Full wwPDB EM Validation Report ⓘ

Apr 23, 2022 – 07:19 am BST

PDB ID	:	7QL5
EMDB ID	:	EMD-14064
Title	:	Torpedo muscle-type nicotinic acetylcholine receptor - nicotine-bound conformation
Authors	:	Zarkadas, E.; Pebay-Peyroula, E.; Baenziger, J.; Nury, H.
Deposited on	:	2021-12-19
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

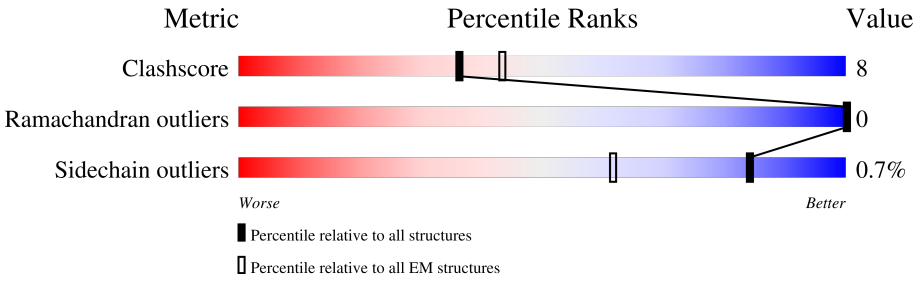
EMDB validation analysis	:	0.0.1.dev7
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 2.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	437	8% 69% 20% 11%
1	D	437	9% 62% 22% 15%
2	B	469	5% 68% 16% 15%
3	C	501	9% 71% 14% 16%
4	E	489	8% 71% 12% 17%
5	F	7	29% 43% 57%
6	G	5	60% 40% 60%
6	H	5	60% 40% 60%

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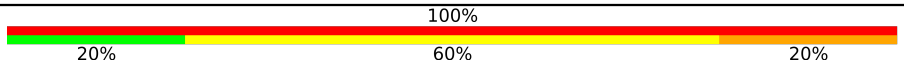
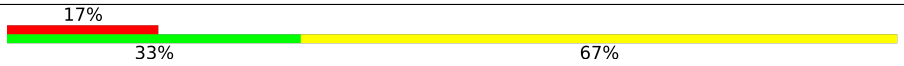
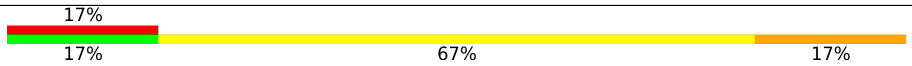
Mol	Chain	Length	Quality of chain
6	I	5	
7	J	2	
8	K	6	
8	L	6	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17028 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 Acetylcholine receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	390	Total	C	N	O	S	1	0
			3173	2081	507	563	22		
1	D	371	Total	C	N	O	S	0	0
			3010	1972	481	537	20		

- Molecule 2 is a protein called Acetylcholine receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total	C	N	O	S	0	0
			3239	2122	515	588	14		

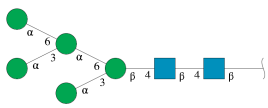
- Molecule 3 is a protein called Acetylcholine receptor subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	423	Total	C	N	O	S	0	0
			3430	2238	557	619	16		

- Molecule 4 is a protein called Acetylcholine receptor subunit gamma.

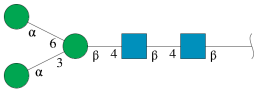
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	406	Total	C	N	O	S	0	0
			3297	2163	524	598	12		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	7	Total	C	N	O	0	0
			83	46	2	35		

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

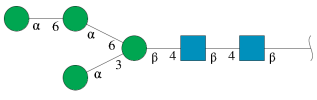


Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	5	Total	C	N	O	0	0
			61	34	2	25		
6	H	5	Total	C	N	O	0	0
			61	34	2	25		
6	I	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 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
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	6	Total	C	N	O	0	0
			72	40	2	30		

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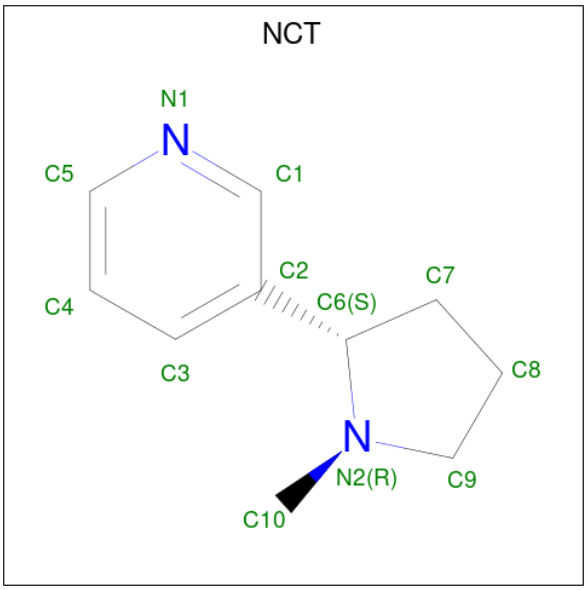
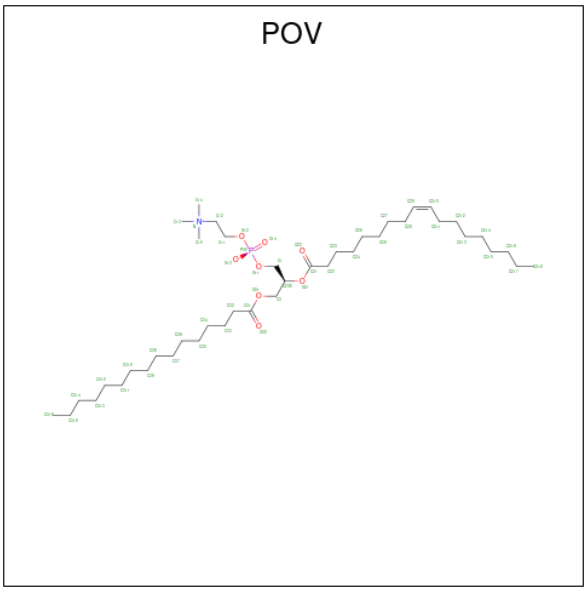
Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$) (labeled as "Ligand of Interest" by depositor).



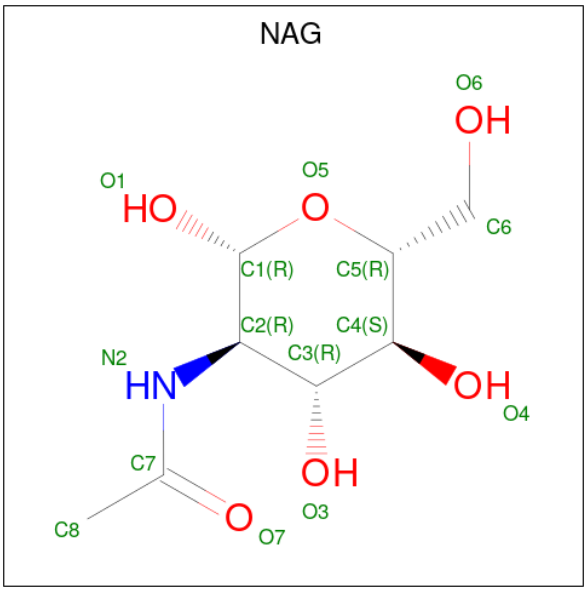
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	N	0
			12	10	2	
9	D	1	Total	C	N	0
			12	10	2	

- Molecule 10 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			123	93	3	24	3	
10	A	1	Total	C	N	O	P	0
			123	93	3	24	3	
10	A	1	Total	C	N	O	P	0
			123	93	3	24	3	
10	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
10	C	1	Total	C	N	O	P	0
			79	59	2	16	2	
10	C	1	Total	C	N	O	P	0
			79	59	2	16	2	
10	D	1	Total	C	N	O	P	0
			66	46	2	16	2	
10	D	1	Total	C	N	O	P	0
			66	46	2	16	2	
10	E	1	Total	C	N	O	P	0
			92	62	3	24	3	
10	E	1	Total	C	N	O	P	0
			92	62	3	24	3	
10	E	1	Total	C	N	O	P	0
			92	62	3	24	3	

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
11	E	1	Total	C	N	O	0
			14	8	1	5	

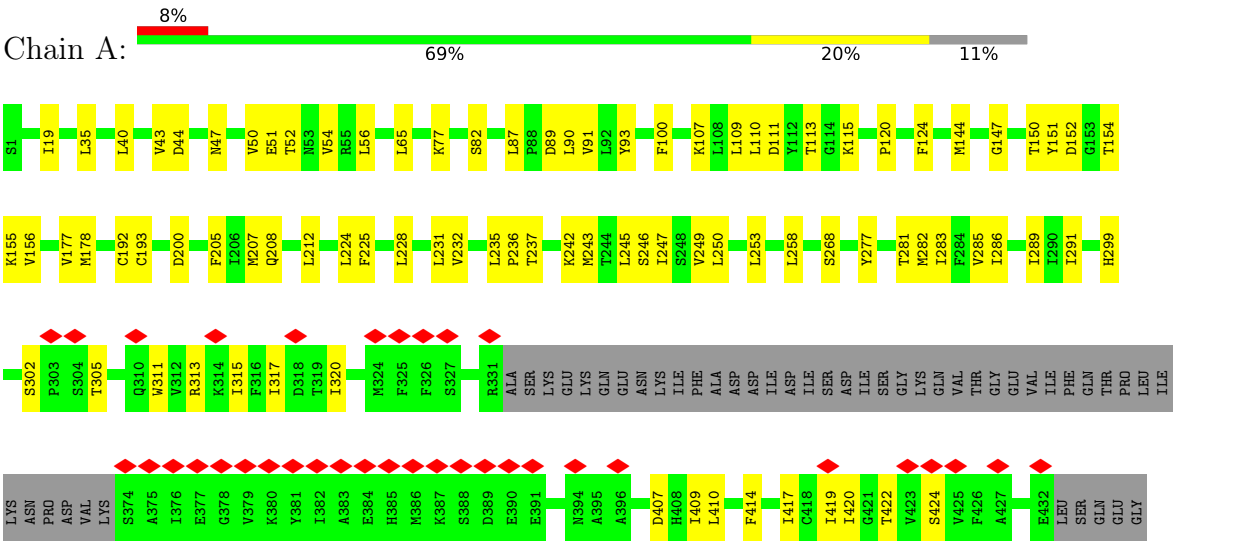
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	C	1	Total	O	0
			1	1	
12	E	1	Total	O	0
			1	1	

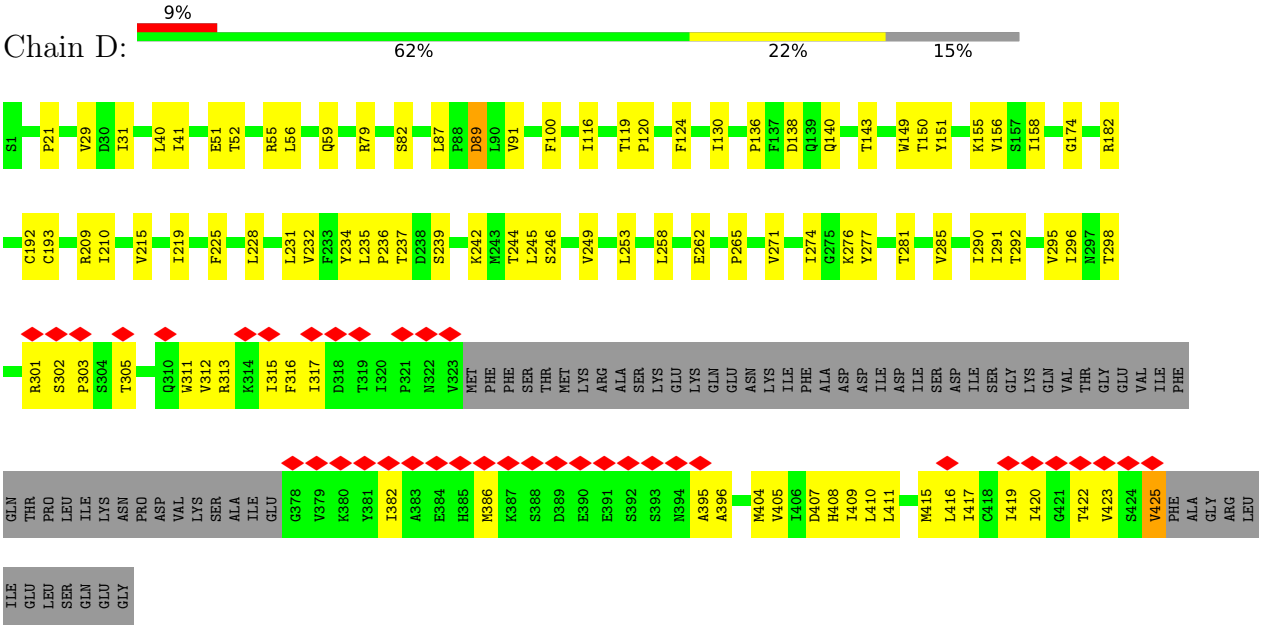
3 Residue-property plots (i)

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: Acetylcholine receptor subunit alpha

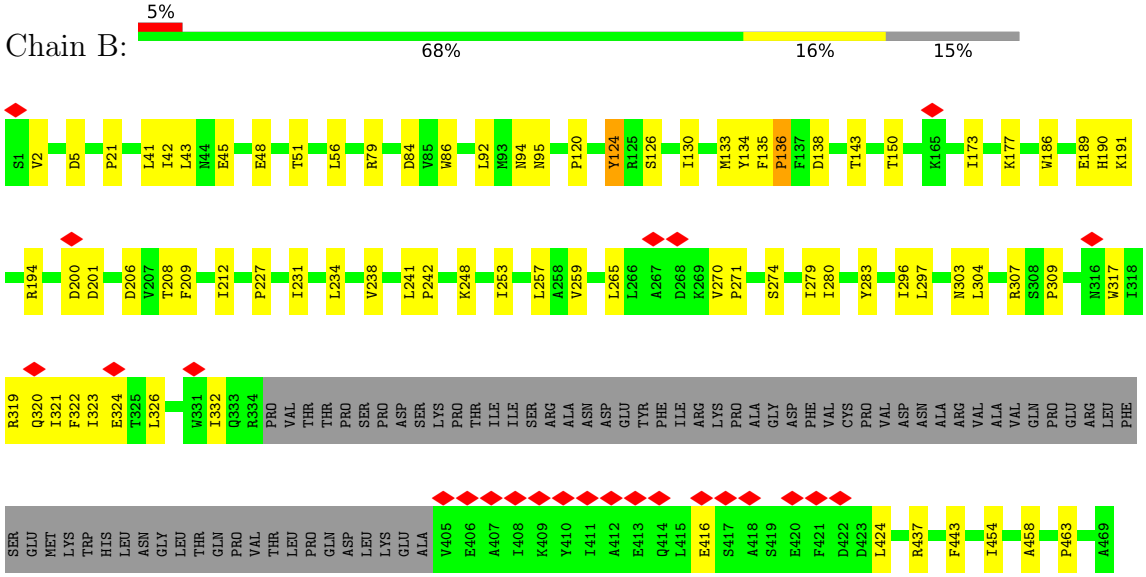


• Molecule 1: Acetylcholine receptor subunit alpha



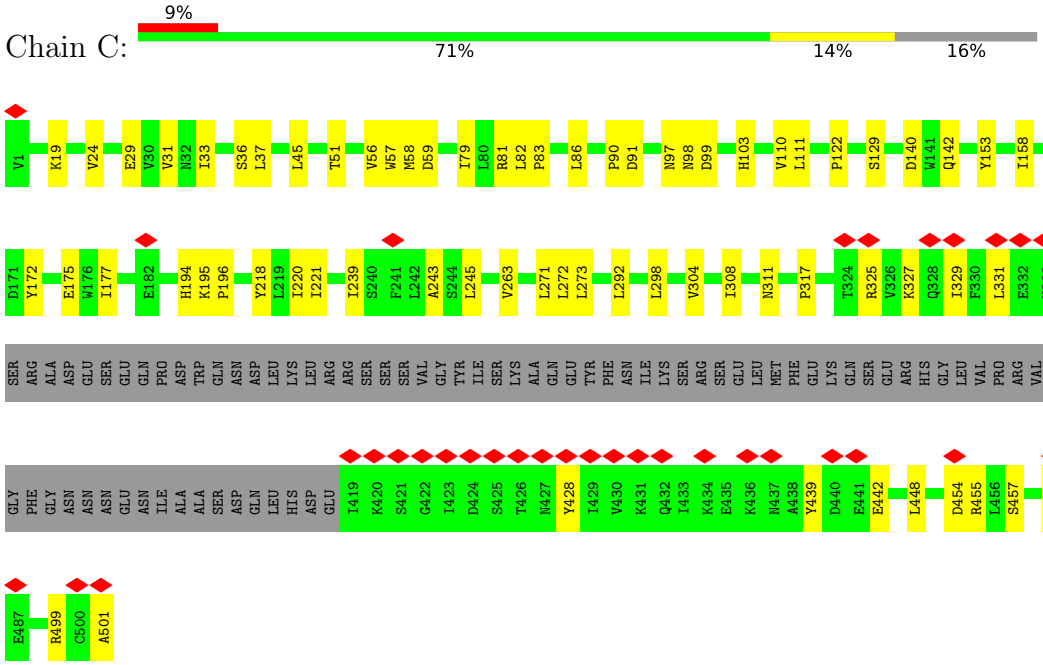
• Molecule 2: Acetylcholine receptor subunit beta

Chain B:



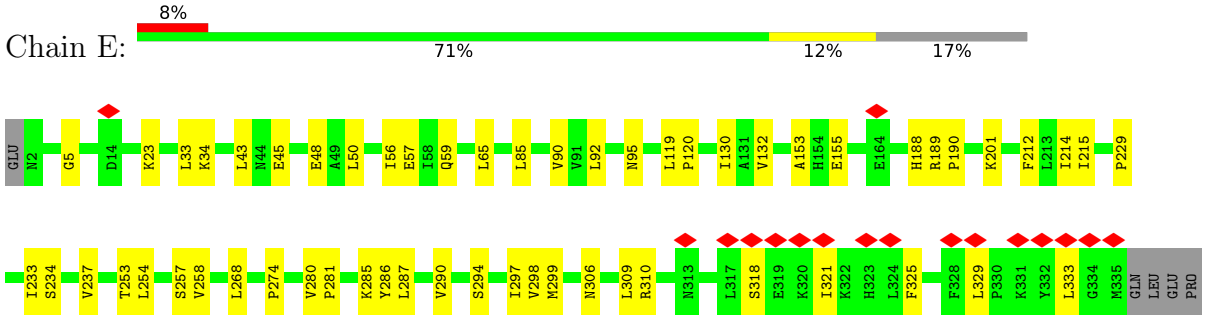
• Molecule 3: Acetylcholine receptor subunit delta

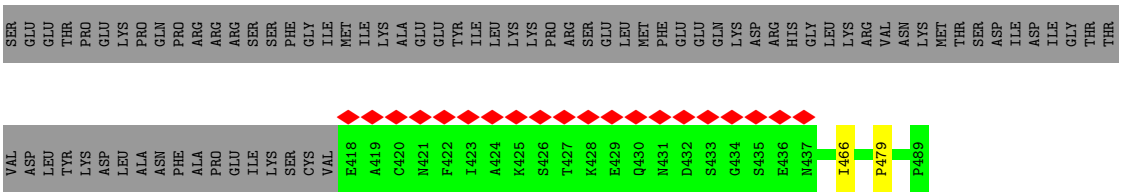
Chain C:



• Molecule 4: Acetylcholine receptor subunit gamma

Chain E:



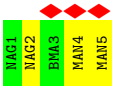


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

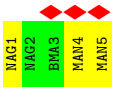
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



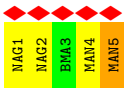
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:

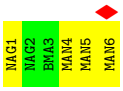


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

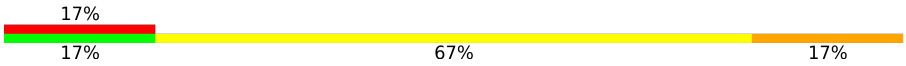
• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

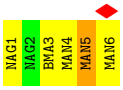
Chain K:



• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70577	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.503	Depositor
Minimum map value	-1.066	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	291.104, 291.104, 291.104	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, NCT, BMA, MAN, 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	0.28	0/3262	0.48	0/4447
1	D	0.30	0/3092	0.49	1/4222 (0.0%)
2	B	0.27	0/3325	0.47	0/4542
3	C	0.27	0/3525	0.45	0/4813
4	E	0.30	0/3384	0.47	0/4617
All	All	0.28	0/16588	0.47	1/22641 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	405	VAL	O-C-N	-5.93	113.22	122.70

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	3173	0	3201	66	0
1	D	3010	0	3033	75	0
2	B	3239	0	3252	57	0
3	C	3430	0	3419	56	0
4	E	3297	0	3295	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	83	0	70	0	0
6	G	61	0	52	2	0
6	H	61	0	52	1	0
6	I	61	0	52	2	0
7	J	28	0	25	0	0
8	K	72	0	61	1	0
8	L	72	0	61	2	0
9	A	12	0	14	0	0
9	D	12	0	14	2	0
10	A	123	0	162	10	0
10	B	41	0	54	1	0
10	C	79	0	103	2	0
10	D	66	0	80	7	0
10	E	92	0	104	3	0
11	E	14	0	13	0	0
12	C	1	0	0	0	0
12	E	1	0	0	0	0
All	All	17028	0	17117	287	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 8.

All (287) 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)
3:C:273:LEU:HD11	1:D:258:LEU:CD2	1.97	0.94
3:C:273:LEU:HD11	1:D:258:LEU:HD21	1.54	0.90
2:B:332:ILE:HG22	2:B:332:ILE:O	1.72	0.88
2:B:194:ARG:HH22	6:G:2:NAG:H2	1.43	0.84
3:C:298:LEU:HD23	3:C:465:MET:HG3	1.60	0.83
3:C:82:LEU:O	3:C:110:VAL:HG12	1.81	0.80
1:D:130:ILE:HD11	1:D:265:PRO:HG3	1.65	0.79
4:E:233:ILE:HG22	4:E:258:VAL:HG13	1.65	0.79
1:A:243:MET:O	1:A:247:ILE:HG12	1.83	0.78
1:D:277:TYR:HB2	10:D:603:POV:H27A	1.64	0.77
3:C:51:THR:HG23	3:C:98:ASN:HD22	1.51	0.75
1:A:19:ILE:HG12	4:E:5:GLY:HA2	1.72	0.72
3:C:455:ARG:HH12	10:D:602:POV:H13	1.55	0.72
4:E:237:VAL:HG22	4:E:258:VAL:HG11	1.70	0.72
2:B:92:LEU:O	2:B:95:ASN:ND2	2.21	0.71
2:B:241:LEU:O	2:B:248:LYS:NZ	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:286:TYR:HB2	4:E:466:ILE:HG21	1.71	0.71
3:C:37:LEU:HD11	3:C:56:VAL:HB	1.73	0.70
3:C:196:PRO:HD2	3:C:218:TYR:HB2	1.72	0.70
2:B:265:LEU:HD12	3:C:272:LEU:HD13	1.72	0.69
2:B:332:ILE:HD11	2:B:437:ARG:CB	2.22	0.69
3:C:243:ALA:HB2	3:C:263:VAL:HG11	1.75	0.68
4:E:92:LEU:O	4:E:95:ASN:ND2	2.27	0.67
1:A:247:ILE:HD11	4:E:254:LEU:HD13	1.78	0.66
3:C:448:LEU:HD21	1:D:305:THR:HG21	1.76	0.66
1:A:237:THR:HA	1:A:242:LYS:HD2	1.77	0.66
10:C:601:POV:H33	10:C:601:POV:H28	1.76	0.65
1:A:107:LYS:HB2	2:B:150:THR:HG21	1.77	0.65
1:A:151:TYR:HB3	1:A:155:LYS:HB2	1.78	0.65
2:B:332:ILE:O	2:B:332:ILE:CG2	2.44	0.64
2:B:45:GLU:HB3	2:B:271:PRO:HG3	1.78	0.64
4:E:57:GLU:OE2	4:E:59:GLN:NE2	2.30	0.64
2:B:133:MET:O	2:B:134:TYR:HB2	1.97	0.64
1:D:91:VAL:HG13	1:D:100:PHE:HB3	1.79	0.64
3:C:97:ASN:ND2	3:C:99:ASP:O	2.31	0.63
10:C:602:POV:H27	10:C:602:POV:H36	1.81	0.63
4:E:237:VAL:HG12	4:E:297:ILE:HD12	1.80	0.63
2:B:332:ILE:HD11	2:B:437:ARG:HB3	1.80	0.62
1:D:416:LEU:O	1:D:420:ILE:HG23	1.99	0.62
1:A:91:VAL:HG13	1:A:100:PHE:HB3	1.80	0.62
2:B:319:ARG:HG3	2:B:323:ILE:HD12	1.81	0.62
2:B:322:PHE:HA	2:B:326:LEU:HD23	1.81	0.62
1:A:313:ARG:HG3	1:A:317:ILE:HD12	1.82	0.62
2:B:194:ARG:NH2	6:G:2:NAG:O7	2.31	0.62
1:D:274:ILE:HD13	10:D:603:POV:H35A	1.81	0.62
1:D:303:PRO:HB3	1:D:395:ALA:HB3	1.82	0.61
1:D:130:ILE:HD11	1:D:265:PRO:CG	2.31	0.61
1:A:246:SER:HB3	1:A:289:ILE:HG12	1.82	0.60
1:D:235:LEU:HD12	1:D:236:PRO:HD2	1.83	0.60
2:B:41:LEU:HB2	2:B:51:THR:HG23	1.82	0.60
1:D:79:ARG:NH1	4:E:155:GLU:OE2	2.34	0.59
1:A:35:LEU:HD21	1:A:144:MET:CE	2.32	0.59
1:D:151:TYR:HB3	1:D:155:LYS:HB2	1.84	0.59
1:A:89:ASP:OD2	1:A:150:THR:OG1	2.20	0.59
1:A:420:ILE:HD11	10:A:604:POV:H27	1.85	0.59
3:C:271:LEU:HA	3:C:292:LEU:HD13	1.83	0.59
1:A:420:ILE:O	1:A:424:SER:OG	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:VAL:HG22	1:D:245:LEU:HD11	1.84	0.58
1:A:144:MET:HE2	1:A:205:PHE:HE1	1.69	0.58
2:B:136:PRO:HD3	2:B:280:ILE:HB	1.85	0.57
1:A:35:LEU:HD11	1:A:54:VAL:HB	1.87	0.57
1:A:152:ASP:OD2	1:A:154:THR:OG1	2.20	0.57
4:E:188:HIS:HB2	4:E:214:ILE:HD12	1.85	0.57
1:A:320:ILE:HG21	1:A:409:ILE:HD11	1.87	0.57
4:E:306:ASN:OD1	4:E:310:ARG:NH2	2.31	0.57
1:A:253:LEU:HD12	1:A:285:VAL:HG21	1.86	0.57
3:C:327:LYS:O	3:C:331:LEU:HB2	2.05	0.56
1:D:138:ASP:OD2	1:D:140:GLN:NE2	2.37	0.56
1:A:82:SER:HB2	1:A:87:LEU:HD11	1.87	0.56
4:E:153:ALA:HB3	4:E:201:LYS:HB2	1.88	0.56
10:A:603:POV:H33	2:B:304:LEU:HD11	1.87	0.56
2:B:317:TRP:O	2:B:321:ILE:HG22	2.05	0.56
4:E:229:PRO:O	4:E:233:ILE:HG12	2.04	0.56
3:C:273:LEU:CD1	1:D:258:LEU:HD21	2.33	0.56
3:C:51:THR:CG2	3:C:98:ASN:HD22	2.16	0.56
3:C:37:LEU:CD1	3:C:56:VAL:HB	2.34	0.56
1:D:192:CYS:SG	1:D:193:CYS:N	2.79	0.56
3:C:37:LEU:HD11	3:C:56:VAL:CB	2.34	0.55
1:A:247:ILE:HG21	4:E:257:SER:CB	2.37	0.55
3:C:457:SER:HA	3:C:460:ILE:HG22	1.88	0.55
3:C:31:VAL:HB	3:C:158:ILE:HG22	1.87	0.55
1:D:302:SER:OG	1:D:305:THR:OG1	2.20	0.55
4:E:280:VAL:O	4:E:285:LYS:NZ	2.29	0.55
1:A:250:LEU:HD21	4:E:233:ILE:HD12	1.89	0.55
1:D:232:VAL:HG21	1:D:246:SER:OG	2.07	0.54
3:C:175:GLU:OE1	3:C:499:ARG:NH2	2.40	0.54
1:A:44:ASP:OD2	1:A:47:ASN:ND2	2.39	0.54
1:A:192:CYS:SG	1:A:193:CYS:N	2.81	0.54
2:B:332:ILE:HD11	2:B:437:ARG:HG2	1.88	0.54
2:B:94:ASN:ND2	2:B:143:THR:O	2.39	0.54
4:E:318:SER:HB3	4:E:321:ILE:HD12	1.89	0.54
2:B:332:ILE:HD11	2:B:437:ARG:CG	2.38	0.54
1:A:212:LEU:HB3	2:B:274:SER:HB3	1.90	0.54
1:A:258:LEU:HD12	4:E:268:LEU:HB2	1.89	0.53
1:A:311:TRP:O	1:A:315:ILE:HG22	2.08	0.53
1:A:237:THR:HG21	1:A:299:HIS:CG	2.44	0.53
3:C:51:THR:HG23	3:C:98:ASN:ND2	2.19	0.53
1:A:302:SER:HB3	1:A:305:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:THR:HG21	8:K:1:NAG:H62	1.90	0.53
3:C:273:LEU:HD11	1:D:258:LEU:HD23	1.86	0.53
1:D:277:TYR:HB2	10:D:603:POV:C27	2.34	0.53
3:C:194:HIS:HB2	3:C:220:ILE:HD12	1.91	0.53
1:D:232:VAL:HG22	1:D:245:LEU:CD1	2.37	0.53
3:C:98:ASN:OD1	3:C:129:SER:HB3	2.09	0.53
3:C:220:ILE:HD13	6:H:1:NAG:H82	1.91	0.53
1:A:35:LEU:CD2	1:A:144:MET:HE3	2.39	0.52
1:A:35:LEU:HD21	1:A:144:MET:HE1	1.91	0.52
4:E:189:ARG:O	4:E:189:ARG:HG3	2.10	0.52
1:D:244:THR:HG21	4:E:253:THR:HG22	1.90	0.52
1:D:313:ARG:HG3	1:D:317:ILE:HD12	1.91	0.52
1:A:235:LEU:HD12	1:A:236:PRO:HD2	1.90	0.52
1:D:21:PRO:HD2	1:D:29:VAL:HG21	1.91	0.52
3:C:91:ASP:OD1	3:C:103:HIS:CE1	2.63	0.52
2:B:189:GLU:HG3	2:B:463:PRO:HG3	1.92	0.52
1:A:247:ILE:HD11	4:E:254:LEU:CD1	2.40	0.51
1:A:291:ILE:HG21	1:A:410:LEU:HG	1.93	0.51
2:B:283:TYR:HB2	2:B:454:ILE:HG21	1.92	0.51
3:C:140:ASP:OD2	3:C:142:GLN:NE2	2.44	0.51
1:D:236:PRO:HG2	4:E:309:LEU:HD12	1.93	0.51
2:B:135:PHE:CE1	2:B:270:VAL:HG12	2.46	0.50
1:A:225:PHE:HB3	1:A:249:VAL:HG13	1.93	0.50
2:B:297:LEU:HD12	2:B:443:PHE:HE1	1.76	0.50
1:A:89:ASP:OD1	1:A:89:ASP:N	2.43	0.50
1:A:93:TYR:HE1	1:A:147:GLY:HA3	1.77	0.50
3:C:83:PRO:HD2	3:C:86:LEU:HD12	1.93	0.49
1:D:242:LYS:HE3	1:D:292:THR:HG23	1.94	0.49
1:D:234:TYR:O	4:E:306:ASN:ND2	2.39	0.49
1:D:411:LEU:O	1:D:415:MET:HG3	2.13	0.49
4:E:65:LEU:HD11	4:E:85:LEU:HD22	1.95	0.49
3:C:79:ILE:HD11	3:C:111:LEU:HD23	1.93	0.49
3:C:304:VAL:O	3:C:308:ILE:HG12	2.12	0.49
4:E:56:ILE:O	4:E:120:PRO:HD2	2.13	0.49
1:D:89:ASP:OD1	1:D:89:ASP:N	2.42	0.49
1:A:419:ILE:HG13	1:A:420:ILE:N	2.27	0.49
4:E:45:GLU:HB3	4:E:274:PRO:HD3	1.94	0.49
1:D:225:PHE:HB3	1:D:249:VAL:HG13	1.95	0.49
3:C:245:LEU:HD21	1:D:290:ILE:HA	1.95	0.49
4:E:45:GLU:O	4:E:274:PRO:HB3	2.12	0.49
4:E:48:GLU:HG2	4:E:130:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:O	1:D:120:PRO:HD2	2.12	0.48
1:D:215:VAL:HG22	1:D:219:ILE:HD12	1.95	0.48
2:B:303:ASN:O	2:B:307:ARG:HG3	2.13	0.48
1:D:228:LEU:HD23	1:D:231:LEU:HD12	1.95	0.48
3:C:58:MET:O	3:C:122:PRO:HD2	2.13	0.48
1:A:281:THR:O	1:A:285:VAL:HG23	2.13	0.48
3:C:317:PRO:HD3	3:C:442:GLU:HG2	1.95	0.48
2:B:309:PRO:HG3	2:B:424:LEU:HB2	1.95	0.48
4:E:132:VAL:O	4:E:281:PRO:HA	2.14	0.48
1:D:239:SER:HB3	4:E:309:LEU:HD11	1.96	0.48
1:A:177:VAL:HG13	1:A:208:GLN:HB3	1.96	0.48
2:B:2:VAL:HG13	2:B:5:ASP:H	1.78	0.48
1:A:232:VAL:HG23	1:A:245:LEU:HD23	1.96	0.48
3:C:36:SER:HB3	3:C:59:ASP:HB3	1.96	0.48
6:I:1:NAG:H61	6:I:2:NAG:O5	2.14	0.48
4:E:190:PRO:HG3	4:E:479:PRO:HB3	1.96	0.47
10:D:603:POV:H3	10:D:603:POV:O12	2.14	0.47
1:A:144:MET:CE	1:A:205:PHE:HE1	2.26	0.47
3:C:317:PRO:HG2	3:C:439:TYR:CE1	2.49	0.47
1:D:417:ILE:O	1:D:420:ILE:HG12	2.14	0.47
2:B:42:ILE:HB	2:B:51:THR:HG22	1.95	0.47
2:B:48:GLU:HG2	2:B:130:ILE:HG12	1.95	0.47
2:B:190:HIS:HB2	2:B:212:ILE:HD12	1.97	0.47
1:D:422:THR:O	1:D:425:VAL:HG12	2.14	0.47
4:E:190:PRO:HG2	4:E:212:PHE:HB2	1.95	0.47
3:C:24:VAL:CG2	3:C:29:GLU:HB2	2.45	0.47
3:C:239:ILE:HG22	3:C:263:VAL:HG13	1.96	0.47
3:C:325:ARG:O	3:C:329:ILE:HG12	2.15	0.47
1:D:237:THR:HA	1:D:242:LYS:HD2	1.96	0.47
1:D:301:ARG:HH12	10:D:602:POV:H1	1.78	0.47
1:D:303:PRO:HG3	1:D:396:ALA:HB2	1.95	0.47
2:B:79:ARG:HD2	3:C:153:TYR:HA	1.97	0.47
2:B:201:ASP:OD1	2:B:201:ASP:N	2.48	0.47
1:A:417:ILE:HD12	10:A:604:POV:H211	1.96	0.47
3:C:81:ARG:HD2	1:D:151:TYR:CE2	2.50	0.47
1:A:277:TYR:CE1	1:A:422:THR:HG22	2.50	0.46
1:D:236:PRO:CG	4:E:309:LEU:HD12	2.44	0.46
10:D:603:POV:H15A	10:D:603:POV:H11	1.53	0.46
10:A:602:POV:H28A	10:A:602:POV:H211	1.74	0.46
3:C:33:ILE:HD12	3:C:90:PRO:HG3	1.96	0.46
1:D:31:ILE:HB	1:D:158:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:234:SER:HA	4:E:237:VAL:HG23	1.97	0.46
1:A:268:SER:O	1:A:268:SER:OG	2.30	0.46
2:B:227:PRO:O	2:B:231:ILE:HG12	2.15	0.46
1:D:40:LEU:HD12	1:D:52:THR:HG22	1.97	0.46
1:A:51:GLU:HA	1:A:124:PHE:O	2.15	0.46
1:A:277:TYR:HE1	1:A:422:THR:HG22	1.80	0.46
4:E:325:PHE:HA	4:E:329:LEU:HD23	1.97	0.46
1:A:111:ASP:OD1	1:A:113:THR:OG1	2.26	0.45
2:B:279:ILE:HD13	2:B:458:ALA:HB2	1.98	0.45
3:C:177:ILE:HB	3:C:195:LYS:HB2	1.98	0.45
1:D:174:GLY:O	1:D:210:ILE:HD12	2.16	0.45
1:A:65:LEU:HB3	1:A:110:LEU:HD21	1.97	0.45
2:B:92:LEU:HD21	2:B:126:SER:HB3	1.99	0.45
2:B:320:GLN:O	2:B:324:GLU:HB2	2.16	0.45
1:D:311:TRP:O	1:D:315:ILE:HG12	2.17	0.45
4:E:237:VAL:CG2	4:E:258:VAL:HG11	2.45	0.45
2:B:95:ASN:HA	2:B:126:SER:HA	1.98	0.45
1:D:51:GLU:HA	1:D:124:PHE:O	2.16	0.45
1:D:228:LEU:HA	1:D:231:LEU:HD12	1.99	0.45
1:D:298:THR:HA	1:D:301:ARG:HG2	1.98	0.45
1:A:178:MET:SD	1:A:207:MET:HG2	2.57	0.45
2:B:321:ILE:HG23	2:B:322:PHE:N	2.32	0.45
1:D:82:SER:HB2	1:D:87:LEU:HD11	1.98	0.45
1:A:56:LEU:O	1:A:120:PRO:HD2	2.17	0.44
1:A:410:LEU:HD12	1:A:414:PHE:CE1	2.53	0.44
2:B:177:LYS:HB2	2:B:177:LYS:HE2	1.74	0.44
2:B:416:GLU:OE1	3:C:428:TYR:OH	2.21	0.44
2:B:242:PRO:HG3	3:C:311:ASN:HA	1.99	0.44
3:C:273:LEU:CD1	1:D:258:LEU:CD2	2.85	0.44
10:A:603:POV:H28A	10:A:603:POV:H21A	1.76	0.44
1:D:237:THR:HG23	1:D:296:ILE:HG12	2.00	0.44
1:A:231:LEU:HD22	2:B:296:ILE:HG12	1.99	0.44
2:B:206:ASP:OD1	2:B:208:THR:OG1	2.35	0.43
1:A:282:MET:O	1:A:286:ILE:HG12	2.18	0.43
4:E:43:LEU:HD12	4:E:50:LEU:HD13	2.00	0.43
1:D:258:LEU:O	1:D:262:GLU:HG2	2.18	0.43
1:D:136:PRO:O	1:D:209:ARG:HD2	2.18	0.43
2:B:138:ASP:OD1	2:B:138:ASP:N	2.50	0.43
1:A:111:ASP:OD2	1:A:115:LYS:HB3	2.19	0.43
2:B:173:ILE:HB	2:B:191:LYS:HB2	2.00	0.43
1:D:182:ARG:HH11	1:D:182:ARG:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:PRO:HD3	2:B:86:TRP:CD2	2.54	0.43
2:B:42:ILE:HD12	2:B:51:THR:HG21	2.00	0.43
1:D:281:THR:O	1:D:285:VAL:HG23	2.18	0.43
1:D:382:ILE:O	1:D:386:MET:HG3	2.19	0.43
4:E:294:SER:O	4:E:298:VAL:HG23	2.18	0.43
1:A:40:LEU:HD12	1:A:52:THR:HG22	2.00	0.43
2:B:297:LEU:HD12	2:B:443:PHE:CE1	2.54	0.43
10:A:603:POV:H35	10:A:603:POV:H38A	1.38	0.42
2:B:56:LEU:O	2:B:120:PRO:HD2	2.19	0.42
10:A:603:POV:H37	10:A:603:POV:H31A	1.73	0.42
3:C:81:ARG:NE	1:D:150:THR:O	2.48	0.42
10:E:504:POV:H11A	10:E:504:POV:H14A	1.82	0.42
10:A:604:POV:H15A	10:A:604:POV:H11A	1.73	0.42
3:C:57:TRP:CH2	9:D:601:NCT:HC81	2.55	0.42
3:C:57:TRP:NE1	1:D:149:TRP:HH2	2.17	0.42
2:B:43:LEU:HD22	2:B:186:TRP:CZ2	2.54	0.42
1:D:404:MET:CE	1:D:408:HIS:CE1	3.03	0.42
4:E:57:GLU:HB2	4:E:119:LEU:HD13	2.00	0.42
1:A:35:LEU:CD2	1:A:144:MET:CE	2.97	0.42
1:A:43:VAL:HG22	1:A:50:VAL:HG22	2.02	0.42
1:A:237:THR:CG2	1:A:299:HIS:CG	3.03	0.42
10:A:604:POV:H211	10:A:604:POV:H28	1.69	0.42
2:B:51:THR:HA	2:B:124:TYR:O	2.19	0.42
1:A:283:ILE:HG23	10:E:503:POV:H37A	2.01	0.42
1:A:247:ILE:CG2	4:E:257:SER:HB3	2.50	0.41
10:B:501:POV:H37A	10:B:501:POV:H310	1.70	0.41
1:D:271:VAL:HB	1:D:276:LYS:HE3	2.01	0.41
6:I:2:NAG:H62	6:I:5:MAN:H2	2.02	0.41
1:A:144:MET:HE2	1:A:205:PHE:CE1	2.51	0.41
1:D:416:LEU:O	1:D:419:ILE:HG13	2.19	0.41
10:E:503:POV:H3A	10:E:503:POV:H32A	1.81	0.41
2:B:253:ILE:O	2:B:257:LEU:HG	2.20	0.41
3:C:172:TYR:HB3	3:C:501:ALA:HB3	2.01	0.41
1:D:41:ILE:HB	1:D:51:GLU:HG3	2.01	0.41
1:A:156:VAL:HG12	1:A:156:VAL:O	2.20	0.41
3:C:45:LEU:HD22	3:C:221:ILE:HD11	2.02	0.41
1:D:253:LEU:HD12	1:D:285:VAL:HG21	2.02	0.41
1:D:291:ILE:HG21	1:D:410:LEU:HG	2.02	0.41
1:D:295:VAL:HG11	1:D:407:ASP:OD1	2.20	0.41
4:E:23:LYS:HD2	4:E:23:LYS:HA	1.93	0.41
4:E:287:LEU:HA	4:E:290:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:5:MAN:O6	8:L:5:MAN:O4	2.29	0.41
3:C:81:ARG:HA	3:C:110:VAL:O	2.21	0.41
4:E:33:LEU:HD21	4:E:90:VAL:HG11	2.01	0.41
1:A:283:ILE:HD12	10:A:604:POV:H32	2.03	0.41
1:D:156:VAL:HG12	1:D:156:VAL:O	2.21	0.41
1:D:312:VAL:HG23	1:D:316:PHE:HD2	1.85	0.41
4:E:214:ILE:HD13	8:L:1:NAG:H82	2.03	0.41
1:A:90:LEU:HA	1:A:147:GLY:O	2.21	0.41
1:D:312:VAL:HG23	1:D:316:PHE:CD2	2.56	0.41
4:E:34:LYS:HB3	4:E:57:GLU:HB3	2.03	0.41
1:D:55:ARG:HB3	1:D:119:THR:HG22	2.02	0.40
1:D:409:ILE:HD13	1:D:409:ILE:HA	1.92	0.40
2:B:234:LEU:O	2:B:238:VAL:HG23	2.21	0.40
3:C:37:LEU:HD11	3:C:56:VAL:CG1	2.51	0.40
3:C:57:TRP:CZ3	9:D:601:NCT:HC81	2.57	0.40
4:E:56:ILE:HG23	4:E:120:PRO:HG2	2.03	0.40
2:B:231:ILE:HG21	2:B:259:VAL:HG23	2.03	0.40
3:C:19:LYS:HB2	3:C:19:LYS:HE2	1.93	0.40
3:C:298:LEU:HD12	3:C:298:LEU:HA	1.79	0.40
1:A:77:LYS:HB3	1:A:109:LEU:HD11	2.03	0.40
1:A:224:LEU:O	1:A:228:LEU:HG	2.21	0.40
2:B:173:ILE:HD11	2:B:209:PHE:HB3	2.04	0.40
1:D:59:GLN:HA	1:D:116:ILE:O	2.21	0.40
1:D:404:MET:HE2	1:D:408:HIS:CE1	2.56	0.40
4:E:43:LEU:HD13	4:E:215:ILE:HD11	2.04	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	387/437 (89%)	375 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	367/437 (84%)	356 (97%)	11 (3%)	0	100	100
2	B	395/469 (84%)	379 (96%)	16 (4%)	0	100	100
3	C	419/501 (84%)	405 (97%)	14 (3%)	0	100	100
4	E	402/489 (82%)	383 (95%)	19 (5%)	0	100	100
All	All	1970/2333 (84%)	1898 (96%)	72 (4%)	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	364/405 (90%)	362 (100%)	2 (0%)	88	96
1	D	347/405 (86%)	344 (99%)	3 (1%)	78	92
2	B	368/431 (85%)	364 (99%)	4 (1%)	73	89
3	C	388/458 (85%)	387 (100%)	1 (0%)	92	97
4	E	369/446 (83%)	367 (100%)	2 (0%)	88	96
All	All	1836/2145 (86%)	1824 (99%)	12 (1%)	84	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ASP
1	A	407	ASP
2	B	84	ASP
2	B	124	TYR
2	B	136	PRO
2	B	200	ASP
3	C	454	ASP
1	D	89	ASP
1	D	423	VAL
1	D	425	VAL

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Mol	Chain	Res	Type
4	E	299	MET
4	E	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	98	ASN
3	C	103	HIS
1	D	408	HIS

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)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	F	1	5,1	14,14,15	0.35	0	17,19,21	0.47	0
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.52	0
5	BMA	F	3	5	11,11,12	0.54	0	15,15,17	0.75	0
5	MAN	F	4	5	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
5	MAN	F	5	5	11,11,12	0.54	0	15,15,17	1.01	2 (13%)
5	MAN	F	6	5	11,11,12	0.88	0	15,15,17	1.11	1 (6%)
5	MAN	F	7	5	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
6	NAG	G	1	2,6	14,14,15	0.20	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	G	2	6	14,14,15	0.30	0	17,19,21	0.53	0
6	BMA	G	3	6	11,11,12	0.53	0	15,15,17	0.71	0
6	MAN	G	4	6	11,11,12	0.74	0	15,15,17	1.03	2 (13%)
6	MAN	G	5	6	11,11,12	0.70	0	15,15,17	0.95	1 (6%)
6	NAG	H	1	3,6	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	H	2	6	14,14,15	0.19	0	17,19,21	0.55	0
6	BMA	H	3	6	11,11,12	0.56	0	15,15,17	0.82	0
6	MAN	H	4	6	11,11,12	0.70	0	15,15,17	0.91	1 (6%)
6	MAN	H	5	6	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
6	NAG	I	1	3,6	14,14,15	0.45	0	17,19,21	0.49	0
6	NAG	I	2	6	14,14,15	0.43	0	17,19,21	0.49	0
6	BMA	I	3	6	11,11,12	0.61	0	15,15,17	0.84	0
6	MAN	I	4	6	11,11,12	0.77	1 (9%)	15,15,17	1.21	2 (13%)
6	MAN	I	5	6	11,11,12	0.63	0	15,15,17	1.16	2 (13%)
7	NAG	J	1	3,7	14,14,15	1.17	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	J	2	7	14,14,15	0.39	0	17,19,21	0.40	0
8	NAG	K	1	8,1	14,14,15	0.42	0	17,19,21	0.52	0
8	NAG	K	2	8	14,14,15	0.28	0	17,19,21	0.52	0
8	BMA	K	3	8	11,11,12	0.54	0	15,15,17	0.82	0
8	MAN	K	4	8	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
8	MAN	K	5	8	11,11,12	0.85	1 (9%)	15,15,17	1.29	3 (20%)
8	MAN	K	6	8	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
8	NAG	L	1	4,8	14,14,15	0.31	0	17,19,21	0.48	0
8	NAG	L	2	8	14,14,15	0.22	0	17,19,21	0.48	0
8	BMA	L	3	8	11,11,12	0.58	0	15,15,17	0.93	1 (6%)
8	MAN	L	4	8	11,11,12	0.59	0	15,15,17	1.02	2 (13%)
8	MAN	L	5	8	11,11,12	0.73	0	15,15,17	1.33	2 (13%)
8	MAN	L	6	8	11,11,12	0.62	0	15,15,17	0.95	2 (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	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	2/2/19/22	0/1/1/1
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	0/2/19/22	0/1/1/1
6	NAG	H	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	1/2/19/22	0/1/1/1
6	MAN	H	5	6	-	1/2/19/22	0/1/1/1
6	NAG	I	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	1/2/19/22	0/1/1/1
7	NAG	J	1	3,7	-	1/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
8	NAG	K	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	2/2/19/22	0/1/1/1
8	MAN	K	4	8	-	1/2/19/22	0/1/1/1
8	MAN	K	5	8	-	0/2/19/22	0/1/1/1
8	MAN	K	6	8	-	0/2/19/22	0/1/1/1
8	NAG	L	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
8	BMA	L	3	8	-	0/2/19/22	0/1/1/1
8	MAN	L	4	8	-	2/2/19/22	0/1/1/1
8	MAN	L	5	8	-	1/2/19/22	0/1/1/1
8	MAN	L	6	8	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	1	NAG	O5-C1	-4.10	1.37	1.43
8	K	5	MAN	C1-C2	2.60	1.58	1.52
6	I	4	MAN	C1-C2	2.18	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	5	MAN	C1-O5-C5	3.62	117.10	112.19
6	I	4	MAN	C1-O5-C5	3.27	116.62	112.19
6	I	5	MAN	C1-O5-C5	3.08	116.37	112.19
8	K	5	MAN	C1-O5-C5	2.79	115.97	112.19
8	L	4	MAN	C1-O5-C5	2.56	115.66	112.19
5	F	6	MAN	O2-C2-C3	-2.54	105.05	110.14
5	F	5	MAN	C1-O5-C5	2.53	115.62	112.19
7	J	1	NAG	C4-C3-C2	2.49	114.66	111.02
8	K	5	MAN	O2-C2-C3	-2.34	105.46	110.14
8	K	4	MAN	O2-C2-C3	-2.33	105.47	110.14
5	F	4	MAN	O2-C2-C3	-2.33	105.47	110.14
6	H	5	MAN	C1-O5-C5	2.31	115.32	112.19
8	L	5	MAN	O2-C2-C3	-2.29	105.56	110.14
6	H	5	MAN	O2-C2-C3	-2.28	105.58	110.14
6	G	5	MAN	O2-C2-C3	-2.27	105.58	110.14
6	G	4	MAN	O2-C2-C3	-2.27	105.58	110.14
8	L	4	MAN	O2-C2-C3	-2.27	105.60	110.14
5	F	7	MAN	O2-C2-C3	-2.26	105.62	110.14
6	I	5	MAN	O2-C2-C3	-2.24	105.65	110.14
5	F	4	MAN	C1-O5-C5	2.24	115.22	112.19
8	K	6	MAN	O2-C2-C3	-2.22	105.70	110.14
8	L	6	MAN	O2-C2-C3	-2.21	105.72	110.14
6	I	4	MAN	O2-C2-C3	-2.20	105.73	110.14
6	G	4	MAN	C1-O5-C5	2.18	115.14	112.19
5	F	5	MAN	O2-C2-C3	-2.17	105.80	110.14
8	K	5	MAN	C1-C2-C3	2.16	112.32	109.67
6	H	4	MAN	O2-C2-C3	-2.14	105.86	110.14
8	K	4	MAN	C1-O5-C5	2.13	115.07	112.19
8	L	6	MAN	C1-O5-C5	2.07	115.00	112.19
8	L	3	BMA	C1-O5-C5	2.05	114.97	112.19
8	K	6	MAN	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	1	NAG	O5-C5-C6-O6
8	L	4	MAN	C4-C5-C6-O6
6	G	3	BMA	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	J	2	NAG	C4-C5-C6-O6
8	L	4	MAN	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
6	G	3	BMA	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
8	K	3	BMA	C4-C5-C6-O6
8	K	2	NAG	O5-C5-C6-O6
5	F	7	MAN	O5-C5-C6-O6
8	L	5	MAN	O5-C5-C6-O6
5	F	7	MAN	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
8	K	2	NAG	C4-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
8	K	3	BMA	O5-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
6	H	4	MAN	O5-C5-C6-O6
6	I	2	NAG	C1-C2-N2-C7
6	I	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
8	K	4	MAN	O5-C5-C6-O6
7	J	1	NAG	C1-C2-N2-C7
5	F	1	NAG	O5-C5-C6-O6
6	H	2	NAG	C3-C2-N2-C7
6	H	2	NAG	C1-C2-N2-C7

There are no ring outliers.

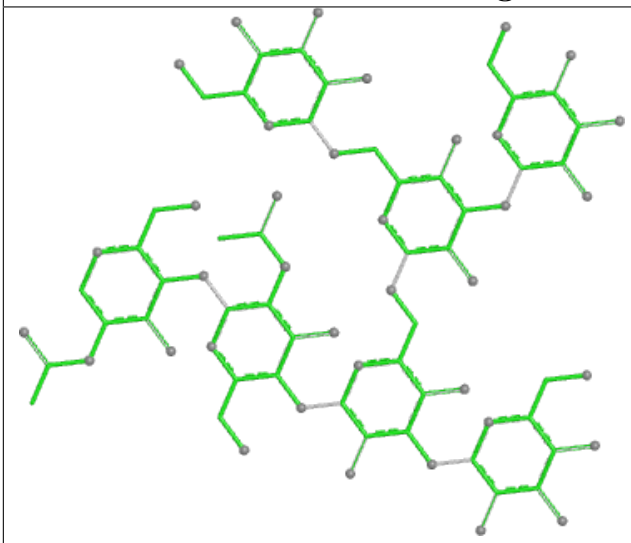
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	5	MAN	1	0
8	K	1	NAG	1	0
6	I	2	NAG	2	0
8	L	1	NAG	1	0
6	I	1	NAG	1	0
8	L	5	MAN	1	0
6	G	2	NAG	2	0
6	H	1	NAG	1	0

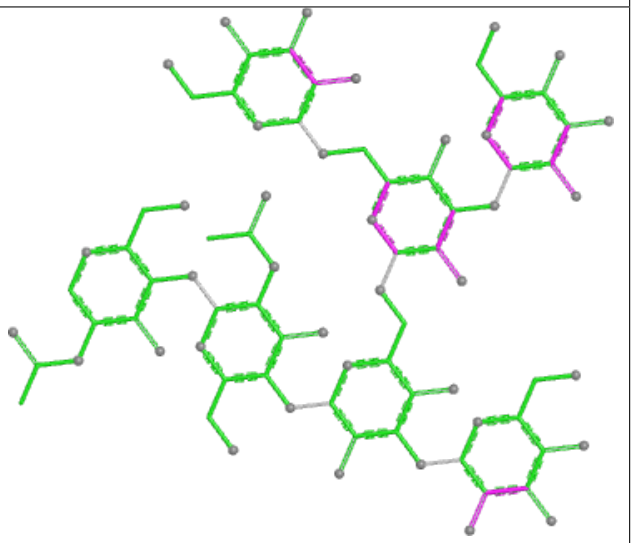
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

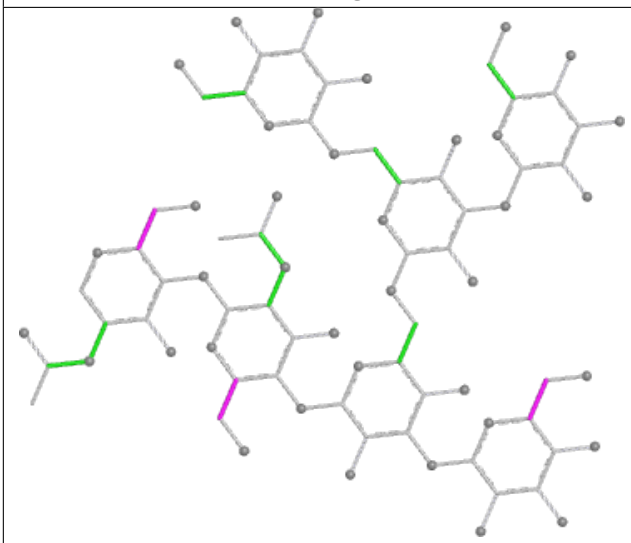
Oligosaccharide Chain F



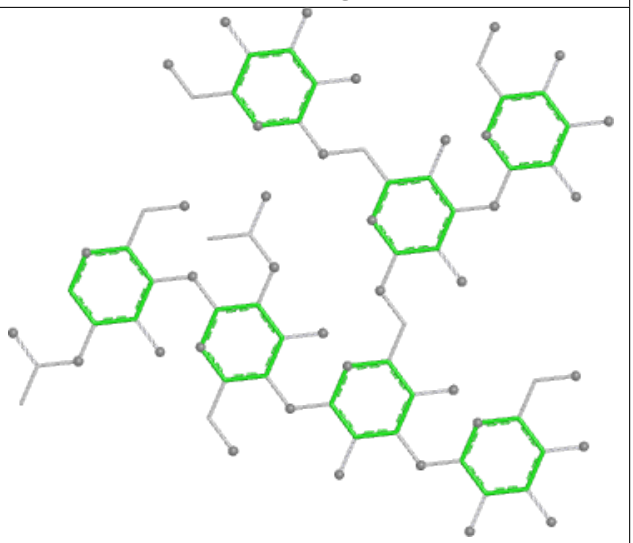
Bond lengths



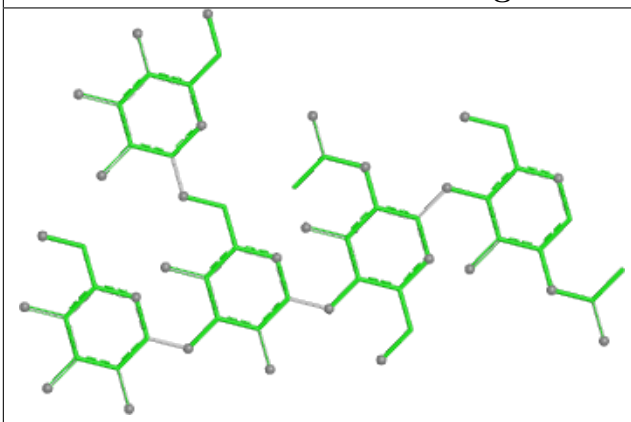
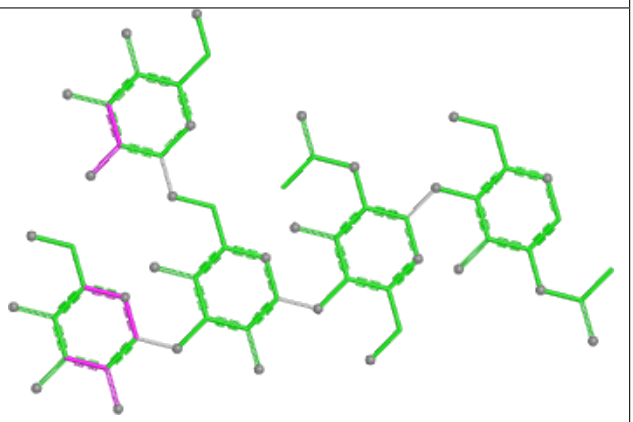
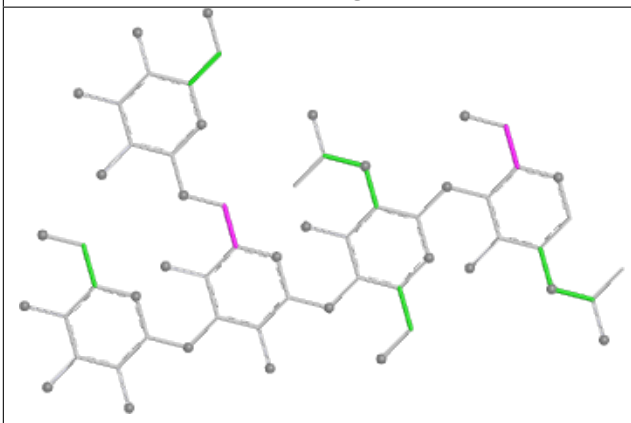
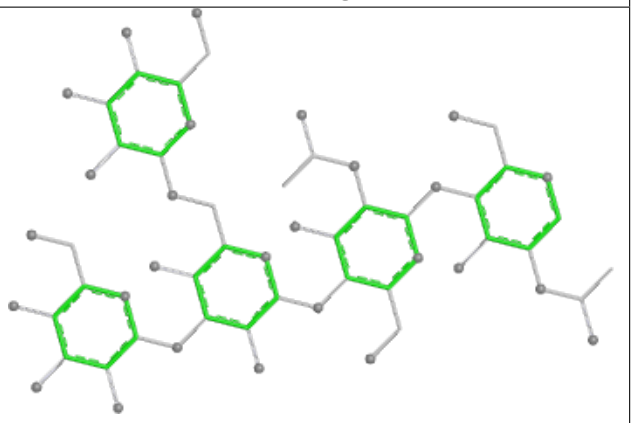
Bond angles

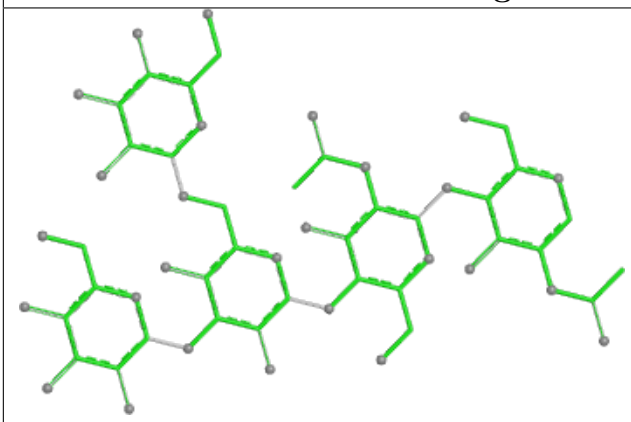
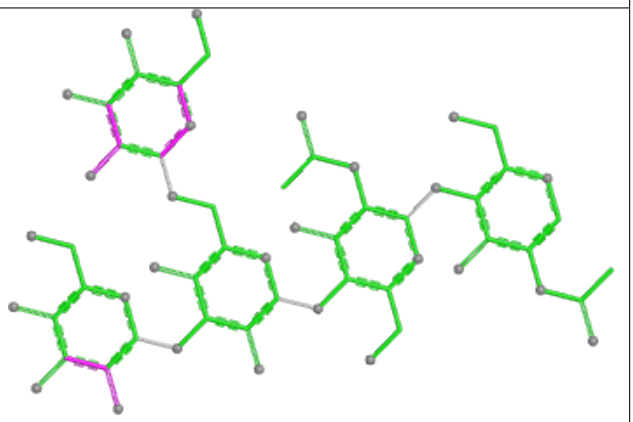
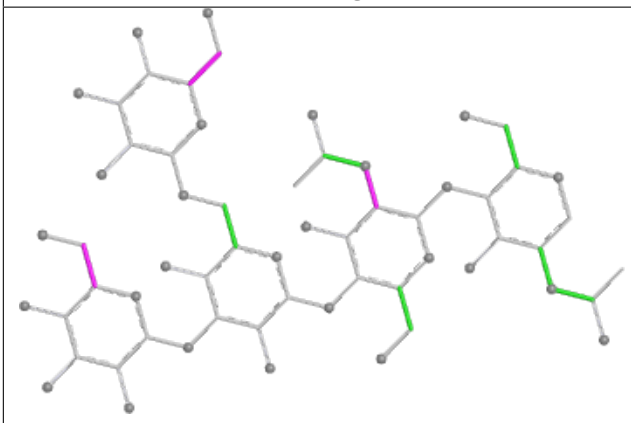
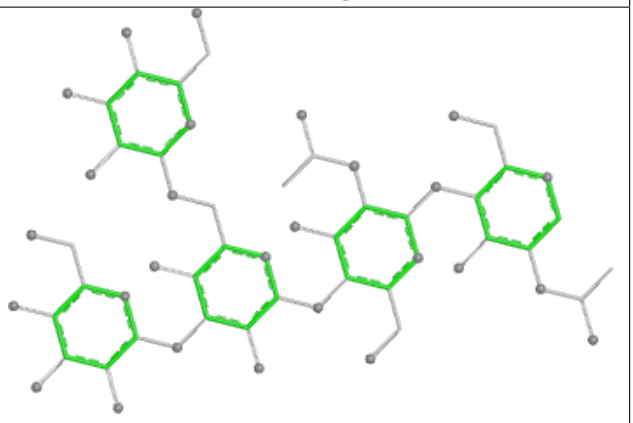


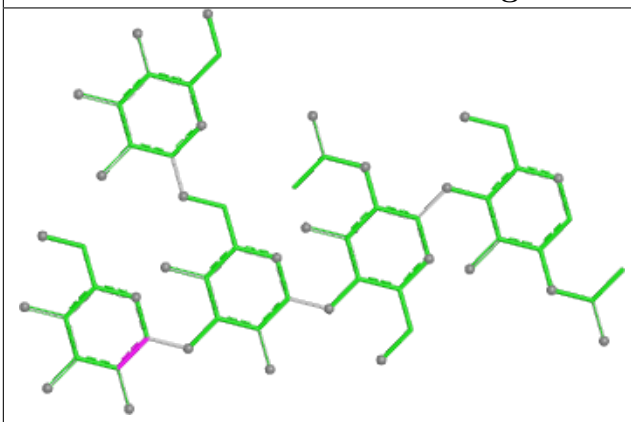
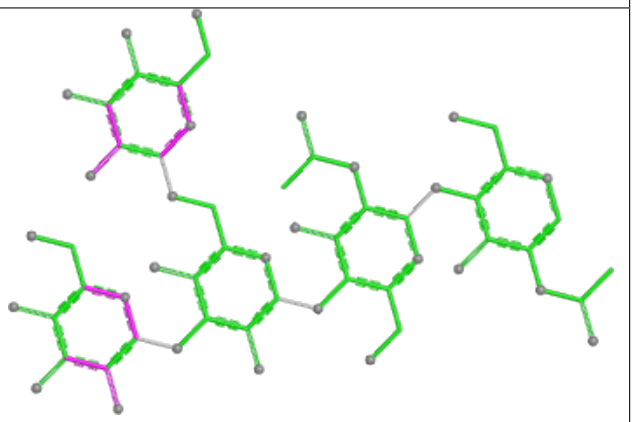
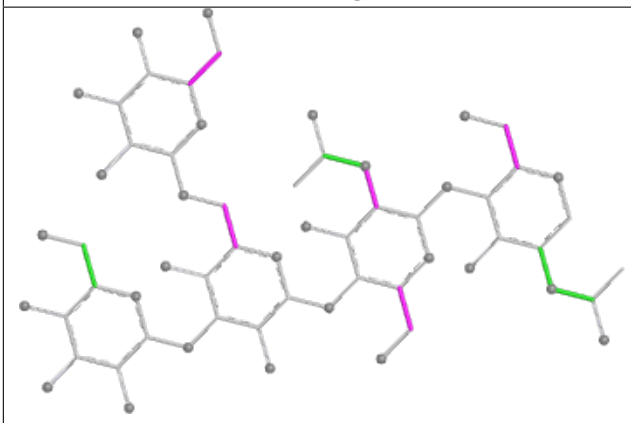
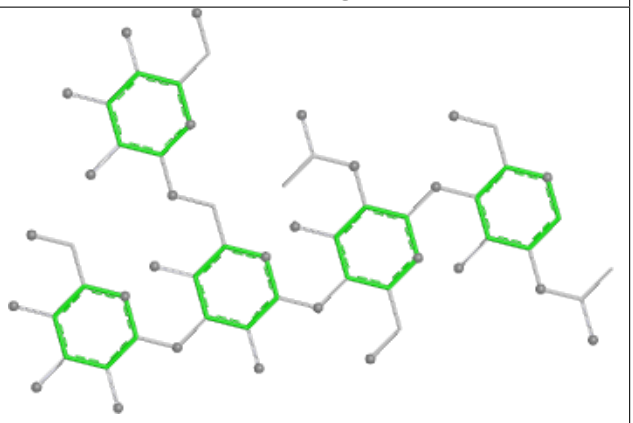
Torsions



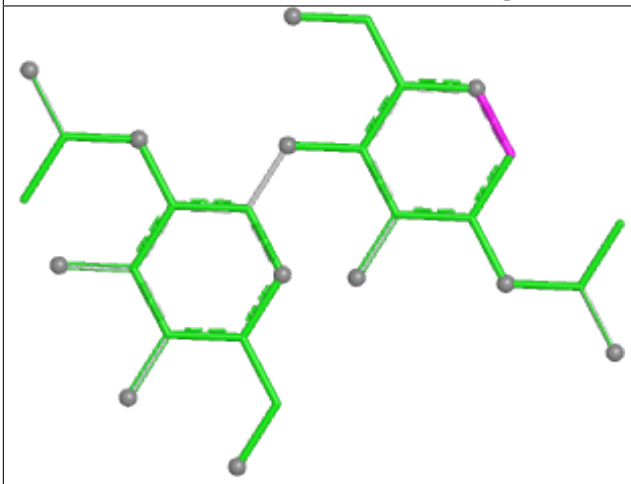
Rings

Oligosaccharide Chain G	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

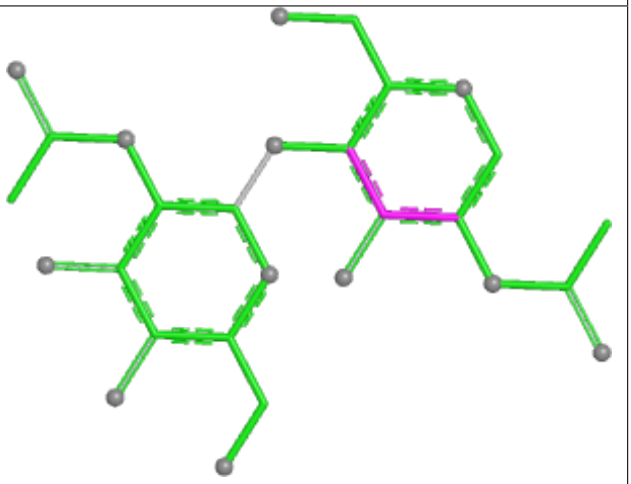
Oligosaccharide Chain H	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain I	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

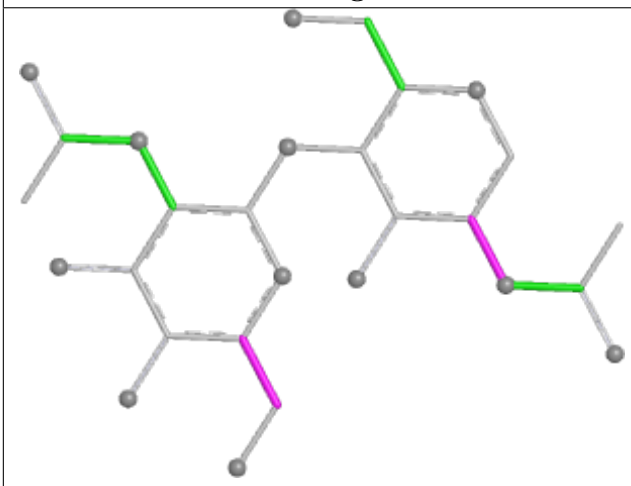
Oligosaccharide Chain J



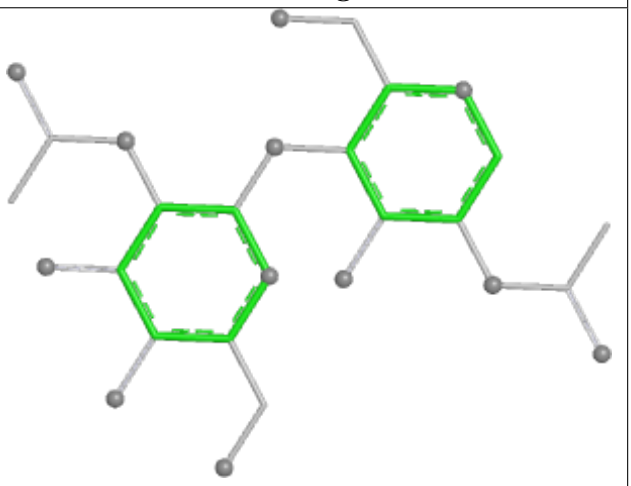
Bond lengths



Bond angles

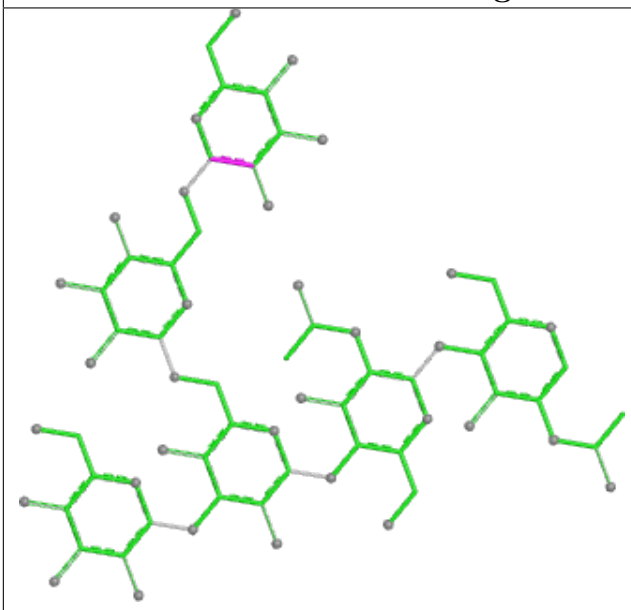


Torsions

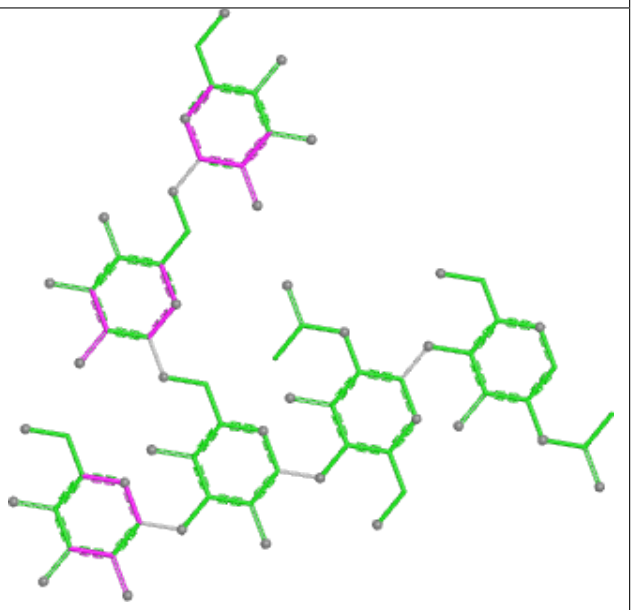


Rings

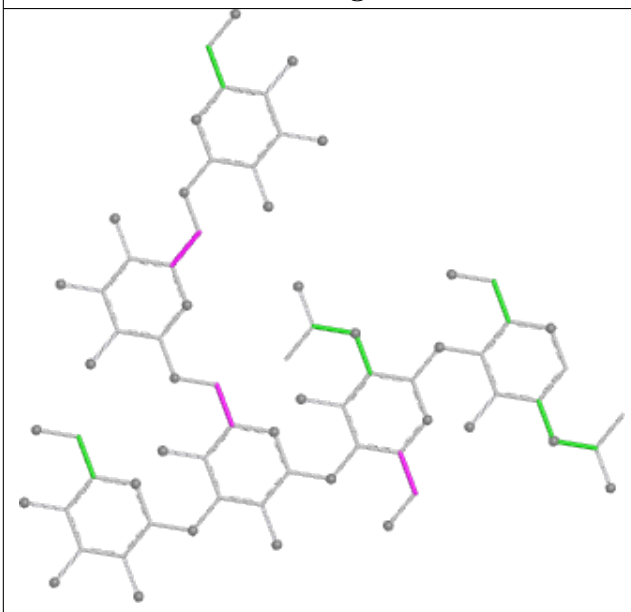
Oligosaccharide Chain K



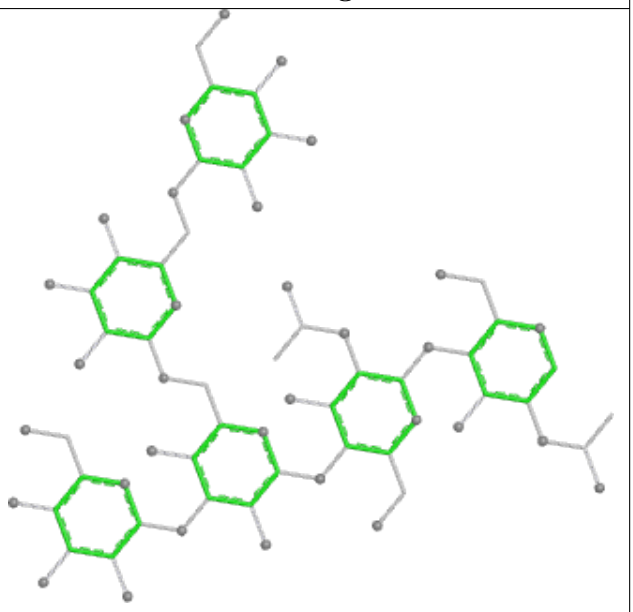
Bond lengths



Bond angles

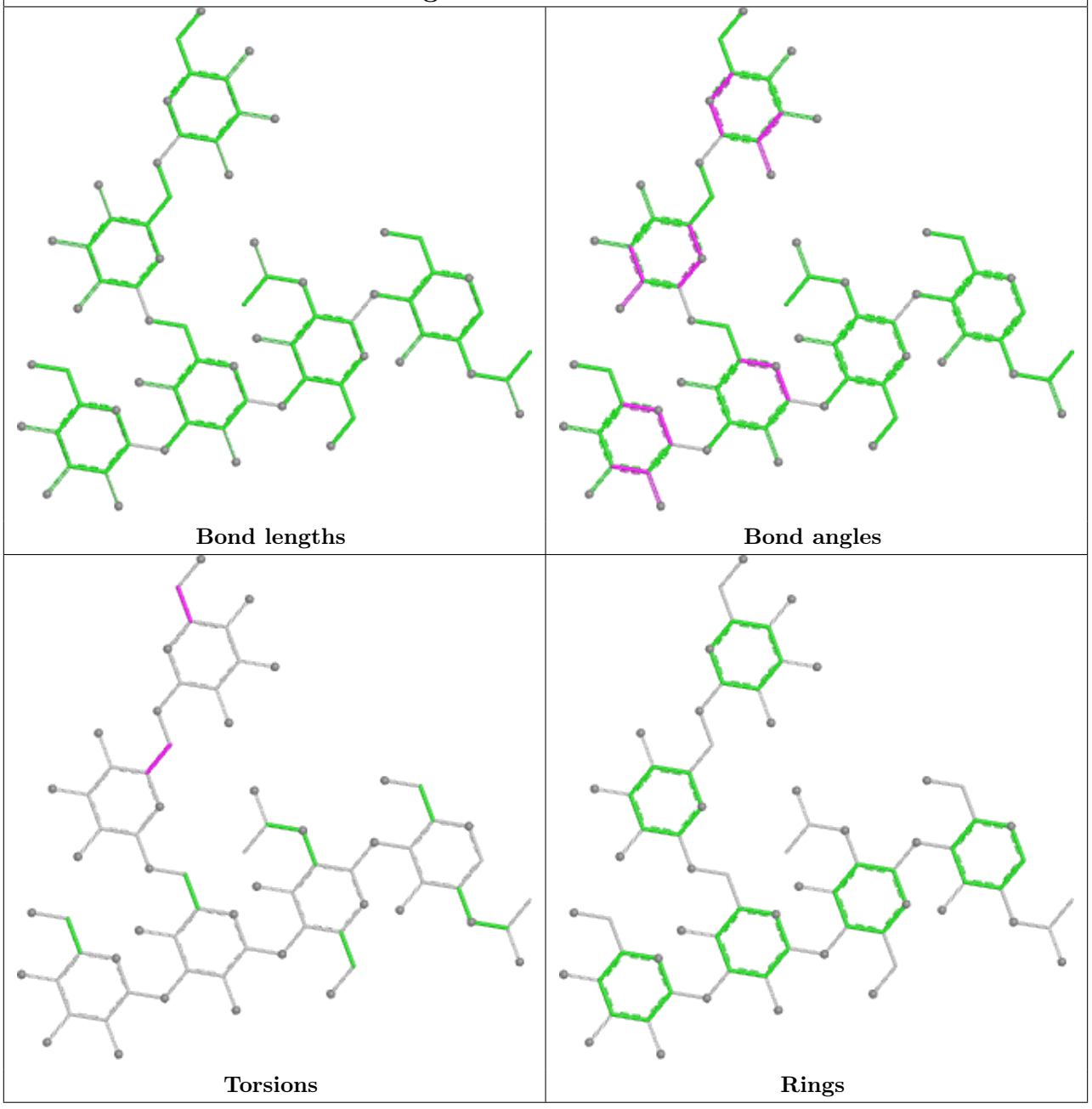


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

14 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	$\#\|Z\|>2$
10	POV	A	602	-	40,40,51	1.23	3 (7%)	46,48,59	1.03	3 (6%)
10	POV	A	603	-	40,40,51	1.24	3 (7%)	45,48,59	1.02	3 (6%)
10	POV	C	602	-	37,37,51	1.28	3 (8%)	43,45,59	1.05	3 (6%)
10	POV	E	502	-	36,36,51	1.29	3 (8%)	42,44,59	1.08	3 (7%)
10	POV	C	601	-	40,40,51	1.25	3 (7%)	45,48,59	1.03	3 (6%)
10	POV	D	603	-	32,32,51	1.30	3 (9%)	38,40,59	1.19	3 (7%)
9	NCT	D	601	-	13,13,13	2.88	7 (53%)	17,17,17	1.37	3 (17%)
10	POV	A	604	-	40,40,51	1.25	3 (7%)	45,48,59	1.04	4 (8%)
11	NAG	E	501	4	14,14,15	0.21	0	17,19,21	0.44	0
10	POV	E	503	-	29,29,51	1.35	3 (10%)	35,37,59	1.06	3 (8%)
9	NCT	A	601	-	13,13,13	2.91	7 (53%)	17,17,17	1.38	2 (11%)
10	POV	E	504	-	24,24,51	1.34	2 (8%)	30,32,59	1.16	2 (6%)
10	POV	D	602	-	32,32,51	1.32	3 (9%)	38,40,59	1.08	3 (7%)
10	POV	B	501	-	40,40,51	1.26	3 (7%)	46,48,59	1.03	3 (6%)

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
10	POV	A	602	-	-	28/44/44/55	-
10	POV	A	603	-	-	23/44/44/55	-
10	POV	C	602	-	-	25/41/41/55	-
10	POV	E	502	-	-	15/40/40/55	-
10	POV	C	601	-	-	17/44/44/55	-
10	POV	D	603	-	-	21/36/36/55	-
9	NCT	D	601	-	-	2/4/14/14	0/2/2/2
10	POV	A	604	-	-	27/44/44/55	-
11	NAG	E	501	4	-	0/6/23/26	0/1/1/1
10	POV	E	503	-	-	17/33/33/55	-
9	NCT	A	601	-	-	0/4/14/14	0/2/2/2
10	POV	E	504	-	-	16/27/27/55	-
10	POV	D	602	-	-	23/36/36/55	-
10	POV	B	501	-	-	23/44/44/55	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	NCT	C9-N2	6.64	1.65	1.46
9	D	601	NCT	C9-N2	6.52	1.65	1.46
9	A	601	NCT	C8-C9	-4.62	1.35	1.51
9	D	601	NCT	C8-C9	-4.60	1.35	1.51
9	D	601	NCT	C6-N2	-3.88	1.33	1.46
9	A	601	NCT	C6-N2	-3.84	1.33	1.46
9	A	601	NCT	C2-C6	3.36	1.57	1.51
10	E	503	POV	O31-C31	3.24	1.42	1.33
10	A	602	POV	O31-C31	3.22	1.42	1.33
10	A	604	POV	O31-C31	3.22	1.42	1.33
10	C	601	POV	O31-C31	3.21	1.42	1.33
9	D	601	NCT	C2-C6	3.21	1.56	1.51
10	B	501	POV	O31-C31	3.19	1.42	1.33
10	D	602	POV	O31-C31	3.19	1.42	1.33
10	C	602	POV	O31-C31	3.18	1.42	1.33
10	A	603	POV	O31-C31	3.14	1.42	1.33
10	E	502	POV	O31-C31	3.10	1.42	1.33
10	D	603	POV	O31-C31	3.08	1.42	1.33
10	B	501	POV	O21-C21	2.88	1.42	1.34
10	E	502	POV	O21-C21	2.85	1.42	1.34
10	A	603	POV	O21-C21	2.83	1.42	1.34
10	C	602	POV	O21-C21	2.82	1.42	1.34
10	D	602	POV	O21-C21	2.81	1.42	1.34
10	D	603	POV	O21-C21	2.80	1.42	1.34
10	A	602	POV	O21-C21	2.80	1.42	1.34
10	C	601	POV	O21-C21	2.80	1.42	1.34
10	E	503	POV	O21-C21	2.80	1.42	1.34
10	E	504	POV	O21-C21	2.79	1.42	1.34
10	A	604	POV	O21-C21	2.71	1.41	1.34
10	A	602	POV	O21-C2	-2.59	1.40	1.46
10	A	604	POV	O21-C2	-2.57	1.40	1.46
10	E	504	POV	O21-C2	-2.51	1.40	1.46
10	C	601	POV	O21-C2	-2.50	1.40	1.46
10	A	603	POV	O21-C2	-2.49	1.40	1.46
10	B	501	POV	O21-C2	-2.49	1.40	1.46
10	D	602	POV	O21-C2	-2.48	1.40	1.46
10	E	503	POV	O21-C2	-2.47	1.40	1.46
10	C	602	POV	O21-C2	-2.47	1.40	1.46
10	E	502	POV	O21-C2	-2.42	1.40	1.46
9	A	601	NCT	C7-C6	2.33	1.60	1.54
9	D	601	NCT	C7-C6	2.31	1.60	1.54
10	D	603	POV	O21-C2	-2.24	1.41	1.46
9	D	601	NCT	C10-N2	2.10	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	NCT	C10-N2	2.10	1.51	1.46
9	A	601	NCT	C3-C2	-2.03	1.35	1.39
9	D	601	NCT	C3-C2	-2.01	1.35	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	603	POV	O21-C21-C22	4.19	120.52	111.50
10	E	502	POV	O21-C21-C22	4.11	120.35	111.50
10	B	501	POV	O21-C21-C22	4.05	120.22	111.50
10	E	504	POV	O21-C21-C22	4.04	120.21	111.50
10	D	602	POV	O21-C21-C22	4.02	120.16	111.50
10	A	604	POV	O21-C21-C22	4.00	120.12	111.50
10	C	602	POV	O21-C21-C22	4.00	120.11	111.50
10	A	602	POV	O21-C21-C22	3.96	120.03	111.50
10	A	603	POV	O21-C21-C22	3.94	119.99	111.50
10	C	601	POV	O21-C21-C22	3.88	119.86	111.50
10	E	503	POV	O21-C21-C22	3.33	120.09	110.80
9	D	601	NCT	C3-C2-C1	2.92	119.99	116.88
10	D	603	POV	O31-C31-C32	2.89	120.96	111.91
9	A	601	NCT	C3-C2-C1	2.78	119.84	116.88
9	D	601	NCT	C2-C1-N1	-2.74	119.84	124.14
10	A	604	POV	O31-C31-C32	2.69	120.35	111.91
10	A	602	POV	O31-C31-C32	2.64	120.19	111.91
10	C	601	POV	O31-C31-C32	2.63	120.15	111.91
10	E	503	POV	O31-C31-C32	2.62	120.12	111.91
10	D	602	POV	O31-C31-C32	2.61	120.10	111.91
9	A	601	NCT	C2-C1-N1	-2.60	120.06	124.14
10	C	602	POV	O31-C31-C32	2.59	120.03	111.91
10	B	501	POV	O31-C31-C32	2.53	119.85	111.91
10	A	603	POV	O31-C31-C32	2.50	119.77	111.91
10	E	502	POV	O31-C31-C32	2.48	119.69	111.91
10	D	603	POV	C13-N-C12	2.42	119.82	109.92
10	A	603	POV	C13-N-C12	2.35	119.54	109.92
10	E	502	POV	C13-N-C12	2.27	119.19	109.92
10	A	602	POV	C13-N-C12	2.26	119.15	109.92
10	C	601	POV	C13-N-C12	2.25	119.10	109.92
10	E	503	POV	C13-N-C12	2.21	118.96	109.92
10	E	504	POV	C13-N-C12	2.20	118.94	109.92
10	B	501	POV	C13-N-C12	2.20	118.92	109.92
10	C	602	POV	C13-N-C12	2.18	118.85	109.92
10	A	604	POV	C13-N-C12	2.12	118.61	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	602	POV	C13-N-C12	2.05	118.30	109.92
10	A	604	POV	C2-O21-C21	-2.01	112.84	117.79
9	D	601	NCT	C7-C6-C2	-2.00	109.73	113.61

There are no chirality outliers.

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	602	POV	C1-O11-P-O12
10	A	602	POV	C1-O11-P-O14
10	A	602	POV	C11-O12-P-O13
10	A	602	POV	O21-C2-C3-O31
10	A	602	POV	O12-C11-C12-N
10	A	603	POV	C1-O11-P-O14
10	A	603	POV	C11-O12-P-O11
10	A	603	POV	C11-O12-P-O13
10	A	603	POV	C11-O12-P-O14
10	A	603	POV	O12-C11-C12-N
10	A	603	POV	C22-C21-O21-C2
10	A	603	POV	O32-C31-O31-C3
10	A	604	POV	C1-O11-P-O13
10	A	604	POV	C1-O11-P-O14
10	A	604	POV	C11-O12-P-O13
10	A	604	POV	C11-O12-P-O14
10	A	604	POV	O12-C11-C12-N
10	A	604	POV	O22-C21-O21-C2
10	B	501	POV	O12-C11-C12-N
10	B	501	POV	C22-C21-O21-C2
10	C	601	POV	C1-O11-P-O12
10	C	601	POV	C1-O11-P-O13
10	C	601	POV	C1-O11-P-O14
10	C	601	POV	O12-C11-C12-N
10	C	601	POV	O22-C21-O21-C2
10	C	602	POV	C11-O12-P-O11
10	C	602	POV	C11-O12-P-O13
10	C	602	POV	C11-O12-P-O14
10	C	602	POV	O12-C11-C12-N
10	D	602	POV	C1-O11-P-O13
10	D	602	POV	C1-O11-P-O14
10	D	602	POV	O12-C11-C12-N
10	D	603	POV	C22-C21-O21-C2
10	E	502	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
10	E	502	POV	C1-O11-P-O14
10	E	502	POV	O21-C2-C3-O31
10	E	503	POV	O12-C11-C12-N
10	E	503	POV	C22-C21-O21-C2
10	E	504	POV	C1-O11-P-O13
10	E	504	POV	O12-C11-C12-N
10	E	504	POV	O22-C21-O21-C2
10	A	604	POV	O32-C31-O31-C3
10	E	503	POV	O32-C31-O31-C3
10	A	604	POV	C32-C31-O31-C3
10	E	503	POV	C32-C31-O31-C3
10	A	603	POV	O22-C21-O21-C2
10	B	501	POV	O22-C21-O21-C2
10	D	603	POV	O22-C21-O21-C2
10	E	503	POV	O22-C21-O21-C2
10	A	603	POV	C32-C31-O31-C3
10	A	604	POV	C22-C21-O21-C2
10	C	601	POV	C22-C21-O21-C2
10	E	504	POV	C22-C21-O21-C2
10	A	603	POV	C35-C36-C37-C38
10	A	602	POV	C32-C31-O31-C3
10	D	602	POV	C32-C33-C34-C35
10	C	602	POV	C24-C25-C26-C27
10	A	603	POV	C25-C26-C27-C28
10	A	602	POV	O32-C31-O31-C3
10	D	603	POV	C32-C31-O31-C3
10	C	602	POV	C22-C23-C24-C25
10	A	602	POV	C21-C22-C23-C24
10	A	603	POV	C21-C22-C23-C24
10	C	601	POV	C21-C22-C23-C24
10	E	502	POV	C21-C22-C23-C24
10	A	604	POV	C21-C22-C23-C24
10	B	501	POV	C21-C22-C23-C24
10	E	504	POV	C21-C22-C23-C24
10	C	602	POV	C27-C28-C29-C210
10	C	601	POV	C34-C35-C36-C37
10	D	603	POV	O32-C31-O31-C3
10	A	602	POV	C11-O12-P-O11
10	A	603	POV	C1-O11-P-O12
10	A	604	POV	C1-O11-P-O12
10	A	604	POV	C11-O12-P-O11
10	B	501	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
10	C	602	POV	C1-O11-P-O12
10	D	602	POV	C1-O11-P-O12
10	D	602	POV	C11-O12-P-O11
10	E	502	POV	C1-O11-P-O12
10	E	503	POV	C11-O12-P-O11
10	E	504	POV	C1-O11-P-O12
10	E	502	POV	C32-C31-O31-C3
10	D	603	POV	C11-C12-N-C14
10	D	603	POV	C11-C12-N-C15
10	A	602	POV	C22-C21-O21-C2
10	A	602	POV	C24-C25-C26-C27
10	E	502	POV	C32-C33-C34-C35
10	A	603	POV	C36-C37-C38-C39
10	C	602	POV	C35-C36-C37-C38
10	A	602	POV	O22-C21-O21-C2
10	A	604	POV	C24-C25-C26-C27
10	C	602	POV	C33-C34-C35-C36
10	A	602	POV	C35-C36-C37-C38
10	A	602	POV	C32-C33-C34-C35
10	C	602	POV	C21-C22-C23-C24
10	A	604	POV	C35-C36-C37-C38
10	A	603	POV	C32-C33-C34-C35
10	E	503	POV	C32-C33-C34-C35
10	A	603	POV	C34-C35-C36-C37
10	C	601	POV	C36-C37-C38-C39
10	B	501	POV	C24-C25-C26-C27
10	E	503	POV	C35-C36-C37-C38
10	D	603	POV	C11-C12-N-C13
10	B	501	POV	C33-C34-C35-C36
10	B	501	POV	C37-C38-C39-C310
10	B	501	POV	C36-C37-C38-C39
10	B	501	POV	C32-C31-O31-C3
10	C	601	POV	C32-C33-C34-C35
10	E	502	POV	O32-C31-O31-C3
10	A	602	POV	C25-C26-C27-C28
10	A	604	POV	C32-C33-C34-C35
10	E	502	POV	C33-C34-C35-C36
10	A	603	POV	C37-C38-C39-C310
10	B	501	POV	C35-C36-C37-C38
10	C	601	POV	C25-C26-C27-C28
10	C	602	POV	C34-C35-C36-C37
10	B	501	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
10	A	604	POV	C34-C35-C36-C37
10	C	602	POV	C25-C26-C27-C28
10	A	602	POV	C22-C23-C24-C25
10	A	604	POV	C25-C26-C27-C28
10	D	603	POV	C21-C22-C23-C24
10	D	602	POV	C22-C21-O21-C2
10	D	602	POV	O22-C21-O21-C2
10	A	604	POV	C22-C23-C24-C25
10	A	604	POV	C33-C34-C35-C36
10	B	501	POV	O21-C2-C3-O31
10	C	601	POV	C27-C28-C29-C210
10	B	501	POV	C311-C310-C39-C38
10	D	602	POV	C26-C27-C28-C29
10	B	501	POV	C25-C26-C27-C28
10	D	603	POV	C23-C24-C25-C26
10	A	602	POV	C36-C37-C38-C39
10	C	602	POV	C1-C2-C3-O31
10	E	503	POV	C1-C2-C3-O31
10	D	603	POV	C22-C23-C24-C25
10	A	602	POV	C211-C212-C213-C214
10	A	604	POV	C36-C37-C38-C39
10	E	502	POV	C34-C35-C36-C37
10	C	601	POV	C32-C31-O31-C3
10	D	603	POV	C33-C34-C35-C36
10	D	602	POV	C21-C22-C23-C24
10	D	602	POV	C24-C25-C26-C27
10	D	603	POV	C26-C27-C28-C29
10	E	503	POV	C34-C35-C36-C37
10	E	503	POV	C36-C37-C38-C39
10	A	602	POV	O11-C1-C2-C3
10	A	602	POV	C1-C2-C3-O31
10	B	501	POV	C1-C2-C3-O31
10	D	602	POV	C1-C2-C3-O31
10	D	603	POV	C1-C2-C3-O31
10	E	504	POV	C1-C2-C3-O31
10	A	602	POV	C33-C34-C35-C36
10	C	601	POV	C35-C36-C37-C38
10	E	504	POV	O11-C1-C2-O21
10	C	601	POV	O32-C31-O31-C3
10	D	602	POV	O21-C2-C3-O31
10	E	503	POV	O21-C2-C3-O31
10	E	502	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
10	D	602	POV	C23-C24-C25-C26
10	B	501	POV	O11-C1-C2-C3
10	C	602	POV	O11-C1-C2-C3
10	D	602	POV	O11-C1-C2-C3
10	E	502	POV	C27-C28-C29-C210
10	B	501	POV	C39-C310-C311-C312
10	E	503	POV	C33-C34-C35-C36
10	A	602	POV	O11-C1-C2-O21
10	C	602	POV	O11-C1-C2-O21
10	A	604	POV	C311-C310-C39-C38
10	C	602	POV	O21-C2-C3-O31
10	D	603	POV	O21-C2-C3-O31
10	E	504	POV	O21-C2-C3-O31
10	A	603	POV	C311-C310-C39-C38
10	C	602	POV	C23-C24-C25-C26
10	A	602	POV	C11-O12-P-O14
10	B	501	POV	C1-O11-P-O14
10	C	602	POV	C1-O11-P-O13
10	D	602	POV	C11-O12-P-O13
10	D	602	POV	C11-O12-P-O14
10	E	503	POV	C11-O12-P-O13
10	E	504	POV	C1-O11-P-O14
10	E	503	POV	O11-C1-C2-C3
10	E	504	POV	O11-C1-C2-C3
10	D	602	POV	C12-C11-O12-P
10	B	501	POV	C32-C33-C34-C35
10	A	603	POV	O11-C1-C2-O21
10	D	602	POV	O11-C1-C2-O21
10	E	503	POV	O11-C1-C2-O21
10	D	603	POV	O21-C21-C22-C23
10	D	602	POV	C25-C26-C27-C28
10	D	603	POV	O12-C11-C12-N
10	E	502	POV	C1-C2-C3-O31
10	E	502	POV	O12-C11-C12-N
10	D	602	POV	C2-C1-O11-P
10	A	602	POV	C23-C24-C25-C26
10	D	603	POV	C25-C26-C27-C28
10	C	601	POV	C311-C310-C39-C38
10	D	603	POV	C3-C2-O21-C21
10	B	501	POV	O11-C1-C2-O21
10	B	501	POV	C11-O12-P-O11
10	D	603	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
10	E	502	POV	C11-O12-P-O11
10	E	503	POV	C1-O11-P-O12
10	E	504	POV	C11-O12-P-O11
10	D	602	POV	C22-C23-C24-C25
10	C	602	POV	C37-C38-C39-C310
10	C	602	POV	C32-C31-O31-C3
10	C	602	POV	O32-C31-O31-C3
10	A	604	POV	O21-C2-C3-O31
10	A	604	POV	C23-C24-C25-C26
9	D	601	NCT	C1-C2-C6-C7
10	E	504	POV	C22-C23-C24-C25
10	C	602	POV	O31-C31-C32-C33
9	D	601	NCT	C3-C2-C6-N2
10	A	603	POV	O21-C21-C22-C23
10	C	602	POV	C26-C27-C28-C29
10	A	604	POV	C1-C2-C3-O31
10	A	603	POV	C33-C34-C35-C36
10	A	603	POV	O11-C1-C2-C3
10	B	501	POV	C27-C28-C29-C210
10	C	602	POV	O32-C31-C32-C33
10	E	504	POV	O21-C21-C22-C23
10	A	603	POV	O22-C21-C22-C23
10	D	603	POV	C2-C1-O11-P
10	A	604	POV	C31-C32-C33-C34
10	D	603	POV	C11-O12-P-O14
10	D	602	POV	O21-C21-C22-C23
10	A	602	POV	C31-C32-C33-C34
10	A	602	POV	C12-C11-O12-P
10	A	604	POV	C1-C2-O21-C21
10	C	601	POV	C12-C11-O12-P
10	E	504	POV	C12-C11-O12-P
10	A	604	POV	C11-C12-N-C15
10	E	504	POV	O22-C21-C22-C23
10	A	602	POV	C34-C35-C36-C37
10	A	602	POV	O21-C21-C22-C23

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	602	POV	1	0
10	A	603	POV	4	0

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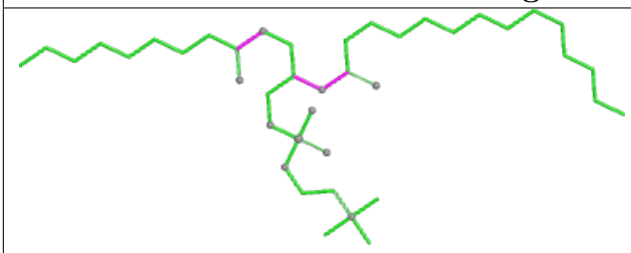
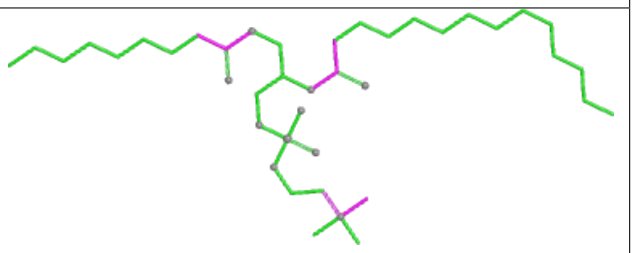
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	602	POV	1	0
10	C	601	POV	1	0
10	D	603	POV	5	0
9	D	601	NCT	2	0
10	A	604	POV	5	0
10	E	503	POV	2	0
10	E	504	POV	1	0
10	D	602	POV	2	0
10	B	501	POV	1	0

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

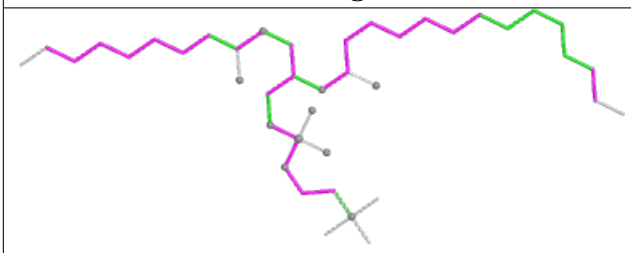
Ligand POV A 602



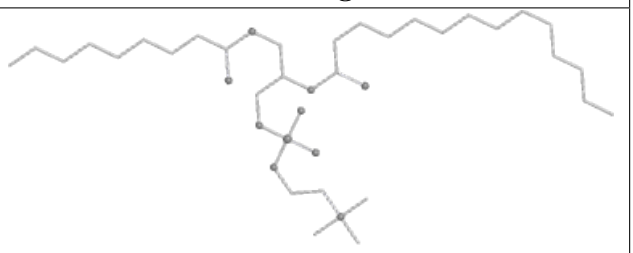
Bond lengths



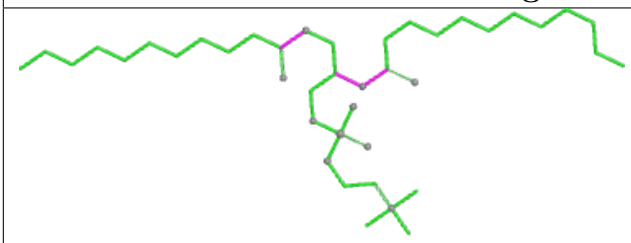
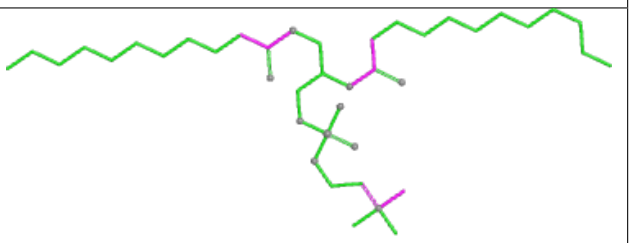
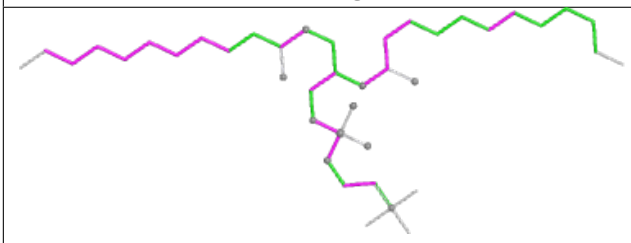
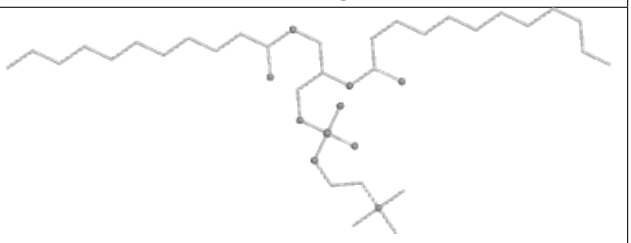
Bond angles

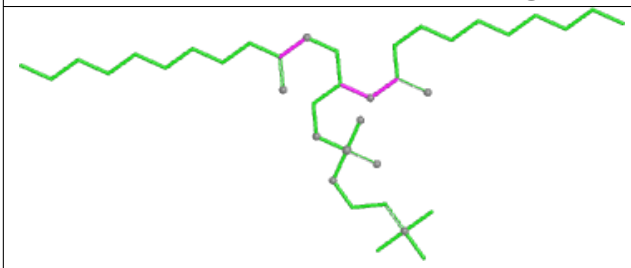
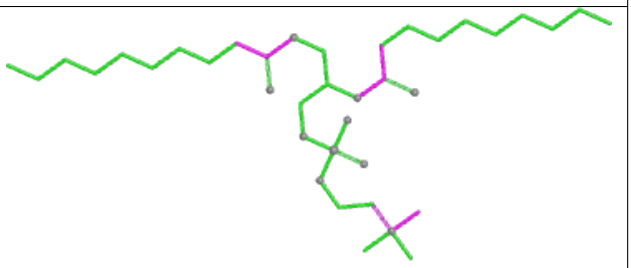
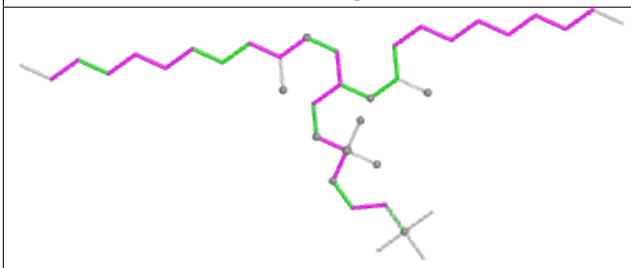
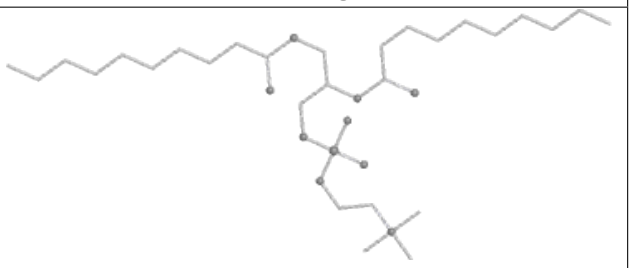


Torsions

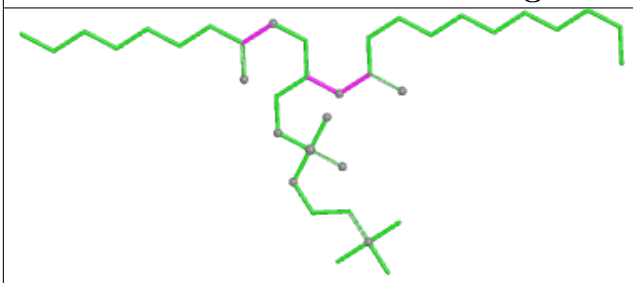


Rings

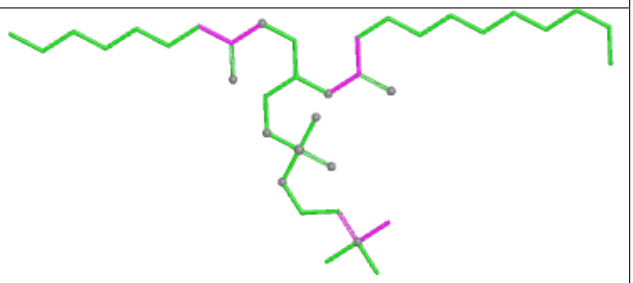
Ligand POV A 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV C 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

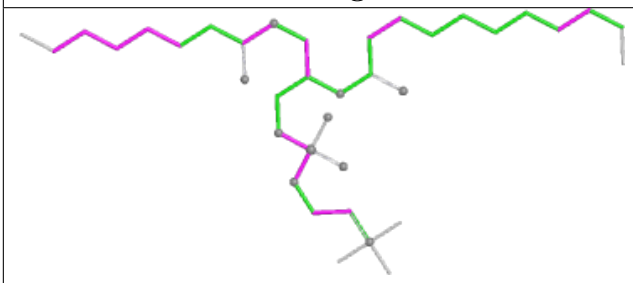
Ligand POV E 502



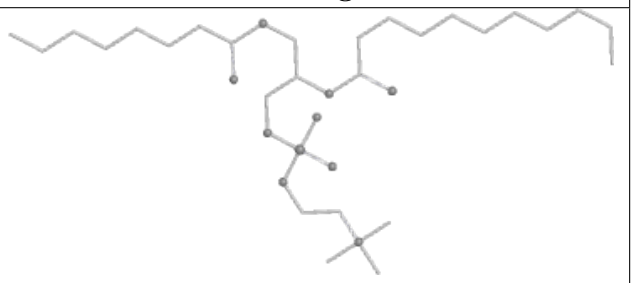
Bond lengths



Bond angles

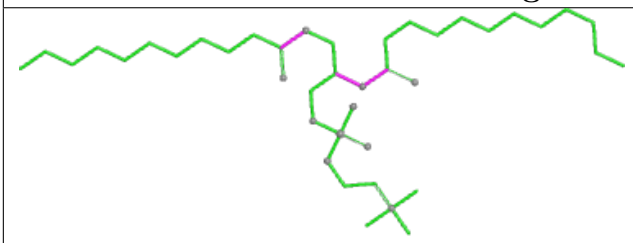


Torsions

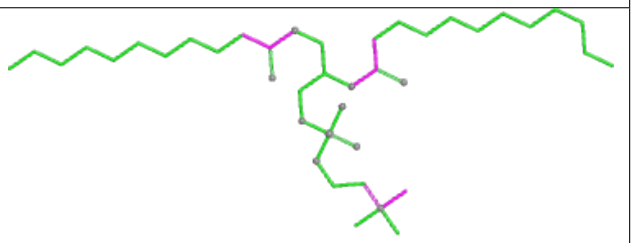


Rings

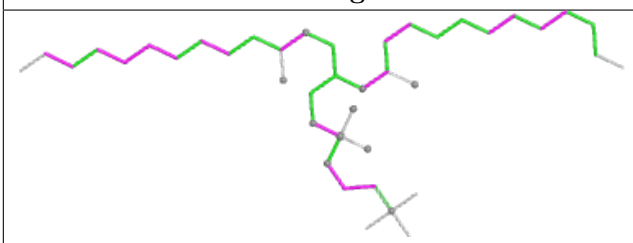
Ligand POV C 601



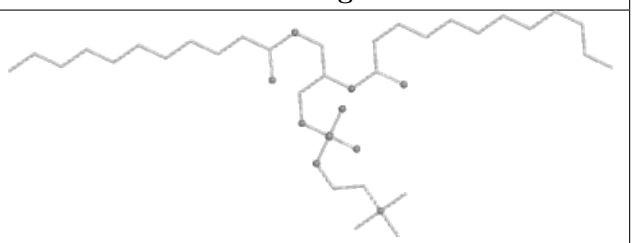
Bond lengths



Bond angles

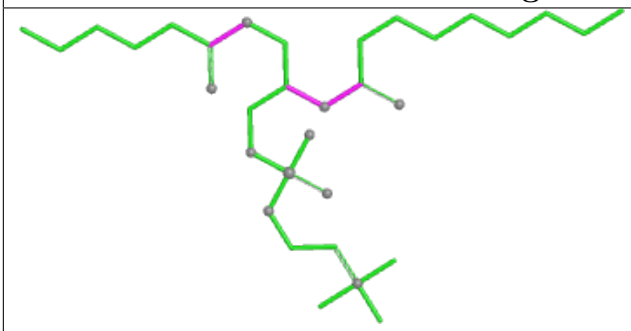


Torsions

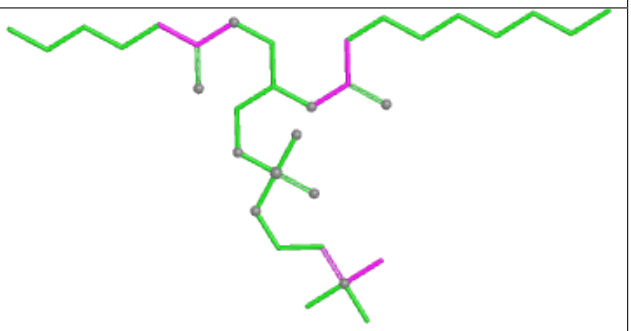


Rings

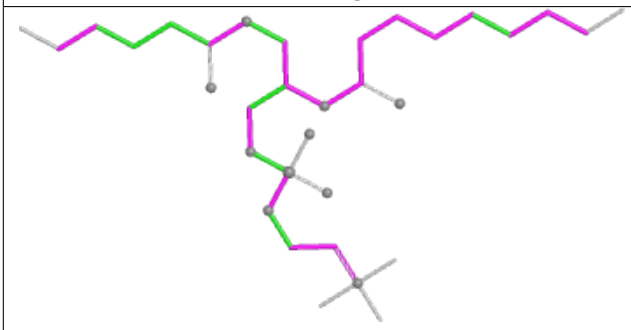
Ligand POV D 603



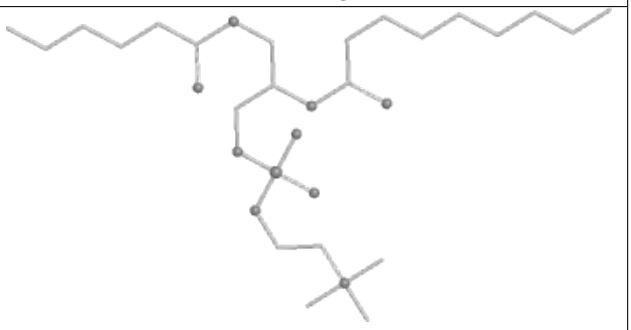
Bond lengths



Bond angles

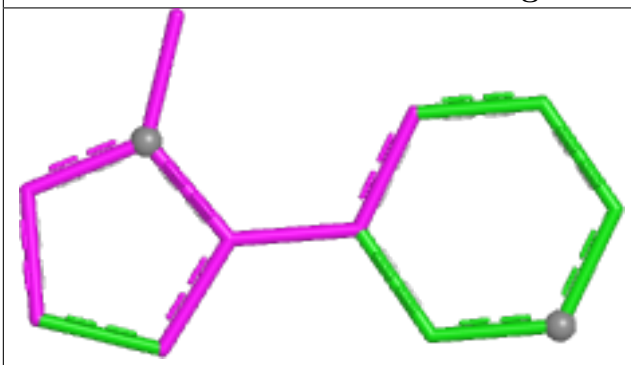


Torsions

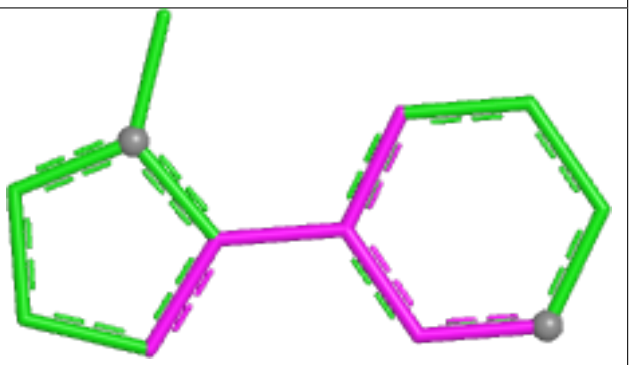


Rings

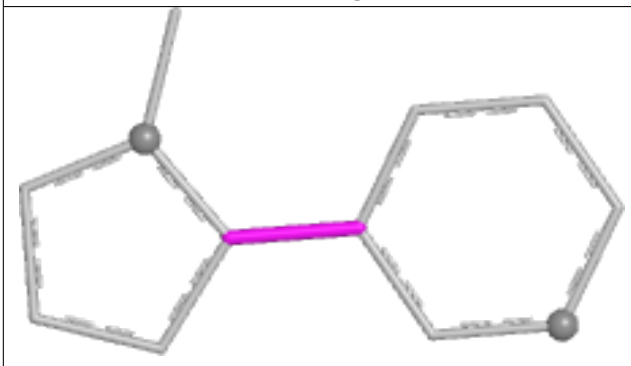
Ligand NCT D 601



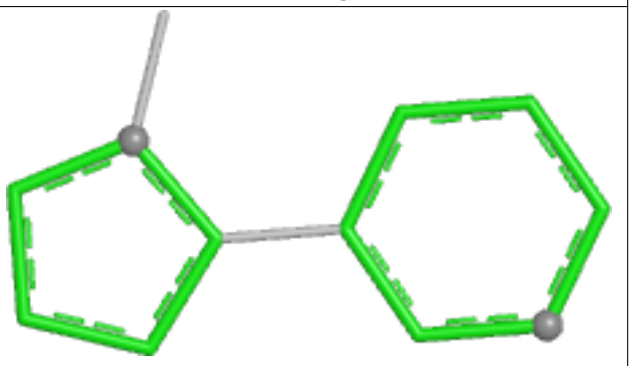
Bond lengths



Bond angles

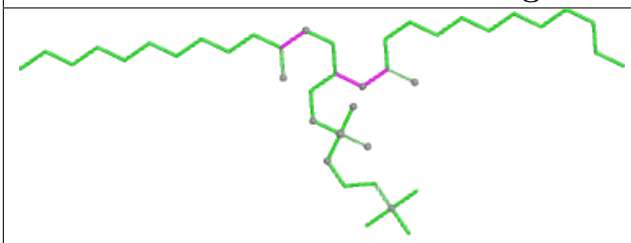


Torsions

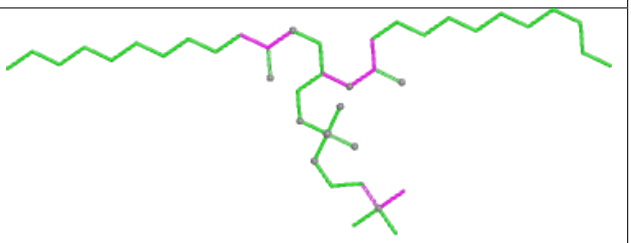


Rings

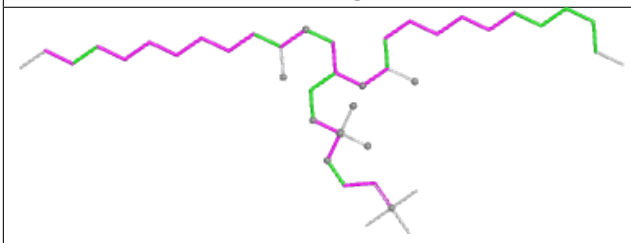
Ligand POV A 604



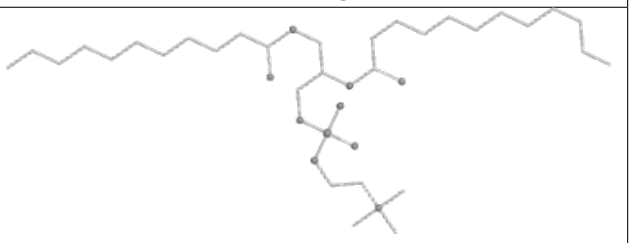
Bond lengths



Bond angles

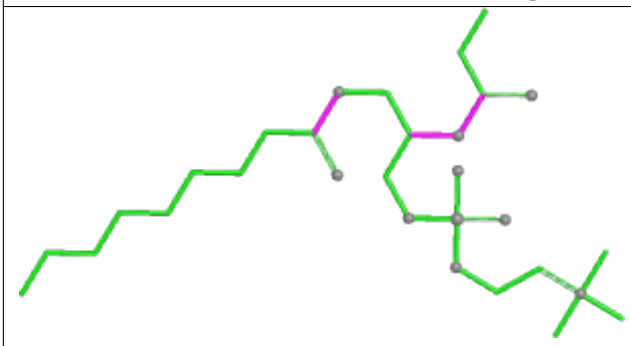


Torsions

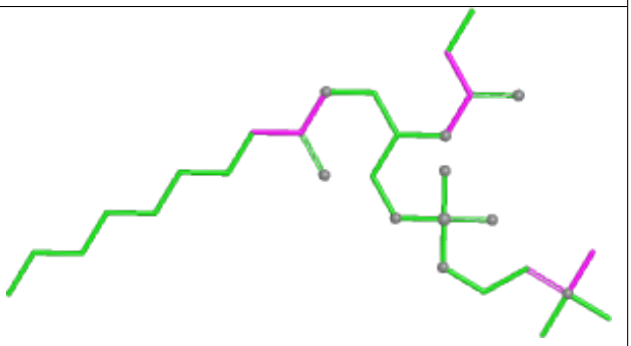


Rings

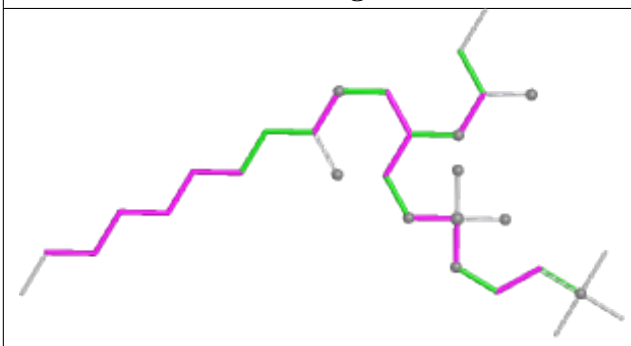
Ligand POV E 503



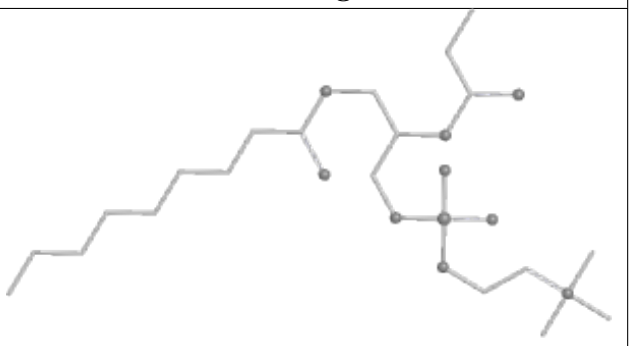
Bond lengths



Bond angles

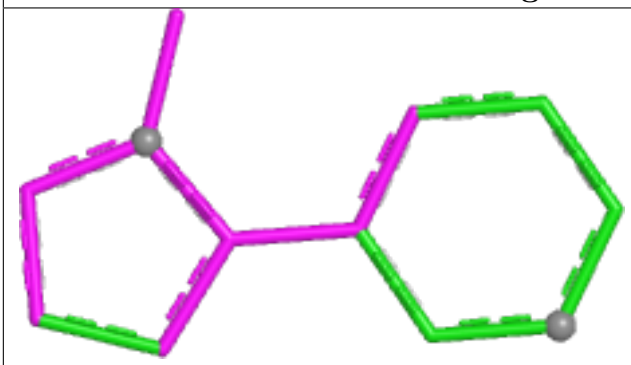


Torsions

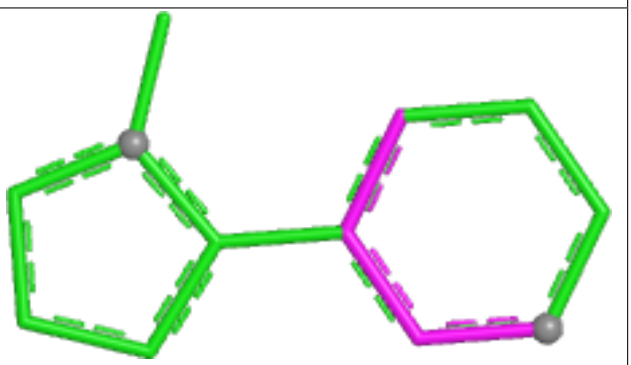


Rings

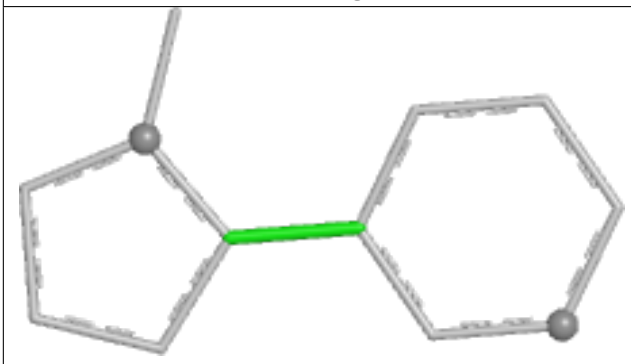
Ligand NCT A 601



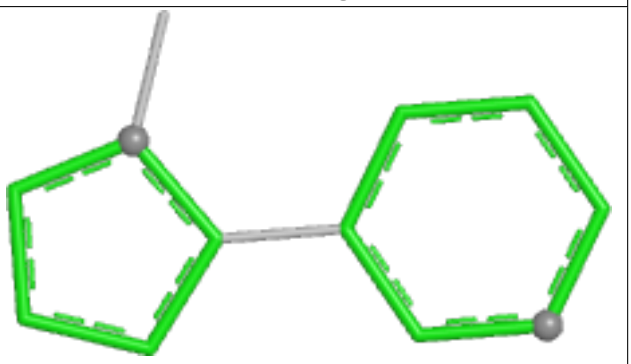
Bond lengths



Bond angles

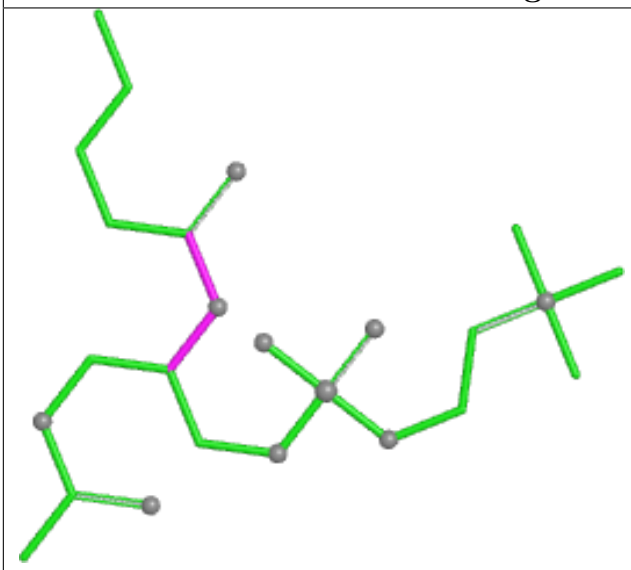


Torsions

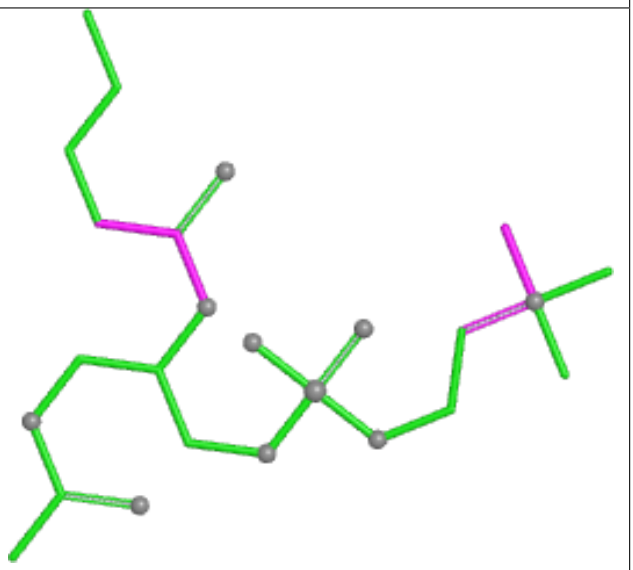


Rings

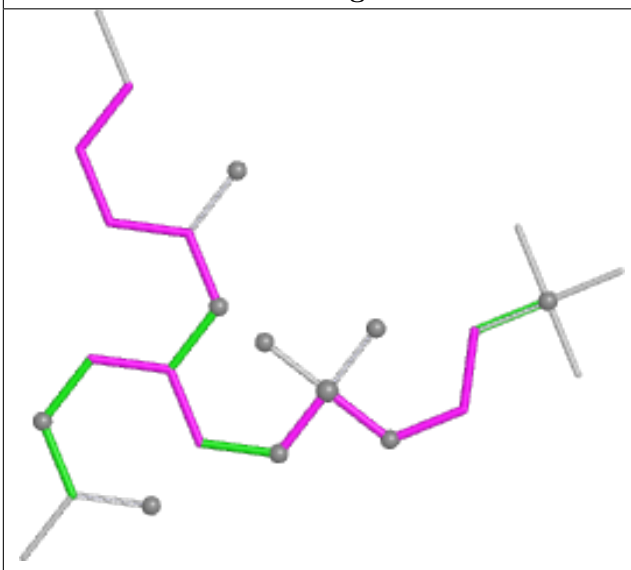
Ligand POV E 504



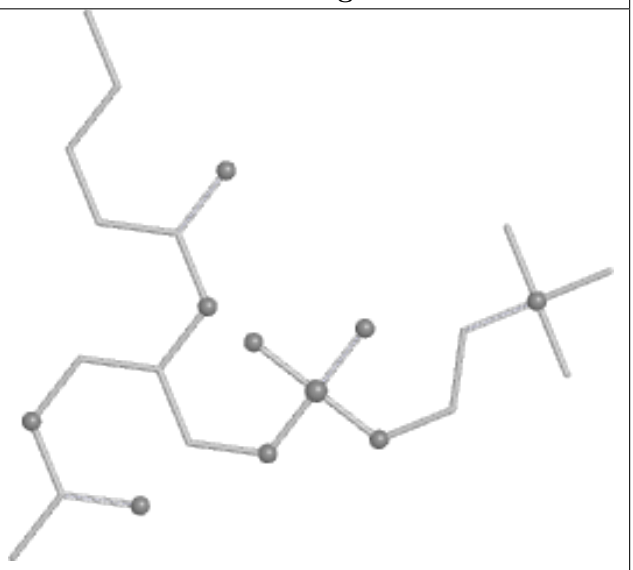
Bond lengths



Bond angles

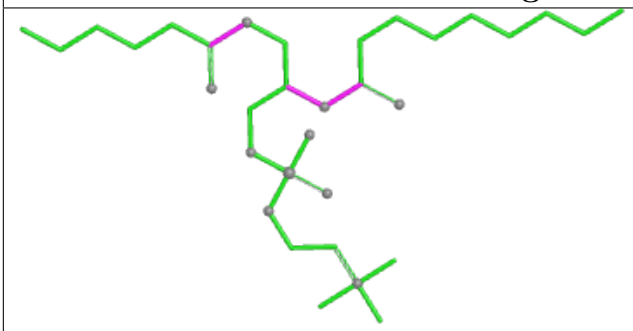


Torsions

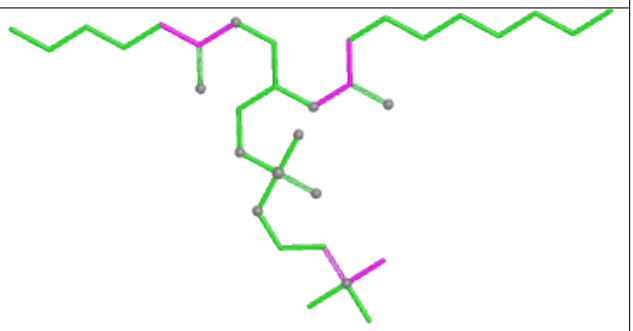


Rings

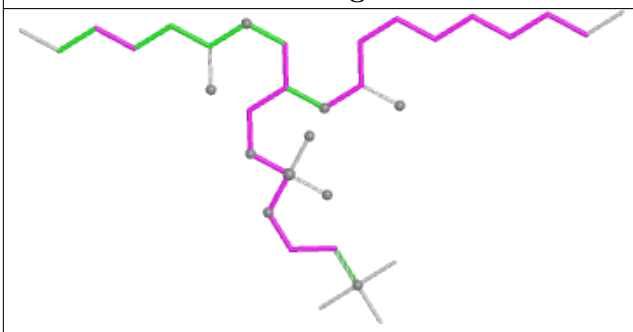
Ligand POV D 602



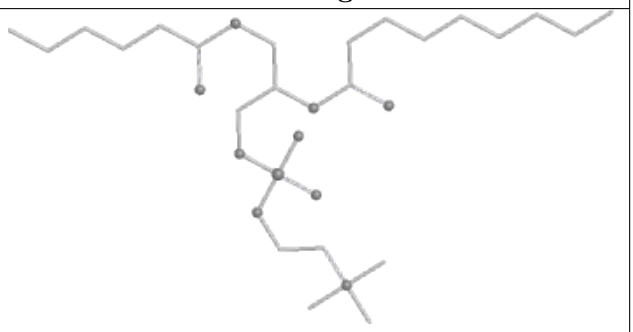
Bond lengths



Bond angles

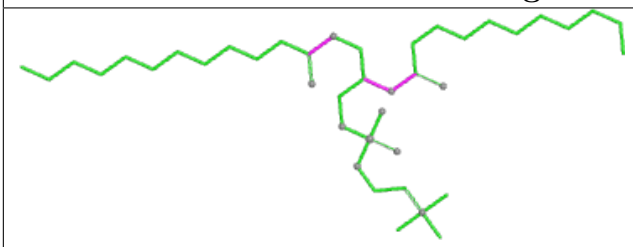


Torsions

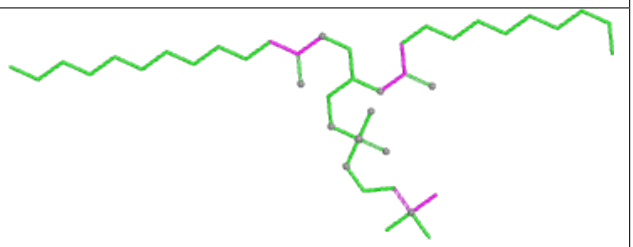


Rings

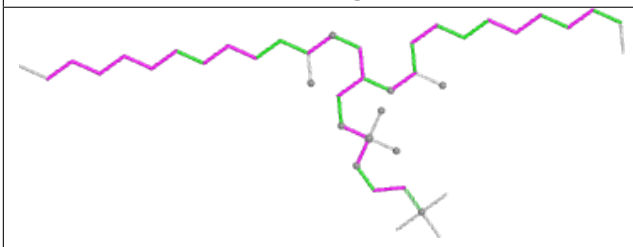
Ligand POV B 501



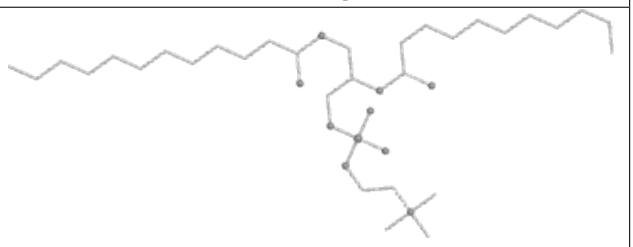
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

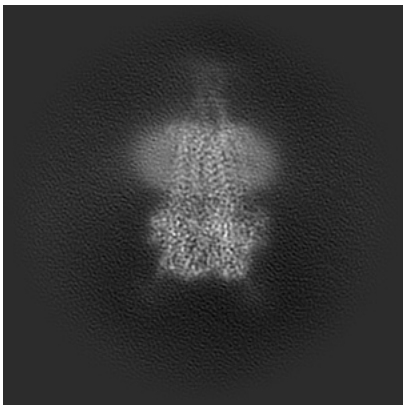
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14064. These allow visual inspection of the internal detail of the map and identification of artifacts.

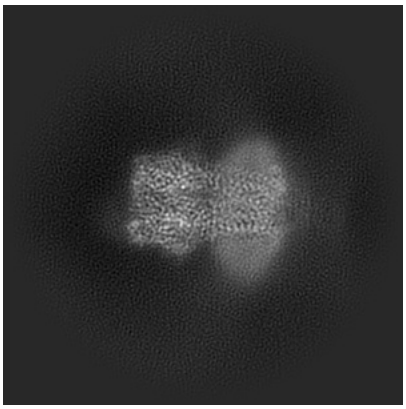
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

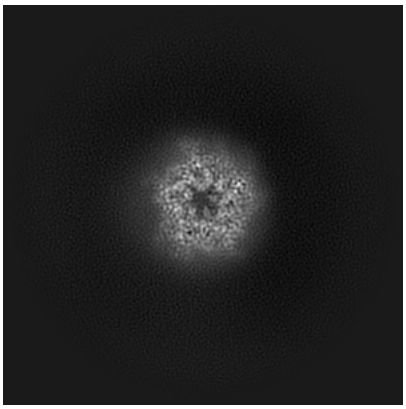
6.1.1 Primary map



X

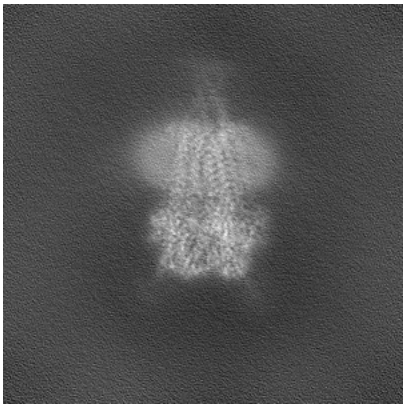


Y

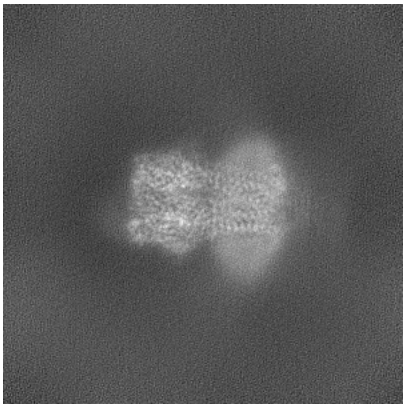


Z

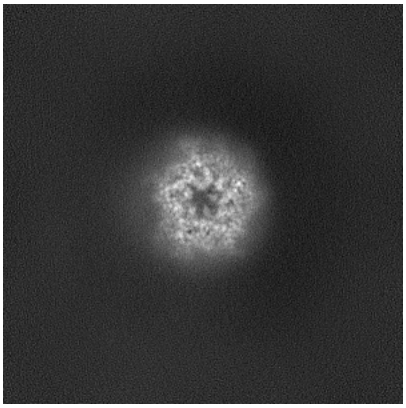
6.1.2 Raw map



X



Y



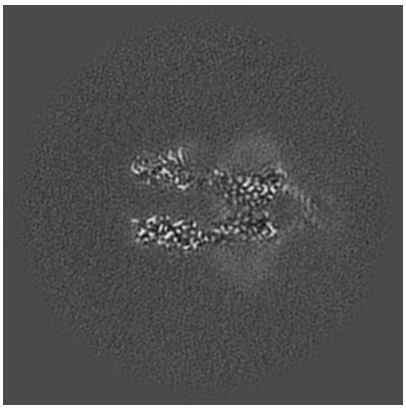
Z

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

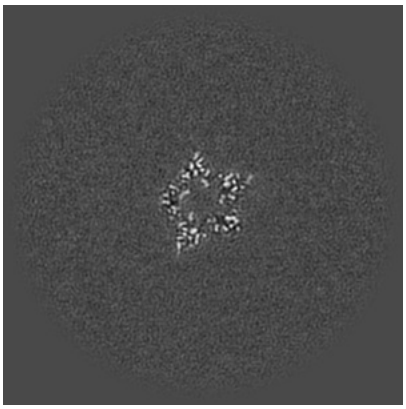
6.2 Central slices (i)

6.2.1 Primary map

X Index: 176

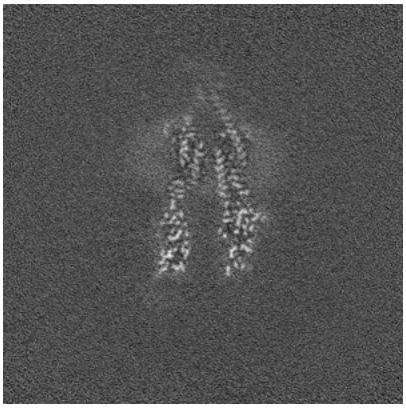


Y Index: 176

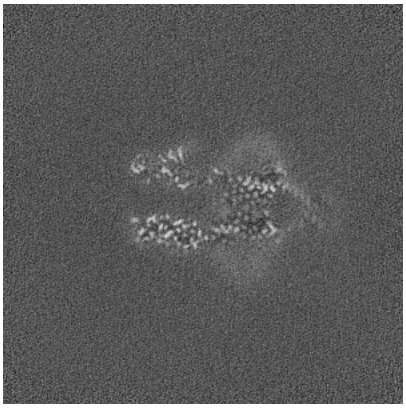


Z Index: 176

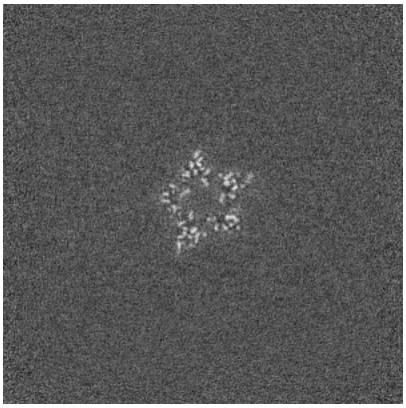
6.2.2 Raw map



X Index: 176



Y Index: 176

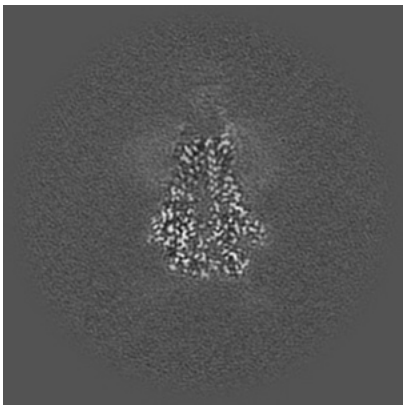


Z Index: 176

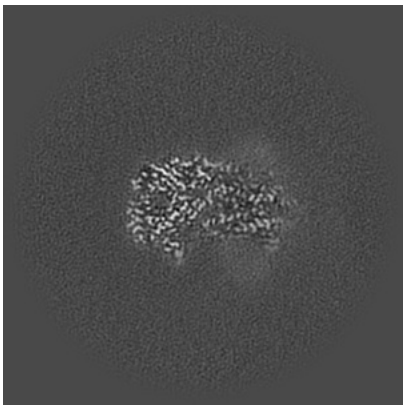
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

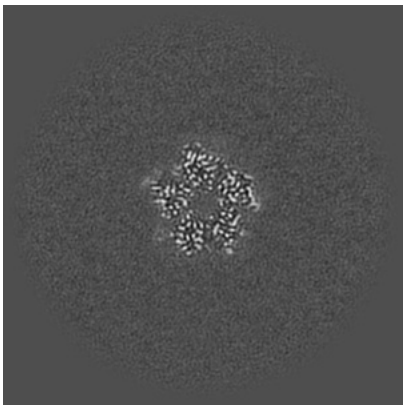
6.3.1 Primary map



X Index: 162

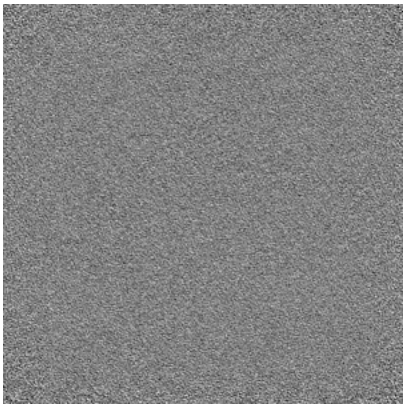


Y Index: 196

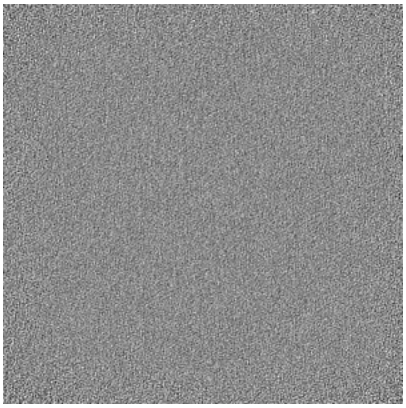


Z Index: 155

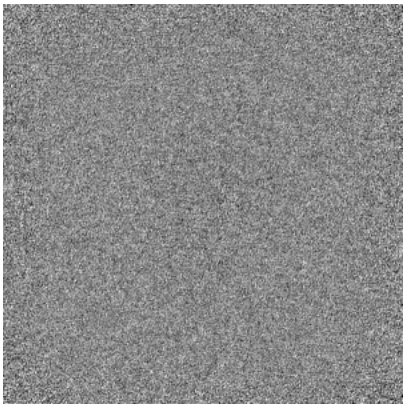
6.3.2 Raw map



X Index: 0



Y Index: 0

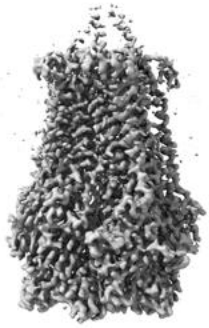


Z Index: 0

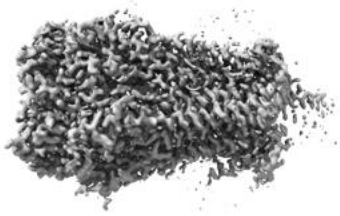
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

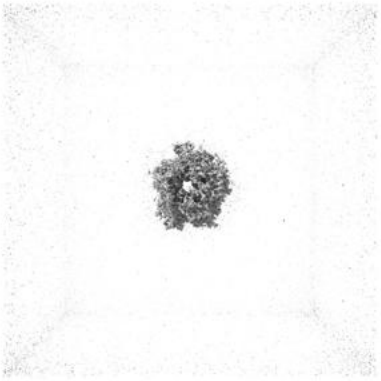
Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

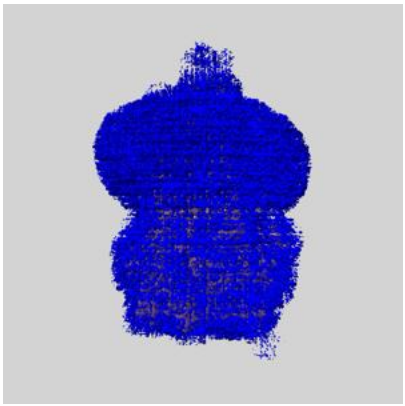
6.5 Mask visualisation (i)

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

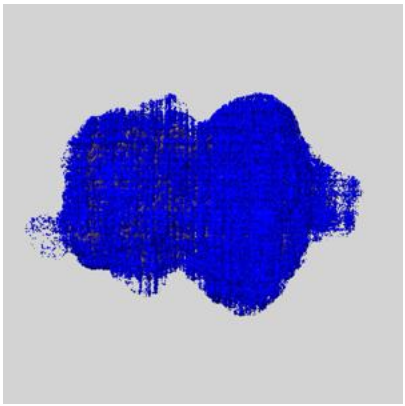
A mask typically either:

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

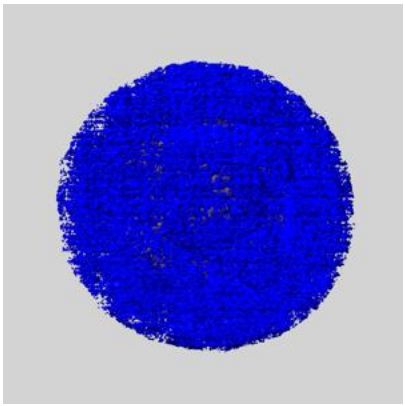
6.5.1 emd_14064_msk_1.map (i)



X

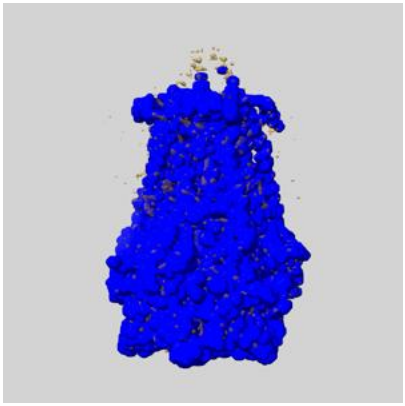


Y

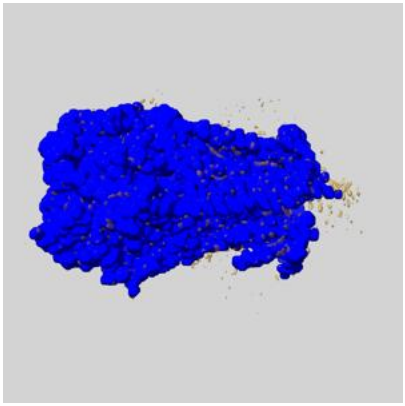


Z

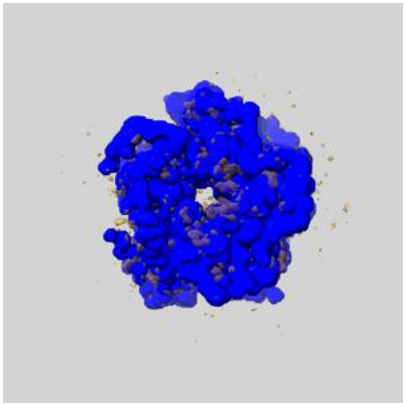
6.5.2 emd_14064_msk_2.map (i)



X



Y

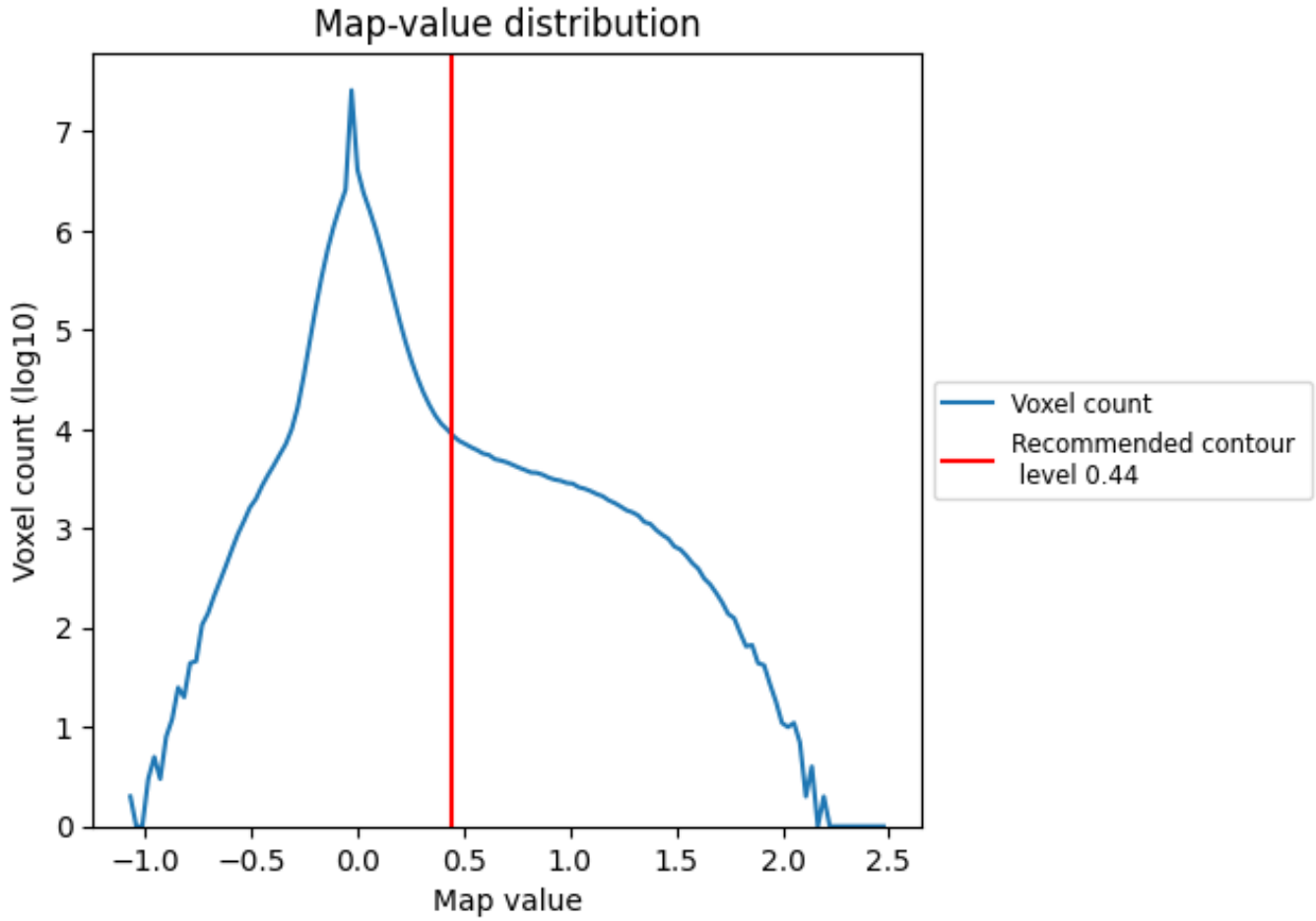


Z

7 Map analysis

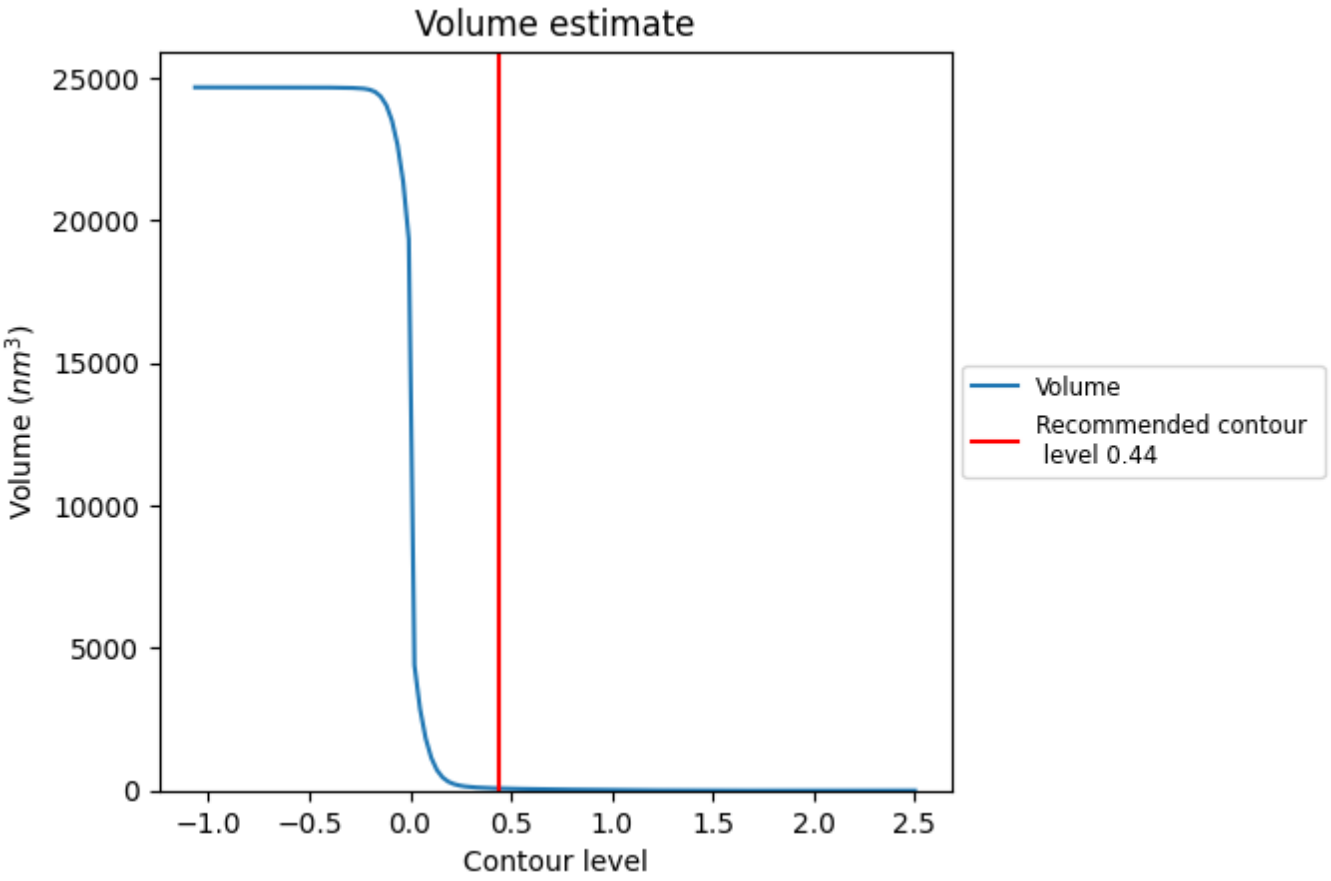
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

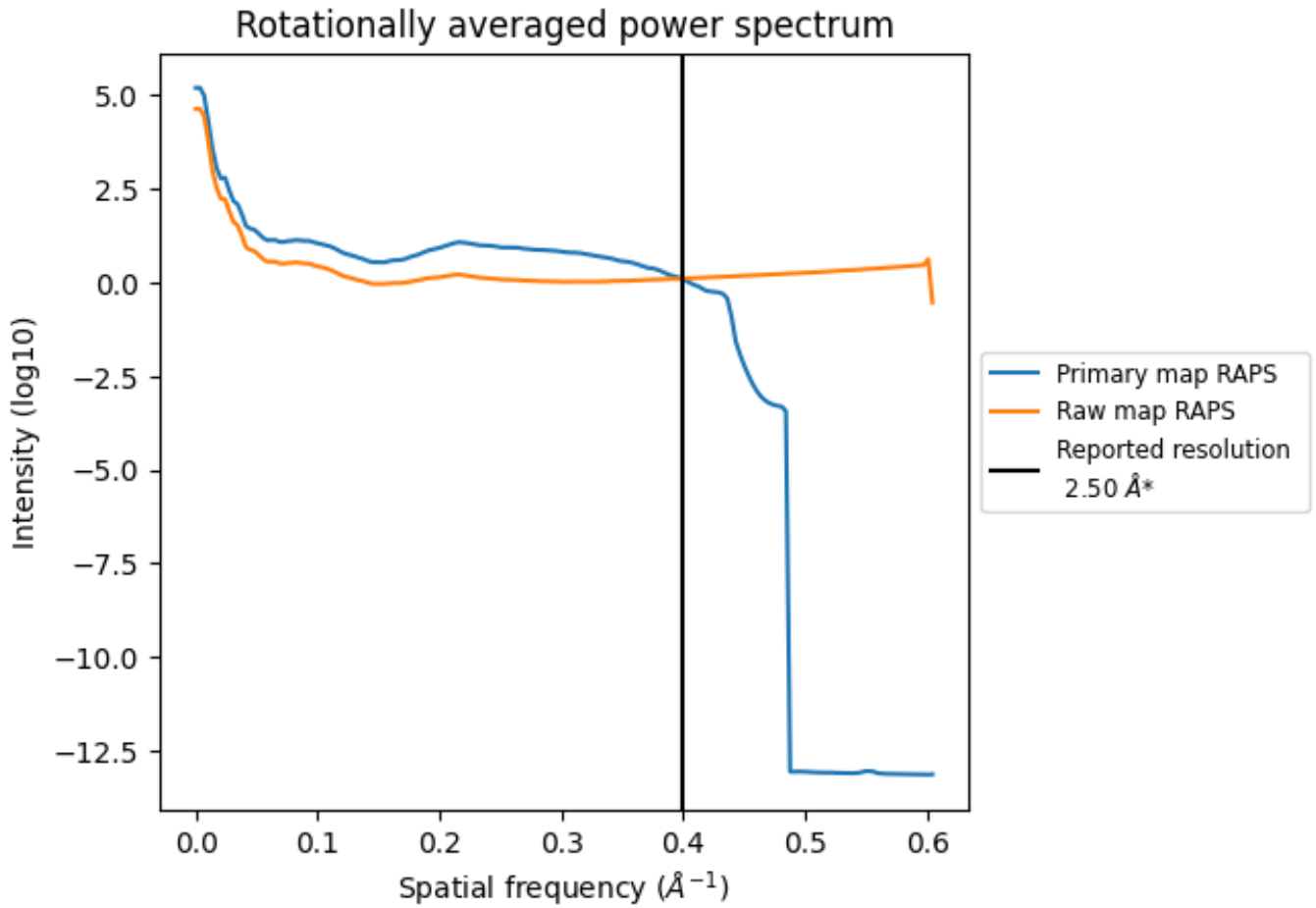
7.2 Volume estimate



The volume at the recommended contour level is 76 nm^3; this corresponds to an approximate mass of 69 kDa.

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

7.3 Rotationally averaged power spectrum (i)

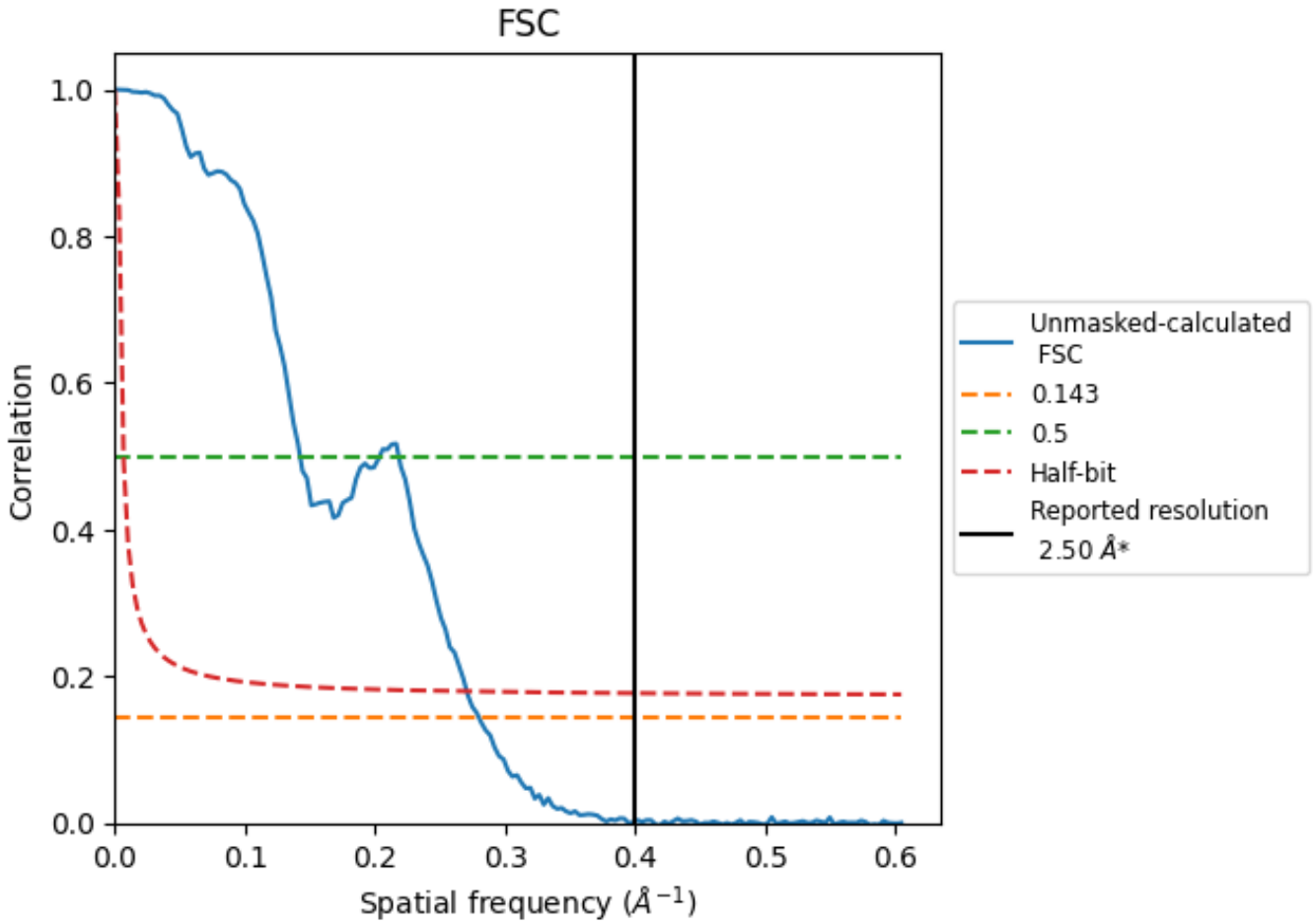


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

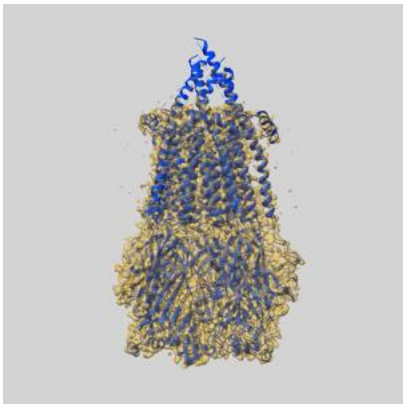
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	7.02	3.70

*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 3.57 differs from the reported value 2.5 by more than 10 %

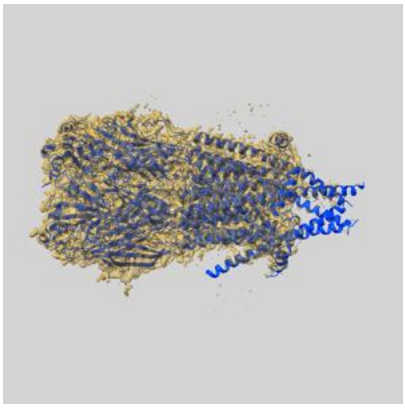
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14064 and PDB model 7QL5. Per-residue inclusion information can be found in section 3 on page 9.

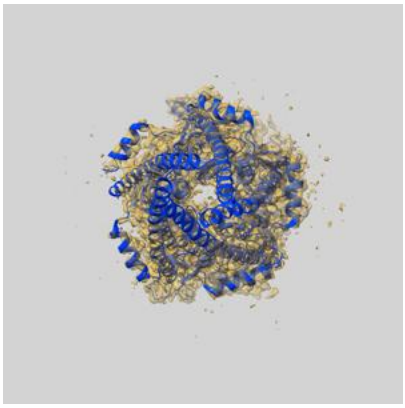
9.1 Map-model overlay



X



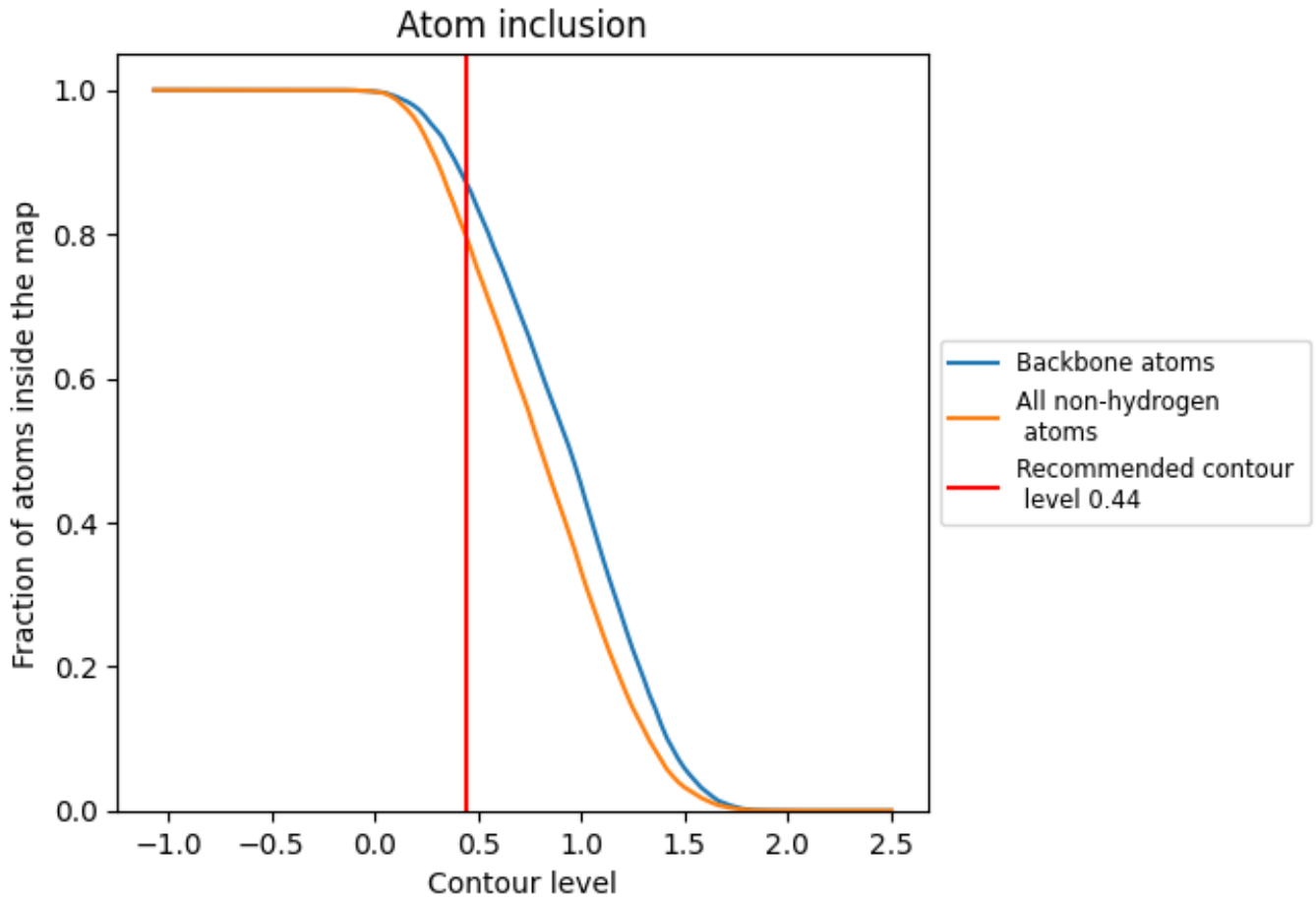
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.44 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 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.