



Full wwPDB EM Validation Report ⓘ

May 27, 2025 – 04:59 pm BST

PDB ID : 9HLA / pdb_00009hla
EMDB ID : EMD-52248
Title : TRPML1 in complex with compound 9a
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 : 2.40 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : **FAILED**
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 2.40 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16180 atoms, of which 276 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	457	Total	C	N	O	S	2	0
			3694	2425	610	634	25		
1	B	457	Total	C	N	O	S	2	0
			3694	2425	610	634	25		
1	C	457	Total	C	N	O	S	2	0
			3694	2425	610	634	25		
1	D	457	Total	C	N	O	S	2	0
			3694	2425	610	634	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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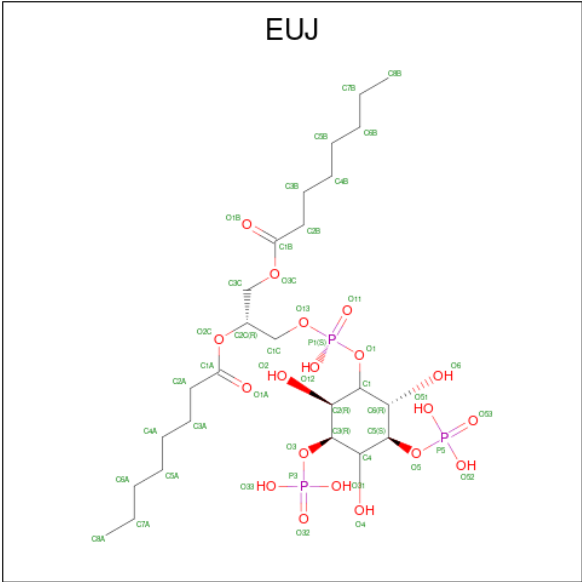
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	TYR	-	expression tag	UNP Q9GZU1
D	-3	PHE	-	expression tag	UNP Q9GZU1
D	-2	GLN	-	expression tag	UNP Q9GZU1
D	-1	GLY	-	expression tag	UNP Q9GZU1
D	0	PRO	-	expression tag	UNP Q9GZU1
D	1	GLY	-	expression tag	UNP Q9GZU1

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



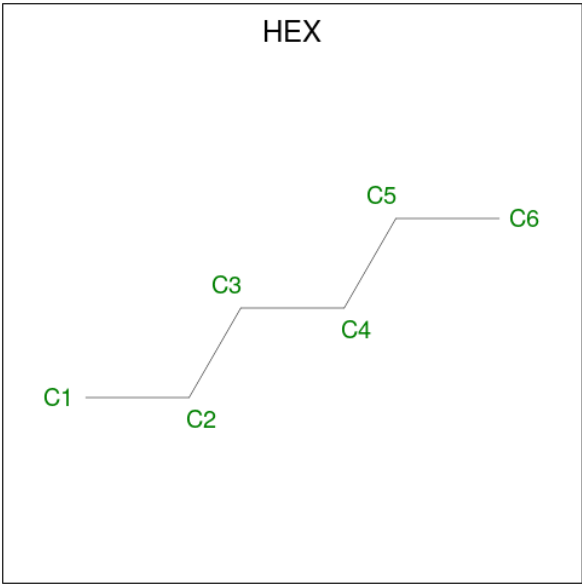
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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: C₂₅H₄₉O₁₉P₃).



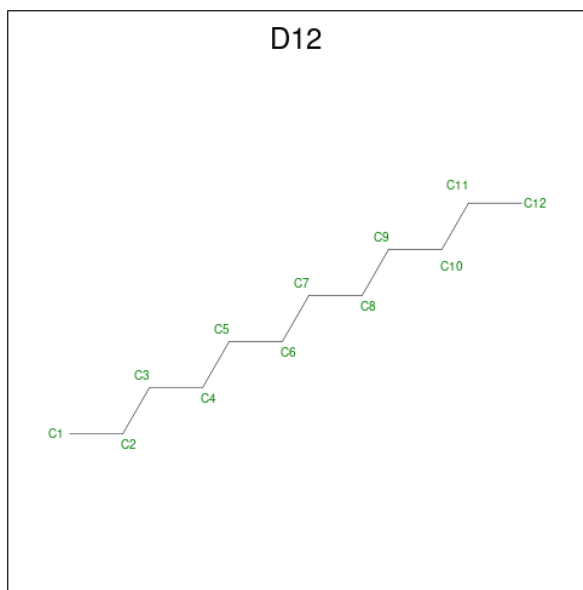
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			47	25	19	3	
3	B	1	Total	C	O	P	0
			47	25	19	3	
3	C	1	Total	C	O	P	0
			47	25	19	3	
3	D	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 4 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



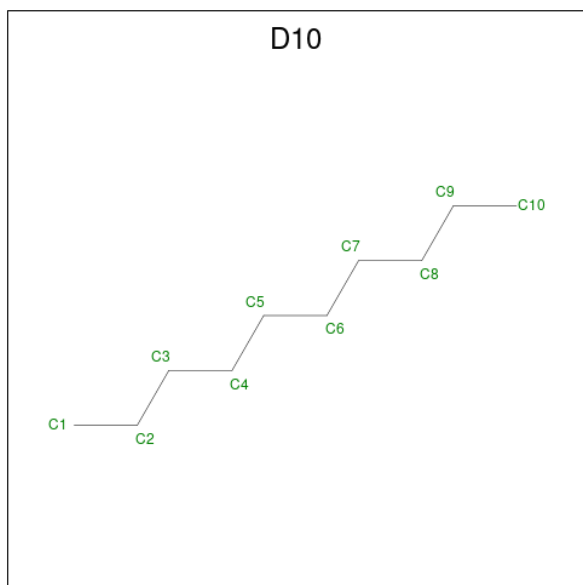
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 6 6	0
4	A	1	Total C 6 6	0
4	A	1	Total C 6 6	0
4	B	1	Total C 6 6	0
4	B	1	Total C 6 6	0
4	B	1	Total C 6 6	0
4	C	1	Total C 6 6	0
4	C	1	Total C 6 6	0
4	C	1	Total C 6 6	0
4	D	1	Total C 6 6	0
4	D	1	Total C 6 6	0
4	D	1	Total C 6 6	0

- Molecule 5 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



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

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



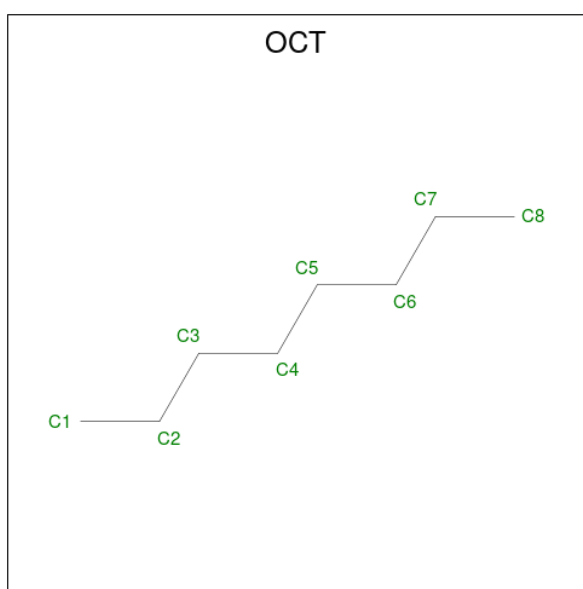
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C 10 10	0
6	A	1	Total C 10 10	0
6	A	1	Total C 10 10	0
6	B	1	Total C 10 10	0
6	B	1	Total C 10 10	0
6	B	1	Total C 10 10	0
6	C	1	Total C 10 10	0
6	C	1	Total C 10 10	0

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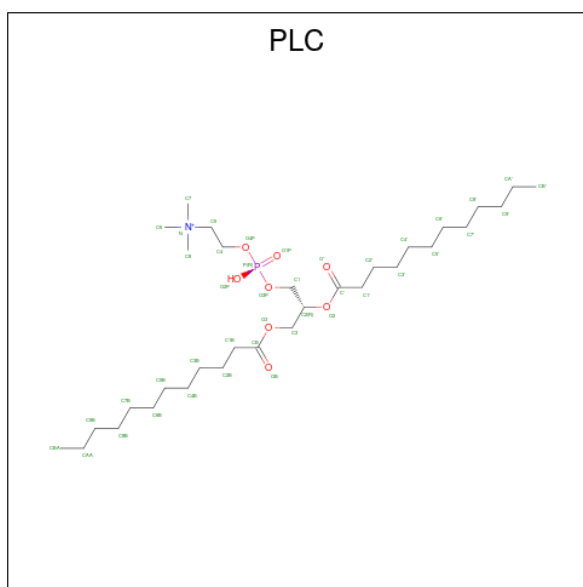
Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total C 10 10	0
6	D	1	Total C 10 10	0
6	D	1	Total C 10 10	0
6	D	1	Total C 10 10	0

- Molecule 7 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



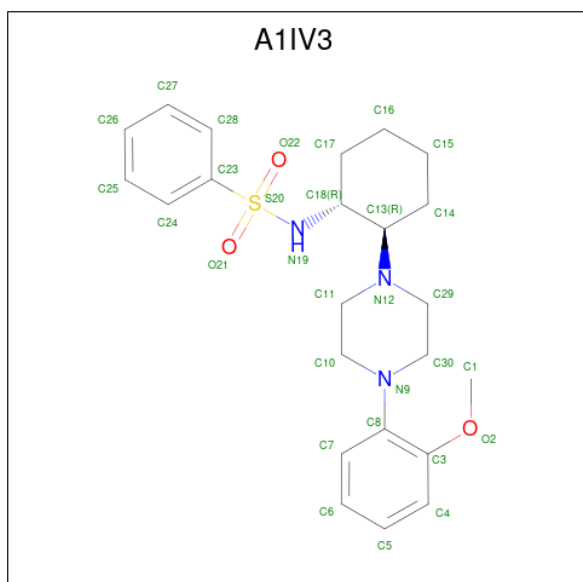
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 8 8	0
7	B	1	Total C 8 8	0
7	C	1	Total C 8 8	0
7	D	1	Total C 8 8	0

- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



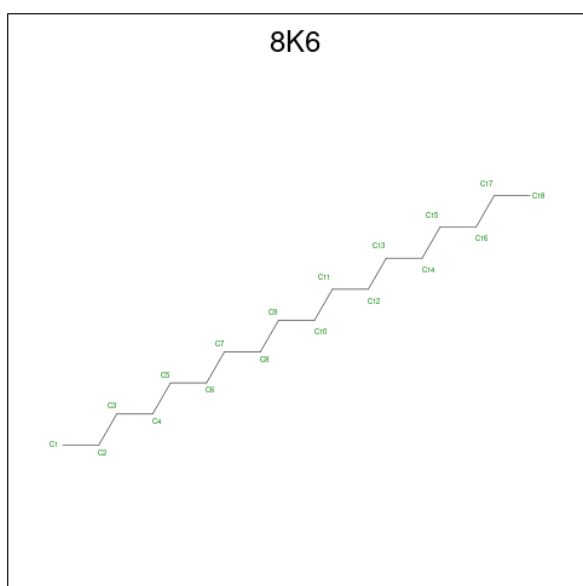
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
8	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
8	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
8	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 9 is N-[(1R,2R)-2-[4-(2-methoxyphenyl)piperazin-1-yl]cyclohexyl]benzenesulfonamide (CCD ID: A1IV3) (formula: $C_{23}H_{31}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
9	A	1	Total 61	C 23	H 31	N 3	O 3	S 1	0
9	A	1	Total 61	C 23	H 31	N 3	O 3	S 1	0
9	B	1	Total 61	C 23	H 31	N 3	O 3	S 1	0
9	C	1	Total 61	C 23	H 31	N 3	O 3	S 1	0

- Molecule 10 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	H	0
			56	18	38	
10	B	1	Total	C	H	0
			56	18	38	
10	C	1	Total	C	H	0
			56	18	38	
10	D	1	Total	C	H	0
			56	18	38	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	49	Total	O	0
			49	49	
11	B	49	Total	O	0
			49	49	

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Mol	Chain	Residues	Atoms		AltConf
11	C	49	Total 49	O 49	0
11	D	49	Total 49	O 49	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	151041	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 ($e^-/\text{\AA}^2$)	39.30	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	2.552	Depositor
Minimum map value	-1.326	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.417	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 [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.75	0	17,19,21	1.54	3 (17%)
2	NAG	E	2	2	14,14,15	0.74	0	17,19,21	1.18	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.77	0	17,19,21	1.54	3 (17%)
2	NAG	F	2	2	14,14,15	0.75	0	17,19,21	1.19	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.75	0	17,19,21	1.52	3 (17%)
2	NAG	G	2	2	14,14,15	0.74	0	17,19,21	1.19	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.75	0	17,19,21	1.54	3 (17%)
2	NAG	H	2	2	14,14,15	0.73	0	17,19,21	1.19	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(°)	Ideal(°)
2	H	1	NAG	C1-O5-C5	4.01	117.62	112.19
2	E	1	NAG	C1-O5-C5	3.99	117.59	112.19
2	F	1	NAG	C1-O5-C5	3.97	117.56	112.19
2	G	1	NAG	C1-O5-C5	3.88	117.45	112.19
2	H	1	NAG	C2-N2-C7	3.14	127.38	122.90
2	F	1	NAG	C2-N2-C7	3.14	127.37	122.90
2	E	1	NAG	C2-N2-C7	3.13	127.36	122.90
2	G	1	NAG	C2-N2-C7	3.09	127.31	122.90
2	F	2	NAG	C2-N2-C7	3.07	127.28	122.90
2	H	2	NAG	C2-N2-C7	3.06	127.25	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C2-N2-C7	3.05	127.25	122.90
2	E	2	NAG	C2-N2-C7	3.05	127.25	122.90
2	G	1	NAG	O4-C4-C5	2.28	114.95	109.30
2	F	1	NAG	O4-C4-C5	2.26	114.91	109.30
2	H	1	NAG	O4-C4-C5	2.26	114.91	109.30
2	E	1	NAG	O4-C4-C5	2.23	114.83	109.30
2	G	2	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

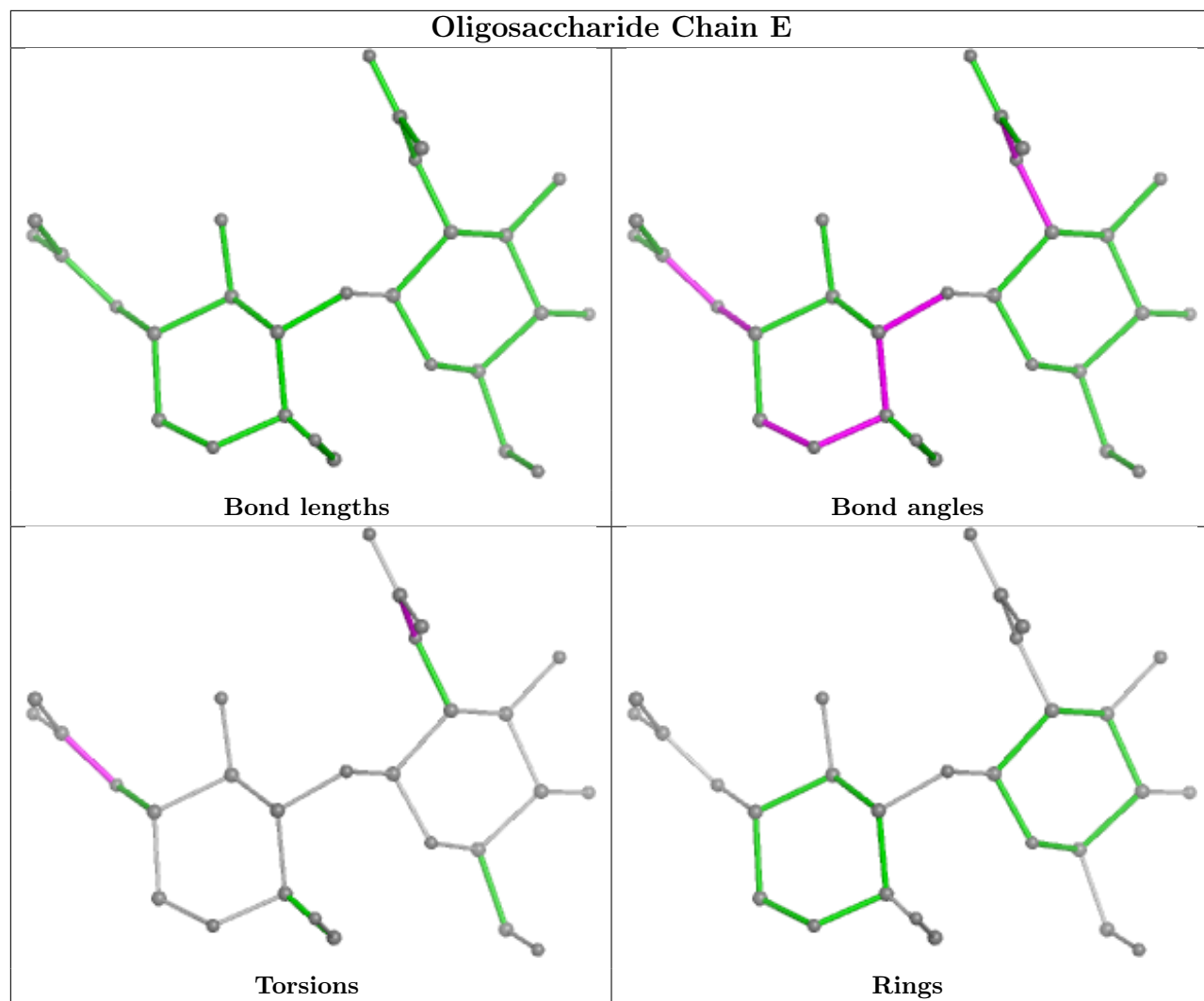
All (16) torsion outliers are listed below:

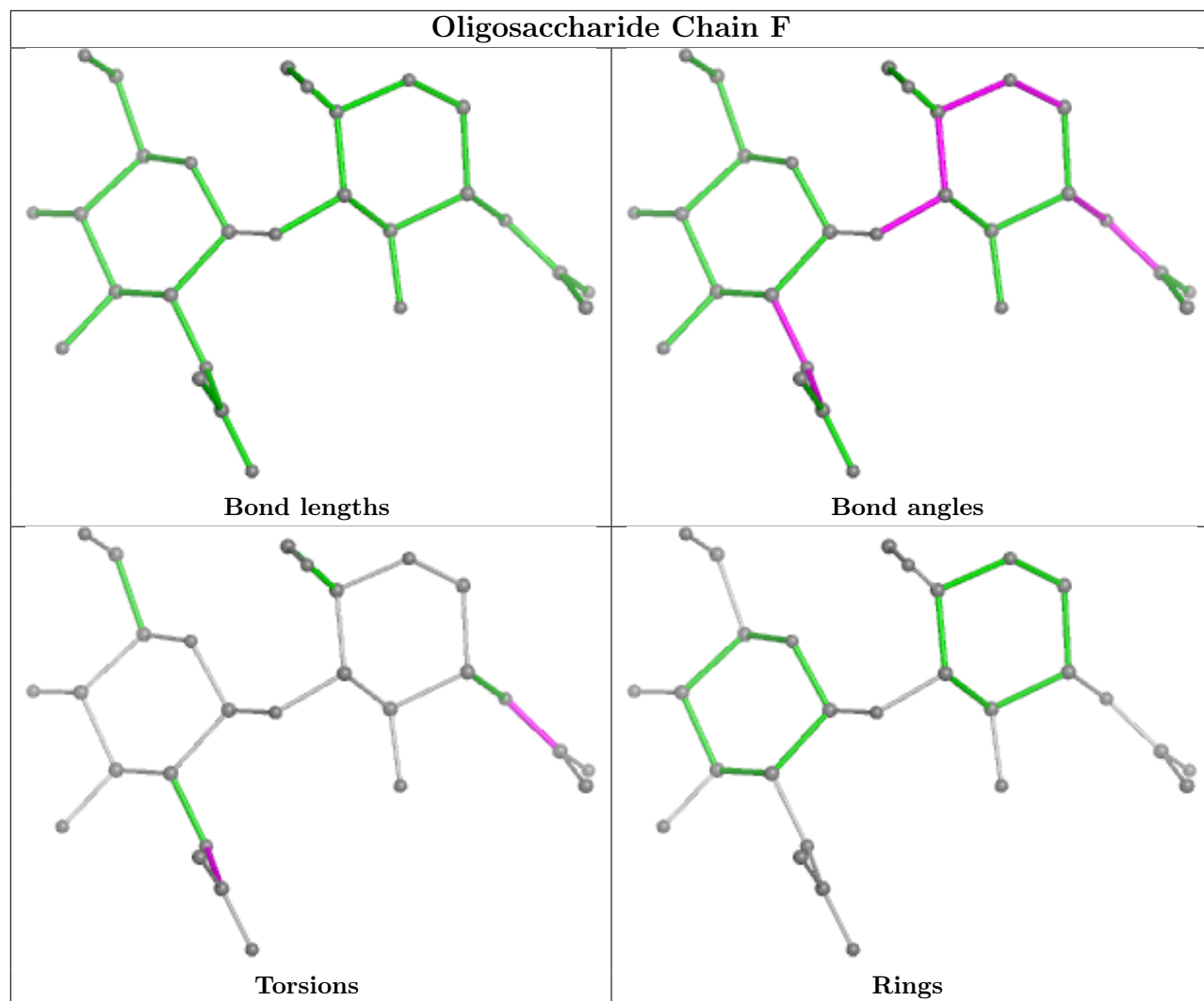
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2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

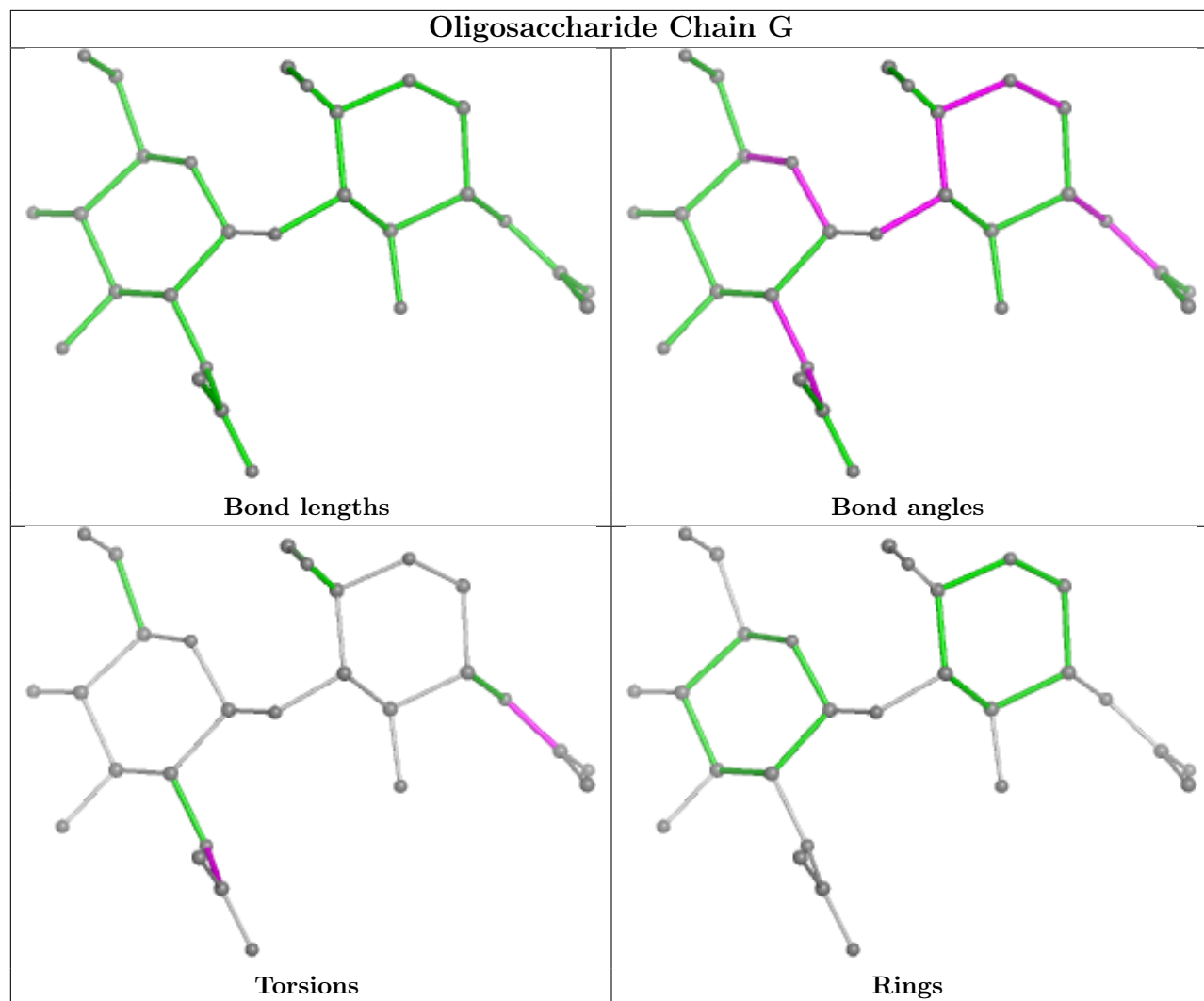
There are no ring outliers.

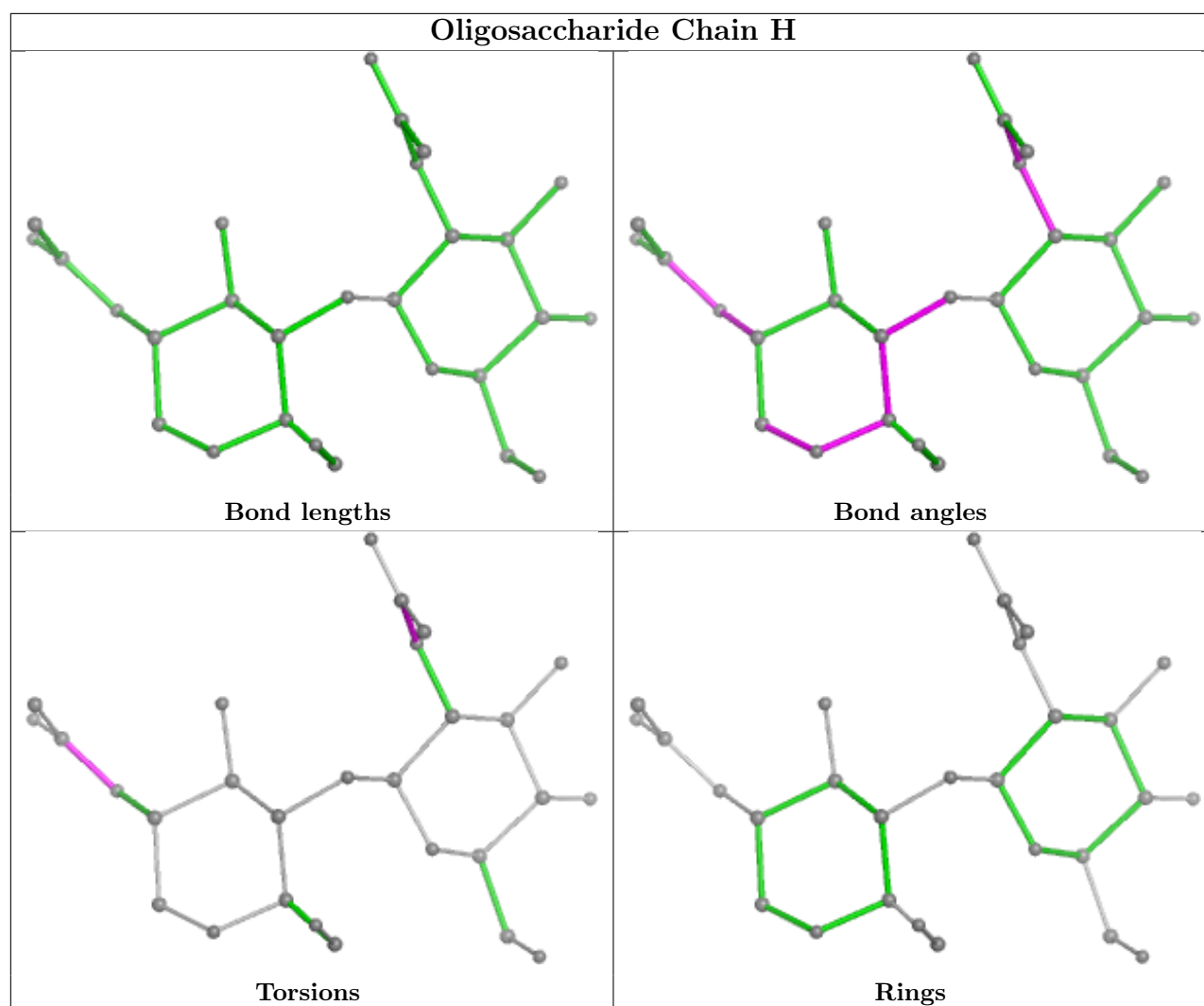
No monomer is involved in short contacts.

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









4.6 Ligand geometry [i](#)

48 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	$\# Z > 2$
9	A1IV3	A	613	-	33,33,33	0.31	0	45,46,46	0.52	0
4	HEX	B	603	-	5,5,5	0.26	0	4,4,4	0.17	0
6	D10	A	606	-	9,9,9	0.24	0	8,8,8	0.19	0
6	D10	D	607	-	9,9,9	0.24	0	8,8,8	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OCT	D	610	-	7,7,7	0.24	0	6,6,6	0.19	0
6	D10	C	608	-	9,9,9	0.23	0	8,8,8	0.18	0
4	HEX	B	602	-	5,5,5	0.26	0	4,4,4	0.16	0
4	HEX	C	602	-	5,5,5	0.26	0	4,4,4	0.16	0
3	EUJ	A	601	-	47,47,47	0.48	0	61,65,65	0.95	3 (4%)
10	8K6	D	601	-	17,17,17	0.08	0	16,16,16	0.09	0
4	HEX	A	602	-	5,5,5	0.26	0	4,4,4	0.16	0
3	EUJ	B	601	-	47,47,47	0.48	0	61,65,65	0.95	2 (3%)
8	PLC	C	610	-	41,41,41	0.51	0	47,49,49	0.56	0
5	D12	C	605	-	11,11,11	0.23	0	10,10,10	0.20	0
6	D10	C	607	-	9,9,9	0.24	0	8,8,8	0.19	0
10	8K6	C	611	-	17,17,17	0.08	0	16,16,16	0.09	0
4	HEX	D	604	-	5,5,5	0.26	0	4,4,4	0.17	0
6	D10	D	609	-	9,9,9	0.22	0	8,8,8	0.18	0
9	A1IV3	C	612	-	33,33,33	0.31	0	45,46,46	0.52	0
3	EUJ	D	602	-	47,47,47	0.48	0	61,65,65	0.95	2 (3%)
6	D10	B	608	-	9,9,9	0.23	0	8,8,8	0.18	0
4	HEX	B	604	-	5,5,5	0.26	0	4,4,4	0.16	0
7	OCT	C	609	-	7,7,7	0.23	0	6,6,6	0.18	0
3	EUJ	C	601	-	47,47,47	0.48	0	61,65,65	0.95	3 (4%)
5	D12	B	605	-	11,11,11	0.23	0	10,10,10	0.20	0
4	HEX	A	603	-	5,5,5	0.26	0	4,4,4	0.17	0
6	D10	C	606	-	9,9,9	0.24	0	8,8,8	0.19	0
4	HEX	A	604	-	5,5,5	0.26	0	4,4,4	0.16	0
8	PLC	D	611	-	41,41,41	0.51	0	47,49,49	0.56	0
4	HEX	D	605	-	5,5,5	0.26	0	4,4,4	0.16	0
8	PLC	B	610	-	41,41,41	0.51	0	47,49,49	0.56	0
7	OCT	B	609	-	7,7,7	0.24	0	6,6,6	0.19	0
6	D10	A	608	-	9,9,9	0.22	0	8,8,8	0.18	0
4	HEX	C	604	-	5,5,5	0.26	0	4,4,4	0.16	0
6	D10	B	607	-	9,9,9	0.24	0	8,8,8	0.18	0
9	A1IV3	B	612	-	33,33,33	0.31	0	45,46,46	0.52	0
5	D12	A	605	-	11,11,11	0.23	0	10,10,10	0.20	0
4	HEX	C	603	-	5,5,5	0.26	0	4,4,4	0.16	0
4	HEX	D	603	-	5,5,5	0.25	0	4,4,4	0.16	0
5	D12	D	606	-	11,11,11	0.23	0	10,10,10	0.20	0
10	8K6	A	612	-	17,17,17	0.08	0	16,16,16	0.08	0
6	D10	B	606	-	9,9,9	0.24	0	8,8,8	0.19	0
8	PLC	A	610	-	41,41,41	0.51	0	47,49,49	0.56	0
7	OCT	A	609	-	7,7,7	0.24	0	6,6,6	0.19	0
10	8K6	B	611	-	17,17,17	0.08	0	16,16,16	0.09	0
6	D10	D	608	-	9,9,9	0.25	0	8,8,8	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A1IV3	A	611	-	33,33,33	0.31	0	45,46,46	0.52	0
6	D10	A	607	-	9,9,9	0.24	0	8,8,8	0.18	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
9	A1IV3	A	613	-	-	2/21/42/42	0/4/4/4
4	HEX	B	603	-	-	0/3/3/3	-
6	D10	A	606	-	-	2/7/7/7	-
6	D10	D	607	-	-	2/7/7/7	-
7	OCT	D	610	-	-	1/5/5/5	-
6	D10	C	608	-	-	5/7/7/7	-
4	HEX	B	602	-	-	0/3/3/3	-
4	HEX	C	602	-	-	0/3/3/3	-
3	EUJ	A	601	-	-	11/44/68/68	0/1/1/1
10	8K6	D	601	-	-	2/15/15/15	-
4	HEX	A	602	-	-	0/3/3/3	-
3	EUJ	B	601	-	-	11/44/68/68	0/1/1/1
8	PLC	C	610	-	-	17/45/45/45	-
5	D12	C	605	-	-	4/9/9/9	-
6	D10	C	607	-	-	2/7/7/7	-
10	8K6	C	611	-	-	2/15/15/15	-
4	HEX	D	604	-	-	0/3/3/3	-
6	D10	D	609	-	-	5/7/7/7	-
9	A1IV3	C	612	-	-	2/21/42/42	0/4/4/4
3	EUJ	D	602	-	-	11/44/68/68	0/1/1/1
6	D10	B	608	-	-	3/7/7/7	-
4	HEX	B	604	-	-	0/3/3/3	-
7	OCT	C	609	-	-	1/5/5/5	-
3	EUJ	C	601	-	-	11/44/68/68	0/1/1/1
5	D12	B	605	-	-	4/9/9/9	-
4	HEX	A	603	-	-	0/3/3/3	-
6	D10	C	606	-	-	2/7/7/7	-
4	HEX	A	604	-	-	0/3/3/3	-
8	PLC	D	611	-	-	17/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEX	D	605	-	-	0/3/3/3	-
8	PLC	B	610	-	-	17/45/45/45	-
7	OCT	B	609	-	-	1/5/5/5	-
6	D10	A	608	-	-	5/7/7/7	-
4	HEX	C	604	-	-	0/3/3/3	-
6	D10	B	607	-	-	2/7/7/7	-
9	A1IV3	B	612	-	-	2/21/42/42	0/4/4/4
5	D12	A	605	-	-	4/9/9/9	-
4	HEX	C	603	-	-	0/3/3/3	-
4	HEX	D	603	-	-	0/3/3/3	-
5	D12	D	606	-	-	4/9/9/9	-
10	8K6	A	612	-	-	2/15/15/15	-
6	D10	B	606	-	-	2/7/7/7	-
8	PLC	A	610	-	-	17/45/45/45	-
7	OCT	A	609	-	-	1/5/5/5	-
10	8K6	B	611	-	-	2/15/15/15	-
6	D10	D	608	-	-	2/7/7/7	-
9	A1IV3	A	611	-	-	2/21/42/42	0/4/4/4
6	D10	A	607	-	-	2/7/7/7	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	EUJ	O2C-C1A-C2A	5.71	123.80	111.50
3	C	601	EUJ	O2C-C1A-C2A	5.69	123.76	111.50
3	A	601	EUJ	O2C-C1A-C2A	5.68	123.75	111.50
3	B	601	EUJ	O2C-C1A-C2A	5.68	123.74	111.50
3	D	602	EUJ	O2C-C1A-O1A	-2.60	117.42	123.70
3	A	601	EUJ	O2C-C1A-O1A	-2.59	117.44	123.70
3	B	601	EUJ	O2C-C1A-O1A	-2.58	117.46	123.70
3	C	601	EUJ	O2C-C1A-O1A	-2.58	117.47	123.70
3	A	601	EUJ	C2C-O2C-C1A	2.01	122.74	117.79
3	C	601	EUJ	C2C-O2C-C1A	2.01	122.73	117.79

There are no chirality outliers.

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	EUJ	C2-C1-O1-P1
3	A	601	EUJ	C6-C1-O1-P1
3	A	601	EUJ	C2-C3-O3-P3
3	A	601	EUJ	C4-C3-O3-P3
3	A	601	EUJ	C2A-C1A-O2C-C2C
3	A	601	EUJ	O1A-C1A-O2C-C2C
3	B	601	EUJ	C6-C1-O1-P1
3	B	601	EUJ	C2-C3-O3-P3
3	B	601	EUJ	C4-C3-O3-P3
3	B	601	EUJ	C2A-C1A-O2C-C2C
3	B	601	EUJ	O1A-C1A-O2C-C2C
3	C	601	EUJ	C2-C1-O1-P1
3	C	601	EUJ	C6-C1-O1-P1
3	C	601	EUJ	C2-C3-O3-P3
3	C	601	EUJ	C4-C3-O3-P3
3	C	601	EUJ	C2A-C1A-O2C-C2C
3	C	601	EUJ	O1A-C1A-O2C-C2C
3	D	602	EUJ	C6-C1-O1-P1
3	D	602	EUJ	C2-C3-O3-P3
3	D	602	EUJ	C4-C3-O3-P3
3	D	602	EUJ	C2A-C1A-O2C-C2C
3	D	602	EUJ	O1A-C1A-O2C-C2C
8	A	610	PLC	O'-C'-O2-C2
8	B	610	PLC	O'-C'-O2-C2
8	C	610	PLC	O'-C'-O2-C2
8	D	611	PLC	O'-C'-O2-C2
8	A	610	PLC	C1'-C'-O2-C2
8	B	610	PLC	C1'-C'-O2-C2
8	C	610	PLC	C1'-C'-O2-C2
8	D	611	PLC	C1'-C'-O2-C2
3	A	601	EUJ	C1-O1-P1-O13
3	B	601	EUJ	C1-O1-P1-O13
3	C	601	EUJ	C1-O1-P1-O13
3	D	602	EUJ	C1-O1-P1-O13
6	A	608	D10	C4-C5-C6-C7
6	B	608	D10	C4-C5-C6-C7
6	C	608	D10	C4-C5-C6-C7
6	D	609	D10	C4-C5-C6-C7
3	B	601	EUJ	C2-C1-O1-P1
3	D	602	EUJ	C2-C1-O1-P1
5	D	606	D12	C6-C7-C8-C9
5	A	605	D12	C6-C7-C8-C9
5	B	605	D12	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	C	605	D12	C6-C7-C8-C9
8	A	610	PLC	C4'-C5'-C6'-C7'
8	B	610	PLC	C4'-C5'-C6'-C7'
8	C	610	PLC	C4'-C5'-C6'-C7'
8	D	611	PLC	C4'-C5'-C6'-C7'
8	A	610	PLC	C1'-C2'-C3'-C4'
8	B	610	PLC	C1'-C2'-C3'-C4'
8	C	610	PLC	C1'-C2'-C3'-C4'
8	D	611	PLC	C1'-C2'-C3'-C4'
5	A	605	D12	C3-C4-C5-C6
5	B	605	D12	C3-C4-C5-C6
5	D	606	D12	C3-C4-C5-C6
5	C	605	D12	C3-C4-C5-C6
8	A	610	PLC	C1B-CB-O3-C3
8	B	610	PLC	C1B-CB-O3-C3
8	C	610	PLC	C1B-CB-O3-C3
8	D	611	PLC	C1B-CB-O3-C3
9	A	611	A1IV3	C18-N19-S20-O21
9	A	613	A1IV3	C18-N19-S20-O21
9	B	612	A1IV3	C18-N19-S20-O21
9	C	612	A1IV3	C18-N19-S20-O21
6	B	608	D10	C2-C3-C4-C5
6	C	606	D10	C6-C7-C8-C9
6	A	606	D10	C6-C7-C8-C9
6	D	607	D10	C6-C7-C8-C9
8	A	610	PLC	OB-CB-O3-C3
8	C	610	PLC	OB-CB-O3-C3
6	B	606	D10	C6-C7-C8-C9
8	A	610	PLC	C1B-C2B-C3B-C4B
8	B	610	PLC	C1B-C2B-C3B-C4B
8	C	610	PLC	C1B-C2B-C3B-C4B
8	D	611	PLC	C1B-C2B-C3B-C4B
8	B	610	PLC	OB-CB-O3-C3
8	D	611	PLC	OB-CB-O3-C3
8	A	610	PLC	C5B-C6B-C7B-C8B
8	D	611	PLC	C5B-C6B-C7B-C8B
8	B	610	PLC	C5B-C6B-C7B-C8B
8	C	610	PLC	C5B-C6B-C7B-C8B
6	D	609	D10	C2-C3-C4-C5
6	A	608	D10	C2-C3-C4-C5
6	C	608	D10	C2-C3-C4-C5
6	A	608	D10	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	C	608	D10	C6-C7-C8-C9
6	D	609	D10	C6-C7-C8-C9
6	B	607	D10	C1-C2-C3-C4
6	C	607	D10	C1-C2-C3-C4
6	D	608	D10	C1-C2-C3-C4
6	A	607	D10	C1-C2-C3-C4
6	B	608	D10	C6-C7-C8-C9
8	A	610	PLC	C7'-C8'-C9'-CA'
8	D	611	PLC	C7'-C8'-C9'-CA'
8	B	610	PLC	C7'-C8'-C9'-CA'
8	C	610	PLC	C7'-C8'-C9'-CA'
8	D	611	PLC	C2'-C3'-C4'-C5'
8	A	610	PLC	C2'-C3'-C4'-C5'
8	B	610	PLC	C2'-C3'-C4'-C5'
6	A	607	D10	C3-C4-C5-C6
6	B	607	D10	C3-C4-C5-C6
6	C	607	D10	C3-C4-C5-C6
6	D	608	D10	C3-C4-C5-C6
8	C	610	PLC	C2'-C3'-C4'-C5'
5	C	605	D12	C5-C6-C7-C8
5	A	605	D12	C5-C6-C7-C8
5	D	606	D12	C5-C6-C7-C8
10	D	601	8K6	C12-C13-C14-C15
5	B	605	D12	C5-C6-C7-C8
10	B	611	8K6	C12-C13-C14-C15
10	A	612	8K6	C12-C13-C14-C15
10	C	611	8K6	C12-C13-C14-C15
8	D	611	PLC	O3P-C1-C2-O2
9	A	611	A1IV3	C18-N19-S20-C23
9	A	613	A1IV3	C18-N19-S20-C23
9	B	612	A1IV3	C18-N19-S20-C23
9	C	612	A1IV3	C18-N19-S20-C23
8	A	610	PLC	O3P-C1-C2-C3
8	B	610	PLC	O3P-C1-C2-C3
8	C	610	PLC	O3P-C1-C2-C3
8	D	611	PLC	O3P-C1-C2-C3
8	A	610	PLC	O3P-C1-C2-O2
8	B	610	PLC	O3P-C1-C2-O2
8	C	610	PLC	O3P-C1-C2-O2
8	D	611	PLC	C4B-C5B-C6B-C7B
8	A	610	PLC	C4B-C5B-C6B-C7B
8	B	610	PLC	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
8	C	610	PLC	C8B-C9B-CAA-CBA
8	D	611	PLC	C3'-C4'-C5'-C6'
8	B	610	PLC	C3'-C4'-C5'-C6'
8	C	610	PLC	C4B-C5B-C6B-C7B
8	A	610	PLC	C3'-C4'-C5'-C6'
8	C	610	PLC	C3'-C4'-C5'-C6'
8	C	610	PLC	C3B-C4B-C5B-C6B
8	D	611	PLC	C3B-C4B-C5B-C6B
5	C	605	D12	C4-C5-C6-C7
8	A	610	PLC	C3B-C4B-C5B-C6B
8	B	610	PLC	C3B-C4B-C5B-C6B
8	A	610	PLC	C1-O3P-P-O4P
8	B	610	PLC	C1-O3P-P-O4P
8	C	610	PLC	C1-O3P-P-O4P
8	D	611	PLC	C1-O3P-P-O4P
5	A	605	D12	C4-C5-C6-C7
5	B	605	D12	C4-C5-C6-C7
5	D	606	D12	C4-C5-C6-C7
3	A	601	EUJ	O3C-C1B-C2B-C3B
3	D	602	EUJ	O3C-C1B-C2B-C3B
8	A	610	PLC	C8B-C9B-CAA-CBA
8	D	611	PLC	C8B-C9B-CAA-CBA
3	C	601	EUJ	O3C-C1B-C2B-C3B
8	B	610	PLC	C8B-C9B-CAA-CBA
3	B	601	EUJ	O3C-C1B-C2B-C3B
6	B	606	D10	C1-C2-C3-C4
6	A	606	D10	C1-C2-C3-C4
6	C	606	D10	C1-C2-C3-C4
6	D	607	D10	C1-C2-C3-C4
3	B	601	EUJ	C1A-C2A-C3A-C4A
3	A	601	EUJ	C1A-C2A-C3A-C4A
3	D	602	EUJ	C1A-C2A-C3A-C4A
10	C	611	8K6	C3-C4-C5-C6
10	D	601	8K6	C3-C4-C5-C6
3	C	601	EUJ	C1A-C2A-C3A-C4A
10	A	612	8K6	C3-C4-C5-C6
10	B	611	8K6	C3-C4-C5-C6
6	C	608	D10	C1-C2-C3-C4
6	A	608	D10	C1-C2-C3-C4
6	D	609	D10	C1-C2-C3-C4
3	A	601	EUJ	C1C-O13-P1-O1
3	B	601	EUJ	C1C-O13-P1-O1

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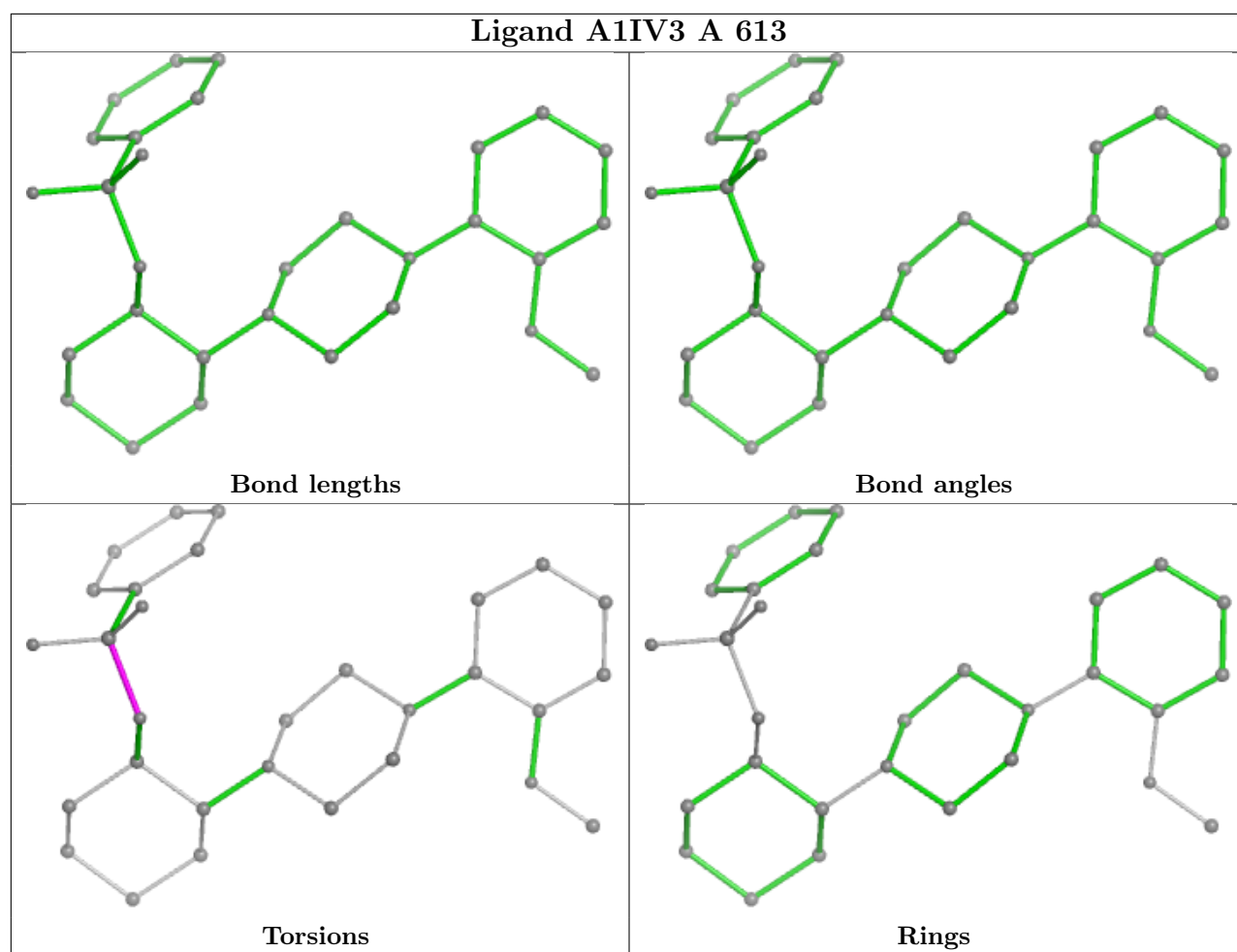
Continued from previous page...

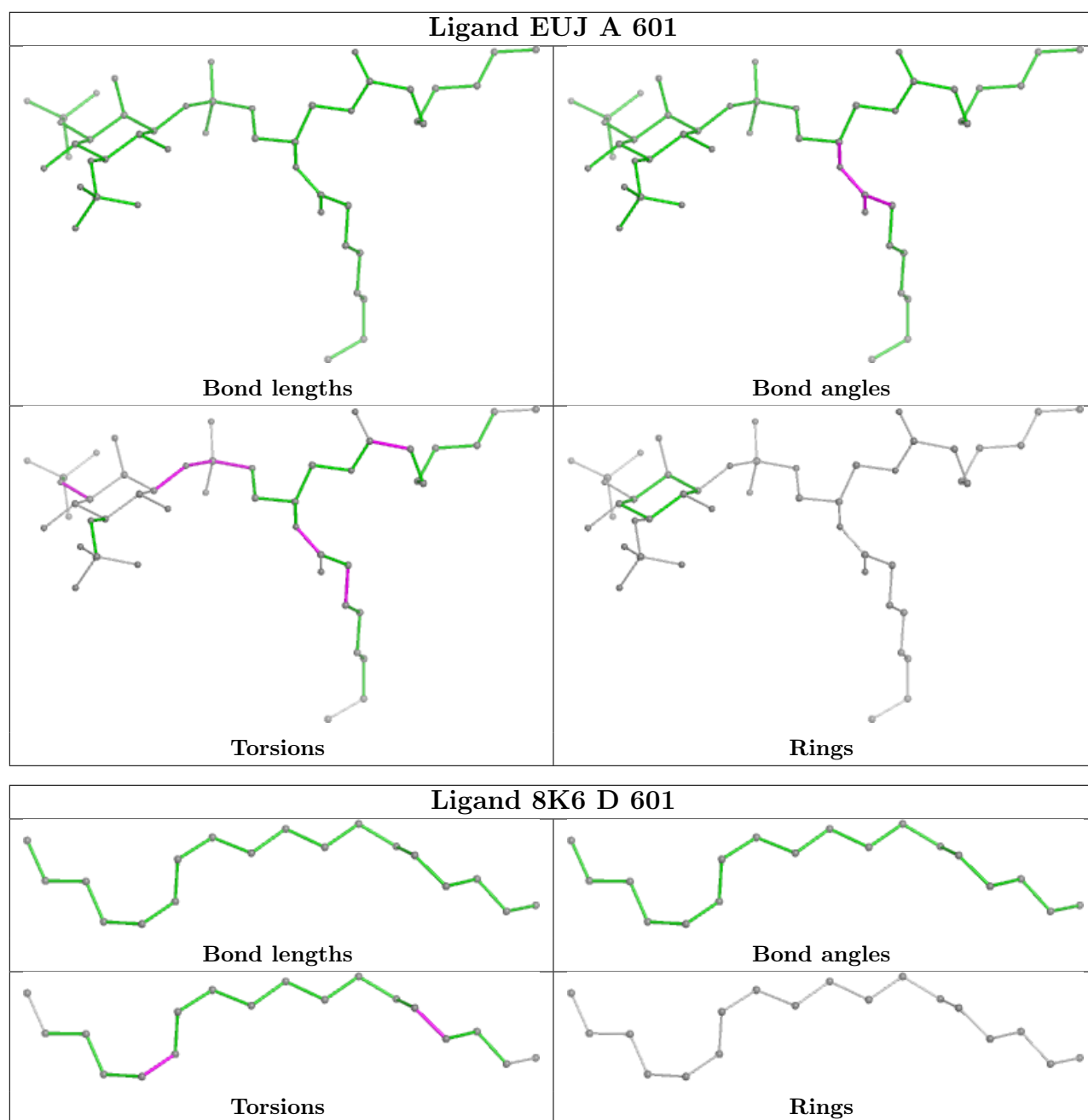
Mol	Chain	Res	Type	Atoms
3	C	601	EUJ	C1C-O13-P1-O1
3	D	602	EUJ	C1C-O13-P1-O1
7	A	609	OCT	C5-C6-C7-C8
7	C	609	OCT	C5-C6-C7-C8
7	B	609	OCT	C5-C6-C7-C8
7	D	610	OCT	C5-C6-C7-C8
6	A	608	D10	C3-C4-C5-C6
6	C	608	D10	C3-C4-C5-C6
6	D	609	D10	C3-C4-C5-C6
3	A	601	EUJ	C1C-O13-P1-O11
3	B	601	EUJ	C1C-O13-P1-O11
3	C	601	EUJ	C1C-O13-P1-O11
3	D	602	EUJ	C1C-O13-P1-O11

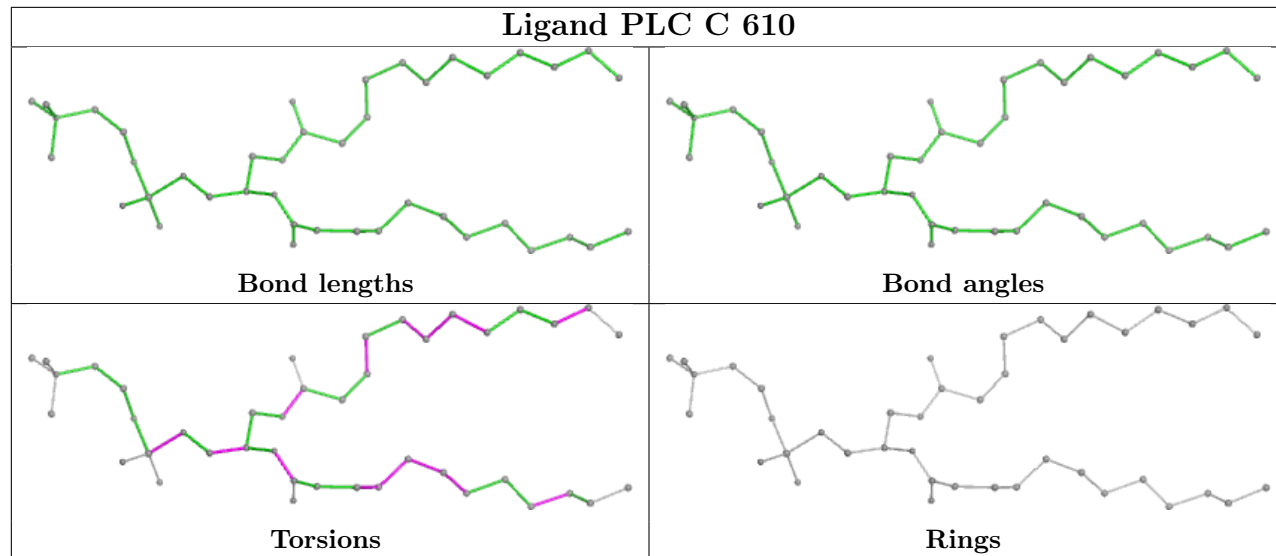
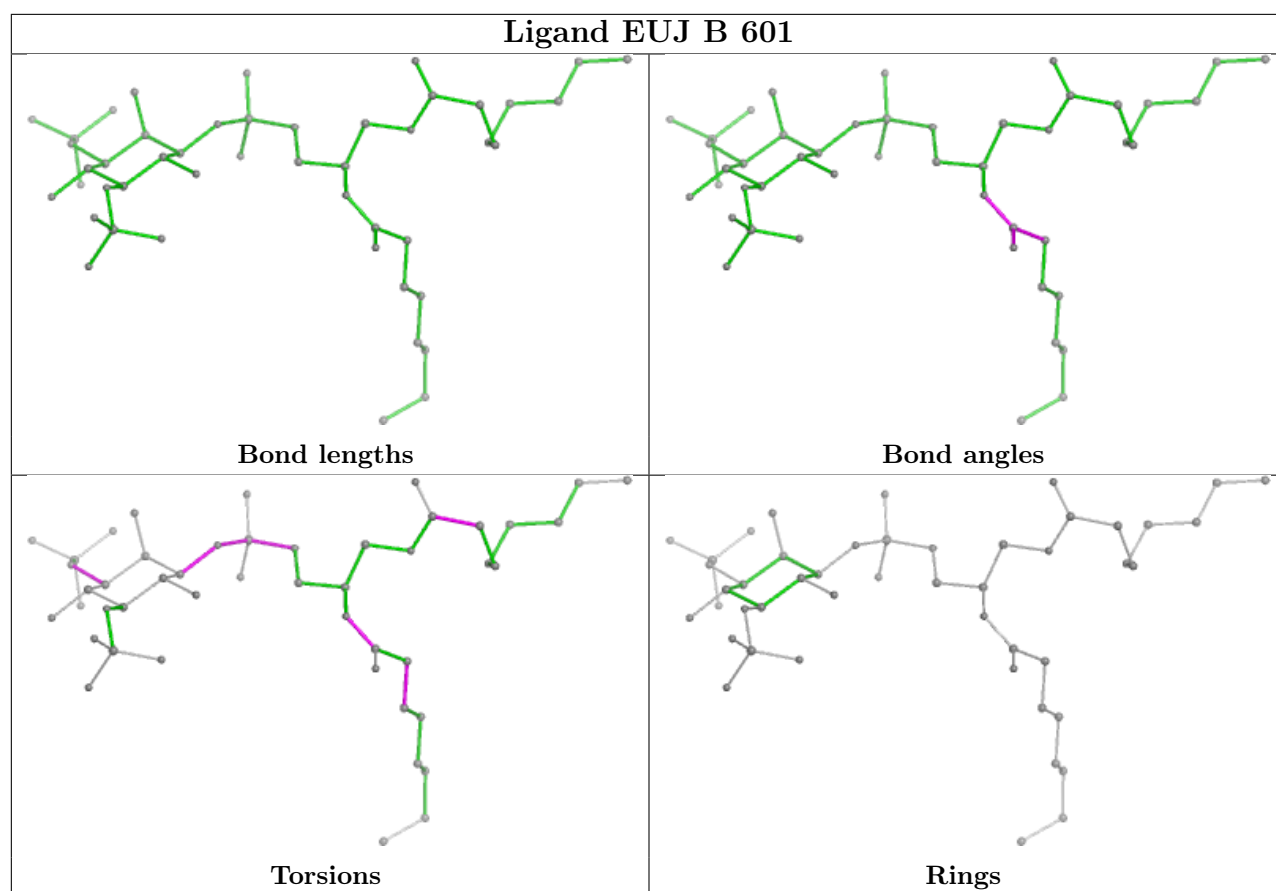
There are no ring outliers.

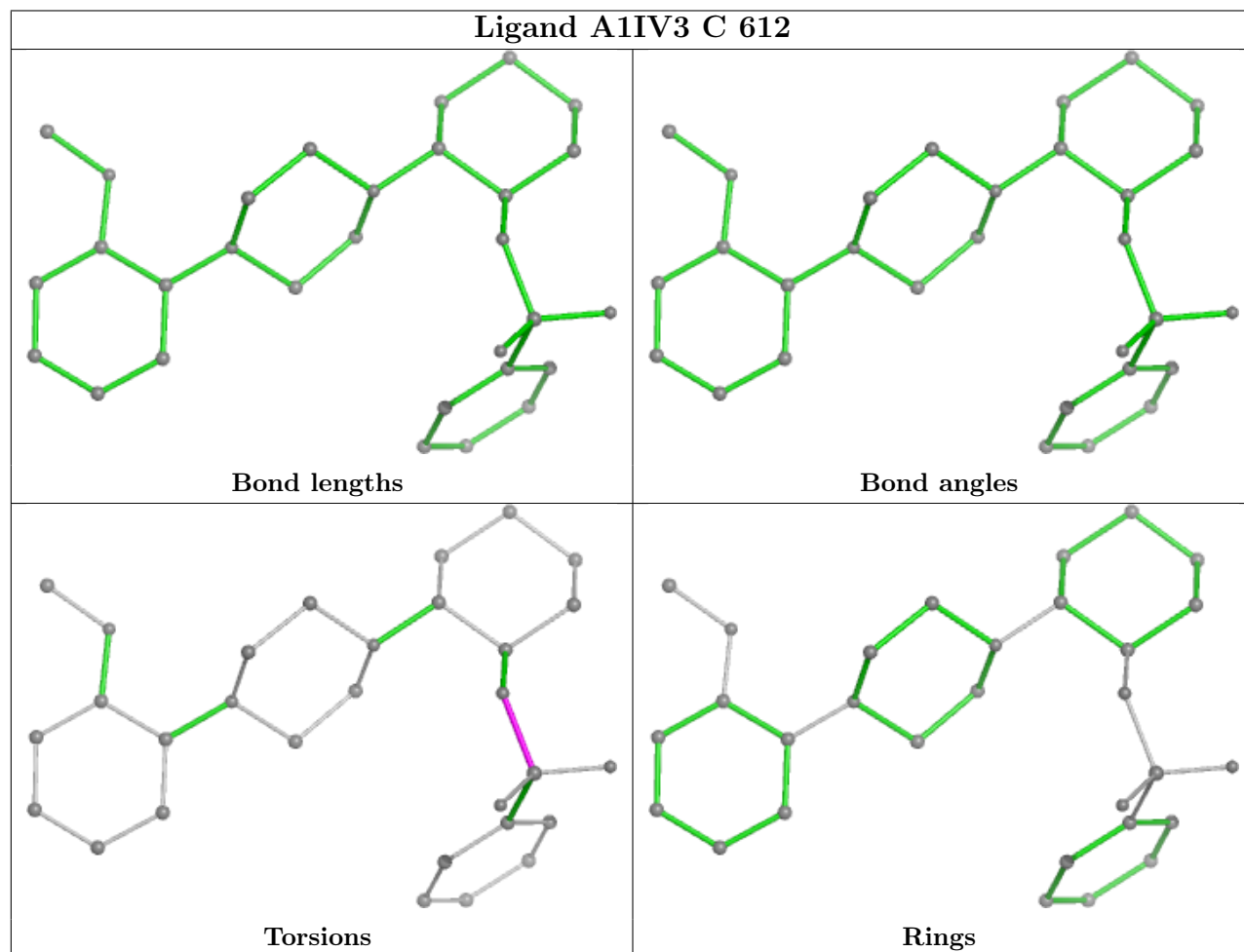
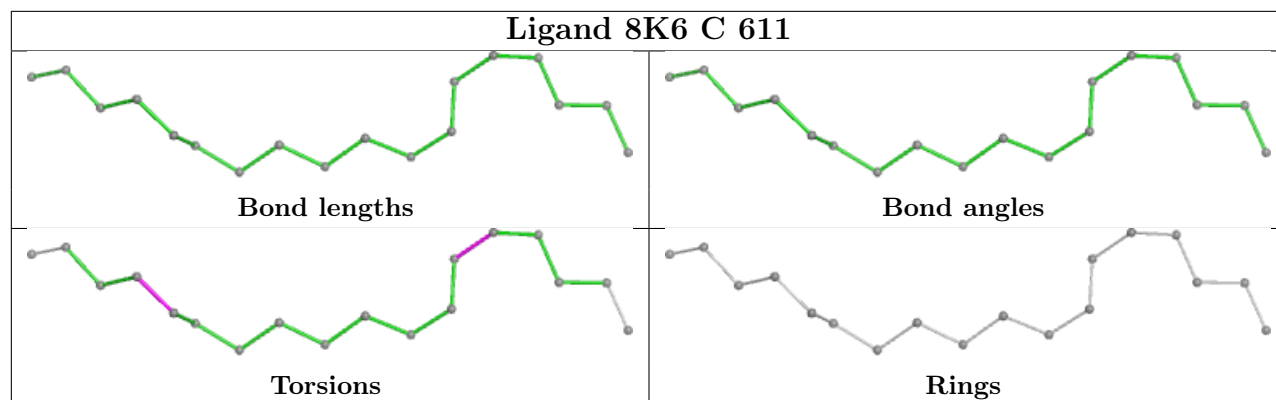
No monomer is involved in short contacts.

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 than 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.

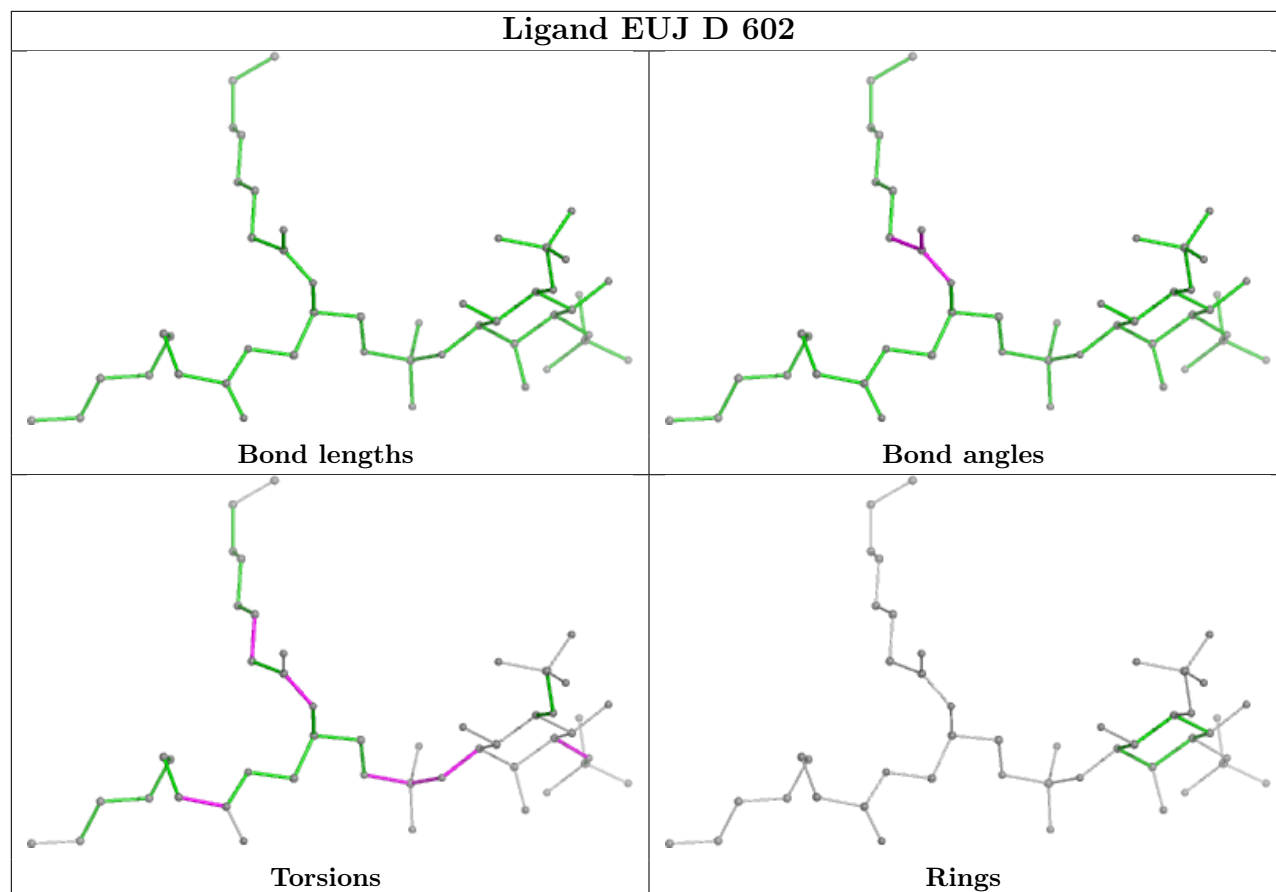




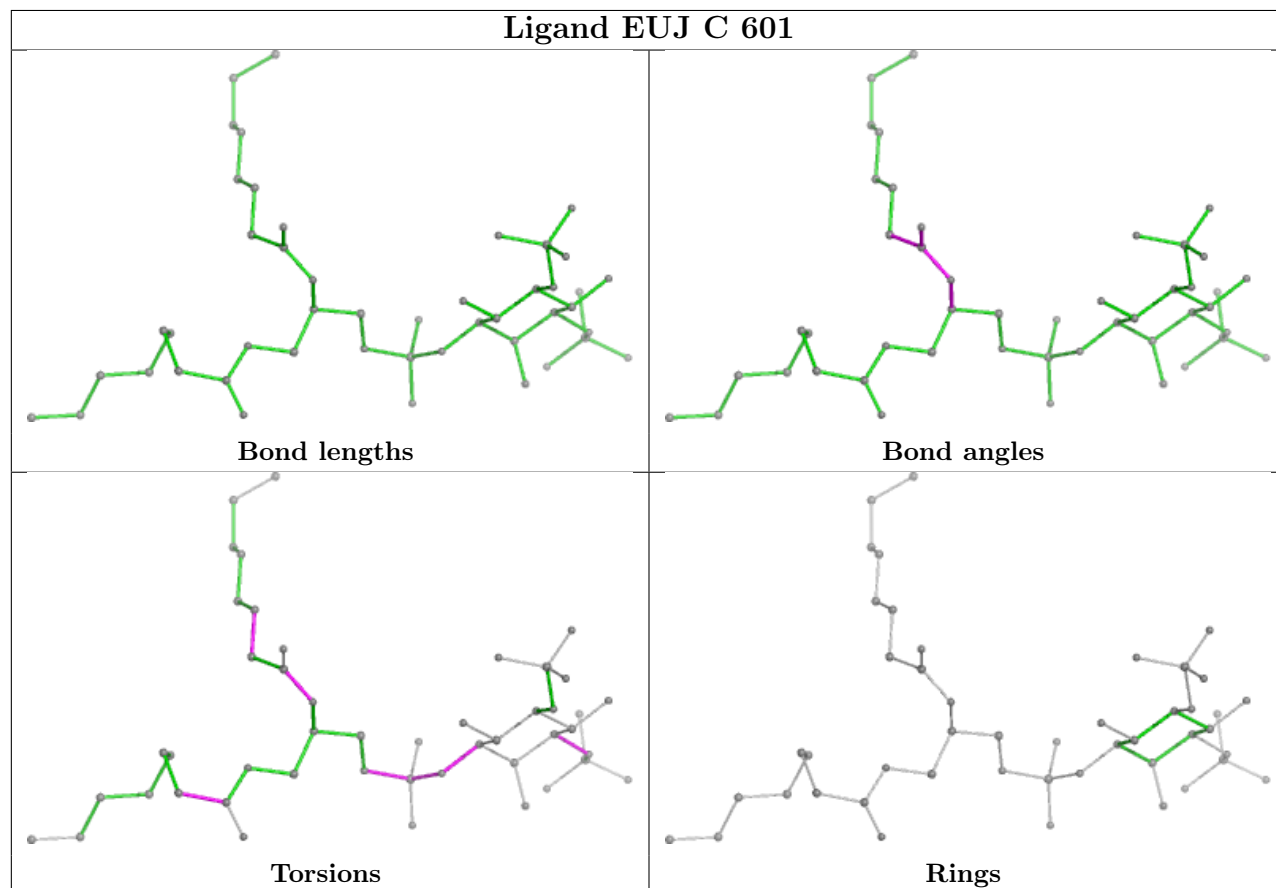


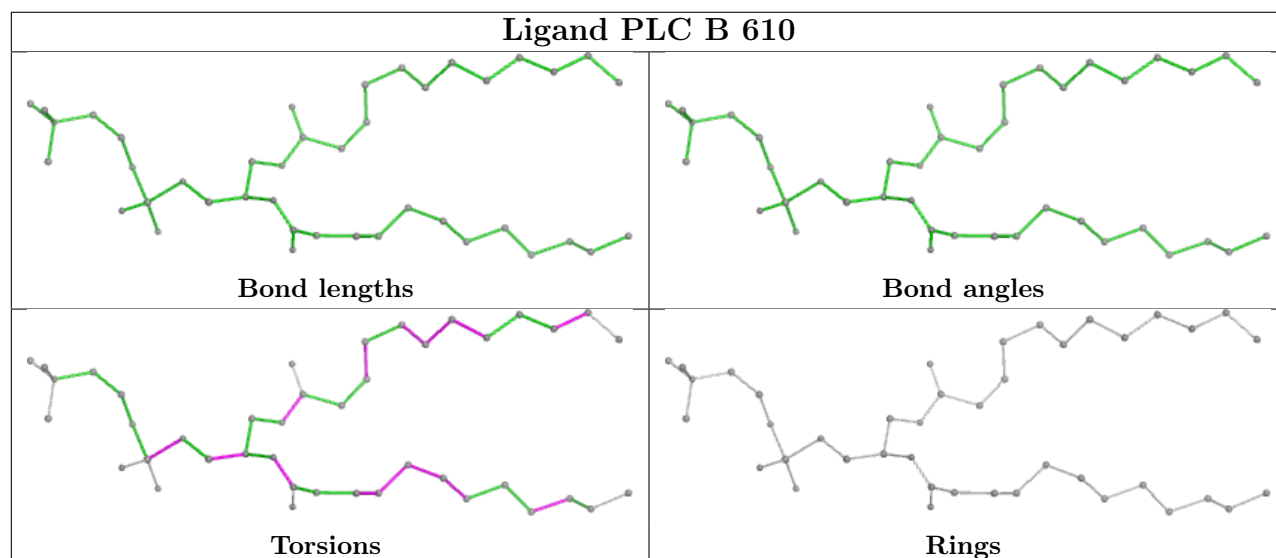
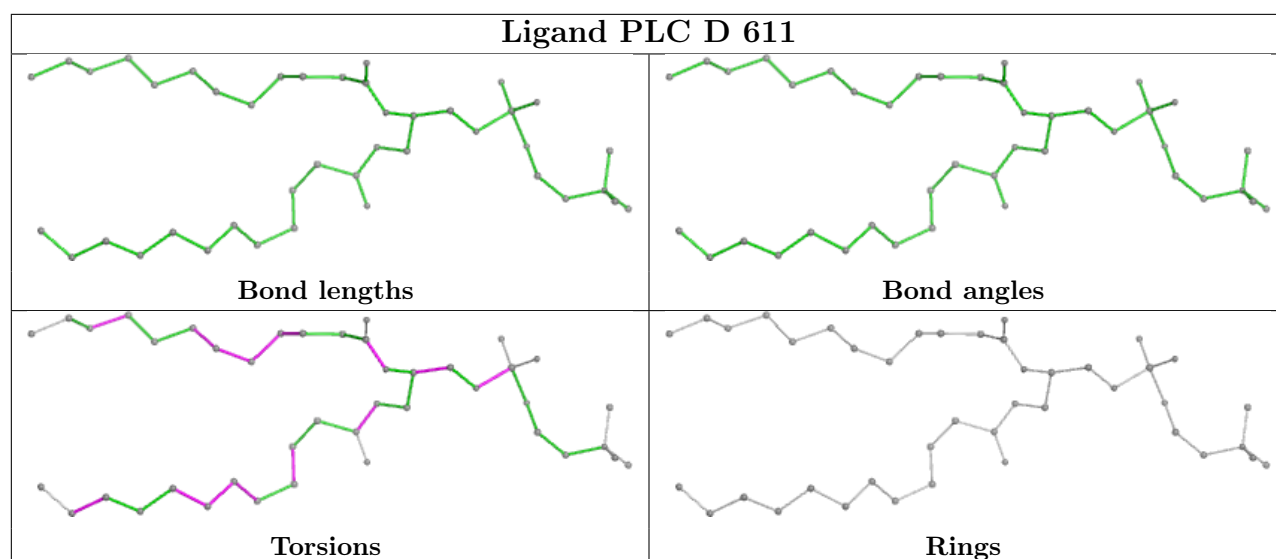


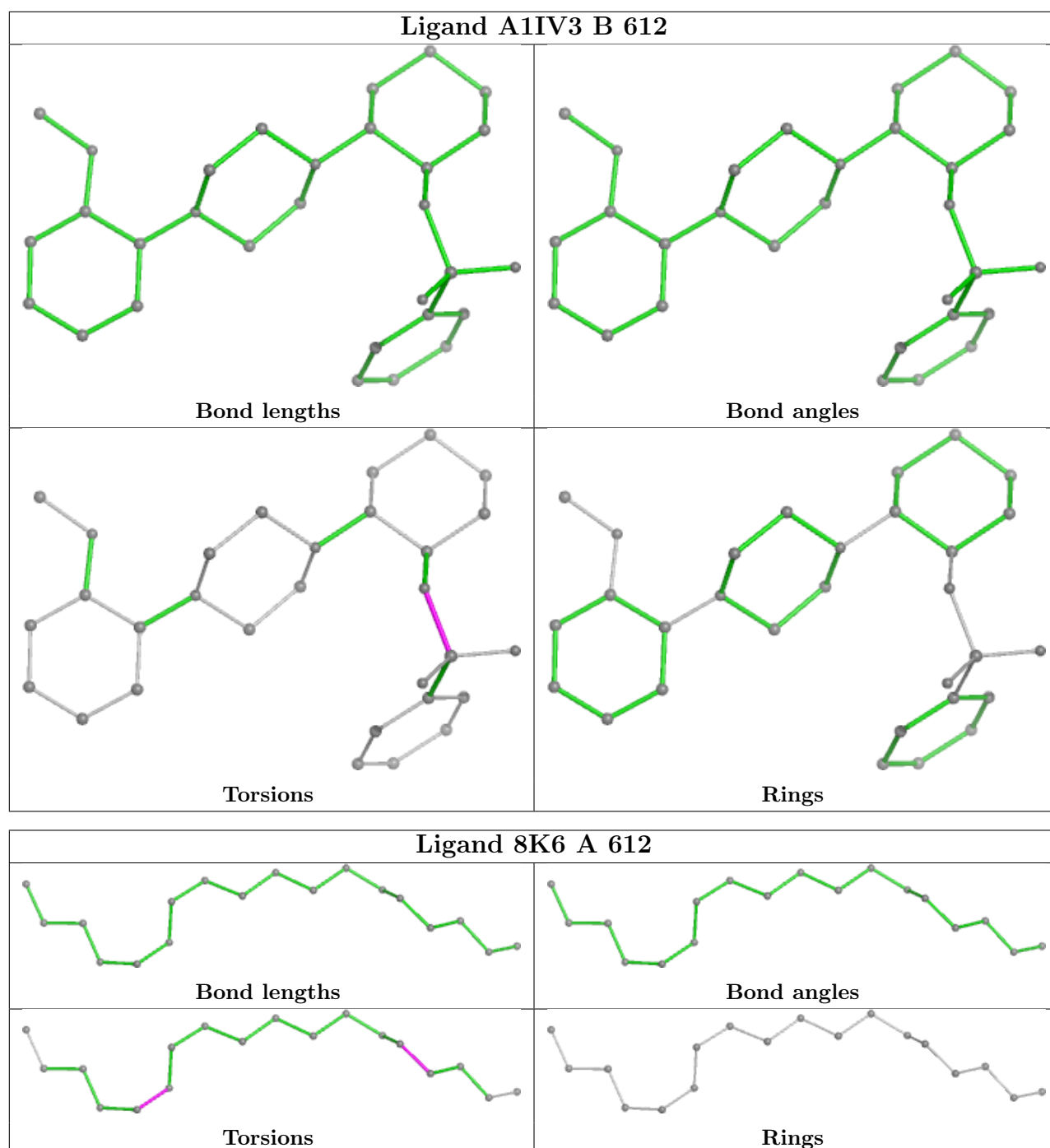
Ligand EUJ D 602

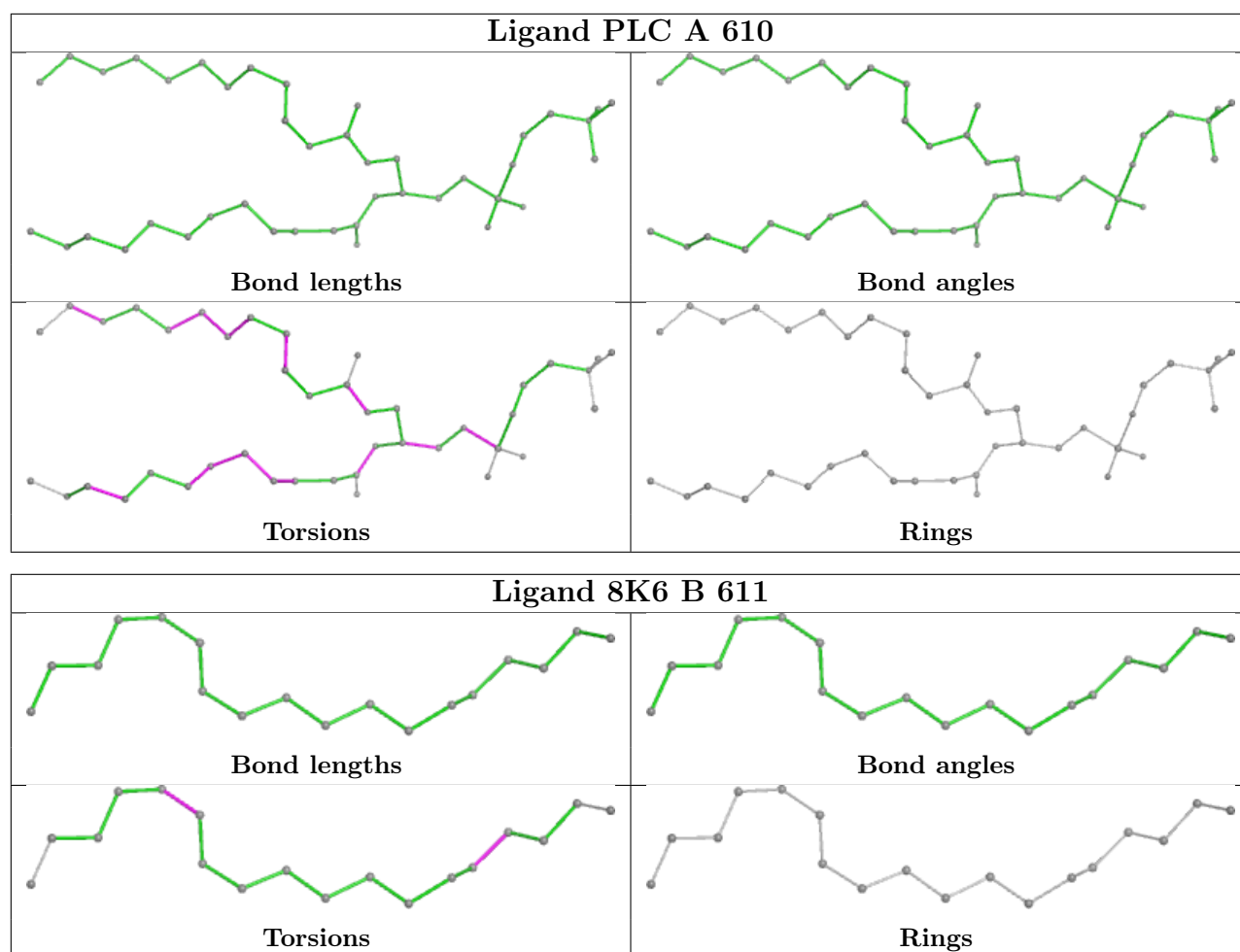


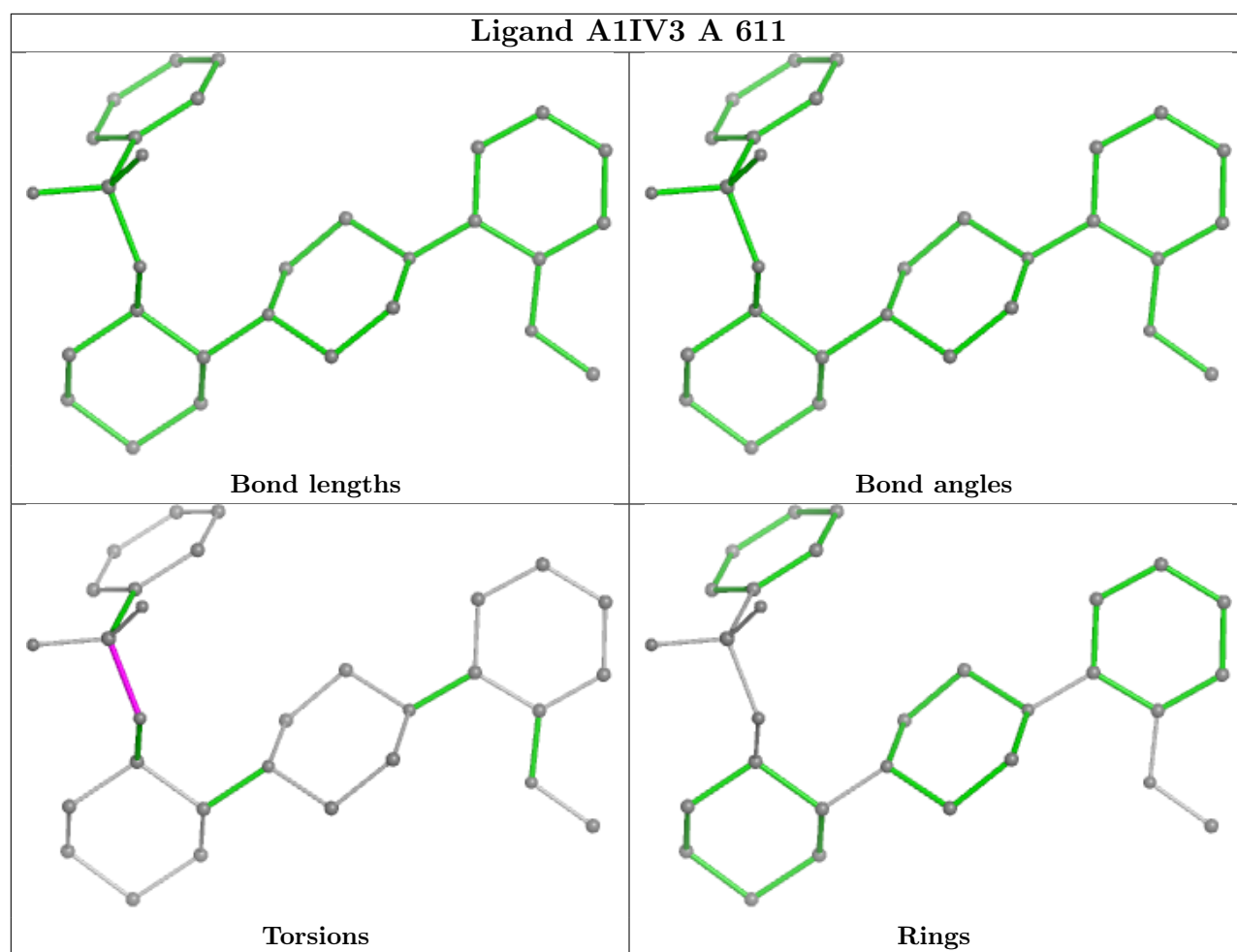
Ligand EUJ C 601











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.

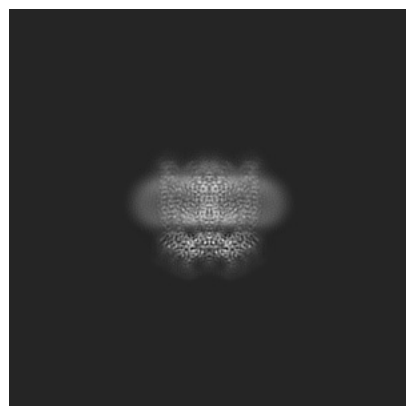
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52248. These allow visual inspection of the internal detail of the map and identification of artifacts.

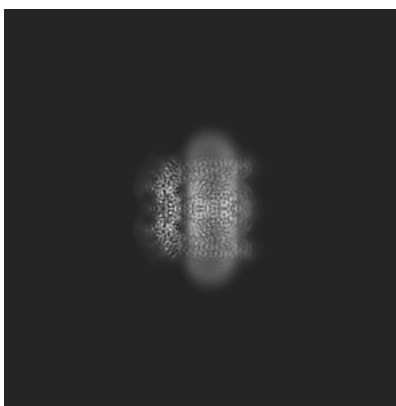
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

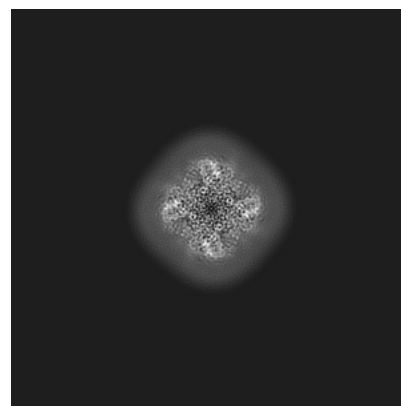
5.1.1 Primary map



X

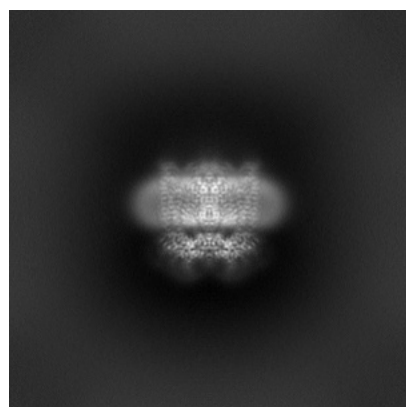


Y

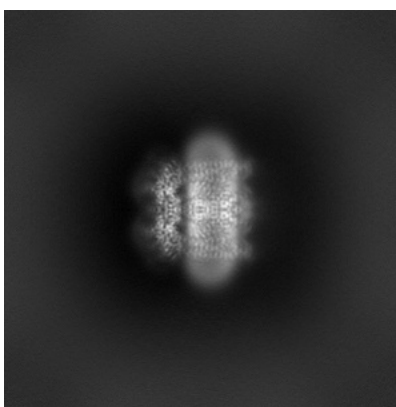


Z

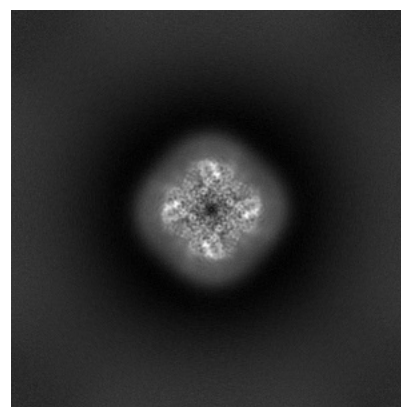
5.1.2 Raw map



X



Y

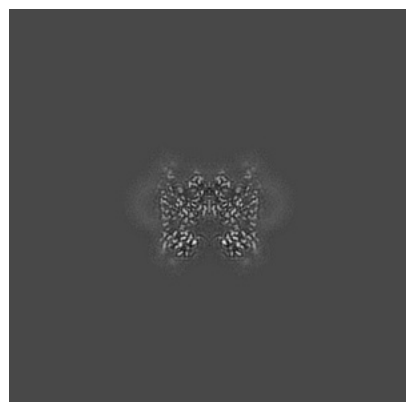


Z

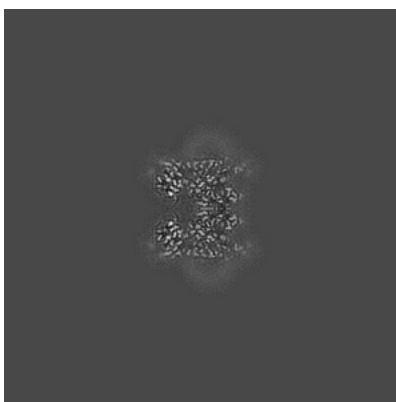
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

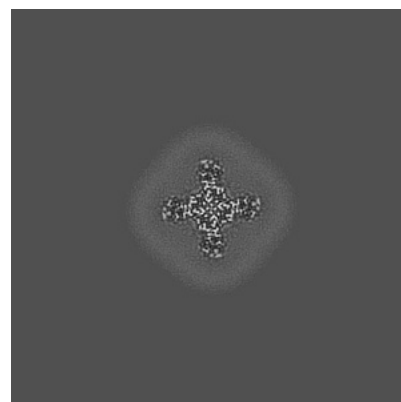
5.2.1 Primary map



X Index: 295

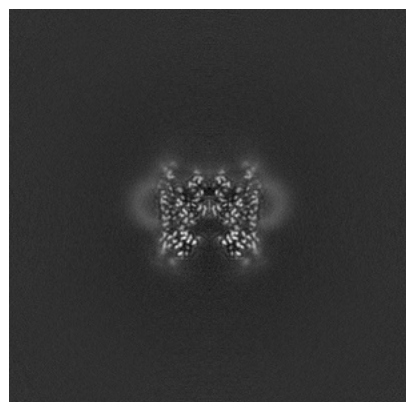


Y Index: 295

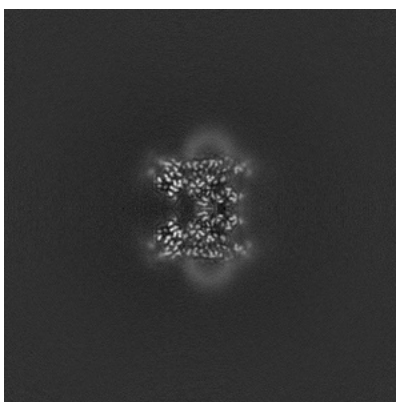


Z Index: 295

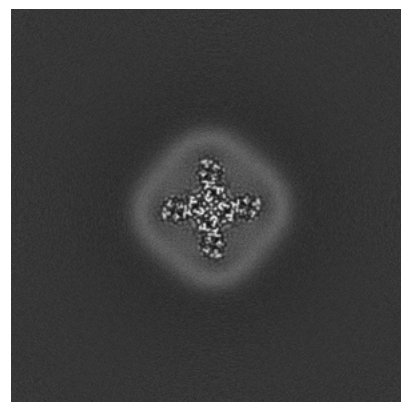
5.2.2 Raw map



X Index: 295



Y Index: 295

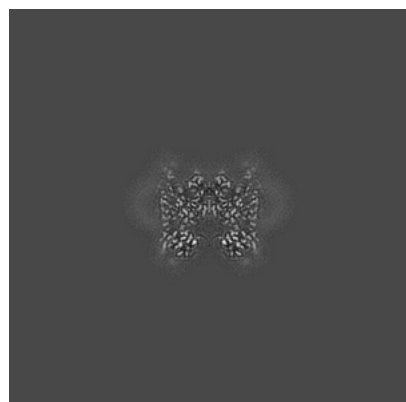


Z Index: 295

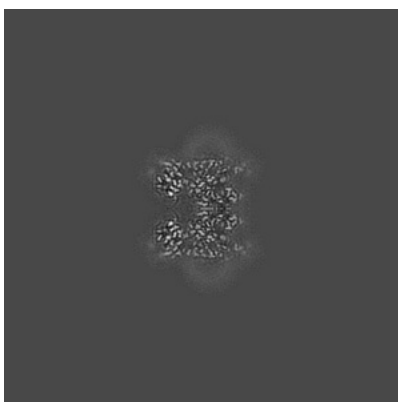
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

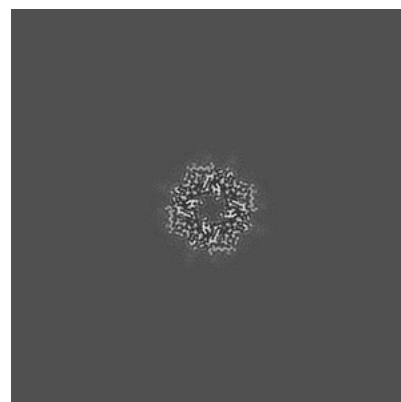
5.3.1 Primary map



X Index: 295

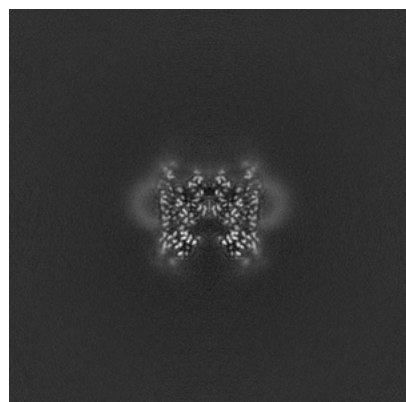


Y Index: 295

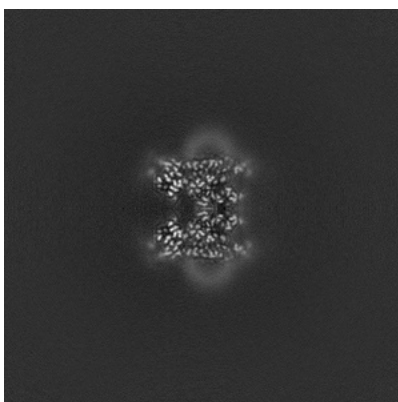


Z Index: 239

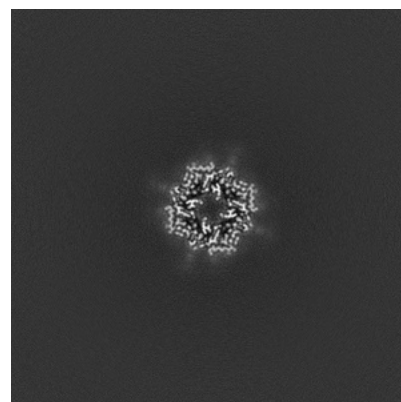
5.3.2 Raw map



X Index: 295



Y Index: 295

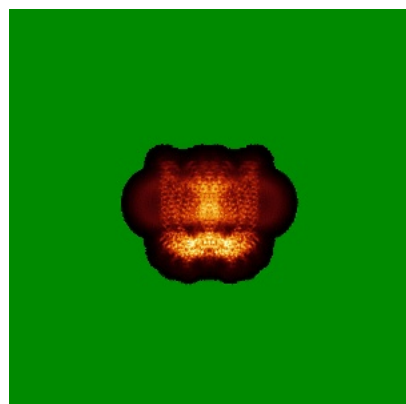


Z Index: 239

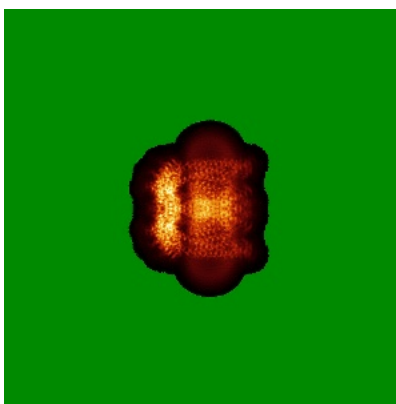
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

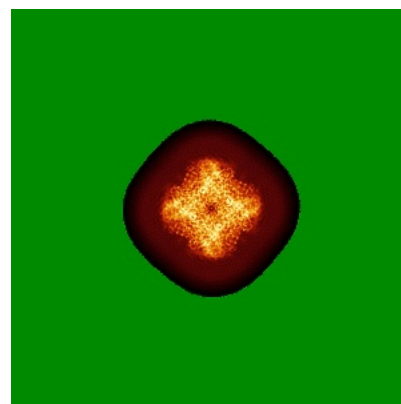
5.4.1 Primary map



X

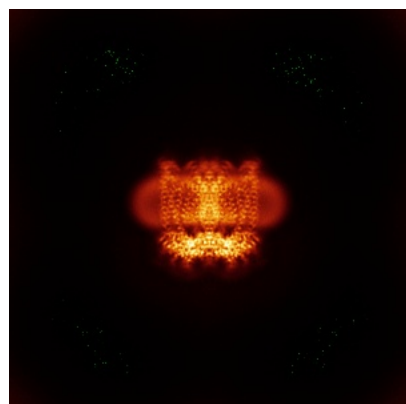


Y

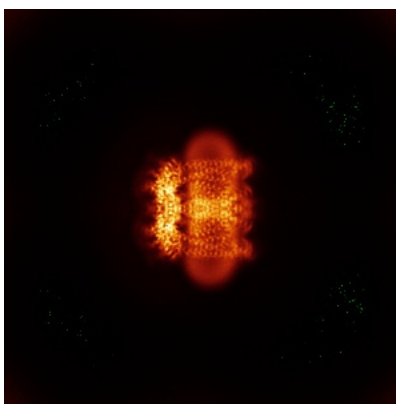


Z

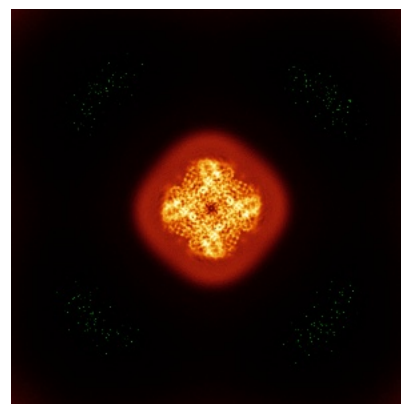
5.4.2 Raw map



X



Y

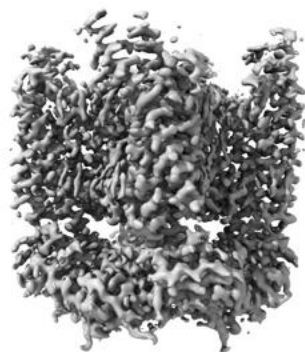


Z

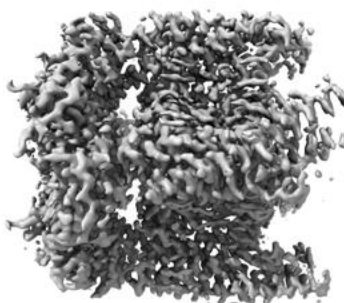
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

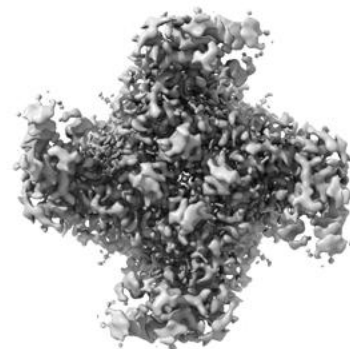
5.5.1 Primary map



X



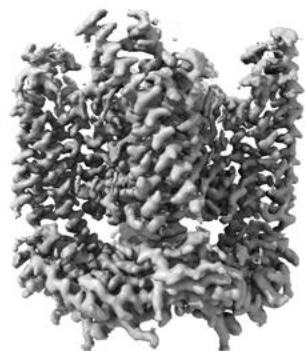
Y



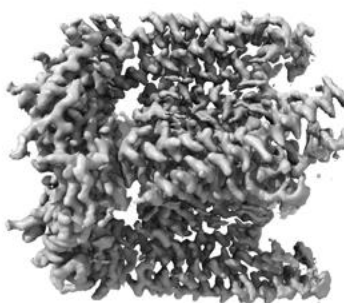
Z

The images above show the 3D surface view of the map at the recommended contour level 0.417. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

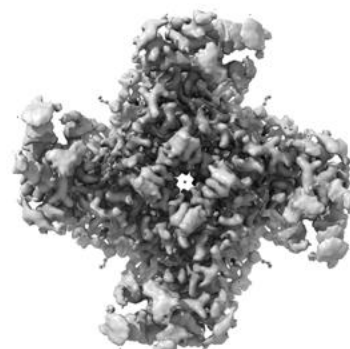
5.5.2 Raw map



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.

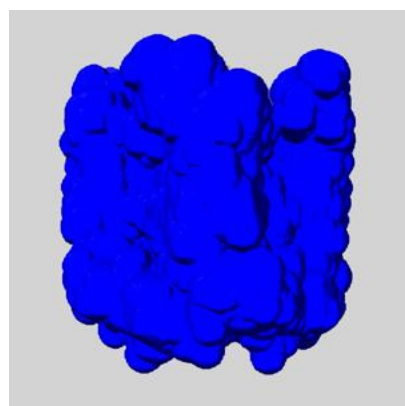
5.6 Mask visualisation [i](#)

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

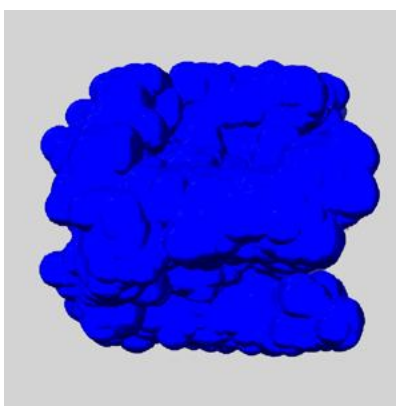
A mask typically either:

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

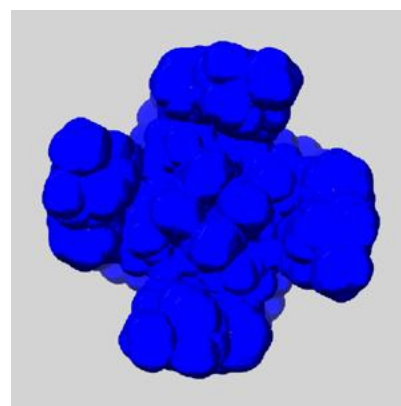
5.6.1 emd_52248_msk_1.map [i](#)



X



Y

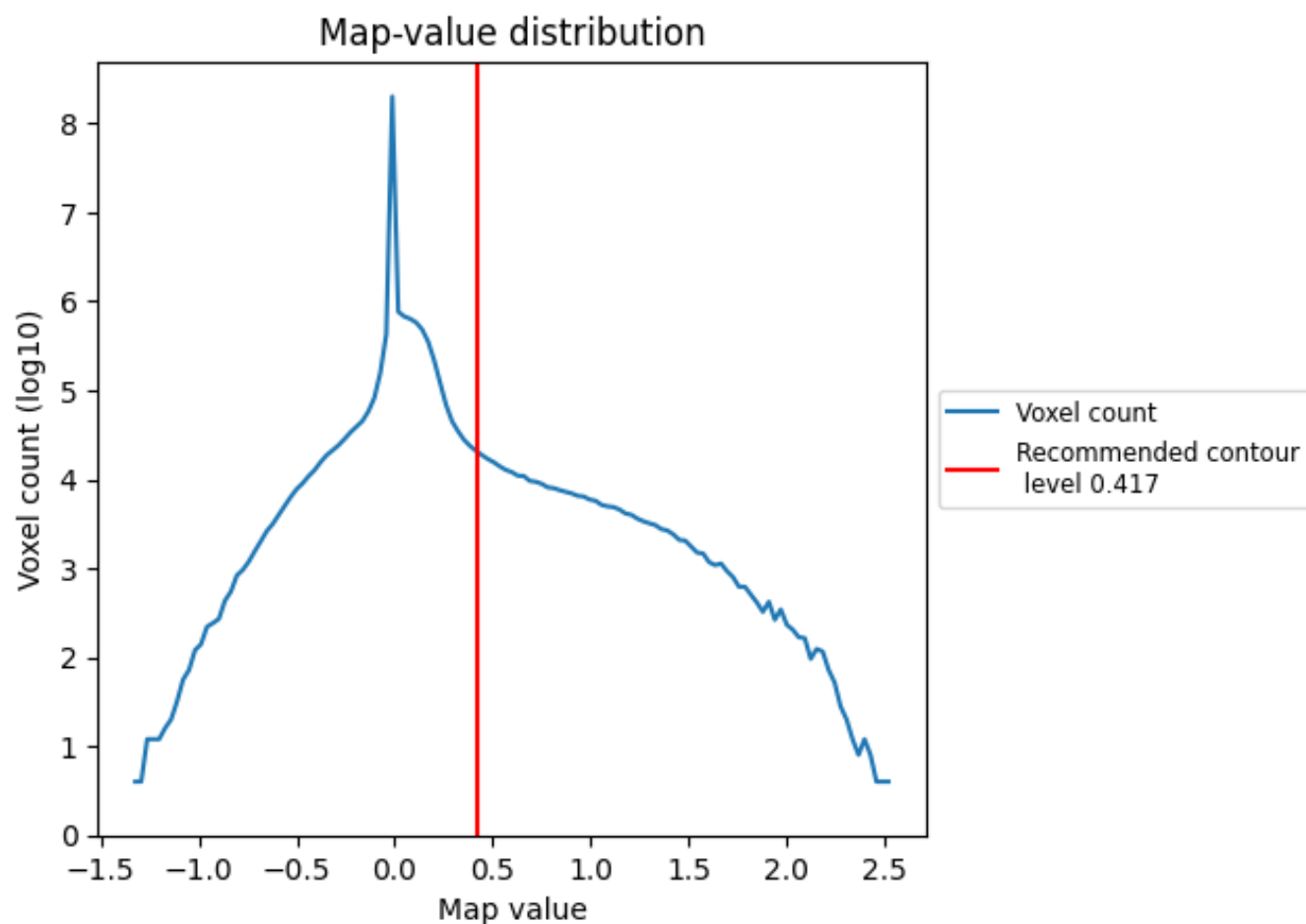


Z

6 Map analysis [i](#)

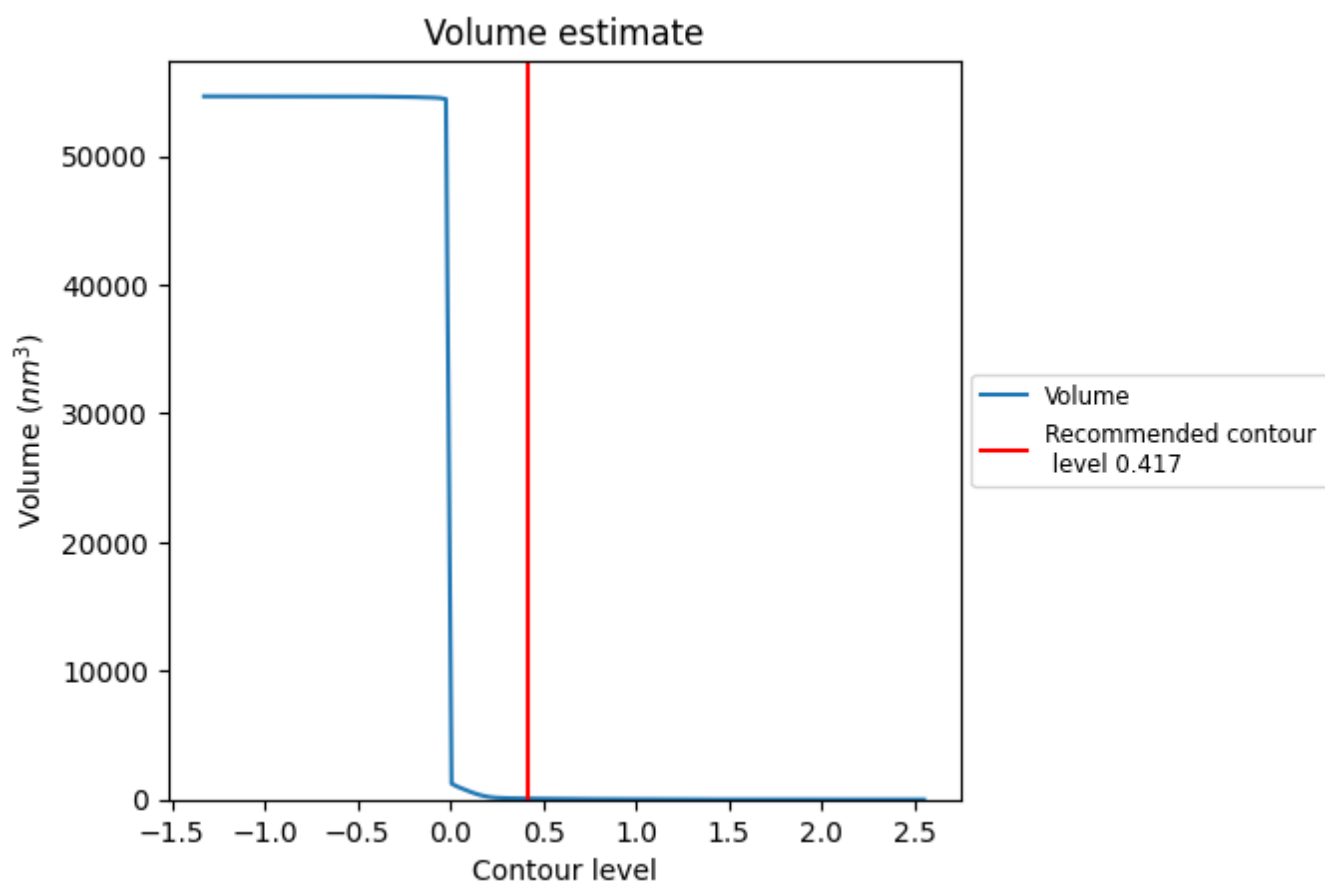
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



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.

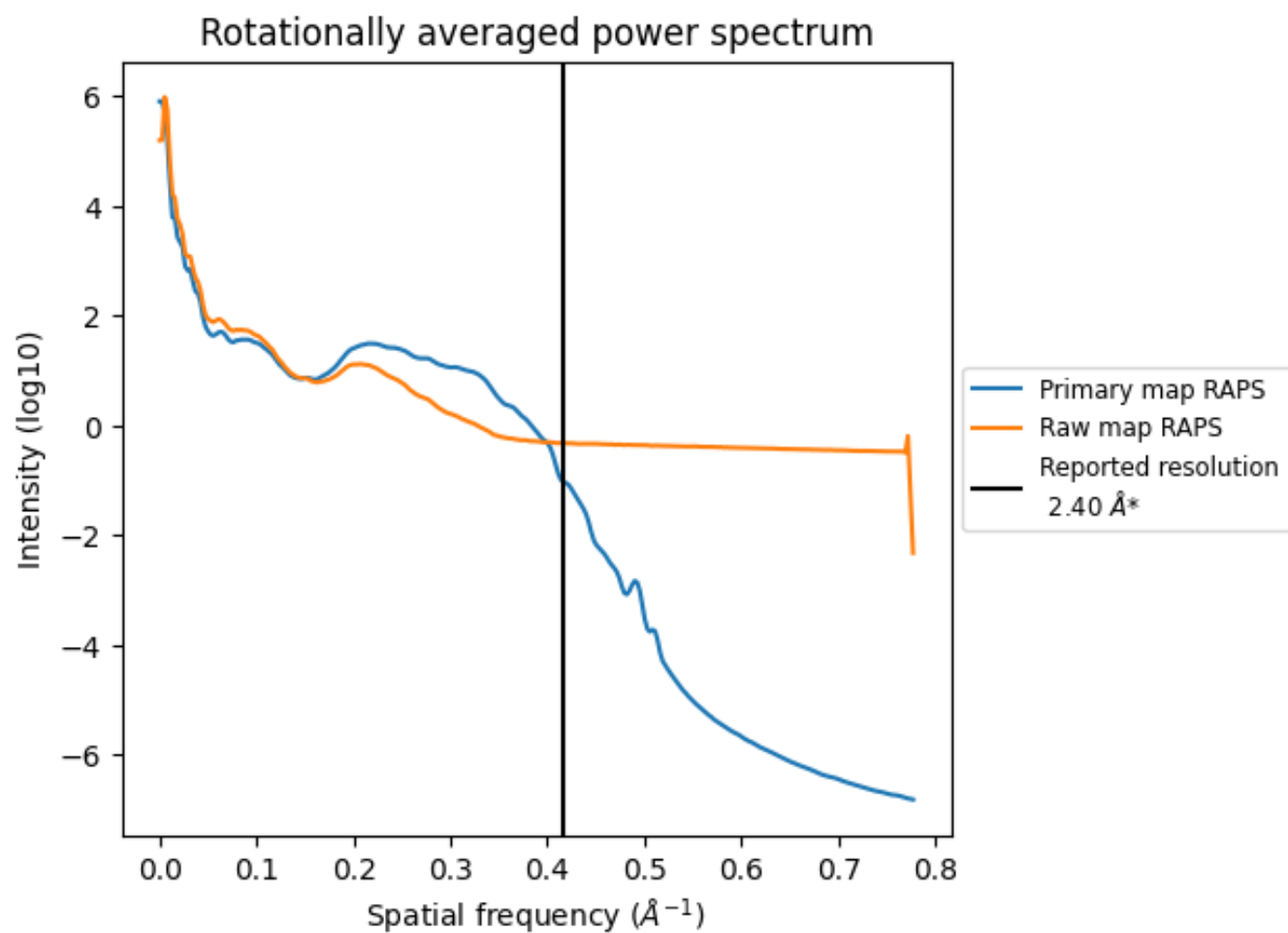
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 69 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](#)

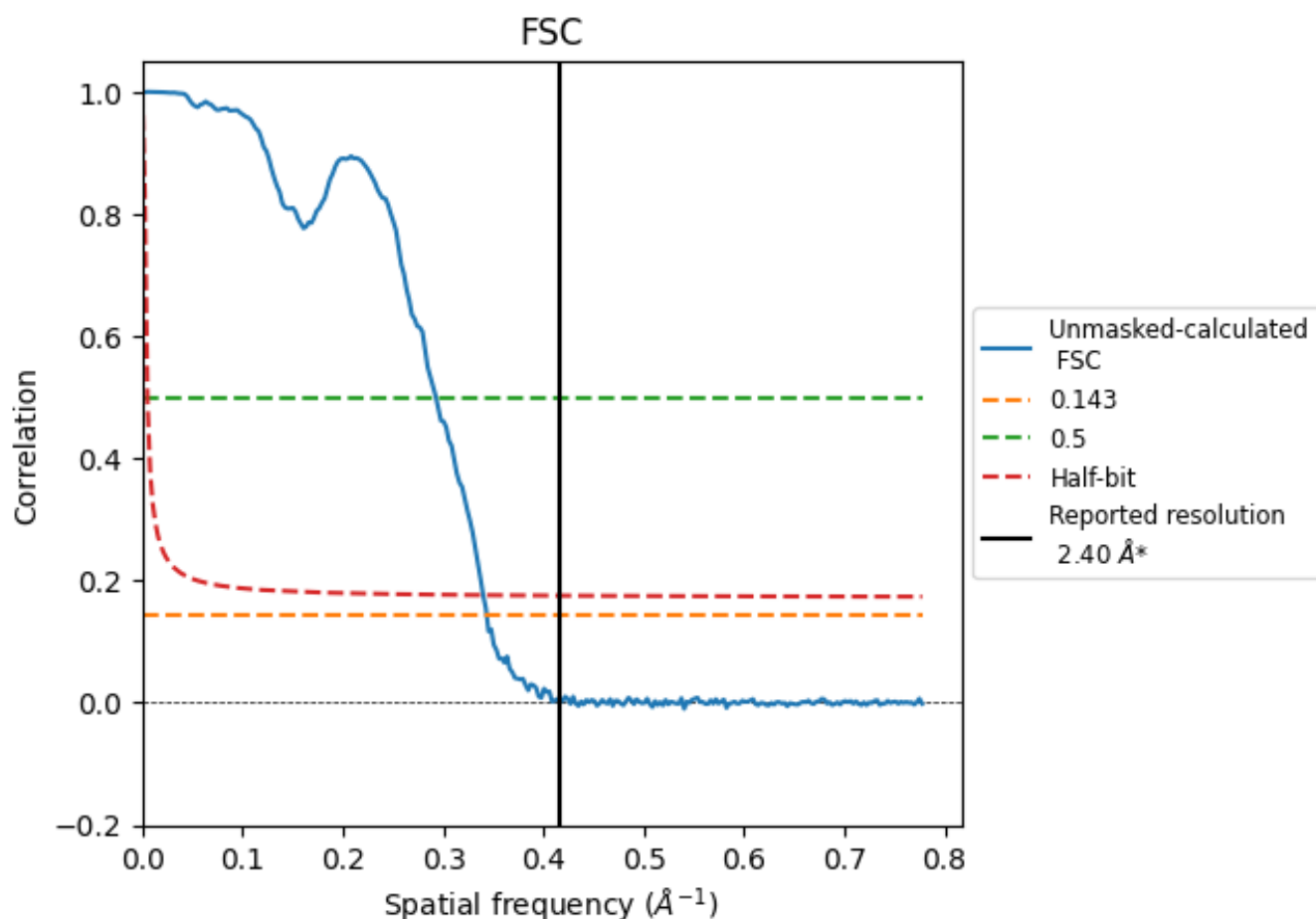


*Reported resolution corresponds to spatial frequency of 0.417\AA^{-1}

7 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

7.2 Resolution estimates [i](#)

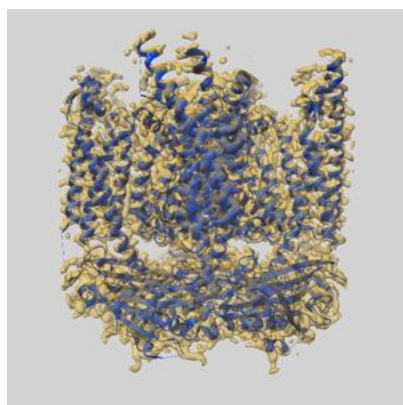
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.91	3.42	2.94

*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 2.91 differs from the reported value 2.4 by more than 10 %

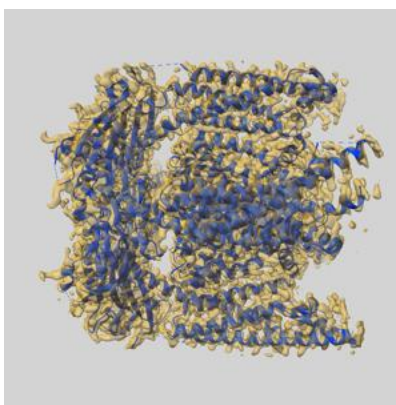
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52248 and PDB model 9HLA. Per-residue inclusion information can be found in section ?? on page ??.

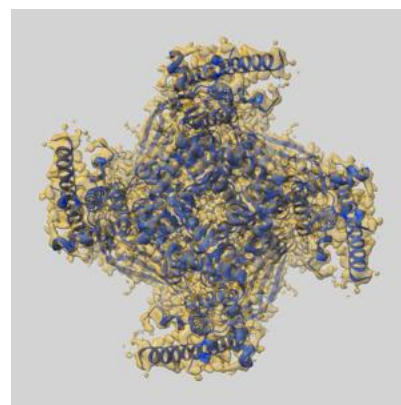
8.1 Map-model overlay [i](#)



X



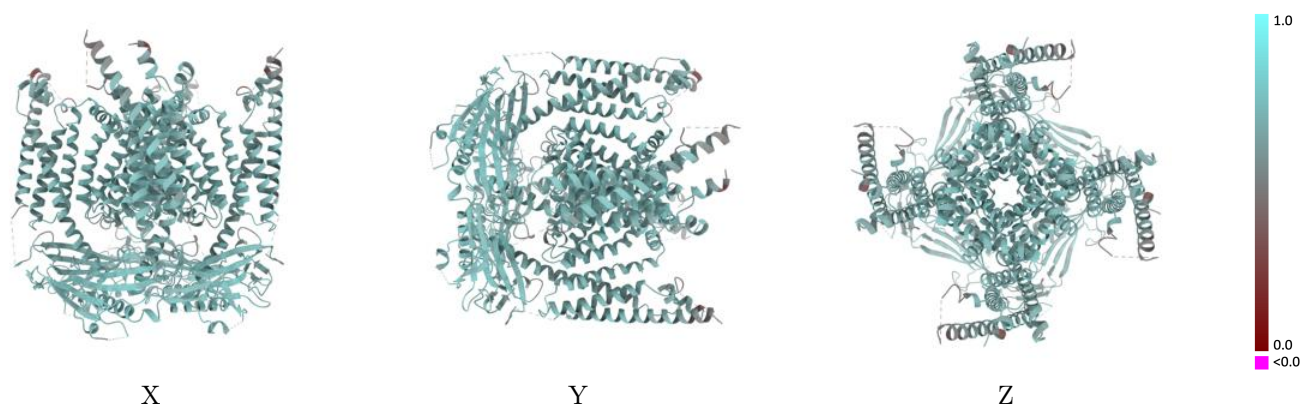
Y



Z

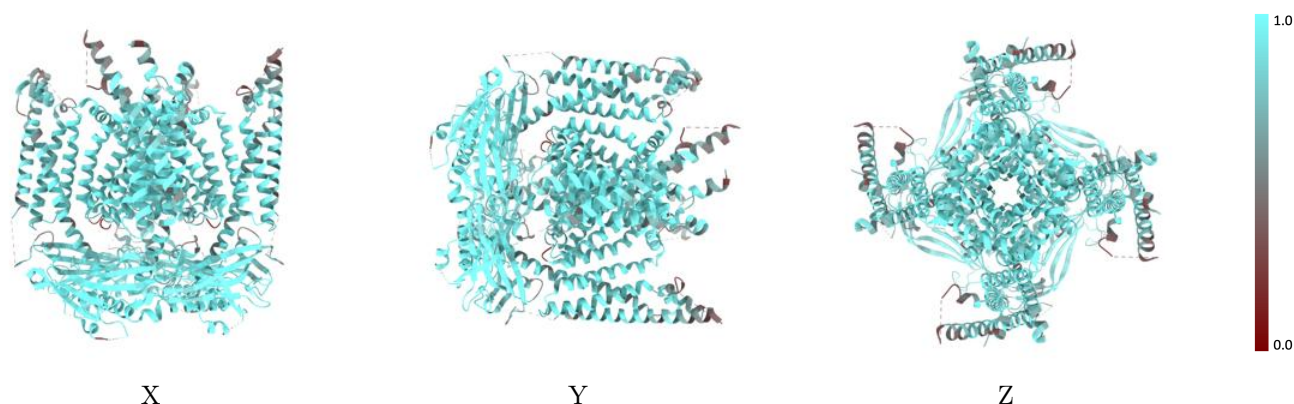
The images above show the 3D surface view of the map at the recommended contour level 0.417 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model [i](#)



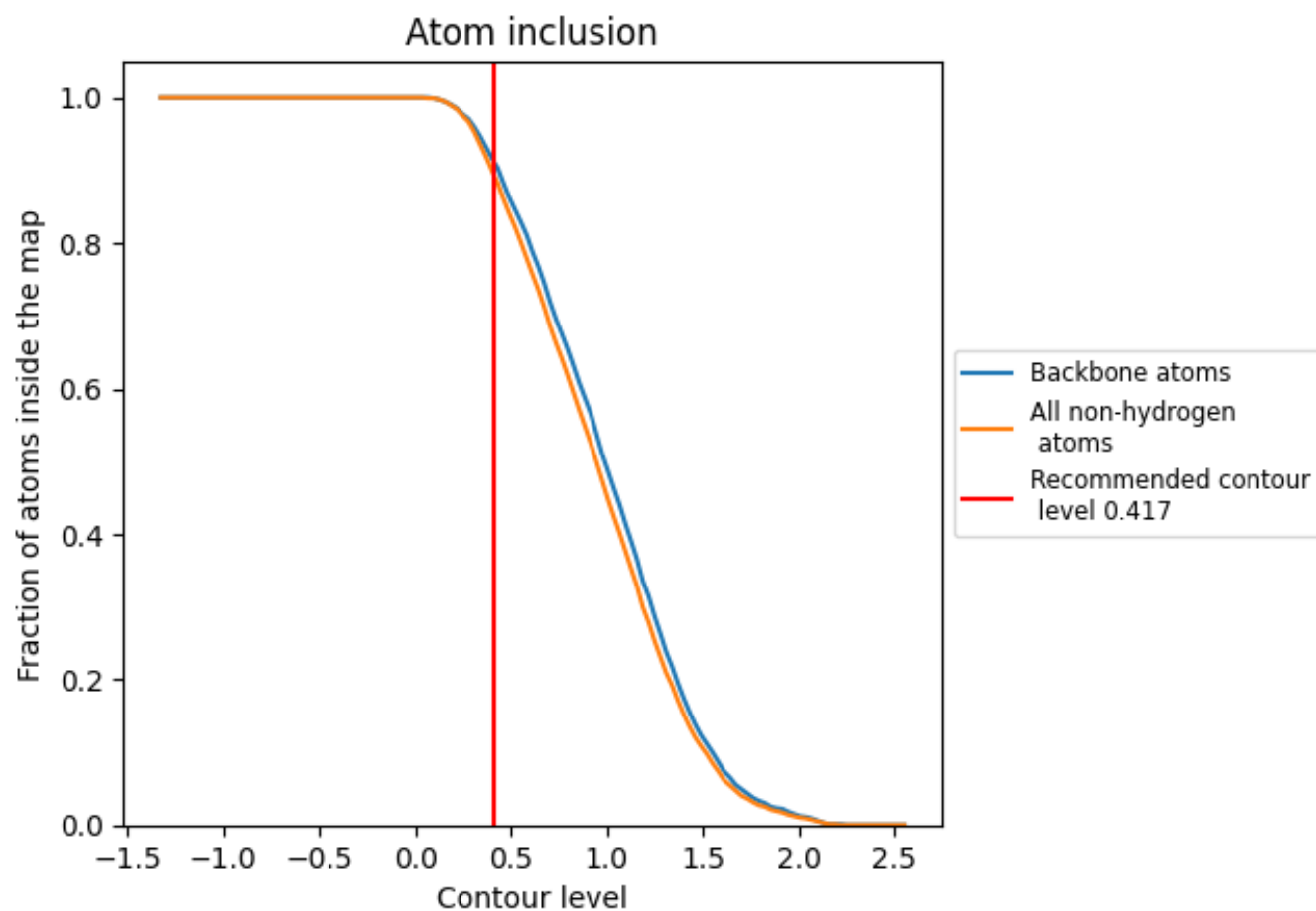
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.417).

8.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.417) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8910	<div><div></div></div> 0.6590
A	<div><div></div></div> 0.8940	<div><div></div></div> 0.6600
B	<div><div></div></div> 0.8940	<div><div></div></div> 0.6590
C	<div><div></div></div> 0.8930	<div><div></div></div> 0.6600
D	<div><div></div></div> 0.8930	<div><div></div></div> 0.6590
E	<div><div></div></div> 0.8930	<div><div></div></div> 0.6230
F	<div><div></div></div> 0.8930	<div><div></div></div> 0.6210
G	<div><div></div></div> 0.8930	<div><div></div></div> 0.6210
H	<div><div></div></div> 0.8930	<div><div></div></div> 0.6200

