



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:07 PM UTC

PDB ID : 7TJ9 / pdb_00007tj9
EMDB ID : EMD-25920
Title : Cryo-EM structure of the human Nax channel in complex with beta3 solved in GDN
Authors : Noland, C.L.; Kschonsak, M.; Ciferri, C.; Payandeh, J.
Deposited on : 2022-01-14
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

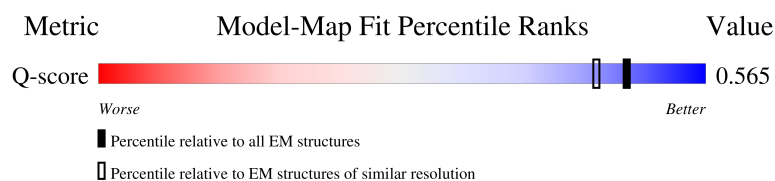
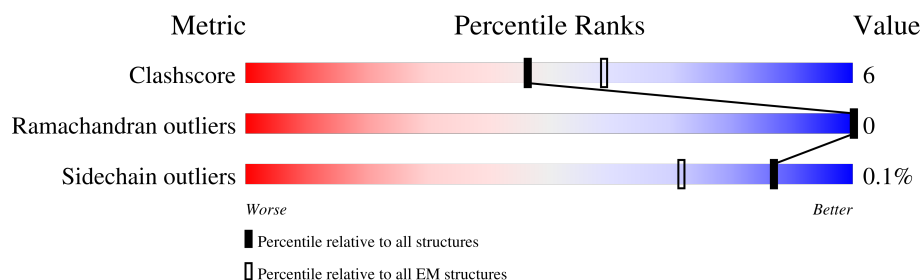
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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 $\leq 5\%$. 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	1737	
2	B	215	
3	C	2	

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	POV	A	2402	-	X	-	-
5	POV	A	2403	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10975 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 Sodium channel protein type 7 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1111	9054	6059	1415	1498	82	0	0

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-54	MET	-	expression tag	UNP Q01118
A	-53	TRP	-	expression tag	UNP Q01118
A	-52	SER	-	expression tag	UNP Q01118
A	-51	HIS	-	expression tag	UNP Q01118
A	-50	PRO	-	expression tag	UNP Q01118
A	-49	GLN	-	expression tag	UNP Q01118
A	-48	PHE	-	expression tag	UNP Q01118
A	-47	GLU	-	expression tag	UNP Q01118
A	-46	LYS	-	expression tag	UNP Q01118
A	-45	GLY	-	expression tag	UNP Q01118
A	-44	GLY	-	expression tag	UNP Q01118
A	-43	GLY	-	expression tag	UNP Q01118
A	-42	SER	-	expression tag	UNP Q01118
A	-41	GLY	-	expression tag	UNP Q01118
A	-40	GLY	-	expression tag	UNP Q01118
A	-39	GLY	-	expression tag	UNP Q01118
A	-38	SER	-	expression tag	UNP Q01118
A	-37	GLY	-	expression tag	UNP Q01118
A	-36	GLY	-	expression tag	UNP Q01118
A	-35	SER	-	expression tag	UNP Q01118
A	-34	ALA	-	expression tag	UNP Q01118
A	-33	TRP	-	expression tag	UNP Q01118
A	-32	SER	-	expression tag	UNP Q01118
A	-31	HIS	-	expression tag	UNP Q01118
A	-30	PRO	-	expression tag	UNP Q01118
A	-29	GLN	-	expression tag	UNP Q01118
A	-28	PHE	-	expression tag	UNP Q01118
A	-27	GLU	-	expression tag	UNP Q01118

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	LYS	-	expression tag	UNP Q01118
A	-25	PHE	-	expression tag	UNP Q01118
A	-24	PHE	-	expression tag	UNP Q01118
A	-23	SER	-	expression tag	UNP Q01118
A	-22	PHE	-	expression tag	UNP Q01118
A	-21	PHE	-	expression tag	UNP Q01118
A	-20	ASP	-	expression tag	UNP Q01118
A	-19	TYR	-	expression tag	UNP Q01118
A	-18	LYS	-	expression tag	UNP Q01118
A	-17	ASP	-	expression tag	UNP Q01118
A	-16	ASP	-	expression tag	UNP Q01118
A	-15	ASP	-	expression tag	UNP Q01118
A	-14	ASP	-	expression tag	UNP Q01118
A	-13	LYS	-	expression tag	UNP Q01118
A	-12	GLY	-	expression tag	UNP Q01118
A	-11	GLY	-	expression tag	UNP Q01118
A	-10	SER	-	expression tag	UNP Q01118
A	-9	GLY	-	expression tag	UNP Q01118
A	-8	GLY	-	expression tag	UNP Q01118
A	-7	ASP	-	expression tag	UNP Q01118
A	-6	TYR	-	expression tag	UNP Q01118
A	-5	LYS	-	expression tag	UNP Q01118
A	-4	ASP	-	expression tag	UNP Q01118
A	-3	ASP	-	expression tag	UNP Q01118
A	-2	ASP	-	expression tag	UNP Q01118
A	-1	ASP	-	expression tag	UNP Q01118
A	0	LYS	-	expression tag	UNP Q01118

- Molecule 2 is a protein called Sodium channel subunit beta-3.

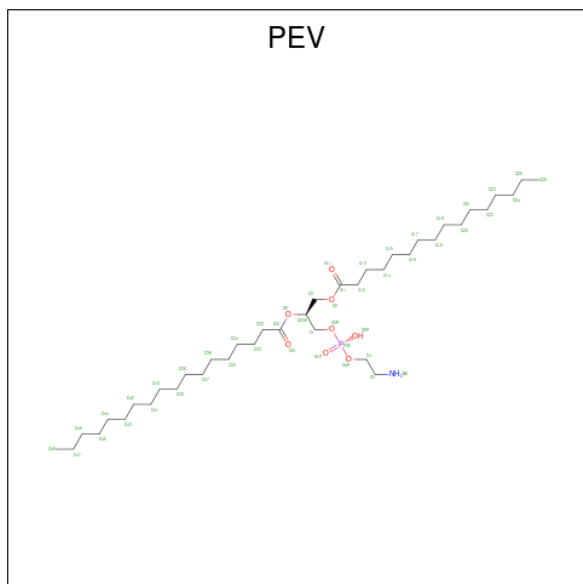
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1322	846	217	249	10		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



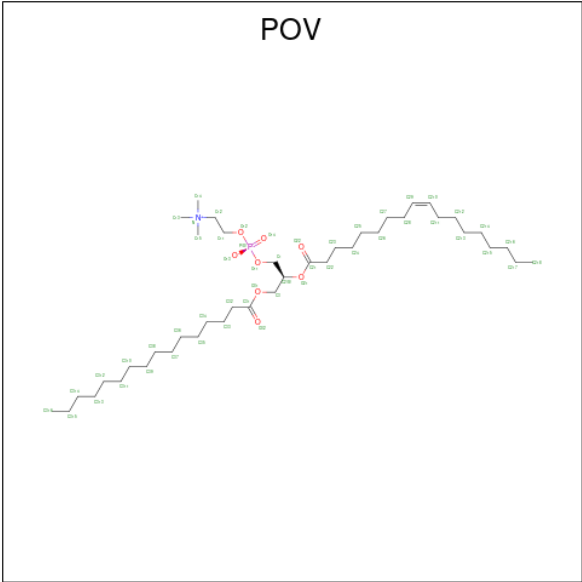
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



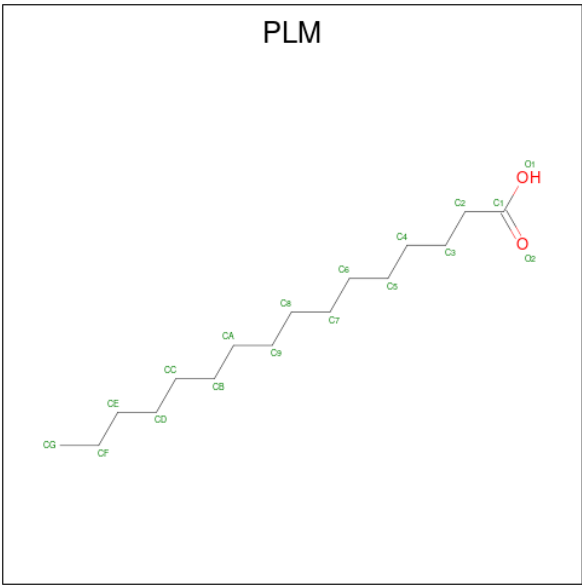
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	0	
			42	37	5		
5	A	1	Total	C		0	
			16	16			
5	A	1	Total	C	O	P	0
			26	19	6	1	

- Molecule 6 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



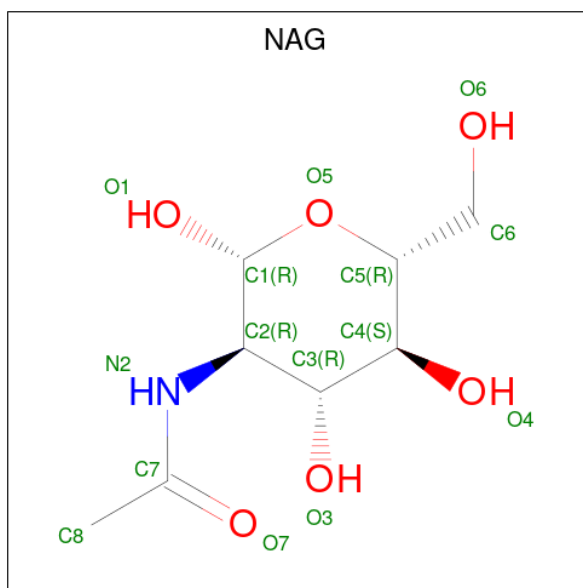
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C		0
			10	10		
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			15	13	2	
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			18	16	2	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



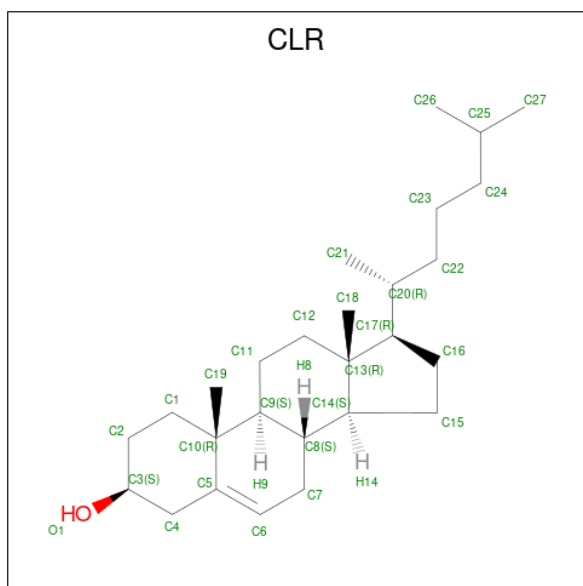
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	

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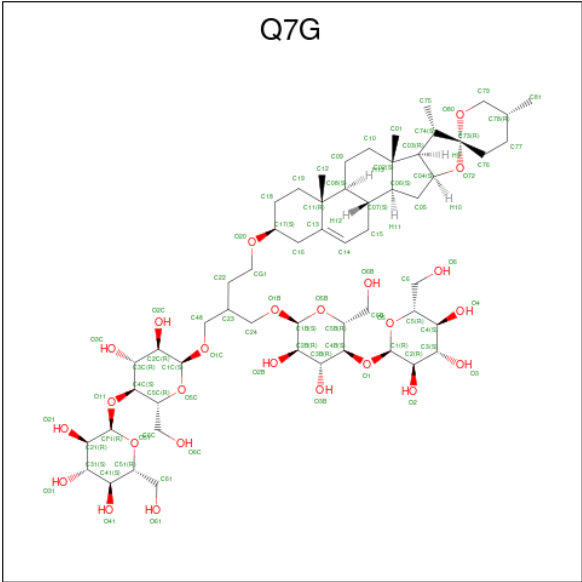
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O		0
			28	27	1		
8	A	1	Total	C	O		0
			28	27	1		

- Molecule 9 is 2-[[[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl]-4-[[[(3b eta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: $C_{56}H_{92}O_{25}$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			81	56	25	

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1420422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.067	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.969	Depositor
Minimum map value	-0.576	Depositor
Average map value	0.036	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.202	Depositor
Map size (Å)	298.1888, 298.1888, 298.1888	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1648, 1.1648, 1.1648	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PEV, CLR, PLM, POV, Q7G

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	0.27	0/9302	0.35	1/12611 (0.0%)
2	B	0.30	0/1350	0.45	0/1829
All	All	0.27	0/10652	0.37	1/14440 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1308	PHE	N-CA-C	-5.14	106.79	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9054	0	9251	119	0
2	B	1322	0	1299	16	0
3	C	28	0	25	1	0
4	A	147	0	231	1	0
5	A	84	0	130	1	0
6	A	133	0	227	0	0
7	A	14	0	13	0	0
7	B	56	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	56	0	92	4	0
9	A	81	0	0	2	0
All	All	10975	0	11320	135	0

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

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:MET:HE1	1:A:1355:HIS:HB3	1.72	0.72
2:B:93:GLN:NE2	7:B:302:NAG:H5	2.07	0.70
1:A:1485:LEU:HD21	5:A:2402:POV:H26	1.80	0.63
1:A:616:LEU:HD13	1:A:1187:MET:CE	2.29	0.62
1:A:1274:VAL:O	1:A:1274:VAL:HG23	2.01	0.61
1:A:207:THR:O	1:A:210:THR:OG1	2.17	0.59
1:A:616:LEU:HD22	1:A:1187:MET:HE3	1.83	0.59
1:A:1445:ASN:OD1	1:A:1446:SER:N	2.37	0.58
2:B:84:VAL:O	2:B:84:VAL:HG13	2.04	0.57
1:A:149:ASN:OD1	1:A:196:TYR:OH	2.21	0.57
1:A:1073:SER:O	1:A:1077:VAL:HG23	2.04	0.57
1:A:1241:GLN:O	1:A:1243:PHE:N	2.38	0.57
1:A:1287:ASN:O	1:A:1291:VAL:HG23	2.05	0.56
1:A:237:LEU:HD23	1:A:392:ILE:HG21	1.87	0.56
1:A:525:GLU:OE1	1:A:596:ARG:NH2	2.39	0.56
1:A:265:HIS:CE1	3:C:1:NAG:H81	2.41	0.56
2:B:111:THR:O	2:B:114:ASP:OD1	2.25	0.55
1:A:1258:MET:HE1	1:A:1355:HIS:CB	2.37	0.54
1:A:253:LEU:HD22	1:A:1268:MET:HB3	1.90	0.54
1:A:185:PHE:O	1:A:189:VAL:HG23	2.08	0.54
1:A:1171:CYS:O	1:A:1175:ASN:ND2	2.38	0.54
1:A:1091:THR:HG23	1:A:1092:SER:N	2.23	0.53
1:A:1091:THR:HG23	1:A:1092:SER:H	1.72	0.53
1:A:1318:ASP:OD1	1:A:1352:ARG:NE	2.42	0.53
1:A:1185:LEU:HD11	1:A:1484:TRP:HZ2	1.74	0.53
1:A:1408:GLU:HG2	1:A:1409:ALA:H	1.74	0.53
1:A:1187:MET:O	1:A:1190:THR:HG22	2.08	0.53
1:A:1350:LEU:O	1:A:1353:ILE:HG22	2.08	0.53
1:A:117:HIS:ND1	1:A:118:PRO:HD2	2.24	0.52
1:A:263:LEU:HD12	1:A:335:ASN:HA	1.90	0.52
1:A:353:ASP:OD1	1:A:688:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:PHE:O	1:A:1015:LEU:HD23	2.09	0.52
1:A:616:LEU:HD13	1:A:1187:MET:HE3	1.91	0.52
1:A:351:ALA:O	4:A:2411:PEV:N6	2.43	0.51
1:A:1383:ILE:HG21	1:A:1490:MET:HG3	1.93	0.51
1:A:600:MET:N	1:A:600:MET:SD	2.84	0.51
2:B:140:LEU:H	2:B:140:LEU:HD23	1.75	0.51
8:A:2417:CLR:H183	8:A:2417:CLR:H212	1.93	0.51
8:A:2416:CLR:H212	8:A:2416:CLR:H121	1.93	0.51
2:B:113:ASN:OD1	2:B:113:ASN:C	2.53	0.50
2:B:107:VAL:HG13	2:B:110:VAL:HG22	1.93	0.50
1:A:583:GLU:O	1:A:587:ALA:HB2	2.12	0.50
1:A:1166:ASN:HD21	1:A:1169:MET:HE2	1.76	0.50
1:A:982:GLU:OE2	1:A:1036:ARG:NH2	2.45	0.49
1:A:1061:VAL:HG21	1:A:1191:VAL:HG21	1.94	0.49
1:A:125:LEU:HD23	1:A:129:LEU:HD23	1.93	0.49
1:A:268:PHE:HB2	1:A:323:VAL:HG22	1.93	0.49
1:A:240:VAL:HG21	1:A:392:ILE:HG13	1.94	0.49
1:A:1374:MET:SD	8:A:2417:CLR:H212	2.53	0.49
1:A:616:LEU:HD13	1:A:1187:MET:HE1	1.93	0.49
1:A:1072:PHE:O	1:A:1172:TYR:OH	2.30	0.49
1:A:582:ILE:HG22	1:A:582:ILE:O	2.12	0.49
1:A:1260:LEU:HD13	1:A:1293:LEU:HD23	1.95	0.49
1:A:1055:THR:HG21	1:A:1485:LEU:HD22	1.95	0.49
1:A:1271:ASP:OD1	1:A:1272:THR:N	2.45	0.49
1:A:1291:VAL:HG21	1:A:1329:LEU:HD22	1.94	0.49
1:A:519:VAL:HG22	1:A:603:ILE:HG12	1.94	0.48
1:A:1055:THR:O	1:A:1055:THR:HG22	2.13	0.48
1:A:1225:MET:HE2	1:A:1371:LEU:HD23	1.94	0.48
1:A:1043:ARG:O	1:A:1046:VAL:HG22	2.13	0.48
1:A:1261:ILE:HD13	1:A:1294:TYR:OH	2.12	0.48
1:A:1005:PHE:CE2	1:A:1009:ILE:HD11	2.49	0.48
2:B:172:TRP:NE1	2:B:176:GLU:OE2	2.45	0.48
2:B:69:GLY:C	2:B:70:LYS:HD3	2.39	0.47
1:A:253:LEU:HD23	1:A:256:MET:CE	2.45	0.47
1:A:586:LEU:HD23	1:A:586:LEU:O	2.15	0.46
1:A:1452:ASP:OD2	1:A:1455:LYS:N	2.48	0.46
1:A:268:PHE:N	1:A:321:VAL:O	2.48	0.46
1:A:560:HIS:HB3	1:A:561:PRO:HD3	1.96	0.46
1:A:996:PHE:O	1:A:1002:ARG:NH1	2.48	0.46
1:A:1270:ILE:O	1:A:1270:ILE:HG22	2.15	0.46
1:A:1123:MET:HE1	1:A:1133:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1488:VAL:O	1:A:1492:ILE:HG12	2.15	0.46
1:A:1465:ASP:OD1	1:A:1465:ASP:O	2.34	0.46
2:B:121:ASN:HD22	7:B:301:NAG:H62	1.81	0.46
1:A:107:ILE:HG23	1:A:108:ARG:N	2.31	0.46
1:A:140:LEU:N	1:A:141:PRO:HD3	2.32	0.45
1:A:573:ASP:O	1:A:577:VAL:HG23	2.17	0.45
1:A:1122:LYS:NZ	1:A:1441:ASP:OD1	2.48	0.45
1:A:1013:LEU:HA	1:A:1016:ILE:HG12	1.97	0.45
1:A:662:LYS:O	1:A:663:ASP:HB2	2.16	0.44
1:A:974:ILE:HD11	2:B:162:MET:HG3	2.00	0.44
1:A:240:VAL:HG23	9:A:2418:Q7G:O6B	2.17	0.44
1:A:1157:VAL:HG12	1:A:1157:VAL:O	2.18	0.44
1:A:372:ILE:HD12	1:A:372:ILE:H	1.82	0.44
1:A:597:LEU:O	1:A:597:LEU:HD23	2.18	0.44
1:A:642:ALA:O	1:A:677:SER:OG	2.24	0.44
1:A:1228:ASP:OD1	1:A:1229:SER:N	2.51	0.44
1:A:1252:ALA:O	1:A:1256:ILE:HG12	2.18	0.44
2:B:73:LEU:H	2:B:73:LEU:HD23	1.83	0.44
1:A:139:ASN:C	1:A:141:PRO:HD3	2.43	0.43
1:A:683:ARG:HE	1:A:688:GLU:HB3	1.84	0.43
1:A:1003:LEU:O	1:A:1007:VAL:HG23	2.18	0.43
1:A:105:ASN:OD1	1:A:106:CYS:N	2.51	0.43
1:A:523:THR:HG22	1:A:523:THR:O	2.18	0.43
1:A:1327:THR:O	1:A:1331:LEU:N	2.50	0.43
1:A:1004:ASP:OD1	1:A:1036:ARG:NH1	2.52	0.43
1:A:991:GLY:O	1:A:992:PHE:C	2.61	0.43
1:A:1282:ALA:O	1:A:1286:ILE:HG12	2.18	0.43
1:A:125:LEU:O	1:A:129:LEU:HD23	2.19	0.43
1:A:625:VAL:HG13	1:A:626:ALA:N	2.33	0.43
1:A:991:GLY:O	1:A:994:ALA:N	2.52	0.43
1:A:1088:ILE:HD11	1:A:1119:GLU:OE2	2.18	0.43
1:A:126:ILE:O	1:A:130:ILE:HG12	2.19	0.43
1:A:197:SER:OG	1:A:198:PRO:HD2	2.19	0.42
1:A:1274:VAL:O	1:A:1274:VAL:CG2	2.67	0.42
1:A:1408:GLU:O	1:A:1409:ALA:C	2.63	0.42
1:A:582:ILE:O	1:A:585:CYS:O	2.37	0.42
1:A:239:GLY:HA3	9:A:2418:Q7G:C6B	2.49	0.42
1:A:1018:LYS:CG	1:A:1027:ILE:HD11	2.50	0.42
1:A:1137:GLN:HG3	1:A:1142:ASN:O	2.19	0.42
2:B:121:ASN:ND2	7:B:301:NAG:H62	2.34	0.42
1:A:131:ASP:OD1	1:A:209:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:O	1:A:513:ILE:HG12	2.20	0.42
1:A:1024:LYS:N	1:A:1025:PRO:HD2	2.34	0.42
2:B:48:CYS:HB2	2:B:101:GLN:NE2	2.35	0.42
1:A:1162:HIS:HB2	1:A:1165:VAL:HG21	2.01	0.42
1:A:148:GLU:OE2	1:A:209:ARG:NH2	2.53	0.41
1:A:1223:LYS:HE3	1:A:1224:LEU:HD12	2.02	0.41
1:A:1268:MET:HE3	1:A:1346:GLN:HG2	2.02	0.41
1:A:1305:PHE:O	1:A:1307:CYS:N	2.52	0.41
1:A:1337:SER:O	1:A:1338:TYR:C	2.62	0.41
1:A:1110:LEU:HD12	1:A:1110:LEU:O	2.19	0.41
1:A:1038:LEU:HD22	1:A:1048:VAL:HG21	2.02	0.41
1:A:1491:TYR:O	1:A:1495:VAL:HG23	2.20	0.41
1:A:1007:VAL:HG11	1:A:1036:ARG:HD3	2.02	0.41
1:A:1225:MET:HG2	8:A:2417:CLR:C19	2.51	0.41
1:A:583:GLU:O	1:A:584:LEU:C	2.64	0.41
1:A:1183:LEU:HB3	1:A:1184:PRO:HD3	2.02	0.41
2:B:112:LEU:H	2:B:112:LEU:HD23	1.85	0.41
1:A:216:ILE:O	1:A:220:ASN:ND2	2.49	0.40
1:A:1069:TRP:NE1	1:A:1180:GLY:O	2.52	0.40
2:B:65:ARG:HB2	2:B:71:ASP:OD1	2.20	0.40
1:A:318:GLU:HG2	2:B:135:VAL:HG21	2.04	0.40
1:A:1031:PHE:CE2	1:A:1400:TYR:HB2	2.55	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	1103/1737 (64%)	1047 (95%)	56 (5%)	0	100	100
2	B	160/215 (74%)	153 (96%)	7 (4%)	0	100	100
All	All	1263/1952 (65%)	1200 (95%)	63 (5%)	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	1003/1561 (64%)	1003 (100%)	0	100	100
2	B	150/195 (77%)	149 (99%)	1 (1%)	76	92
All	All	1153/1756 (66%)	1152 (100%)	1 (0%)	87	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	113	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	ASN
1	A	1166	ASN
1	A	1207	ASN
2	B	93	GLN

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](#)

2 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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.64	0	17,19,21	1.19	1 (5%)
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	0.88	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	3.60	117.02	112.19
3	C	2	NAG	C4-C3-C2	-2.32	107.61	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

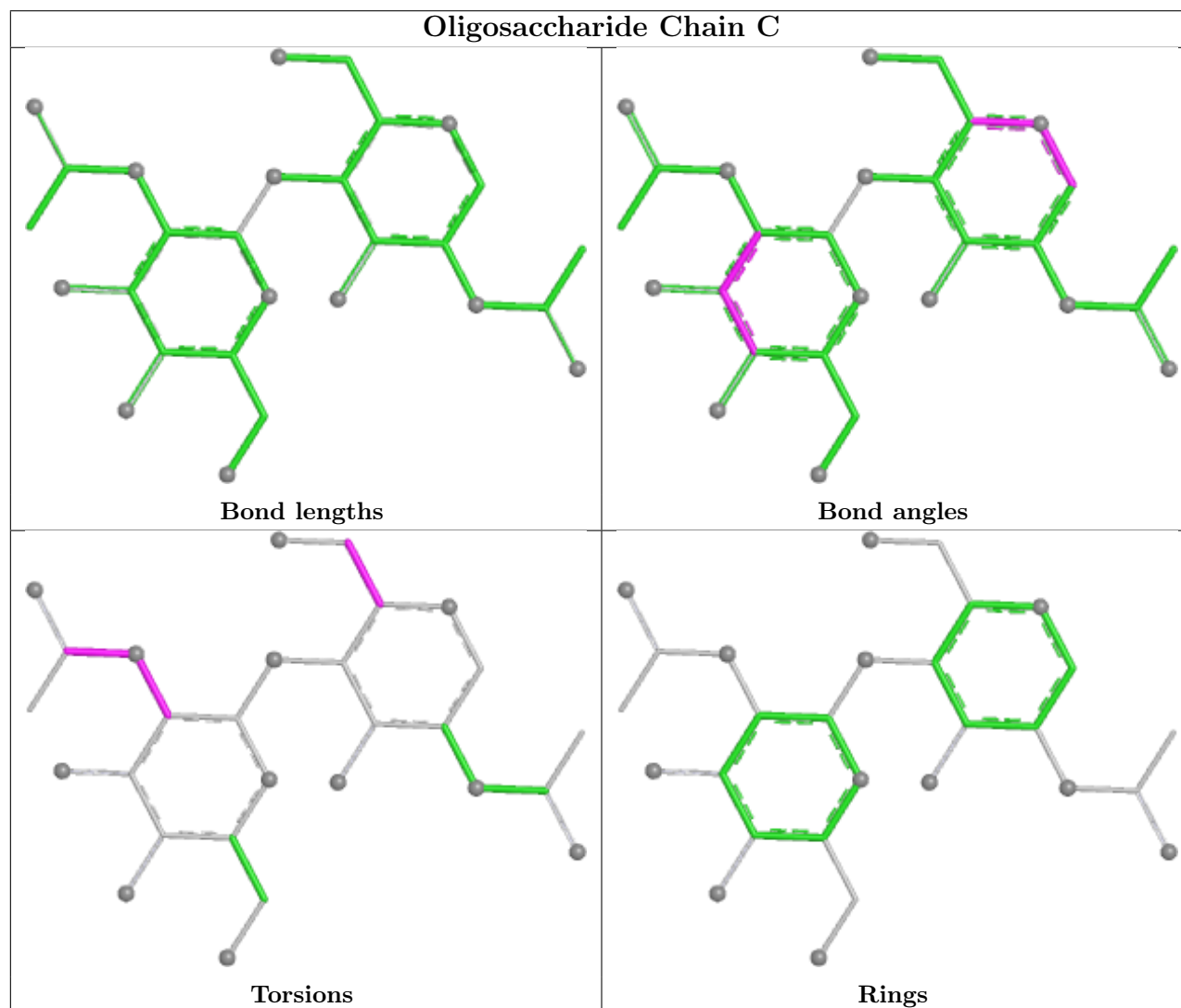
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	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.



5.6 Ligand geometry [i](#)

22 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
7	NAG	A	2412	1	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
8	CLR	A	2416	-	31,31,31	1.92	7 (22%)	48,48,48	1.86	12 (25%)
6	PLM	A	2415	-	17,17,17	0.86	1 (5%)	17,17,17	0.76	2 (11%)
4	PEV	A	2411	-	48,48,48	2.14	11 (22%)	51,53,53	1.20	2 (3%)
7	NAG	B	301	2	14,14,15	0.45	0	17,19,21	1.15	1 (5%)
5	POV	A	2408	-	25,25,51	3.14	18 (72%)	28,28,59	0.92	1 (3%)
8	CLR	A	2417	-	31,31,31	2.22	9 (29%)	48,48,48	2.05	19 (39%)
7	NAG	B	303	2	14,14,15	0.32	0	17,19,21	1.07	2 (11%)
6	PLM	A	2407	-	9,9,17	0.28	0	8,8,17	0.15	0
6	PLM	A	2413	-	17,17,17	0.87	1 (5%)	17,17,17	0.76	2 (11%)
6	PLM	A	2414	-	17,17,17	0.88	1 (5%)	17,17,17	0.75	2 (11%)
4	PEV	A	2401	-	48,48,48	2.17	11 (22%)	51,53,53	1.15	2 (3%)
6	PLM	A	2410	-	14,14,17	1.05	1 (7%)	14,14,17	0.96	2 (14%)
6	PLM	A	2409	-	17,17,17	0.83	1 (5%)	17,17,17	0.73	2 (11%)
6	PLM	A	2406	-	17,17,17	0.78	1 (5%)	17,17,17	0.76	2 (11%)
6	PLM	A	2404	-	17,17,17	0.72	1 (5%)	17,17,17	0.75	2 (11%)
5	POV	A	2403	-	15,15,51	2.70	13 (86%)	14,14,59	0.70	0
4	PEV	A	2405	-	48,48,48	2.18	11 (22%)	51,53,53	1.16	2 (3%)
7	NAG	B	304	2	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
5	POV	A	2402	-	41,41,51	2.89	32 (78%)	43,43,59	1.01	2 (4%)
9	Q7G	A	2418	-	90,90,90	2.26	18 (20%)	134,138,138	1.87	24 (17%)
7	NAG	B	302	2	14,14,15	0.34	0	17,19,21	0.90	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
7	NAG	A	2412	1	-	2/6/23/26	0/1/1/1
8	CLR	A	2416	-	-	3/10/68/68	0/4/4/4
6	PLM	A	2415	-	-	8/15/15/15	-
4	PEV	A	2411	-	-	28/52/52/52	-
7	NAG	B	301	2	-	5/6/23/26	0/1/1/1
5	POV	A	2408	-	-	9/24/24/55	-
8	CLR	A	2417	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	303	2	-	5/6/23/26	0/1/1/1
6	PLM	A	2407	-	-	2/7/7/15	-
6	PLM	A	2413	-	-	4/15/15/15	-
6	PLM	A	2414	-	-	2/15/15/15	-
4	PEV	A	2401	-	-	24/52/52/52	-
6	PLM	A	2410	-	-	7/12/12/15	-
6	PLM	A	2409	-	-	6/15/15/15	-
6	PLM	A	2406	-	-	6/15/15/15	-
6	PLM	A	2404	-	-	6/15/15/15	-
5	POV	A	2403	-	-	4/13/13/55	-
4	PEV	A	2405	-	-	21/52/52/52	-
7	NAG	B	304	2	-	3/6/23/26	0/1/1/1
5	POV	A	2402	-	-	18/43/43/55	-
9	Q7G	A	2418	-	-	18/32/200/200	0/10/10/10
7	NAG	B	302	2	-	0/6/23/26	0/1/1/1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2418	Q7G	C10-C09	9.34	1.72	1.53
5	A	2408	POV	P-O14	7.95	1.75	1.50
9	A	2418	Q7G	O72-C73	7.39	1.58	1.42
8	A	2417	CLR	C10-C9	7.09	1.67	1.56
9	A	2418	Q7G	C02-C06	-6.74	1.42	1.55
9	A	2418	Q7G	C15-C14	6.56	1.63	1.50
5	A	2402	POV	O31-C31	6.07	1.51	1.33
5	A	2408	POV	O31-C31	6.02	1.50	1.33
5	A	2402	POV	O21-C21	5.93	1.51	1.34
5	A	2403	POV	C29-C210	5.73	1.64	1.31
9	A	2418	Q7G	C07-C06	-5.43	1.43	1.53
5	A	2408	POV	P-O11	5.19	1.76	1.60
5	A	2402	POV	C32-C31	5.12	1.65	1.50
4	A	2405	PEV	O2-C2	-5.11	1.34	1.46
4	A	2411	PEV	O2-C2	-5.06	1.34	1.46
5	A	2402	POV	C22-C21	4.79	1.64	1.50
4	A	2401	PEV	O2-C2	-4.76	1.35	1.46
4	A	2405	PEV	O3-C11	4.75	1.47	1.33
4	A	2401	PEV	O2-C31	4.74	1.47	1.34
4	A	2401	PEV	O3-C11	4.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2416	CLR	C10-C9	4.69	1.63	1.56
5	A	2408	POV	C32-C31	4.67	1.64	1.50
4	A	2411	PEV	O3-C11	4.67	1.46	1.33
8	A	2417	CLR	C13-C17	4.66	1.63	1.55
4	A	2411	PEV	O2-C31	4.63	1.47	1.34
4	A	2405	PEV	O2-C31	4.54	1.47	1.34
8	A	2416	CLR	C13-C17	4.24	1.62	1.55
5	A	2402	POV	C1-C2	4.20	1.61	1.51
9	A	2418	Q7G	C03-C74	-4.11	1.42	1.54
9	A	2418	Q7G	C05-C06	3.70	1.61	1.54
8	A	2417	CLR	C4-C3	3.70	1.58	1.52
9	A	2418	Q7G	C05-C04	3.69	1.60	1.52
8	A	2416	CLR	C4-C3	3.67	1.58	1.52
4	A	2405	PEV	P-O4P	3.61	1.73	1.59
4	A	2401	PEV	C32-C31	3.60	1.61	1.50
4	A	2405	PEV	P-O3P	3.57	1.73	1.59
5	A	2402	POV	C3-C2	3.57	1.62	1.50
8	A	2417	CLR	C12-C11	3.56	1.60	1.53
4	A	2401	PEV	P-O4P	3.55	1.73	1.59
4	A	2401	PEV	P-O3P	3.54	1.73	1.59
5	A	2402	POV	C23-C22	3.53	1.65	1.52
4	A	2411	PEV	P-O4P	3.43	1.72	1.59
4	A	2411	PEV	C12-C11	3.41	1.60	1.50
4	A	2405	PEV	C32-C31	3.39	1.60	1.50
4	A	2405	PEV	C12-C11	3.39	1.60	1.50
5	A	2402	POV	C33-C32	3.37	1.64	1.52
9	A	2418	Q7G	C75-C74	3.37	1.60	1.53
4	A	2411	PEV	P-O3P	3.33	1.72	1.59
4	A	2401	PEV	C12-C11	3.30	1.60	1.50
9	A	2418	Q7G	C11-C13	3.30	1.59	1.52
9	A	2418	Q7G	C16-C13	3.29	1.58	1.51
4	A	2411	PEV	C32-C31	3.28	1.60	1.50
9	A	2418	Q7G	C22-CG1	3.28	1.62	1.50
5	A	2408	POV	C33-C32	3.27	1.64	1.52
8	A	2416	CLR	C8-C14	3.26	1.59	1.53
6	A	2410	PLM	C2-C1	3.23	1.58	1.50
9	A	2418	Q7G	C02-C03	3.19	1.61	1.56
9	A	2418	Q7G	C12-C11	-3.08	1.49	1.54
5	A	2402	POV	C27-C28	2.96	1.64	1.52
8	A	2417	CLR	C8-C14	2.90	1.59	1.53
9	A	2418	Q7G	C48-C23	2.89	1.62	1.51
5	A	2403	POV	C212-C211	2.88	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2413	PLM	C2-C1	2.84	1.57	1.50
5	A	2403	POV	C27-C28	2.81	1.64	1.52
6	A	2414	PLM	C2-C1	2.79	1.57	1.50
5	A	2402	POV	C24-C23	2.73	1.65	1.51
8	A	2416	CLR	C8-C9	2.72	1.58	1.53
5	A	2402	POV	C212-C211	2.71	1.63	1.52
6	A	2415	PLM	C2-C1	2.65	1.56	1.50
4	A	2411	PEV	C5-C4	2.64	1.60	1.49
4	A	2401	PEV	C5-C4	2.64	1.60	1.49
5	A	2402	POV	C25-C24	2.63	1.64	1.51
6	A	2409	PLM	C2-C1	2.61	1.56	1.50
5	A	2402	POV	C36-C35	2.61	1.64	1.51
5	A	2402	POV	O31-C3	2.60	1.51	1.45
5	A	2402	POV	C26-C25	2.60	1.64	1.51
4	A	2405	PEV	C5-C4	2.58	1.60	1.49
5	A	2403	POV	C28-C29	2.58	1.64	1.50
9	A	2418	Q7G	C76-C73	2.54	1.55	1.51
5	A	2408	POV	C38-C37	2.53	1.64	1.51
9	A	2418	Q7G	C19-C18	2.53	1.58	1.53
5	A	2402	POV	C27-C26	2.52	1.64	1.51
5	A	2402	POV	C38-C37	2.52	1.64	1.51
5	A	2408	POV	C36-C35	2.51	1.64	1.51
5	A	2403	POV	C213-C212	2.50	1.64	1.51
5	A	2402	POV	C35-C34	2.50	1.64	1.51
5	A	2403	POV	C211-C210	2.49	1.63	1.50
5	A	2402	POV	C34-C33	2.49	1.64	1.51
5	A	2402	POV	C214-C213	2.48	1.64	1.51
5	A	2408	POV	C2-C3	2.48	1.61	1.51
5	A	2402	POV	C39-C38	2.47	1.64	1.51
5	A	2402	POV	C39-C310	2.45	1.64	1.51
5	A	2408	POV	C2-C1	2.45	1.61	1.51
6	A	2406	PLM	C2-C1	2.44	1.56	1.50
5	A	2408	POV	C39-C38	2.44	1.63	1.51
5	A	2402	POV	C215-C214	2.44	1.63	1.51
5	A	2408	POV	C39-C310	2.44	1.63	1.51
5	A	2408	POV	C34-C33	2.43	1.63	1.51
5	A	2403	POV	C214-C213	2.43	1.63	1.51
5	A	2408	POV	C35-C34	2.43	1.63	1.51
9	A	2418	Q7G	C03-C04	-2.41	1.50	1.54
5	A	2402	POV	C311-C310	2.41	1.63	1.51
8	A	2417	CLR	C11-C9	2.38	1.57	1.53
5	A	2402	POV	C37-C36	2.37	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2402	POV	C213-C212	2.36	1.63	1.51
5	A	2408	POV	C37-C36	2.35	1.63	1.51
5	A	2403	POV	C27-C26	2.34	1.63	1.51
5	A	2408	POV	C311-C310	2.34	1.63	1.51
5	A	2402	POV	C313-C312	2.32	1.63	1.51
4	A	2405	PEV	C13-C12	2.31	1.60	1.52
8	A	2417	CLR	C1-C10	2.30	1.58	1.54
5	A	2403	POV	C25-C24	2.30	1.63	1.51
5	A	2403	POV	C26-C25	2.30	1.63	1.51
5	A	2402	POV	C211-C210	2.29	1.62	1.50
4	A	2411	PEV	P-O1P	2.29	1.58	1.50
5	A	2408	POV	C314-C313	2.29	1.63	1.51
5	A	2402	POV	C312-C311	2.28	1.63	1.51
5	A	2402	POV	C216-C215	2.27	1.63	1.51
5	A	2408	POV	C313-C312	2.27	1.63	1.51
4	A	2405	PEV	C33-C32	2.27	1.60	1.52
5	A	2402	POV	C314-C313	2.26	1.63	1.51
4	A	2405	PEV	P-O1P	2.26	1.58	1.50
4	A	2401	PEV	P-O1P	2.26	1.58	1.50
5	A	2403	POV	C24-C23	2.25	1.63	1.51
8	A	2416	CLR	C4-C5	2.25	1.56	1.51
5	A	2408	POV	C312-C311	2.25	1.63	1.51
4	A	2401	PEV	C33-C32	2.24	1.60	1.52
8	A	2417	CLR	C4-C5	2.23	1.56	1.51
4	A	2401	PEV	C13-C12	2.23	1.60	1.52
4	A	2411	PEV	C13-C12	2.21	1.60	1.52
5	A	2402	POV	C28-C29	2.20	1.62	1.50
8	A	2416	CLR	C1-C10	2.18	1.58	1.54
8	A	2417	CLR	C8-C9	2.13	1.57	1.53
6	A	2404	PLM	C2-C1	2.12	1.55	1.50
5	A	2403	POV	C216-C215	2.11	1.65	1.50
4	A	2411	PEV	C33-C32	2.10	1.59	1.52
5	A	2403	POV	C215-C214	2.09	1.64	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2418	Q7G	C76-C73-C74	8.69	131.39	115.66
9	A	2418	Q7G	O80-C73-O72	-6.91	93.43	109.88
8	A	2417	CLR	C3-C4-C5	6.19	121.92	112.05
8	A	2416	CLR	C3-C4-C5	6.02	121.64	112.05
9	A	2418	Q7G	O61-C61-C51	5.75	130.90	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2418	Q7G	O80-C73-C74	-5.65	90.40	107.26
9	A	2418	Q7G	O72-C73-C76	4.57	117.81	108.54
9	A	2418	Q7G	C05-C06-C07	-4.39	111.02	119.53
4	A	2405	PEV	O2-C31-C32	4.23	120.64	111.48
8	A	2417	CLR	C18-C13-C12	-4.15	104.49	110.61
4	A	2401	PEV	O2-C31-C32	4.14	120.43	111.48
8	A	2416	CLR	C18-C13-C12	-4.12	104.53	110.61
8	A	2417	CLR	C11-C9-C8	-4.12	106.03	111.78
9	A	2418	Q7G	O1-C4B-C3B	4.08	117.60	107.23
4	A	2411	PEV	O2-C31-C32	3.96	120.05	111.48
5	A	2402	POV	O21-C21-C22	3.92	119.96	111.48
8	A	2416	CLR	C1-C10-C9	3.88	113.88	108.74
9	A	2418	Q7G	CF1-O11-C4C	-3.51	109.66	117.98
9	A	2418	Q7G	C09-C10-C02	-3.47	106.89	112.74
9	A	2418	Q7G	C15-C07-C06	-3.44	106.06	110.93
9	A	2418	Q7G	C09-C08-C11	-3.34	108.97	113.08
8	A	2416	CLR	C13-C17-C20	-3.30	114.40	119.50
8	A	2417	CLR	C15-C14-C8	3.20	124.20	119.10
9	A	2418	Q7G	C3C-C4C-C5C	3.18	117.97	110.93
4	A	2411	PEV	O3-C11-C12	3.17	121.51	111.83
8	A	2417	CLR	C4-C5-C6	3.15	124.84	120.57
8	A	2416	CLR	C4-C5-C6	3.13	124.81	120.57
7	B	303	NAG	C1-O5-C5	3.08	116.32	112.19
4	A	2401	PEV	O3-C11-C12	3.01	121.02	111.83
5	A	2408	POV	O31-C31-C32	3.00	120.99	111.83
5	A	2402	POV	O31-C31-C32	2.98	120.92	111.83
9	A	2418	Q7G	C75-C74-C73	-2.96	110.16	114.94
8	A	2417	CLR	C2-C1-C10	2.89	118.95	112.78
9	A	2418	Q7G	O72-C04-C03	2.80	108.92	105.12
8	A	2417	CLR	C17-C13-C14	2.79	103.30	100.10
4	A	2405	PEV	O3-C11-C12	2.77	120.27	111.83
9	A	2418	Q7G	C73-C74-C03	2.73	107.38	103.37
6	A	2410	PLM	O2-C1-C2	-2.72	114.48	123.09
8	A	2417	CLR	C10-C5-C6	-2.70	118.98	122.93
9	A	2418	Q7G	O5C-C1C-C2C	-2.69	104.83	110.37
8	A	2417	CLR	C13-C17-C20	-2.67	115.38	119.50
8	A	2417	CLR	C7-C8-C14	2.63	114.65	110.93
9	A	2418	Q7G	C10-C02-C03	-2.60	111.66	115.36
8	A	2417	CLR	C1-C10-C9	2.60	112.17	108.74
8	A	2417	CLR	C11-C9-C10	2.59	116.28	113.08
8	A	2417	CLR	C12-C11-C9	2.54	117.45	113.14
7	B	301	NAG	C1-O5-C5	2.47	115.50	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2416	CLR	C2-C1-C10	2.46	118.02	112.78
8	A	2417	CLR	C19-C10-C9	-2.44	108.92	111.66
7	B	303	NAG	C1-C2-N2	-2.43	106.60	110.43
9	A	2418	Q7G	C77-C76-C73	-2.43	108.12	111.93
9	A	2418	Q7G	C11-C08-C07	-2.40	109.21	112.71
7	B	304	NAG	C4-C3-C2	-2.38	107.53	111.02
8	A	2417	CLR	C15-C14-C13	-2.38	101.04	103.84
8	A	2416	CLR	C15-C14-C13	-2.38	101.05	103.84
8	A	2416	CLR	C19-C10-C9	-2.37	109.00	111.66
8	A	2417	CLR	C19-C10-C5	-2.30	104.86	108.38
8	A	2417	CLR	C1-C10-C5	2.30	112.72	108.74
9	A	2418	Q7G	O1-C1-O5	-2.30	104.63	110.69
7	A	2412	NAG	C4-C3-C2	-2.28	107.68	111.02
9	A	2418	Q7G	C74-C03-C04	2.27	107.92	104.27
9	A	2418	Q7G	C75-C74-C03	-2.26	109.98	114.50
8	A	2416	CLR	C14-C8-C9	2.26	112.04	109.09
8	A	2416	CLR	C15-C14-C8	2.23	122.66	119.10
6	A	2406	PLM	O1-C1-O2	2.23	129.06	123.33
8	A	2417	CLR	C10-C9-C8	2.22	115.97	112.71
9	A	2418	Q7G	C06-C05-C04	-2.21	98.55	102.40
6	A	2404	PLM	O1-C1-O2	2.21	129.02	123.33
9	A	2418	Q7G	C18-C17-C16	-2.20	107.92	110.97
6	A	2415	PLM	O1-C1-O2	2.19	128.96	123.33
8	A	2416	CLR	C12-C11-C9	2.18	116.84	113.14
6	A	2413	PLM	O1-C1-O2	2.18	128.94	123.33
8	A	2416	CLR	C7-C8-C14	2.17	114.01	110.93
6	A	2414	PLM	O1-C1-O2	2.14	128.82	123.33
6	A	2409	PLM	O1-C1-O2	2.11	128.75	123.33
6	A	2406	PLM	O2-C1-C2	-2.09	116.45	123.09
6	A	2415	PLM	O2-C1-C2	-2.06	116.56	123.09
6	A	2404	PLM	O2-C1-C2	-2.05	116.60	123.09
6	A	2409	PLM	O2-C1-C2	-2.04	116.61	123.09
6	A	2414	PLM	O2-C1-C2	-2.02	116.68	123.09
6	A	2413	PLM	O2-C1-C2	-2.02	116.70	123.09
6	A	2410	PLM	O1-C1-O2	2.01	128.50	123.33
8	A	2417	CLR	C19-C10-C1	-2.00	106.38	109.43

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2401	PEV	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	2401	PEV	O31-C31-O2-C2
4	A	2401	PEV	C4-O4P-P-O3P
4	A	2401	PEV	O4P-C4-C5-N6
4	A	2405	PEV	C32-C31-O2-C2
4	A	2411	PEV	C32-C31-O2-C2
4	A	2411	PEV	C1-O3P-P-O1P
4	A	2411	PEV	C1-O3P-P-O2P
4	A	2411	PEV	C1-O3P-P-O4P
4	A	2411	PEV	O4P-C4-C5-N6
5	A	2402	POV	O11-C1-C2-O21
5	A	2402	POV	C22-C21-O21-C2
7	B	301	NAG	C1-C2-N2-C7
7	B	301	NAG	C8-C7-N2-C2
7	B	301	NAG	O7-C7-N2-C2
7	B	303	NAG	C3-C2-N2-C7
7	B	303	NAG	C8-C7-N2-C2
7	B	303	NAG	O7-C7-N2-C2
9	A	2418	Q7G	C16-C17-O20-CG1
9	A	2418	Q7G	O5C-C1C-O1C-C48
9	A	2418	Q7G	C48-C23-C24-O1B
9	A	2418	Q7G	C3B-C4B-O1-C1
4	A	2401	PEV	O11-C11-O3-C3
4	A	2401	PEV	C12-C11-O3-C3
4	A	2405	PEV	O31-C31-O2-C2
4	A	2411	PEV	O31-C31-O2-C2
4	A	2405	PEV	C12-C11-O3-C3
5	A	2402	POV	O22-C21-O21-C2
7	A	2412	NAG	C8-C7-N2-C2
7	A	2412	NAG	O7-C7-N2-C2
4	A	2405	PEV	O11-C11-O3-C3
7	B	301	NAG	O5-C5-C6-O6
9	A	2418	Q7G	O51-C51-C61-O61
9	A	2418	Q7G	C41-C51-C61-O61
5	A	2402	POV	C32-C31-O31-C3
5	A	2408	POV	C32-C31-O31-C3
9	A	2418	Q7G	C22-C23-C24-O1B
9	A	2418	Q7G	C2C-C1C-O1C-C48
7	B	303	NAG	O5-C5-C6-O6
7	B	303	NAG	C4-C5-C6-O6
7	B	301	NAG	C4-C5-C6-O6
4	A	2411	PEV	C12-C11-O3-C3
6	A	2404	PLM	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
7	B	304	NAG	C8-C7-N2-C2
5	A	2402	POV	O32-C31-O31-C3
8	A	2417	CLR	C22-C23-C24-C25
5	A	2408	POV	O32-C31-O31-C3
4	A	2411	PEV	O11-C11-O3-C3
8	A	2417	CLR	C21-C20-C22-C23
7	B	304	NAG	O7-C7-N2-C2
4	A	2401	PEV	C31-C32-C33-C34
9	A	2418	Q7G	O5C-C5C-C6C-O6C
9	A	2418	Q7G	C4C-C5C-C6C-O6C
6	A	2410	PLM	C4-C5-C6-C7
4	A	2405	PEV	C18-C19-C20-C21
4	A	2411	PEV	C16-C17-C18-C19
6	A	2404	PLM	CB-CC-CD-CE
5	A	2408	POV	C39-C310-C311-C312
4	A	2405	PEV	C11-C12-C13-C14
8	A	2416	CLR	C20-C22-C23-C24
5	A	2402	POV	C31-C32-C33-C34
6	A	2409	PLM	C8-C9-CA-CB
4	A	2401	PEV	C18-C19-C20-C21
4	A	2411	PEV	C13-C14-C15-C16
6	A	2410	PLM	C5-C6-C7-C8
4	A	2401	PEV	C39-C40-C41-C42
6	A	2409	PLM	CA-CB-CC-CD
6	A	2415	PLM	C7-C8-C9-CA
4	A	2401	PEV	C32-C33-C34-C35
6	A	2406	PLM	CA-CB-CC-CD
4	A	2401	PEV	C21-C22-C23-C24
4	A	2405	PEV	C42-C43-C44-C45
4	A	2405	PEV	C33-C34-C35-C36
4	A	2405	PEV	C16-C17-C18-C19
4	A	2401	PEV	C11-C12-C13-C14
4	A	2411	PEV	C14-C15-C16-C17
5	A	2403	POV	C26-C27-C28-C29
6	A	2409	PLM	C1-C2-C3-C4
4	A	2401	PEV	C35-C36-C37-C38
5	A	2408	POV	C34-C35-C36-C37
6	A	2415	PLM	C6-C7-C8-C9
6	A	2404	PLM	C8-C9-CA-CB
4	A	2401	PEV	C14-C15-C16-C17
5	A	2402	POV	C210-C211-C212-C213
4	A	2401	PEV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	A	2418	Q7G	O5B-C5B-C6B-O6B
5	A	2402	POV	C3-C2-O21-C21
5	A	2402	POV	C26-C27-C28-C29
4	A	2411	PEV	C36-C37-C38-C39
5	A	2408	POV	C312-C313-C314-C315
4	A	2401	PEV	C37-C38-C39-C40
5	A	2408	POV	C313-C314-C315-C316
4	A	2411	PEV	C21-C22-C23-C24
5	A	2408	POV	C33-C34-C35-C36
6	A	2409	PLM	C3-C4-C5-C6
4	A	2411	PEV	C23-C24-C25-C26
4	A	2411	PEV	C20-C21-C22-C23
5	A	2402	POV	C212-C213-C214-C215
5	A	2403	POV	C25-C26-C27-C28
6	A	2406	PLM	C8-C9-CA-CB
4	A	2405	PEV	C31-C32-C33-C34
4	A	2401	PEV	C44-C45-C46-C47
4	A	2401	PEV	C19-C20-C21-C22
6	A	2410	PLM	C6-C7-C8-C9
4	A	2411	PEV	O3P-C1-C2-O2
4	A	2411	PEV	C33-C34-C35-C36
4	A	2401	PEV	C38-C39-C40-C41
6	A	2413	PLM	C1-C2-C3-C4
5	A	2403	POV	C23-C24-C25-C26
4	A	2405	PEV	C44-C45-C46-C47
5	A	2402	POV	C25-C26-C27-C28
4	A	2411	PEV	C44-C45-C46-C47
5	A	2402	POV	C37-C38-C39-C310
4	A	2411	PEV	C40-C41-C42-C43
6	A	2410	PLM	C8-C9-CA-CB
5	A	2408	POV	C1-C2-C3-O31
4	A	2405	PEV	C39-C40-C41-C42
4	A	2405	PEV	C34-C35-C36-C37
4	A	2405	PEV	C35-C36-C37-C38
4	A	2401	PEV	O2-C2-C3-O3
4	A	2411	PEV	C45-C46-C47-C48
9	A	2418	Q7G	O51-CF1-O11-C4C
4	A	2401	PEV	C1-O3P-P-O1P
4	A	2405	PEV	C4-O4P-P-O3P
4	A	2405	PEV	C4-O4P-P-O1P
4	A	2405	PEV	C4-O4P-P-O2P
6	A	2409	PLM	CD-CE-CF-CG

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Mol	Chain	Res	Type	Atoms
6	A	2413	PLM	C2-C3-C4-C5
4	A	2411	PEV	C1-C2-O2-C31
4	A	2401	PEV	C15-C16-C17-C18
8	A	2416	CLR	C23-C24-C25-C27
6	A	2404	PLM	C3-C4-C5-C6
4	A	2411	PEV	C31-C32-C33-C34
4	A	2411	PEV	C17-C18-C19-C20
6	A	2406	PLM	CB-CC-CD-CE
9	A	2418	Q7G	C23-C22-CG1-O20
4	A	2401	PEV	C1-C2-C3-O3
5	A	2402	POV	C23-C24-C25-C26
6	A	2407	PLM	C8-C9-CA-CB
8	A	2417	CLR	C23-C24-C25-C26
9	A	2418	Q7G	CG1-C22-C23-C48
5	A	2402	POV	C213-C214-C215-C216
4	A	2411	PEV	C18-C19-C20-C21
5	A	2403	POV	C213-C214-C215-C216
5	A	2408	POV	C32-C33-C34-C35
4	A	2405	PEV	C3-C2-O2-C31
9	A	2418	Q7G	C21-CF1-O11-C4C
6	A	2404	PLM	O2-C1-C2-C3
6	A	2415	PLM	CB-CC-CD-CE
6	A	2406	PLM	O2-C1-C2-C3
6	A	2410	PLM	O2-C1-C2-C3
6	A	2407	PLM	CA-CB-CC-CD
6	A	2404	PLM	O1-C1-C2-C3
6	A	2410	PLM	O1-C1-C2-C3
5	A	2402	POV	C33-C34-C35-C36
6	A	2415	PLM	O2-C1-C2-C3
4	A	2411	PEV	O3-C11-C12-C13
7	B	304	NAG	C1-C2-N2-C7
9	A	2418	Q7G	C22-CG1-O20-C17
6	A	2410	PLM	C3-C4-C5-C6
6	A	2415	PLM	O1-C1-C2-C3
4	A	2411	PEV	C42-C43-C44-C45
6	A	2406	PLM	C4-C5-C6-C7
6	A	2406	PLM	O1-C1-C2-C3
4	A	2411	PEV	O3P-C1-C2-C3
4	A	2401	PEV	C23-C24-C25-C26
6	A	2413	PLM	O1-C1-C2-C3
6	A	2413	PLM	O2-C1-C2-C3
6	A	2415	PLM	C5-C6-C7-C8

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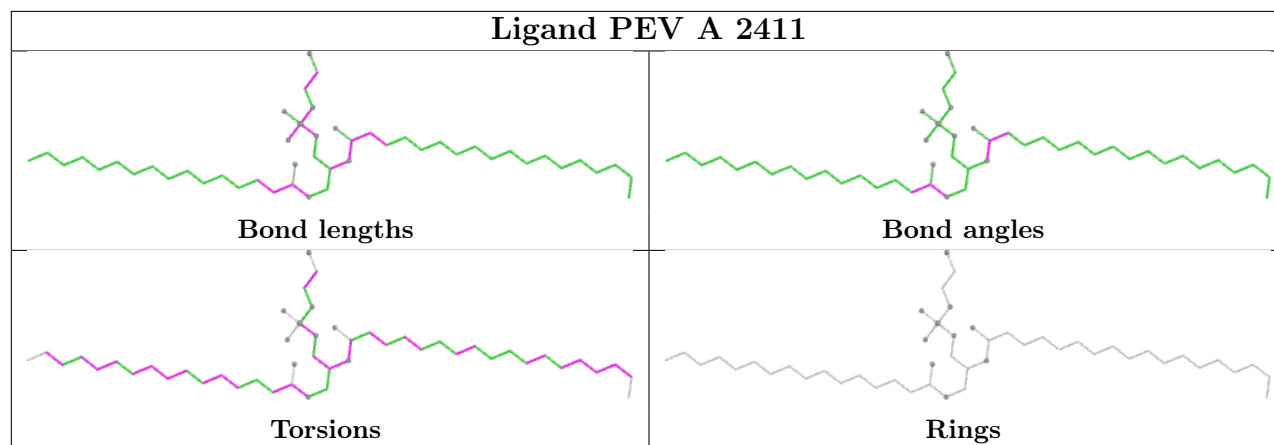
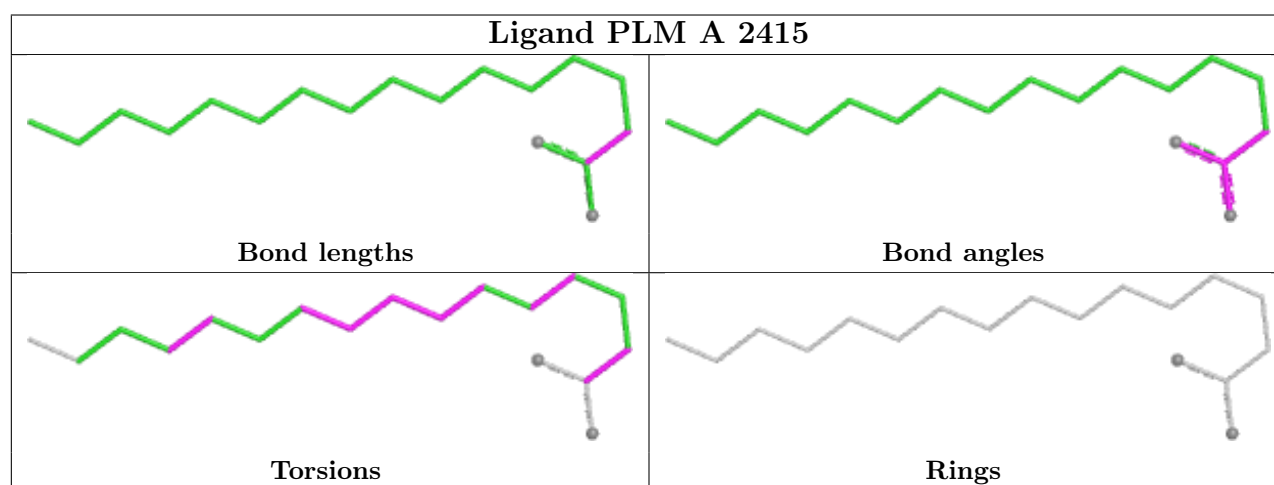
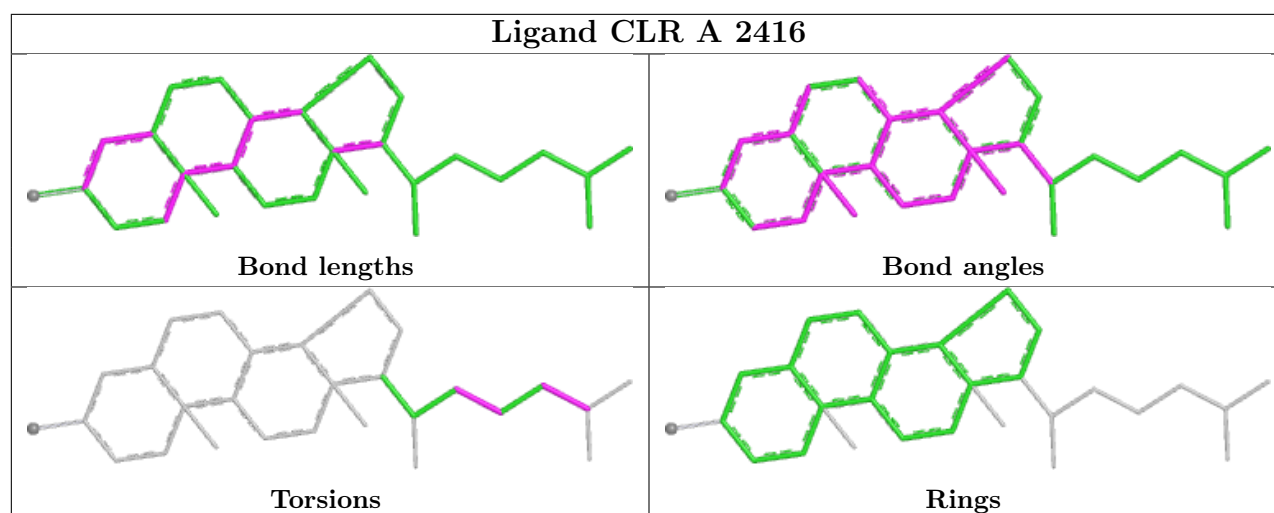
Mol	Chain	Res	Type	Atoms
4	A	2405	PEV	O3P-C1-C2-O2
6	A	2414	PLM	C3-C4-C5-C6
9	A	2418	Q7G	C4-C5-C6-O6
9	A	2418	Q7G	O5B-C1B-O1B-C24
5	A	2402	POV	C27-C28-C29-C210
6	A	2414	PLM	C4-C5-C6-C7
6	A	2415	PLM	C8-C9-CA-CB
4	A	2411	PEV	C43-C44-C45-C46
8	A	2416	CLR	C23-C24-C25-C26
4	A	2405	PEV	C20-C21-C22-C23
6	A	2409	PLM	O2-C1-C2-C3
4	A	2405	PEV	C40-C41-C42-C43
6	A	2415	PLM	C3-C4-C5-C6
5	A	2402	POV	O31-C31-C32-C33
5	A	2402	POV	O11-C1-C2-C3

There are no ring outliers.

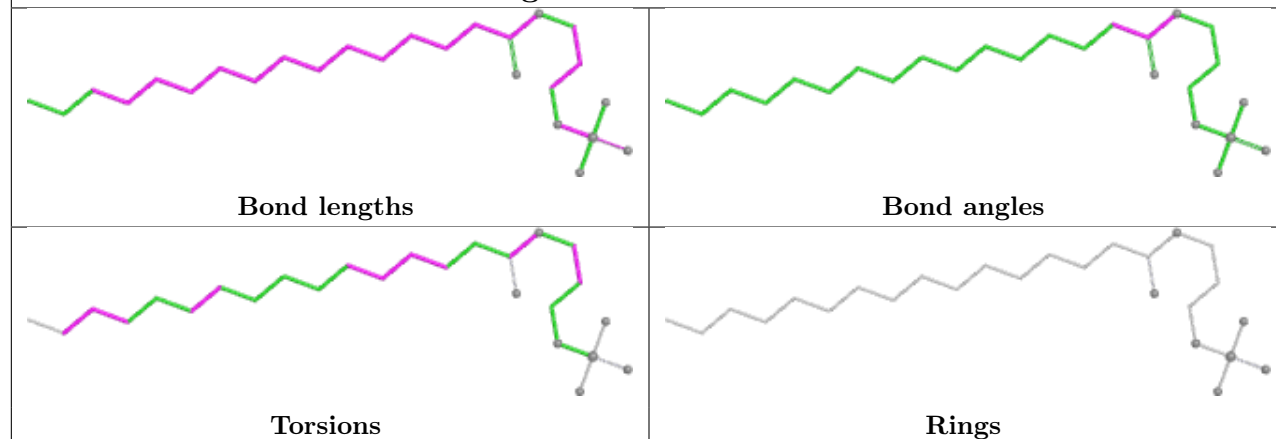
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2416	CLR	1	0
4	A	2411	PEV	1	0
7	B	301	NAG	2	0
8	A	2417	CLR	3	0
5	A	2402	POV	1	0
9	A	2418	Q7G	2	0
7	B	302	NAG	1	0

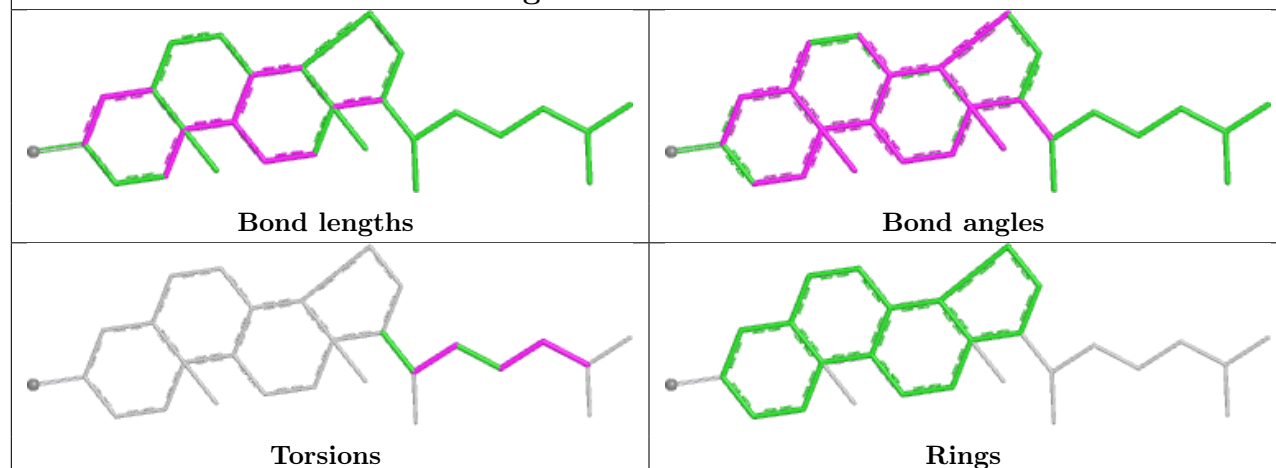
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



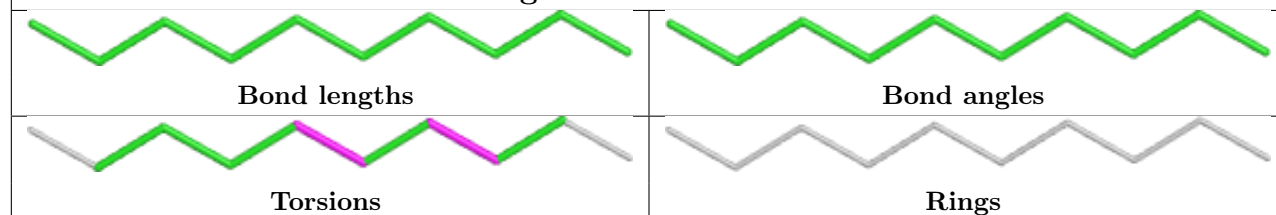
Ligand POV A 2408



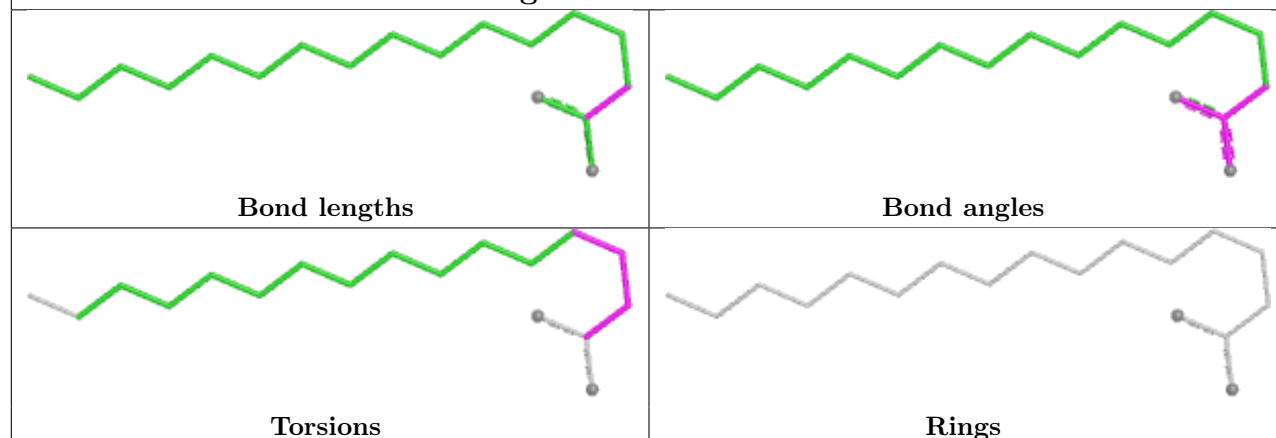
Ligand CLR A 2417

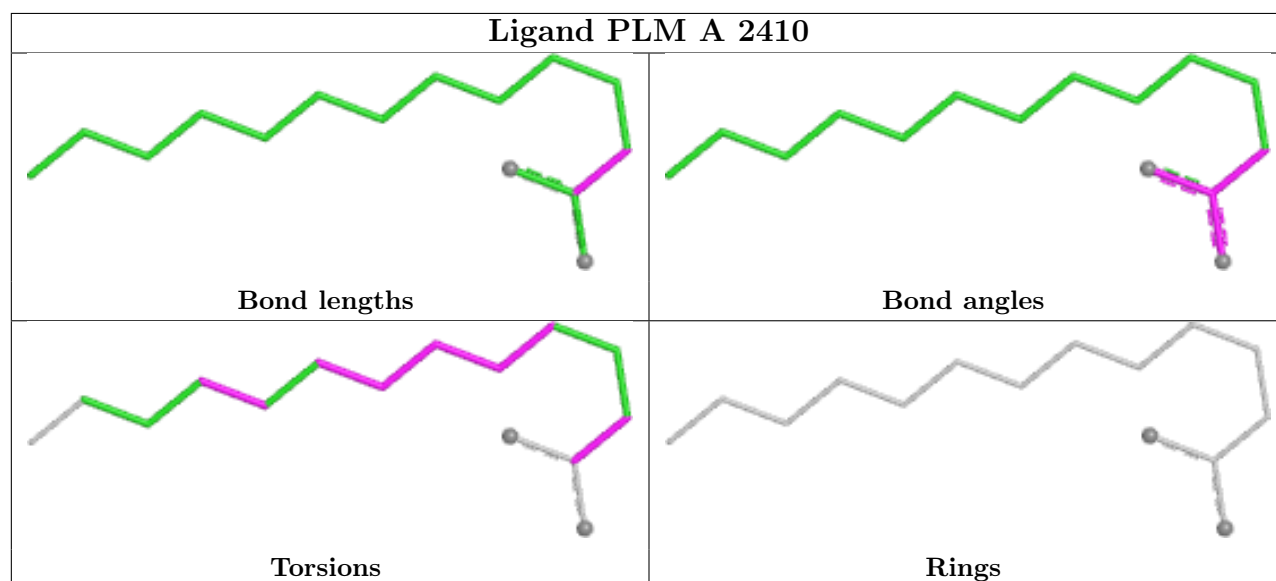
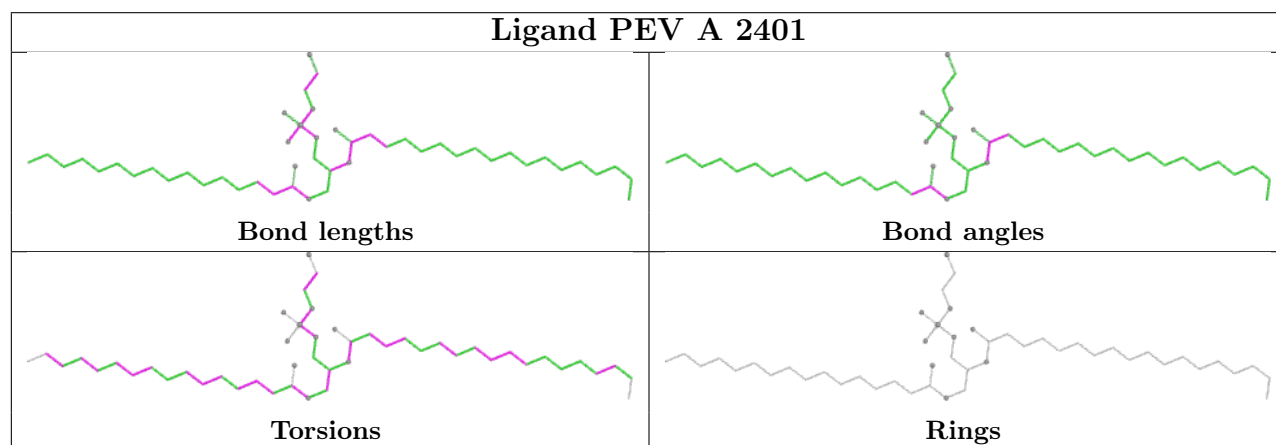
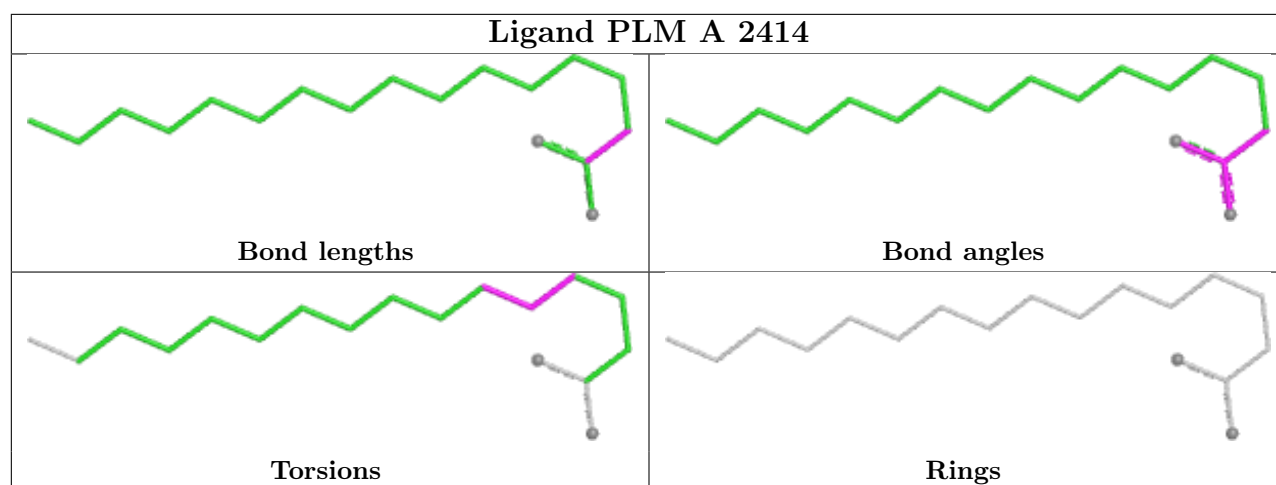


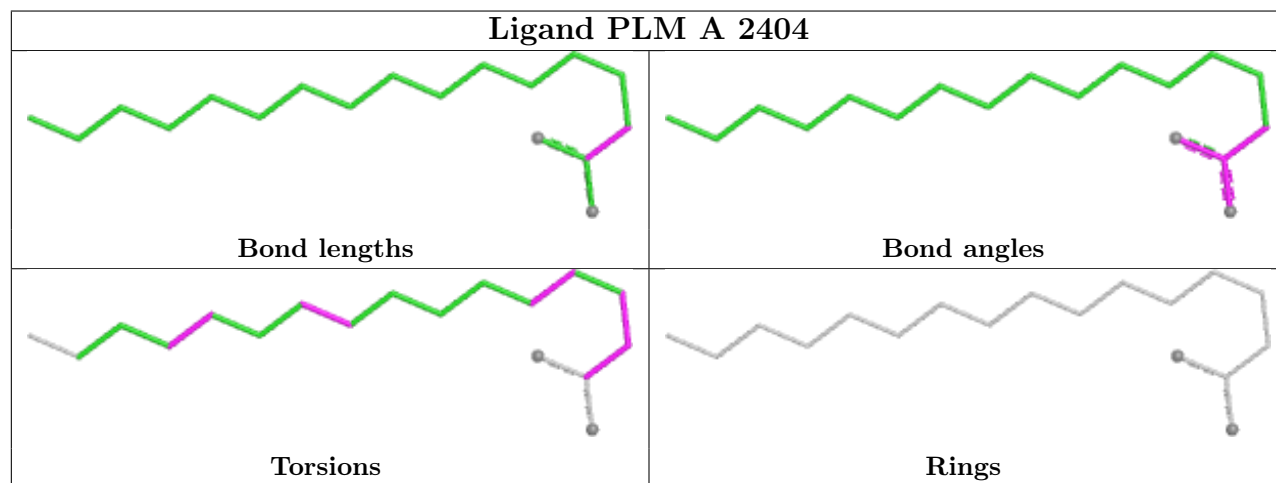
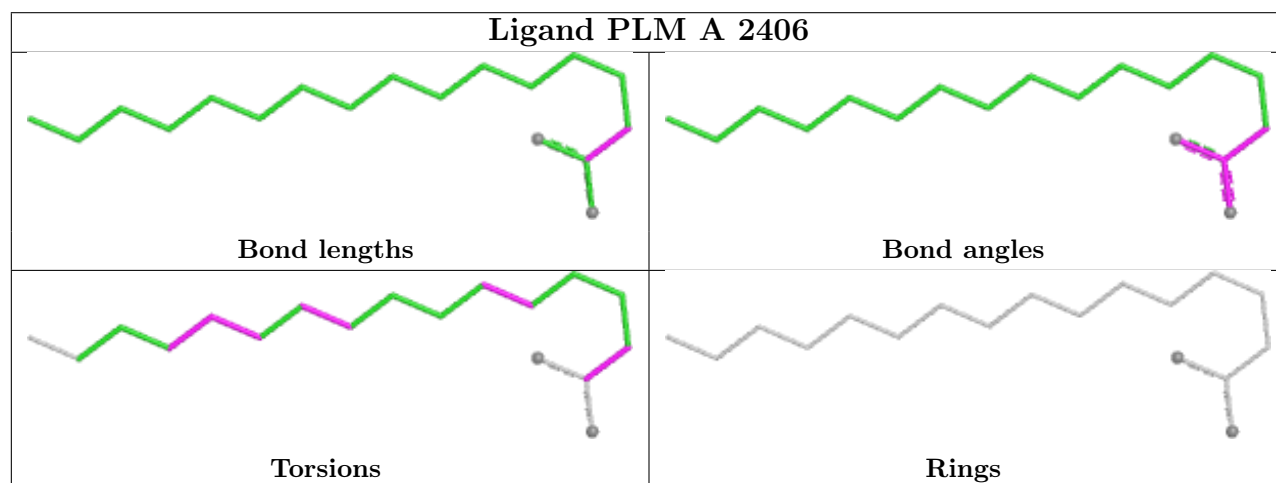
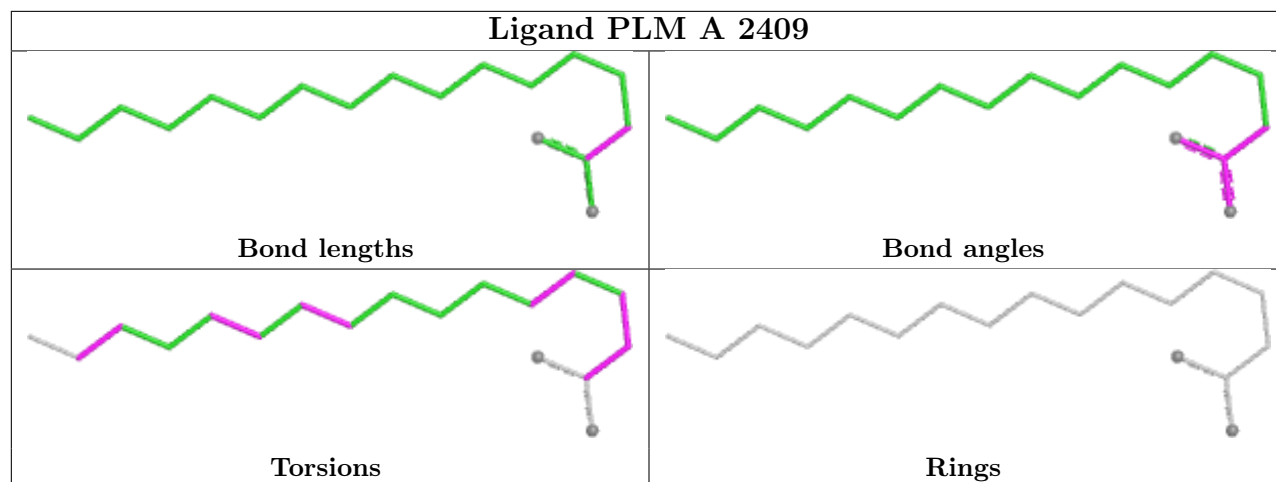
Ligand PLM A 2407

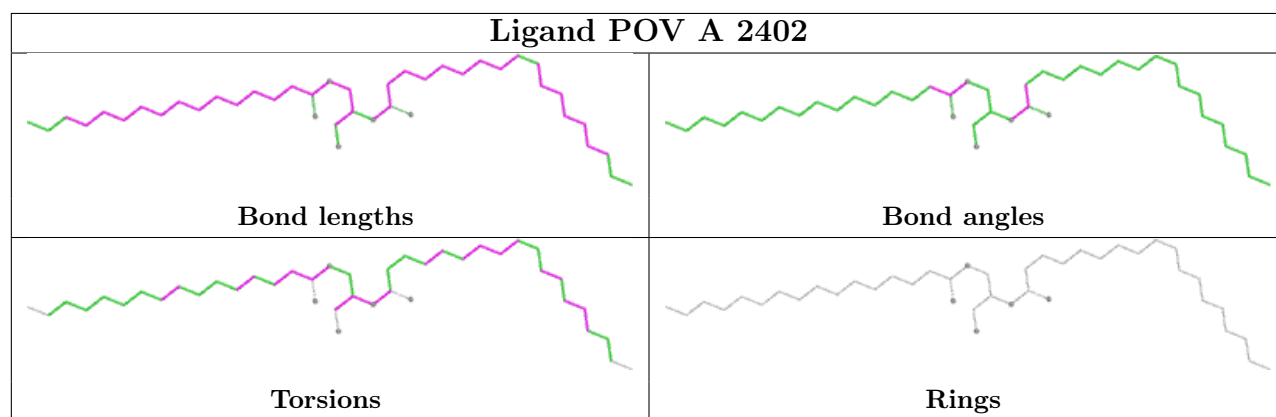
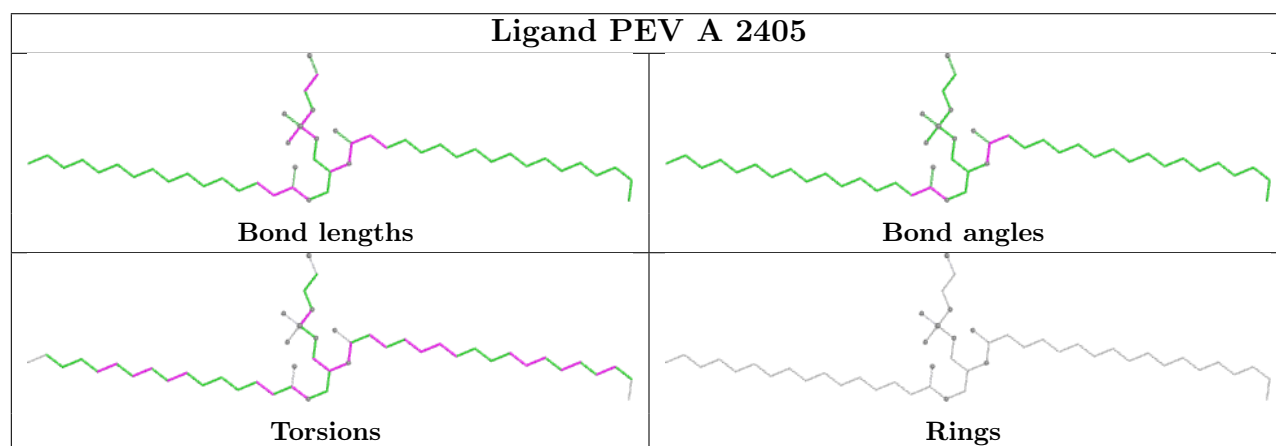
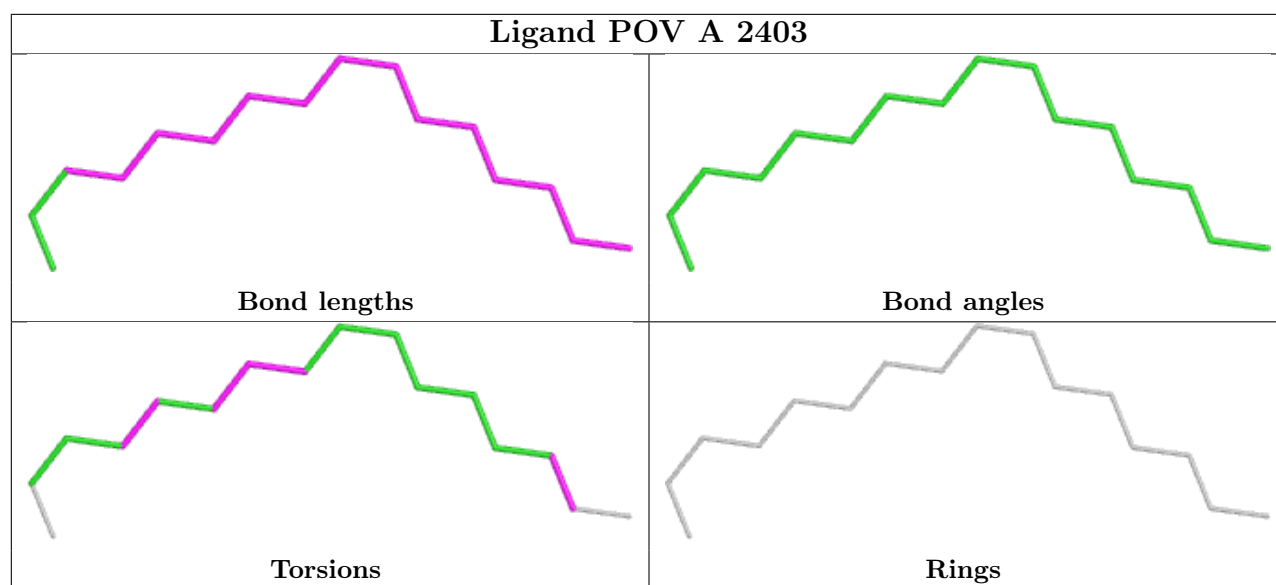


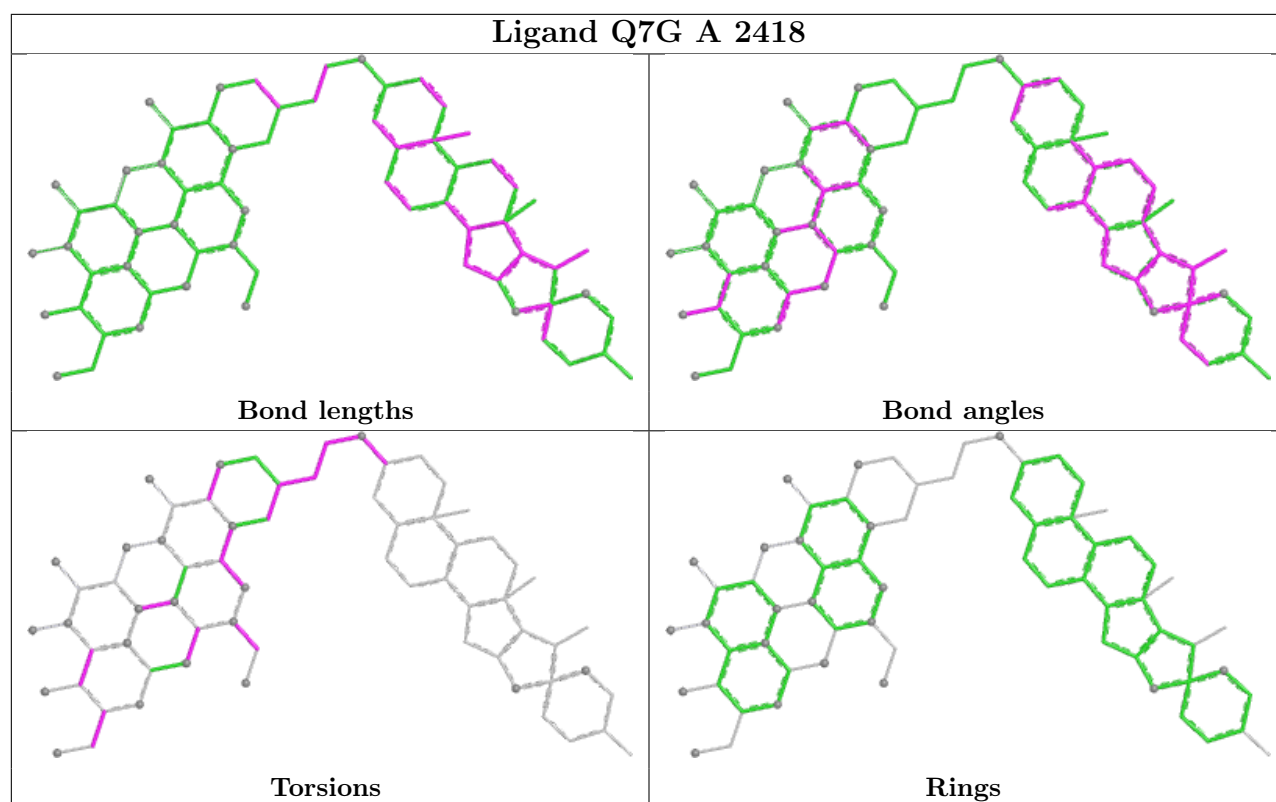
Ligand PLM A 2413











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

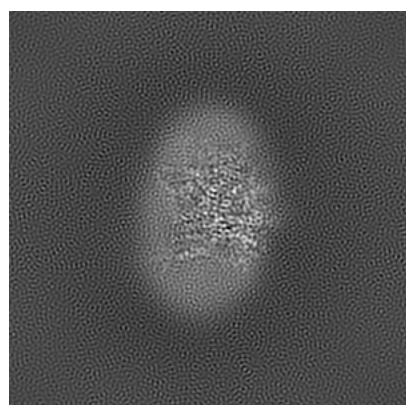
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25920. These allow visual inspection of the internal detail of the map and identification of artifacts.

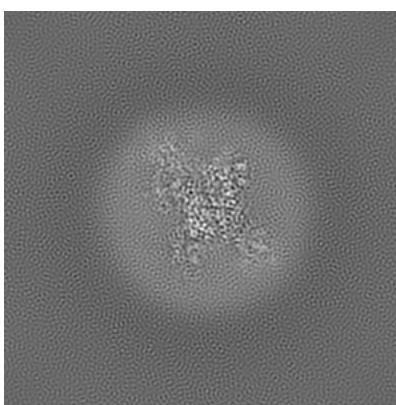
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

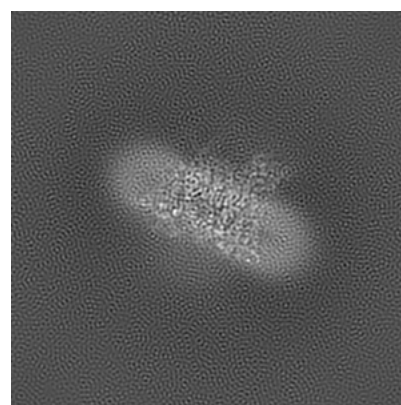
6.1.1 Primary map



X



Y

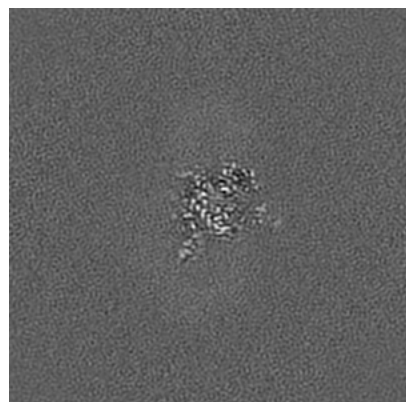


Z

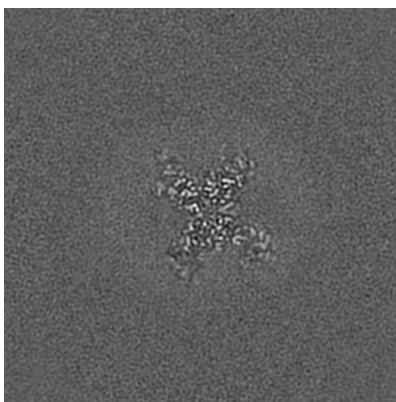
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

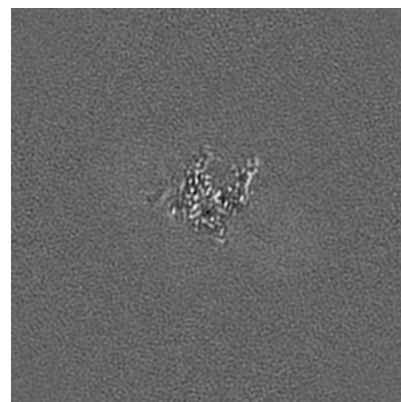
6.2.1 Primary map



X Index: 128



Y Index: 128

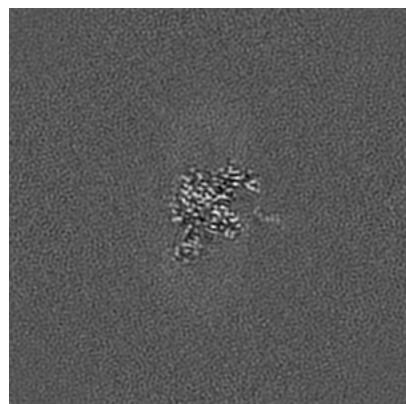


Z Index: 128

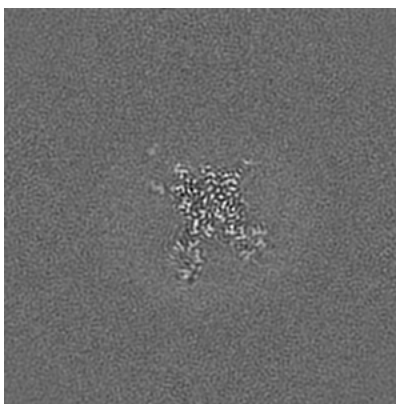
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

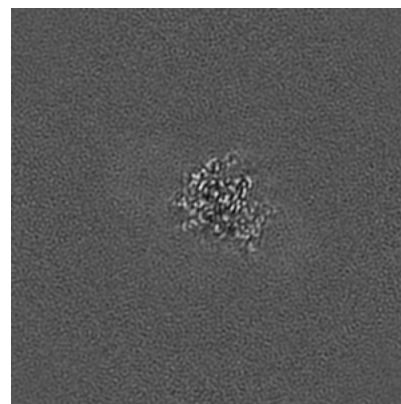
6.3.1 Primary map



X Index: 132



Y Index: 136

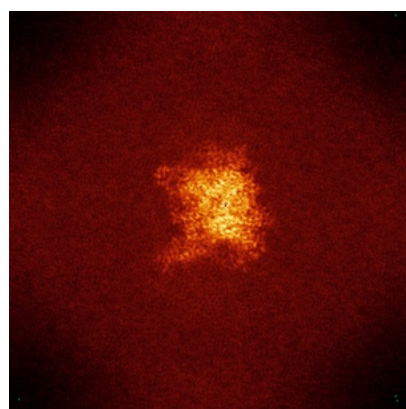


Z Index: 141

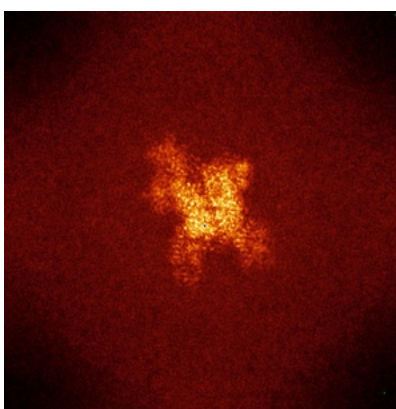
The images above show the largest variance slices of the map in three orthogonal directions.

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

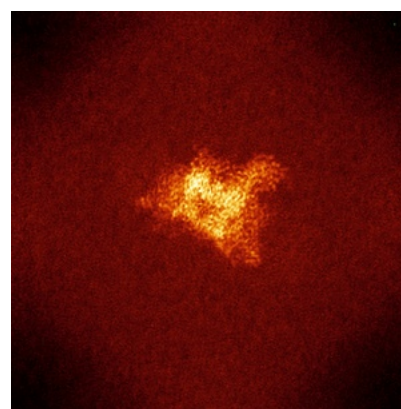
6.4.1 Primary map



X



Y

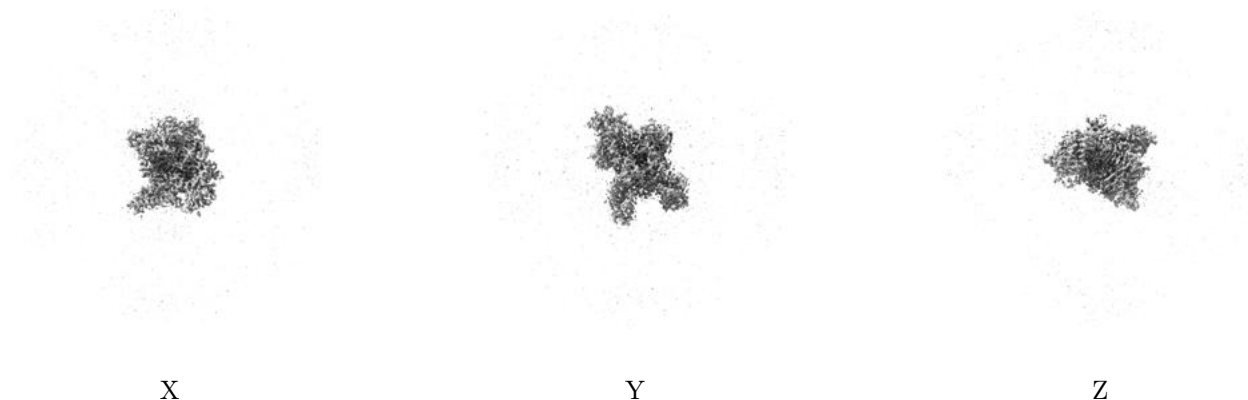


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.202. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

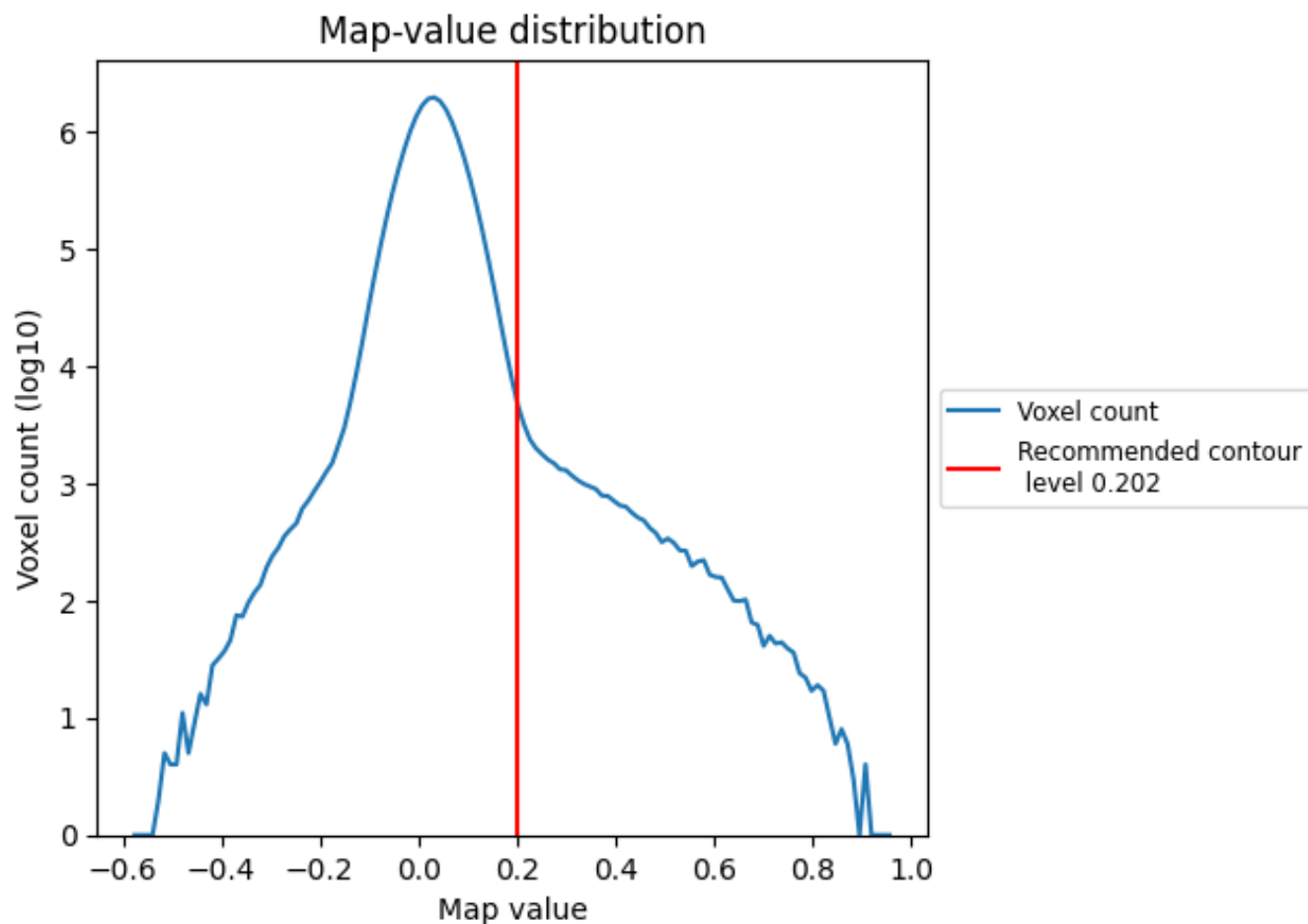
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

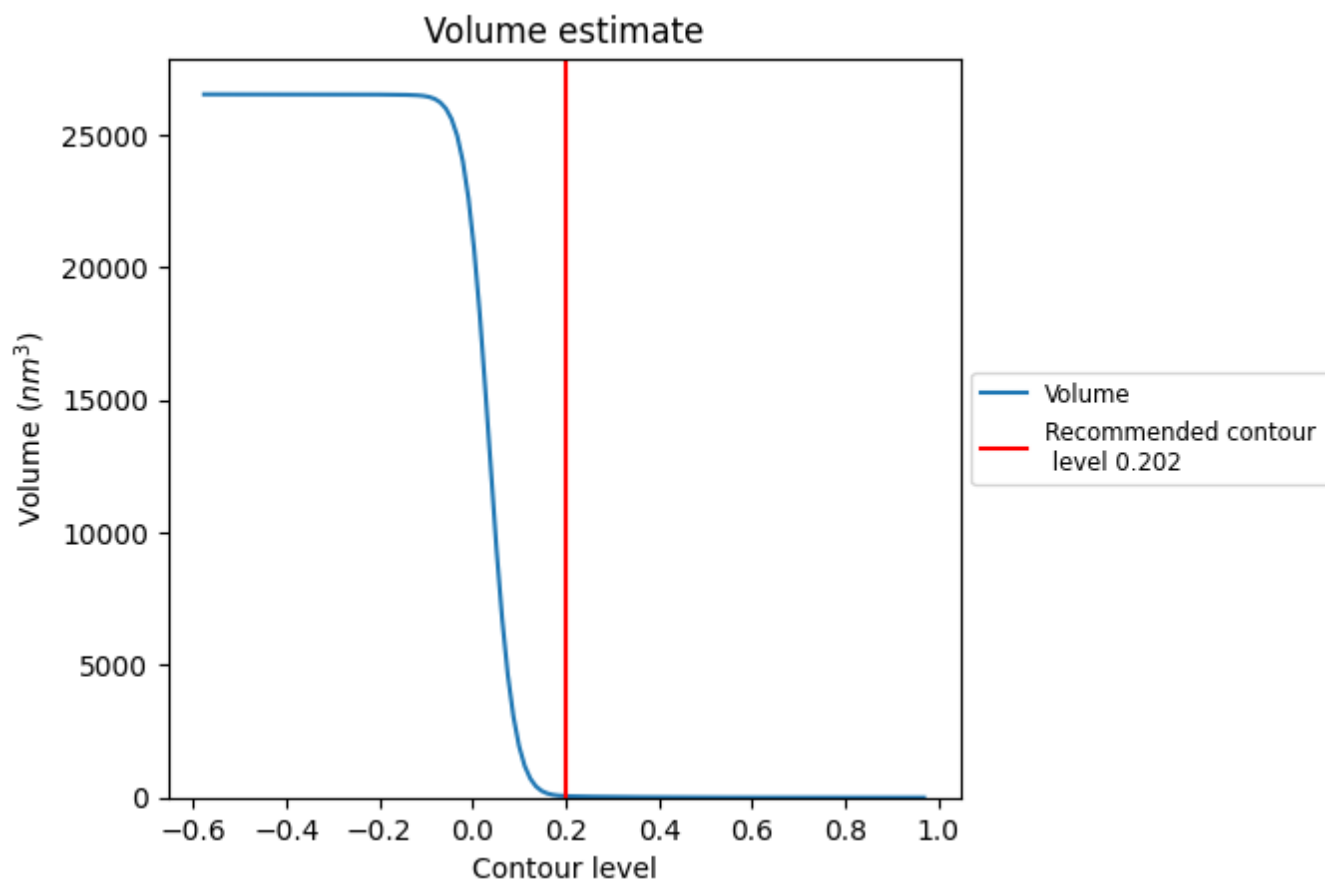
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

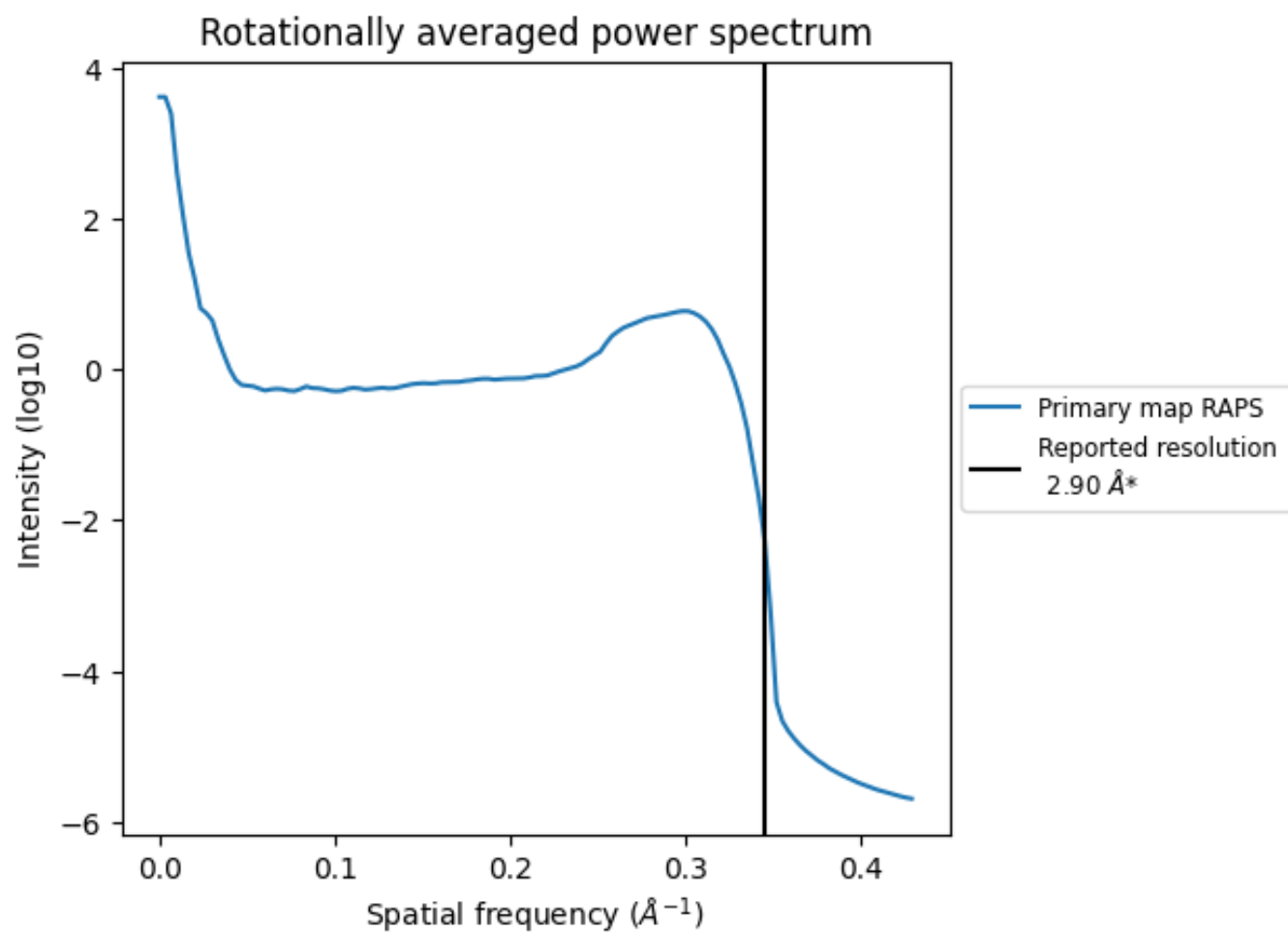
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm³; this corresponds to an approximate mass of 49 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

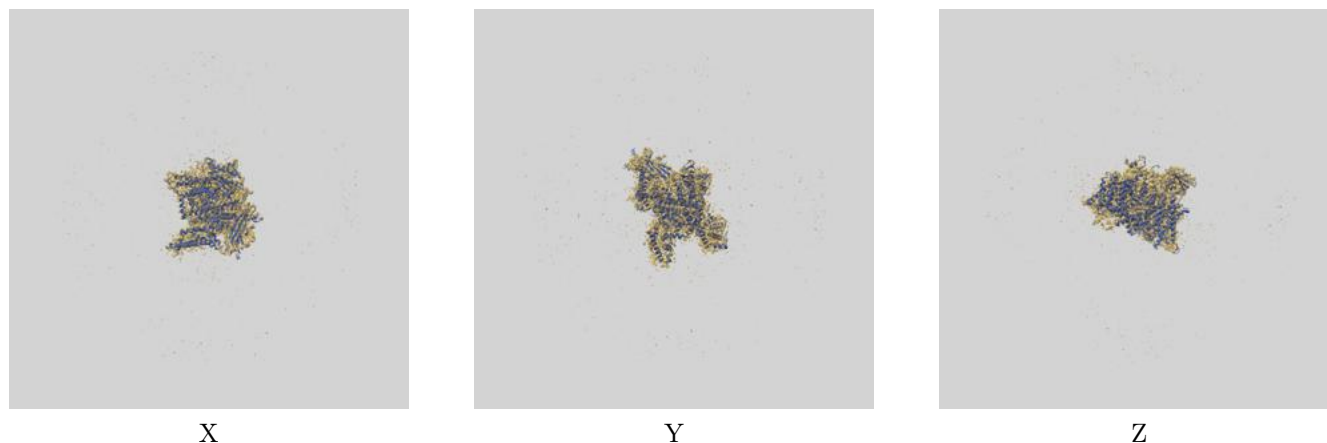
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

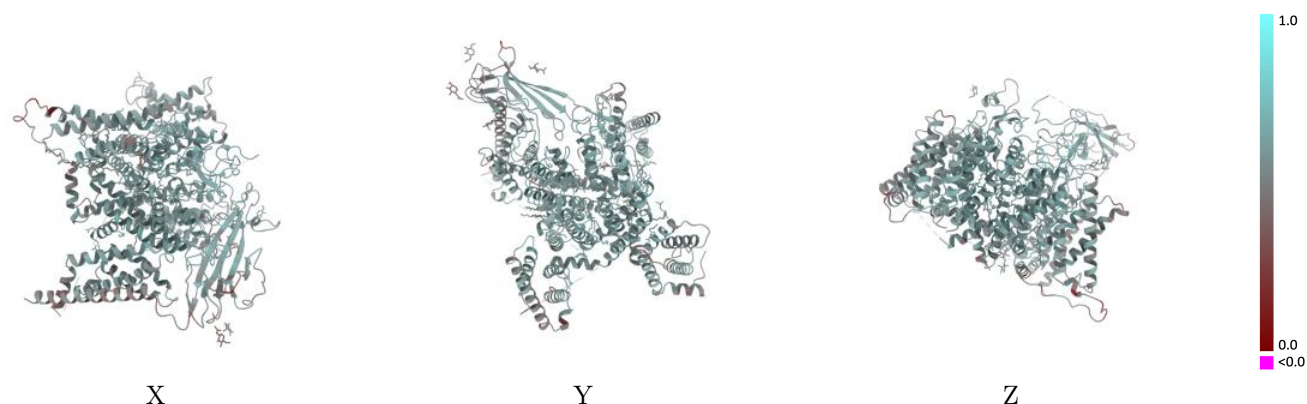
This section contains information regarding the fit between EMDB map EMD-25920 and PDB model 7TJ9. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



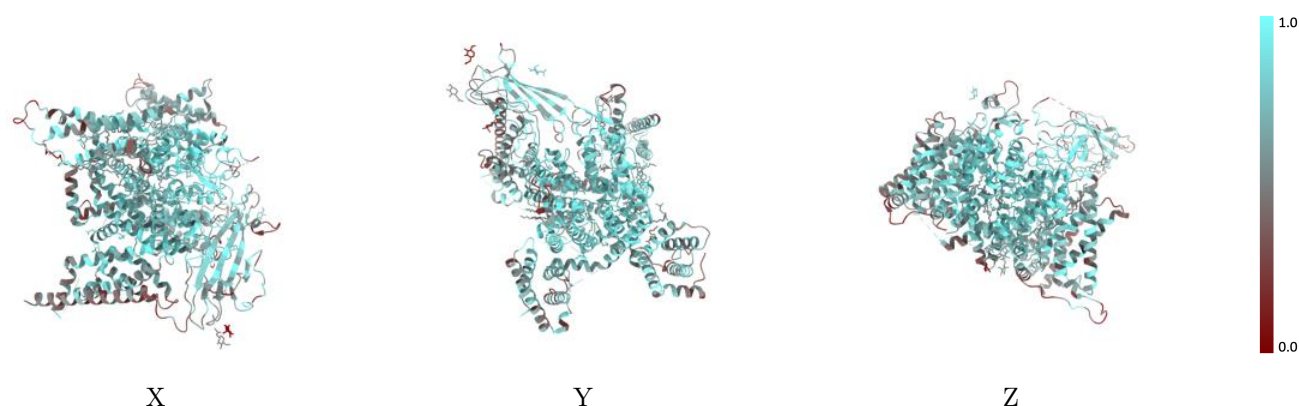
The images above show the 3D surface view of the map at the recommended contour level 0.202 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



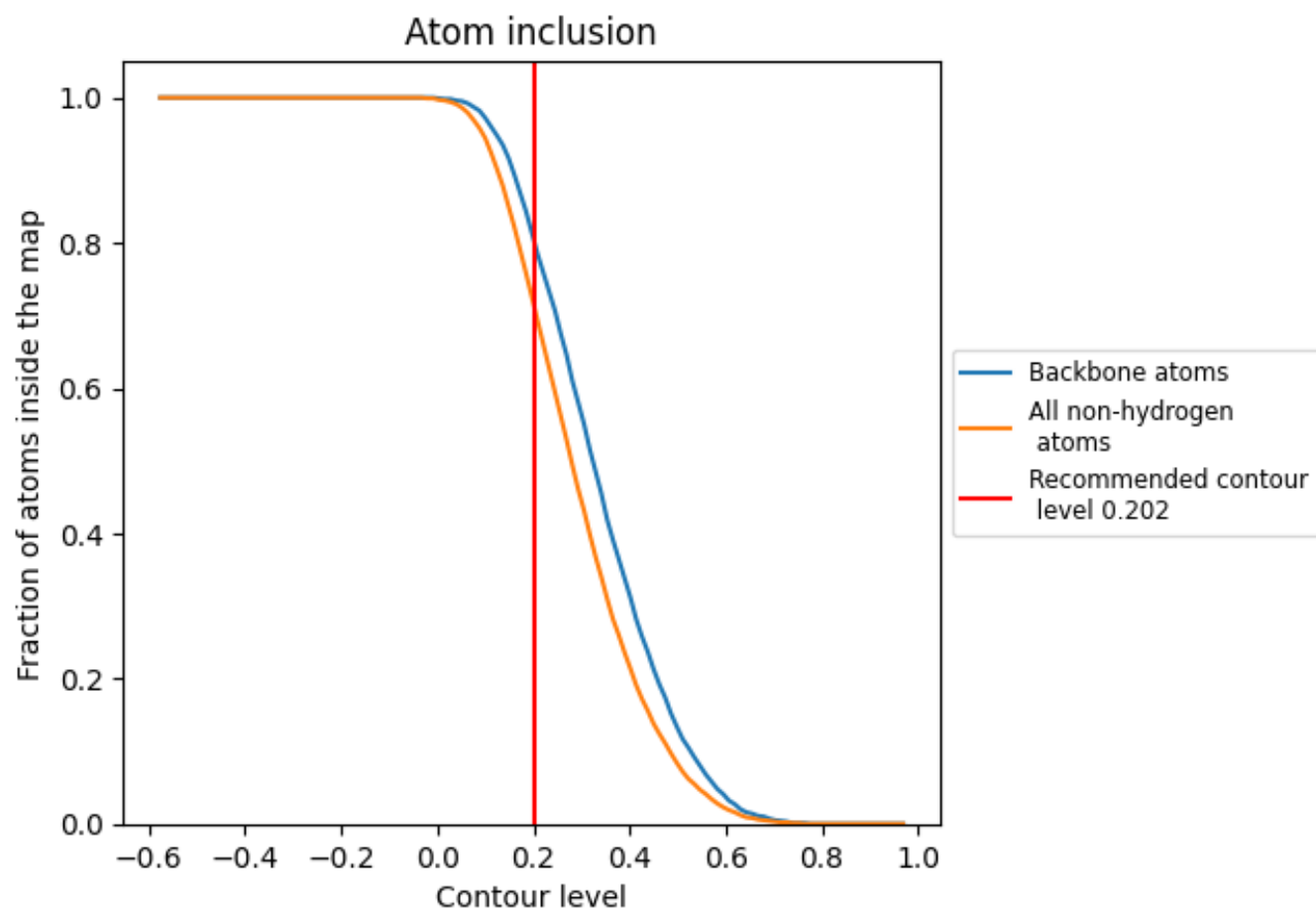
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.202).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.202) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.5650
A	0.7290	0.5730
B	0.5890	0.5150
C	0.6070	0.5160

