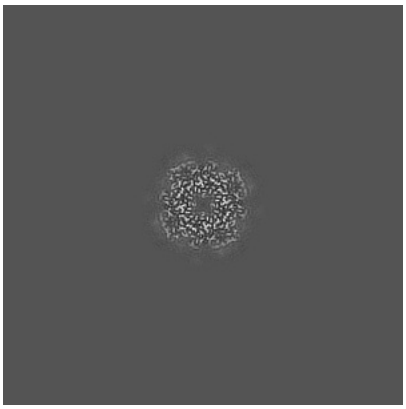
5.3.1 Primary map



X Index: 284

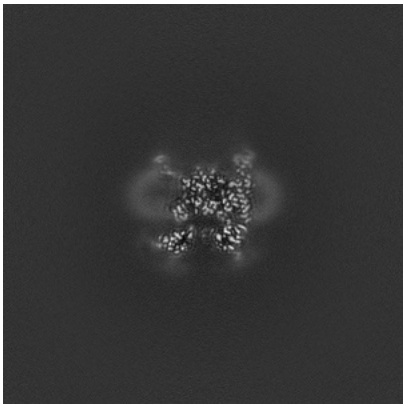


Y Index: 306

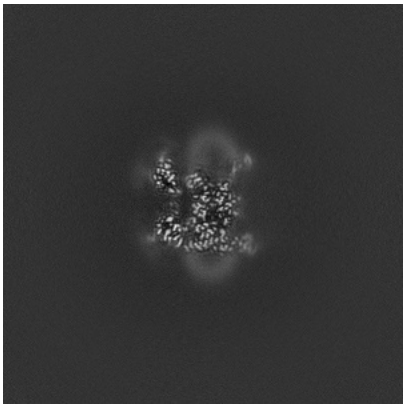


Z Index: 247

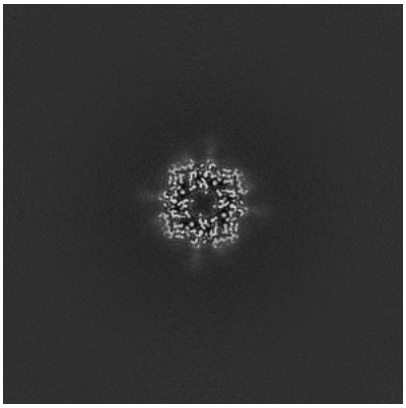
5.3.2 Raw map



X Index: 284



Y Index: 284

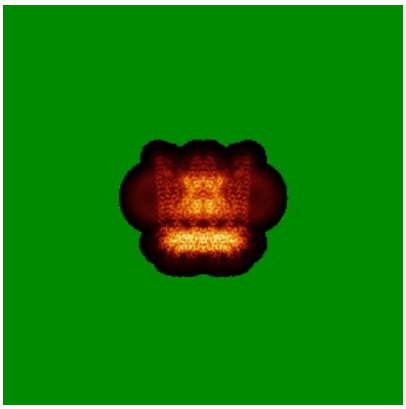


Z Index: 241

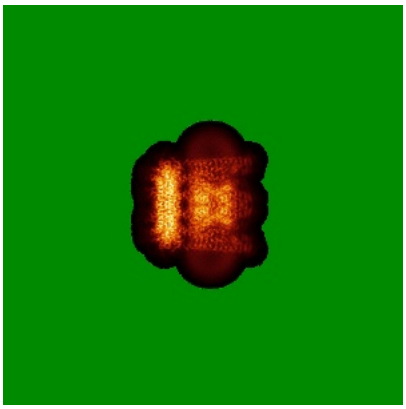
The images above show the largest variance slices of the map in three orthogonal directions.

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

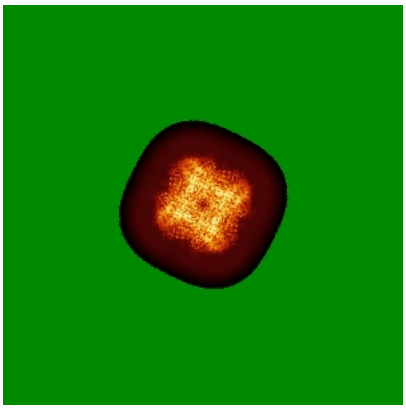
5.4.1 Primary map



X

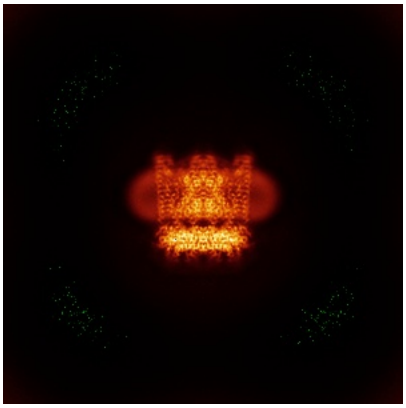


Y

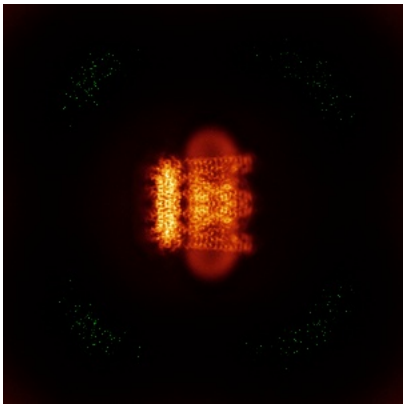


Z

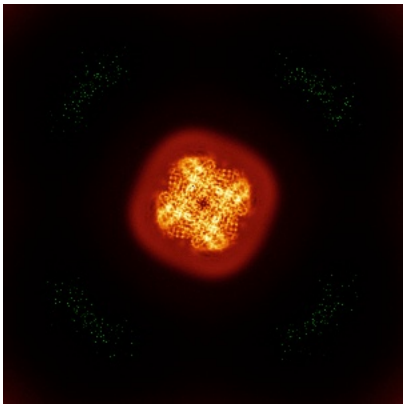
5.4.2 Raw map



X



Y

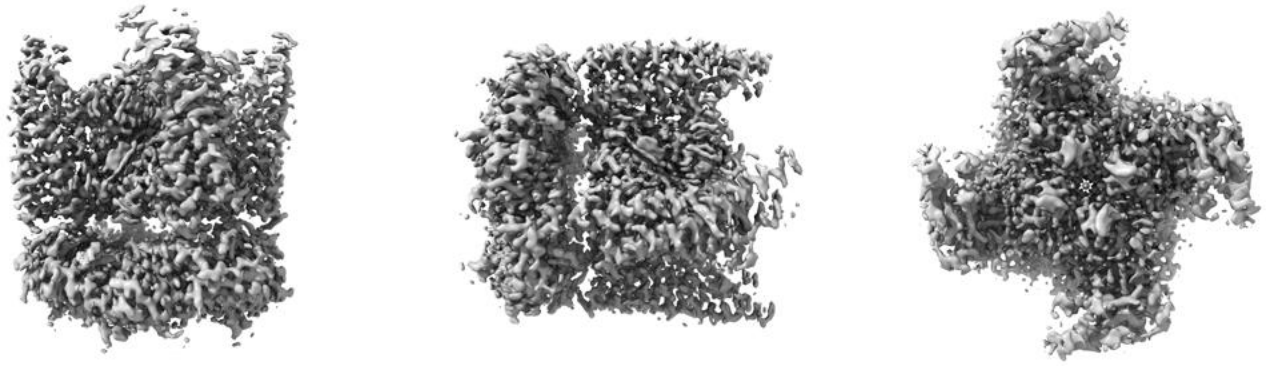


Z

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.

5.5 Orthogonal surface views (i)

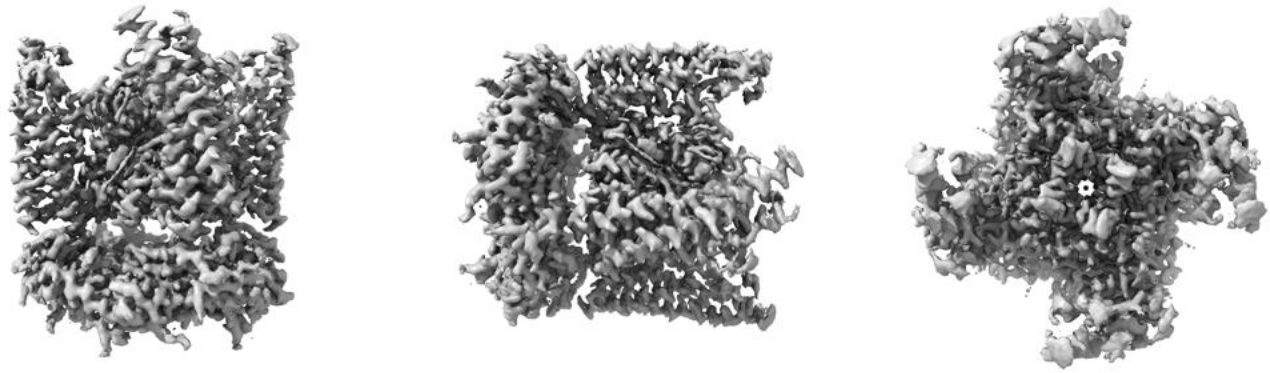
5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.397. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

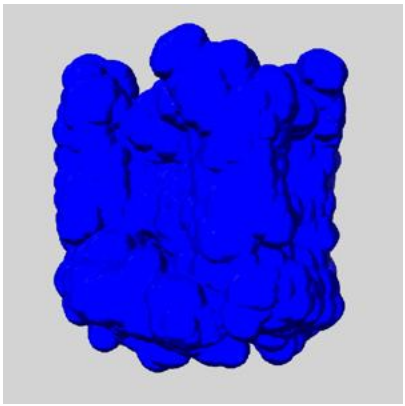
5.6 Mask visualisation (i)

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

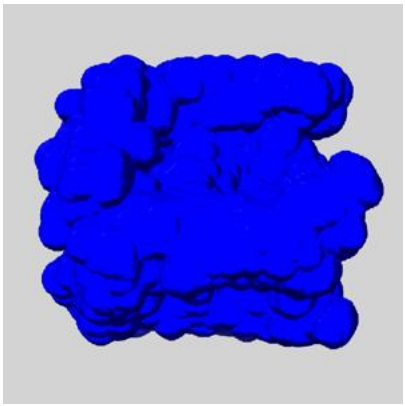
A mask typically either:

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

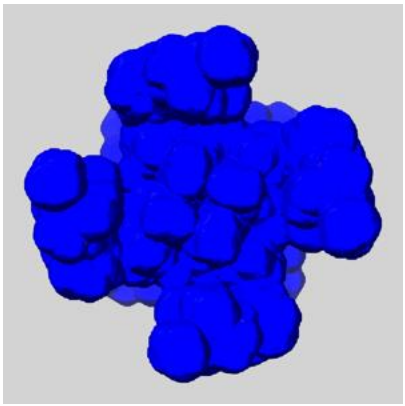
5.6.1 emd_52250_msk_1.map (i)



X



Y

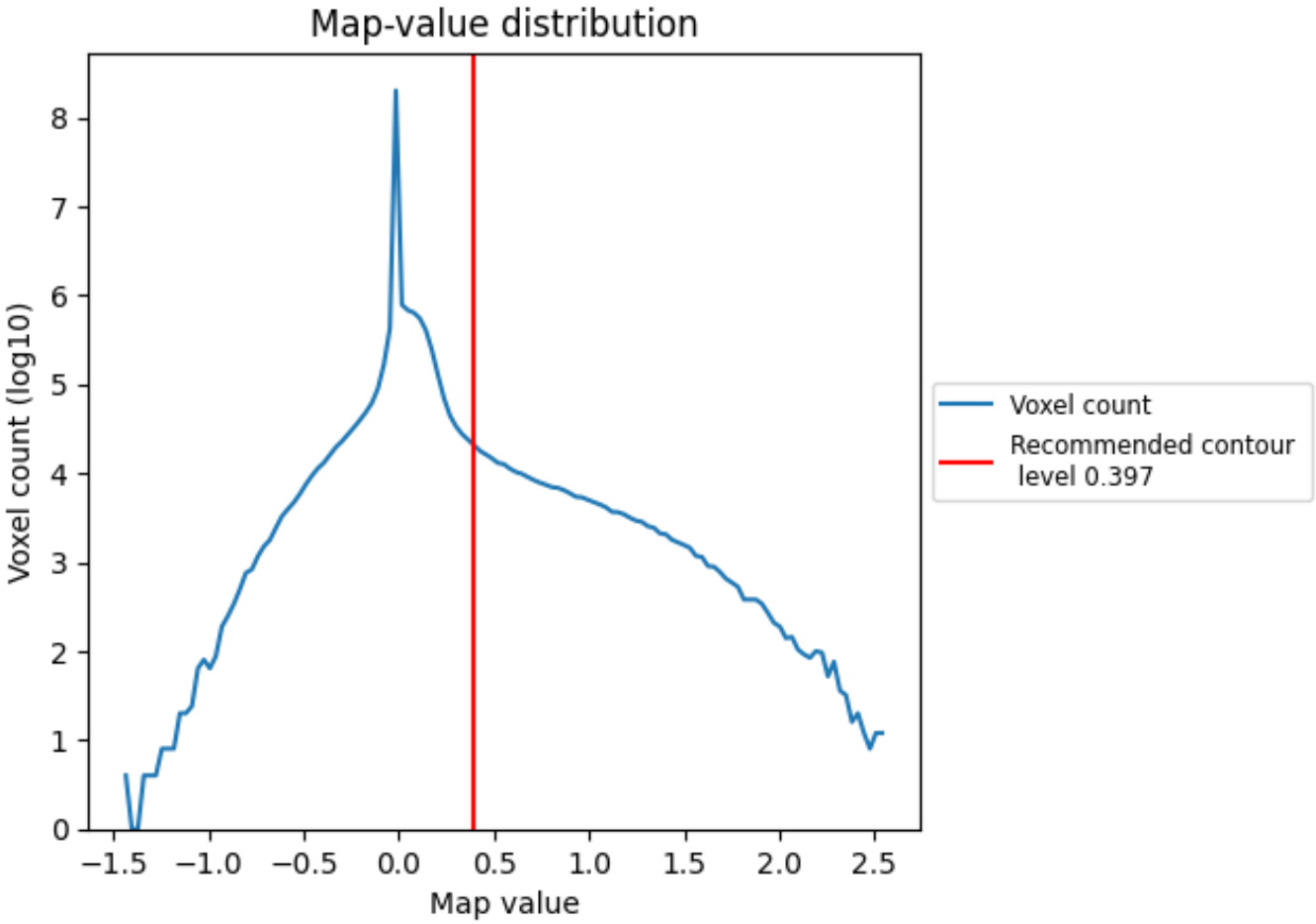


Z

6 Map analysis

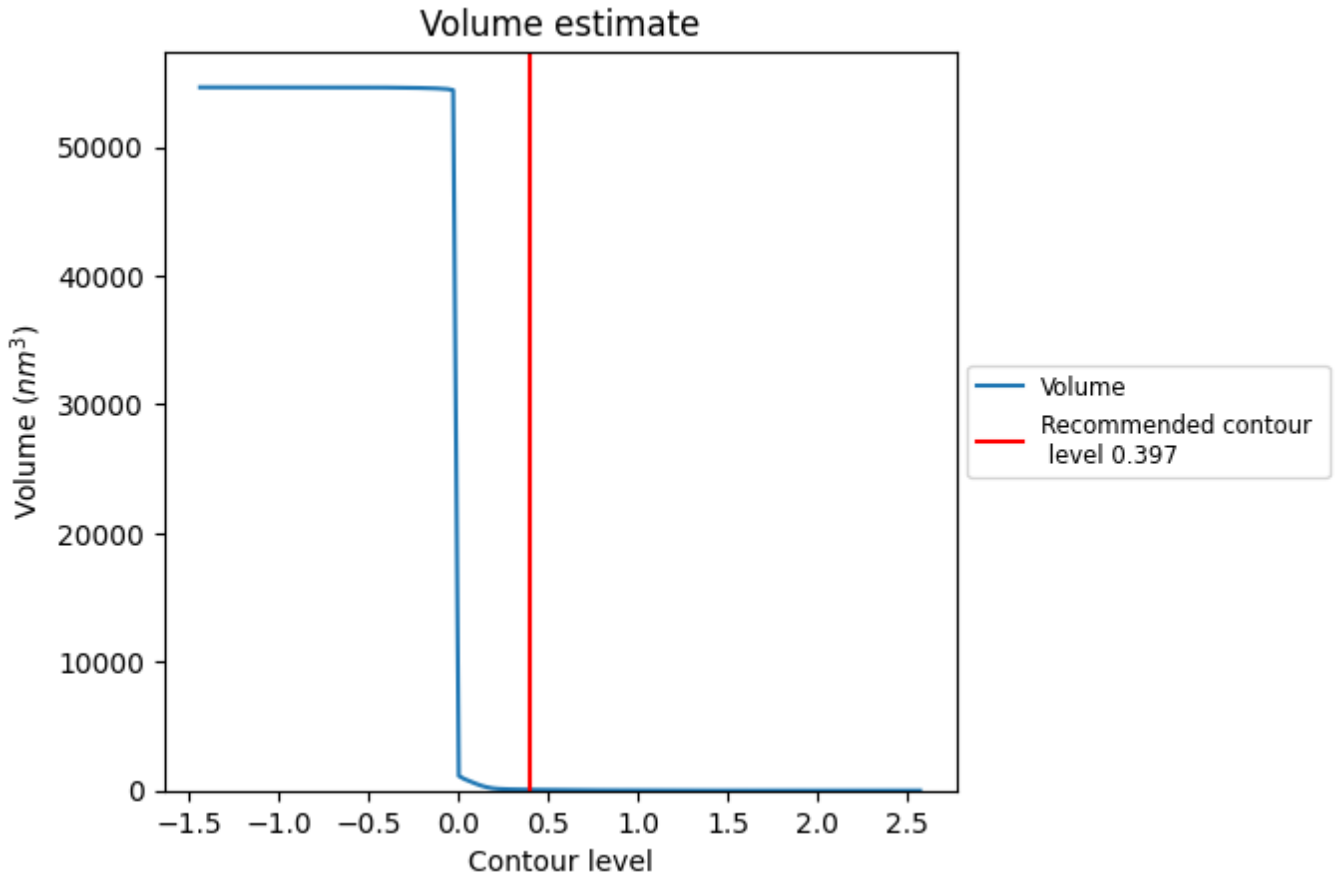
This section contains the results of statistical analysis of the map.

6.1 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.

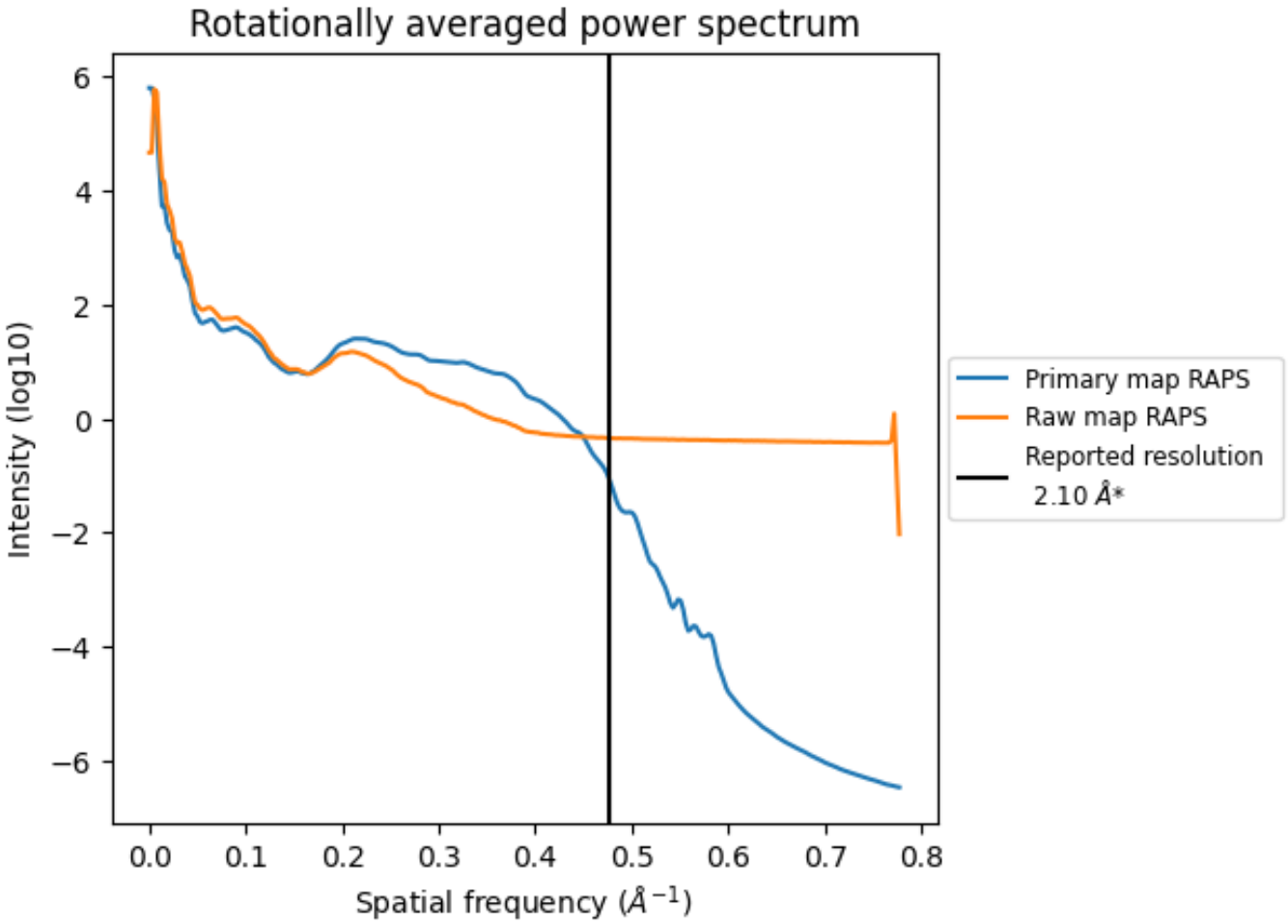
6.2 Volume estimate



The volume at the recommended contour level is 69 nm^3; this corresponds to an approximate mass of 62 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.

6.3 Rotationally averaged power spectrum (i)

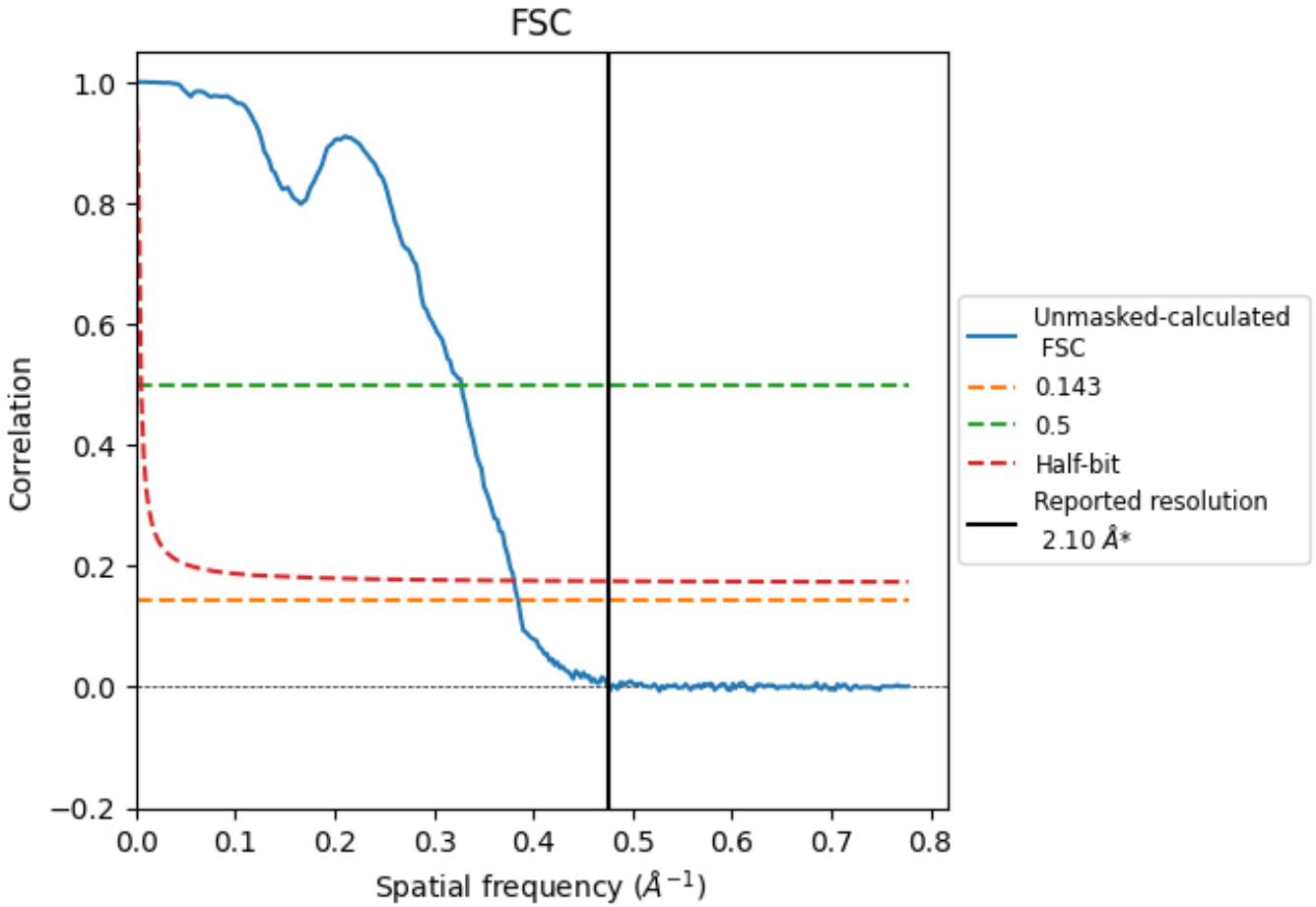


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

7 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.

7.1 FSC



*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

7.2 Resolution estimates (i)

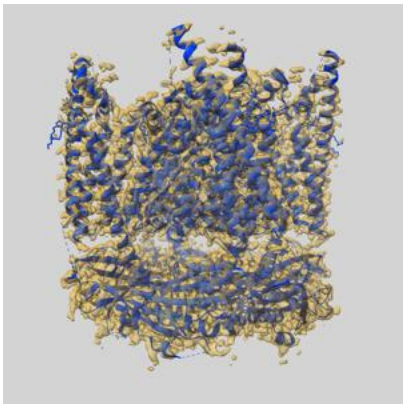
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.60	3.05	2.63

*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 2.60 differs from the reported value 2.1 by more than 10 %

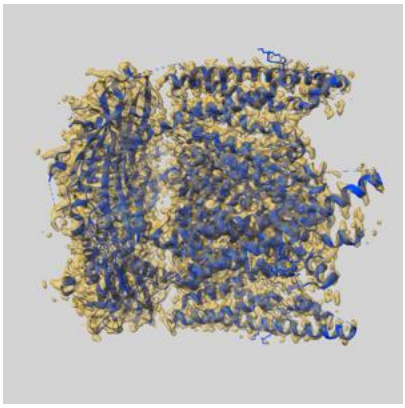
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52250 and PDB model 9HLC. Per-residue inclusion information can be found in section ?? on page ??.

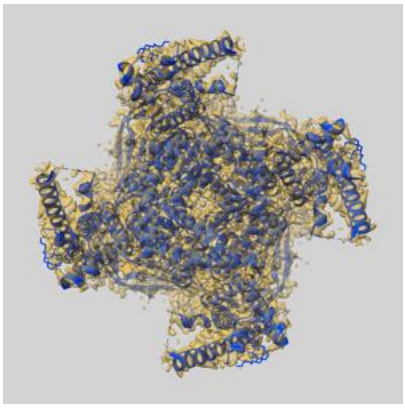
8.1 Map-model overlay



X



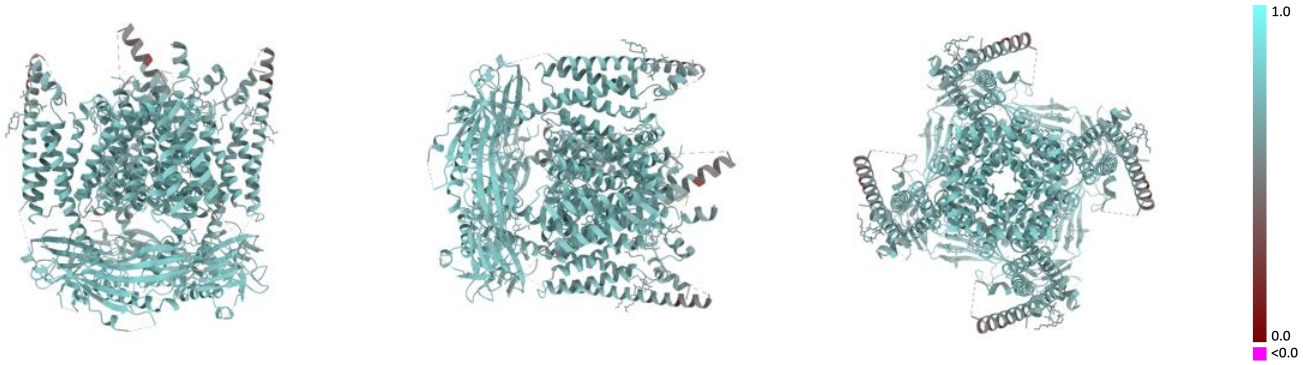
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.397 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.

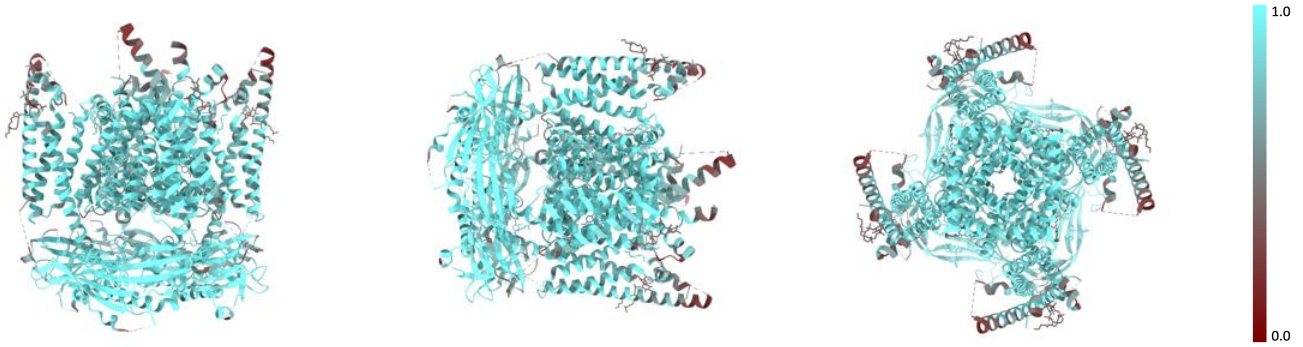
8.2 Q-score mapped to coordinate model (i)



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.

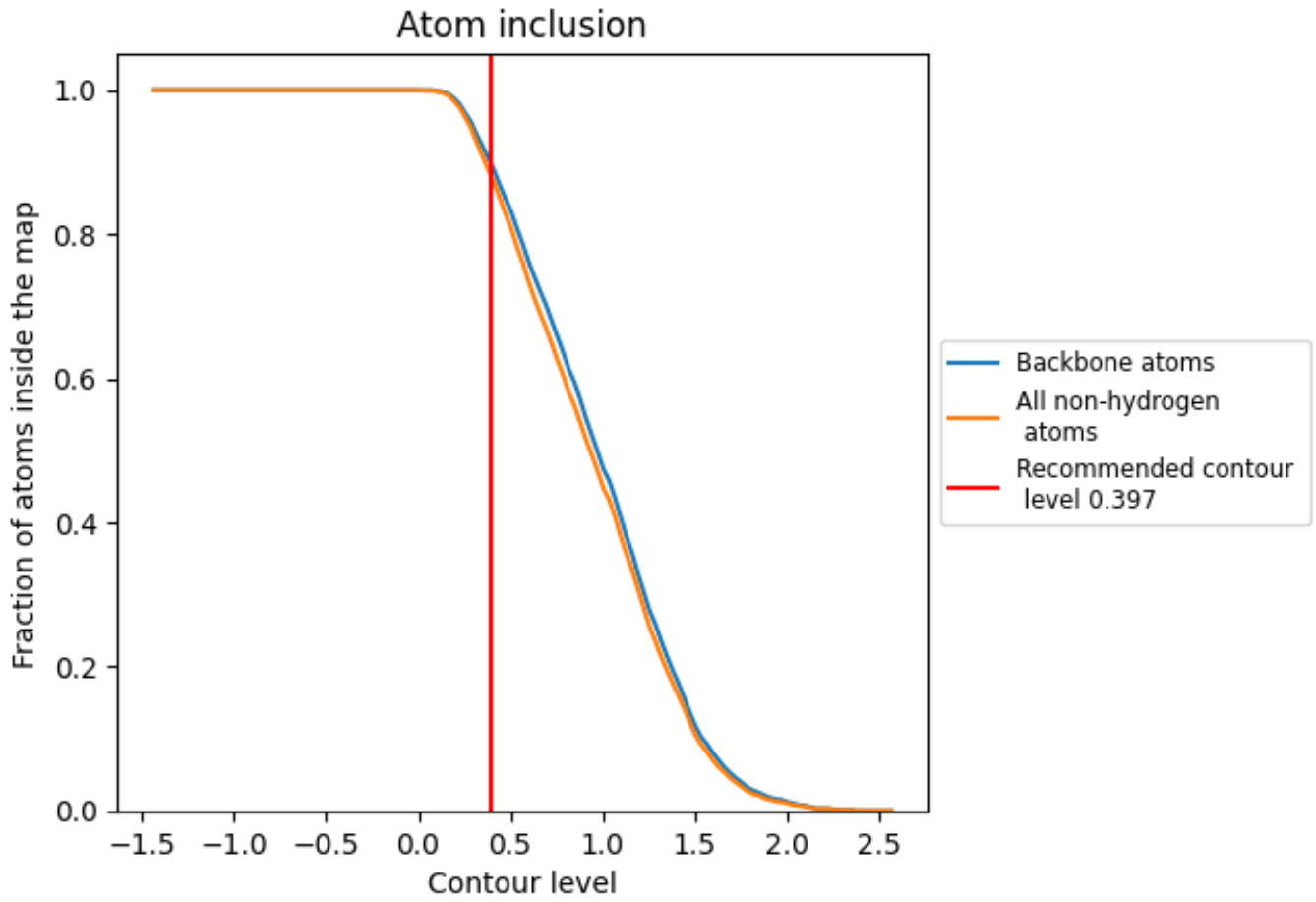
8.3 Atom inclusion mapped to coordinate model (i)



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 (0.397).

8.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.397) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.6980
A	0.8820	0.6980
B	0.8840	0.6980
C	0.8820	0.6980
D	0.8820	0.6980
E	0.9640	0.6540
F	0.9640	0.6510
G	0.9640	0.6510
H	0.9640	0.6490

