Full wwPDB EM Validation Report

Oct 14, 2024 – 07:51 PM JST

PDB ID	:	7Y6I
EMDB ID	:	EMD-33641
Title	:	Cryo-EM structure of human sodium-chloride cotransporter
Authors	:	Nan, J.; Yang, X.; Shan, Z.; Yuan, Y.; Zhang, Y.Q.
Deposited on	:	2022-06-20
Resolution	:	2.85 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 ⓘ symbol.

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

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

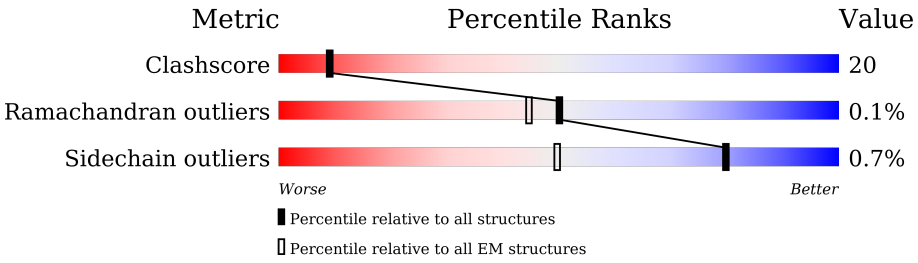
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1053	33% 11% 55%
1	B	1053	33% 12% 55%
2	C	2	50% 50%
2	D	2	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
5	Y01	B	1109	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8176 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 Solute carrier family 12 member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	469	Total	C	N	O	S	0	0
			3564	2362	557	624	21		
1	B	469	Total	C	N	O	S	0	0
			3564	2362	557	624	21		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P55017
A	264	GLY	ALA	engineered mutation	UNP P55017
A	1022	LEU	-	expression tag	UNP P55017
A	1023	GLU	-	expression tag	UNP P55017
A	1024	GLY	-	expression tag	UNP P55017
A	1025	SER	-	expression tag	UNP P55017
A	1026	ASP	-	expression tag	UNP P55017
A	1027	GLU	-	expression tag	UNP P55017
A	1028	VAL	-	expression tag	UNP P55017
A	1029	ASP	-	expression tag	UNP P55017
A	1030	ALA	-	expression tag	UNP P55017
A	1031	GLY	-	expression tag	UNP P55017
A	1032	SER	-	expression tag	UNP P55017
A	1033	HIS	-	expression tag	UNP P55017
A	1034	HIS	-	expression tag	UNP P55017
A	1035	HIS	-	expression tag	UNP P55017
A	1036	HIS	-	expression tag	UNP P55017
A	1037	HIS	-	expression tag	UNP P55017
A	1038	HIS	-	expression tag	UNP P55017
A	1039	HIS	-	expression tag	UNP P55017
A	1040	HIS	-	expression tag	UNP P55017
A	1041	HIS	-	expression tag	UNP P55017
A	1042	HIS	-	expression tag	UNP P55017
A	1043	GLY	-	expression tag	UNP P55017
A	1044	SER	-	expression tag	UNP P55017
A	1045	VAL	-	expression tag	UNP P55017

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1046	GLU	-	expression tag	UNP P55017
A	1047	ASP	-	expression tag	UNP P55017
A	1048	TYR	-	expression tag	UNP P55017
A	1049	LYS	-	expression tag	UNP P55017
A	1050	ASP	-	expression tag	UNP P55017
A	1051	ASP	-	expression tag	UNP P55017
A	1052	ASP	-	expression tag	UNP P55017
A	1053	ASP	-	expression tag	UNP P55017
A	1054	LYS	-	expression tag	UNP P55017
B	?	-	GLN	deletion	UNP P55017
B	264	GLY	ALA	engineered mutation	UNP P55017
B	1022	LEU	-	expression tag	UNP P55017
B	1023	GLU	-	expression tag	UNP P55017
B	1024	GLY	-	expression tag	UNP P55017
B	1025	SER	-	expression tag	UNP P55017
B	1026	ASP	-	expression tag	UNP P55017
B	1027	GLU	-	expression tag	UNP P55017
B	1028	VAL	-	expression tag	UNP P55017
B	1029	ASP	-	expression tag	UNP P55017
B	1030	ALA	-	expression tag	UNP P55017
B	1031	GLY	-	expression tag	UNP P55017
B	1032	SER	-	expression tag	UNP P55017
B	1033	HIS	-	expression tag	UNP P55017
B	1034	HIS	-	expression tag	UNP P55017
B	1035	HIS	-	expression tag	UNP P55017
B	1036	HIS	-	expression tag	UNP P55017
B	1037	HIS	-	expression tag	UNP P55017
B	1038	HIS	-	expression tag	UNP P55017
B	1039	HIS	-	expression tag	UNP P55017
B	1040	HIS	-	expression tag	UNP P55017
B	1041	HIS	-	expression tag	UNP P55017
B	1042	HIS	-	expression tag	UNP P55017
B	1043	GLY	-	expression tag	UNP P55017
B	1044	SER	-	expression tag	UNP P55017
B	1045	VAL	-	expression tag	UNP P55017
B	1046	GLU	-	expression tag	UNP P55017
B	1047	ASP	-	expression tag	UNP P55017
B	1048	TYR	-	expression tag	UNP P55017
B	1049	LYS	-	expression tag	UNP P55017
B	1050	ASP	-	expression tag	UNP P55017
B	1051	ASP	-	expression tag	UNP P55017
B	1052	ASP	-	expression tag	UNP P55017

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1053	ASP	-	expression tag	UNP P55017
B	1054	LYS	-	expression tag	UNP P55017

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

Mol	Chain	Residues	Atoms	AltConf	Trace
2	C	2	Total C N O 28 16 2 10	0	0
2	D	2	Total C N O 28 16 2 10	0	0

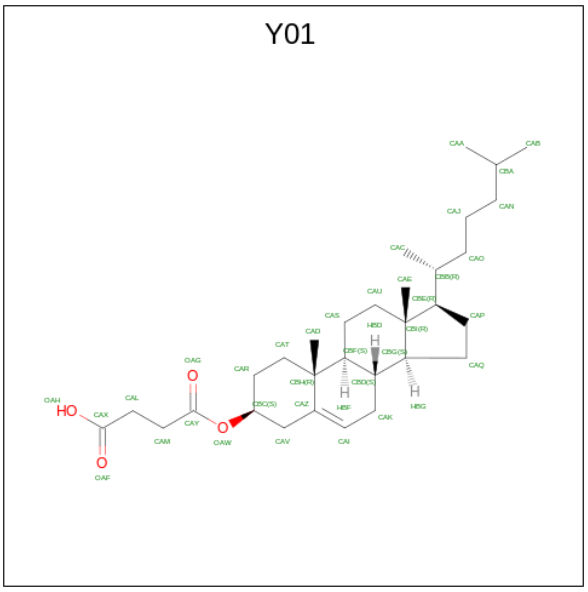
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	2	Total Cl 2 2	0
3	B	2	Total Cl 2 2	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

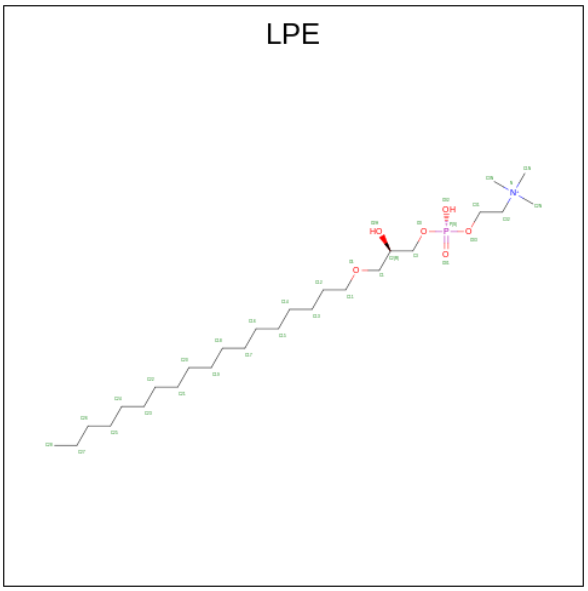
Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Na 2 2	0
4	B	2	Total Na 2 2	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



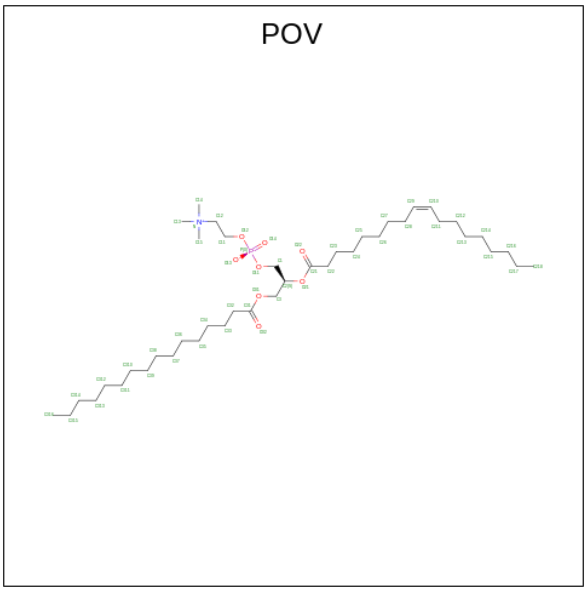
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	B	1	Total C O 35 31 4	0
5	B	1	Total C O 35 31 4	0
5	B	1	Total C O 35 31 4	0

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



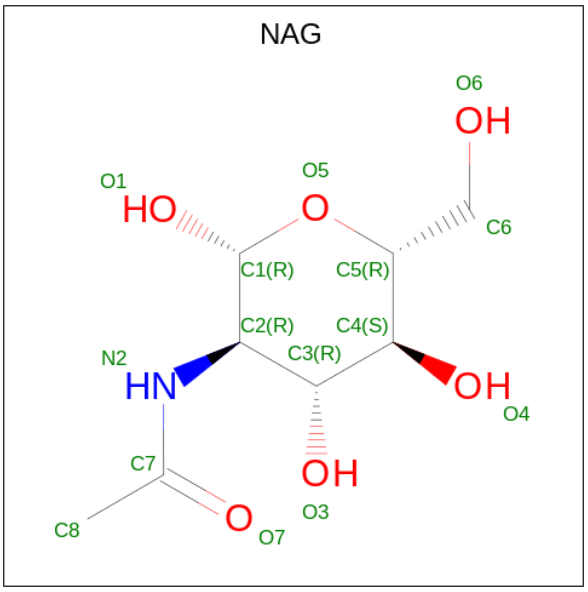
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	B	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	B	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	B	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	B	1	Total	C	N	O	P	0
			34	26	1	6	1	

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



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0

- Molecule 9 is water.

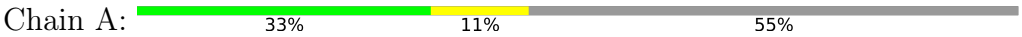
Mol	Chain	Residues	Atoms	AltConf
9	A	3	Total O 3 3	0
9	B	3	Total O 3 3	0

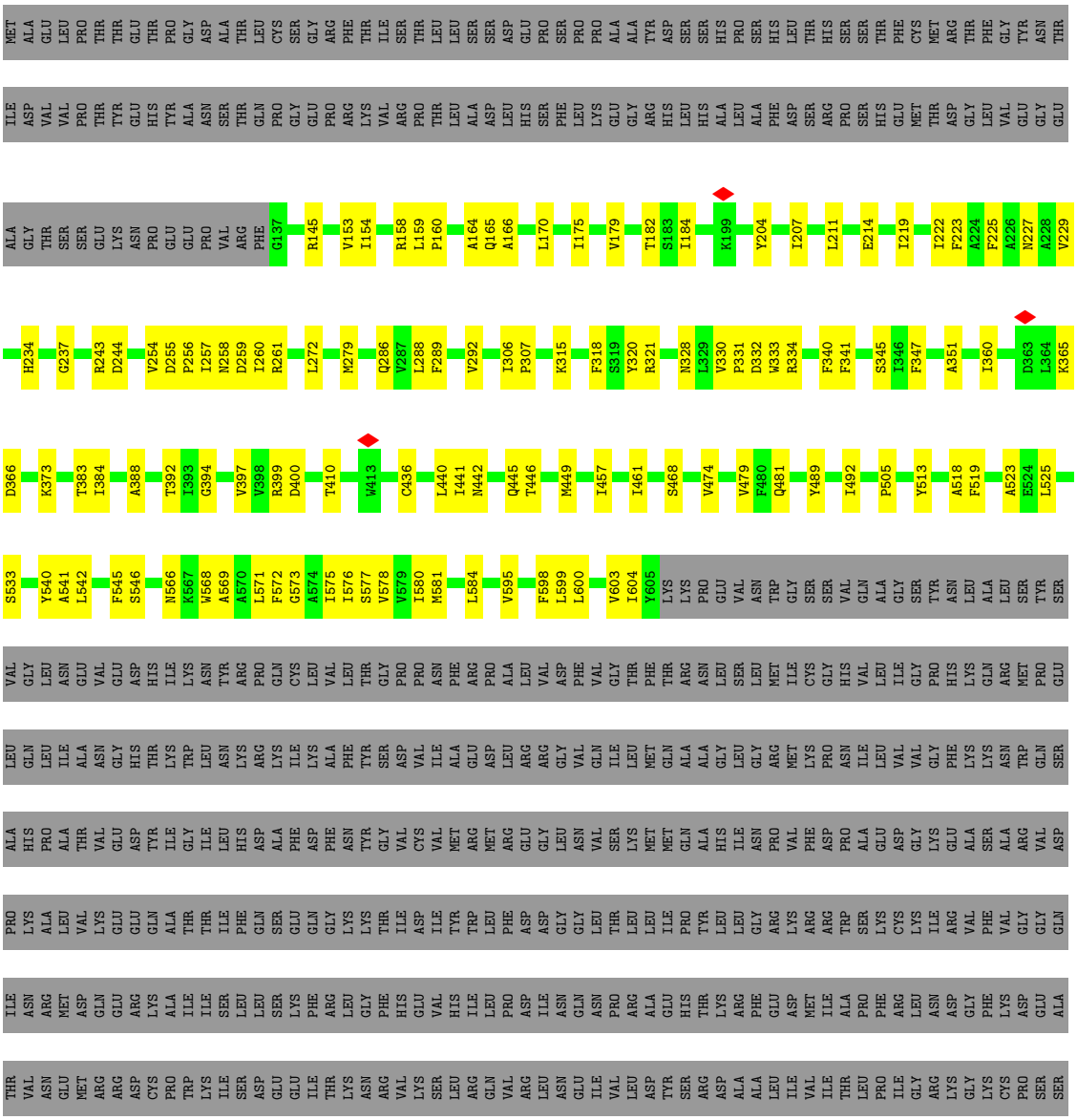
3 Residue-property plots (i)

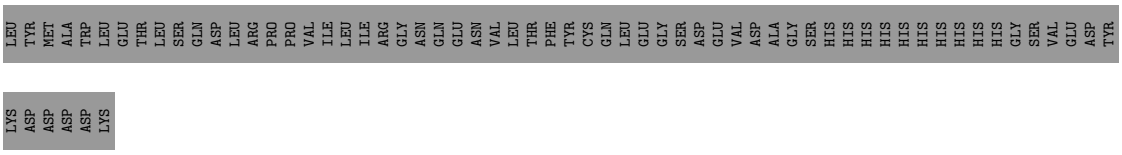
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Solute carrier family 12 member 3

Chain A:

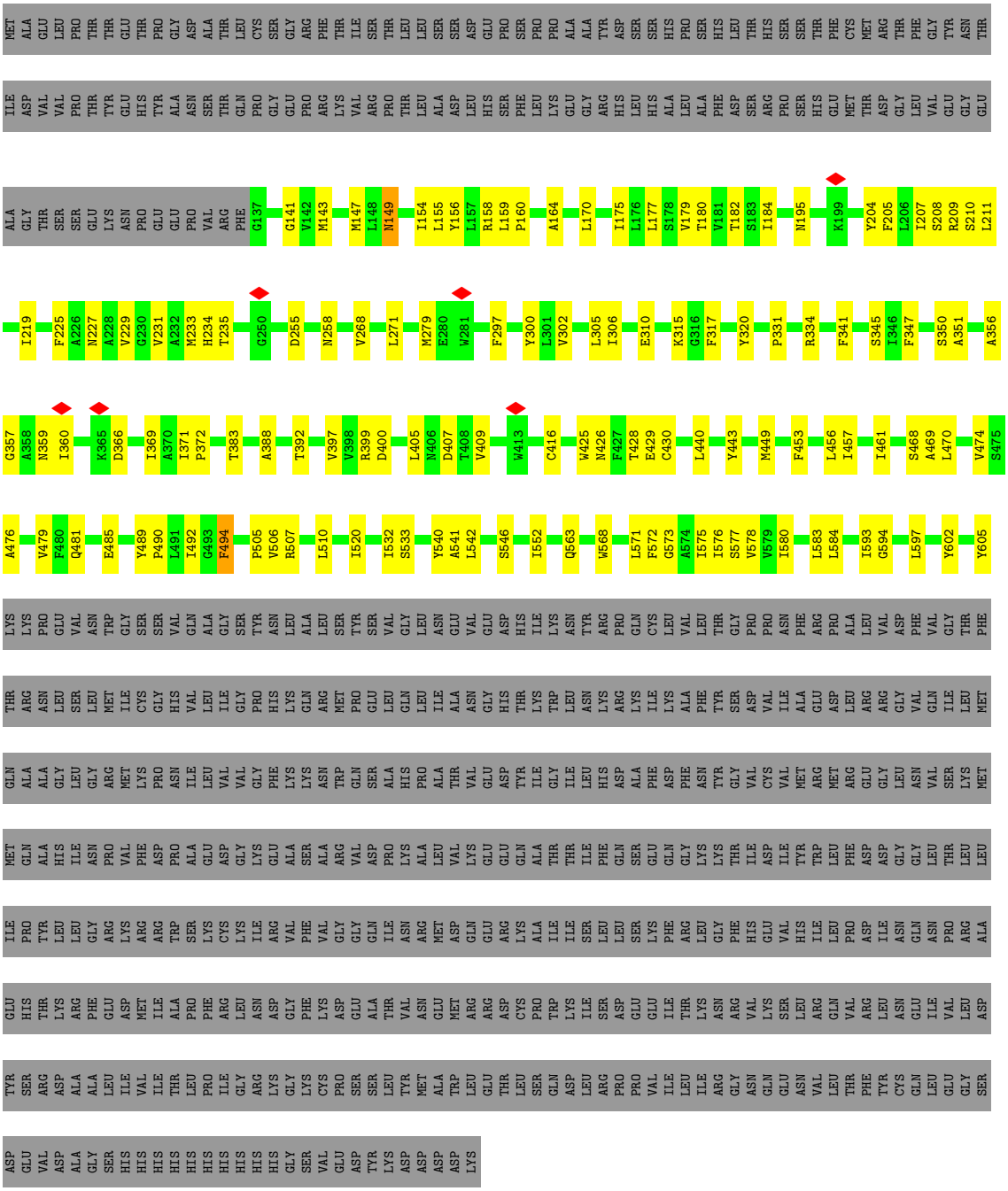






• Molecule 1: Solute carrier family 12 member 3

Chain B:



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

Chain C:

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

Chain D:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	382235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.307	Depositor
Minimum map value	-3.732	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.282	Depositor
Map size (Å)	267.776, 267.776, 267.776	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.046, 1.046, 1.046	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, POV, Y01, LPE, CL, 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	0.30	0/3659	0.44	0/4996
1	B	0.34	0/3659	0.45	0/4996
All	All	0.32	0/7318	0.44	0/9992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3564	0	3605	102	0
1	B	3564	0	3605	98	0
2	C	28	0	25	4	0
2	D	28	0	25	3	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	105	0	147	41	0
5	B	105	0	147	55	0
6	A	136	0	224	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	136	0	223	32	0
7	A	260	0	410	52	0
7	B	208	0	328	38	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
9	A	3	0	0	0	0
9	B	3	0	0	0	0
All	All	8176	0	8765	342	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 20.

All (342) 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)
5:A:1105:Y01:HAI	5:A:1107:Y01:HAK2	1.22	1.09
5:B:1109:Y01:HAJ1	6:B:1112:LPE:H281	1.38	1.04
5:B:1107:Y01:HAS1	5:B:1109:Y01:HAK1	1.40	1.02
5:B:1107:Y01:HAT2	5:B:1109:Y01:HAI	1.47	0.93
5:B:1109:Y01:HAA3	6:B:1112:LPE:H232	1.53	0.91
7:A:1112:POV:H218	1:B:597:LEU:HB3	1.53	0.90
5:B:1109:Y01:HAJ1	6:B:1112:LPE:C28	2.00	0.90
7:B:1114:POV:H310	7:B:1114:POV:H26A	1.54	0.89
5:B:1109:Y01:HAC3	6:B:1112:LPE:H281	1.53	0.88
5:B:1109:Y01:HAS1	7:B:1114:POV:H34A	1.54	0.88
1:A:410:THR:HG23	2:C:1:NAG:H81	1.56	0.86
1:A:410:THR:HG23	2:C:1:NAG:C8	2.08	0.84
1:B:571:LEU:HD11	7:B:1114:POV:H28	1.58	0.84
7:A:1112:POV:H3A	7:A:1112:POV:H25	1.60	0.83
5:B:1107:Y01:HAT2	5:B:1109:Y01:CAI	2.08	0.83
5:B:1109:Y01:HAV2	5:B:1109:Y01:HAL1	1.60	0.82
5:A:1105:Y01:HAA3	6:A:1108:LPE:C25	2.10	0.81
1:A:410:THR:H	2:C:1:NAG:H81	1.43	0.81
5:A:1105:Y01:HAA3	6:A:1108:LPE:C24	2.11	0.81
5:A:1105:Y01:CAI	5:A:1107:Y01:HAK2	2.09	0.81
5:B:1107:Y01:CAS	5:B:1109:Y01:HAK1	2.11	0.81
5:B:1109:Y01:CAB	6:B:1112:LPE:H231	2.11	0.80
5:B:1109:Y01:CAA	6:B:1112:LPE:H232	2.12	0.80
5:B:1109:Y01:HAA3	6:B:1112:LPE:C23	2.11	0.79
1:A:243:ARG:HH21	1:A:260:ILE:HD11	1.48	0.78
5:A:1105:Y01:HAA3	6:A:1108:LPE:H252	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1110:LPE:O2H	6:B:1110:LPE:O31	2.03	0.77
6:B:1111:LPE:H212	6:B:1111:LPE:H172	1.65	0.77
5:B:1109:Y01:HAT2	7:B:1114:POV:H34	1.66	0.77
5:B:1109:Y01:HAB2	6:B:1112:LPE:H283	1.67	0.76
1:A:572:PHE:CE2	5:A:1105:Y01:HAP1	2.21	0.75
5:A:1106:Y01:HAR1	5:A:1106:Y01:HAM1	1.66	0.75
5:B:1109:Y01:HAB2	6:B:1112:LPE:H231	1.68	0.74
7:B:1115:POV:H21H	7:B:1115:POV:H21D	1.69	0.74
6:A:1109:LPE:O31	6:A:1109:LPE:H11	1.86	0.74
7:A:1112:POV:H36A	7:A:1112:POV:H21J	1.70	0.74
1:A:572:PHE:CZ	5:A:1105:Y01:HAP1	2.22	0.74
7:A:1116:POV:H21H	7:A:1116:POV:H313	1.68	0.74
7:A:1116:POV:H315	7:A:1116:POV:H31B	1.70	0.74
7:B:1115:POV:H21H	7:B:1115:POV:C214	2.19	0.73
1:B:300:TYR:OH	1:B:392:THR:HG23	1.87	0.72
1:B:576:ILE:HG22	5:B:1109:Y01:HAA1	1.71	0.72
1:A:397:VAL:HB	1:A:440:LEU:HG	1.72	0.71
1:B:568:TRP:HB3	5:B:1109:Y01:HAK2	1.72	0.71
7:A:1116:POV:H315	7:A:1116:POV:C311	2.20	0.71
1:B:388:ALA:O	1:B:392:THR:HG22	1.91	0.71
7:A:1115:POV:H25	7:A:1115:POV:H29	1.71	0.70
1:B:578:VAL:HG21	7:B:1114:POV:H213	1.74	0.70
1:B:300:TYR:HB2	1:B:457:ILE:HD11	1.73	0.70
5:B:1107:Y01:HAS1	5:B:1109:Y01:CAK	2.20	0.69
1:B:572:PHE:CE2	5:B:1107:Y01:HAJ1	2.28	0.69
1:B:409:VAL:HG22	1:B:426:ASN:HB2	1.75	0.69
1:A:222:ILE:HD13	7:A:1114:POV:H218	1.75	0.68
1:A:153:VAL:HG21	1:A:237:GLY:HA3	1.74	0.68
5:A:1105:Y01:HAJ2	5:A:1106:Y01:HAB3	1.74	0.68
5:B:1109:Y01:CAA	6:B:1112:LPE:C23	2.70	0.68
7:A:1115:POV:O14	7:A:1115:POV:H12	1.94	0.68
1:A:576:ILE:HG22	5:A:1107:Y01:HAB2	1.75	0.67
1:A:568:TRP:CE2	5:A:1107:Y01:HAT1	2.29	0.67
7:B:1101:POV:H3	7:B:1101:POV:O14	1.95	0.66
1:B:331:PRO:HG2	5:B:1108:Y01:HAL2	1.77	0.66
1:B:164:ALA:HB2	1:B:440:LEU:HB3	1.77	0.65
1:B:593:ILE:HD13	7:B:1114:POV:H21H	1.79	0.65
1:A:566:ASN:OD1	5:A:1105:Y01:HAD1	1.96	0.65
7:B:1101:POV:O31	7:B:1101:POV:H35A	1.97	0.65
1:A:595:VAL:HG11	7:A:1114:POV:H21J	1.79	0.64
5:A:1106:Y01:HAM1	5:A:1106:Y01:CAR	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:O	1:A:399:ARG:NH2	2.31	0.64
6:A:1111:LPE:H171	6:A:1111:LPE:H132	1.80	0.63
1:B:305:LEU:HD23	1:B:320:TYR:HE1	1.64	0.63
5:B:1107:Y01:HAA3	6:B:1110:LPE:H171	1.81	0.63
1:A:572:PHE:HE1	5:A:1107:Y01:HAA3	1.62	0.62
7:A:1116:POV:H31H	7:A:1116:POV:H311	1.80	0.62
1:B:492:ILE:HD12	1:B:492:ILE:O	2.00	0.62
1:A:572:PHE:CD1	5:A:1107:Y01:HAN1	2.35	0.61
5:A:1107:Y01:HAT2	7:A:1112:POV:H24	1.81	0.61
6:B:1113:LPE:H172	6:B:1113:LPE:H132	1.80	0.61
1:B:572:PHE:HB2	5:B:1109:Y01:HAP2	1.82	0.61
1:B:568:TRP:CB	5:B:1109:Y01:HAK2	2.30	0.61
5:B:1107:Y01:HAU2	5:B:1109:Y01:CAQ	2.31	0.60
7:A:1116:POV:H31H	7:A:1116:POV:C312	2.32	0.60
7:A:1116:POV:H311	7:A:1116:POV:C316	2.31	0.60
5:B:1107:Y01:CAT	5:B:1109:Y01:HAI	2.27	0.60
7:B:1114:POV:H36A	7:B:1114:POV:H22A	1.84	0.60
1:A:204:TYR:HB2	1:A:479:VAL:HG13	1.85	0.59
1:B:143:MET:O	1:B:147:MET:HG3	2.03	0.59
1:B:572:PHE:HD1	5:B:1109:Y01:HAO1	1.66	0.59
5:B:1107:Y01:HAU2	5:B:1109:Y01:HAQ2	1.84	0.59
1:B:234:HIS:CD2	1:B:468:SER:HB2	2.37	0.59
1:A:255:ASP:OD1	1:A:256:PRO:HD2	2.02	0.59
7:A:1115:POV:H21H	7:B:1114:POV:H313	1.84	0.58
1:A:145:ARG:HH11	1:A:360:ILE:HD13	1.68	0.58
1:A:154:ILE:HG23	1:A:158:ARG:HB2	1.85	0.58
7:A:1116:POV:H314	7:B:1102:POV:H316	1.86	0.58
1:A:388:ALA:O	1:A:392:THR:HG23	2.03	0.58
1:B:575:ILE:CG2	5:B:1109:Y01:HAN2	2.34	0.58
1:A:518:ALA:O	7:A:1114:POV:H35	2.03	0.58
1:B:572:PHE:CD1	5:B:1109:Y01:HAN1	2.39	0.58
7:A:1112:POV:H218	1:B:597:LEU:CB	2.30	0.57
5:A:1105:Y01:HAN1	5:A:1105:Y01:HAC3	1.85	0.57
5:A:1105:Y01:HAA3	6:A:1108:LPE:H242	1.83	0.57
7:A:1112:POV:O32	1:B:605:TYR:HD2	1.87	0.57
7:B:1115:POV:C214	7:B:1115:POV:C218	2.81	0.57
1:A:575:ILE:HG21	5:A:1107:Y01:HAN2	1.86	0.57
1:B:154:ILE:HG23	1:B:158:ARG:HB2	1.84	0.57
1:B:397:VAL:HB	1:B:440:LEU:HG	1.85	0.57
6:A:1110:LPE:H251	7:B:1102:POV:H38A	1.85	0.57
5:B:1109:Y01:HAL1	5:B:1109:Y01:CAV	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:VAL:HA	1:A:581:MET:HE3	1.86	0.57
1:B:575:ILE:HG21	5:B:1109:Y01:HAN2	1.85	0.57
1:B:568:TRP:HE1	7:B:1114:POV:H15B	1.70	0.57
1:A:328:ASN:ND2	1:A:394:GLY:O	2.33	0.56
1:B:279:MET:HE2	1:B:474:VAL:HG11	1.87	0.56
1:A:234:HIS:CD2	1:A:468:SER:HB2	2.39	0.56
7:A:1116:POV:C311	7:A:1116:POV:C315	2.84	0.56
1:A:334:ARG:NH2	1:A:400:ASP:OD2	2.30	0.56
7:A:1115:POV:H315	1:B:578:VAL:HG11	1.88	0.55
1:A:519:PHE:CE2	7:A:1114:POV:H31A	2.40	0.55
6:A:1109:LPE:H31	6:A:1109:LPE:C31	2.36	0.55
1:B:428:THR:HB	2:D:1:NAG:H5	1.88	0.55
6:B:1111:LPE:C3	6:B:1111:LPE:C31	2.84	0.55
1:A:243:ARG:HG3	1:A:259:ASP:HB3	1.90	0.54
7:A:1116:POV:C311	7:A:1116:POV:H31H	2.38	0.54
1:A:164:ALA:HB2	1:A:440:LEU:HB3	1.88	0.54
1:A:571:LEU:HG	5:A:1107:Y01:HAC2	1.88	0.54
7:A:1112:POV:H1	7:A:1112:POV:H22	1.90	0.54
1:B:457:ILE:O	1:B:461:ILE:HG13	2.08	0.53
1:B:357:GLY:HA2	1:B:360:ILE:HD11	1.88	0.53
1:A:481:GLN:HB2	1:A:505:PRO:HB3	1.90	0.53
1:A:257:ILE:HG13	1:A:523:ALA:HB3	1.90	0.53
7:B:1114:POV:H35	7:B:1114:POV:O31	2.08	0.53
7:B:1101:POV:H27A	7:B:1101:POV:H23	1.89	0.53
1:B:345:SER:O	1:B:533:SER:OG	2.23	0.52
1:A:345:SER:O	1:A:533:SER:OG	2.22	0.52
6:B:1111:LPE:C31	6:B:1111:LPE:H32	2.38	0.52
1:B:568:TRP:CG	5:B:1109:Y01:HAK2	2.44	0.52
1:A:575:ILE:CD1	5:A:1107:Y01:HAC3	2.40	0.51
6:A:1111:LPE:H132	6:A:1111:LPE:C17	2.41	0.51
7:A:1115:POV:O22	7:A:1115:POV:H1	2.10	0.51
7:A:1116:POV:C311	7:A:1116:POV:C316	2.88	0.51
5:B:1107:Y01:HAT2	5:B:1109:Y01:CAK	2.40	0.51
7:B:1115:POV:H31C	7:B:1115:POV:H38	1.92	0.51
1:A:540:TYR:OH	3:A:1103:CL:CL	2.59	0.51
1:A:541:ALA:HB2	1:A:577:SER:HB2	1.92	0.51
1:A:255:ASP:HB3	1:A:258:ASN:HB2	1.92	0.51
7:B:1101:POV:H27A	7:B:1101:POV:C23	2.41	0.51
1:B:208:SER:OG	1:B:209:ARG:NH1	2.44	0.51
1:B:341:PHE:CZ	5:B:1108:Y01:HAQ2	2.45	0.51
1:A:320:TYR:CZ	7:A:1113:POV:H35	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1107:Y01:HAT2	7:A:1112:POV:C24	2.41	0.50
5:B:1109:Y01:CAU	7:B:1114:POV:H37	2.41	0.50
6:B:1111:LPE:H141	6:B:1111:LPE:H182	1.92	0.50
6:B:1113:LPE:H282	6:B:1113:LPE:C24	2.40	0.50
1:A:595:VAL:HG11	7:A:1114:POV:C218	2.41	0.50
1:B:541:ALA:HB2	1:B:577:SER:HB2	1.93	0.50
1:A:145:ARG:NH1	1:A:360:ILE:HD13	2.27	0.50
1:A:219:ILE:HG12	1:A:542:LEU:HB3	1.93	0.50
1:A:489:TYR:HB2	1:A:492:ILE:HG12	1.94	0.50
1:A:223:PHE:O	1:A:227:ASN:ND2	2.42	0.50
7:B:1115:POV:O22	7:B:1115:POV:H24	2.11	0.50
1:B:182:THR:HG21	1:B:351:ALA:HB1	1.93	0.50
6:B:1113:LPE:H251	6:B:1113:LPE:C21	2.42	0.49
7:A:1116:POV:O31	7:A:1116:POV:H34A	2.10	0.49
5:A:1107:Y01:HAU2	5:A:1107:Y01:HAC1	1.93	0.49
1:B:177:LEU:HD13	5:B:1108:Y01:HAO1	1.95	0.49
1:B:334:ARG:HH12	1:B:400:ASP:CG	2.15	0.49
1:B:405:LEU:HD12	1:B:425:TRP:HH2	1.77	0.49
1:A:315:LYS:HD3	1:A:449:MET:HG3	1.95	0.49
1:A:207:ILE:HG23	1:A:211:LEU:HD12	1.95	0.48
1:B:315:LYS:HD3	1:B:449:MET:HG3	1.96	0.48
5:B:1107:Y01:CAM	5:B:1107:Y01:HAV2	2.43	0.48
5:B:1107:Y01:CAU	5:B:1109:Y01:HAQ2	2.43	0.48
7:A:1112:POV:H21J	7:A:1112:POV:C36	2.41	0.48
1:B:227:ASN:HB2	1:B:476:ALA:HB2	1.94	0.48
1:B:271:LEU:HG	1:B:470:LEU:HD13	1.96	0.48
1:A:569:ALA:HB2	5:A:1105:Y01:CAD	2.44	0.48
7:A:1113:POV:H21B	7:A:1113:POV:H313	1.95	0.48
6:A:1109:LPE:C31	6:A:1109:LPE:C3	2.92	0.48
1:B:481:GLN:HB2	1:B:505:PRO:HB3	1.95	0.47
1:A:341:PHE:CZ	5:A:1106:Y01:HAQ2	2.49	0.47
1:B:233:MET:HB2	1:B:532:ILE:CD1	2.44	0.47
5:B:1108:Y01:HAU2	5:B:1108:Y01:HAC1	1.96	0.47
1:A:440:LEU:HD23	1:A:446:THR:HG21	1.95	0.47
5:B:1109:Y01:CAA	6:B:1112:LPE:H231	2.44	0.47
7:A:1114:POV:H210	7:A:1114:POV:H21D	1.96	0.47
1:B:219:ILE:HG12	1:B:542:LEU:HB3	1.95	0.47
1:A:279:MET:HE1	1:A:474:VAL:HG11	1.97	0.47
1:B:184:ILE:HG21	1:B:573:GLY:HA3	1.97	0.47
1:B:341:PHE:HZ	5:B:1108:Y01:HAQ2	1.79	0.47
7:A:1115:POV:H25	7:A:1115:POV:C29	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:HG2	1:A:604:ILE:HG13	1.97	0.47
1:A:254:VAL:HG12	1:A:255:ASP:HB2	1.98	0.46
1:A:318:PHE:O	1:A:321:ARG:NH1	2.44	0.46
1:A:545:PHE:CD1	7:A:1112:POV:H39	2.50	0.46
6:A:1110:LPE:C25	7:B:1102:POV:H38A	2.45	0.46
1:A:184:ILE:HG21	1:A:573:GLY:HA3	1.97	0.46
1:A:289:PHE:HA	1:A:292:VAL:HG22	1.97	0.46
1:A:457:ILE:O	1:A:461:ILE:HG13	2.14	0.46
1:B:235:THR:HG21	1:B:268:VAL:HB	1.97	0.46
1:A:256:PRO:O	1:A:260:ILE:HG13	2.16	0.46
1:A:332:ASP:OD2	1:A:334:ARG:NE	2.45	0.46
1:B:141:GLY:O	1:B:360:ILE:HD13	2.15	0.46
1:A:366:ASP:N	1:A:366:ASP:OD1	2.49	0.46
1:B:211:LEU:HD13	1:B:546:SER:HB2	1.97	0.46
1:A:244:ASP:OD2	1:A:445:GLN:NE2	2.49	0.46
7:A:1112:POV:H38A	7:A:1112:POV:H216	1.96	0.46
1:B:207:ILE:HG23	1:B:211:LEU:HD12	1.98	0.46
1:A:170:LEU:HD12	1:A:331:PRO:HG3	1.96	0.46
7:A:1114:POV:H25A	7:A:1114:POV:H28	1.75	0.46
5:A:1106:Y01:HAP1	5:A:1106:Y01:HAO1	1.81	0.45
6:A:1111:LPE:C17	6:A:1111:LPE:C13	2.92	0.45
1:B:310:GLU:HB3	1:B:405:LEU:HD11	1.98	0.45
1:A:234:HIS:CD2	1:A:468:SER:CB	3.00	0.45
1:A:340:PHE:CD1	5:A:1106:Y01:HAK2	2.51	0.45
6:A:1109:LPE:H152	6:A:1109:LPE:H122	1.74	0.45
1:B:170:LEU:HD11	5:B:1108:Y01:HAR1	1.98	0.45
1:A:331:PRO:HG2	5:A:1106:Y01:HAL2	1.98	0.45
1:A:572:PHE:CD2	5:A:1105:Y01:HAE3	2.50	0.45
5:A:1105:Y01:CAK	5:A:1107:Y01:HAQ2	2.46	0.45
6:B:1112:LPE:H142	6:B:1112:LPE:H111	1.42	0.45
1:B:154:ILE:HB	1:B:350:SER:OG	2.17	0.45
1:A:388:ALA:HA	7:A:1113:POV:H21A	1.98	0.45
1:A:580:ILE:O	1:A:584:LEU:HG	2.17	0.45
5:A:1107:Y01:HAB3	6:A:1110:LPE:C24	2.47	0.45
6:A:1109:LPE:C3	6:A:1109:LPE:H312	2.47	0.45
1:A:575:ILE:CG2	5:A:1107:Y01:HAN2	2.45	0.45
7:A:1112:POV:H21G	1:B:594:GLY:HA2	1.98	0.45
1:B:541:ALA:HB1	7:B:1114:POV:H216	1.99	0.45
5:B:1107:Y01:HAU2	5:B:1109:Y01:HAQ1	1.99	0.45
7:B:1115:POV:H34A	7:B:1115:POV:H37A	1.73	0.45
1:A:384:ILE:HD12	7:A:1113:POV:H216	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1107:Y01:HAO2	5:B:1107:Y01:HAP1	1.40	0.45
1:A:179:VAL:HG21	1:A:383:THR:HG23	1.98	0.44
1:B:175:ILE:HG12	1:B:347:PHE:CZ	2.52	0.44
1:A:214:GLU:HB3	1:A:600:LEU:HD12	1.98	0.44
7:A:1115:POV:H34	6:B:1112:LPE:H181	1.98	0.44
7:B:1101:POV:H21G	7:B:1101:POV:H214	1.63	0.44
1:A:598:PHE:HD1	7:B:1114:POV:H25A	1.83	0.44
1:B:255:ASP:OD2	1:B:258:ASN:ND2	2.51	0.44
1:B:540:TYR:OH	3:B:1105:CL:CL	2.66	0.44
6:B:1113:LPE:H181	6:B:1113:LPE:H222	1.99	0.44
1:A:566:ASN:OD1	5:A:1105:Y01:HAV1	2.17	0.44
6:A:1110:LPE:O31	6:A:1110:LPE:H321	2.17	0.44
1:B:489:TYR:HD2	1:B:492:ILE:HD11	1.82	0.44
7:A:1112:POV:O14	7:A:1112:POV:H12A	2.17	0.44
5:B:1107:Y01:HAQ2	6:B:1110:LPE:H112	1.98	0.44
5:B:1109:Y01:HAC3	6:B:1112:LPE:C28	2.35	0.44
1:A:333:TRP:NE1	5:A:1106:Y01:OAG	2.48	0.44
1:A:572:PHE:CG	5:A:1105:Y01:HAQ1	2.52	0.44
1:B:580:ILE:O	1:B:584:LEU:HG	2.18	0.44
1:B:195:ASN:HD22	1:B:210:SER:HB3	1.82	0.43
7:B:1114:POV:H28A	7:B:1114:POV:H312	2.00	0.43
1:B:234:HIS:HB2	1:B:469:ALA:HB2	2.00	0.43
6:B:1113:LPE:H172	6:B:1113:LPE:C13	2.47	0.43
7:B:1114:POV:H35	7:B:1114:POV:C31	2.48	0.43
7:B:1115:POV:H21H	7:B:1115:POV:H214	1.99	0.43
1:B:317:PHE:HB2	1:B:397:VAL:HG22	2.00	0.43
1:B:453:PHE:HD2	1:B:456:LEU:HG	1.84	0.43
1:B:576:ILE:HG22	5:B:1109:Y01:CAA	2.43	0.43
6:B:1113:LPE:H132	6:B:1113:LPE:C17	2.45	0.43
7:B:1115:POV:H22A	7:B:1115:POV:H25	1.74	0.43
1:A:175:ILE:HG12	1:A:347:PHE:CZ	2.53	0.43
7:A:1112:POV:O13	7:A:1112:POV:H15B	2.18	0.43
1:B:179:VAL:HG21	1:B:383:THR:HG23	2.01	0.43
1:B:490:PRO:HD3	1:B:602:TYR:CZ	2.53	0.43
1:B:429:GLU:HG3	2:D:1:NAG:C6	2.49	0.43
5:B:1109:Y01:HAA2	6:B:1112:LPE:H232	1.97	0.43
1:B:234:HIS:CD2	1:B:468:SER:CB	3.01	0.43
1:A:410:THR:CG2	2:C:1:NAG:H81	2.39	0.43
7:A:1115:POV:H26A	7:A:1115:POV:H23A	1.76	0.43
1:B:225:PHE:O	1:B:229:VAL:HG23	2.19	0.43
1:B:481:GLN:O	1:B:485:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1105:Y01:CAA	6:A:1108:LPE:H242	2.48	0.43
1:A:440:LEU:HD23	1:A:440:LEU:HA	1.88	0.43
6:A:1111:LPE:H171	6:A:1111:LPE:C13	2.49	0.43
6:B:1111:LPE:H32	6:B:1111:LPE:H311	2.01	0.42
1:A:243:ARG:NH1	1:A:244:ASP:OD1	2.52	0.42
1:A:288:LEU:O	1:A:292:VAL:HG22	2.19	0.42
1:A:365:LYS:HE3	1:A:365:LYS:HB2	1.60	0.42
6:A:1109:LPE:H231	6:A:1109:LPE:H192	2.01	0.42
7:A:1116:POV:H34A	7:A:1116:POV:H1A	2.01	0.42
1:B:159:LEU:HB3	1:B:160:PRO:HD3	2.01	0.42
1:B:164:ALA:O	1:B:399:ARG:NE	2.43	0.42
1:B:366:ASP:HB2	1:B:369:ILE:HD12	2.01	0.42
6:B:1110:LPE:O2H	6:B:1110:LPE:P	2.78	0.42
1:A:145:ARG:NE	1:A:286:GLN:HE22	2.17	0.42
1:A:272:LEU:HD22	1:A:513:TYR:CG	2.55	0.42
6:A:1111:LPE:H141	6:A:1111:LPE:H111	1.72	0.42
5:A:1106:Y01:CAR	5:A:1106:Y01:CAM	2.94	0.42
7:A:1112:POV:H36A	7:A:1112:POV:H214	2.02	0.42
7:A:1113:POV:H11A	7:A:1113:POV:H13B	1.73	0.42
1:B:149:ASN:OD1	1:B:356:ALA:HB2	2.20	0.42
1:B:302:VAL:O	1:B:306:ILE:HG13	2.19	0.42
1:B:597:LEU:HD23	1:B:597:LEU:HA	1.88	0.42
1:A:211:LEU:HD13	1:A:546:SER:HB2	2.02	0.42
1:B:371:ILE:HB	1:B:372:PRO:HD3	2.01	0.42
7:B:1115:POV:O22	7:B:1115:POV:C24	2.67	0.42
1:A:568:TRP:CD2	5:A:1107:Y01:HAT1	2.54	0.42
1:A:578:VAL:HG11	7:B:1102:POV:H314	2.01	0.42
7:A:1115:POV:C29	7:A:1115:POV:C25	2.97	0.42
1:B:360:ILE:H	1:B:360:ILE:HG13	1.70	0.42
7:B:1101:POV:H3	7:B:1101:POV:P	2.60	0.42
1:A:159:LEU:HB3	1:A:160:PRO:HD3	2.00	0.42
1:A:243:ARG:HD3	1:A:256:PRO:HA	2.02	0.42
1:B:156:TYR:CG	1:B:461:ILE:HG12	2.55	0.42
7:B:1114:POV:H13B	7:B:1114:POV:H11A	1.85	0.42
1:A:525:LEU:HD12	1:A:525:LEU:HA	1.95	0.42
1:A:599:LEU:O	1:A:603:VAL:HG23	2.20	0.42
1:A:166:ALA:O	1:A:170:LEU:HB2	2.20	0.41
6:A:1111:LPE:H1N2	6:A:1111:LPE:H311	1.83	0.41
1:B:416:CYS:HB2	2:D:1:NAG:O7	2.20	0.41
1:B:552:ILE:HD11	7:B:1114:POV:O11	2.20	0.41
5:B:1109:Y01:HAT2	7:B:1114:POV:C34	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HG21	1:A:351:ALA:HB1	2.03	0.41
1:B:155:LEU:HD21	1:B:297:PHE:CZ	2.55	0.41
1:B:170:LEU:HD21	5:B:1108:Y01:HAT2	2.01	0.41
1:A:341:PHE:HZ	5:A:1106:Y01:HAQ2	1.86	0.41
5:A:1105:Y01:HAK2	5:A:1107:Y01:HAQ2	2.02	0.41
1:B:180:THR:HG23	5:B:1107:Y01:HAB3	2.00	0.41
1:A:436:CYS:HB2	1:A:442:ASN:ND2	2.35	0.41
1:B:204:TYR:HB2	1:B:479:VAL:HG13	2.02	0.41
1:B:576:ILE:CG2	5:B:1109:Y01:HAA1	2.46	0.41
1:A:165:GLN:HG2	1:A:441:ILE:HG13	2.01	0.41
7:A:1116:POV:H21B	7:A:1116:POV:H21E	1.82	0.41
1:B:205:PHE:O	1:B:209:ARG:HG2	2.21	0.41
1:A:179:VAL:HG11	6:A:1109:LPE:H252	2.02	0.41
1:A:257:ILE:O	1:A:261:ARG:HG3	2.21	0.41
1:A:578:VAL:HG21	7:A:1112:POV:H31B	2.02	0.41
1:B:227:ASN:O	1:B:231:VAL:HG23	2.21	0.41
1:B:341:PHE:CZ	1:B:583:LEU:HD13	2.56	0.41
5:B:1109:Y01:CAB	6:B:1112:LPE:H283	2.43	0.41
1:A:225:PHE:O	1:A:229:VAL:HG23	2.21	0.41
1:B:494:PHE:CZ	1:B:507:ARG:HD3	2.56	0.41
7:A:1115:POV:O22	7:A:1115:POV:C1	2.69	0.40
1:B:506:VAL:O	1:B:510:LEU:HG	2.22	0.40
7:B:1115:POV:H27	7:B:1115:POV:H24A	1.79	0.40
5:A:1105:Y01:HAN2	6:A:1108:LPE:H261	2.04	0.40
1:A:373:LYS:HB2	1:A:373:LYS:HE3	1.79	0.40
7:A:1113:POV:H211	7:A:1113:POV:H28A	1.66	0.40
1:B:563:GLN:NE2	6:B:1110:LPE:H3N3	2.36	0.40
1:A:306:ILE:HG23	1:A:307:PRO:HD2	2.03	0.40
1:B:235:THR:HB	1:B:520:ILE:HD11	2.03	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	467/1053 (44%)	455 (97%)	12 (3%)	0	100	100
1	B	467/1053 (44%)	448 (96%)	18 (4%)	1 (0%)	44	63
All	All	934/2106 (44%)	903 (97%)	30 (3%)	1 (0%)	50	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	ASP

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	376/890 (42%)	376 (100%)	0	100	100
1	B	376/890 (42%)	371 (99%)	5 (1%)	65	83
All	All	752/1780 (42%)	747 (99%)	5 (1%)	80	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	B	359	ASN
1	B	430	CYS
1	B	443	TYR
1	B	494	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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	C	1	2,1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	0.74	0
2	NAG	D	1	2,1	14,14,15	0.47	0	17,19,21	0.67	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.88	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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7

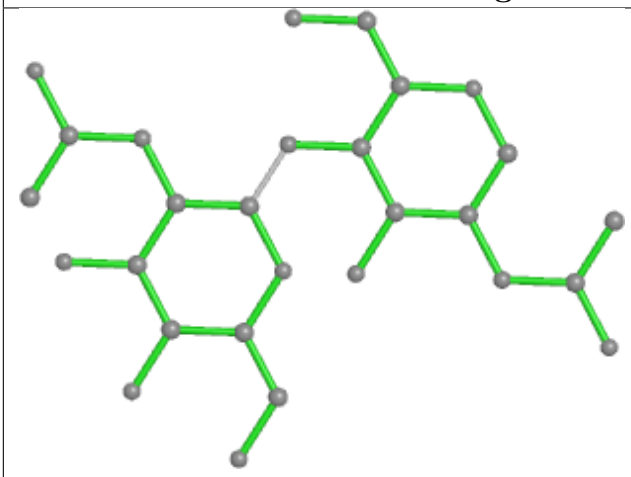
There are no ring outliers.

2 monomers are involved in 7 short contacts:

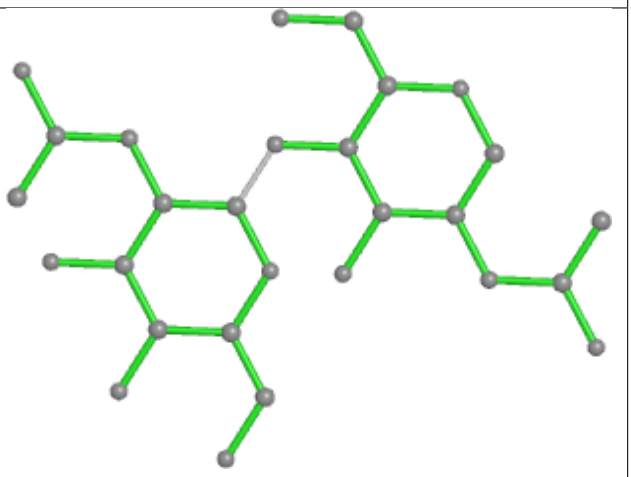
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	4	0
2	D	1	NAG	3	0

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

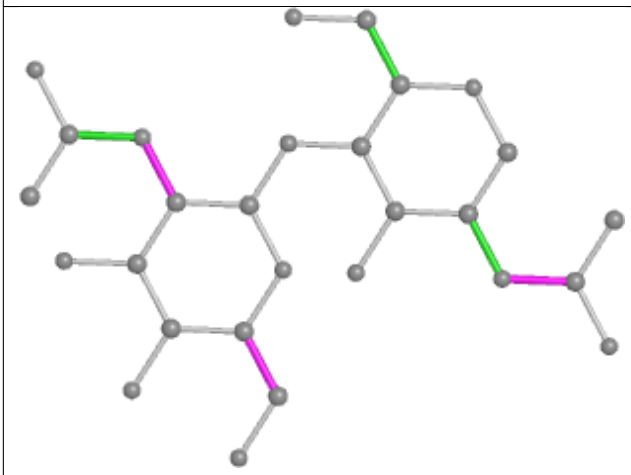
Oligosaccharide Chain C



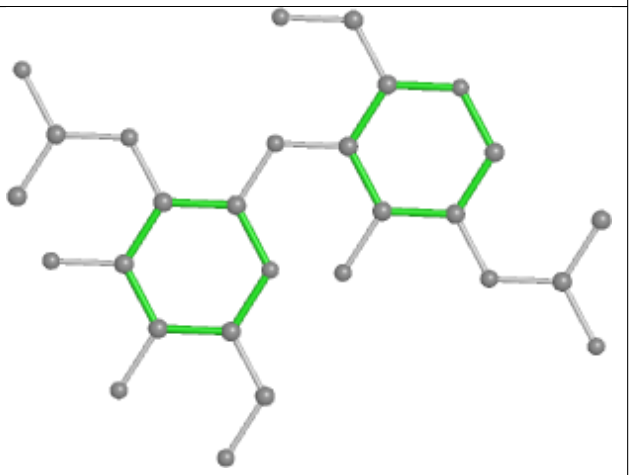
Bond lengths



Bond angles

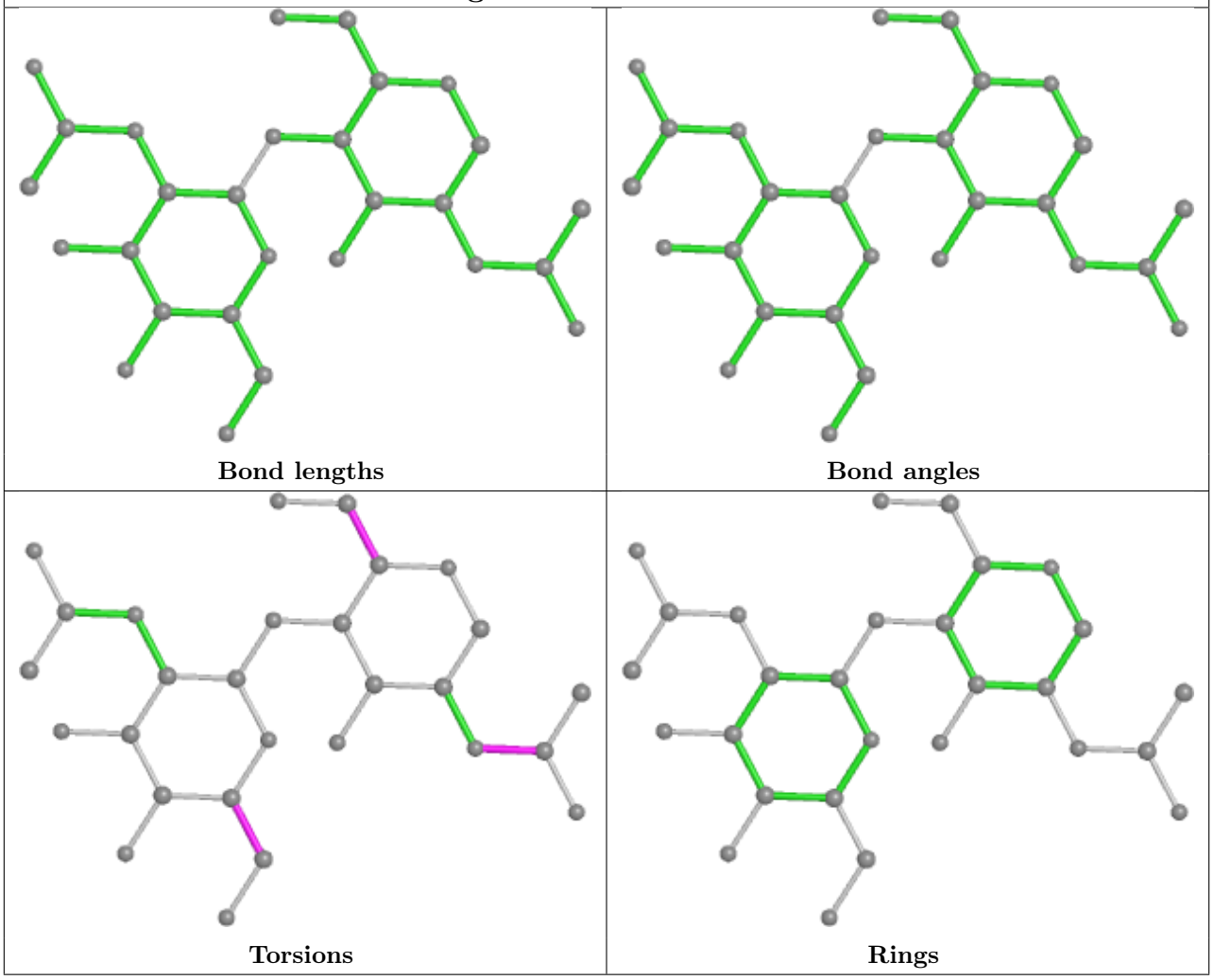


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 8 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	Y01	A	1105	-	38,38,38	0.17	0	57,57,57	0.45	0
5	Y01	B	1108	-	38,38,38	0.21	0	57,57,57	0.43	0
5	Y01	A	1107	-	38,38,38	0.20	0	57,57,57	0.56	0
8	NAG	B	1116	1	14,14,15	0.31	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	POV	B	1115	-	51,51,51	1.20	2 (3%)	57,59,59	1.92	12 (21%)
7	POV	B	1101	-	51,51,51	1.28	6 (11%)	57,59,59	2.10	23 (40%)
7	POV	A	1112	-	51,51,51	0.93	2 (3%)	57,59,59	1.09	4 (7%)
6	LPE	A	1108	-	33,33,33	0.98	2 (6%)	37,39,39	1.14	3 (8%)
6	LPE	B	1113	-	33,33,33	0.97	0	37,39,39	1.63	7 (18%)
5	Y01	B	1109	-	38,38,38	0.24	0	57,57,57	0.37	0
6	LPE	B	1110	-	33,33,33	1.45	5 (15%)	37,39,39	2.32	16 (43%)
6	LPE	A	1110	-	33,33,33	0.94	1 (3%)	37,39,39	1.42	6 (16%)
5	Y01	A	1106	-	38,38,38	0.22	0	57,57,57	0.50	0
6	LPE	B	1112	-	33,33,33	0.45	0	37,39,39	0.79	1 (2%)
7	POV	B	1102	-	51,51,51	1.06	4 (7%)	57,59,59	1.81	12 (21%)
7	POV	A	1113	-	51,51,51	0.94	2 (3%)	57,59,59	1.03	5 (8%)
7	POV	A	1116	-	51,51,51	1.14	4 (7%)	57,59,59	1.89	15 (26%)
7	POV	B	1114	-	51,51,51	0.94	2 (3%)	57,59,59	1.09	4 (7%)
8	NAG	A	1117	1	14,14,15	0.29	0	17,19,21	0.63	0
6	LPE	A	1109	-	33,33,33	0.97	1 (3%)	37,39,39	1.97	14 (37%)
6	LPE	A	1111	-	33,33,33	1.02	0	37,39,39	1.87	8 (21%)
7	POV	A	1115	-	51,51,51	1.11	4 (7%)	57,59,59	1.83	10 (17%)
7	POV	A	1114	-	51,51,51	0.96	2 (3%)	57,59,59	1.04	2 (3%)
5	Y01	B	1107	-	38,38,38	0.24	0	57,57,57	0.67	1 (1%)
6	LPE	B	1111	-	33,33,33	1.13	1 (3%)	37,39,39	1.45	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	Y01	A	1105	-	-	7/19/77/77	0/4/4/4
5	Y01	B	1108	-	-	7/19/77/77	0/4/4/4
5	Y01	A	1107	-	-	7/19/77/77	0/4/4/4
8	NAG	B	1116	1	-	1/6/23/26	0/1/1/1
7	POV	B	1115	-	-	26/55/55/55	-
7	POV	B	1101	-	-	34/55/55/55	-
7	POV	A	1112	-	-	17/55/55/55	-
6	LPE	A	1108	-	-	14/34/34/34	-
6	LPE	B	1113	-	-	19/34/34/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	Y01	B	1109	-	-	9/19/77/77	0/4/4/4
6	LPE	B	1110	-	-	16/34/34/34	-
6	LPE	A	1110	-	-	23/34/34/34	-
5	Y01	A	1106	-	-	8/19/77/77	0/4/4/4
6	LPE	B	1112	-	-	15/34/34/34	-
7	POV	B	1102	-	-	26/55/55/55	-
7	POV	A	1113	-	-	10/55/55/55	-
7	POV	A	1116	-	-	32/55/55/55	-
7	POV	B	1114	-	-	22/55/55/55	-
8	NAG	A	1117	1	-	2/6/23/26	0/1/1/1
6	LPE	A	1109	-	-	15/34/34/34	-
6	LPE	A	1111	-	-	17/34/34/34	-
7	POV	A	1115	-	-	29/55/55/55	-
7	POV	A	1114	-	-	17/55/55/55	-
5	Y01	B	1107	-	-	10/19/77/77	0/4/4/4
6	LPE	B	1111	-	-	15/34/34/34	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1115	POV	O31-C31	4.85	1.47	1.33
7	B	1101	POV	O31-C31	4.73	1.47	1.33
7	A	1116	POV	O21-C21	4.46	1.46	1.34
7	B	1102	POV	O21-C21	4.45	1.46	1.34
7	A	1115	POV	O21-C21	4.45	1.46	1.34
7	A	1114	POV	O31-C31	4.38	1.46	1.33
6	B	1110	LPE	O2H-C2	-4.26	1.30	1.43
7	B	1114	POV	O31-C31	4.26	1.45	1.33
7	A	1114	POV	O21-C21	4.22	1.46	1.34
7	A	1113	POV	O31-C31	4.22	1.45	1.33
7	A	1112	POV	O21-C21	4.14	1.46	1.34
7	A	1112	POV	O31-C31	4.01	1.45	1.33
7	A	1113	POV	O21-C21	4.01	1.45	1.34
7	B	1114	POV	O21-C21	3.94	1.45	1.34
6	B	1110	LPE	P-O32	-3.32	1.39	1.55
6	A	1110	LPE	C32-C31	3.15	1.61	1.51
6	B	1110	LPE	O1-C1	-3.13	1.34	1.42
7	A	1116	POV	O31-C3	-2.74	1.38	1.45
7	A	1115	POV	O32-C31	-2.71	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1110	LPE	P-O31	-2.71	1.41	1.50
7	B	1102	POV	O32-C31	-2.57	1.14	1.22
7	A	1115	POV	O31-C3	-2.57	1.39	1.45
6	A	1109	LPE	P-O33	2.50	1.69	1.59
6	A	1108	LPE	O1-C1	-2.47	1.36	1.42
7	A	1116	POV	C311-C310	-2.43	1.37	1.51
6	B	1111	LPE	O1-C1	-2.41	1.36	1.42
7	B	1101	POV	C3-C2	2.40	1.58	1.50
7	B	1101	POV	O11-C1	-2.38	1.35	1.44
7	A	1116	POV	O31-C31	2.37	1.40	1.33
6	A	1108	LPE	P-O32	-2.33	1.44	1.55
7	B	1102	POV	C33-C32	-2.21	1.44	1.52
7	A	1115	POV	C12-N	-2.13	1.44	1.51
7	B	1115	POV	O21-C21	2.13	1.40	1.34
7	B	1101	POV	C214-C213	-2.10	1.39	1.51
7	B	1102	POV	O31-C31	2.09	1.39	1.33
7	B	1101	POV	O21-C21	2.03	1.40	1.34
6	B	1110	LPE	C1-C2	-2.02	1.44	1.51
7	B	1101	POV	P-O11	-2.01	1.51	1.59

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1115	POV	O31-C31-O32	-6.93	106.10	123.59
7	B	1115	POV	O31-C3-C2	6.02	125.96	108.43
7	A	1115	POV	O21-C21-C22	5.71	123.81	111.50
7	B	1102	POV	C3-C2-C1	-5.63	98.48	111.79
7	B	1115	POV	C3-C2-C1	-5.57	98.61	111.79
7	B	1102	POV	O31-C31-O32	-5.34	110.11	123.59
6	B	1110	LPE	O32-P-O33	-4.98	84.61	107.75
7	A	1116	POV	C39-C38-C37	-4.93	89.39	114.42
7	B	1101	POV	O31-C3-C2	4.82	122.45	108.43
6	A	1111	LPE	C23-C22-C21	-4.63	90.93	114.42
7	A	1115	POV	O31-C31-C32	4.56	126.21	111.91
6	A	1111	LPE	C19-C18-C17	-4.54	91.39	114.42
7	B	1115	POV	O21-C21-C22	4.46	121.12	111.50
7	B	1101	POV	O21-C2-C1	-4.45	92.28	108.40
7	B	1115	POV	O21-C2-C3	4.45	124.51	108.40
6	A	1109	LPE	C3N-N-C1N	-4.43	97.59	108.97
6	B	1113	LPE	C23-C22-C21	-4.43	91.94	114.42
6	A	1111	LPE	C22-C21-C20	-4.42	91.97	114.42
7	B	1101	POV	C215-C214-C213	-4.42	91.98	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1111	LPE	C13-C12-C11	-4.40	94.00	113.49
7	A	1116	POV	C37-C36-C35	-4.38	92.20	114.42
7	B	1115	POV	C27-C28-C29	-4.32	87.68	112.43
7	A	1114	POV	O21-C21-C22	4.31	120.78	111.50
7	B	1102	POV	O21-C21-C22	4.24	120.64	111.50
7	A	1116	POV	O21-C21-C22	4.23	120.62	111.50
7	B	1114	POV	O21-C21-C22	4.19	120.54	111.50
6	B	1110	LPE	O2H-C2-C3	-4.05	95.35	109.56
6	B	1110	LPE	O33-P-O31	4.04	124.86	109.07
6	B	1110	LPE	O32-P-O3	4.03	126.46	107.75
7	A	1113	POV	O21-C21-C22	4.00	120.11	111.50
7	A	1112	POV	O21-C21-C22	3.99	120.11	111.50
7	A	1116	POV	O31-C31-O32	-3.90	113.75	123.59
7	B	1102	POV	O31-C31-C32	3.83	123.94	111.91
6	B	1111	LPE	C23-C22-C21	-3.77	95.30	114.42
6	A	1110	LPE	C19-C18-C17	-3.76	95.32	114.42
7	A	1116	POV	C213-C212-C211	-3.76	97.41	113.79
7	B	1101	POV	C26-C25-C24	-3.69	95.68	114.42
7	A	1115	POV	C313-C312-C311	3.62	132.79	114.42
6	A	1109	LPE	O1-C1-C2	-3.61	97.31	109.52
6	B	1110	LPE	C3N-N-C32	3.60	124.63	109.92
6	A	1109	LPE	O2H-C2-C1	3.59	122.14	109.56
7	B	1101	POV	P-O11-C1	-3.54	100.92	121.68
7	B	1102	POV	C25-C24-C23	-3.52	96.57	114.42
6	B	1110	LPE	C2N-N-C1N	3.51	118.00	108.97
6	B	1110	LPE	O2H-C2-C1	-3.51	97.26	109.56
6	A	1109	LPE	O2H-C2-C3	-3.50	97.28	109.56
7	B	1101	POV	C3-O31-C31	3.49	130.03	117.12
7	B	1101	POV	C34-C33-C32	3.45	125.58	113.19
7	B	1115	POV	O31-C31-C32	3.41	122.61	111.91
6	B	1111	LPE	C15-C14-C13	-3.39	97.19	114.42
6	B	1110	LPE	C3N-N-C1N	-3.33	100.41	108.97
6	A	1111	LPE	C20-C19-C18	-3.33	97.52	114.42
7	B	1101	POV	O21-C21-C22	3.26	118.53	111.50
7	B	1101	POV	C33-C32-C31	3.22	125.33	113.62
6	B	1113	LPE	C22-C21-C20	-3.21	98.12	114.42
7	B	1101	POV	C214-C213-C212	-3.20	98.17	114.42
7	A	1116	POV	C314-C313-C312	3.13	130.31	114.42
6	B	1113	LPE	C20-C19-C18	-3.11	98.65	114.42
6	A	1110	LPE	C2N-N-C1N	-3.09	101.03	108.97
6	A	1109	LPE	C21-C20-C19	-3.08	98.78	114.42
6	A	1109	LPE	P-O3-C3	-3.08	103.61	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1102	POV	O21-C2-C1	3.06	119.49	108.40
6	B	1113	LPE	C28-C27-C26	-3.03	90.40	113.42
6	B	1110	LPE	C21-C20-C19	-3.00	99.19	114.42
6	A	1111	LPE	C25-C24-C23	-2.99	99.26	114.42
6	A	1109	LPE	C31-C32-N	2.98	125.74	115.78
7	B	1101	POV	C27-C26-C25	-2.97	99.35	114.42
6	A	1111	LPE	C28-C27-C26	-2.96	90.95	113.42
7	B	1102	POV	C216-C215-C214	-2.95	99.44	114.42
7	B	1115	POV	C33-C32-C31	-2.94	102.91	113.62
6	A	1109	LPE	C20-C19-C18	2.93	129.31	114.42
7	B	1101	POV	C2-O21-C21	-2.93	110.58	117.79
7	A	1112	POV	O31-C31-C32	2.91	121.04	111.91
7	B	1114	POV	C2-O21-C21	-2.91	110.64	117.79
5	B	1107	Y01	CAP-CAQ-CBG	-2.89	99.41	105.13
7	B	1114	POV	O31-C31-C32	2.86	120.88	111.91
7	A	1116	POV	C313-C312-C311	2.85	128.91	114.42
6	B	1110	LPE	C3N-N-C2N	-2.85	101.64	108.97
6	A	1111	LPE	C21-C20-C19	-2.83	100.06	114.42
7	A	1116	POV	O12-P-O14	-2.83	98.01	109.07
7	B	1102	POV	C213-C212-C211	-2.83	101.47	113.79
7	A	1115	POV	C3-C2-C1	-2.82	105.11	111.79
6	A	1111	LPE	C18-C17-C16	-2.81	100.16	114.42
6	B	1111	LPE	C11-O1-C1	-2.76	101.27	113.61
6	B	1110	LPE	C31-C32-N	-2.75	106.59	115.78
7	A	1114	POV	O31-C31-C32	2.74	120.50	111.91
6	B	1113	LPE	C19-C18-C17	-2.73	100.55	114.42
6	A	1109	LPE	C24-C23-C22	-2.72	100.62	114.42
6	B	1110	LPE	C25-C24-C23	-2.70	100.70	114.42
6	B	1113	LPE	C21-C20-C19	-2.66	100.92	114.42
7	B	1101	POV	C26-C27-C28	2.65	125.34	113.79
7	B	1101	POV	C3-C2-C1	2.63	118.00	111.79
7	A	1113	POV	C2-O21-C21	-2.60	111.38	117.79
6	B	1110	LPE	O1-C1-C2	-2.60	100.72	109.52
7	A	1113	POV	O31-C31-C32	2.58	120.00	111.91
7	B	1102	POV	C313-C312-C311	2.55	127.39	114.42
7	A	1112	POV	C3-C2-C1	-2.54	105.77	111.79
6	A	1110	LPE	C18-C17-C16	-2.54	101.52	114.42
7	A	1115	POV	O22-C21-C22	-2.53	113.87	123.73
6	A	1109	LPE	O33-C31-C32	2.52	122.40	109.16
7	B	1102	POV	C23-C22-C21	-2.51	104.49	113.62
7	A	1116	POV	O31-C3-C2	-2.47	101.23	108.43
7	B	1115	POV	C214-C213-C212	-2.47	101.90	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1101	POV	O13-P-O12	2.46	119.16	107.75
6	A	1110	LPE	C16-C15-C14	-2.41	102.17	114.42
7	B	1101	POV	O31-C31-C32	2.41	119.47	111.91
6	B	1110	LPE	C11-O1-C1	-2.40	102.85	113.61
7	A	1115	POV	C33-C32-C31	-2.39	104.93	113.62
7	A	1116	POV	C13-N-C12	2.36	119.58	109.92
7	B	1101	POV	O21-C2-C3	2.31	116.76	108.40
7	A	1116	POV	O21-C21-O22	-2.31	118.13	123.70
7	A	1115	POV	C14-N-C12	-2.30	100.50	109.92
6	A	1108	LPE	O32-P-O33	-2.26	97.25	107.75
7	B	1101	POV	O21-C21-O22	-2.25	118.27	123.70
6	A	1110	LPE	C17-C16-C15	-2.24	103.05	114.42
7	A	1116	POV	C24-C23-C22	-2.23	105.17	113.19
6	B	1113	LPE	P-O3-C3	2.23	134.75	121.68
7	B	1101	POV	C11-C12-N	2.23	123.21	115.78
6	A	1109	LPE	C14-C13-C12	-2.22	103.17	114.42
7	A	1116	POV	C315-C314-C313	-2.21	94.79	115.30
7	B	1101	POV	C218-C217-C216	-2.21	96.66	113.42
6	A	1109	LPE	C3N-N-C32	2.20	118.91	109.92
7	A	1116	POV	C214-C213-C212	2.19	125.57	114.42
7	B	1102	POV	P-O11-C1	2.19	134.54	121.68
7	B	1101	POV	C24-C23-C22	-2.17	105.38	113.19
6	B	1111	LPE	C3-C2-C1	2.17	119.16	112.79
7	B	1101	POV	C15-N-C13	-2.16	103.41	108.97
6	A	1109	LPE	C19-C18-C17	2.14	125.29	114.42
6	A	1110	LPE	C25-C24-C23	2.14	125.29	114.42
6	B	1112	LPE	C31-C32-N	-2.12	108.69	115.78
7	B	1101	POV	C35-C34-C33	2.12	125.16	114.42
7	B	1102	POV	C3-O31-C31	2.11	124.95	117.12
7	B	1114	POV	C11-C12-N	-2.11	108.75	115.78
7	A	1112	POV	O31-C31-O32	-2.10	118.28	123.59
6	B	1110	LPE	C2N-N-C32	-2.10	101.31	109.92
7	B	1115	POV	O21-C21-O22	-2.10	118.63	123.70
7	A	1116	POV	C11-C12-N	2.09	122.76	115.78
6	A	1108	LPE	C3-C2-C1	-2.06	106.73	112.79
6	B	1110	LPE	C19-C18-C17	-2.06	103.98	114.42
7	B	1115	POV	C312-C311-C310	-2.05	104.00	114.42
7	B	1115	POV	C3-O31-C31	2.05	124.71	117.12
7	A	1115	POV	C37-C36-C35	-2.04	104.07	114.42
7	B	1115	POV	C14-N-C12	-2.04	101.57	109.92
7	A	1113	POV	O31-C31-O32	-2.04	118.44	123.59
7	A	1115	POV	O21-C2-C3	2.02	115.72	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1109	LPE	P-O33-C31	2.02	131.51	121.59
6	A	1108	LPE	O32-P-O31	2.02	122.20	112.24
7	A	1113	POV	C11-C12-N	-2.01	109.08	115.78

There are no chirality outliers.

All (398) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1106	Y01	OAG-CAY-OAW-CBC
5	A	1106	Y01	CAM-CAY-OAW-CBC
5	B	1107	Y01	OAG-CAY-OAW-CBC
5	B	1107	Y01	CAM-CAY-OAW-CBC
5	B	1108	Y01	CAM-CAY-OAW-CBC
5	B	1109	Y01	OAG-CAY-OAW-CBC
5	B	1109	Y01	CAM-CAY-OAW-CBC
6	A	1108	LPE	C3-O3-P-O31
6	A	1108	LPE	C3-O3-P-O32
6	A	1108	LPE	C3-O3-P-O33
6	A	1109	LPE	C31-O33-P-O31
6	A	1110	LPE	O1-C1-C2-O2H
6	A	1110	LPE	O1-C1-C2-C3
6	A	1110	LPE	C3-O3-P-O31
6	A	1110	LPE	C32-C31-O33-P
6	A	1111	LPE	O33-C31-C32-N
6	B	1110	LPE	C3-O3-P-O32
6	B	1110	LPE	O33-C31-C32-N
6	B	1111	LPE	O33-C31-C32-N
6	B	1112	LPE	C3-O3-P-O33
6	B	1112	LPE	C31-O33-P-O32
6	B	1113	LPE	C3-O3-P-O31
7	A	1112	POV	C11-O12-P-O14
7	A	1112	POV	O12-C11-C12-N
7	A	1112	POV	C12-C11-O12-P
7	A	1112	POV	C22-C21-O21-C2
7	A	1113	POV	C1-O11-P-O14
7	A	1113	POV	C11-O12-P-O14
7	A	1114	POV	C1-O11-P-O13
7	A	1114	POV	C1-O11-P-O14
7	A	1115	POV	C11-O12-P-O14
7	A	1115	POV	C12-C11-O12-P
7	A	1116	POV	C1-O11-P-O12
7	A	1116	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
7	A	1116	POV	C1-O11-P-O14
7	A	1116	POV	C2-C1-O11-P
7	A	1116	POV	O12-C11-C12-N
7	A	1116	POV	C22-C21-O21-C2
7	A	1116	POV	O22-C21-O21-C2
7	B	1101	POV	C11-O12-P-O11
7	B	1101	POV	C11-O12-P-O14
7	B	1101	POV	O22-C21-O21-C2
7	B	1102	POV	C11-O12-P-O14
7	B	1102	POV	O21-C2-C3-O31
7	B	1102	POV	O12-C11-C12-N
7	B	1114	POV	C1-O11-P-O14
7	B	1114	POV	C11-O12-P-O13
7	B	1114	POV	C2-C1-O11-P
7	B	1114	POV	C22-C21-O21-C2
7	B	1115	POV	C1-O11-P-O12
7	B	1115	POV	C1-O11-P-O13
7	B	1115	POV	C1-O11-P-O14
7	B	1115	POV	O12-C11-C12-N
8	A	1117	NAG	C8-C7-N2-C2
8	A	1117	NAG	O7-C7-N2-C2
7	A	1114	POV	O32-C31-O31-C3
5	B	1108	Y01	OAG-CAY-OAW-CBC
7	A	1112	POV	O22-C21-O21-C2
7	B	1114	POV	O22-C21-O21-C2
7	A	1114	POV	C32-C31-O31-C3
7	B	1101	POV	C22-C21-O21-C2
5	B	1107	Y01	CAJ-CAO-CBB-CAC
5	B	1107	Y01	CAC-CBB-CBE-CAP
5	B	1107	Y01	CAC-CBB-CBE-CBI
5	B	1107	Y01	CAO-CBB-CBE-CBI
6	A	1111	LPE	C11-C12-C13-C14
5	B	1107	Y01	CAO-CBB-CBE-CAP
6	A	1108	LPE	O2H-C2-C3-O3
7	A	1112	POV	O32-C31-O31-C3
6	A	1108	LPE	C23-C24-C25-C26
7	A	1116	POV	C212-C213-C214-C215
6	A	1109	LPE	C14-C15-C16-C17
6	A	1110	LPE	C22-C23-C24-C25
6	A	1111	LPE	C13-C14-C15-C16
7	A	1115	POV	C23-C24-C25-C26
7	B	1101	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
5	B	1107	Y01	CAJ-CAO-CBB-CBE
7	A	1112	POV	C32-C31-O31-C3
7	B	1115	POV	C32-C33-C34-C35
6	B	1111	LPE	C14-C15-C16-C17
7	A	1115	POV	C32-C31-O31-C3
7	A	1116	POV	C311-C312-C313-C314
5	A	1107	Y01	CAJ-CAO-CBB-CBE
5	B	1108	Y01	CAJ-CAO-CBB-CBE
5	A	1105	Y01	CAV-CBC-OAW-CAY
6	A	1108	LPE	C1-C2-C3-O3
7	A	1116	POV	C11-C12-N-C13
7	B	1101	POV	C11-C12-N-C14
6	B	1111	LPE	C17-C18-C19-C20
5	B	1108	Y01	CAV-CBC-OAW-CAY
6	B	1111	LPE	O2H-C2-C3-O3
5	B	1108	Y01	CAJ-CAO-CBB-CAC
6	A	1109	LPE	C17-C18-C19-C20
6	B	1113	LPE	C2-C1-O1-C11
7	B	1115	POV	C34-C35-C36-C37
5	A	1107	Y01	CAJ-CAO-CBB-CAC
6	B	1112	LPE	C15-C16-C17-C18
7	B	1101	POV	C11-C12-N-C13
5	A	1105	Y01	CAR-CBC-OAW-CAY
5	B	1108	Y01	CAR-CBC-OAW-CAY
7	A	1115	POV	O32-C31-O31-C3
7	A	1113	POV	C32-C33-C34-C35
5	B	1108	Y01	CAN-CAJ-CAO-CBB
6	B	1112	LPE	C13-C14-C15-C16
6	A	1110	LPE	C3-O3-P-O33
6	A	1111	LPE	C31-O33-P-O3
6	B	1113	LPE	C3-O3-P-O33
7	A	1113	POV	C1-O11-P-O12
7	A	1113	POV	C11-O12-P-O11
7	A	1114	POV	C1-O11-P-O12
7	A	1115	POV	C1-O11-P-O12
7	A	1115	POV	C11-O12-P-O11
7	B	1114	POV	C11-O12-P-O11
7	B	1115	POV	C11-O12-P-O11
6	A	1110	LPE	C31-C32-N-C2N
7	A	1112	POV	C11-C12-N-C15
7	A	1115	POV	C11-C12-N-C13
7	A	1115	POV	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
7	A	1116	POV	C11-C12-N-C15
7	A	1116	POV	C34-C35-C36-C37
6	A	1110	LPE	C14-C15-C16-C17
6	B	1113	LPE	C23-C24-C25-C26
6	B	1113	LPE	C21-C22-C23-C24
7	B	1102	POV	C214-C215-C216-C217
6	B	1110	LPE	C2-C3-O3-P
7	A	1114	POV	C211-C212-C213-C214
6	B	1113	LPE	O2H-C2-C3-O3
7	B	1101	POV	C23-C24-C25-C26
6	A	1109	LPE	C23-C24-C25-C26
6	A	1111	LPE	C17-C18-C19-C20
6	A	1111	LPE	C20-C21-C22-C23
5	A	1106	Y01	CAV-CBC-OAW-CAY
6	B	1110	LPE	C22-C23-C24-C25
6	B	1113	LPE	C24-C25-C26-C27
7	A	1116	POV	C23-C24-C25-C26
7	B	1102	POV	C33-C34-C35-C36
6	A	1110	LPE	C20-C21-C22-C23
6	A	1108	LPE	C19-C20-C21-C22
6	A	1110	LPE	C18-C19-C20-C21
6	A	1111	LPE	C23-C24-C25-C26
7	B	1101	POV	C33-C34-C35-C36
6	A	1110	LPE	C31-C32-N-C1N
6	A	1110	LPE	C31-C32-N-C3N
7	A	1112	POV	C11-C12-N-C14
7	A	1115	POV	C11-C12-N-C14
7	B	1102	POV	C11-C12-N-C13
7	B	1102	POV	C11-C12-N-C15
6	A	1108	LPE	C20-C21-C22-C23
7	A	1115	POV	C35-C36-C37-C38
7	A	1116	POV	C311-C310-C39-C38
6	A	1110	LPE	C19-C20-C21-C22
7	B	1102	POV	C32-C33-C34-C35
6	A	1108	LPE	C16-C17-C18-C19
7	A	1115	POV	C311-C310-C39-C38
6	B	1110	LPE	C21-C22-C23-C24
7	A	1115	POV	C33-C34-C35-C36
6	B	1113	LPE	C14-C15-C16-C17
5	A	1106	Y01	CAR-CBC-OAW-CAY
6	A	1109	LPE	C20-C21-C22-C23
6	A	1111	LPE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
6	A	1110	LPE	C17-C18-C19-C20
7	A	1116	POV	C312-C313-C314-C315
7	A	1112	POV	C214-C215-C216-C217
6	A	1108	LPE	C13-C14-C15-C16
7	A	1112	POV	C11-C12-N-C13
7	B	1101	POV	C11-C12-N-C15
7	B	1102	POV	C11-C12-N-C14
7	A	1116	POV	C214-C215-C216-C217
5	A	1105	Y01	CAM-CAY-OAW-CBC
7	B	1102	POV	C215-C216-C217-C218
6	B	1111	LPE	C18-C19-C20-C21
7	B	1115	POV	C39-C310-C311-C312
7	B	1101	POV	C311-C310-C39-C38
7	B	1102	POV	C34-C35-C36-C37
7	A	1113	POV	C22-C21-O21-C2
7	A	1113	POV	O22-C21-O21-C2
6	B	1113	LPE	C18-C19-C20-C21
7	B	1102	POV	C311-C310-C39-C38
6	A	1108	LPE	C25-C26-C27-C28
7	A	1116	POV	C11-C12-N-C14
6	B	1110	LPE	C16-C17-C18-C19
6	B	1113	LPE	C20-C21-C22-C23
7	A	1114	POV	C37-C38-C39-C310
7	A	1116	POV	C210-C211-C212-C213
6	A	1111	LPE	C16-C17-C18-C19
5	A	1105	Y01	OAG-CAY-OAW-CBC
6	A	1109	LPE	C31-O33-P-O3
6	B	1112	LPE	C31-O33-P-O3
6	B	1110	LPE	C23-C24-C25-C26
6	B	1112	LPE	C11-C12-C13-C14
7	B	1115	POV	C35-C36-C37-C38
6	B	1113	LPE	C1-C2-C3-O3
7	A	1114	POV	C39-C310-C311-C312
7	A	1115	POV	C25-C26-C27-C28
6	A	1108	LPE	C22-C23-C24-C25
6	A	1109	LPE	C15-C16-C17-C18
7	B	1115	POV	C311-C310-C39-C38
6	A	1111	LPE	C19-C20-C21-C22
6	B	1111	LPE	C25-C26-C27-C28
7	A	1115	POV	C212-C213-C214-C215
7	A	1115	POV	C22-C21-O21-C2
7	B	1101	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
7	B	1114	POV	O11-C1-C2-O21
6	B	1111	LPE	C22-C23-C24-C25
7	B	1101	POV	C31-C32-C33-C34
7	B	1101	POV	C215-C216-C217-C218
7	A	1112	POV	C21-C22-C23-C24
7	B	1114	POV	C32-C31-O31-C3
6	B	1111	LPE	C16-C17-C18-C19
6	A	1109	LPE	C1-C2-C3-O3
6	A	1110	LPE	C16-C17-C18-C19
7	B	1115	POV	C23-C24-C25-C26
7	A	1115	POV	C39-C310-C311-C312
7	B	1101	POV	C34-C35-C36-C37
7	A	1115	POV	C312-C313-C314-C315
7	B	1102	POV	C312-C313-C314-C315
6	A	1108	LPE	C15-C16-C17-C18
7	B	1115	POV	C25-C26-C27-C28
7	B	1101	POV	C35-C36-C37-C38
7	B	1114	POV	C1-C2-C3-O31
7	B	1115	POV	C312-C313-C314-C315
6	B	1113	LPE	C25-C26-C27-C28
5	A	1106	Y01	CAO-CBB-CBE-CBI
6	B	1113	LPE	O1-C1-C2-C3
6	A	1109	LPE	C13-C14-C15-C16
7	A	1116	POV	O31-C31-C32-C33
6	B	1110	LPE	C17-C18-C19-C20
5	A	1106	Y01	CAO-CBB-CBE-CAP
5	B	1109	Y01	CAJ-CAN-CBA-CAB
7	B	1102	POV	C23-C24-C25-C26
7	B	1115	POV	C214-C215-C216-C217
5	A	1106	Y01	CAC-CBB-CBE-CBI
7	B	1101	POV	C32-C31-O31-C3
7	B	1101	POV	C39-C310-C311-C312
7	B	1101	POV	C32-C33-C34-C35
7	A	1116	POV	C211-C212-C213-C214
6	A	1109	LPE	C18-C19-C20-C21
6	B	1112	LPE	C2-C3-O3-P
6	A	1110	LPE	C11-C12-C13-C14
7	A	1112	POV	C39-C310-C311-C312
7	B	1101	POV	O11-C1-C2-C3
7	B	1115	POV	C215-C216-C217-C218
7	B	1114	POV	O32-C31-O31-C3
5	A	1106	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
6	A	1110	LPE	C12-C13-C14-C15
7	A	1116	POV	C39-C310-C311-C312
7	B	1101	POV	C24-C25-C26-C27
6	B	1113	LPE	C19-C20-C21-C22
7	B	1102	POV	C1-C2-C3-O31
5	B	1109	Y01	CAX-CAL-CAM-CAY
6	B	1110	LPE	C25-C26-C27-C28
7	B	1114	POV	O21-C2-C3-O31
7	B	1115	POV	C32-C31-O31-C3
6	B	1113	LPE	C22-C23-C24-C25
7	B	1102	POV	C36-C37-C38-C39
6	B	1111	LPE	C21-C22-C23-C24
7	B	1114	POV	C35-C36-C37-C38
7	B	1115	POV	O32-C31-O31-C3
7	A	1114	POV	C25-C26-C27-C28
6	B	1111	LPE	O1-C1-C2-O2H
6	B	1113	LPE	O1-C1-C2-O2H
7	B	1102	POV	C213-C214-C215-C216
7	B	1102	POV	C25-C26-C27-C28
7	A	1112	POV	C11-O12-P-O11
7	A	1116	POV	C11-O12-P-O11
7	A	1114	POV	C2-C1-O11-P
7	B	1101	POV	C2-C1-O11-P
6	A	1109	LPE	C31-O33-P-O32
6	A	1110	LPE	C3-O3-P-O32
6	A	1111	LPE	C31-O33-P-O32
6	B	1112	LPE	C3-O3-P-O32
6	B	1112	LPE	C31-O33-P-O31
6	B	1113	LPE	C3-O3-P-O32
7	A	1113	POV	C1-O11-P-O13
7	A	1115	POV	C1-O11-P-O14
7	A	1115	POV	C11-O12-P-O13
7	B	1115	POV	C11-O12-P-O14
7	B	1114	POV	O11-C1-C2-C3
6	B	1112	LPE	O1-C11-C12-C13
7	A	1116	POV	C215-C216-C217-C218
6	B	1110	LPE	C32-C31-O33-P
7	B	1115	POV	C26-C27-C28-C29
7	A	1115	POV	O22-C21-O21-C2
5	B	1109	Y01	CAJ-CAN-CBA-CAA
7	A	1113	POV	C36-C37-C38-C39
6	A	1111	LPE	C2-C1-O1-C11

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Mol	Chain	Res	Type	Atoms
6	B	1111	LPE	C2-C1-O1-C11
7	A	1116	POV	C22-C23-C24-C25
7	A	1114	POV	C11-C12-N-C15
6	A	1110	LPE	O33-C31-C32-N
6	B	1112	LPE	O33-C31-C32-N
7	A	1113	POV	O12-C11-C12-N
7	A	1115	POV	O12-C11-C12-N
7	B	1114	POV	O12-C11-C12-N
6	A	1110	LPE	C12-C11-O1-C1
7	B	1101	POV	O32-C31-O31-C3
6	A	1110	LPE	C13-C14-C15-C16
6	B	1113	LPE	O1-C11-C12-C13
7	A	1112	POV	C3-C2-O21-C21
7	A	1115	POV	C1-C2-O21-C21
7	B	1115	POV	C3-C2-O21-C21
7	B	1115	POV	O31-C31-C32-C33
7	A	1116	POV	C35-C36-C37-C38
7	B	1101	POV	O11-C1-C2-O21
6	B	1110	LPE	C31-C32-N-C2N
6	B	1112	LPE	C12-C11-O1-C1
7	B	1101	POV	C25-C26-C27-C28
6	A	1108	LPE	C31-O33-P-O3
6	A	1110	LPE	C31-O33-P-O3
6	A	1111	LPE	C3-O3-P-O33
6	B	1110	LPE	C3-O3-P-O33
7	A	1112	POV	C1-O11-P-O12
7	B	1101	POV	C1-O11-P-O12
7	B	1102	POV	C1-O11-P-O12
7	B	1102	POV	C11-O12-P-O11
7	B	1114	POV	C1-O11-P-O12
7	A	1116	POV	C37-C38-C39-C310
5	A	1105	Y01	CAN-CAJ-CAO-CBB
8	B	1116	NAG	C3-C2-N2-C7
6	B	1112	LPE	O1-C1-C2-O2H
6	A	1110	LPE	C2-C1-O1-C11
7	A	1112	POV	C29-C210-C211-C212
6	A	1109	LPE	C16-C17-C18-C19
6	B	1111	LPE	C11-C12-C13-C14
7	B	1114	POV	C311-C310-C39-C38
6	B	1113	LPE	C12-C11-O1-C1
6	A	1111	LPE	C14-C15-C16-C17
6	B	1110	LPE	O1-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
6	A	1109	LPE	C2-C3-O3-P
5	A	1105	Y01	CAM-CAL-CAX-OAH
5	B	1109	Y01	CAM-CAL-CAX-OAH
7	A	1114	POV	C11-C12-N-C14
7	B	1114	POV	C27-C28-C29-C210
6	B	1110	LPE	C11-C12-C13-C14
5	A	1105	Y01	CAM-CAL-CAX-OAF
5	B	1107	Y01	CAM-CAL-CAX-OAH
5	B	1107	Y01	CAM-CAL-CAX-OAF
6	A	1111	LPE	C15-C16-C17-C18
7	A	1114	POV	C35-C36-C37-C38
5	B	1109	Y01	CAM-CAL-CAX-OAF
6	A	1109	LPE	C31-C32-N-C3N
7	A	1114	POV	C29-C210-C211-C212
7	A	1114	POV	C311-C310-C39-C38
7	B	1101	POV	C22-C23-C24-C25
5	A	1107	Y01	CAX-CAL-CAM-CAY
7	A	1116	POV	O32-C31-O31-C3
7	A	1115	POV	C32-C33-C34-C35
6	B	1110	LPE	C31-C32-N-C1N
7	A	1116	POV	C36-C37-C38-C39
7	A	1115	POV	C34-C35-C36-C37
7	B	1101	POV	C26-C27-C28-C29
7	B	1101	POV	C29-C210-C211-C212
7	B	1101	POV	C27-C28-C29-C210
7	A	1114	POV	C11-C12-N-C13
7	B	1114	POV	C22-C23-C24-C25
7	A	1116	POV	C32-C31-O31-C3
7	B	1102	POV	O21-C21-C22-C23
7	B	1114	POV	O31-C31-C32-C33
7	A	1114	POV	C214-C215-C216-C217
7	A	1115	POV	C24-C25-C26-C27
7	A	1116	POV	C313-C314-C315-C316
7	B	1102	POV	C27-C28-C29-C210
7	B	1115	POV	C27-C28-C29-C210
7	A	1115	POV	C36-C37-C38-C39
7	B	1101	POV	O21-C21-C22-C23
7	B	1102	POV	C37-C38-C39-C310
7	B	1115	POV	C29-C210-C211-C212
5	A	1107	Y01	CAM-CAL-CAX-OAF
7	B	1114	POV	C29-C210-C211-C212
7	B	1102	POV	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
6	A	1111	LPE	C31-C32-N-C1N
7	B	1115	POV	C22-C23-C24-C25
5	B	1109	Y01	CAO-CBB-CBE-CAP
6	A	1111	LPE	C21-C22-C23-C24
6	B	1111	LPE	C20-C21-C22-C23
7	A	1115	POV	C313-C314-C315-C316
7	A	1116	POV	O32-C31-C32-C33
7	B	1101	POV	O22-C21-C22-C23
7	B	1102	POV	O32-C31-C32-C33
6	B	1112	LPE	C23-C24-C25-C26
7	B	1102	POV	C210-C211-C212-C213
7	B	1114	POV	O32-C31-C32-C33
7	B	1114	POV	C32-C33-C34-C35
5	A	1107	Y01	CAL-CAM-CAY-OAW
6	B	1111	LPE	C3-O3-P-O31
7	B	1101	POV	C21-C22-C23-C24
5	B	1109	Y01	CAC-CBB-CBE-CBI
7	B	1115	POV	C12-C11-O12-P
6	B	1111	LPE	C12-C13-C14-C15
6	B	1112	LPE	C22-C23-C24-C25
5	A	1107	Y01	CAM-CAL-CAX-OAH
6	A	1109	LPE	O1-C11-C12-C13
7	B	1115	POV	O21-C21-C22-C23
7	A	1116	POV	C21-C22-C23-C24
7	A	1115	POV	C311-C312-C313-C314
7	B	1101	POV	C36-C37-C38-C39
6	B	1110	LPE	C2-C1-O1-C11
5	A	1107	Y01	CAL-CAM-CAY-OAG

There are no ring outliers.

23 monomers are involved in 207 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1105	Y01	19	0
5	B	1108	Y01	7	0
5	A	1107	Y01	17	0
7	B	1115	POV	10	0
7	B	1101	POV	6	0
7	A	1112	POV	16	0
6	A	1108	LPE	6	0
6	B	1113	LPE	6	0
5	B	1109	Y01	42	0

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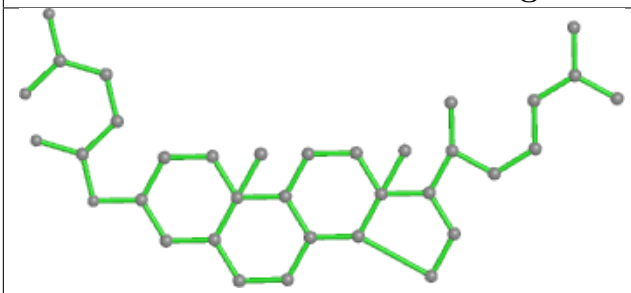
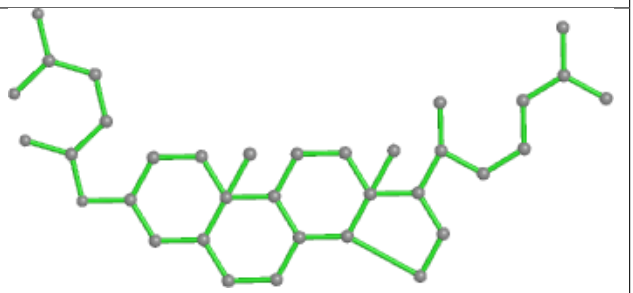
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1110	LPE	5	0
6	A	1110	LPE	4	0
5	A	1106	Y01	10	0
6	B	1112	LPE	16	0
7	B	1102	POV	4	0
7	A	1113	POV	6	0
7	A	1116	POV	13	0
7	B	1114	POV	18	0
6	A	1109	LPE	7	0
6	A	1111	LPE	6	0
7	A	1115	POV	10	0
7	A	1114	POV	7	0
5	B	1107	Y01	17	0
6	B	1111	LPE	5	0

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.

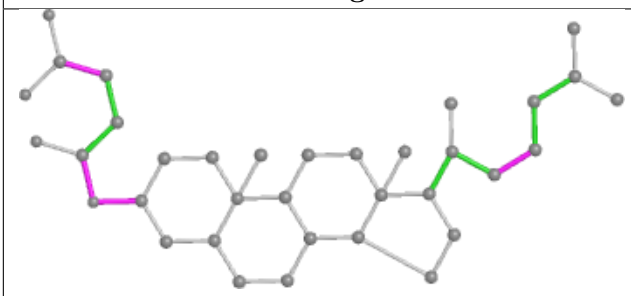
Ligand Y01 A 1105



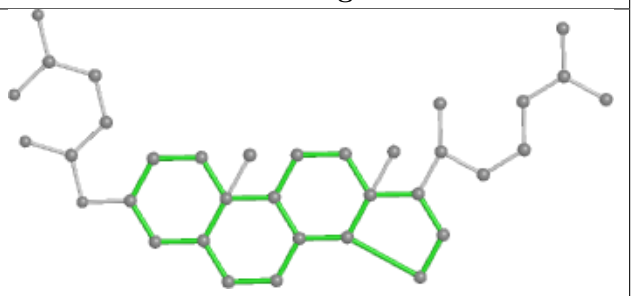
Bond lengths



Bond angles

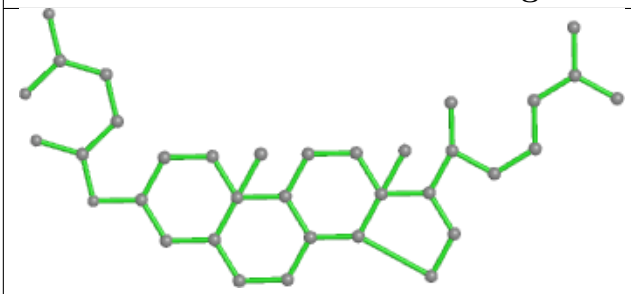


Torsions

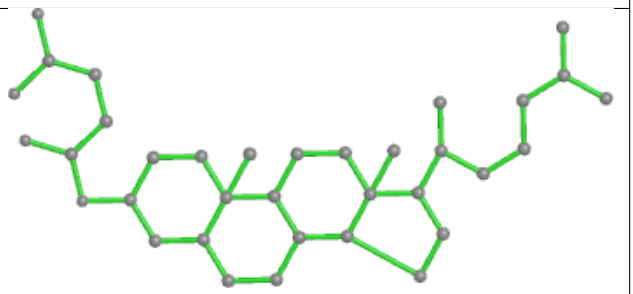


Rings

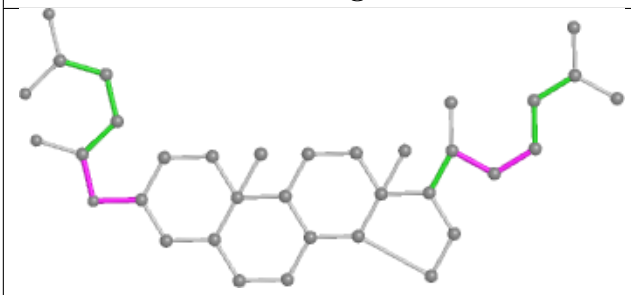
Ligand Y01 B 1108



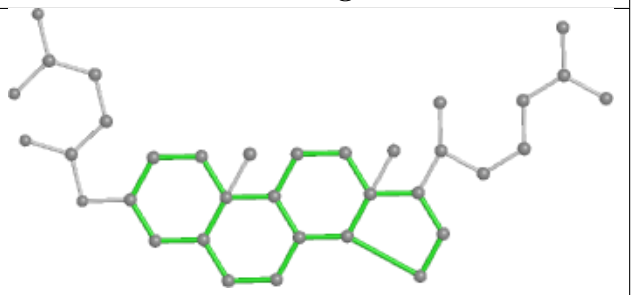
Bond lengths



Bond angles

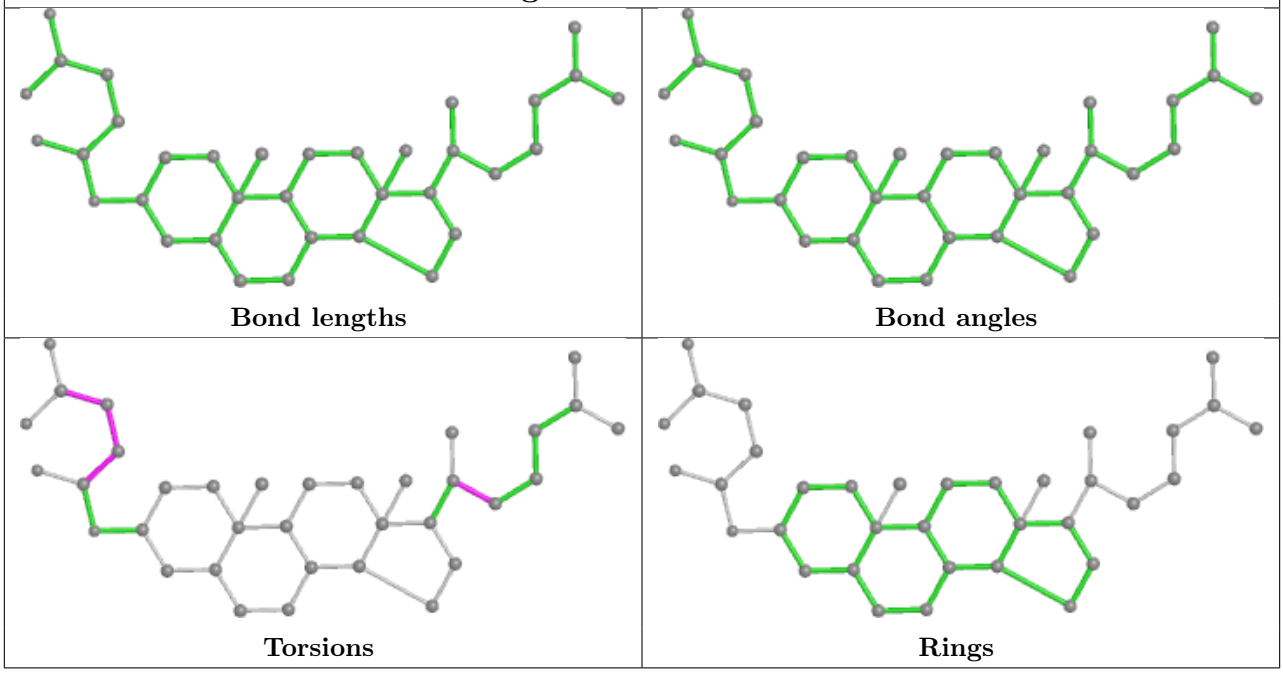


Torsions

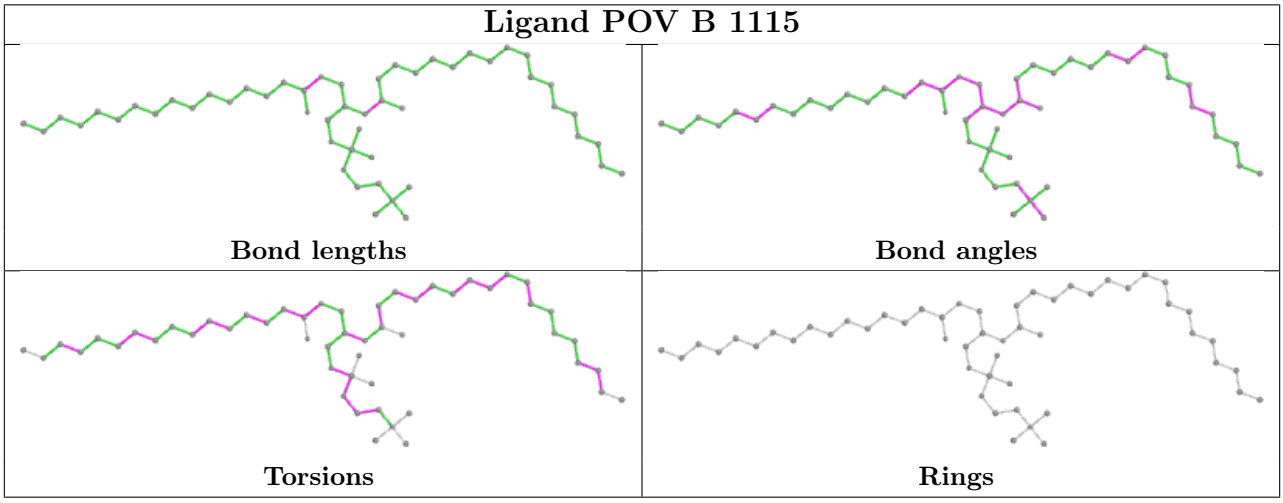


Rings

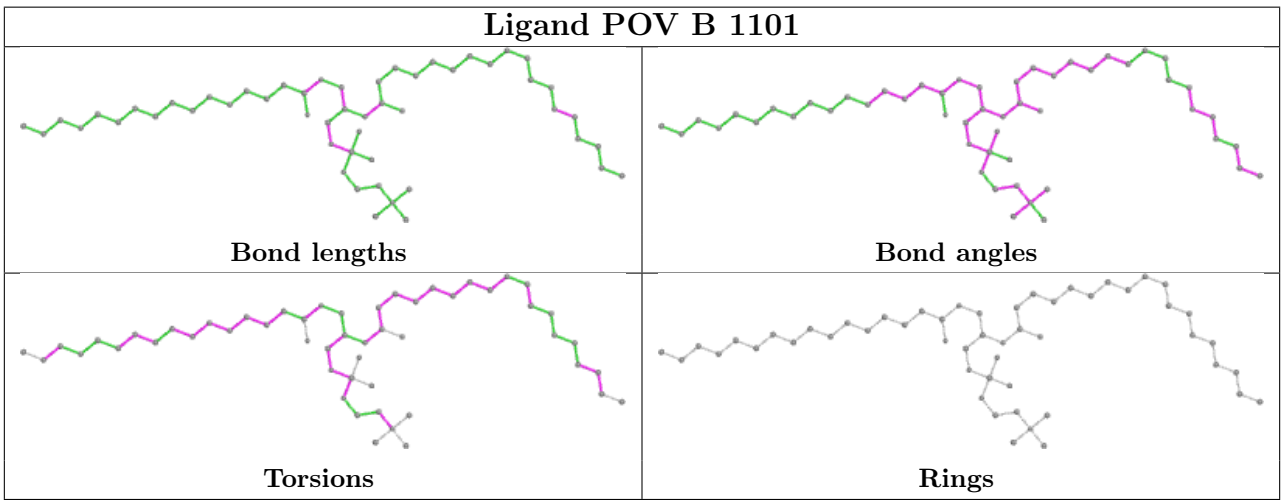
Ligand Y01 A 1107



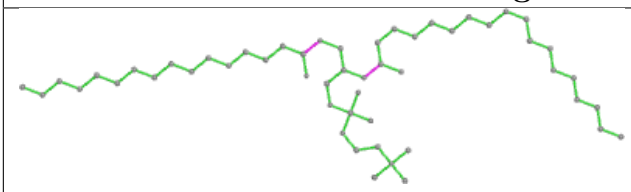
Ligand POV B 1115



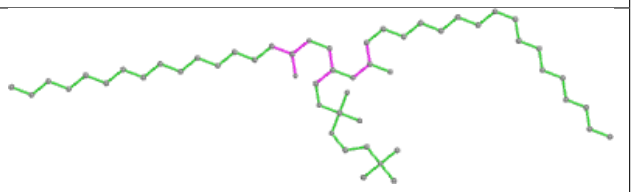
Ligand POV B 1101



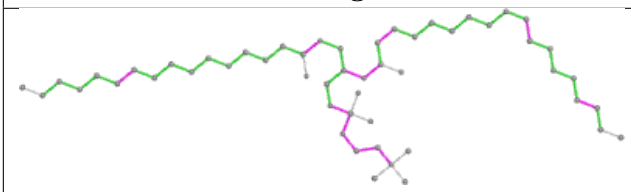
Ligand POV A 1112



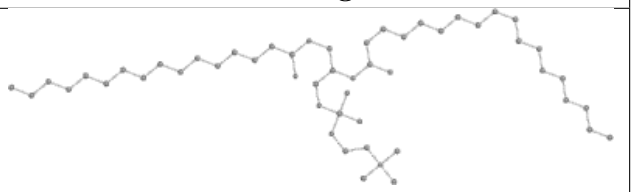
Bond lengths



Bond angles

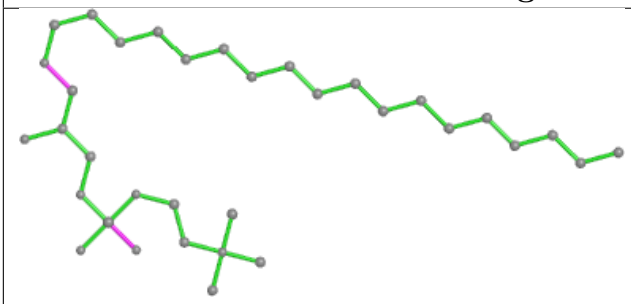


Torsions

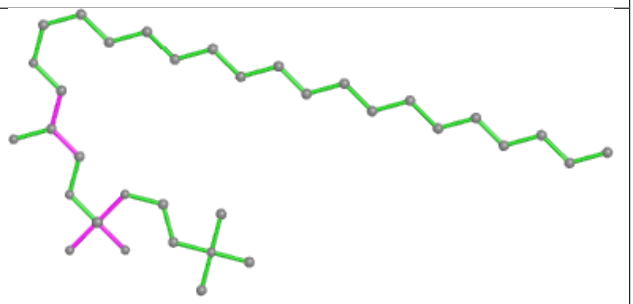


Rings

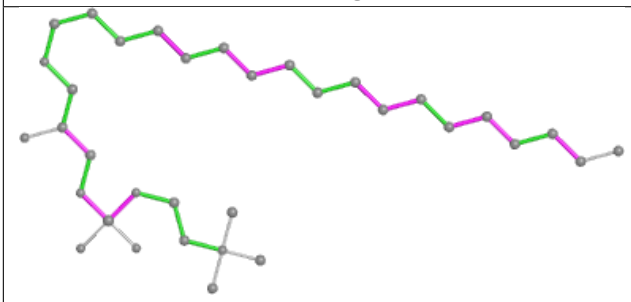
Ligand LPE A 1108



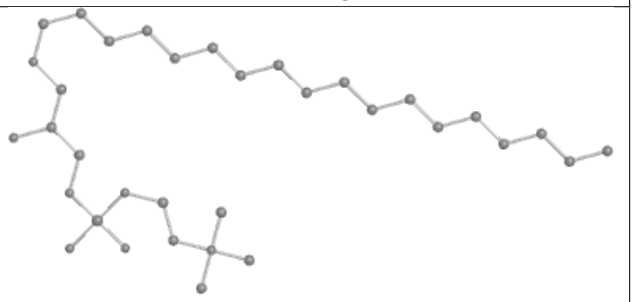
Bond lengths



Bond angles

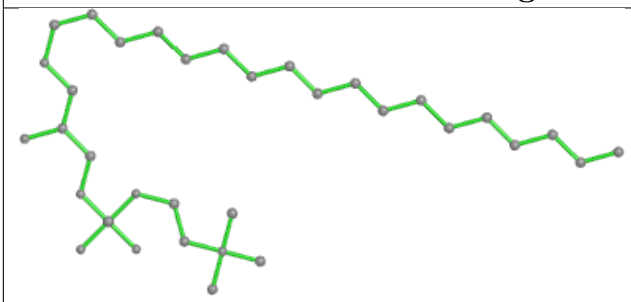


Torsions

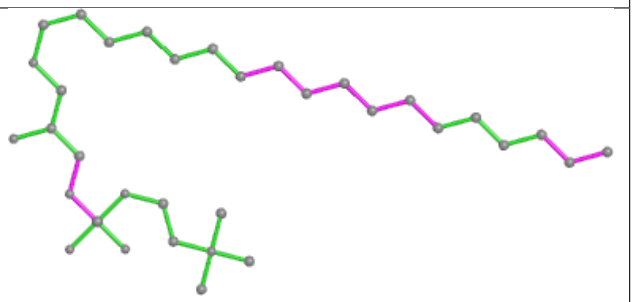


Rings

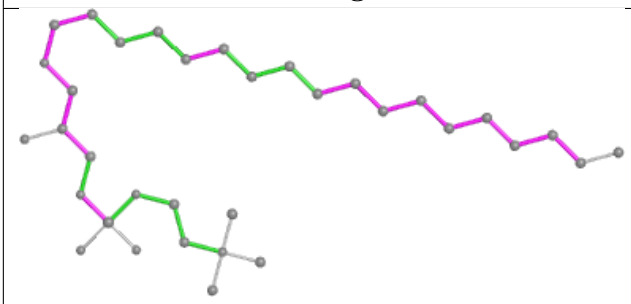
Ligand LPE B 1113



Bond lengths



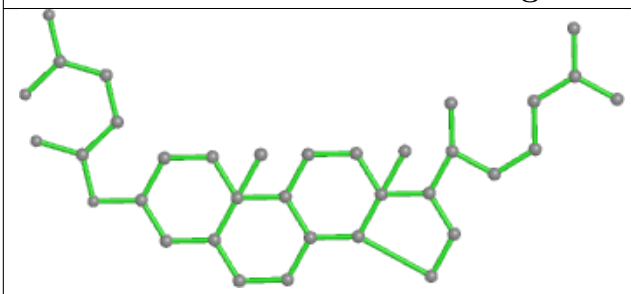
Bond angles



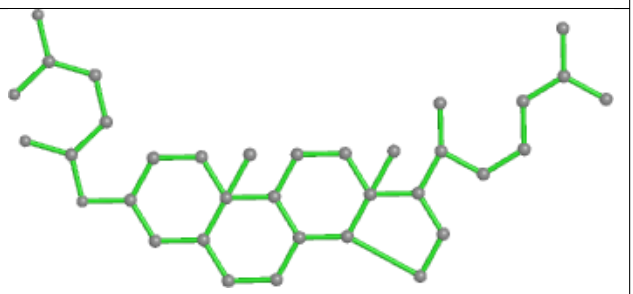
Torsions

Rings

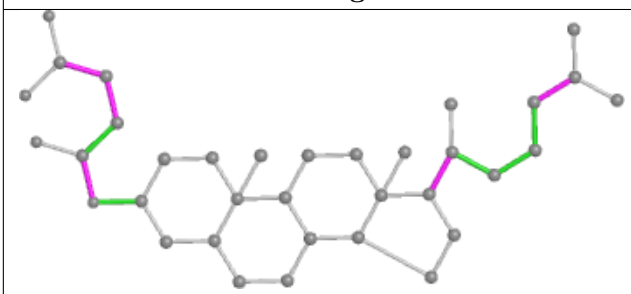
Ligand Y01 B 1109



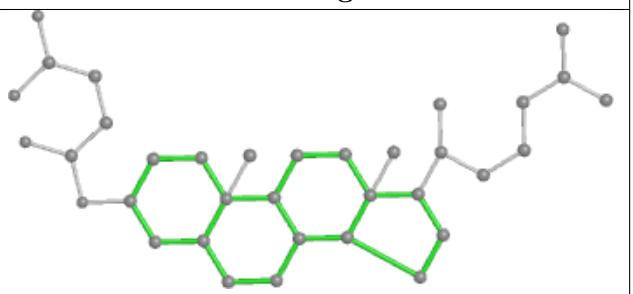
Bond lengths



Bond angles

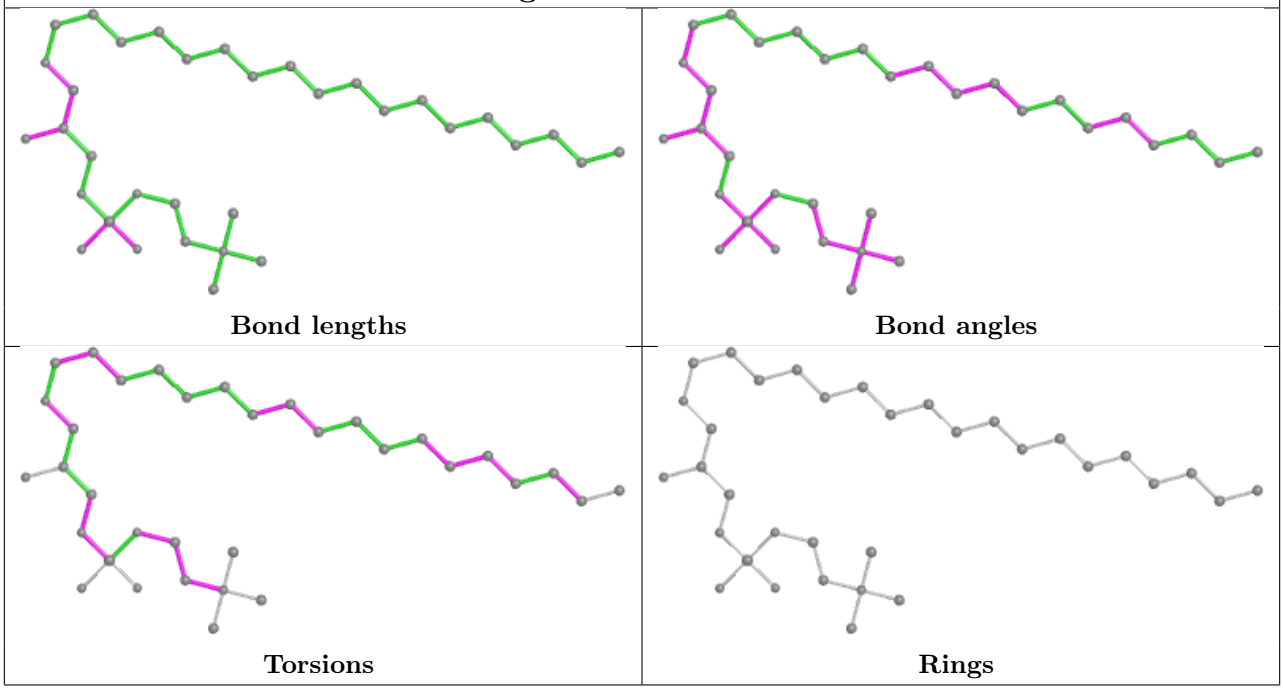


Torsions

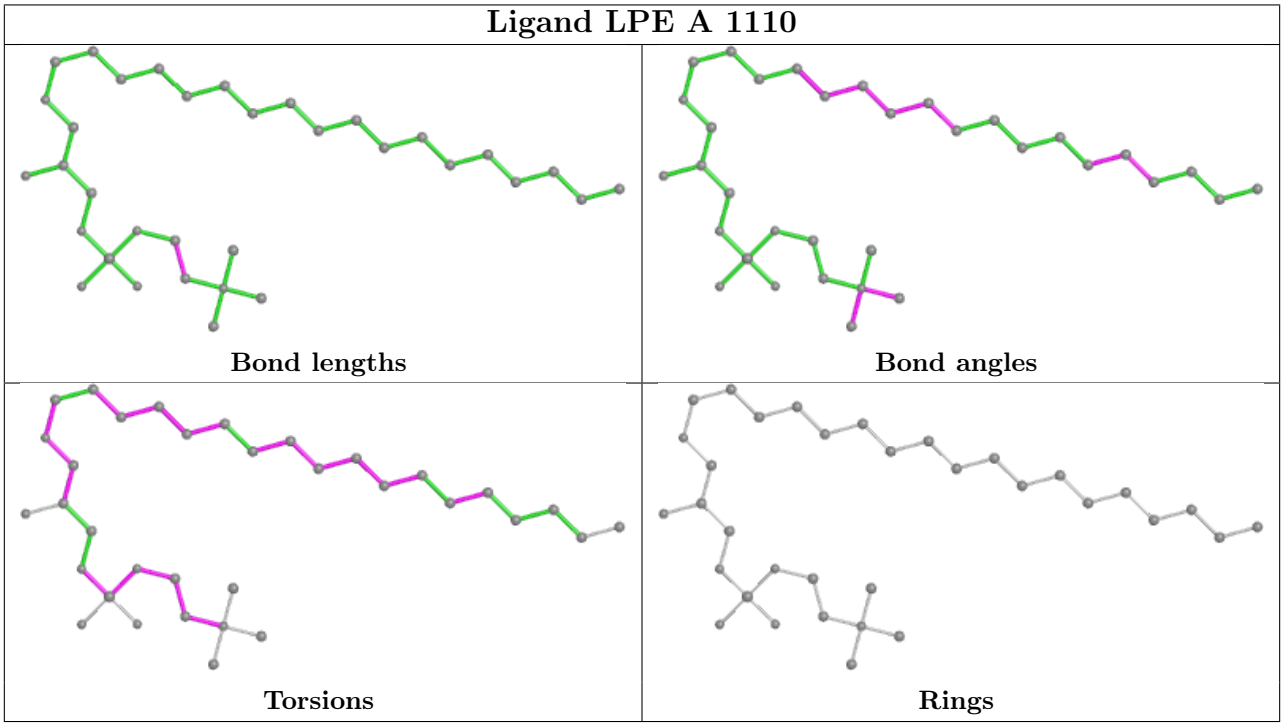


Rings

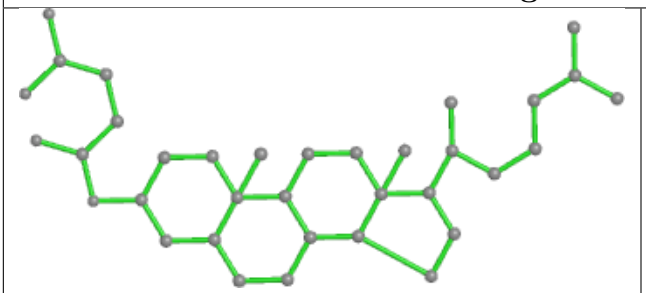
Ligand LPE B 1110



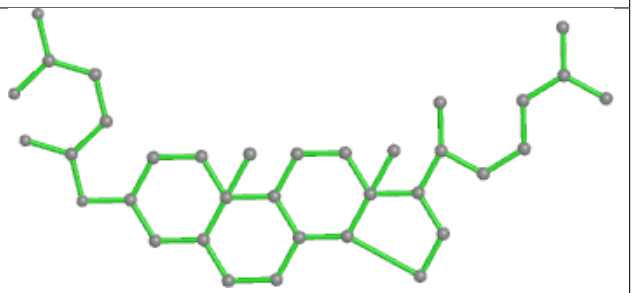
Ligand LPE A 1110



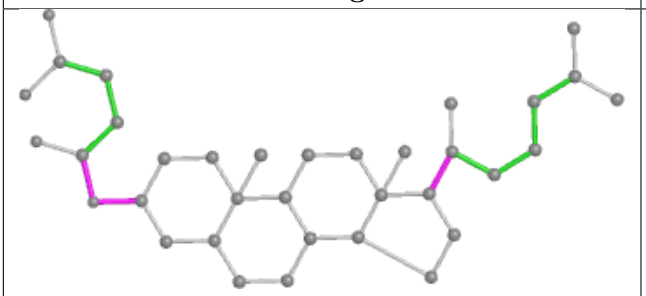
Ligand Y01 A 1106



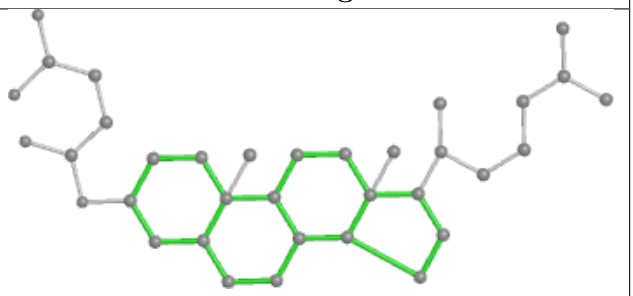
Bond lengths



Bond angles

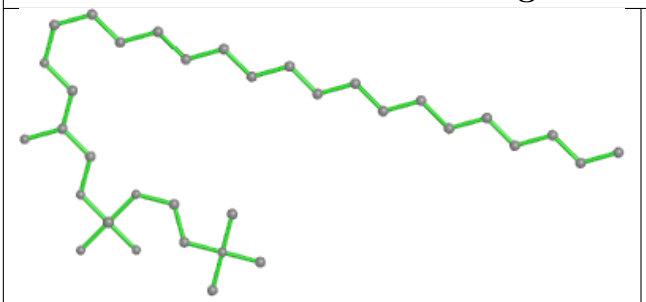


Torsions

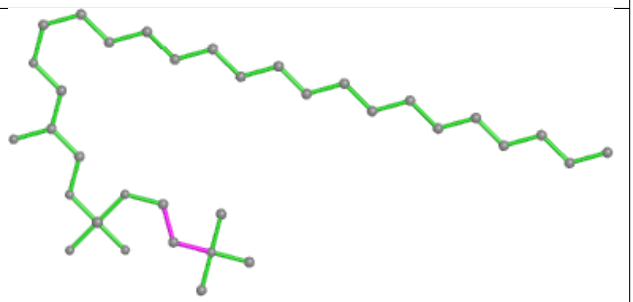


Rings

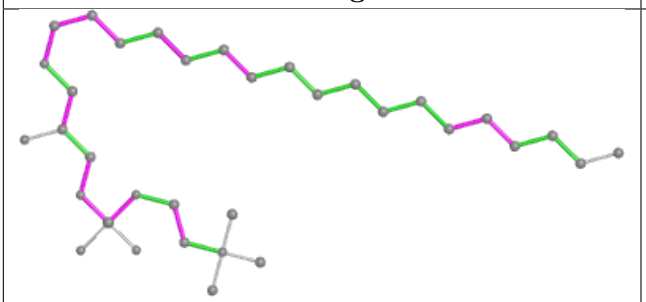
Ligand LPE B 1112



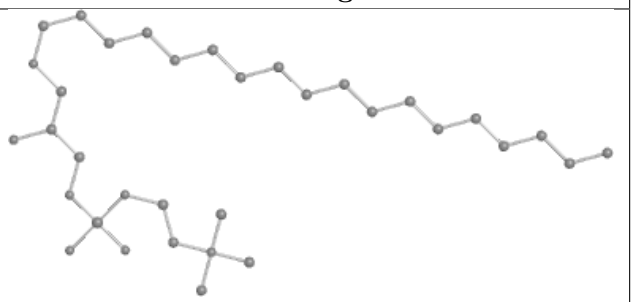
Bond lengths



Bond angles

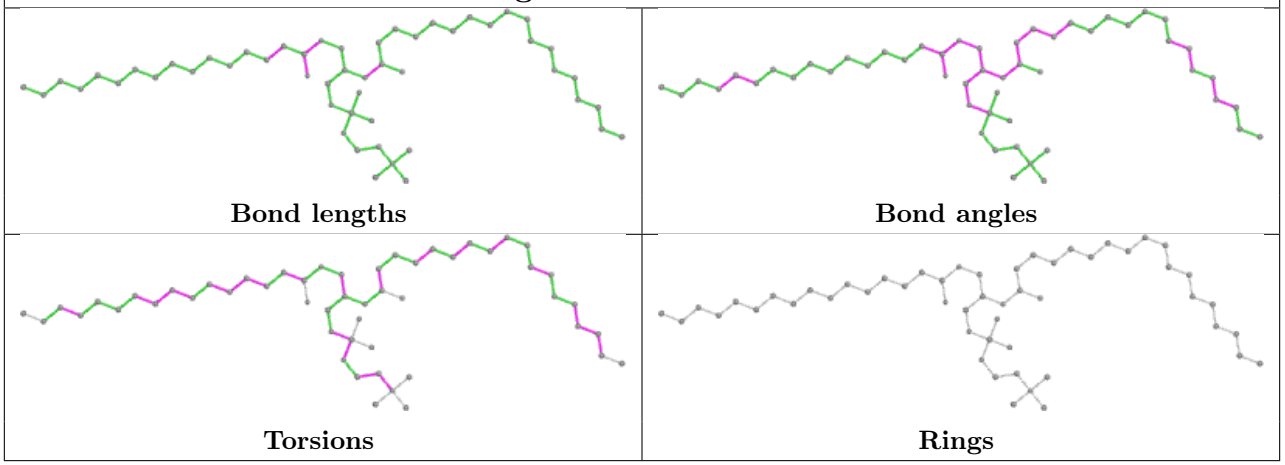


Torsions

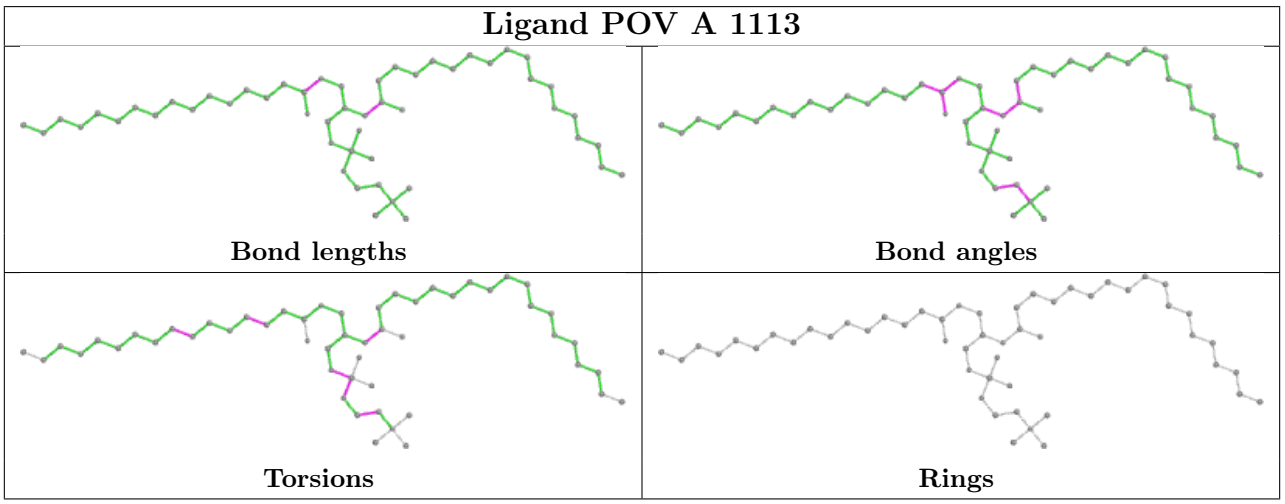


Rings

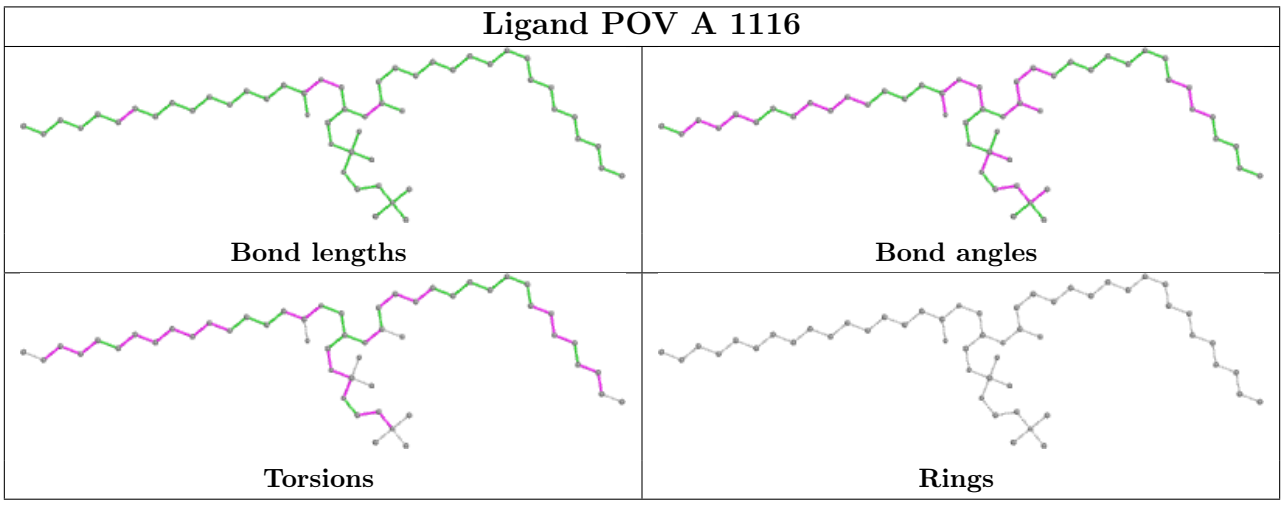
Ligand POV B 1102



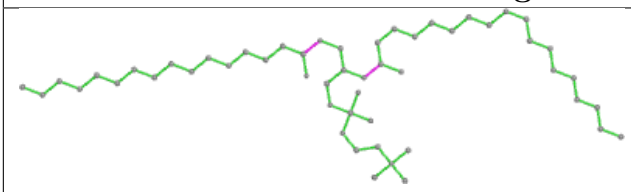
Ligand POV A 1113



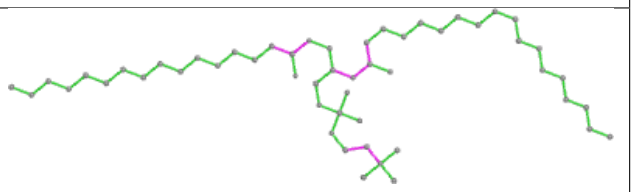
Ligand POV A 1116



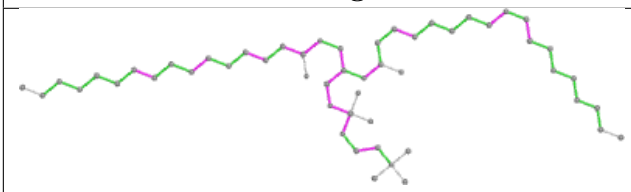
Ligand POV B 1114



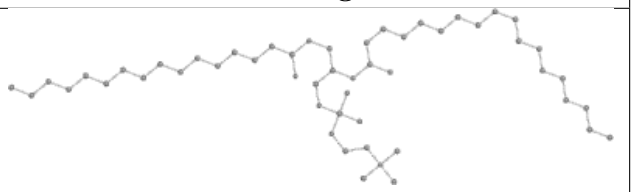
Bond lengths



Bond angles

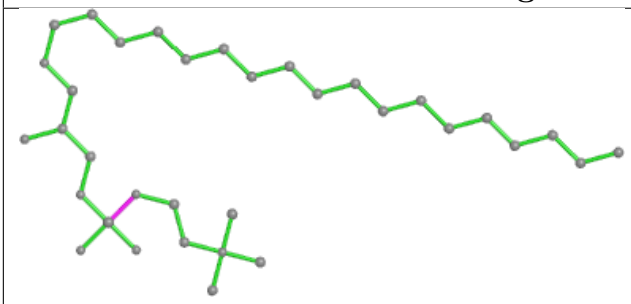


Torsions

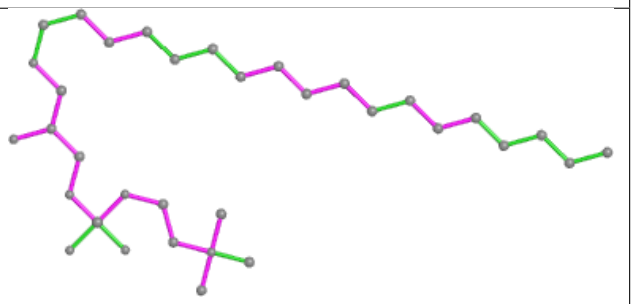


Rings

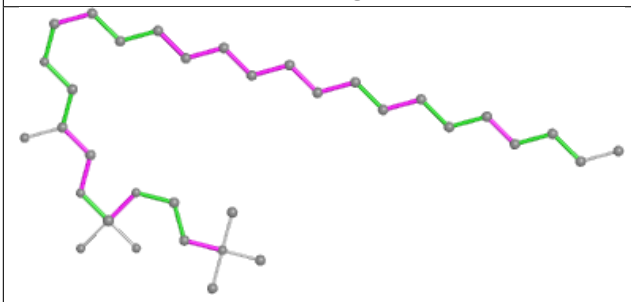
Ligand LPE A 1109



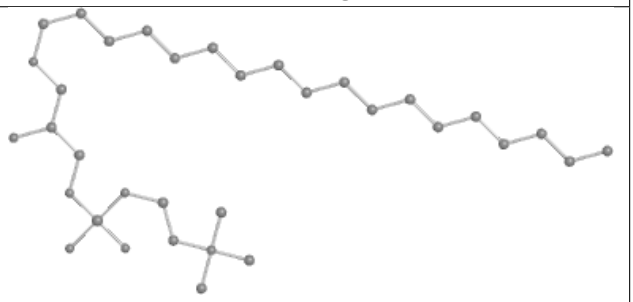
Bond lengths



Bond angles

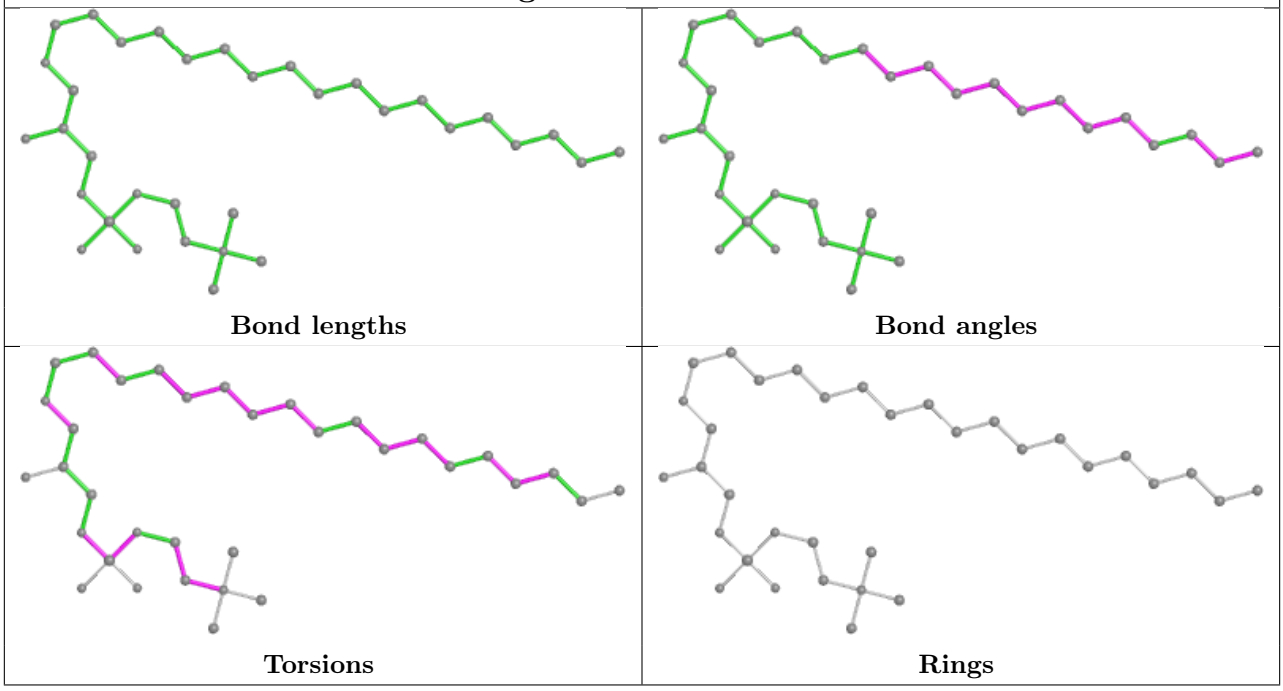


Torsions

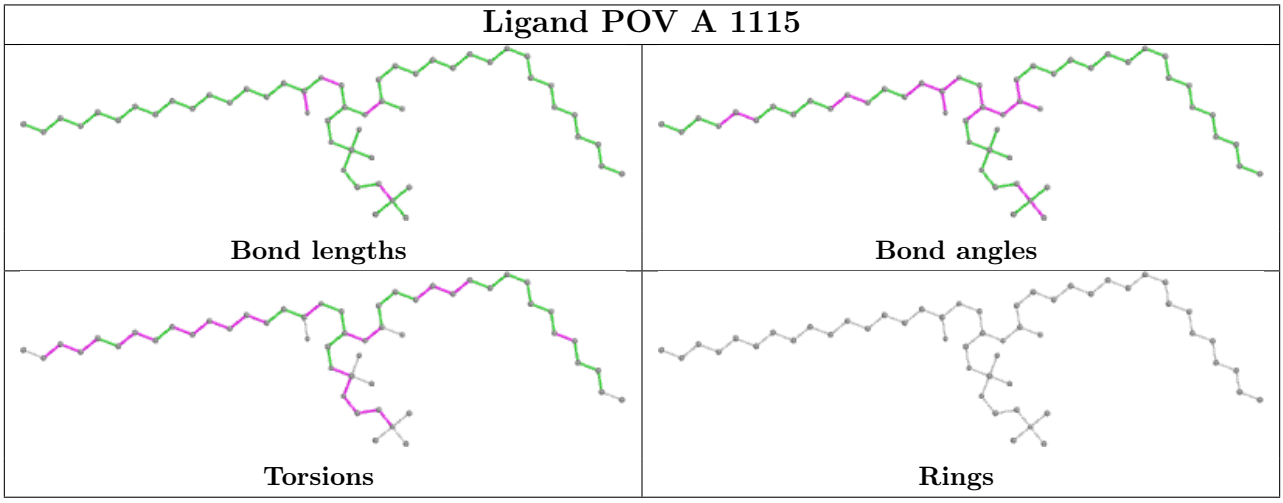


Rings

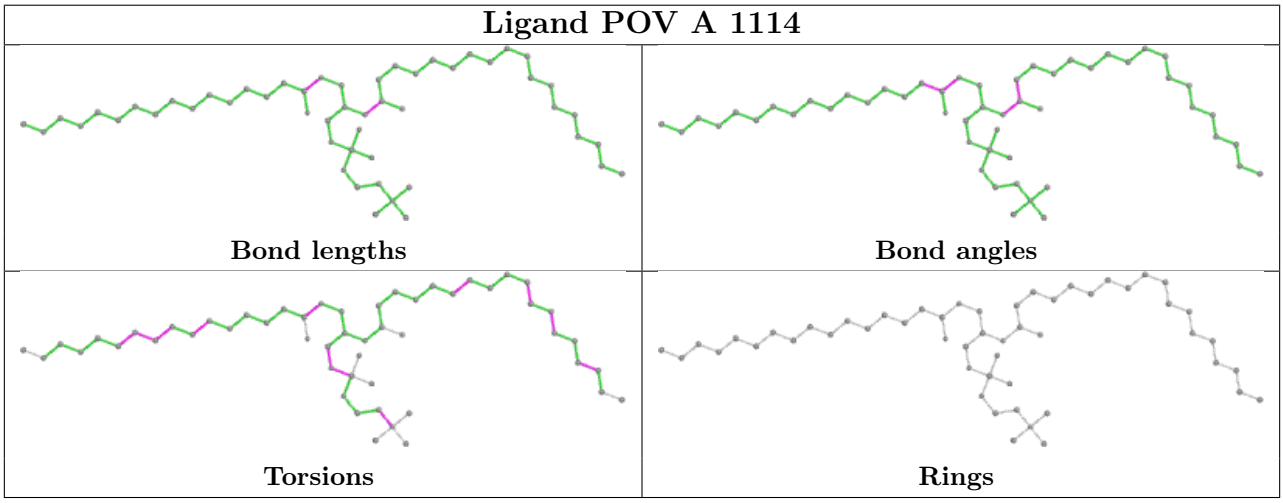
Ligand LPE A 1111



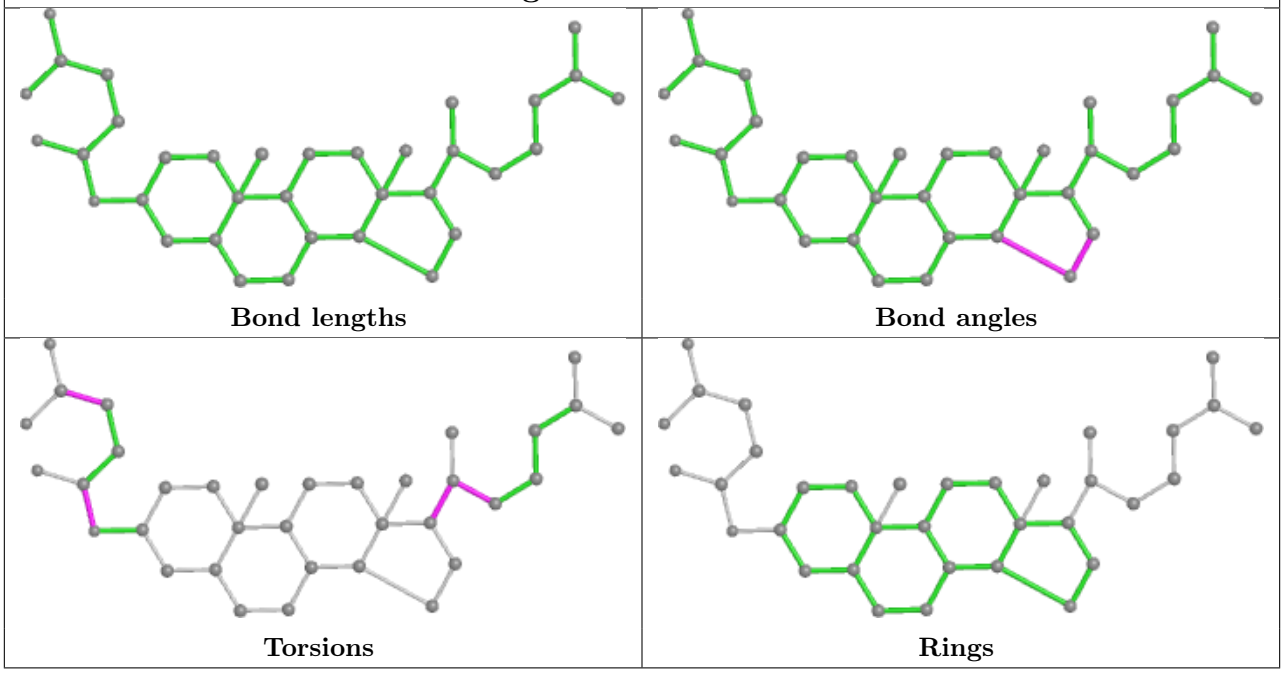
Ligand POV A 1115



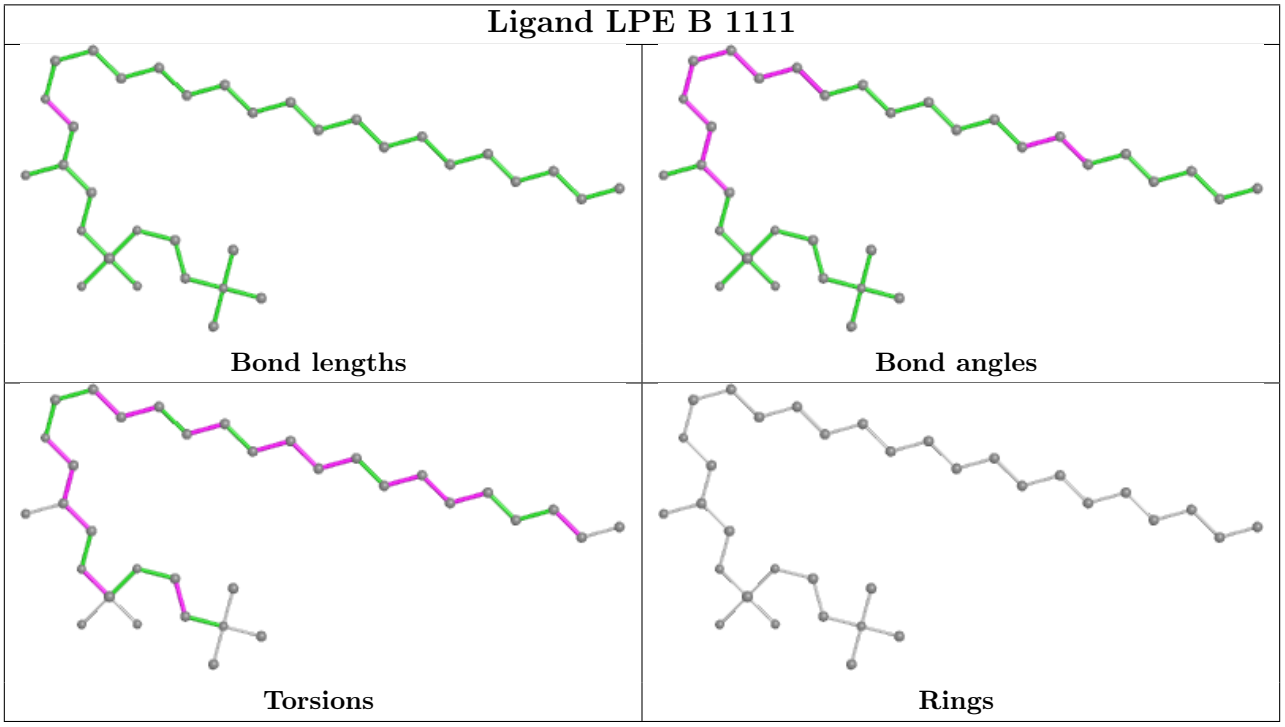
Ligand POV A 1114



Ligand Y01 B 1107



Ligand LPE B 1111



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

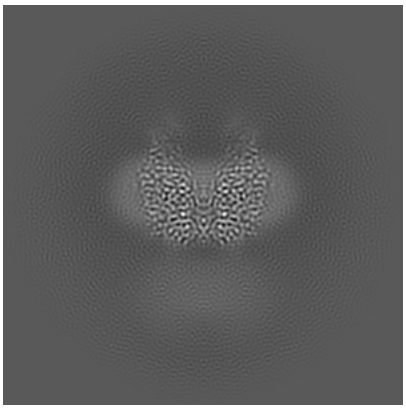
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33641. These allow visual inspection of the internal detail of the map and identification of artifacts.

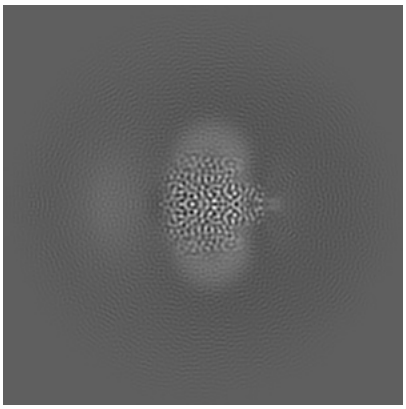
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

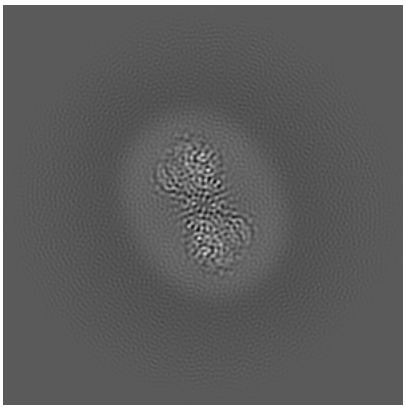
6.1.1 Primary map



X

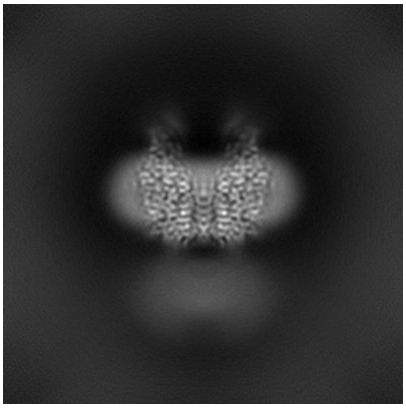


Y

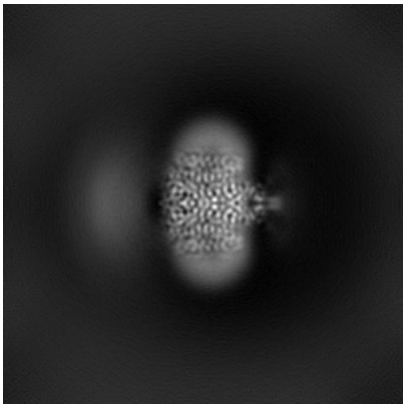


Z

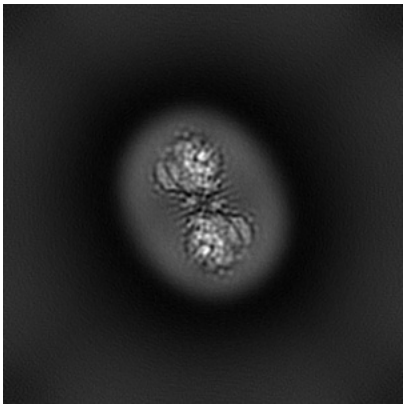
6.1.2 Raw map



X



Y

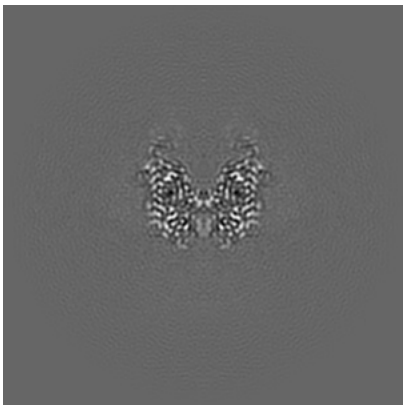


Z

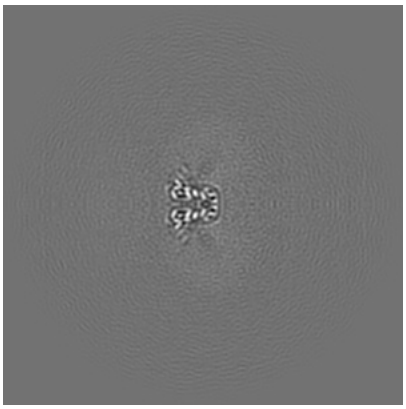
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

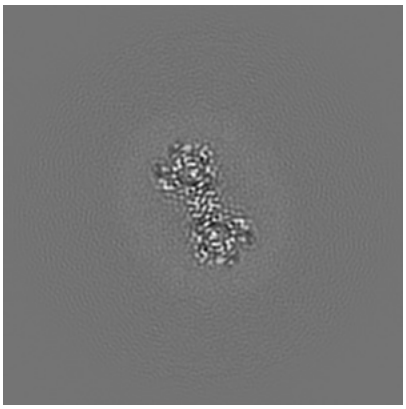
6.2.1 Primary map



X Index: 128

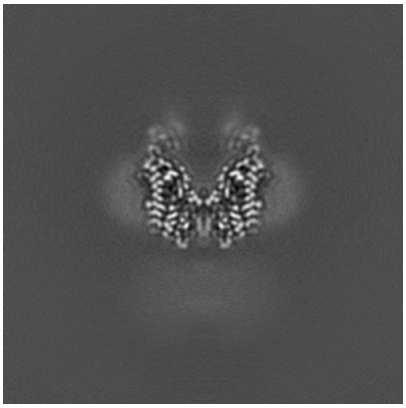


Y Index: 128

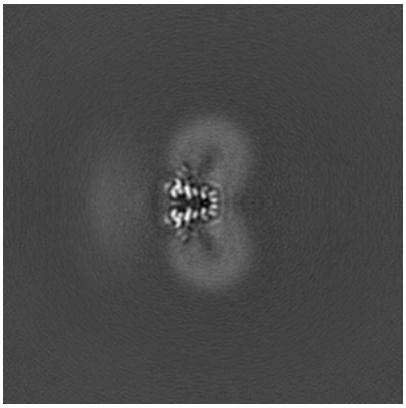


Z Index: 128

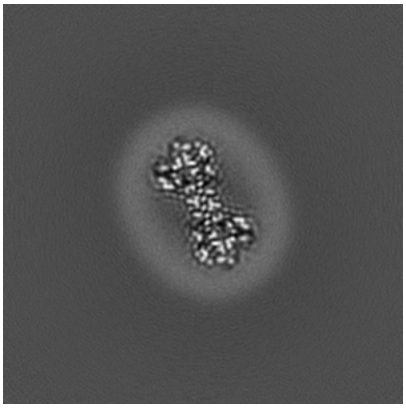
6.2.2 Raw map



X Index: 128



Y Index: 128

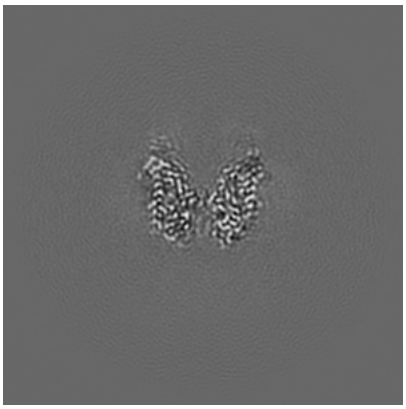


Z Index: 128

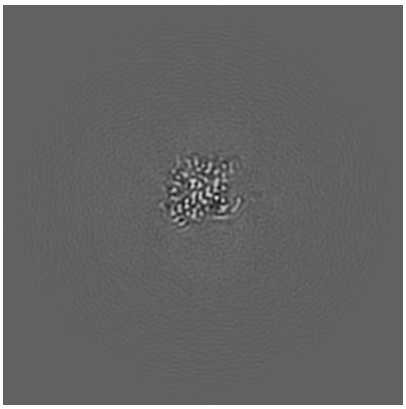
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

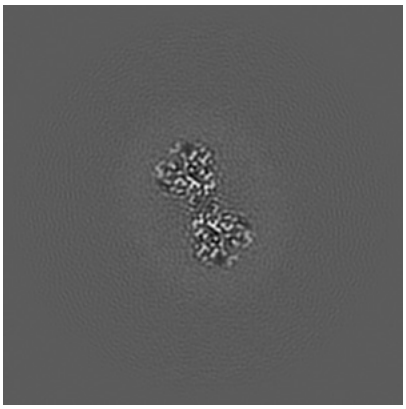
6.3.1 Primary map



X Index: 129

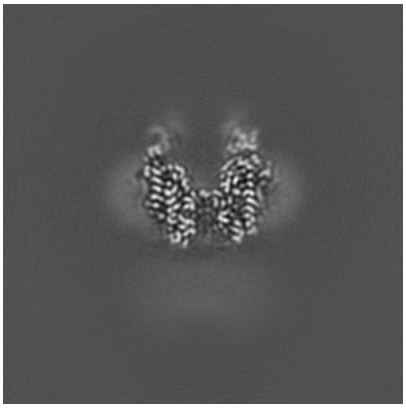


Y Index: 115

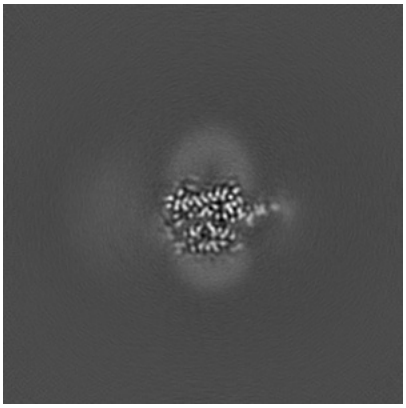


Z Index: 126

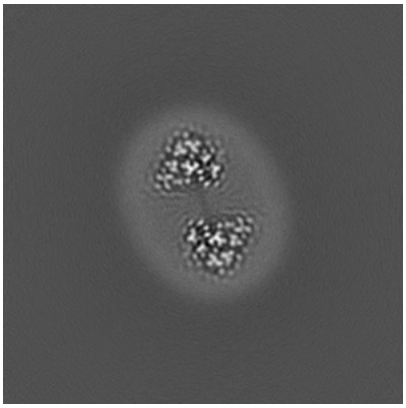
6.3.2 Raw map



X Index: 126



Y Index: 149

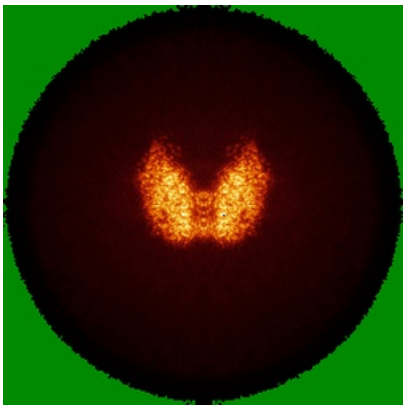


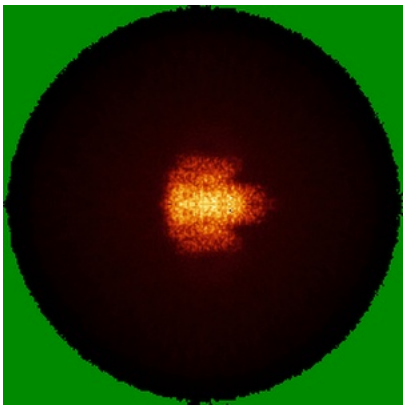
Z Index: 142

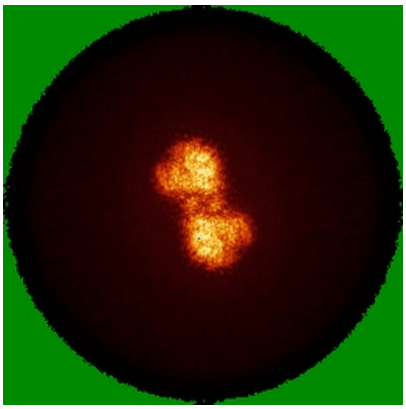
The images above show the largest variance slices of the map in three orthogonal directions.

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

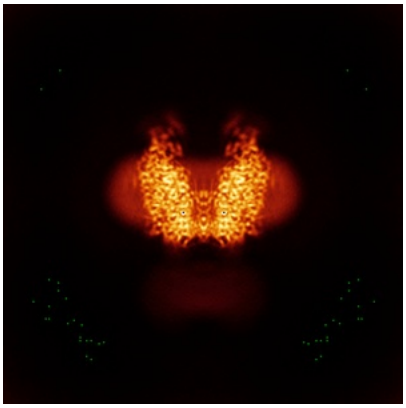
6.4.1 Primary map

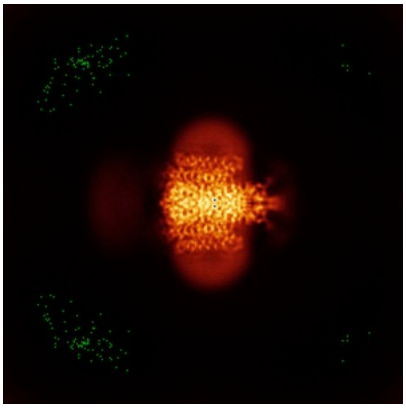

X

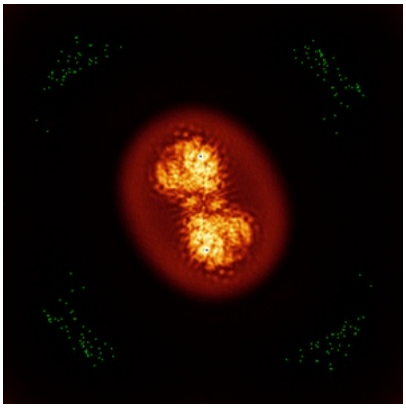

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.282. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

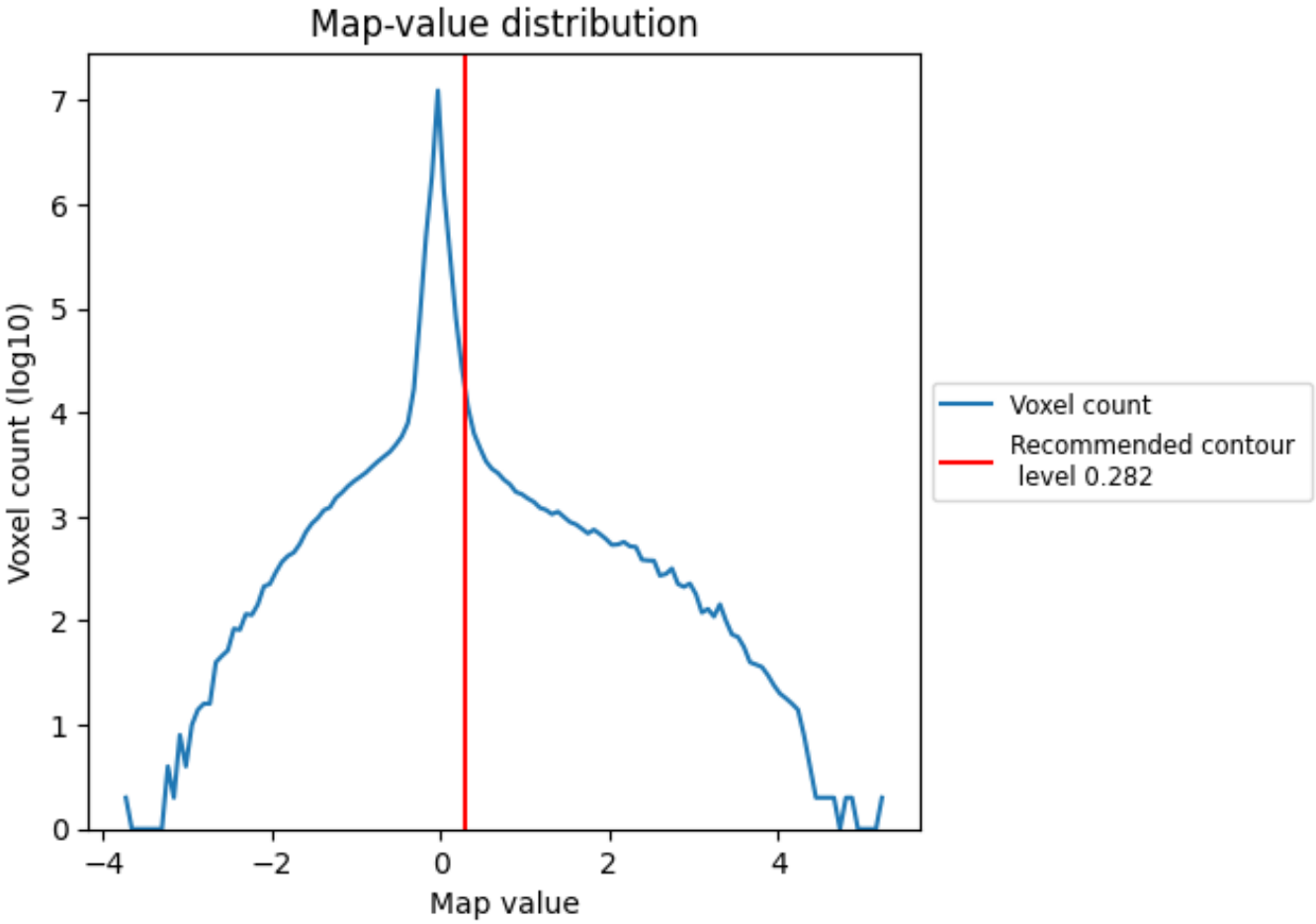
6.6 Mask visualisation (i)

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

7 Map analysis

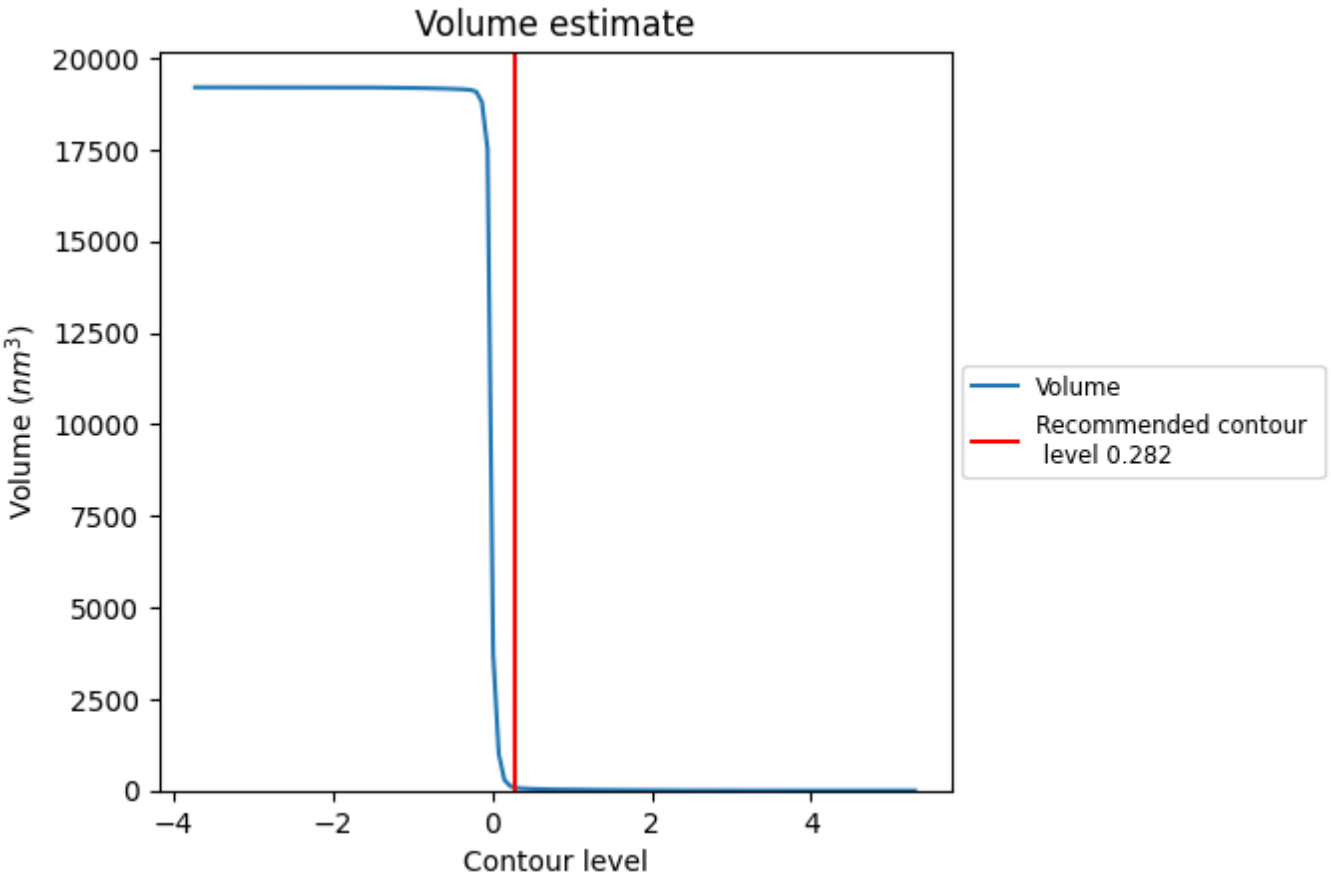
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

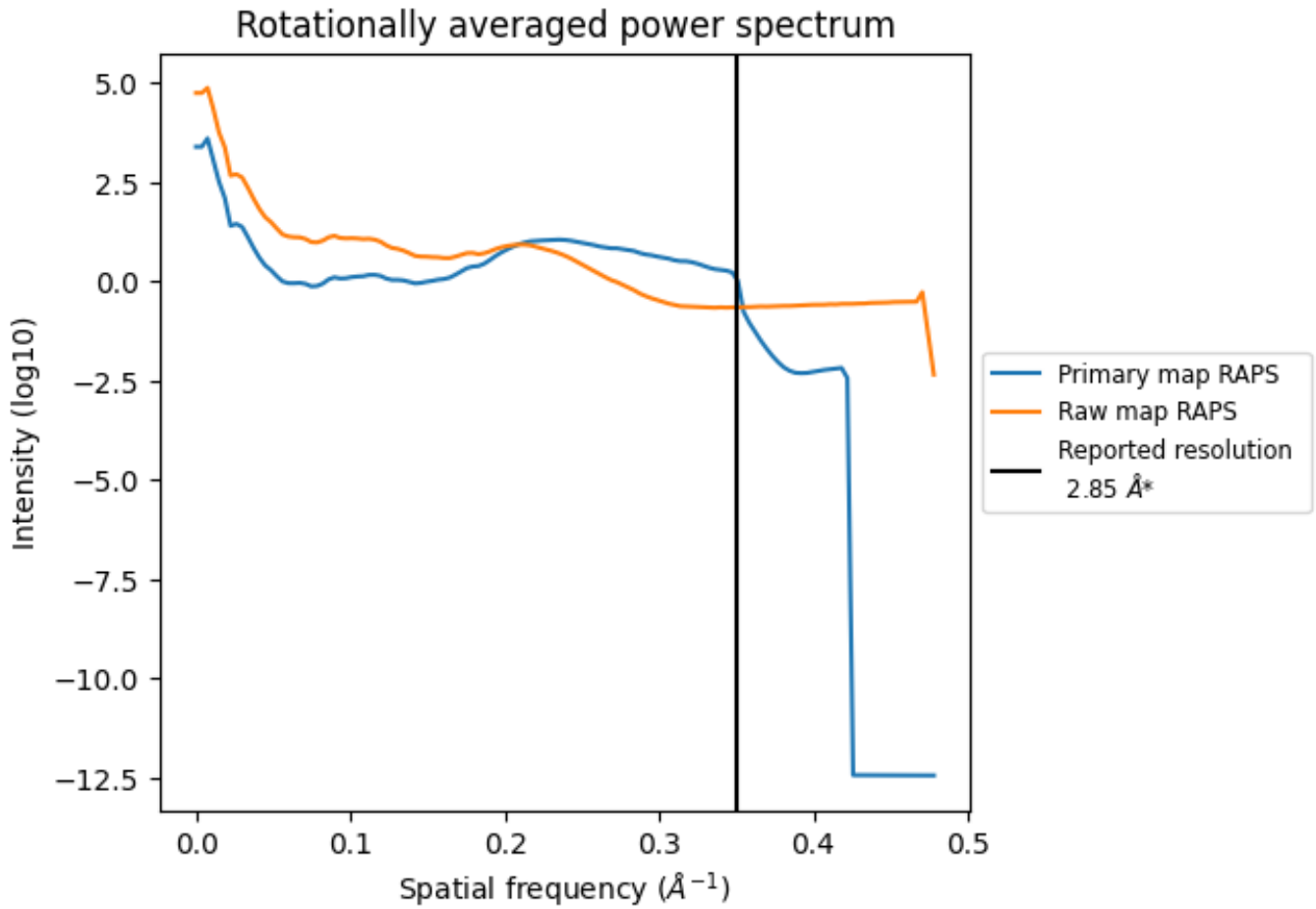
7.2 Volume estimate



The volume at the recommended contour level is 86 nm^3; this corresponds to an approximate mass of 77 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)

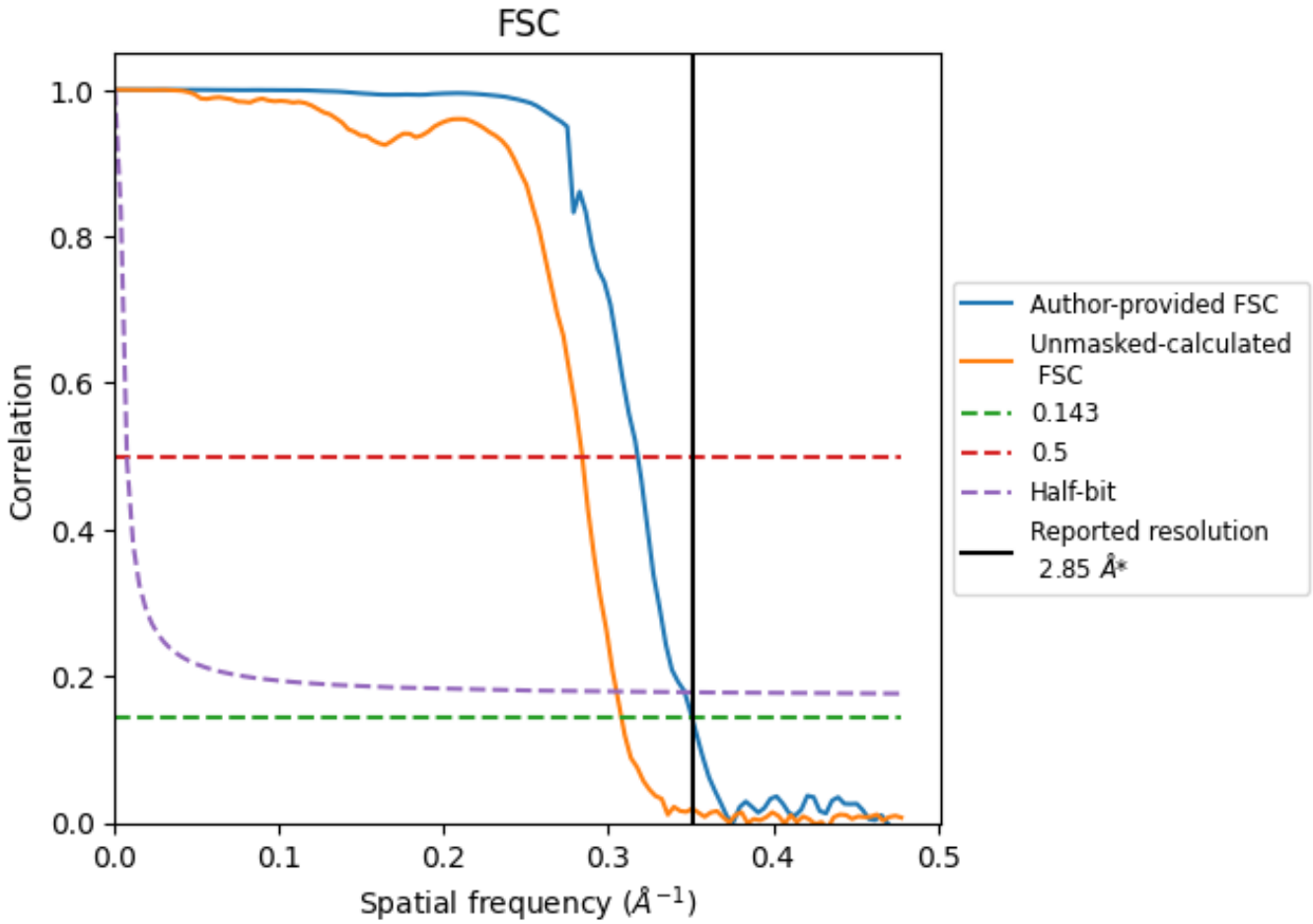


*Reported resolution corresponds to spatial frequency of 0.351 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8.2 Resolution estimates (i)

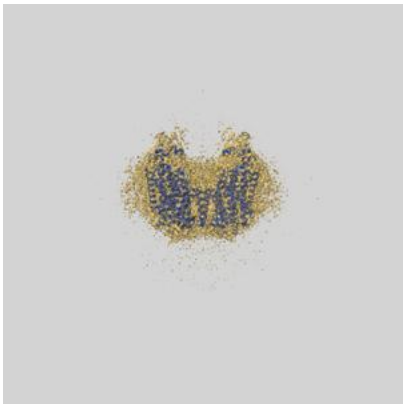
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.15	2.89
Unmasked-calculated*	3.25	3.52	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.85 by more than 10 %

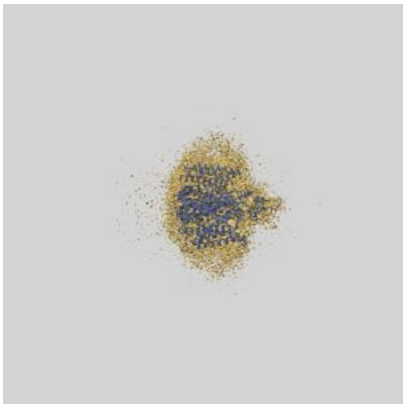
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33641 and PDB model 7Y6I. Per-residue inclusion information can be found in section 3 on page 10.

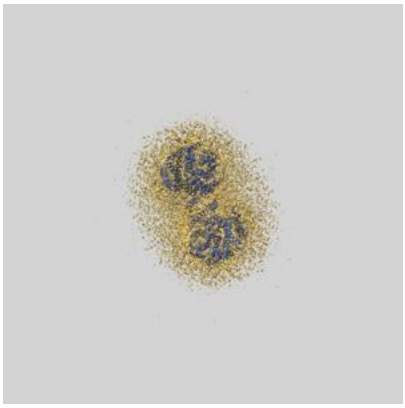
9.1 Map-model overlay



X



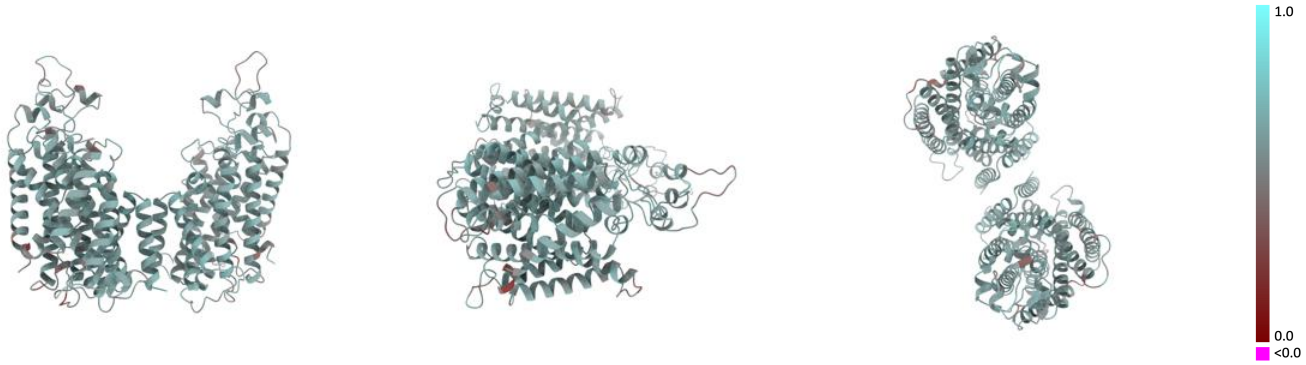
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

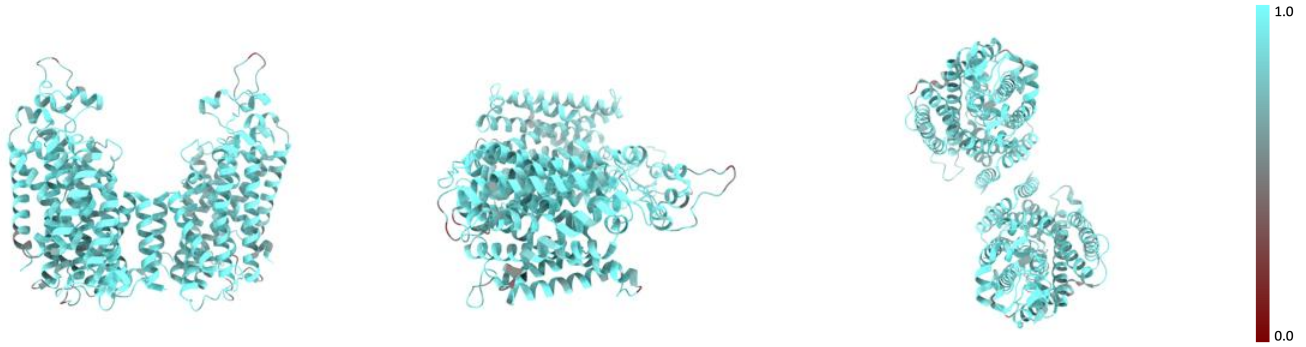
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

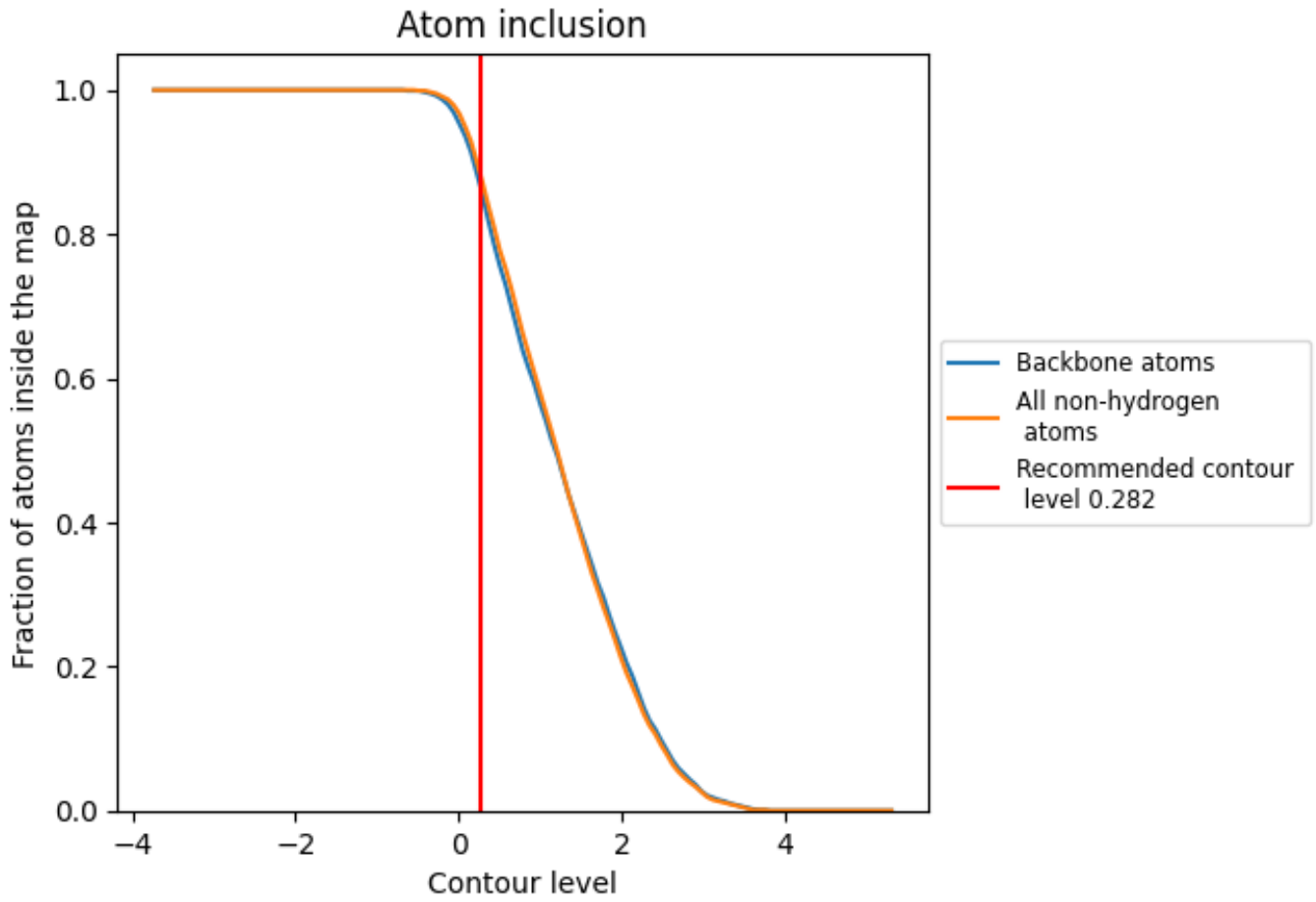
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.282).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.5700
A	0.8790	0.5690
B	0.8790	0.5730
C	0.7500	0.4720
D	0.7140	0.4570