Full wwPDB EM Validation Report (i)

Mar 5, 2026 – 06:44 PM UTC

PDB ID	:	9BVJ / pdb_00009bvj
EMDB ID	:	EMD-44934
Title	:	Homomeric alpha3 glycine receptor in the presence of 1 mM glycine in an desensitized state.
Authors	:	Kindig, K.; Gibbs, E.; Chakrapani, S.
Deposited on	:	2024-05-20
Resolution	:	2.80 Å(reported)

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 (i) symbol.

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

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

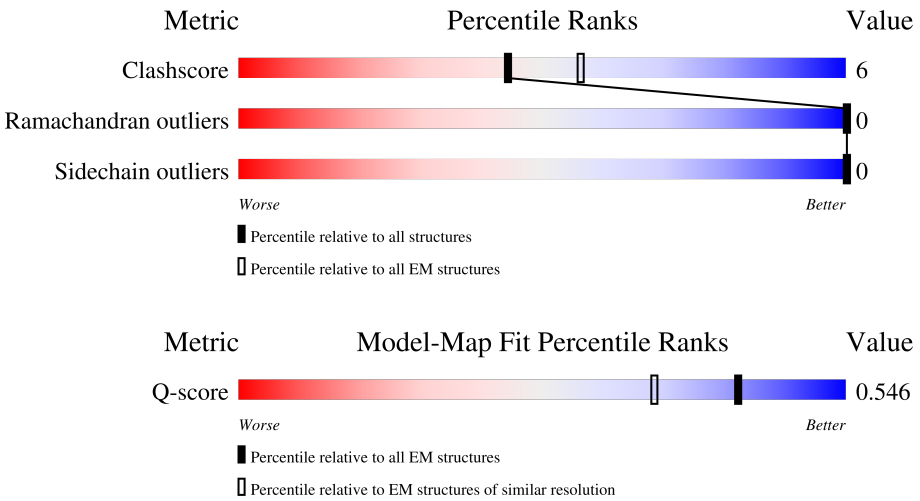
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	59% 12% 28%
1	B	478	59% 13% 28%
1	C	478	59% 12% 28%
1	D	478	59% 13% 28%

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Mol	Chain	Length	Quality of chain
1	E	478	58% 13% 28%
2	F	2	50% 50% 50%
2	G	2	50% 50% 50%
2	H	2	50% 50% 50%
2	I	2	50% 50% 50%
2	J	2	50% 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	A	501	-	X	-	-
3	GLY	A	511	-	X	-	-
3	GLY	B	501	-	X	-	-
3	GLY	C	501	-	X	-	-
3	GLY	D	501	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14620 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycine receptor subunit alpha-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	342	2787	1817	455	495	20	0	0
1	B	342	2787	1817	455	495	20	0	0
1	C	342	2787	1817	455	495	20	0	0
1	D	342	2787	1817	455	495	20	0	0
1	E	342	2787	1817	455	495	20	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	LEU	-	expression tag	UNP O75311
A	433	VAL	-	expression tag	UNP O75311
A	434	PRO	-	expression tag	UNP O75311
A	435	ARG	-	expression tag	UNP O75311
A	436	GLY	-	expression tag	UNP O75311
A	437	SER	-	expression tag	UNP O75311
A	438	HIS	-	expression tag	UNP O75311
A	439	HIS	-	expression tag	UNP O75311
A	440	HIS	-	expression tag	UNP O75311
A	441	HIS	-	expression tag	UNP O75311
A	442	HIS	-	expression tag	UNP O75311
A	443	HIS	-	expression tag	UNP O75311
A	444	HIS	-	expression tag	UNP O75311
A	445	HIS	-	expression tag	UNP O75311
B	432	LEU	-	expression tag	UNP O75311
B	433	VAL	-	expression tag	UNP O75311
B	434	PRO	-	expression tag	UNP O75311
B	435	ARG	-	expression tag	UNP O75311
B	436	GLY	-	expression tag	UNP O75311
B	437	SER	-	expression tag	UNP O75311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	438	HIS	-	expression tag	UNP O75311
B	439	HIS	-	expression tag	UNP O75311
B	440	HIS	-	expression tag	UNP O75311
B	441	HIS	-	expression tag	UNP O75311
B	442	HIS	-	expression tag	UNP O75311
B	443	HIS	-	expression tag	UNP O75311
B	444	HIS	-	expression tag	UNP O75311
B	445	HIS	-	expression tag	UNP O75311
C	432	LEU	-	expression tag	UNP O75311
C	433	VAL	-	expression tag	UNP O75311
C	434	PRO	-	expression tag	UNP O75311
C	435	ARG	-	expression tag	UNP O75311
C	436	GLY	-	expression tag	UNP O75311
C	437	SER	-	expression tag	UNP O75311
C	438	HIS	-	expression tag	UNP O75311
C	439	HIS	-	expression tag	UNP O75311
C	440	HIS	-	expression tag	UNP O75311
C	441	HIS	-	expression tag	UNP O75311
C	442	HIS	-	expression tag	UNP O75311
C	443	HIS	-	expression tag	UNP O75311
C	444	HIS	-	expression tag	UNP O75311
C	445	HIS	-	expression tag	UNP O75311
D	432	LEU	-	expression tag	UNP O75311
D	433	VAL	-	expression tag	UNP O75311
D	434	PRO	-	expression tag	UNP O75311
D	435	ARG	-	expression tag	UNP O75311
D	436	GLY	-	expression tag	UNP O75311
D	437	SER	-	expression tag	UNP O75311
D	438	HIS	-	expression tag	UNP O75311
D	439	HIS	-	expression tag	UNP O75311
D	440	HIS	-	expression tag	UNP O75311
D	441	HIS	-	expression tag	UNP O75311
D	442	HIS	-	expression tag	UNP O75311
D	443	HIS	-	expression tag	UNP O75311
D	444	HIS	-	expression tag	UNP O75311
D	445	HIS	-	expression tag	UNP O75311
E	432	LEU	-	expression tag	UNP O75311
E	433	VAL	-	expression tag	UNP O75311
E	434	PRO	-	expression tag	UNP O75311
E	435	ARG	-	expression tag	UNP O75311
E	436	GLY	-	expression tag	UNP O75311
E	437	SER	-	expression tag	UNP O75311

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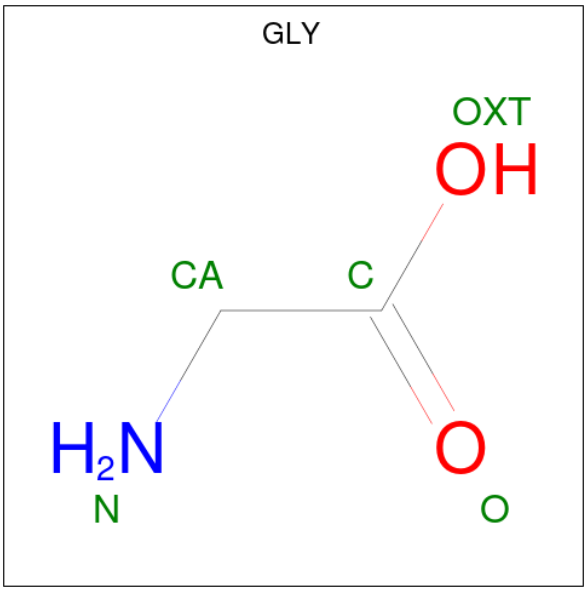
Chain	Residue	Modelled	Actual	Comment	Reference
E	438	HIS	-	expression tag	UNP O75311
E	439	HIS	-	expression tag	UNP O75311
E	440	HIS	-	expression tag	UNP O75311
E	441	HIS	-	expression tag	UNP O75311
E	442	HIS	-	expression tag	UNP O75311
E	443	HIS	-	expression tag	UNP O75311
E	444	HIS	-	expression tag	UNP O75311
E	445	HIS	-	expression tag	UNP O75311

- 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
			Total	C	N	O		
2	F	2	28	16	2	10	0	0
			Total	C	N	O		
2	G	2	28	16	2	10	0	0
			Total	C	N	O		
2	H	2	28	16	2	10	0	0
			Total	C	N	O		
2	I	2	28	16	2	10	0	0
			Total	C	N	O		
2	J	2	28	16	2	10	0	0

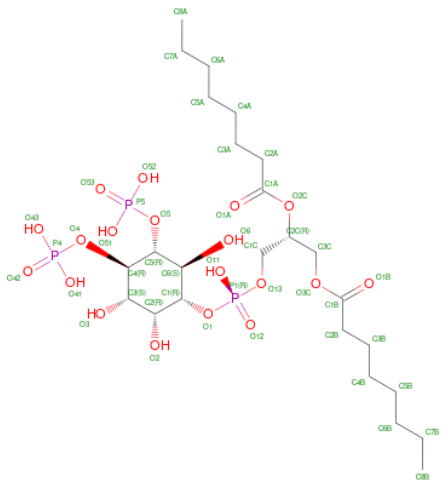
- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: $C_{25}H_{49}O_{19}P_3$).

PIO



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 8	C 6	O 2	0
4	A	1	Total 10	C 8	O 2	0
4	A	1	Total 8	C 6	O 2	0
4	A	1	Total 10	C 8	O 2	0
4	A	1	Total 8	C 6	O 2	0
4	B	1	Total 8	C 6	O 2	0
4	B	1	Total 10	C 8	O 2	0
4	B	1	Total 8	C 6	O 2	0
4	B	1	Total 10	C 8	O 2	0
4	B	1	Total 8	C 6	O 2	0
4	C	1	Total 8	C 6	O 2	0
4	C	1	Total 10	C 8	O 2	0
4	C	1	Total 8	C 6	O 2	0
4	C	1	Total 10	C 8	O 2	0

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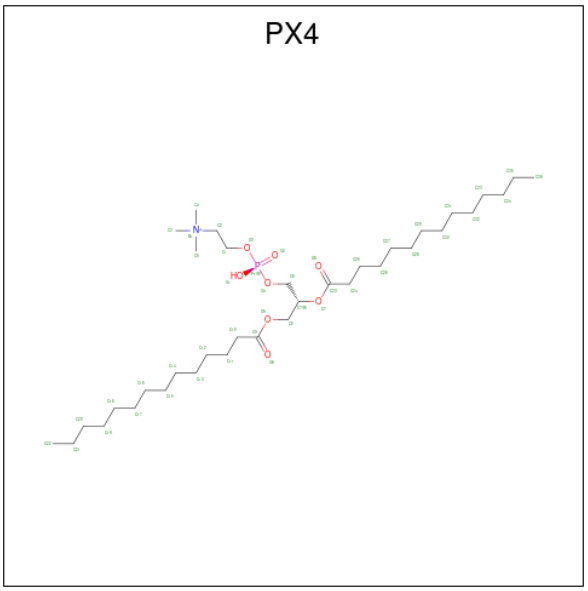
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	O		0
			8	6	2		
4	D	1	Total	C	O		0
			8	6	2		
4	D	1	Total	C	O		0
			10	8	2		
4	D	1	Total	C	O		0
			8	6	2		
4	D	1	Total	C	O		0
			10	8	2		
4	D	1	Total	C	O		0
			8	6	2		
4	E	1	Total	C	O		0
			8	6	2		
4	E	1	Total	C	O		0
			8	6	2		
4	E	1	Total	C	O		0
			10	8	2		
4	E	1	Total	C	O		0
			8	6	2		
4	E	1	Total	C	O		0
			10	8	2		

- Molecule 5 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	14	12	2	0
5	A	1	14	12	2	0
5	A	1	16	14	2	0
5	A	1	14	12	2	0
5	B	1	14	12	2	0
5	B	1	14	12	2	0
5	B	1	16	14	2	0
5	B	1	14	12	2	0
5	C	1	14	12	2	0
5	C	1	14	12	2	0
5	C	1	16	14	2	0
5	C	1	14	12	2	0
5	D	1	14	12	2	0
5	D	1	14	12	2	0
5	D	1	16	14	2	0
5	D	1	14	12	2	0
5	E	1	14	12	2	0
5	E	1	16	14	2	0
5	E	1	14	12	2	0
5	E	1	14	12	2	0

- Molecule 6 is water.

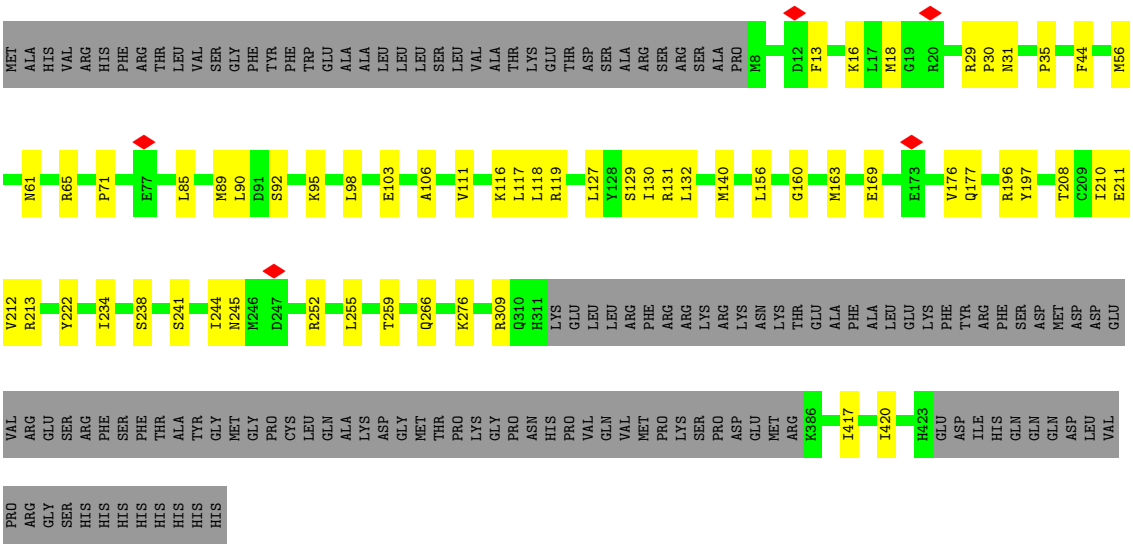
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	A	2	2	2	0
			Total	O	
6	B	2	2	2	0
			Total	O	
6	C	2	2	2	0
			Total	O	
6	D	2	2	2	0
			Total	O	
6	E	2	2	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

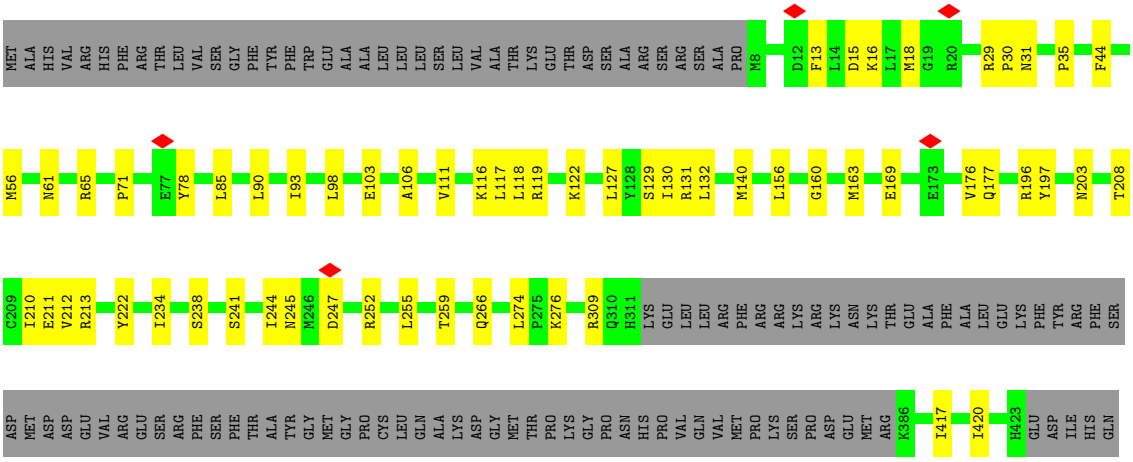
- Molecule 1: Glycine receptor subunit alpha-3

Chain A:



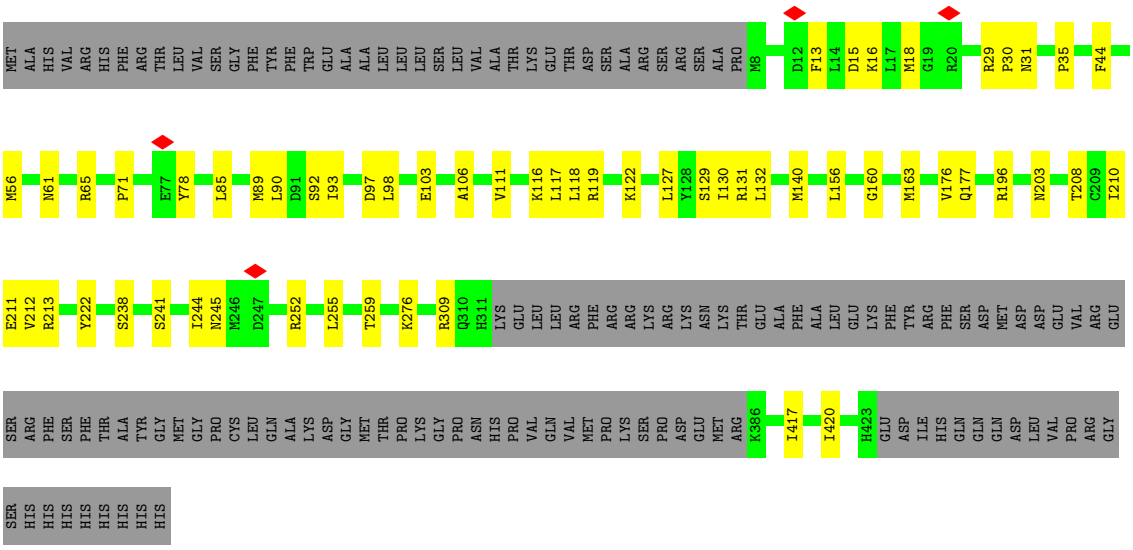
- Molecule 1: Glycine receptor subunit alpha-3

Chain B:



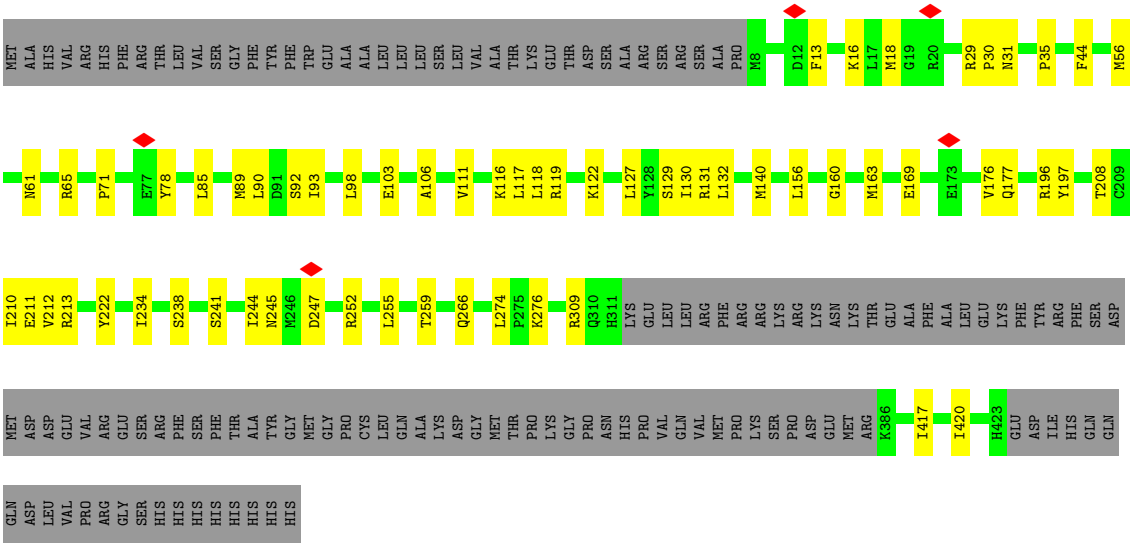
• Molecule 1: Glycine receptor subunit alpha-3

Chain C:



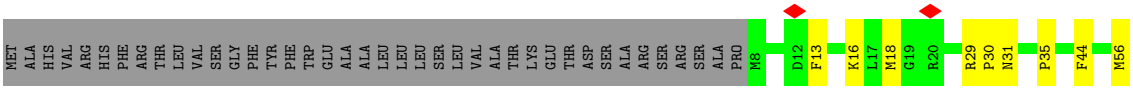
• Molecule 1: Glycine receptor subunit alpha-3

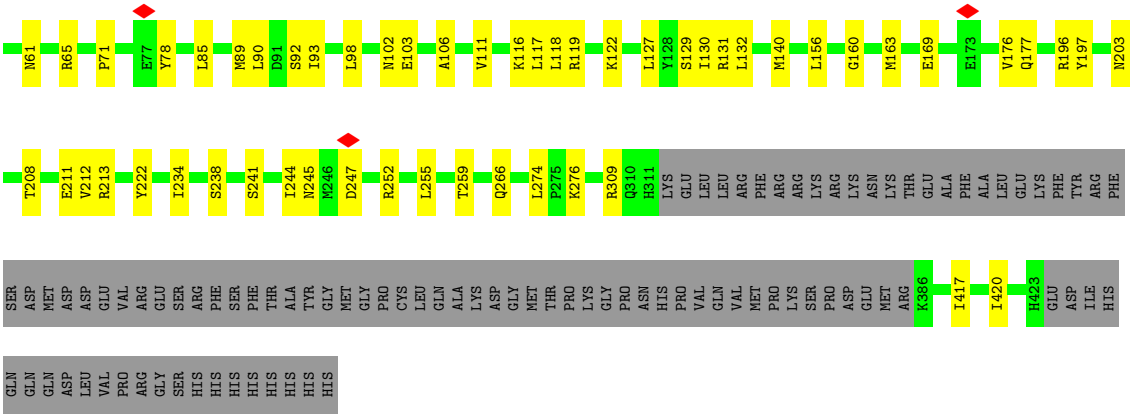
Chain D:



• Molecule 1: Glycine receptor subunit alpha-3

Chain E:





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

Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	435078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0162	Depositor
Map size (Å)	320.7, 320.7, 320.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PX4, PIO, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.22	0/2859	0.49	0/3879
1	B	0.22	0/2859	0.49	0/3879
1	C	0.22	0/2859	0.49	0/3879
1	D	0.22	0/2859	0.49	0/3879
1	E	0.22	0/2859	0.49	0/3879
All	All	0.22	0/14295	0.49	0/19395

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2787	0	2787	40	0
1	B	2787	0	2787	42	0
1	C	2787	0	2787	41	0
1	D	2787	0	2787	43	0
1	E	2787	0	2787	44	0
2	F	28	0	25	1	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	28	0	25	1	0
2	J	28	0	25	1	0
3	A	10	0	4	2	0
3	B	5	0	2	1	0
3	C	5	0	2	1	0
3	D	5	0	2	1	0
4	A	44	0	54	0	0
4	B	44	0	54	0	0
4	C	44	0	54	0	0
4	D	44	0	54	0	0
4	E	44	0	54	0	0
5	A	58	0	87	0	0
5	B	58	0	87	1	0
5	C	58	0	87	1	0
5	D	58	0	87	1	0
5	E	58	0	87	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
All	All	14620	0	14775	189	0

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

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLY:HA2	1:E:117:LEU:HD12	1.77	0.67
1:A:160:GLY:HA2	1:B:117:LEU:HD12	1.76	0.66
1:B:160:GLY:HA2	1:C:117:LEU:HD12	1.76	0.65
1:C:160:GLY:HA2	1:D:117:LEU:HD12	1.78	0.65
1:A:117:LEU:HD12	1:E:160:GLY:HA2	1.79	0.64
1:D:98:LEU:HD11	1:D:156:LEU:HD23	1.80	0.64
1:B:98:LEU:HD11	1:B:156:LEU:HD23	1.80	0.64
1:B:241:SER:HB2	1:B:255:LEU:HD22	1.80	0.64
1:D:241:SER:HB2	1:D:255:LEU:HD22	1.80	0.64
1:C:98:LEU:HD11	1:C:156:LEU:HD23	1.80	0.63
1:A:98:LEU:HD11	1:A:156:LEU:HD23	1.80	0.63
1:C:241:SER:HB2	1:C:255:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LEU:HD11	1:E:156:LEU:HD23	1.80	0.62
1:A:241:SER:HB2	1:A:255:LEU:HD22	1.80	0.62
1:E:241:SER:HB2	1:E:255:LEU:HD22	1.80	0.62
1:A:244:ILE:HB	1:A:252:ARG:HD3	1.82	0.61
1:C:244:ILE:HB	1:C:252:ARG:HD3	1.82	0.61
1:B:244:ILE:HB	1:B:252:ARG:HD3	1.82	0.61
1:E:244:ILE:HB	1:E:252:ARG:HD3	1.82	0.61
1:D:244:ILE:HB	1:D:252:ARG:HD3	1.83	0.60
1:D:176:VAL:HG21	1:D:212:VAL:HG21	1.85	0.59
1:A:176:VAL:HG21	1:A:212:VAL:HG21	1.85	0.58
1:C:176:VAL:HG21	1:C:212:VAL:HG21	1.85	0.58
1:B:176:VAL:HG21	1:B:212:VAL:HG21	1.85	0.57
1:E:176:VAL:HG21	1:E:212:VAL:HG21	1.85	0.57
3:B:501:GLY:OXT	1:C:65:ARG:NH2	2.38	0.57
1:C:103:GLU:OE2	1:D:131:ARG:NH1	2.37	0.57
1:B:13:PHE:HA	1:B:16:LYS:HG2	1.87	0.57
1:A:13:PHE:HA	1:A:16:LYS:HG2	1.87	0.56
3:A:501:GLY:OXT	1:B:65:ARG:NH2	2.39	0.56
1:C:13:PHE:HA	1:C:16:LYS:HG2	1.87	0.56
1:D:103:GLU:OE2	1:E:131:ARG:NH1	2.39	0.56
1:B:103:GLU:OE2	1:C:131:ARG:NH1	2.38	0.55
1:E:13:PHE:HA	1:E:16:LYS:HG2	1.87	0.55
1:A:103:GLU:OE2	1:B:131:ARG:NH1	2.39	0.55
1:C:106:ALA:HB3	1:D:111:VAL:HG12	1.89	0.55
3:D:501:GLY:OXT	1:E:65:ARG:NH2	2.39	0.55
1:D:13:PHE:HA	1:D:16:LYS:HG2	1.87	0.54
1:A:65:ARG:NH2	3:A:511:GLY:OXT	2.41	0.54
3:C:501:GLY:OXT	1:D:65:ARG:NH2	2.41	0.54
1:C:119:ARG:HD2	1:C:127:LEU:HD23	1.90	0.54
1:E:119:ARG:HD2	1:E:127:LEU:HD23	1.90	0.54
1:A:106:ALA:HB3	1:B:111:VAL:HG12	1.90	0.54
1:A:119:ARG:HD2	1:A:127:LEU:HD23	1.90	0.54
1:D:119:ARG:HD2	1:D:127:LEU:HD23	1.90	0.53
1:A:131:ARG:NH1	1:E:103:GLU:OE2	2.40	0.53
1:B:106:ALA:HB3	1:C:111:VAL:HG12	1.91	0.53
1:B:119:ARG:HD2	1:B:127:LEU:HD23	1.90	0.53
1:A:196:ARG:HD2	1:A:213:ARG:HH21	1.75	0.52
1:E:196:ARG:HD2	1:E:213:ARG:HH21	1.75	0.52
1:A:309:ARG:HD3	1:B:245:ASN:HB3	1.92	0.52
1:C:117:LEU:HB3	1:C:129:SER:HB3	1.92	0.52
1:D:106:ALA:HB3	1:E:111:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:HD2	1:D:213:ARG:HH21	1.75	0.52
1:A:111:VAL:HG12	1:E:106:ALA:HB3	1.92	0.52
1:A:117:LEU:HB3	1:A:129:SER:HB3	1.92	0.52
1:B:117:LEU:HB3	1:B:129:SER:HB3	1.92	0.52
1:B:196:ARG:HD2	1:B:213:ARG:HH21	1.75	0.52
1:D:117:LEU:HB3	1:D:129:SER:HB3	1.92	0.51
1:B:116:LYS:HG2	1:B:130:ILE:HG13	1.93	0.51
1:C:116:LYS:HG2	1:C:130:ILE:HG13	1.93	0.51
1:E:117:LEU:HB3	1:E:129:SER:HB3	1.92	0.51
1:C:196:ARG:HD2	1:C:213:ARG:HH21	1.75	0.51
1:C:85:LEU:HG	1:C:118:LEU:HD23	1.94	0.50
1:D:85:LEU:HG	1:D:118:LEU:HD23	1.94	0.50
1:A:90:LEU:HD21	1:A:118:LEU:HB2	1.94	0.50
1:B:90:LEU:HD21	1:B:118:LEU:HB2	1.94	0.50
1:D:116:LYS:HG2	1:D:130:ILE:HG13	1.92	0.50
1:A:85:LEU:HG	1:A:118:LEU:HD23	1.94	0.50
1:A:116:LYS:HG2	1:A:130:ILE:HG13	1.93	0.50
1:B:247:ASP:OD1	1:B:247:ASP:N	2.42	0.49
1:E:90:LEU:HD21	1:E:118:LEU:HB2	1.94	0.49
1:E:61:ASN:ND2	1:E:132:LEU:O	2.45	0.49
1:E:116:LYS:HG2	1:E:130:ILE:HG13	1.93	0.49
1:A:61:ASN:ND2	1:A:132:LEU:O	2.45	0.49
1:C:61:ASN:ND2	1:C:132:LEU:O	2.45	0.49
1:B:85:LEU:HG	1:B:118:LEU:HD23	1.94	0.49
1:E:85:LEU:HG	1:E:118:LEU:HD23	1.94	0.49
1:B:61:ASN:ND2	1:B:132:LEU:O	2.45	0.48
1:C:90:LEU:HD21	1:C:118:LEU:HB2	1.94	0.48
1:D:90:LEU:HD21	1:D:118:LEU:HB2	1.94	0.48
1:D:211:GLU:OE2	1:D:213:ARG:NH2	2.47	0.48
1:C:211:GLU:OE2	1:C:213:ARG:NH2	2.47	0.48
1:A:211:GLU:OE2	1:A:213:ARG:NH2	2.47	0.48
1:D:61:ASN:ND2	1:D:132:LEU:O	2.45	0.48
1:E:211:GLU:OE2	1:E:213:ARG:NH2	2.47	0.48
1:B:211:GLU:OE2	1:B:213:ARG:NH2	2.47	0.47
1:A:244:ILE:O	1:A:252:ARG:NH1	2.48	0.47
1:A:245:ASN:HB3	1:E:309:ARG:HD3	1.96	0.47
1:C:238:SER:HB3	1:C:259:THR:HG21	1.97	0.47
1:D:238:SER:HB3	1:D:259:THR:HG21	1.97	0.47
1:A:30:PRO:HB3	1:A:71:PRO:HD2	1.97	0.47
1:A:238:SER:HB3	1:A:259:THR:HG21	1.97	0.47
1:C:244:ILE:O	1:C:252:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:HE2	1:B:208:THR:HA	1.97	0.47
1:C:163:MET:HE2	1:C:208:THR:HA	1.97	0.47
1:B:244:ILE:O	1:B:252:ARG:NH1	2.48	0.46
1:D:30:PRO:HB3	1:D:71:PRO:HD2	1.97	0.46
1:E:244:ILE:O	1:E:252:ARG:NH1	2.48	0.46
1:C:30:PRO:HB3	1:C:71:PRO:HD2	1.97	0.46
1:D:163:MET:HE2	1:D:208:THR:HA	1.97	0.46
1:A:163:MET:HE2	1:A:208:THR:HA	1.97	0.46
1:C:309:ARG:HD3	1:D:245:ASN:HB3	1.96	0.46
1:E:238:SER:HB3	1:E:259:THR:HG21	1.97	0.46
1:D:244:ILE:O	1:D:252:ARG:NH1	2.48	0.46
1:E:30:PRO:HB3	1:E:71:PRO:HD2	1.97	0.46
1:B:238:SER:HB3	1:B:259:THR:HG21	1.97	0.46
1:D:89:MET:O	1:D:92:SER:OG	2.34	0.46
1:A:56:MET:HE1	1:A:140:MET:H	1.81	0.45
1:B:276:LYS:HD2	1:C:222:TYR:CZ	2.51	0.45
1:B:30:PRO:HB3	1:B:71:PRO:HD2	1.97	0.45
1:B:56:MET:HE1	1:B:140:MET:H	1.81	0.45
1:D:276:LYS:HD2	1:E:222:TYR:CZ	2.51	0.45
1:D:56:MET:HE1	1:D:140:MET:H	1.81	0.45
1:E:163:MET:HE2	1:E:208:THR:HA	1.97	0.45
1:E:56:MET:HE1	1:E:140:MET:H	1.82	0.45
1:A:89:MET:O	1:A:92:SER:OG	2.34	0.45
1:E:89:MET:O	1:E:92:SER:OG	2.34	0.44
1:D:78:TYR:O	1:D:122:LYS:NZ	2.51	0.44
5:E:503:PX4:H33	5:E:503:PX4:H28	1.92	0.43
5:D:509:PX4:H33	5:D:509:PX4:H28	1.92	0.43
1:A:222:TYR:CZ	1:E:276:LYS:HD2	2.53	0.43
1:C:56:MET:HE1	1:C:140:MET:H	1.81	0.43
1:D:247:ASP:OD1	1:D:247:ASP:N	2.42	0.43
1:B:78:TYR:O	1:B:122:LYS:NZ	2.51	0.43
5:B:509:PX4:H33	5:B:509:PX4:H28	1.92	0.43
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.91	0.43
1:C:89:MET:O	1:C:92:SER:OG	2.34	0.43
1:C:417:ILE:HA	1:C:420:ILE:HG12	2.01	0.43
1:B:29:ARG:NH1	1:B:31:ASN:O	2.52	0.42
1:D:417:ILE:HA	1:D:420:ILE:HG12	2.01	0.42
1:E:247:ASP:OD1	1:E:247:ASP:N	2.42	0.42
1:A:276:LYS:HD2	1:B:222:TYR:CZ	2.54	0.42
1:C:29:ARG:NH1	1:C:31:ASN:O	2.52	0.42
1:B:169:GLU:OE1	1:B:197:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ARG:NH1	1:E:31:ASN:O	2.52	0.42
1:B:18:MET:HE3	1:B:93:ILE:HG22	2.02	0.42
1:E:44:PHE:HD1	1:E:177:GLN:HG2	1.84	0.42
1:E:78:TYR:O	1:E:122:LYS:NZ	2.51	0.42
1:A:29:ARG:NH1	1:A:31:ASN:O	2.52	0.42
1:D:18:MET:HE3	1:D:93:ILE:HG22	2.02	0.42
1:D:29:ARG:NH1	1:D:31:ASN:O	2.52	0.42
1:A:44:PHE:HD1	1:A:177:GLN:HG2	1.84	0.42
1:A:169:GLU:OE1	1:A:197:TYR:OH	2.37	0.42
1:C:78:TYR:O	1:C:122:LYS:NZ	2.51	0.42
1:D:276:LYS:HD2	1:E:222:TYR:CE2	2.56	0.41
1:D:309:ARG:HD3	1:E:245:ASN:HB3	2.02	0.41
1:A:95:LYS:HE2	1:A:95:LYS:HB2	1.89	0.41
1:B:15:ASP:OD1	1:B:15:ASP:N	2.51	0.41
1:B:309:ARG:HD3	1:C:245:ASN:HB3	2.00	0.41
1:A:35:PRO:HG2	2:F:1:NAG:H83	2.03	0.41
1:B:35:PRO:HG2	2:G:1:NAG:H83	2.03	0.41
1:B:44:PHE:HD1	1:B:177:GLN:HG2	1.84	0.41
1:C:276:LYS:HD2	1:D:222:TYR:CZ	2.55	0.41
1:D:44:PHE:HD1	1:D:177:GLN:HG2	1.84	0.41
1:A:18:MET:HE1	1:A:92:SER:HB2	2.02	0.41
1:C:44:PHE:HD1	1:C:177:GLN:HG2	1.84	0.41
1:A:417:ILE:HA	1:A:420:ILE:HG12	2.01	0.41
1:B:417:ILE:HA	1:B:420:ILE:HG12	2.01	0.41
1:C:35:PRO:HG2	2:H:1:NAG:H83	2.03	0.41
1:C:156:LEU:HB2	1:C:210:ILE:HG13	2.03	0.41
1:D:35:PRO:HG2	2:I:1:NAG:H83	2.03	0.41
1:E:35:PRO:HG2	2:J:1:NAG:H83	2.03	0.41
1:B:234:ILE:HG13	1:B:266:GLN:HE22	1.86	0.41
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.91	0.41
1:C:18:MET:HE3	1:C:93:ILE:HG22	2.02	0.41
5:C:509:PX4:H31	5:C:509:PX4:H38	1.90	0.41
1:D:156:LEU:HB2	1:D:210:ILE:HG13	2.03	0.41
1:E:102:ASN:OD1	1:E:102:ASN:N	2.54	0.41
1:E:169:GLU:OE1	1:E:197:TYR:OH	2.37	0.41
1:B:203:ASN:OD1	1:B:203:ASN:N	2.54	0.41
1:C:203:ASN:OD1	1:C:203:ASN:N	2.54	0.41
1:B:156:LEU:HB2	1:B:210:ILE:HG13	2.03	0.40
1:D:169:GLU:OE1	1:D:197:TYR:OH	2.37	0.40
1:E:18:MET:HE1	1:E:92:SER:HB2	2.02	0.40
1:E:417:ILE:HA	1:E:420:ILE:HG12	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:503:PX4:H31	5:E:503:PX4:H38	1.90	0.40
1:C:18:MET:HE1	1:C:92:SER:HB2	2.02	0.40
1:D:18:MET:HE1	1:D:92:SER:HB2	2.03	0.40
1:E:18:MET:HE3	1:E:93:ILE:HG22	2.02	0.40
1:E:234:ILE:HG13	1:E:266:GLN:HE22	1.86	0.40
1:D:234:ILE:HG13	1:D:266:GLN:HE22	1.86	0.40
1:A:234:ILE:HG13	1:A:266:GLN:HE22	1.86	0.40
1:A:255:LEU:O	1:A:259:THR:OG1	2.29	0.40
1:C:97:ASP:OD1	1:C:97:ASP:N	2.49	0.40
1:E:274:LEU:HD23	1:E:274:LEU:HA	1.91	0.40
1:A:156:LEU:HB2	1:A:210:ILE:HG13	2.03	0.40
1:C:15:ASP:OD1	1:C:15:ASP:N	2.51	0.40
1:E:203:ASN:OD1	1:E:203:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/478 (71%)	335 (99%)	3 (1%)	0	100	100
1	B	338/478 (71%)	335 (99%)	3 (1%)	0	100	100
1	C	338/478 (71%)	335 (99%)	3 (1%)	0	100	100
1	D	338/478 (71%)	335 (99%)	3 (1%)	0	100	100
1	E	338/478 (71%)	335 (99%)	3 (1%)	0	100	100
All	All	1690/2390 (71%)	1675 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/430 (72%)	310 (100%)	0	100	100
1	B	310/430 (72%)	310 (100%)	0	100	100
1	C	310/430 (72%)	310 (100%)	0	100	100
1	D	310/430 (72%)	310 (100%)	0	100	100
1	E	310/430 (72%)	310 (100%)	0	100	100
All	All	1550/2150 (72%)	1550 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	69	ASN
1	A	186	GLN
1	A	310	GLN
1	A	411	ASN
1	B	66	GLN
1	B	186	GLN
1	B	310	GLN
1	B	411	ASN
1	C	66	GLN
1	C	186	GLN
1	C	310	GLN
1	C	411	ASN
1	D	66	GLN
1	D	69	ASN
1	D	186	GLN
1	D	310	GLN
1	D	411	ASN
1	E	66	GLN
1	E	186	GLN
1	E	310	GLN

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Mol	Chain	Res	Type
1	E	411	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	F	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	G	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	0.46	0
2	NAG	H	1	2,1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.47	0
2	NAG	I	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	I	2	2	14,14,15	0.31	0	17,19,21	0.47	0
2	NAG	J	1	2,1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.47	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
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

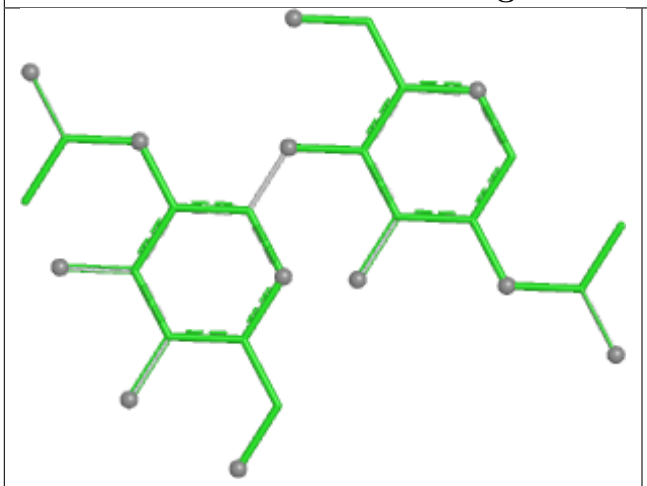
There are no ring outliers.

5 monomers are involved in 5 short contacts:

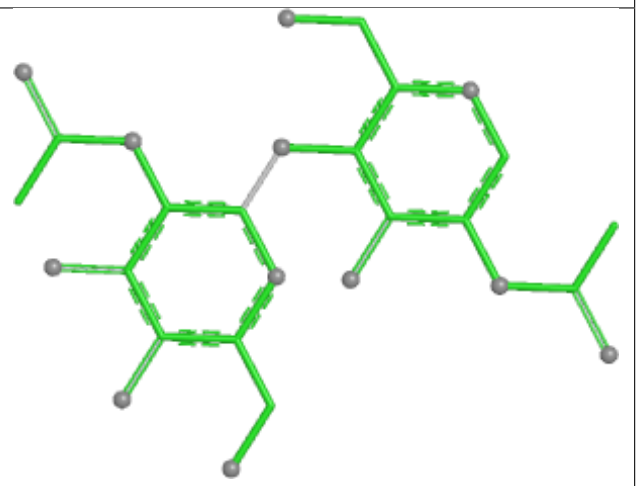
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	1	0
2	H	1	NAG	1	0
2	I	1	NAG	1	0
2	G	1	NAG	1	0
2	F	1	NAG	1	0

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

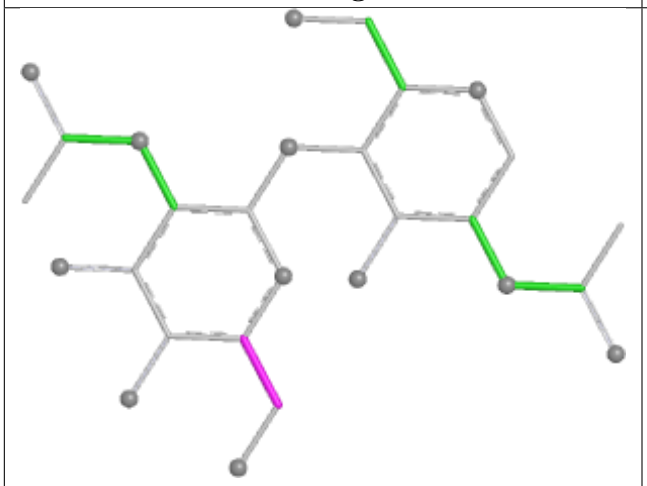
Oligosaccharide Chain F



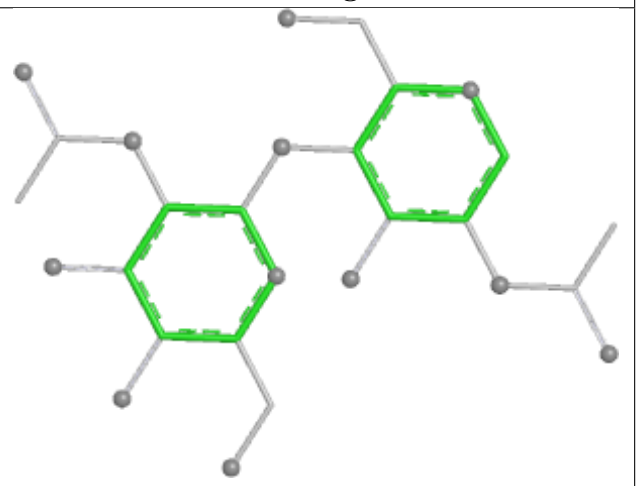
Bond lengths



Bond angles

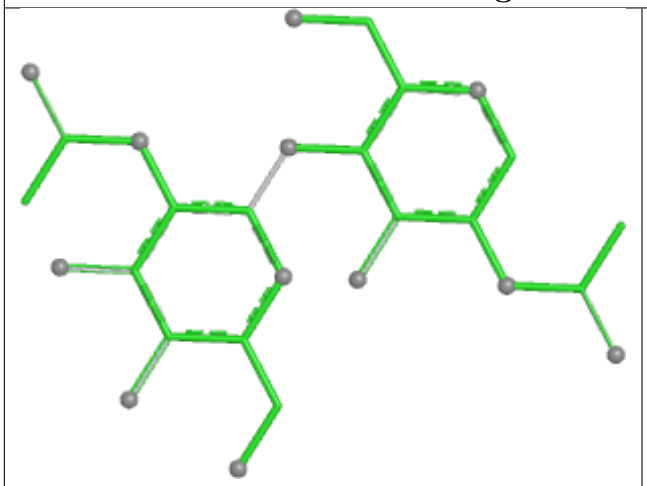


Torsions

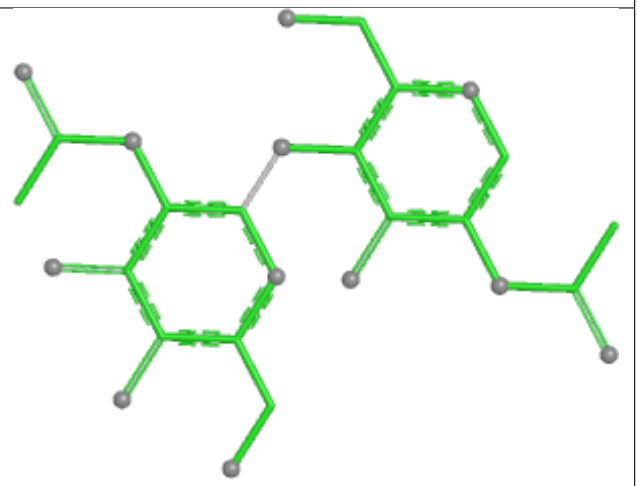


Rings

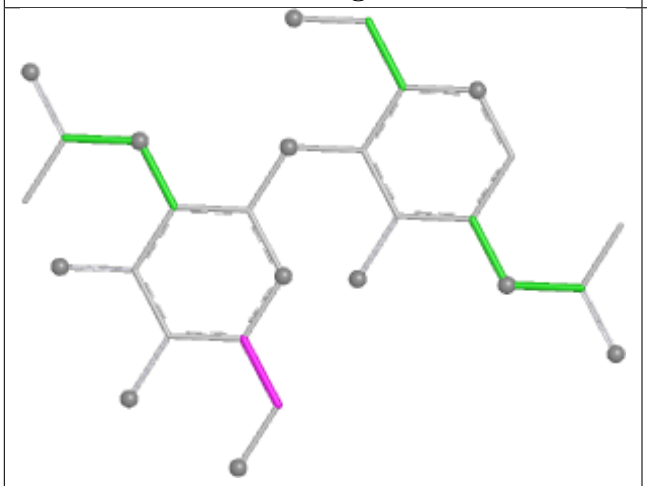
Oligosaccharide Chain G



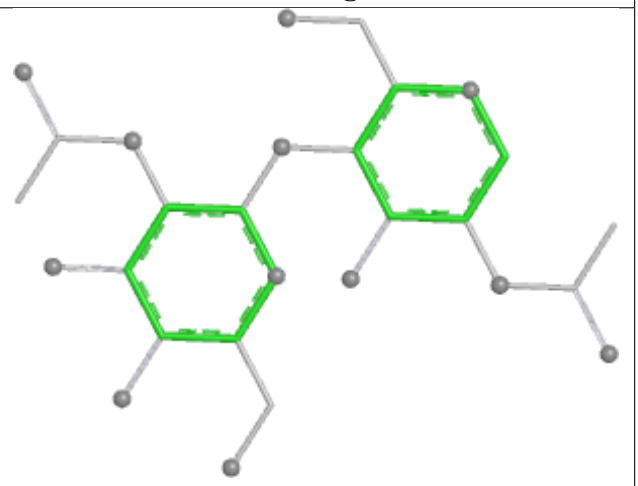
Bond lengths



Bond angles

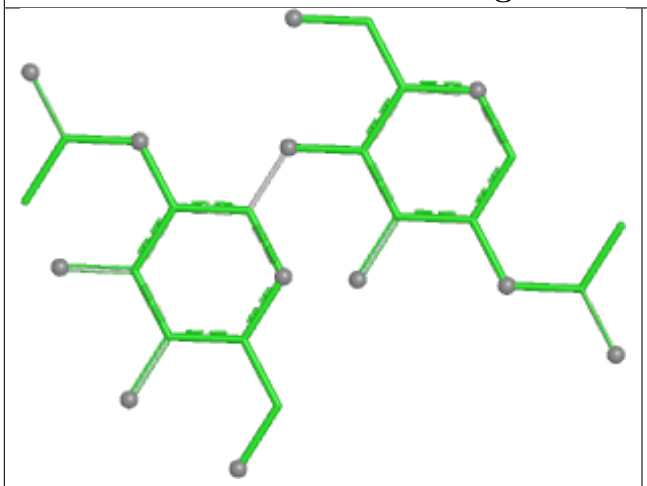


Torsions

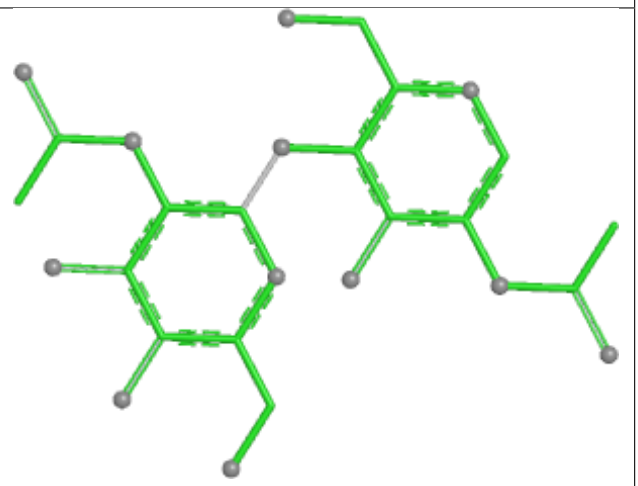


Rings

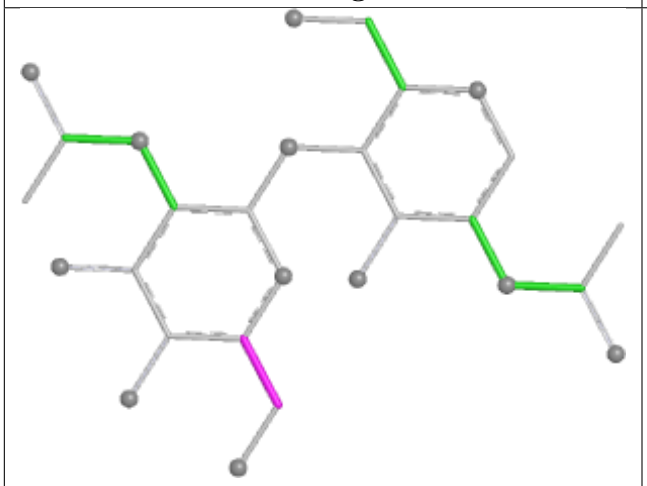
Oligosaccharide Chain H



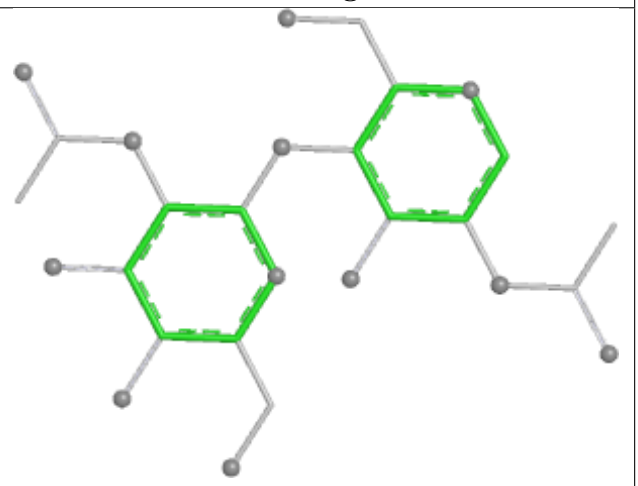
Bond lengths



Bond angles

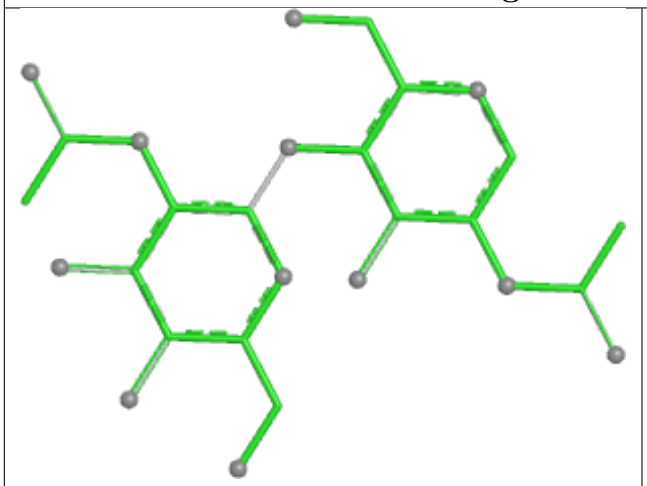


Torsions

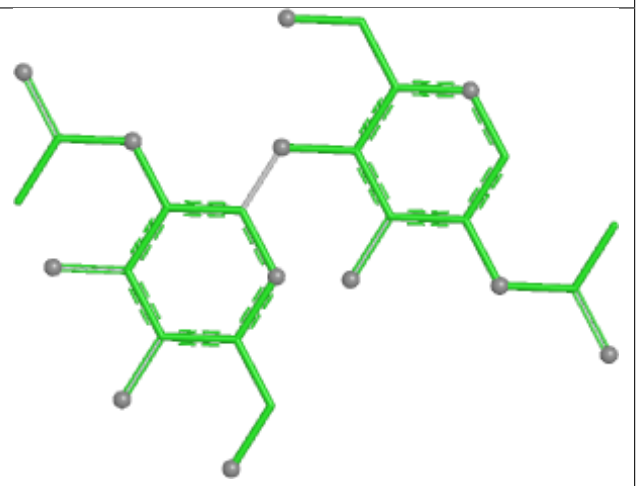


Rings

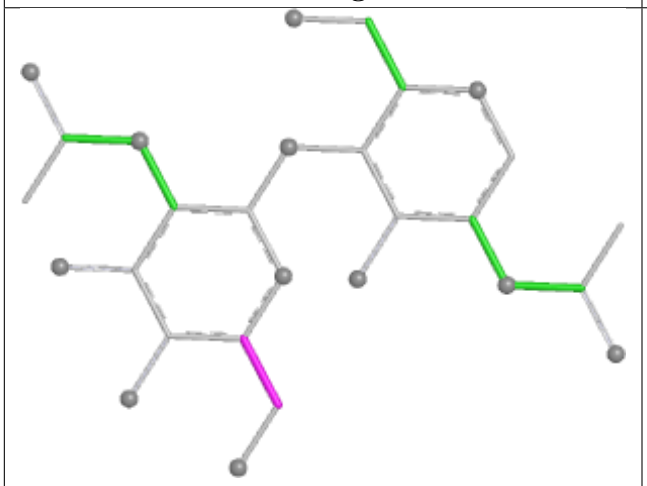
Oligosaccharide Chain I



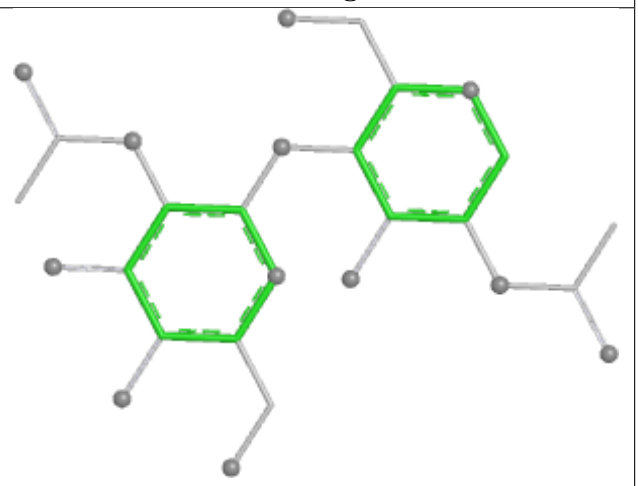
Bond lengths



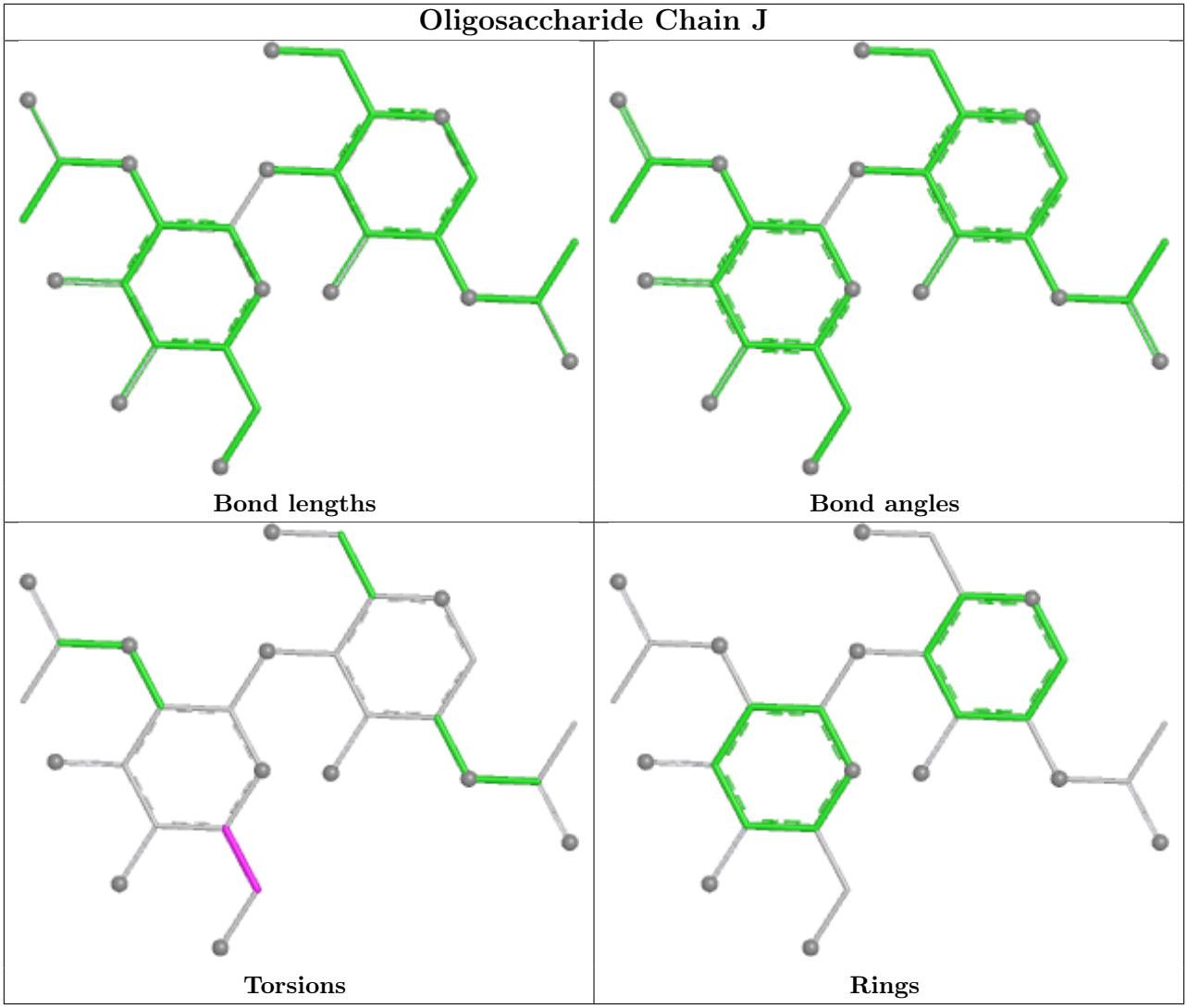
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

50 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	PIO	A	503	-	9,9,47	0.48	0	9,9,65	0.48	0
5	PX4	D	510	-	13,13,45	2.42	3 (23%)	13,13,53	1.17	0
4	PIO	E	507	-	7,7,47	0.53	0	7,7,65	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLY	A	501	-	4,4,4	1.15	1 (25%)	3,4,4	1.84	2 (66%)
4	PIO	E	501	-	7,7,47	0.55	0	7,7,65	0.54	0
5	PX4	C	509	-	15,15,45	2.35	3 (20%)	15,15,53	1.13	0
5	PX4	B	509	-	15,15,45	2.35	3 (20%)	15,15,53	1.14	0
3	GLY	D	501	-	4,4,4	1.14	1 (25%)	3,4,4	1.85	2 (66%)
4	PIO	C	505	-	9,9,47	0.47	0	9,9,65	0.47	0
5	PX4	E	509	-	13,13,45	2.44	3 (23%)	13,13,53	1.14	0
4	PIO	E	505	-	7,7,47	0.53	0	7,7,65	0.55	0
3	GLY	C	501	-	4,4,4	1.16	1 (25%)	3,4,4	1.84	2 (66%)
5	PX4	E	503	-	15,15,45	2.35	3 (20%)	15,15,53	1.14	0
3	GLY	B	501	-	4,4,4	1.15	1 (25%)	3,4,4	1.85	2 (66%)
4	PIO	C	502	-	7,7,47	0.54	0	7,7,65	0.55	0
4	PIO	A	507	-	7,7,47	0.54	0	7,7,65	0.54	0
5	PX4	D	506	-	13,13,45	2.44	3 (23%)	13,13,53	1.14	0
4	PIO	E	506	-	9,9,47	0.48	0	9,9,65	0.48	0
5	PX4	B	508	-	13,13,45	2.42	3 (23%)	13,13,53	1.16	0
4	PIO	D	504	-	7,7,47	0.55	0	7,7,65	0.55	0
5	PX4	B	506	-	13,13,45	2.44	3 (23%)	13,13,53	1.14	0
4	PIO	A	505	-	9,9,47	0.49	0	9,9,65	0.48	0
5	PX4	C	508	-	13,13,45	2.42	3 (23%)	13,13,53	1.16	0
5	PX4	D	509	-	15,15,45	2.34	3 (20%)	15,15,53	1.14	0
3	GLY	A	511	-	4,4,4	1.16	1 (25%)	3,4,4	1.85	2 (66%)
4	PIO	B	502	-	7,7,47	0.55	0	7,7,65	0.56	0
4	PIO	B	507	-	7,7,47	0.54	0	7,7,65	0.55	0
4	PIO	B	504	-	7,7,47	0.55	0	7,7,65	0.54	0
4	PIO	A	502	-	7,7,47	0.54	0	7,7,65	0.56	0
4	PIO	D	507	-	7,7,47	0.54	0	7,7,65	0.53	0
5	PX4	E	502	-	13,13,45	2.42	3 (23%)	13,13,53	1.16	0
5	PX4	C	510	-	13,13,45	2.42	3 (23%)	13,13,53	1.17	1 (7%)
5	PX4	A	510	-	13,13,45	2.42	3 (23%)	13,13,53	1.17	1 (7%)
4	PIO	C	507	-	7,7,47	0.54	0	7,7,65	0.54	0
4	PIO	B	505	-	9,9,47	0.48	0	9,9,65	0.48	0
4	PIO	E	508	-	9,9,47	0.49	0	9,9,65	0.48	0
5	PX4	A	508	-	13,13,45	2.42	3 (23%)	13,13,53	1.16	0
4	PIO	C	504	-	7,7,47	0.54	0	7,7,65	0.54	0
5	PX4	D	508	-	13,13,45	2.42	3 (23%)	13,13,53	1.16	0
4	PIO	D	502	-	7,7,47	0.54	0	7,7,65	0.55	0
5	PX4	A	506	-	13,13,45	2.44	3 (23%)	13,13,53	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PX4	B	510	-	13,13,45	2.42	3 (23%)	13,13,53	1.17	1 (7%)
4	PIO	C	503	-	9,9,47	0.48	0	9,9,65	0.49	0
5	PX4	C	506	-	13,13,45	2.45	3 (23%)	13,13,53	1.14	0
4	PIO	D	505	-	9,9,47	0.49	0	9,9,65	0.48	0
4	PIO	A	504	-	7,7,47	0.54	0	7,7,65	0.54	0
4	PIO	D	503	-	9,9,47	0.49	0	9,9,65	0.48	0
5	PX4	A	509	-	15,15,45	2.35	3 (20%)	15,15,53	1.13	0
5	PX4	E	504	-	13,13,45	2.42	3 (23%)	13,13,53	1.17	1 (7%)
4	PIO	B	503	-	9,9,47	0.49	0	9,9,65	0.49	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	PIO	A	503	-	-	0/7/7/68	-
5	PX4	D	510	-	-	3/11/11/49	-
4	PIO	E	507	-	-	1/5/5/68	-
3	GLY	A	501	-	-	2/2/2/2	-
4	PIO	E	501	-	-	2/5/5/68	-
5	PX4	C	509	-	-	5/13/13/49	-
5	PX4	B	509	-	-	5/13/13/49	-
3	GLY	D	501	-	-	2/2/2/2	-
4	PIO	C	505	-	-	1/7/7/68	-
5	PX4	E	509	-	-	2/11/11/49	-
4	PIO	E	505	-	-	0/5/5/68	-
3	GLY	C	501	-	-	2/2/2/2	-
5	PX4	E	503	-	-	5/13/13/49	-
3	GLY	B	501	-	-	2/2/2/2	-
4	PIO	C	502	-	-	0/5/5/68	-
4	PIO	A	507	-	-	2/5/5/68	-
5	PX4	D	506	-	-	2/11/11/49	-
4	PIO	E	506	-	-	0/7/7/68	-
5	PX4	B	508	-	-	3/11/11/49	-
4	PIO	D	504	-	-	1/5/5/68	-
5	PX4	B	506	-	-	3/11/11/49	-
4	PIO	A	505	-	-	1/7/7/68	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PX4	C	508	-	-	3/11/11/49	-
5	PX4	D	509	-	-	5/13/13/49	-
3	GLY	A	511	-	-	2/2/2/2	-
4	PIO	B	502	-	-	0/5/5/68	-
4	PIO	B	507	-	-	2/5/5/68	-
4	PIO	B	504	-	-	1/5/5/68	-
4	PIO	A	502	-	-	0/5/5/68	-
4	PIO	D	507	-	-	2/5/5/68	-
5	PX4	E	502	-	-	3/11/11/49	-
5	PX4	C	510	-	-	3/11/11/49	-
5	PX4	A	510	-	-	3/11/11/49	-
4	PIO	C	507	-	-	2/5/5/68	-
4	PIO	B	505	-	-	1/7/7/68	-
4	PIO	E	508	-	-	1/7/7/68	-
5	PX4	A	508	-	-	3/11/11/49	-
4	PIO	C	504	-	-	1/5/5/68	-
5	PX4	D	508	-	-	3/11/11/49	-
4	PIO	D	502	-	-	0/5/5/68	-
5	PX4	A	506	-	-	2/11/11/49	-
5	PX4	B	510	-	-	3/11/11/49	-
4	PIO	C	503	-	-	0/7/7/68	-
5	PX4	C	506	-	-	2/11/11/49	-
4	PIO	D	505	-	-	1/7/7/68	-
4	PIO	A	504	-	-	1/5/5/68	-
4	PIO	D	503	-	-	0/7/7/68	-
5	PX4	A	509	-	-	5/13/13/49	-
5	PX4	E	504	-	-	3/11/11/49	-
4	PIO	B	503	-	-	0/7/7/68	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	506	PX4	O7-C23	5.01	1.47	1.30
5	D	506	PX4	O7-C23	4.99	1.47	1.30
5	B	506	PX4	O7-C23	4.99	1.47	1.30
5	A	506	PX4	O7-C23	4.98	1.47	1.30
5	E	509	PX4	O7-C23	4.98	1.47	1.30
5	A	510	PX4	O5-C9	4.97	1.47	1.30
5	E	504	PX4	O5-C9	4.94	1.47	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	510	PX4	O5-C9	4.94	1.47	1.30
5	B	510	PX4	O5-C9	4.94	1.47	1.30
5	B	508	PX4	O5-C9	4.94	1.47	1.30
5	C	510	PX4	O5-C9	4.93	1.47	1.30
5	C	508	PX4	O5-C9	4.93	1.47	1.30
5	E	502	PX4	O5-C9	4.92	1.47	1.30
5	D	508	PX4	O5-C9	4.92	1.47	1.30
5	D	509	PX4	O5-C9	4.92	1.47	1.30
5	B	509	PX4	O5-C9	4.92	1.47	1.30
5	C	509	PX4	O5-C9	4.91	1.47	1.30
5	A	508	PX4	O5-C9	4.91	1.47	1.30
5	A	509	PX4	O5-C9	4.91	1.47	1.30
5	E	503	PX4	O5-C9	4.91	1.47	1.30
5	D	506	PX4	C24-C23	4.44	1.60	1.50
5	B	506	PX4	C24-C23	4.42	1.60	1.50
5	A	506	PX4	C24-C23	4.42	1.60	1.50
5	C	506	PX4	C24-C23	4.42	1.60	1.50
5	E	509	PX4	C24-C23	4.40	1.60	1.50
5	A	508	PX4	C10-C9	4.39	1.60	1.50
5	C	509	PX4	C10-C9	4.39	1.60	1.50
5	E	502	PX4	C10-C9	4.39	1.60	1.50
5	B	508	PX4	C10-C9	4.38	1.60	1.50
5	A	509	PX4	C10-C9	4.38	1.60	1.50
5	C	508	PX4	C10-C9	4.38	1.60	1.50
5	B	510	PX4	C10-C9	4.38	1.60	1.50
5	C	510	PX4	C10-C9	4.38	1.60	1.50
5	D	508	PX4	C10-C9	4.38	1.60	1.50
5	E	504	PX4	C10-C9	4.38	1.60	1.50
5	D	510	PX4	C10-C9	4.37	1.60	1.50
5	E	503	PX4	C10-C9	4.37	1.60	1.50
5	A	510	PX4	C10-C9	4.37	1.60	1.50
5	B	509	PX4	C10-C9	4.36	1.60	1.50
5	D	509	PX4	C10-C9	4.35	1.60	1.50
5	C	506	PX4	C25-C24	2.38	1.60	1.52
5	E	509	PX4	C25-C24	2.38	1.60	1.52
5	A	506	PX4	C25-C24	2.38	1.60	1.52
5	B	506	PX4	C25-C24	2.37	1.60	1.52
5	D	506	PX4	C25-C24	2.36	1.60	1.52
5	D	509	PX4	C11-C10	2.28	1.60	1.52
5	C	508	PX4	C11-C10	2.27	1.60	1.52
5	B	509	PX4	C11-C10	2.27	1.60	1.52
5	C	509	PX4	C11-C10	2.27	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	503	PX4	C11-C10	2.27	1.60	1.52
5	B	508	PX4	C11-C10	2.26	1.60	1.52
5	A	508	PX4	C11-C10	2.25	1.60	1.52
5	A	509	PX4	C11-C10	2.25	1.60	1.52
5	E	502	PX4	C11-C10	2.25	1.60	1.52
5	D	508	PX4	C11-C10	2.24	1.60	1.52
5	B	510	PX4	C11-C10	2.24	1.60	1.52
5	D	510	PX4	C11-C10	2.24	1.60	1.52
5	E	504	PX4	C11-C10	2.23	1.60	1.52
5	A	510	PX4	C11-C10	2.22	1.60	1.52
3	A	511	GLY	OXT-C	-2.21	1.23	1.30
3	C	501	GLY	OXT-C	-2.21	1.23	1.30
5	C	510	PX4	C11-C10	2.21	1.60	1.52
3	A	501	GLY	OXT-C	-2.21	1.23	1.30
3	B	501	GLY	OXT-C	-2.20	1.23	1.30
3	D	501	GLY	OXT-C	-2.18	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	GLY	OXT-C-O	-2.31	117.39	123.33
3	A	511	GLY	OXT-C-O	-2.31	117.40	123.33
3	D	501	GLY	OXT-C-O	-2.31	117.40	123.33
3	A	501	GLY	OXT-C-O	-2.30	117.42	123.33
3	C	501	GLY	OXT-C-O	-2.29	117.45	123.33
3	A	511	GLY	OXT-C-CA	2.19	122.08	113.38
3	B	501	GLY	OXT-C-CA	2.19	122.08	113.38
3	A	501	GLY	OXT-C-CA	2.17	122.03	113.38
3	D	501	GLY	OXT-C-CA	2.17	122.02	113.38
3	C	501	GLY	OXT-C-CA	2.17	122.00	113.38
5	B	510	PX4	C11-C10-C9	-2.02	109.25	114.51
5	A	510	PX4	C11-C10-C9	-2.01	109.27	114.51
5	E	504	PX4	C11-C10-C9	-2.01	109.28	114.51
5	C	510	PX4	C11-C10-C9	-2.00	109.28	114.51

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GLY	O-C-CA-N
3	A	511	GLY	O-C-CA-N
3	B	501	GLY	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	C	501	GLY	O-C-CA-N
3	D	501	GLY	O-C-CA-N
3	A	501	GLY	OXT-C-CA-N
3	A	511	GLY	OXT-C-CA-N
3	B	501	GLY	OXT-C-CA-N
3	C	501	GLY	OXT-C-CA-N
3	D	501	GLY	OXT-C-CA-N
5	C	509	PX4	C10-C11-C12-C13
5	A	509	PX4	C10-C11-C12-C13
5	B	509	PX4	C10-C11-C12-C13
5	D	509	PX4	C10-C11-C12-C13
5	E	503	PX4	C10-C11-C12-C13
5	A	508	PX4	C14-C15-C16-C17
5	B	508	PX4	C14-C15-C16-C17
5	C	508	PX4	C14-C15-C16-C17
5	D	508	PX4	C14-C15-C16-C17
5	E	502	PX4	C14-C15-C16-C17
5	A	508	PX4	C13-C14-C15-C16
5	C	508	PX4	C13-C14-C15-C16
5	E	502	PX4	C13-C14-C15-C16
5	B	508	PX4	C13-C14-C15-C16
5	D	508	PX4	C13-C14-C15-C16
5	C	509	PX4	C14-C15-C16-C17
5	D	509	PX4	C14-C15-C16-C17
5	A	509	PX4	C14-C15-C16-C17
5	B	509	PX4	C14-C15-C16-C17
5	E	503	PX4	C14-C15-C16-C17
5	A	508	PX4	C10-C11-C12-C13
5	B	508	PX4	C10-C11-C12-C13
5	D	508	PX4	C10-C11-C12-C13
5	E	502	PX4	C10-C11-C12-C13
5	C	508	PX4	C10-C11-C12-C13
5	A	509	PX4	C13-C14-C15-C16
5	C	509	PX4	C13-C14-C15-C16
5	D	509	PX4	C13-C14-C15-C16
5	E	503	PX4	C13-C14-C15-C16
5	B	509	PX4	C13-C14-C15-C16
4	C	504	PIO	C2A-C3A-C4A-C5A
4	D	504	PIO	C2A-C3A-C4A-C5A
4	E	507	PIO	C2A-C3A-C4A-C5A
4	A	504	PIO	C2A-C3A-C4A-C5A
4	B	504	PIO	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
5	D	509	PX4	C11-C10-C9-O5
5	A	509	PX4	C11-C10-C9-O5
5	B	509	PX4	C11-C10-C9-O5
5	C	509	PX4	C11-C10-C9-O5
5	E	503	PX4	C11-C10-C9-O5
5	A	506	PX4	C30-C31-C32-C33
5	B	506	PX4	C30-C31-C32-C33
5	E	509	PX4	C30-C31-C32-C33
5	C	506	PX4	C30-C31-C32-C33
5	D	506	PX4	C30-C31-C32-C33
5	A	510	PX4	C10-C11-C12-C13
5	B	510	PX4	C10-C11-C12-C13
5	C	510	PX4	C10-C11-C12-C13
5	E	504	PX4	C10-C11-C12-C13
5	D	510	PX4	C10-C11-C12-C13
5	A	509	PX4	C11-C10-C9-O6
5	B	509	PX4	C11-C10-C9-O6
5	C	509	PX4	C11-C10-C9-O6
5	D	509	PX4	C11-C10-C9-O6
5	E	503	PX4	C11-C10-C9-O6
4	A	507	PIO	O1A-C1A-C2A-C3A
4	B	507	PIO	O1A-C1A-C2A-C3A
4	D	507	PIO	O1A-C1A-C2A-C3A
4	E	501	PIO	O1A-C1A-C2A-C3A
4	C	507	PIO	O1A-C1A-C2A-C3A
4	C	507	PIO	O2C-C1A-C2A-C3A
4	B	507	PIO	O2C-C1A-C2A-C3A
4	D	507	PIO	O2C-C1A-C2A-C3A
4	E	501	PIO	O2C-C1A-C2A-C3A
4	C	505	PIO	C4A-C5A-C6A-C7A
4	B	505	PIO	C4A-C5A-C6A-C7A
4	D	505	PIO	C4A-C5A-C6A-C7A
4	A	505	PIO	C4A-C5A-C6A-C7A
4	A	507	PIO	O2C-C1A-C2A-C3A
4	E	508	PIO	C4A-C5A-C6A-C7A
5	A	506	PX4	O7-C23-C24-C25
5	A	510	PX4	C11-C10-C9-O6
5	B	506	PX4	O7-C23-C24-C25
5	B	510	PX4	C11-C10-C9-O6
5	C	506	PX4	O7-C23-C24-C25
5	C	510	PX4	C11-C10-C9-O6
5	D	506	PX4	O7-C23-C24-C25

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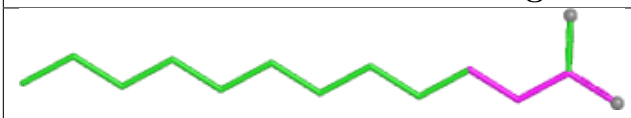
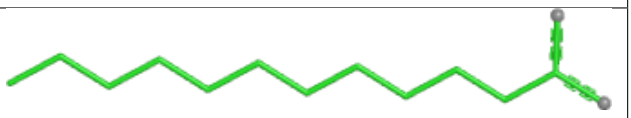
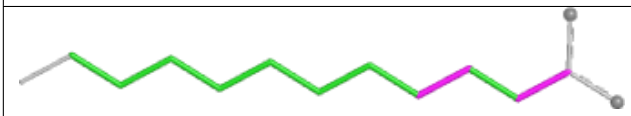
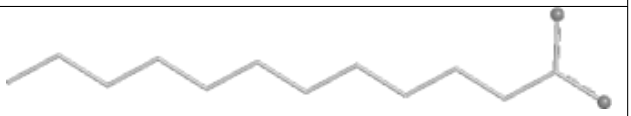
Mol	Chain	Res	Type	Atoms
5	D	510	PX4	C11-C10-C9-O6
5	E	504	PX4	C11-C10-C9-O6
5	E	509	PX4	O7-C23-C24-C25
5	A	510	PX4	C11-C10-C9-O5
5	B	510	PX4	C11-C10-C9-O5
5	E	504	PX4	C11-C10-C9-O5
5	C	510	PX4	C11-C10-C9-O5
5	D	510	PX4	C11-C10-C9-O5
5	B	506	PX4	O8-C23-C24-C25

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GLY	1	0
5	C	509	PX4	1	0
5	B	509	PX4	1	0
3	D	501	GLY	1	0
3	C	501	GLY	1	0
5	E	503	PX4	2	0
3	B	501	GLY	1	0
5	D	509	PX4	1	0
3	A	511	GLY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PX4 D 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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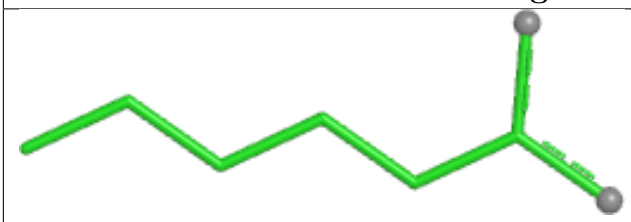
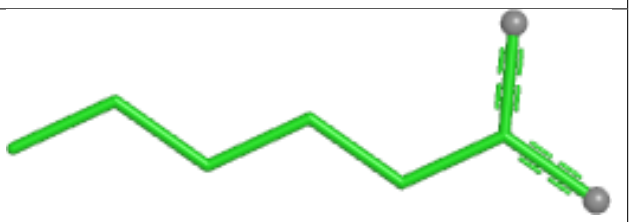
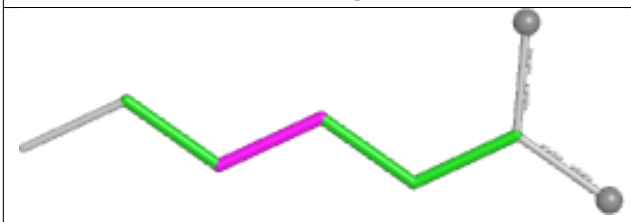
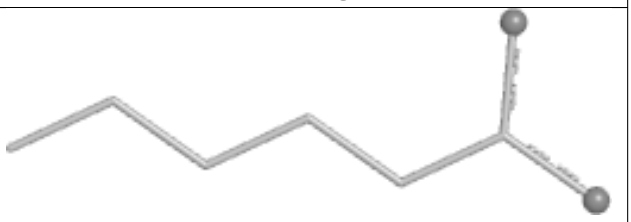
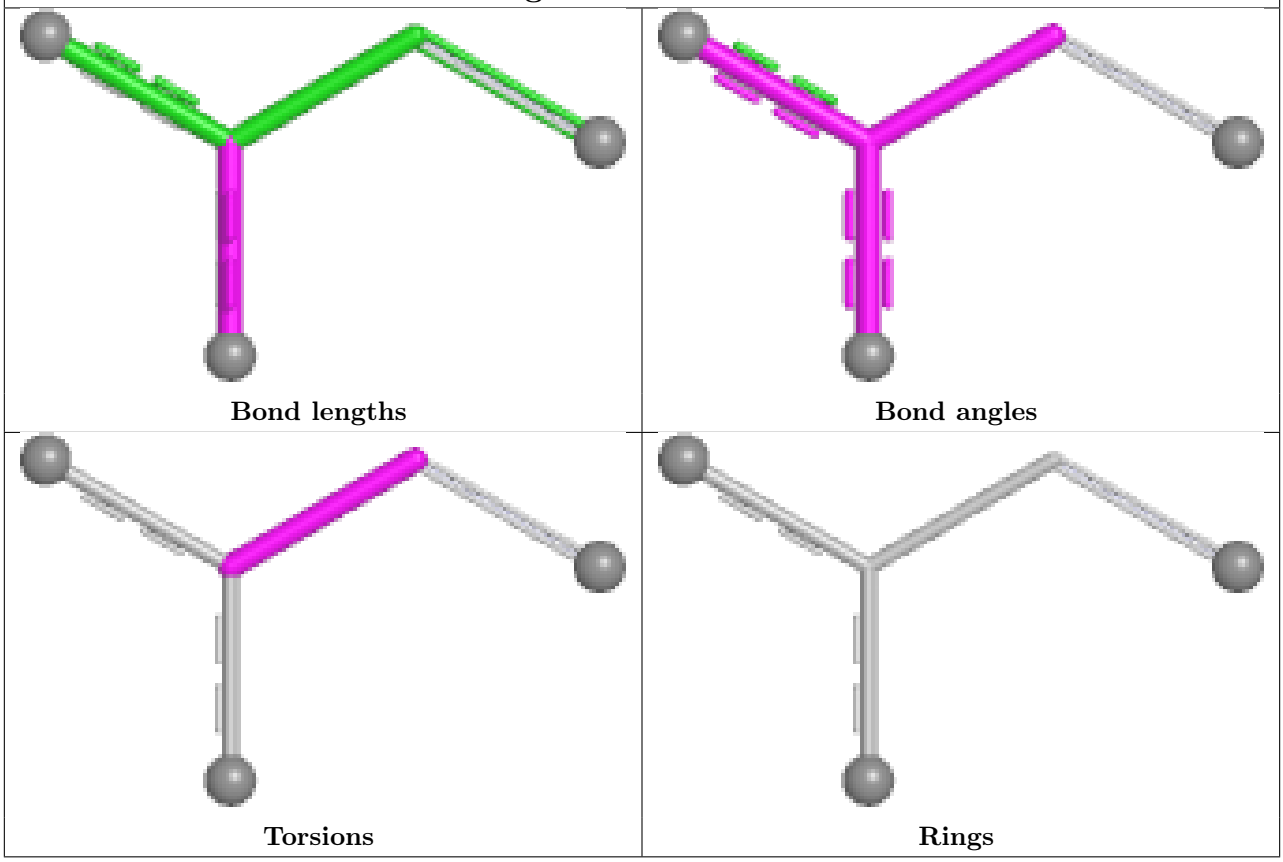
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLY A 501



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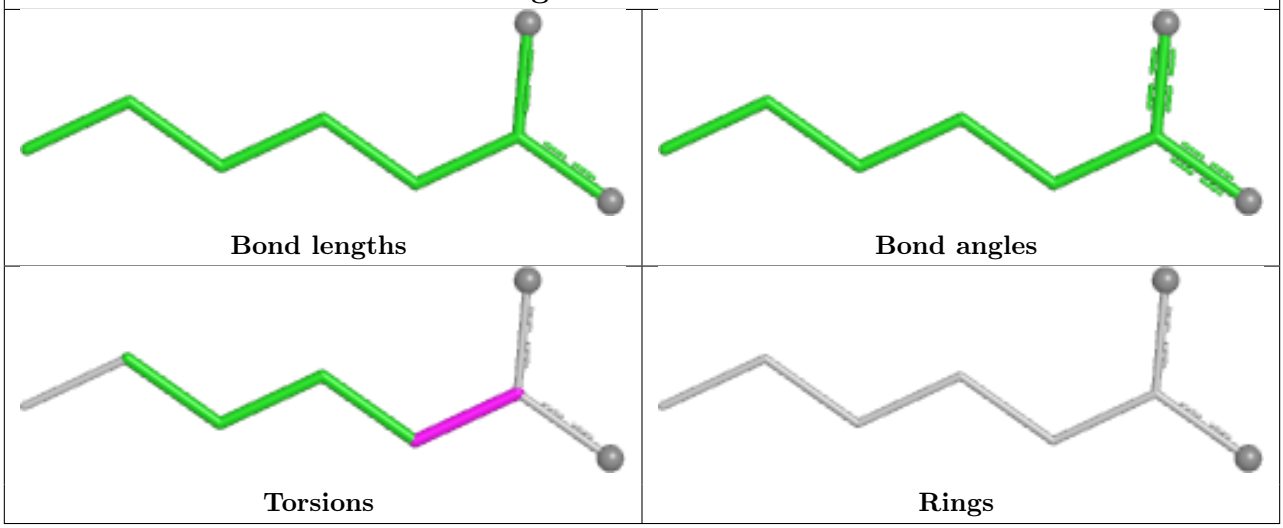
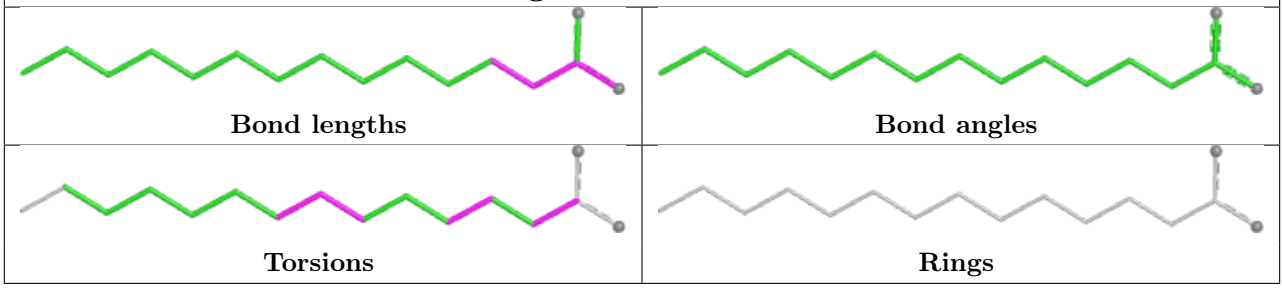
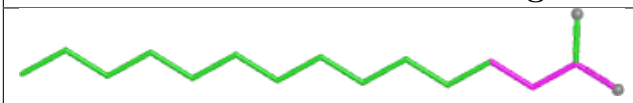


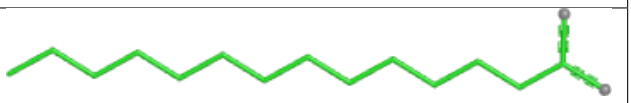
Ligand PX4 C 509



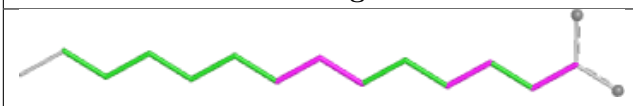
Ligand PX4 B 509



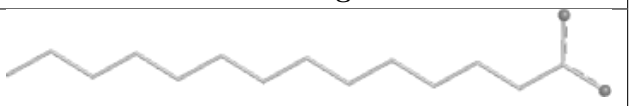
Bond lengths



Bond angles

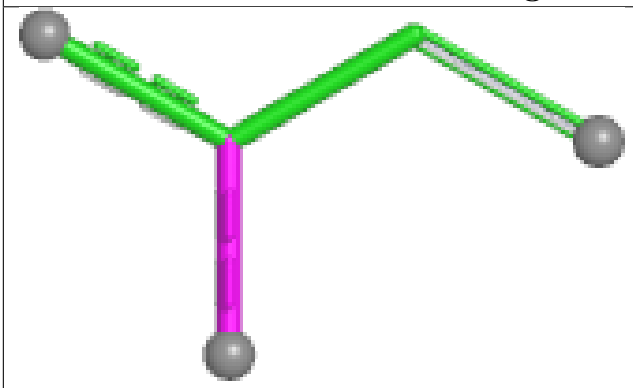


Torsions



Rings

Ligand GLY D 501



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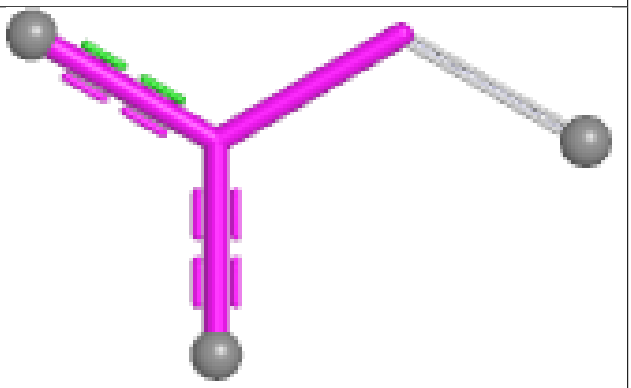

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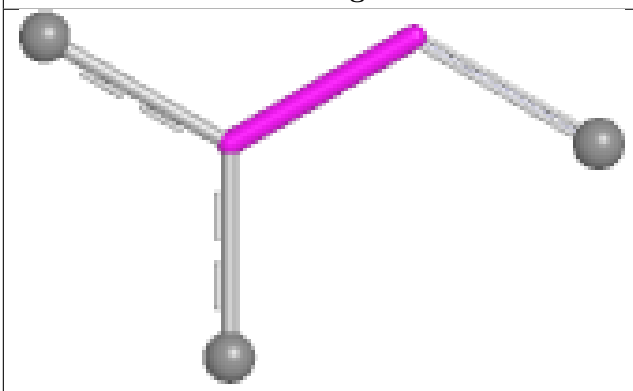

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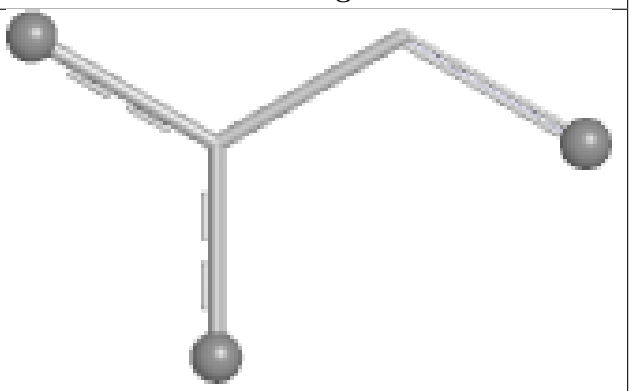
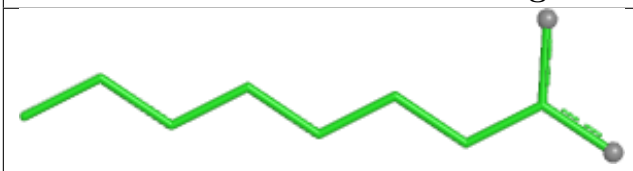


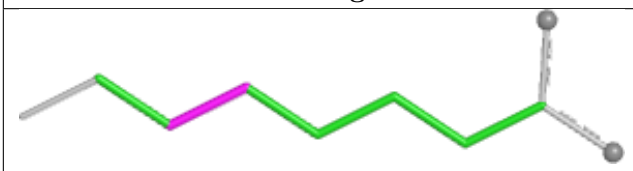
Rings

Ligand PIO C 505



Bond lengths

Bond angles



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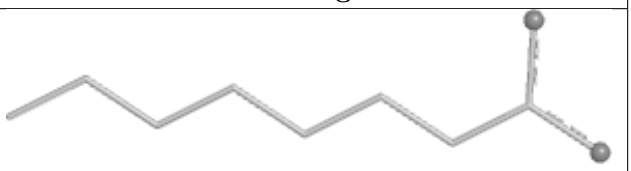
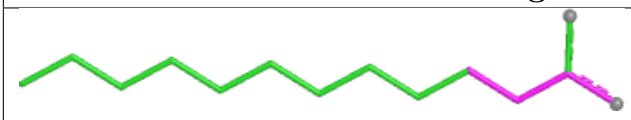


Rings

Ligand PX4 E 509



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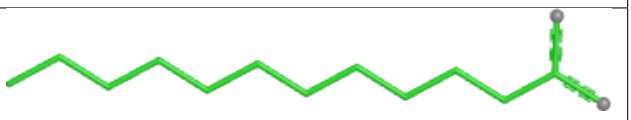

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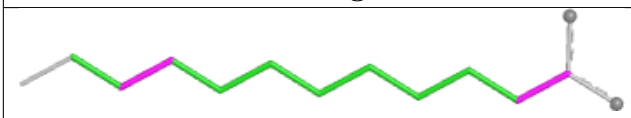

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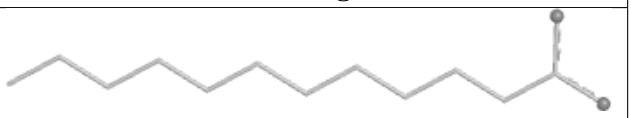
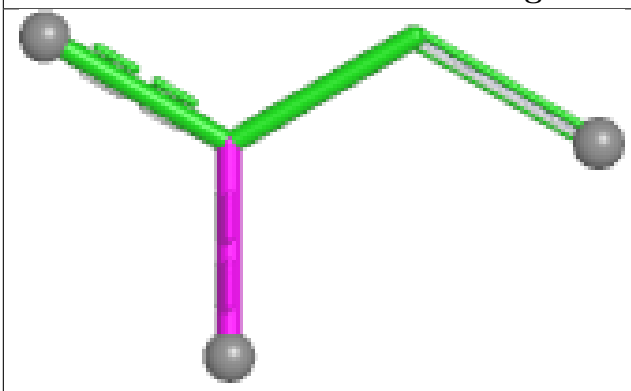


Rings

Ligand GLY C 501



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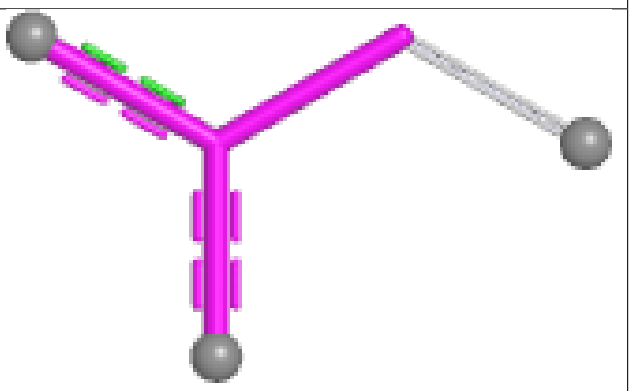
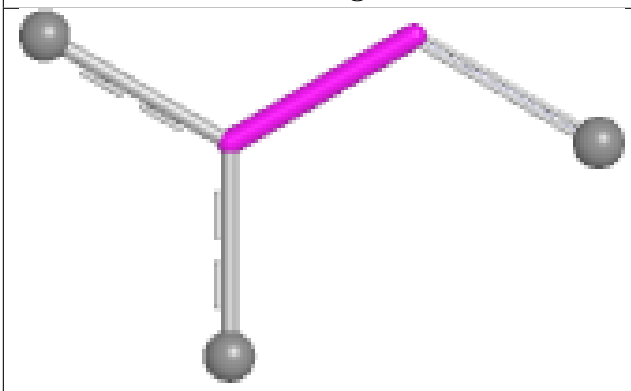


Bond angles



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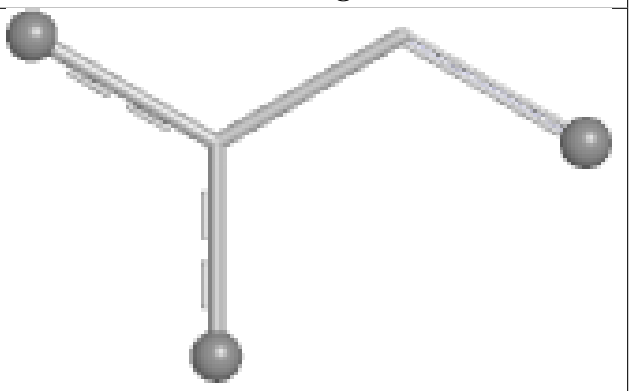
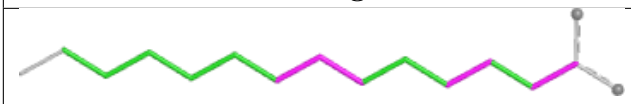


Rings

Ligand PX4 E 503

Bond lengths

Bond angles



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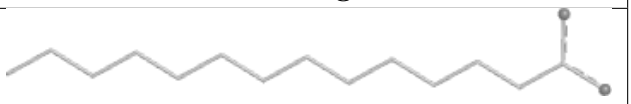
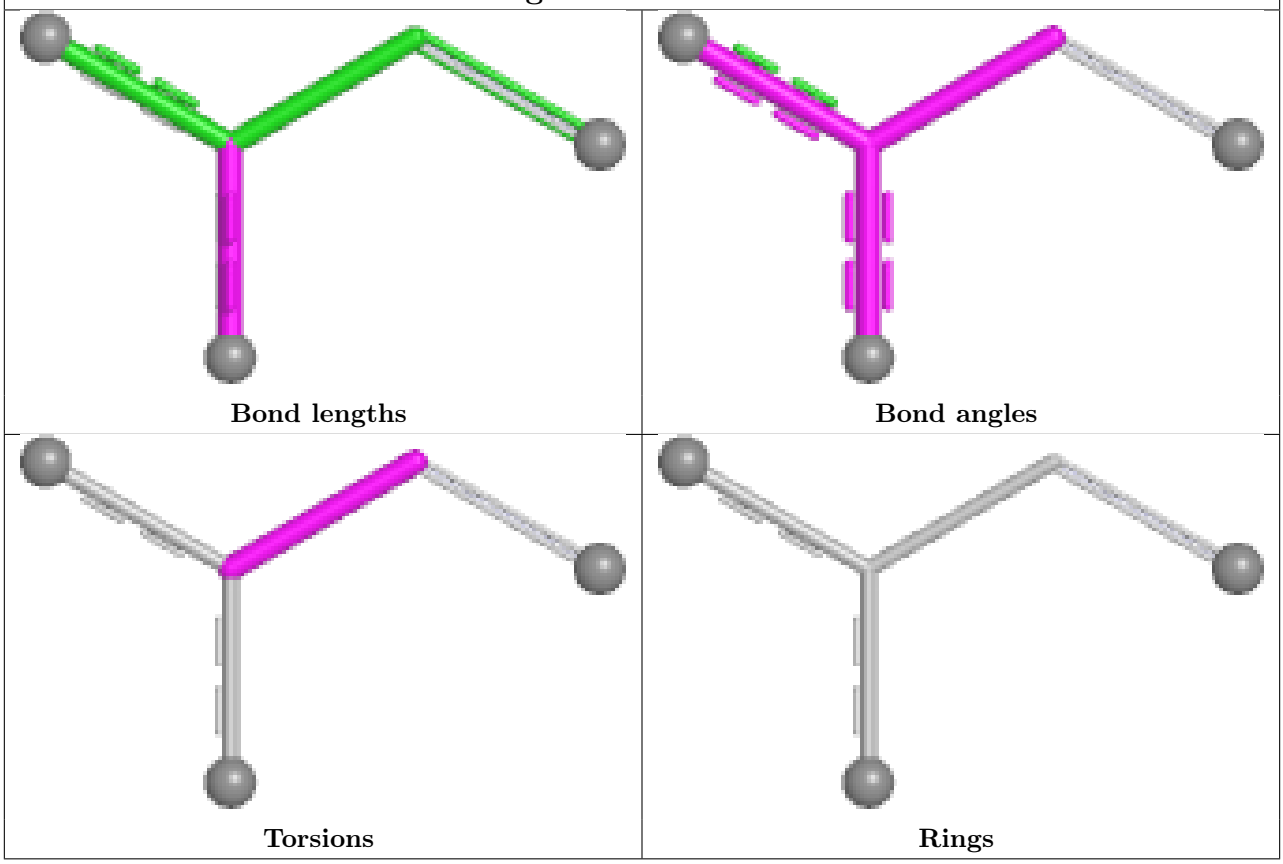
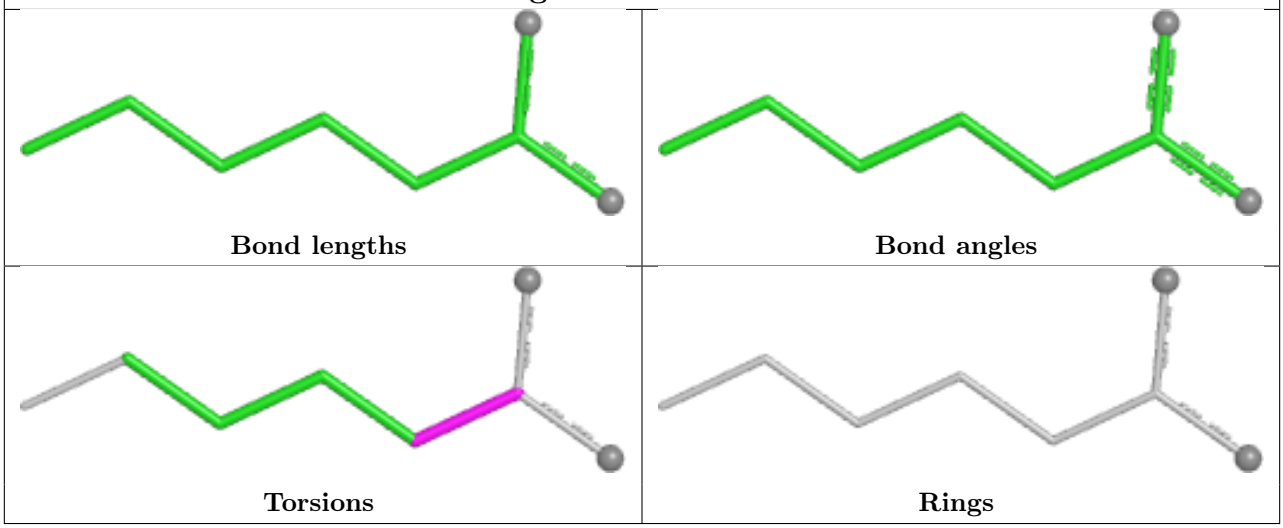


Rings

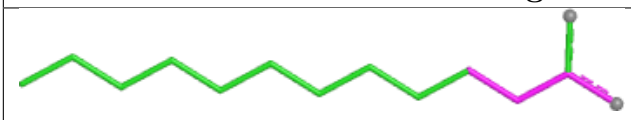
Ligand GLY B 501



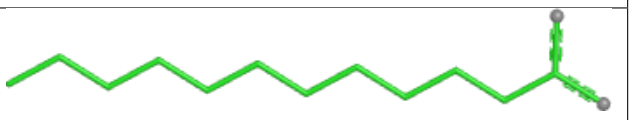
Ligand PIO A 507



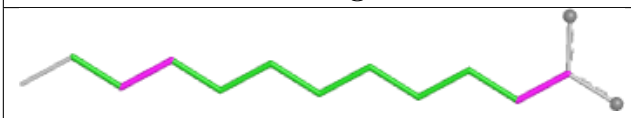
Ligand PX4 D 506



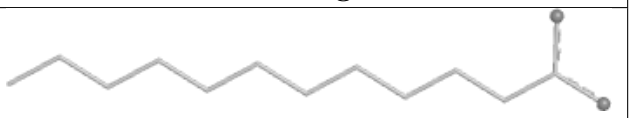
Bond lengths



Bond angles

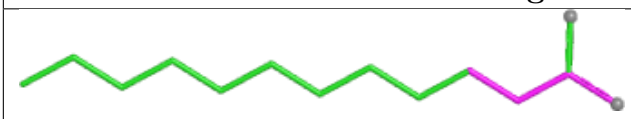


Torsions



Rings

Ligand PX4 B 508



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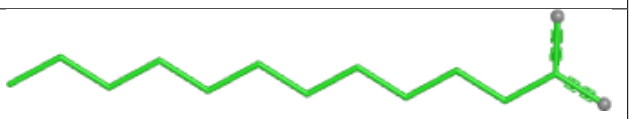
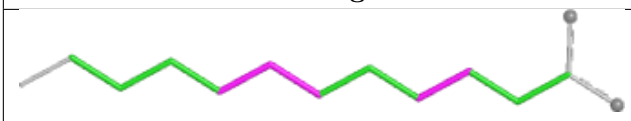


Bond angles



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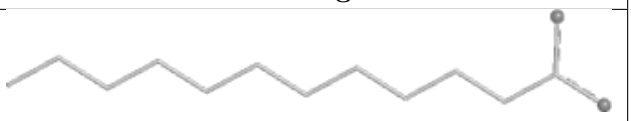
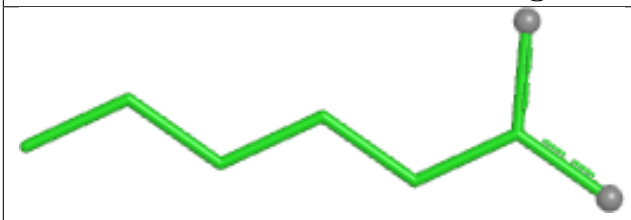


Rings

Ligand PIO D 504



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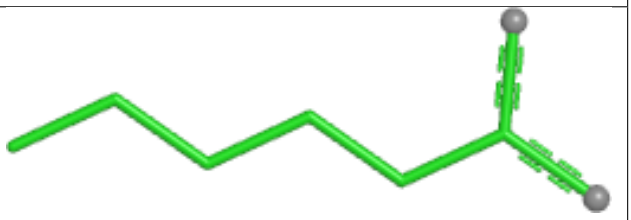
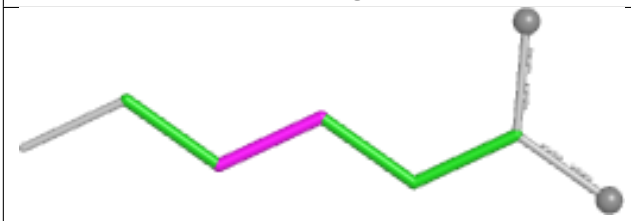


Bond angles



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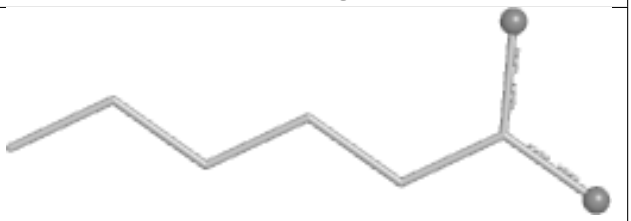
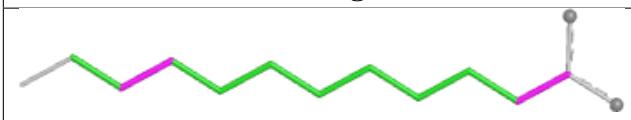


Rings

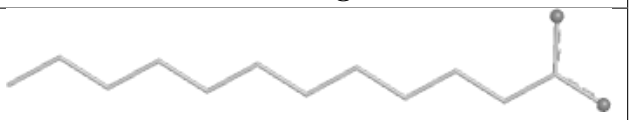
Ligand PX4 B 506

Bond lengths

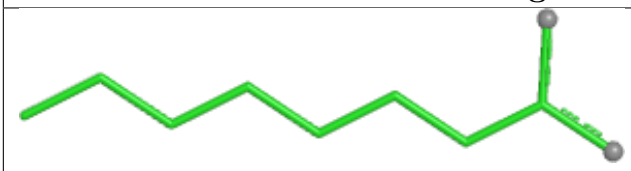
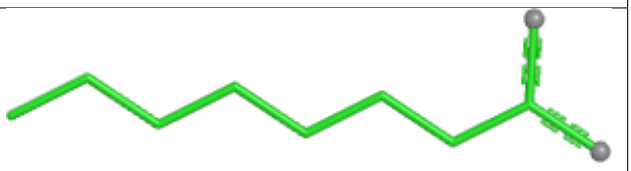
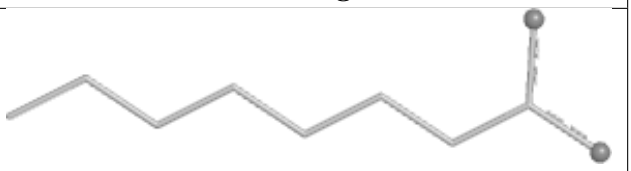
Bond angles

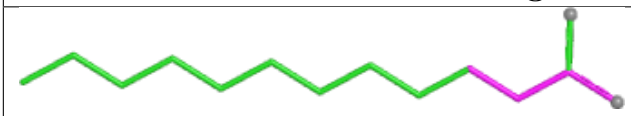
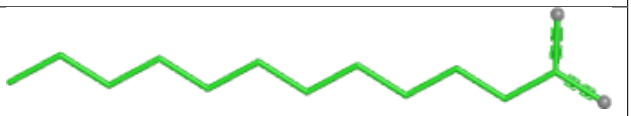
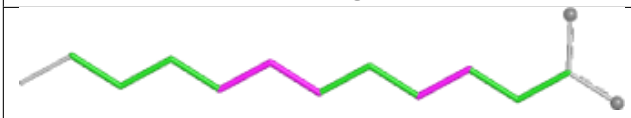
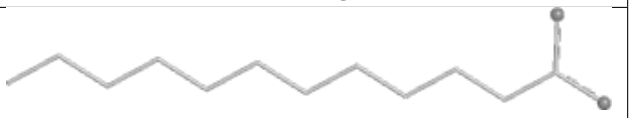


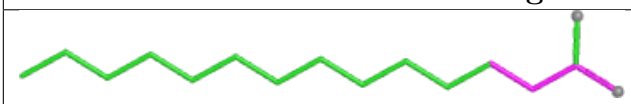
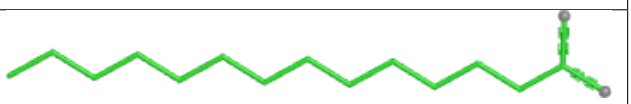
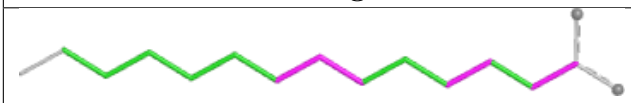
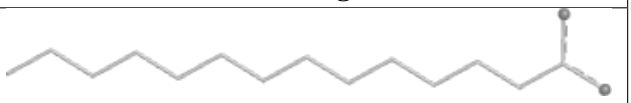
Torsions



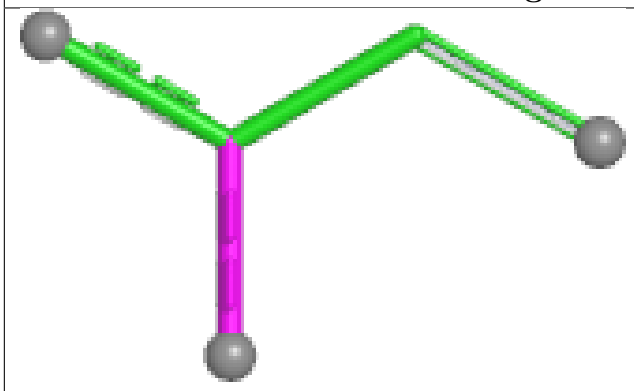
Rings

Ligand PIO A 505	
 Bond lengths	 Bond angles
Torsions	 Rings

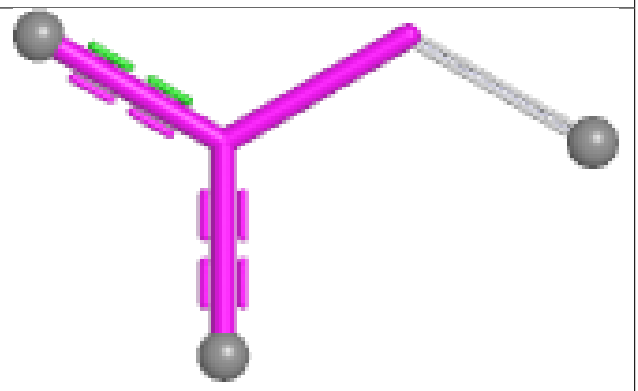
Ligand PX4 C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PX4 D 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

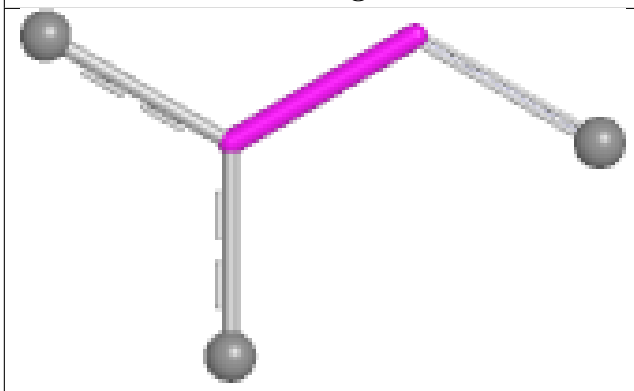
Ligand GLY A 511



Bond lengths



Bond angles



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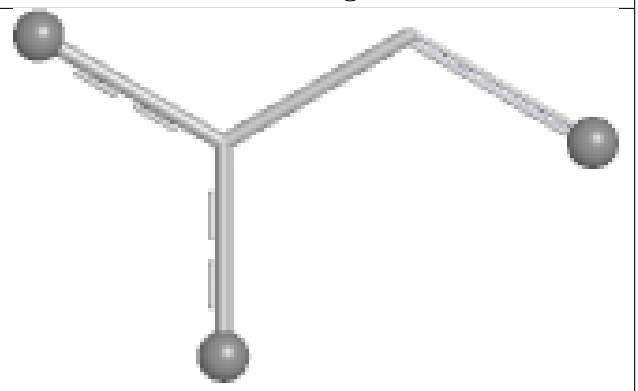
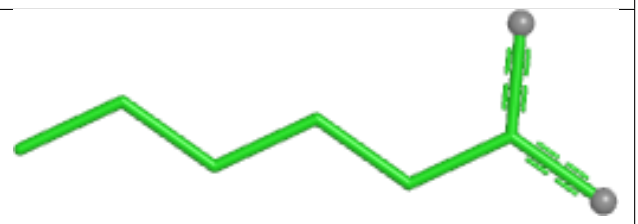


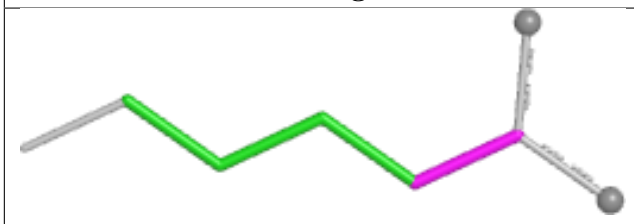
Rings

Ligand PIO B 507

Bond lengths



Bond angles



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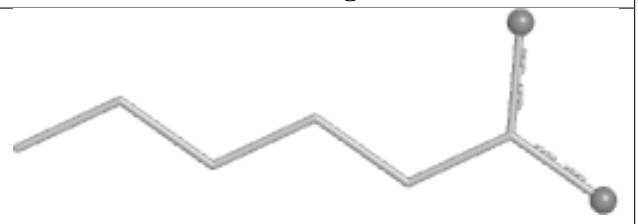
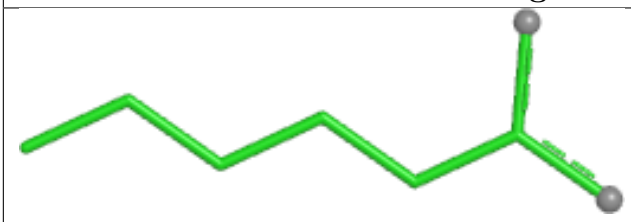
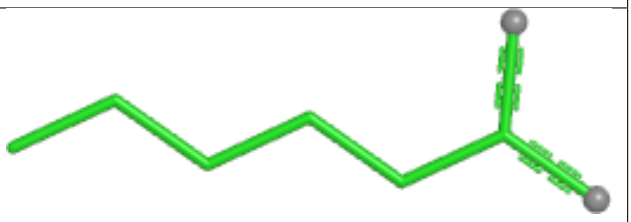


Rings

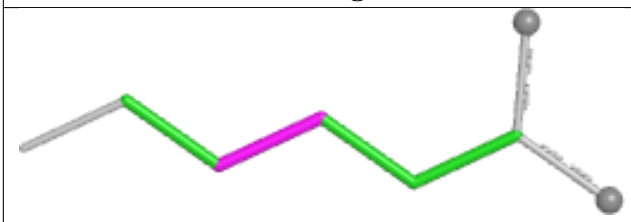
Ligand PIO B 504



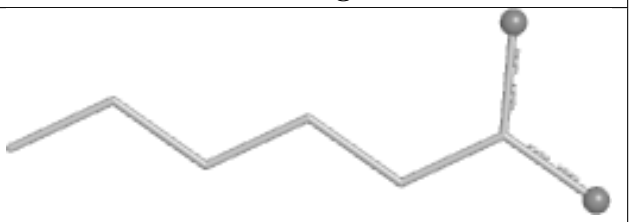
Bond lengths



Bond angles

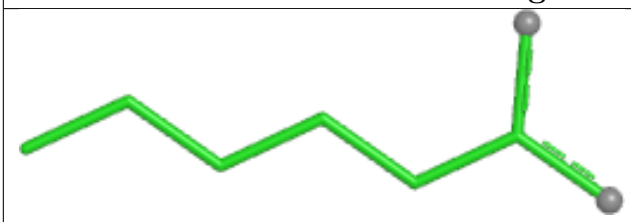


Torsions



Rings

Ligand PIO D 507



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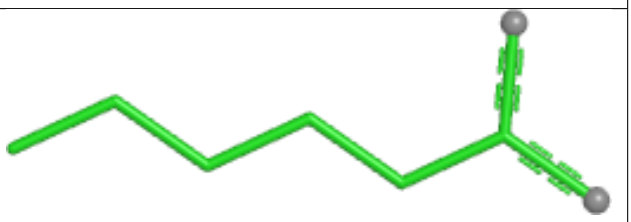
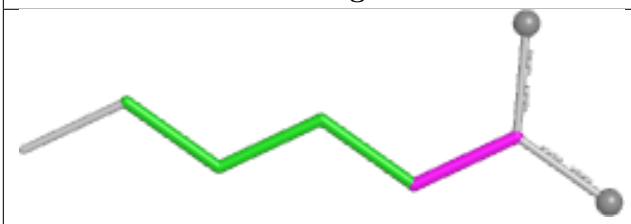


Bond angles



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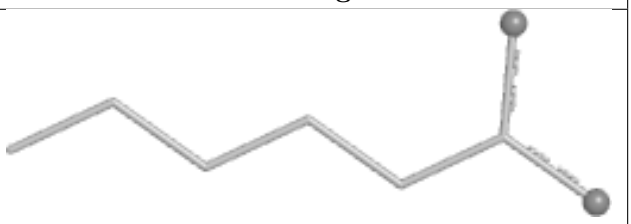
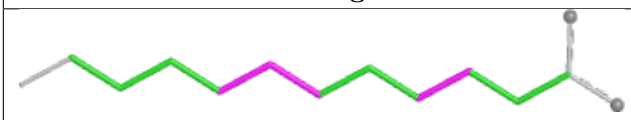


Rings

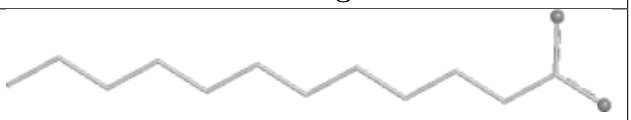
Ligand PX4 E 502

Bond lengths

Bond angles

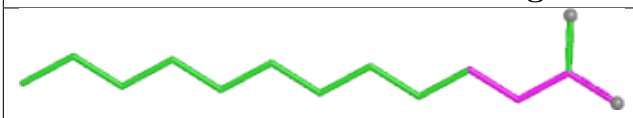


Torsions

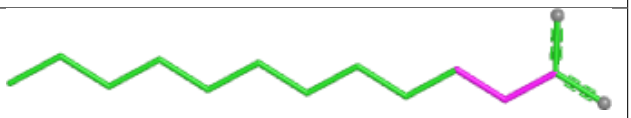


Rings

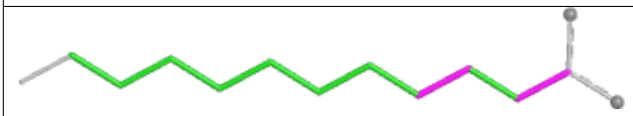
Ligand PX4 C 510



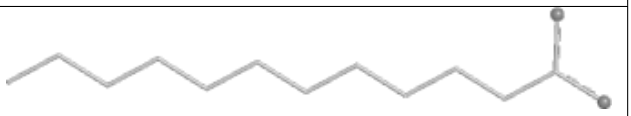
Bond lengths



Bond angles

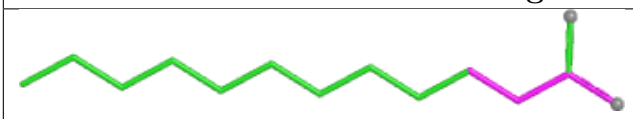


Torsions

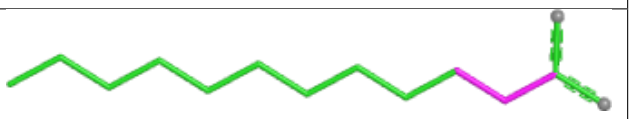


Rings

Ligand PX4 A 510

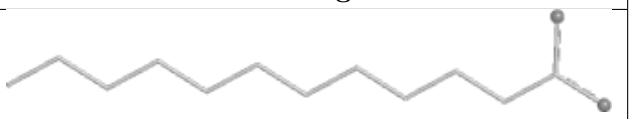


Bond lengths



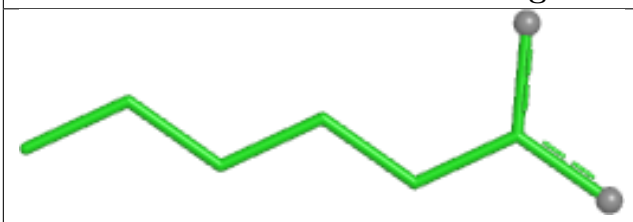
Bond angles

Torsions

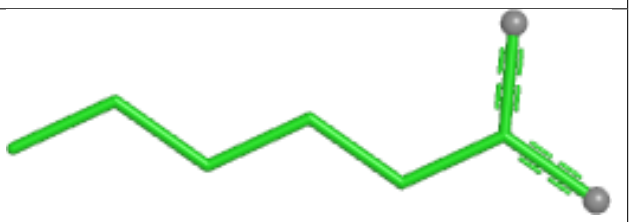


Rings

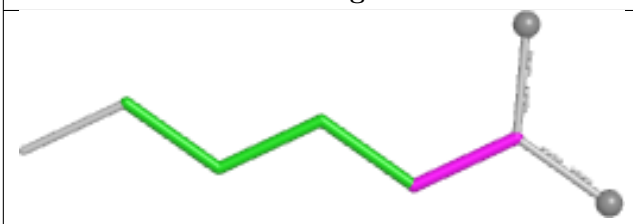
Ligand PIO C 507



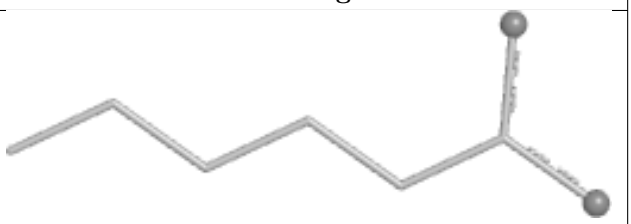
Bond lengths



Bond angles

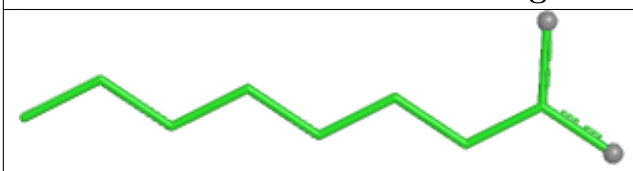


Torsions

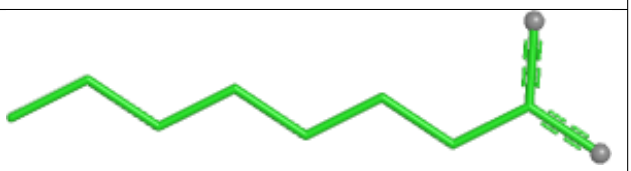


Rings

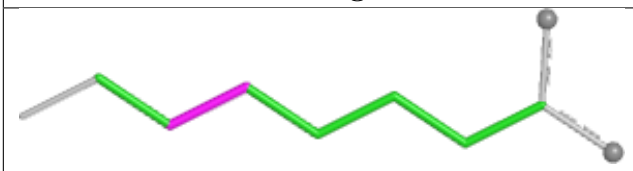
Ligand PIO B 505



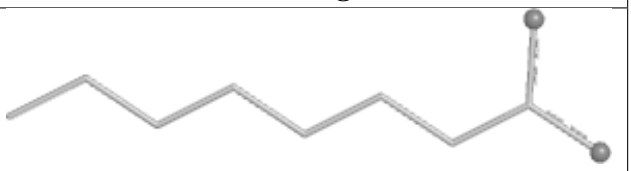
Bond lengths



Bond angles

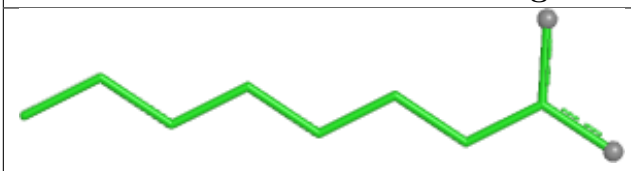


Torsions

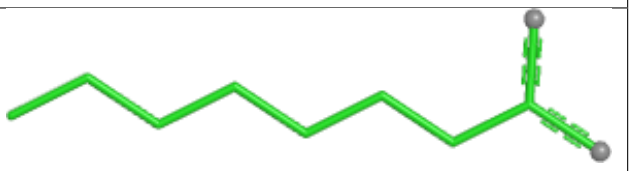


Rings

Ligand PIO E 508

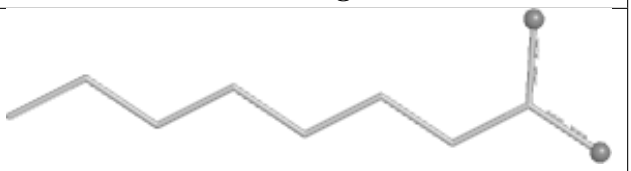


Bond lengths



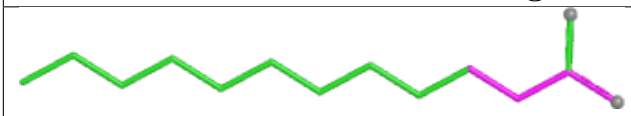
Bond angles

Torsions

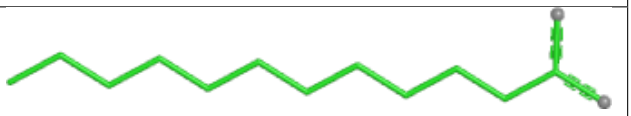


Rings

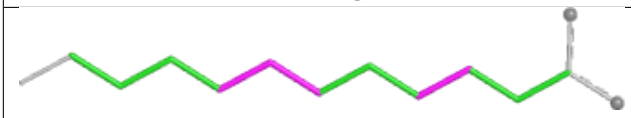
Ligand PX4 A 508



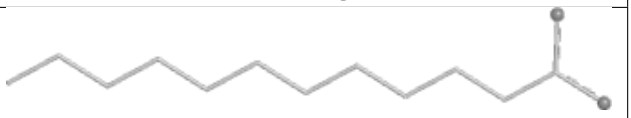
Bond lengths



Bond angles

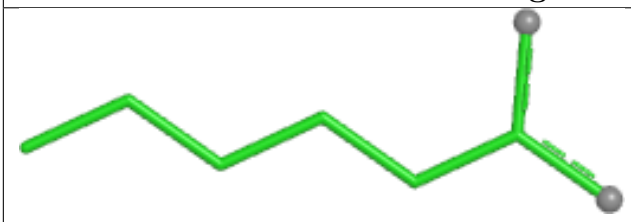


Torsions

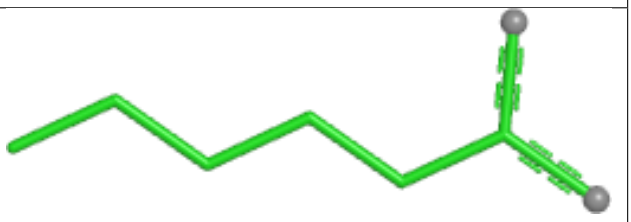


Rings

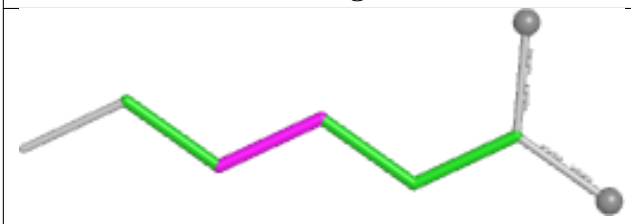
Ligand PIO C 504



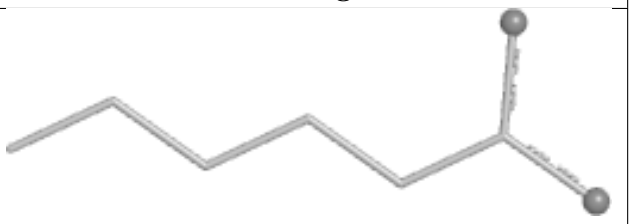
Bond lengths



Bond angles



Torsions

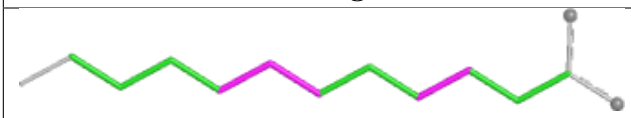


Rings

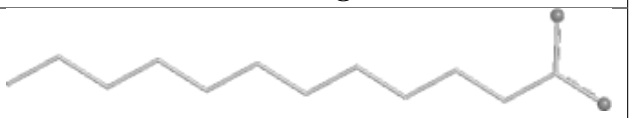
Ligand PX4 D 508

Bond lengths

Bond angles

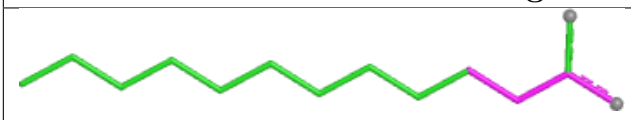


Torsions

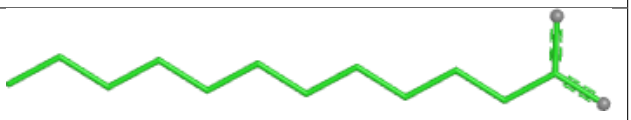


Rings

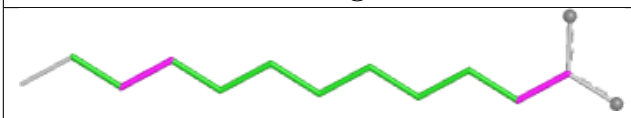
Ligand PX4 A 506



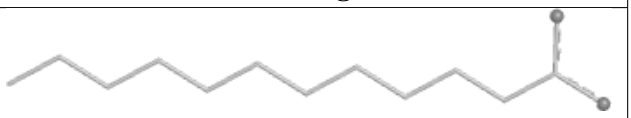
Bond lengths



Bond angles

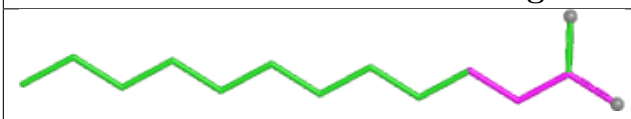


Torsions

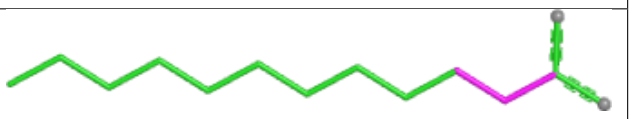


Rings

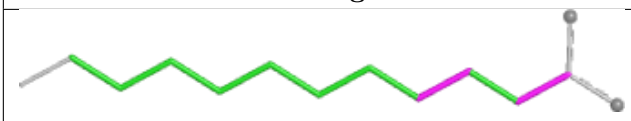
Ligand PX4 B 510



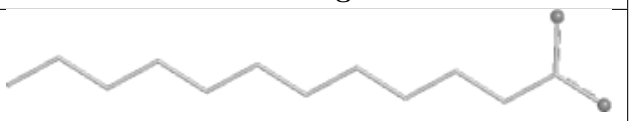
Bond lengths



Bond angles

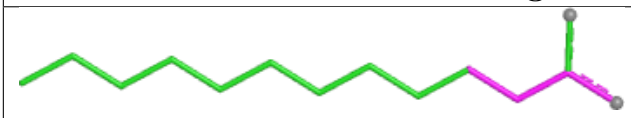


Torsions

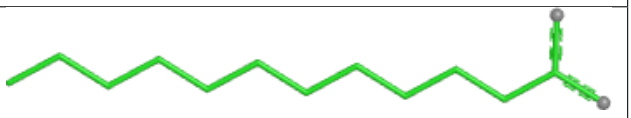


Rings

Ligand PX4 C 506

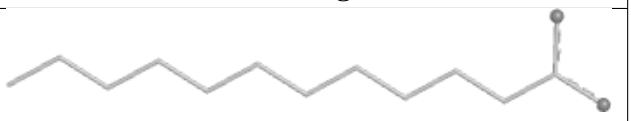


Bond lengths



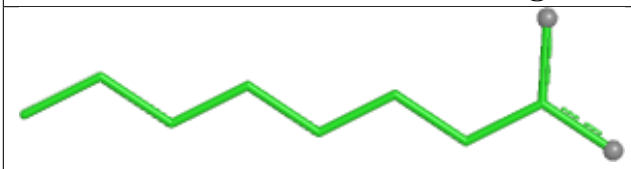
Bond angles

Torsions

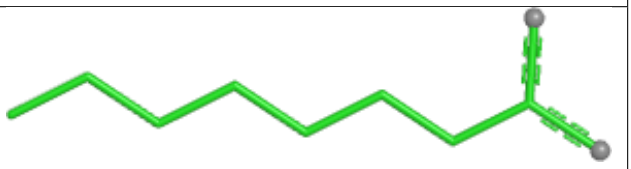


Rings

Ligand PIO D 505

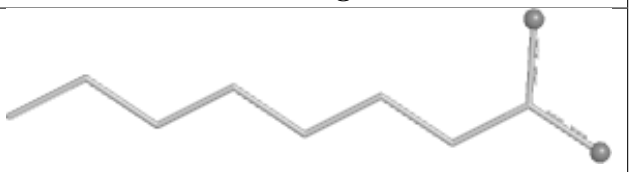


Bond lengths

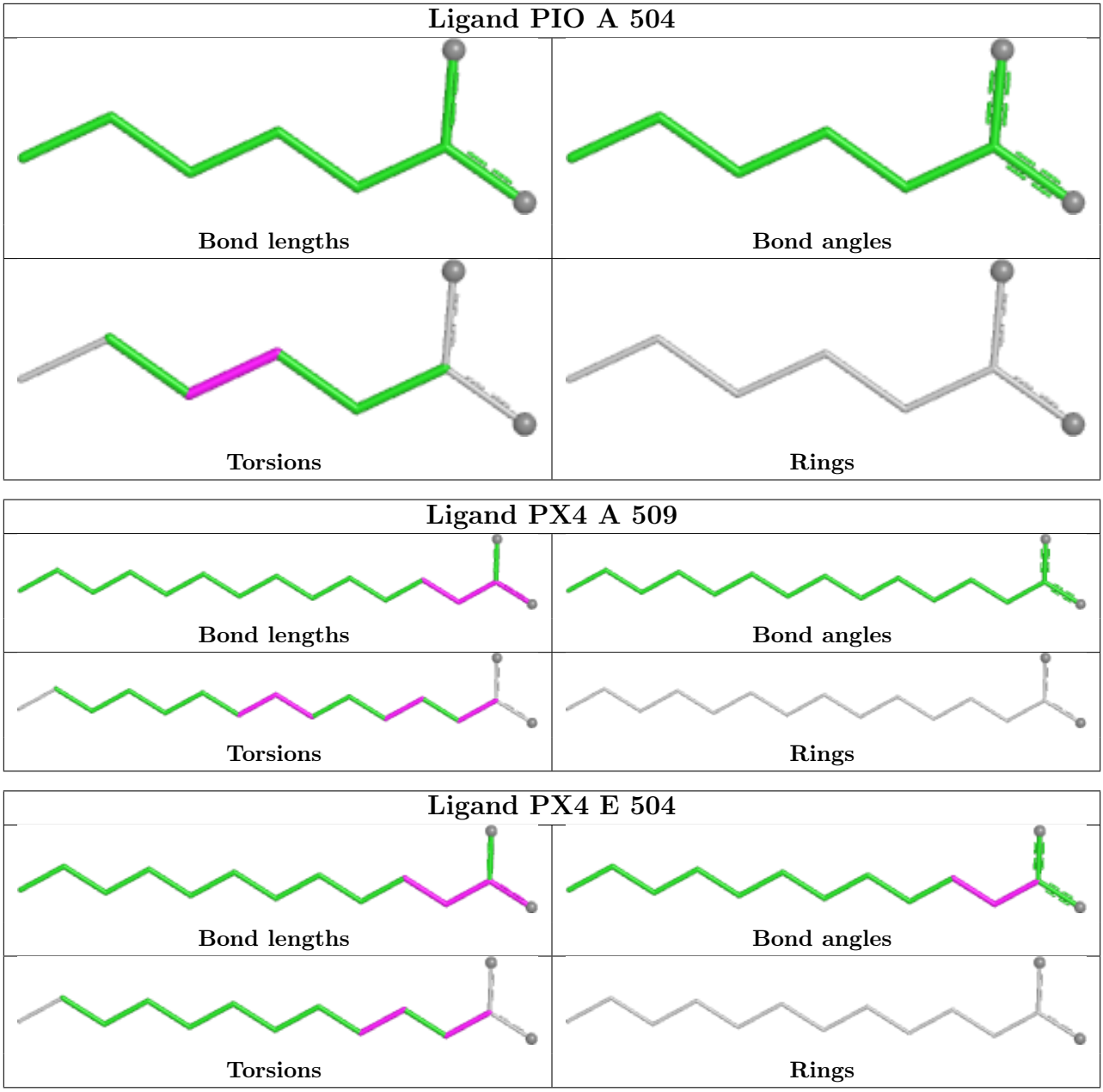


Bond angles

Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

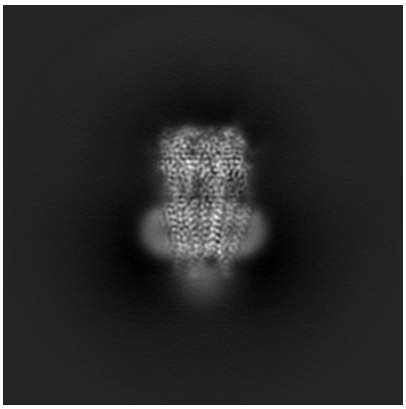
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-44934. These allow visual inspection of the internal detail of the map and identification of artifacts.

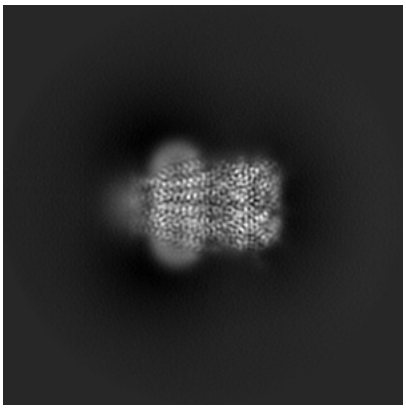
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

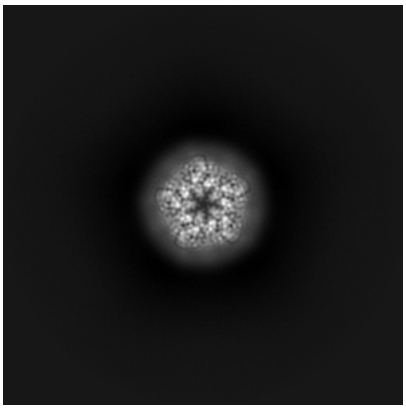
6.1.1 Primary map



X

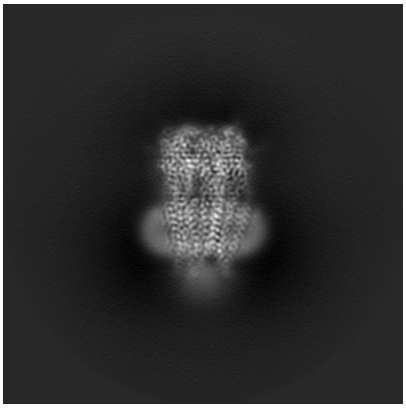


Y

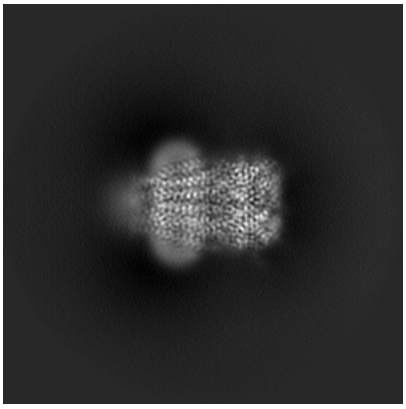


Z

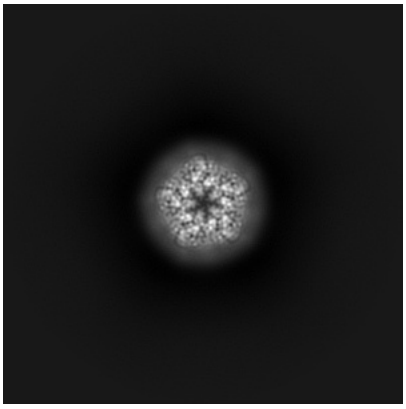
6.1.2 Raw map



X



Y

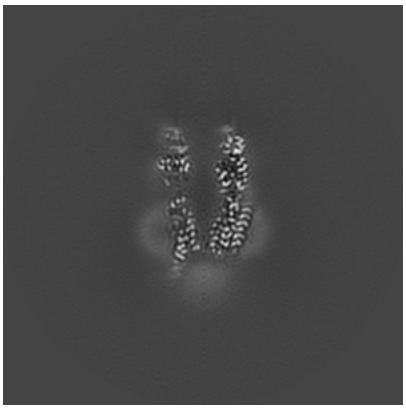


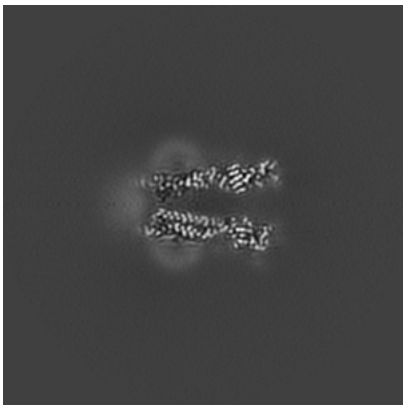
Z

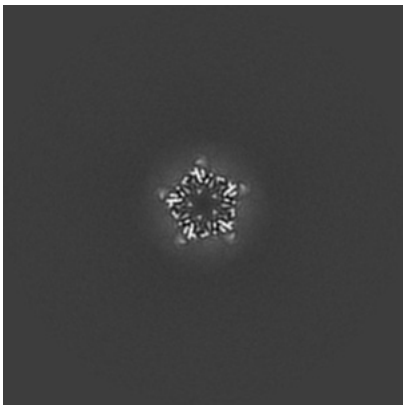
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

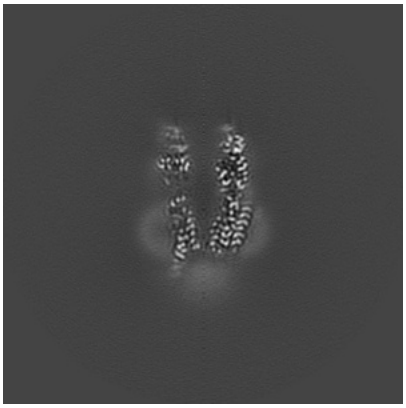
6.2.1 Primary map

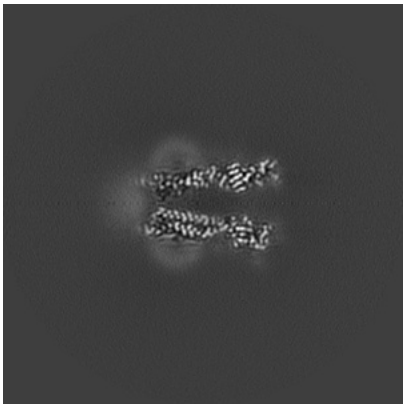

X Index: 150

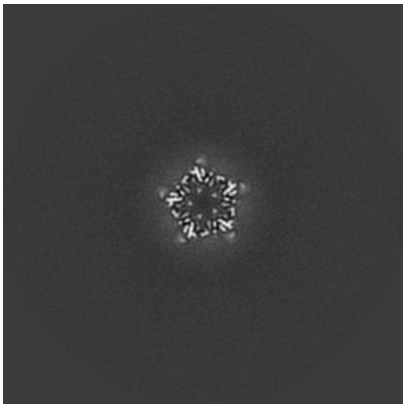

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

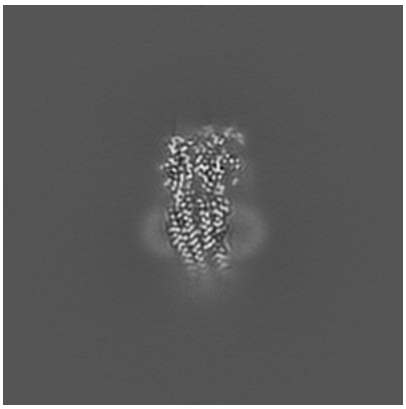

Y Index: 150

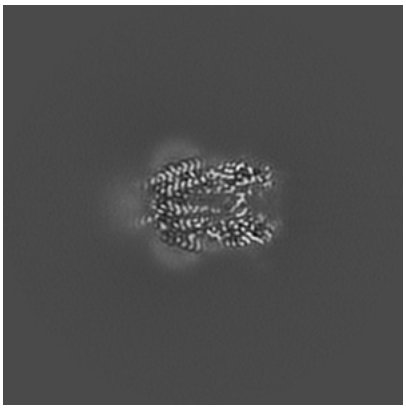

Z Index: 150

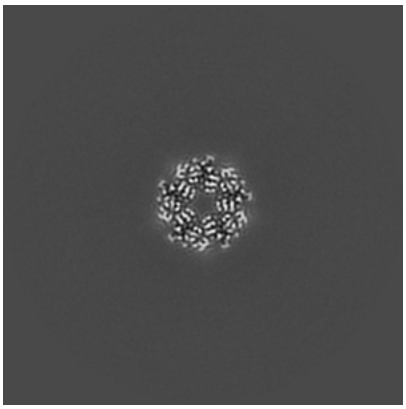
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

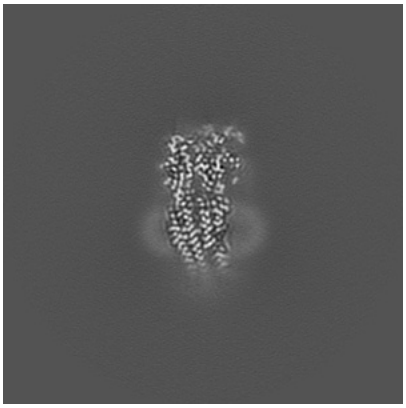
6.3.1 Primary map

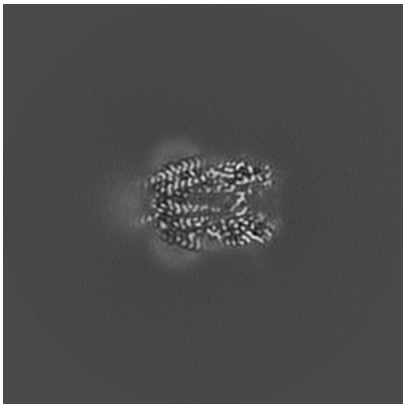

X Index: 166

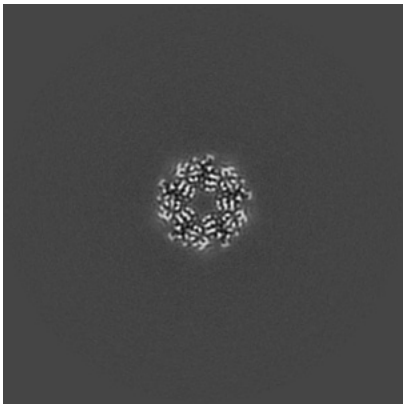

Y Index: 160


Z Index: 178

6.3.2 Raw map


X Index: 166

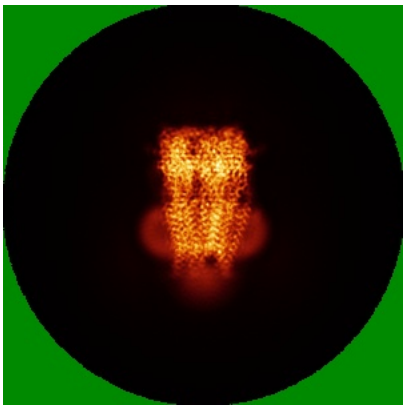

Y Index: 160

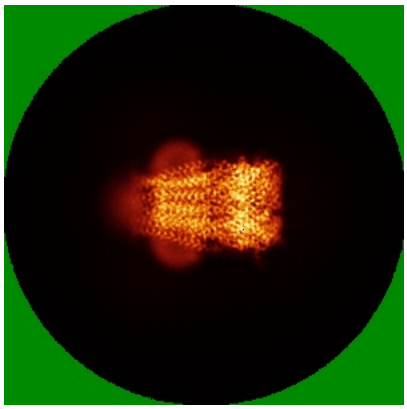

Z Index: 178

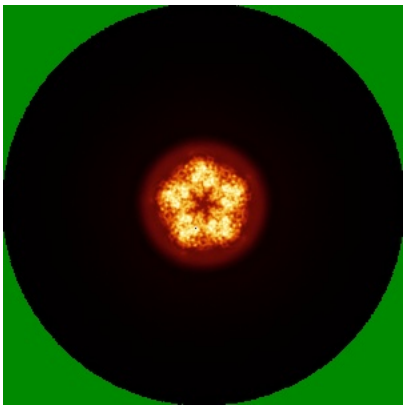
The images above show the largest variance slices of the map in three orthogonal directions.

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

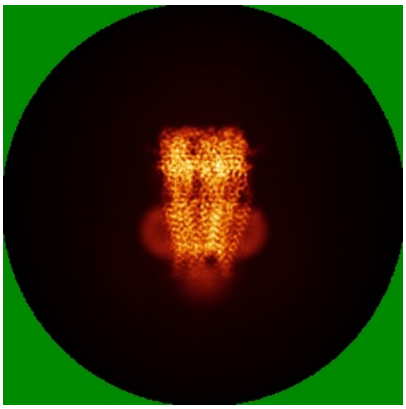
6.4.1 Primary map

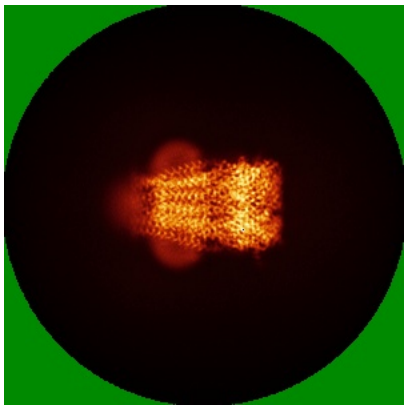

X

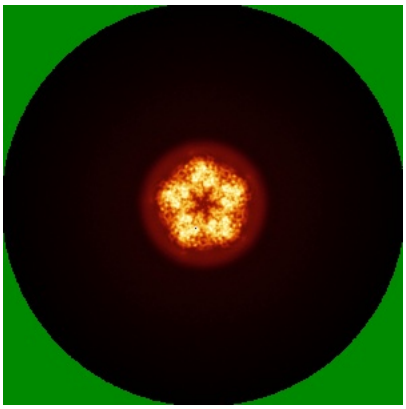

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

This section was not generated.

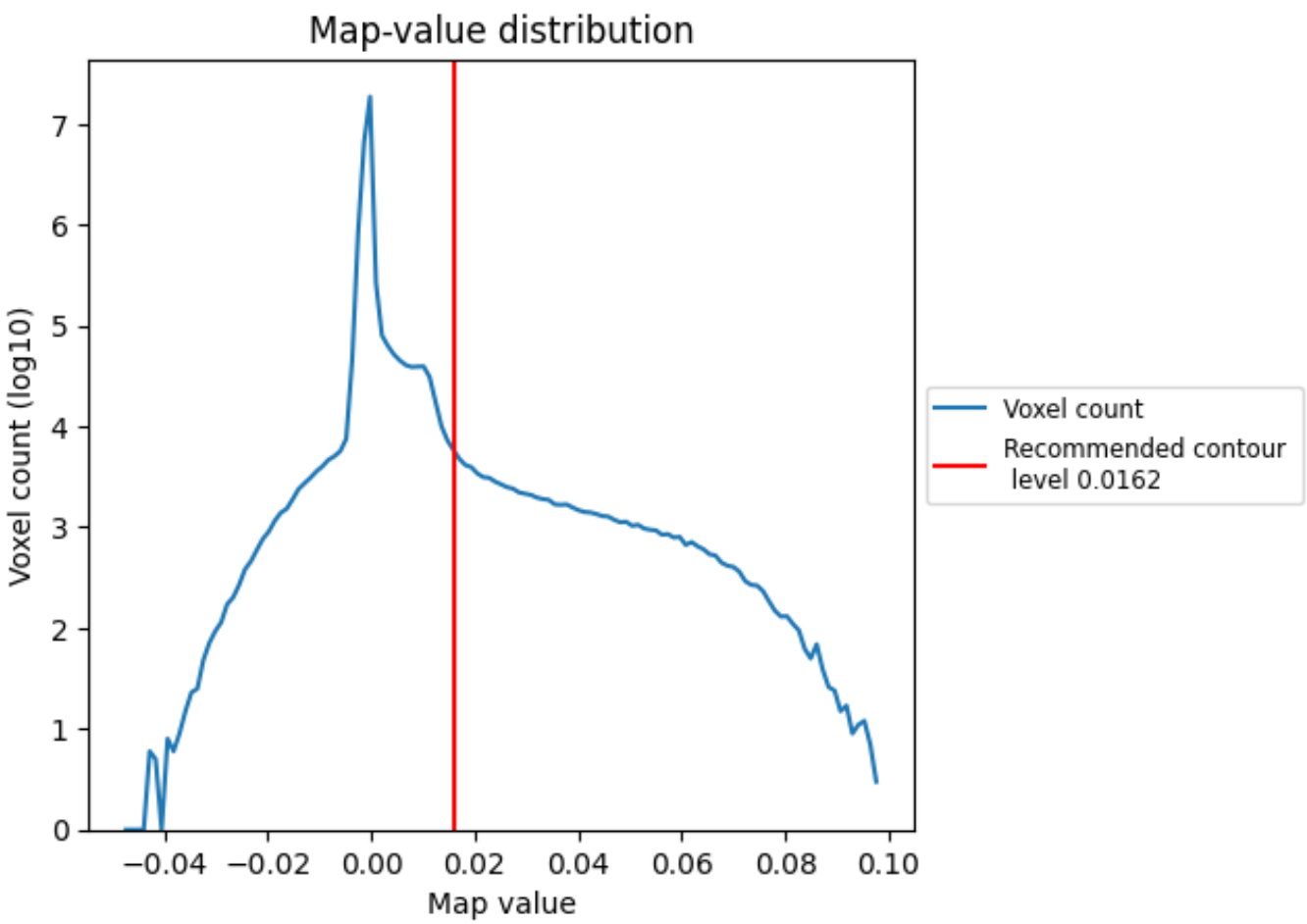
6.6 Mask visualisation (i)

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

7 Map analysis (i)

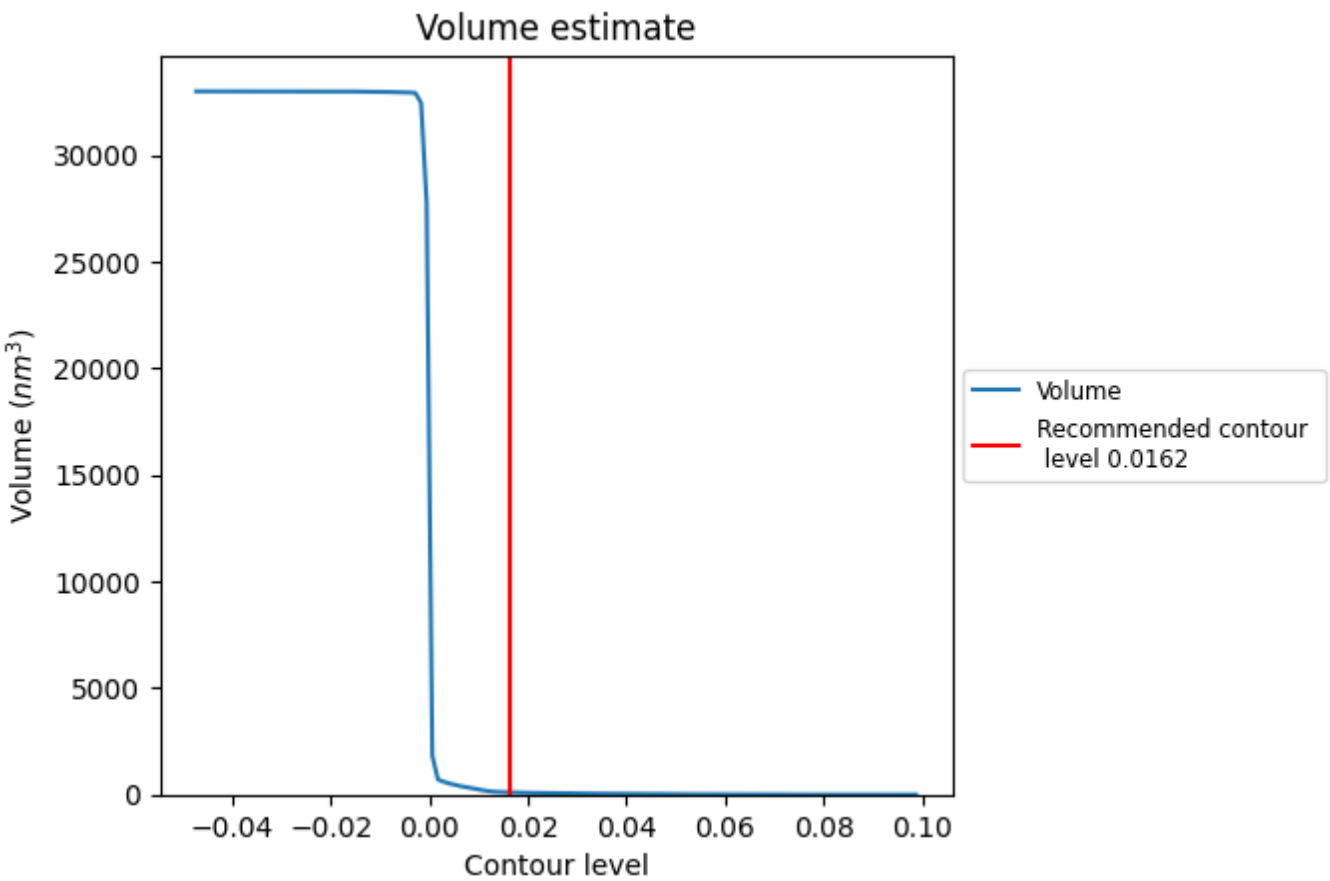
This section contains the results of statistical analysis of the map.

7.1 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.

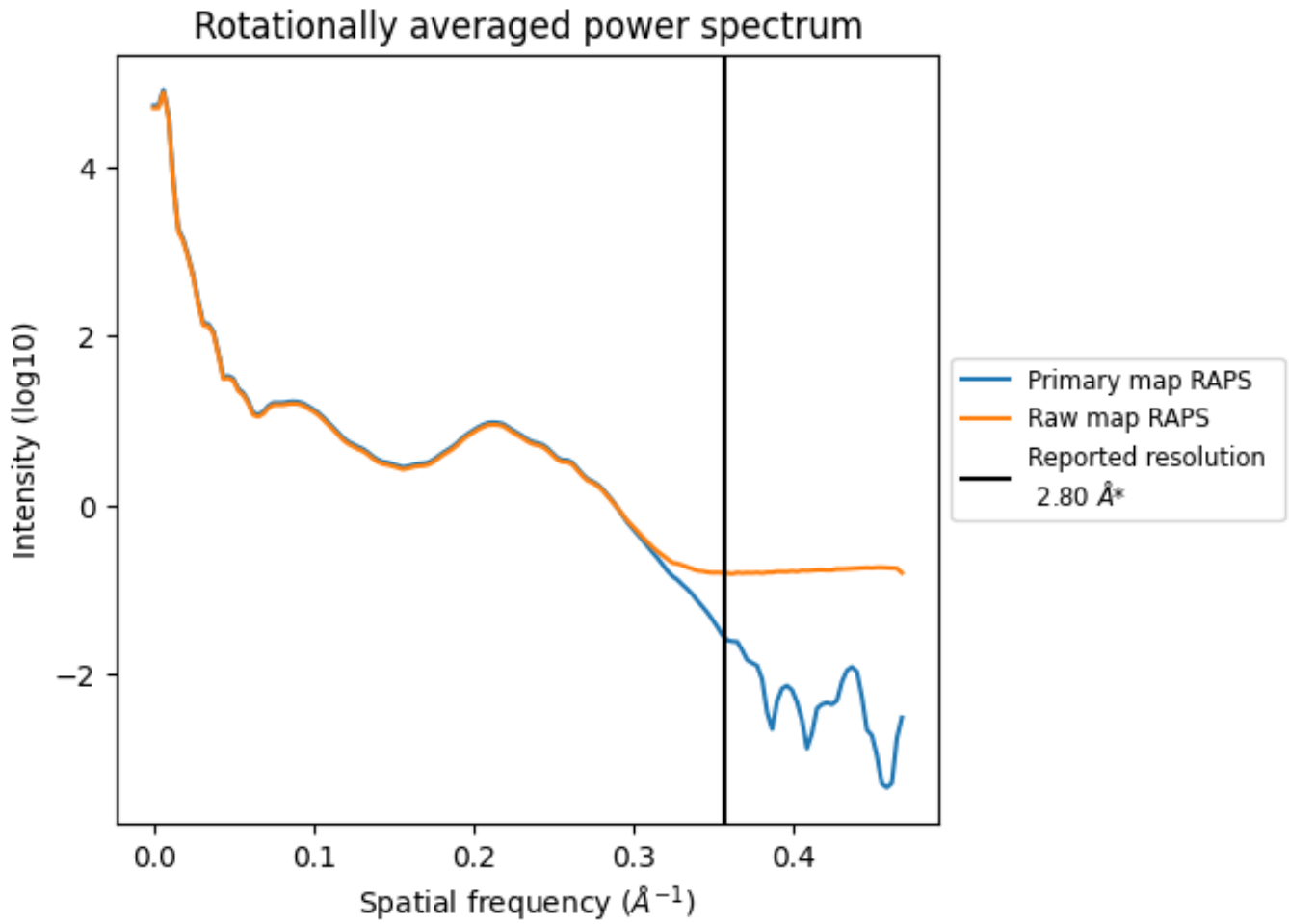
7.2 Volume estimate (i)



The volume at the recommended contour level is 102 nm^3; this corresponds to an approximate mass of 92 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

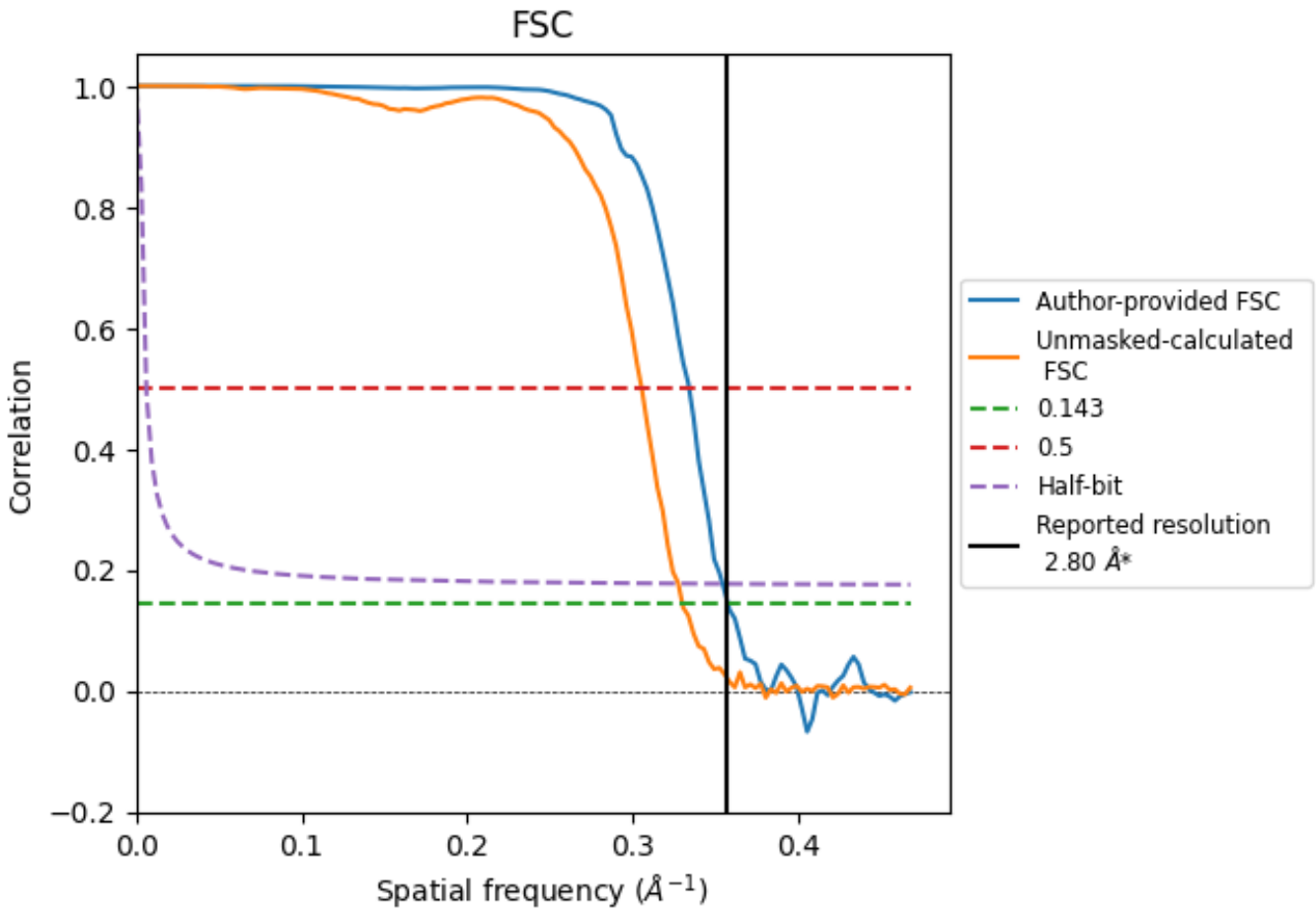


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation (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.

8.1 FSC (i)



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

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	2.99	2.82
Unmasked-calculated*	3.03	3.27	3.05

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

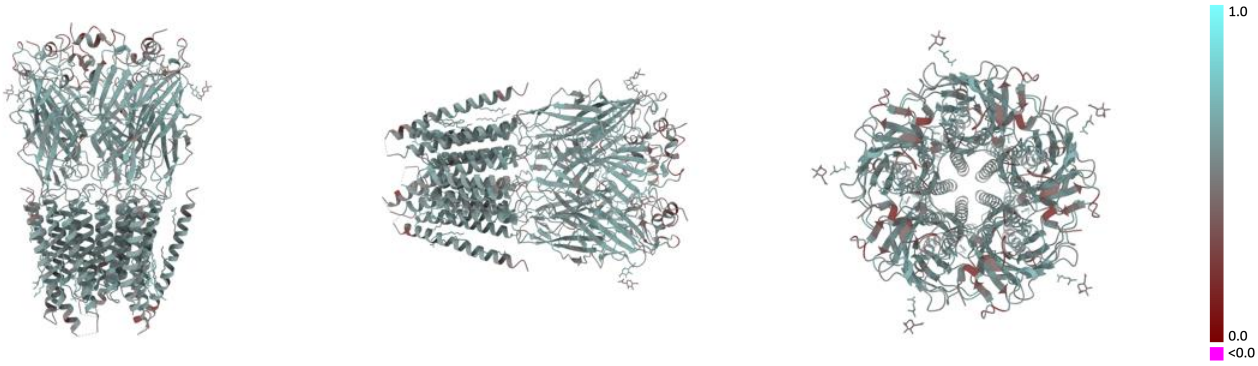
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-44934 and PDB model 9BVJ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay (i)

This section was not generated.

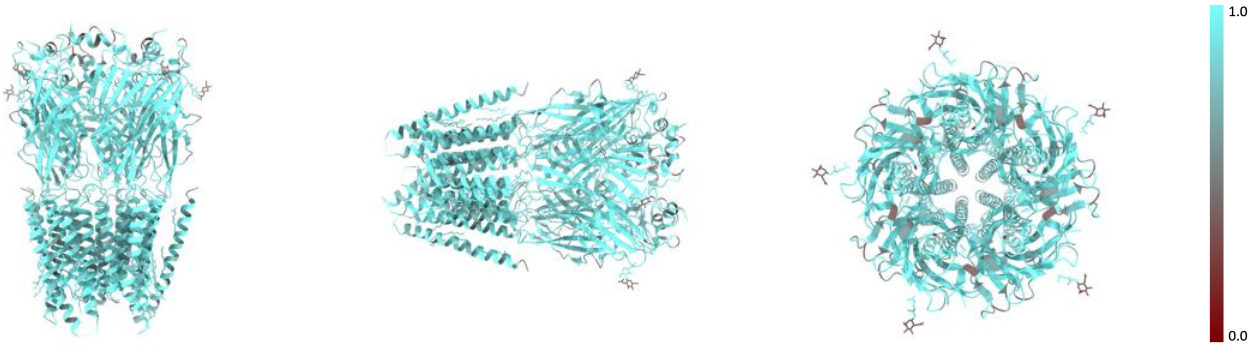
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

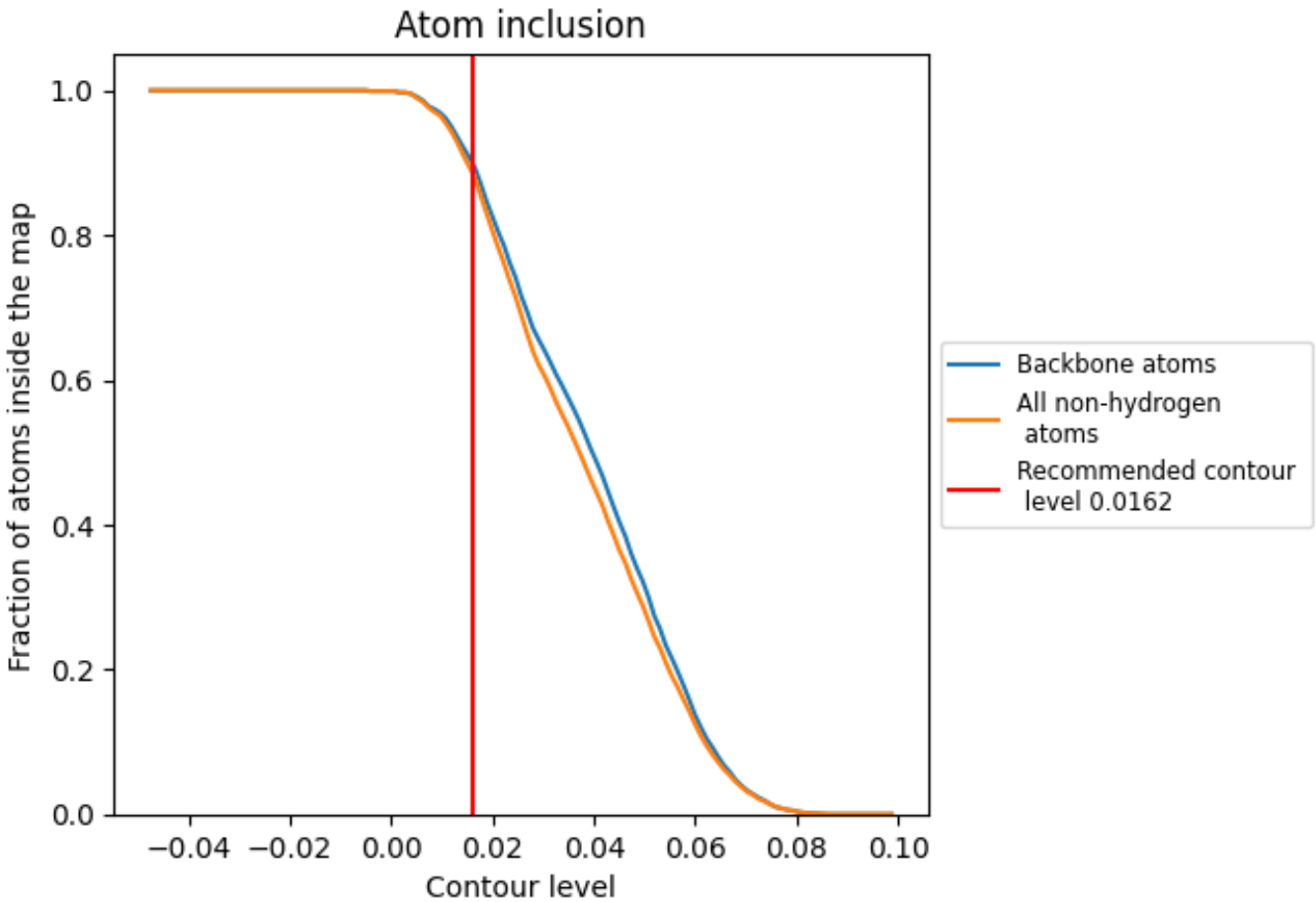
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0162).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0162) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.5460
A	0.8920	0.5480
B	0.8920	0.5460
C	0.8900	0.5480
D	0.8900	0.5460
E	0.8890	0.5460
F	0.6430	0.5040
G	0.6430	0.4980
H	0.6430	0.5010
I	0.6430	0.5020
J	0.6070	0.5000