



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 11:43 AM JST

PDB ID : 7WE4
EMDB ID : EMD-32439
Title : Human Nav1.8 with A-803467, class I
Authors : Yan, N.; Pan, X.J.; Huang, X.S.; Huang, G.X.
Deposited on : 2021-12-22
Resolution : 2.70 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:

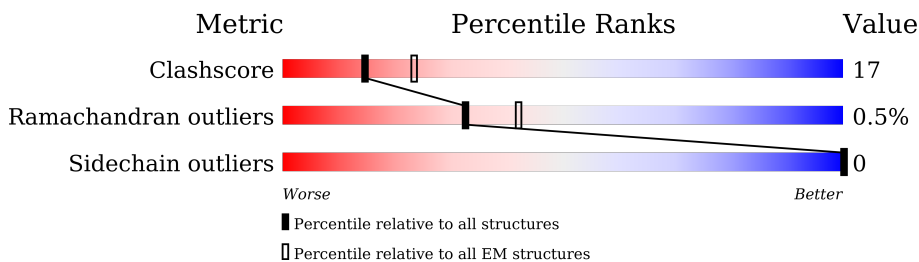
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 2.70 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 $\leq 5\%$. 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	1956	 42% 16% 43%
2	B	2	 50% 100%
2	C	2	 50% 50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9806 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 10 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1122	9019	5988	1441	1527	63	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	894	PHE	SER	conflict	UNP Q9Y5Y9

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



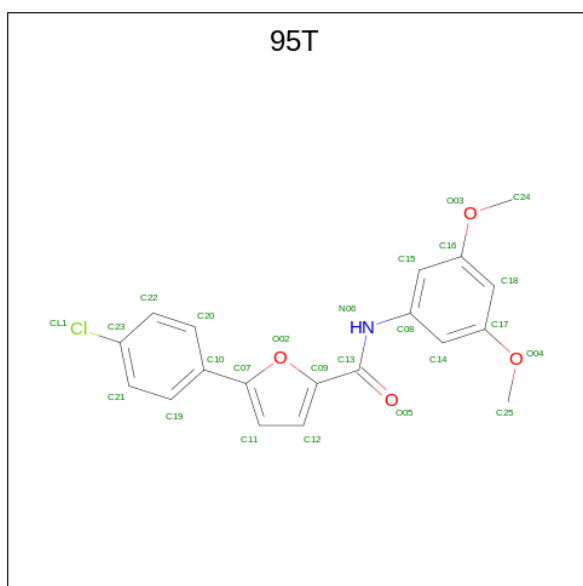
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0
2	C	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



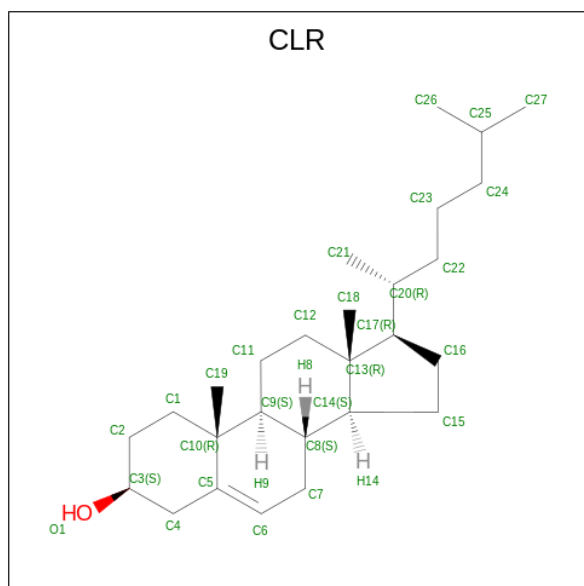
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	42	24	3	15	0
3	A	1	42	24	3	15	0
3	A	1	42	24	3	15	0

- Molecule 4 is 5-(4-chlorophenyl)- {N}-(3,5-dimethoxyphenyl)furan-2-carboxamide (three-letter code: 95T) (formula: C₁₉H₁₆ClNO₄) (labeled as "Ligand of Interest" by depositor).



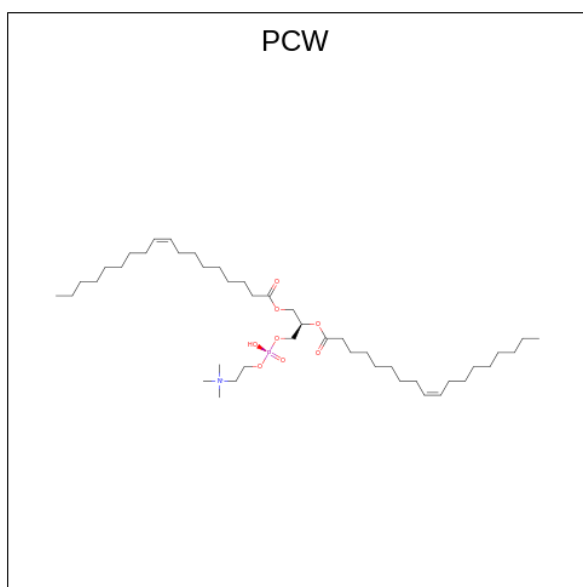
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	N		O
4	A	1	25	19	1	1	4	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



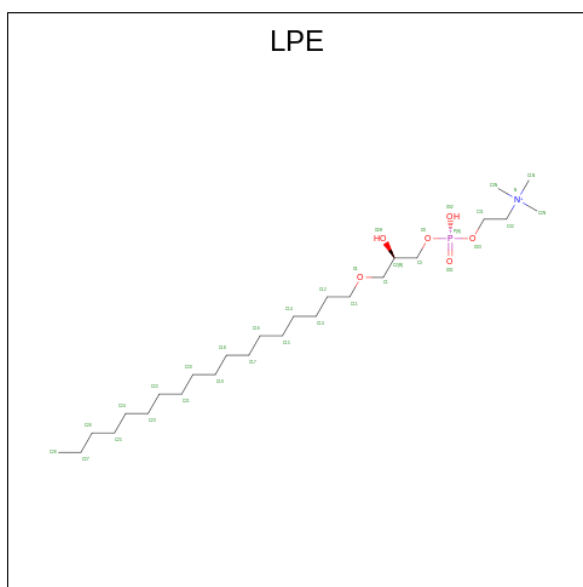
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	112	108	4	0
5	A	1	112	108	4	0
5	A	1	112	108	4	0
5	A	1	112	108	4	0

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



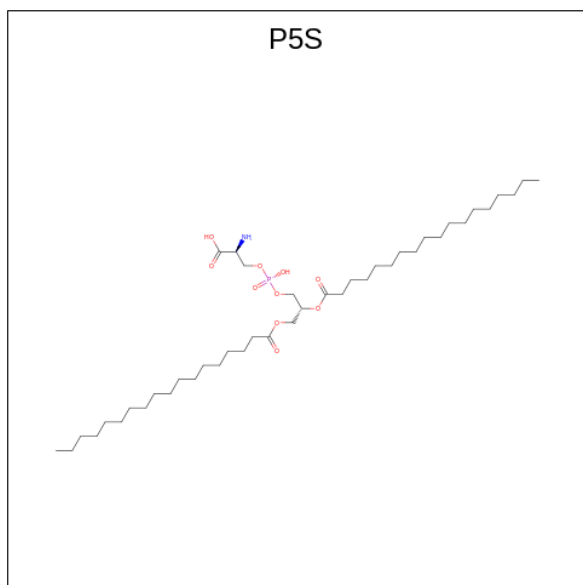
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	Total 207	159	3	40	5	0
6	A	1	Total 207	159	3	40	5	0
6	A	1	Total 207	159	3	40	5	0
6	A	1	Total 207	159	3	40	5	0
6	A	1	Total 207	159	3	40	5	0

- Molecule 7 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0
7	A	1	214	142	9	54	9	0

- Molecule 8 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	Total 131	95	3	30	3	0
8	A	1	Total 131	95	3	30	3	0
8	A	1	Total 131	95	3	30	3	0



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

Chain C: A horizontal progress bar for Chain C. The bar is divided into two segments: a green segment on the left and a yellow segment on the right. The green segment is labeled '50%' and the yellow segment is labeled '50%'.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237316	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.874	Depositor
Minimum map value	-1.920	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.565	Depositor
Map size (Å)	259.8, 259.8, 259.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	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: LPE, P5S, NAG, 95T, PCW, CLR

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	0.44	0/9246	0.63	0/12543

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9019	0	9176	295	0
2	B	28	0	25	0	0
2	C	28	0	25	3	0
3	A	42	0	39	0	0
4	A	25	0	0	1	0
5	A	112	0	184	43	0
6	A	207	0	271	23	0
7	A	214	0	296	40	0
8	A	131	0	163	18	0
All	All	9806	0	10179	340	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 17.

All (340) 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:827:TRP:CE3	1:A:828:PRO:HD2	1.68	1.28
5:A:2021:CLR:H121	5:A:2021:CLR:H212	1.34	1.10
1:A:1428:LEU:HG	1:A:1431:GLN:HB2	1.16	1.09
1:A:1291:PHE:CE2	1:A:1405:GLY:HA2	1.87	1.09
1:A:1291:PHE:CZ	1:A:1295:PHE:HE2	1.70	1.09
1:A:1601:MET:HE3	6:A:2006:PCW:H131	1.19	1.08
1:A:1721:ILE:HD13	5:A:2025:CLR:C18	1.84	1.08
1:A:1714:VAL:HG12	5:A:2025:CLR:H21	1.36	1.03
1:A:1291:PHE:HE2	1:A:1405:GLY:HA2	1.16	1.02
1:A:1425:LYS:HG2	1:A:1430:GLY:HA2	1.41	1.02
1:A:1567:PHE:CE2	7:A:2012:LPE:H322	1.94	1.02
1:A:827:TRP:HE3	1:A:828:PRO:HD2	1.25	0.98
1:A:398:MET:HG2	1:A:1725:PHE:HE1	1.30	0.97
1:A:1567:PHE:CZ	7:A:2012:LPE:H3N2	1.99	0.96
1:A:692:THR:OG1	7:A:2020:LPE:H321	1.65	0.95
1:A:1428:LEU:CG	1:A:1431:GLN:HB2	1.97	0.94
1:A:1475:ARG:NH1	8:A:2023:P5S:HBA	1.83	0.94
5:A:2016:CLR:H121	5:A:2016:CLR:H212	1.49	0.93
1:A:1567:PHE:CZ	7:A:2012:LPE:C3N	2.52	0.93
1:A:1428:LEU:HG	1:A:1431:GLN:CB	2.01	0.89
1:A:827:TRP:CE3	1:A:828:PRO:CD	2.55	0.89
1:A:1418:ILE:HD11	5:A:2025:CLR:H122	1.54	0.89
1:A:1291:PHE:HE2	1:A:1405:GLY:CA	1.84	0.88
1:A:1601:MET:CE	6:A:2006:PCW:H131	2.02	0.88
1:A:1291:PHE:CZ	1:A:1295:PHE:CE2	2.61	0.88
1:A:871:LEU:HD12	8:A:2024:P5S:H29A	1.58	0.85
1:A:124:ILE:O	1:A:128:VAL:HG22	1.75	0.84
1:A:398:MET:HG2	1:A:1725:PHE:CE1	2.12	0.83
1:A:390:ASN:OD1	1:A:1717:TYR:CD2	2.31	0.83
5:A:2021:CLR:H162	5:A:2021:CLR:H231	1.63	0.81
1:A:728:LYS:HD2	6:A:2013:PCW:O1P	1.82	0.80
1:A:827:TRP:HE3	1:A:828:PRO:CD	1.92	0.80
1:A:1721:ILE:HD13	5:A:2025:CLR:H183	1.64	0.79
1:A:680:ILE:HD12	7:A:2020:LPE:H162	1.65	0.79
1:A:1567:PHE:HE2	7:A:2012:LPE:H322	1.47	0.79
1:A:1717:TYR:CD1	5:A:2025:CLR:H22	2.18	0.78
1:A:680:ILE:CD1	7:A:2020:LPE:H162	2.14	0.77
1:A:1567:PHE:HZ	7:A:2012:LPE:H3N2	1.48	0.77
1:A:1721:ILE:CD1	5:A:2025:CLR:C18	2.63	0.76
1:A:390:ASN:OD1	1:A:1717:TYR:HD2	1.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:CG	1:A:1725:PHE:HE1	1.99	0.75
7:A:2015:LPE:H111	7:A:2015:LPE:H31	1.69	0.75
7:A:2018:LPE:H322	8:A:2022:P5S:C	2.18	0.74
7:A:2018:LPE:H322	8:A:2022:P5S:O	1.87	0.73
1:A:1290:ILE:HD12	5:A:2005:CLR:H25	1.71	0.72
1:A:331:ASN:HB2	1:A:335:ASN:HA	1.71	0.72
1:A:398:MET:CG	1:A:1725:PHE:CE1	2.72	0.72
5:A:2016:CLR:H212	5:A:2016:CLR:C12	2.19	0.72
6:A:2014:PCW:H321	6:A:2014:PCW:O1P	1.89	0.72
1:A:829:ARG:HD2	1:A:1374:TYR:CD1	2.25	0.72
1:A:1721:ILE:HD13	5:A:2025:CLR:H182	1.70	0.72
1:A:1721:ILE:CD1	5:A:2025:CLR:H182	2.20	0.72
1:A:172:ILE:HD11	1:A:197:ILE:HD12	1.71	0.72
1:A:871:LEU:CD1	8:A:2024:P5S:H29A	2.21	0.71
1:A:1428:LEU:CD2	1:A:1431:GLN:HB3	2.21	0.70
5:A:2021:CLR:H212	5:A:2021:CLR:C12	2.16	0.69
1:A:728:LYS:CD	6:A:2013:PCW:O1P	2.40	0.69
1:A:1217:ALA:HB3	7:A:2015:LPE:H121	1.73	0.69
1:A:220:LEU:O	1:A:223:LEU:N	2.26	0.69
1:A:664:ASP:HB3	1:A:665:PRO:HD2	1.75	0.69
7:A:2015:LPE:H111	7:A:2015:LPE:C3	2.23	0.69
1:A:1682:LEU:HD12	1:A:1683:PRO:HD2	1.73	0.69
1:A:1428:LEU:CD2	1:A:1431:GLN:CB	2.73	0.67
1:A:390:ASN:OD1	1:A:1717:TYR:CE2	2.48	0.67
5:A:2021:CLR:H121	5:A:2021:CLR:C21	2.20	0.66
1:A:829:ARG:HD2	1:A:1374:TYR:CE1	2.30	0.66
1:A:152:LEU:HD12	1:A:153:PRO:HD2	1.79	0.66
1:A:1377:VAL:HG13	1:A:1392:VAL:HA	1.78	0.66
1:A:1567:PHE:CE2	7:A:2012:LPE:C32	2.76	0.65
1:A:1171:PHE:CE1	7:A:2017:LPE:H2N3	2.32	0.65
1:A:136:ILE:HG12	1:A:171:LYS:HE3	1.78	0.65
1:A:1342:PHE:CE1	2:C:1:NAG:H3	2.32	0.65
1:A:391:LEU:HD23	1:A:1596:LEU:HD13	1.79	0.64
1:A:715:LYS:HD2	1:A:719:PHE:HE2	1.62	0.64
1:A:216:THR:HG21	1:A:808:LEU:HD21	1.80	0.64
1:A:661:LEU:HD12	1:A:718:ALA:HB1	1.80	0.64
1:A:1140:GLN:HA	1:A:1143:LYS:HE2	1.79	0.63
1:A:1428:LEU:HG	1:A:1428:LEU:O	1.99	0.63
1:A:1567:PHE:CZ	7:A:2012:LPE:H3N3	2.33	0.63
1:A:128:VAL:HG11	1:A:178:CYS:SG	2.39	0.63
1:A:871:LEU:HB3	8:A:2024:P5S:H31A	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2014:PCW:H52	6:A:2014:PCW:O2P	1.99	0.62
1:A:168:ALA:HB1	1:A:197:ILE:HG22	1.81	0.62
1:A:816:ASN:HB2	1:A:860:VAL:HG23	1.82	0.62
1:A:153:PRO:HB2	1:A:156:ILE:HG13	1.82	0.61
1:A:692:THR:OG1	7:A:2020:LPE:C32	2.43	0.61
1:A:1595:THR:HG23	6:A:2006:PCW:H73	1.82	0.61
1:A:1428:LEU:HD21	1:A:1431:GLN:HB3	1.82	0.61
1:A:1291:PHE:CE2	1:A:1405:GLY:CA	2.68	0.61
1:A:1171:PHE:CE1	7:A:2017:LPE:C2N	2.84	0.61
1:A:1171:PHE:CD1	7:A:2017:LPE:C2N	2.83	0.61
1:A:387:TYR:CZ	1:A:391:LEU:HD11	2.36	0.61
1:A:355:GLN:NE2	4:A:2004:95T:O05	2.32	0.61
1:A:857:CYS:HA	1:A:860:VAL:HG12	1.83	0.61
1:A:1370:MET:HG3	1:A:1374:TYR:CE2	2.36	0.60
1:A:1717:TYR:HB3	5:A:2025:CLR:H193	1.83	0.60
1:A:871:LEU:CD1	8:A:2024:P5S:C29	2.79	0.60
5:A:2021:CLR:H231	5:A:2021:CLR:C16	2.30	0.60
1:A:684:MET:SD	7:A:2019:LPE:H31	2.41	0.60
1:A:1567:PHE:CZ	7:A:2012:LPE:H322	2.35	0.60
1:A:1342:PHE:CD1	2:C:1:NAG:H3	2.36	0.60
1:A:172:ILE:HD11	1:A:197:ILE:CD1	2.32	0.60
1:A:871:LEU:HD12	8:A:2024:P5S:C29	2.31	0.59
1:A:219:VAL:HG12	1:A:803:LEU:HD23	1.84	0.59
1:A:736:ILE:HG21	1:A:762:ARG:HG3	1.85	0.58
1:A:1696:ALA:O	1:A:1700:ILE:HG13	2.03	0.58
1:A:1567:PHE:CZ	7:A:2012:LPE:C32	2.86	0.58
1:A:1601:MET:HE1	6:A:2007:PCW:C12	2.34	0.58
1:A:1597:LEU:HB3	6:A:2006:PCW:H122	1.86	0.58
7:A:2015:LPE:O31	7:A:2015:LPE:H21	2.04	0.58
1:A:1601:MET:HE1	6:A:2007:PCW:H122	1.84	0.58
1:A:809:LEU:O	1:A:813:TYR:HD2	1.87	0.57
1:A:1291:PHE:HD2	1:A:1292:TRP:HD1	1.51	0.57
1:A:203:GLY:HA2	1:A:207:ASP:HB3	1.87	0.57
1:A:253:THR:HG23	1:A:388:LEU:HD13	1.87	0.57
1:A:801:PHE:CG	1:A:873:VAL:HG22	2.40	0.57
1:A:705:THR:OG1	1:A:759:ARG:NH2	2.38	0.57
1:A:748:LYS:HB2	1:A:751:SER:HB2	1.87	0.57
1:A:1592:GLY:O	1:A:1596:LEU:HG	2.06	0.56
1:A:387:TYR:CZ	1:A:1600:LEU:HB2	2.41	0.56
1:A:1601:MET:CE	6:A:2007:PCW:H122	2.36	0.56
5:A:2025:CLR:H121	5:A:2025:CLR:H212	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HD12	1:A:225:THR:HG22	1.87	0.56
1:A:1522:GLU:HG2	1:A:1526:LYS:HD2	1.88	0.55
1:A:1601:MET:HE3	6:A:2006:PCW:C13	2.13	0.55
1:A:871:LEU:HD13	8:A:2024:P5S:H29	1.88	0.55
1:A:890:LEU:HA	1:A:894:PHE:HD2	1.70	0.54
1:A:732:PHE:O	1:A:736:ILE:HG12	2.07	0.54
1:A:352:LEU:HD23	1:A:358:TRP:HB2	1.89	0.54
7:A:2015:LPE:C3	7:A:2015:LPE:C11	2.86	0.54
1:A:267:LEU:HD21	1:A:1577:LEU:HD11	1.90	0.53
1:A:188:PRO:HA	1:A:191:TRP:CZ3	2.42	0.53
8:A:2022:P5S:H44	8:A:2022:P5S:H22	1.91	0.53
1:A:1522:GLU:HA	1:A:1525:MET:HE2	1.90	0.53
1:A:720:ASP:HB2	1:A:723:TYR:HD2	1.74	0.53
1:A:1377:VAL:O	1:A:1389:GLU:HA	2.09	0.53
1:A:1630:PRO:HD2	1:A:1631[B]:HIS:ND1	2.24	0.53
1:A:252:LEU:HD13	1:A:1593:ILE:HG23	1.91	0.52
1:A:1418:ILE:HD11	5:A:2025:CLR:C12	2.35	0.52
1:A:169:LEU:HD21	1:A:201:TYR:OH	2.10	0.52
1:A:694:GLU:O	1:A:698:GLN:HG2	2.09	0.52
1:A:215:ARG:HD2	1:A:807:GLN:NE2	2.23	0.52
1:A:129:HIS:CD2	1:A:131:TRP:CD1	2.97	0.52
1:A:1139:TRP:NE1	1:A:1143:LYS:HD3	2.24	0.52
1:A:817:ARG:HG3	1:A:818:LYS:HD3	1.90	0.52
1:A:281:MET:SD	1:A:281:MET:N	2.83	0.51
1:A:1217:ALA:HB2	5:A:2016:CLR:H151	1.93	0.51
1:A:203:GLY:HA2	1:A:207:ASP:CB	2.41	0.51
1:A:722:TYR:O	1:A:726:GLN:HG3	2.10	0.51
1:A:757:SER:O	1:A:760:LEU:HG	2.11	0.51
1:A:814:ARG:HA	1:A:827:TRP:CZ2	2.46	0.51
1:A:1243:VAL:HG12	1:A:1245:PRO:HD2	1.91	0.51
1:A:215:ARG:O	1:A:219:VAL:HG13	2.11	0.51
1:A:680:ILE:CD1	7:A:2020:LPE:H182	2.40	0.51
1:A:129:HIS:HD2	1:A:131:TRP:CD1	2.29	0.50
1:A:144:CYS:O	1:A:148:THR:HG23	2.12	0.50
1:A:1380:ARG:HB3	1:A:1384:MET:HE3	1.94	0.50
1:A:685:GLU:OE1	1:A:1301:ASN:ND2	2.44	0.50
1:A:142:VAL:HA	1:A:145:VAL:HG12	1.92	0.50
1:A:148:THR:HG22	1:A:799:PHE:HE1	1.75	0.50
1:A:275:LYS:HE3	1:A:328:THR:OG1	2.12	0.50
1:A:155:LYS:O	1:A:159:VAL:HG23	2.11	0.49
1:A:680:ILE:HD11	7:A:2020:LPE:H162	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:LEU:HG	1:A:1221:LEU:O	2.11	0.49
1:A:194:PHE:O	1:A:197:ILE:HG12	2.12	0.49
1:A:302:ARG:HH11	1:A:302:ARG:HG2	1.77	0.49
1:A:1274:LEU:O	1:A:1278:ILE:HG12	2.12	0.49
1:A:1466:GLN:NE2	1:A:1531:ARG:HH22	2.10	0.49
1:A:1475:ARG:NH1	8:A:2023:P5S:CB	2.68	0.49
1:A:153:PRO:HB2	1:A:156:ILE:CG1	2.42	0.49
1:A:1291:PHE:CE2	1:A:1295:PHE:CE2	3.00	0.49
1:A:1171:PHE:CD1	7:A:2017:LPE:H2N2	2.47	0.49
1:A:216:THR:O	1:A:219:VAL:HG22	2.13	0.49
1:A:1369:TRP:O	1:A:1373:MET:HG3	2.13	0.49
1:A:1413:PHE:O	1:A:1417:ILE:HG12	2.12	0.49
1:A:1475:ARG:CZ	8:A:2023:P5S:HBA	2.41	0.49
1:A:677:VAL:HA	1:A:680:ILE:HG12	1.94	0.48
1:A:1377:VAL:HG11	1:A:1395:TYR:CE2	2.47	0.48
1:A:241:HIS:CE1	1:A:399:ALA:HB1	2.48	0.48
1:A:1618:MET:HG2	1:A:1705:TYR:OH	2.12	0.48
1:A:393:LEU:HD23	5:A:2025:CLR:H191	1.95	0.48
1:A:736:ILE:HD13	1:A:758:PHE:CE2	2.48	0.48
1:A:1345:ASN:HD21	1:A:1349:ASN:HD22	1.60	0.48
1:A:1580:ILE:HA	1:A:1583:ILE:HD12	1.95	0.48
1:A:1363:VAL:HA	1:A:1369:TRP:HB3	1.95	0.48
1:A:167:GLU:O	1:A:171:LYS:HD3	2.14	0.48
1:A:827:TRP:CD2	1:A:828:PRO:HD2	2.37	0.48
5:A:2016:CLR:C12	5:A:2016:CLR:C21	2.91	0.48
5:A:2016:CLR:H182	5:A:2016:CLR:H8	1.62	0.48
1:A:736:ILE:HA	1:A:758:PHE:HE2	1.80	0.47
1:A:1428:LEU:CG	1:A:1431:GLN:CB	2.74	0.47
1:A:1531:ARG:HB2	1:A:1532:GLN:OE1	2.13	0.47
1:A:1670:ILE:CD1	1:A:1702:PHE:HE2	2.27	0.47
6:A:2013:PCW:H372	6:A:2013:PCW:H40	1.52	0.47
1:A:709:THR:O	1:A:713:VAL:HG23	2.14	0.47
1:A:1458:ILE:HG21	1:A:1533:TYR:HB3	1.95	0.47
1:A:1492:THR:HG21	1:A:1511:ILE:HG21	1.95	0.47
1:A:350:PHE:CE1	8:A:2024:P5S:H49A	2.49	0.47
1:A:387:TYR:CE2	1:A:391:LEU:HD11	2.48	0.47
1:A:1401:PHE:O	1:A:1405:GLY:N	2.48	0.47
7:A:2018:LPE:H151	7:A:2018:LPE:H122	1.71	0.47
1:A:871:LEU:HD13	8:A:2024:P5S:C29	2.44	0.47
1:A:1291:PHE:HD2	1:A:1292:TRP:CD1	2.33	0.47
1:A:129:HIS:CG	1:A:130:SER:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:ARG:HA	1:A:827:TRP:CH2	2.49	0.47
1:A:1465:PHE:O	1:A:1469:VAL:HG23	2.15	0.47
7:A:2018:LPE:H322	8:A:2022:P5S:OXT	2.14	0.47
1:A:185:LEU:O	1:A:186:ARG:C	2.51	0.47
1:A:236:VAL:O	1:A:240:ILE:HD12	2.15	0.47
1:A:692:THR:HG1	7:A:2020:LPE:H321	1.73	0.47
1:A:398:MET:HG3	1:A:1725:PHE:CE1	2.49	0.47
1:A:393:LEU:CD2	5:A:2025:CLR:H191	2.45	0.46
1:A:1558:ALA:O	1:A:1561:LYS:HG2	2.15	0.46
1:A:136:ILE:O	1:A:140:ILE:HG12	2.15	0.46
7:A:2012:LPE:H2N3	7:A:2012:LPE:H312	1.75	0.46
1:A:241:HIS:HE1	1:A:399:ALA:HB1	1.81	0.46
1:A:679:THR:HG21	5:A:2005:CLR:H271	1.97	0.46
1:A:1453:LYS:N	1:A:1454:PRO:HD2	2.30	0.46
1:A:1604:LEU:HD21	6:A:2006:PCW:H20	1.97	0.46
5:A:2025:CLR:H183	5:A:2025:CLR:H212	1.97	0.46
1:A:719:PHE:O	1:A:720:ASP:C	2.54	0.46
5:A:2021:CLR:H193	5:A:2021:CLR:H111	1.63	0.46
1:A:184:TYR:CE2	1:A:190:ASN:HB3	2.50	0.46
1:A:871:LEU:CB	8:A:2024:P5S:H31A	2.43	0.46
1:A:1455:GLN:HG2	1:A:1457:PRO:HD3	1.97	0.46
5:A:2021:CLR:C12	5:A:2021:CLR:C21	2.84	0.46
1:A:152:LEU:HB3	1:A:157:GLU:OE1	2.16	0.46
1:A:400:TYR:HD2	1:A:890:LEU:HD22	1.81	0.46
1:A:401:GLU:HG2	1:A:890:LEU:HD21	1.98	0.46
7:A:2009:LPE:H311	7:A:2009:LPE:H2N2	1.65	0.46
1:A:728:LYS:HD2	6:A:2013:PCW:P	2.56	0.46
1:A:1564:GLN:OE1	1:A:1564:GLN:HA	2.16	0.46
1:A:734:CYS:O	1:A:738:THR:HG23	2.15	0.45
1:A:215:ARG:HB3	1:A:807:GLN:HE21	1.80	0.45
1:A:226:VAL:HA	1:A:232:LEU:HD12	1.98	0.45
1:A:844:ARG:HG2	1:A:849:GLU:HB2	1.98	0.45
1:A:1539:TRP:CH2	6:A:2006:PCW:H381	2.52	0.45
1:A:1606:ALA:O	1:A:1610:ILE:HG13	2.15	0.45
6:A:2006:PCW:H421	6:A:2007:PCW:C21	2.47	0.45
1:A:188:PRO:HA	1:A:191:TRP:CE3	2.52	0.45
1:A:393:LEU:HD23	5:A:2025:CLR:H8	1.97	0.45
1:A:1500:GLN:HG3	1:A:1501:SER:H	1.81	0.45
1:A:1699:ILE:HG21	8:A:2022:P5S:H21A	1.98	0.45
1:A:1717:TYR:CG	5:A:2025:CLR:H192	2.52	0.45
6:A:2006:PCW:H341	6:A:2006:PCW:H371	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2008:LPE:H312	7:A:2008:LPE:H3N3	1.63	0.45
1:A:1469:VAL:HA	1:A:1472:ILE:HG12	1.99	0.45
8:A:2022:P5S:H42	8:A:2022:P5S:H20	1.98	0.45
1:A:702:ILE:O	1:A:706:ILE:HG23	2.17	0.44
1:A:1343:TRP:H	2:C:1:NAG:H82	1.83	0.44
1:A:1628:SER:C	1:A:1630:PRO:HD3	2.38	0.44
1:A:1685:SER:O	1:A:1689:ARG:HA	2.17	0.44
1:A:728:LYS:HD3	6:A:2013:PCW:O1P	2.15	0.44
6:A:2014:PCW:P	6:A:2014:PCW:O2	2.75	0.44
1:A:826:ASP:O	1:A:827:TRP:CD1	2.70	0.44
1:A:1460:ARG:HD2	1:A:1461:PRO:HD2	2.00	0.44
1:A:1537:ASN:OD1	1:A:1538:GLY:N	2.50	0.44
1:A:1570:THR:HA	1:A:1573:ARG:HD3	1.99	0.44
1:A:1414:VAL:HG11	5:A:2025:CLR:H9	2.00	0.44
1:A:192:LEU:O	1:A:196:VAL:HG23	2.18	0.43
1:A:667:ALA:O	1:A:671:ILE:HG12	2.18	0.43
1:A:1418:ILE:CD1	5:A:2025:CLR:H17	2.47	0.43
5:A:2005:CLR:H183	5:A:2005:CLR:H20	1.74	0.43
1:A:158:TYR:O	1:A:162:VAL:HG23	2.18	0.43
1:A:1453:LYS:N	1:A:1454:PRO:CD	2.81	0.43
5:A:2016:CLR:H183	5:A:2016:CLR:H20	1.82	0.43
1:A:1198:VAL:HG21	1:A:1230:LEU:HD21	1.99	0.43
1:A:1428:LEU:CD2	1:A:1431:GLN:HB2	2.38	0.43
1:A:1145:CYS:O	1:A:1149:VAL:HG23	2.18	0.43
1:A:1695:PRO:O	1:A:1699:ILE:HG13	2.18	0.43
1:A:196:VAL:HG21	1:A:224:LYS:HD3	2.00	0.43
1:A:758:PHE:O	1:A:761:LEU:HG	2.19	0.43
1:A:816:ASN:HB2	1:A:860:VAL:CG2	2.47	0.43
1:A:653:LYS:O	1:A:657:ILE:HG13	2.19	0.43
1:A:1449:LEU:O	1:A:1452:LYS:HG2	2.18	0.43
1:A:1490:MET:O	1:A:1494:MET:HG3	2.19	0.43
1:A:854:MET:O	1:A:858:MET:HG3	2.19	0.43
1:A:1328:ASN:OD1	1:A:1384:MET:HG2	2.18	0.43
1:A:1699:ILE:O	1:A:1703:THR:OG1	2.24	0.43
1:A:868:ILE:HG13	1:A:869:LEU:N	2.34	0.43
1:A:1619:PHE:O	1:A:1623:ILE:HG12	2.19	0.43
1:A:1713:MET:CE	5:A:2025:CLR:O1	2.67	0.43
1:A:827:TRP:CE3	1:A:828:PRO:CG	3.02	0.43
1:A:1458:ILE:HD11	1:A:1470:PHE:HE1	1.84	0.43
1:A:1560:LEU:HD21	1:A:1571:LEU:HD23	2.00	0.42
5:A:2021:CLR:H183	5:A:2021:CLR:H20	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:LYS:HE2	1:A:1661:ALA:HA	2.00	0.42
1:A:367:ARG:NH2	1:A:1641:MET:HG3	2.34	0.42
1:A:749:LYS:HA	1:A:749:LYS:HD3	1.85	0.42
1:A:1567:PHE:HE2	7:A:2012:LPE:C32	2.24	0.42
5:A:2005:CLR:H221	5:A:2005:CLR:H162	1.41	0.42
7:A:2015:LPE:H2N3	7:A:2015:LPE:H311	1.60	0.42
1:A:129:HIS:CD2	1:A:131:TRP:H	2.37	0.42
1:A:1170:ALA:CB	7:A:2017:LPE:O32	2.67	0.42
1:A:159:VAL:O	1:A:163:ILE:HG13	2.20	0.42
5:A:2021:CLR:H232	5:A:2021:CLR:H262	1.70	0.42
1:A:1265:GLU:O	1:A:1269:VAL:HG13	2.20	0.42
5:A:2025:CLR:H121	5:A:2025:CLR:C21	2.50	0.42
1:A:130:SER:HA	1:A:133:SER:OG	2.19	0.42
1:A:216:THR:HG21	1:A:808:LEU:CD2	2.47	0.42
1:A:136:ILE:HG12	1:A:171:LYS:CE	2.45	0.42
1:A:1552:ALA:HA	1:A:1555:ILE:HG12	2.01	0.42
1:A:1567:PHE:CE1	7:A:2012:LPE:H3N2	2.52	0.42
1:A:1345:ASN:OD1	1:A:1346:VAL:N	2.53	0.42
1:A:1568:SER:CB	7:A:2012:LPE:H2N2	2.49	0.42
5:A:2021:CLR:H111	5:A:2021:CLR:H182	1.68	0.42
1:A:717:ILE:HG22	1:A:717:ILE:O	2.20	0.42
1:A:1377:VAL:O	1:A:1377:VAL:HG12	2.20	0.42
6:A:2006:PCW:H42	6:A:2006:PCW:H72	1.52	0.42
1:A:373:TYR:O	1:A:376:PHE:HB3	2.20	0.41
1:A:770:TRP:CZ2	5:A:2005:CLR:H122	2.55	0.41
1:A:893:PHE:HZ	1:A:1412:LEU:HA	1.84	0.41
6:A:2007:PCW:H63	6:A:2007:PCW:H41	1.63	0.41
7:A:2015:LPE:C11	7:A:2015:LPE:O3	2.68	0.41
1:A:851:ILE:HG12	1:A:855:TRP:CE2	2.54	0.41
1:A:664:ASP:HB3	1:A:665:PRO:CD	2.49	0.41
5:A:2021:CLR:H112	5:A:2021:CLR:H11	1.77	0.41
1:A:219:VAL:CG1	1:A:803:LEU:HD23	2.51	0.41
1:A:817:ARG:HD3	1:A:827:TRP:CE2	2.55	0.41
1:A:736:ILE:HA	1:A:758:PHE:CE2	2.56	0.41
1:A:1436:THR:HG22	1:A:1437:GLU:N	2.35	0.41
5:A:2021:CLR:H192	5:A:2021:CLR:H22	1.64	0.41
1:A:735:ILE:O	1:A:739:VAL:HG23	2.20	0.41
1:A:1396:LEU:O	1:A:1400:ILE:HG13	2.20	0.41
1:A:656:THR:O	1:A:660:GLY:N	2.45	0.41
1:A:659:PHE:HA	1:A:662:VAL:HG23	2.02	0.41
1:A:1188:TYR:O	1:A:1192:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LYS:HB3	1:A:308:LEU:HD13	2.03	0.41
1:A:1324:SER:HB2	1:A:1325:ILE:HD12	2.02	0.41
1:A:351:ARG:HD2	1:A:851:ILE:HD13	2.02	0.41
1:A:680:ILE:HD13	7:A:2020:LPE:H182	2.02	0.41
1:A:1404:PHE:HA	1:A:1408:PHE:HD2	1.86	0.41
1:A:1678:CYS:SG	1:A:1692:CYS:N	2.94	0.40
1:A:128:VAL:HG23	1:A:128:VAL:O	2.21	0.40
1:A:698:GLN:O	1:A:702:ILE:HG12	2.21	0.40
1:A:241:HIS:CG	1:A:403:GLN:HE21	2.40	0.40
1:A:1234:THR:HA	1:A:1237:ILE:HG12	2.02	0.40
1:A:271:ASN:HD22	1:A:271:ASN:HA	1.69	0.40
1:A:862:GLN:HB2	1:A:865:ILE:HD12	2.03	0.40
1:A:1601:MET:SD	6:A:2007:PCW:H122	2.62	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	1115/1956 (57%)	1050 (94%)	59 (5%)	6 (0%)	29 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	A	153	PRO
1	A	181	GLU
1	A	383	LEU
1	A	720	ASP
1	A	1630	PRO

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	983/1727 (57%)	983 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	271	ASN
1	A	390	ASN
1	A	807	GLN
1	A	878	ASN
1	A	1301	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	0.50	0	17,19,21	1.52	2 (11%)
2	NAG	B	2	2	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	3.98	117.58	111.29
2	B	1	NAG	C4-C3-C2	-3.87	105.35	111.02
2	B	2	NAG	C4-C3-C2	-3.61	105.73	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

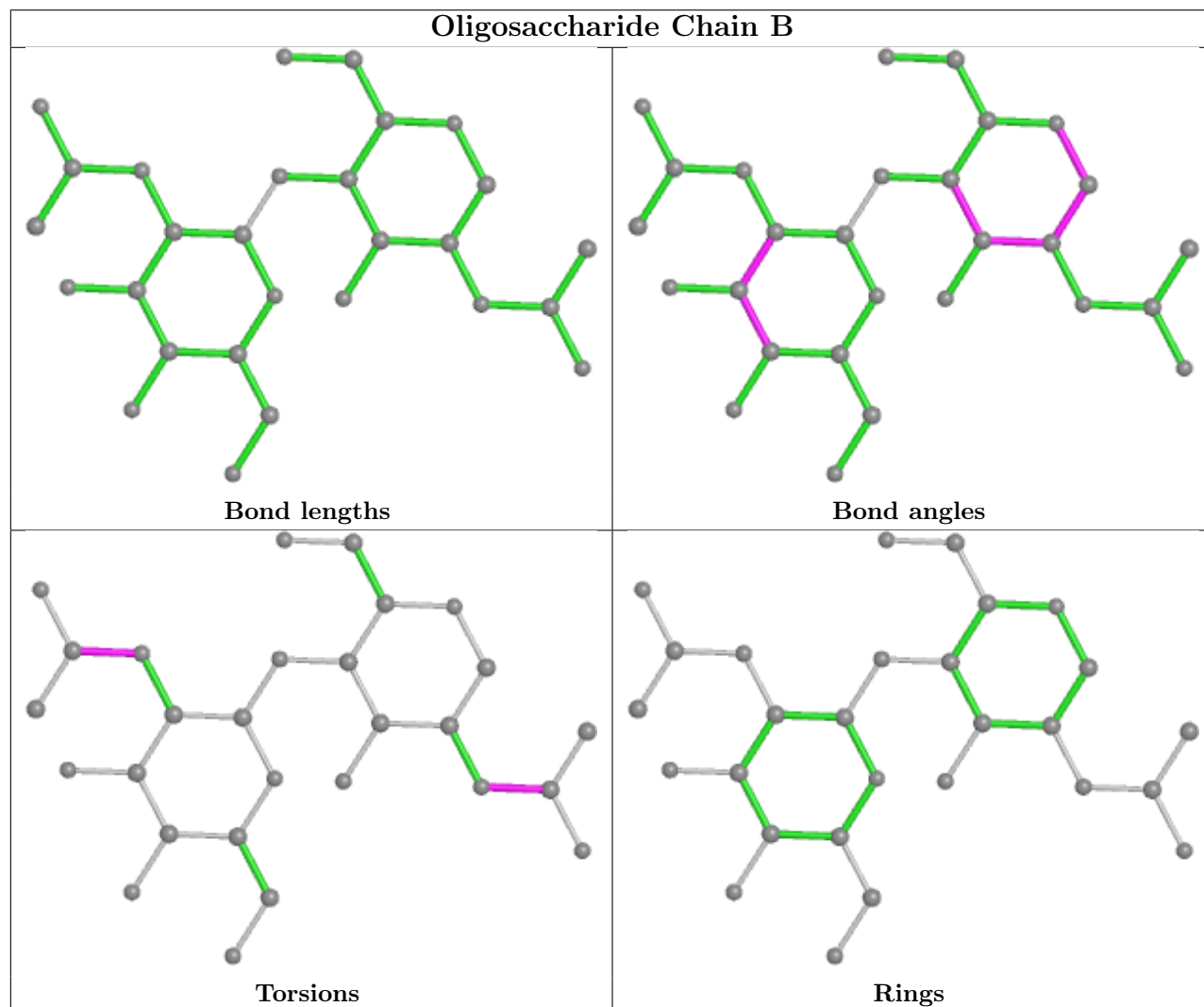
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

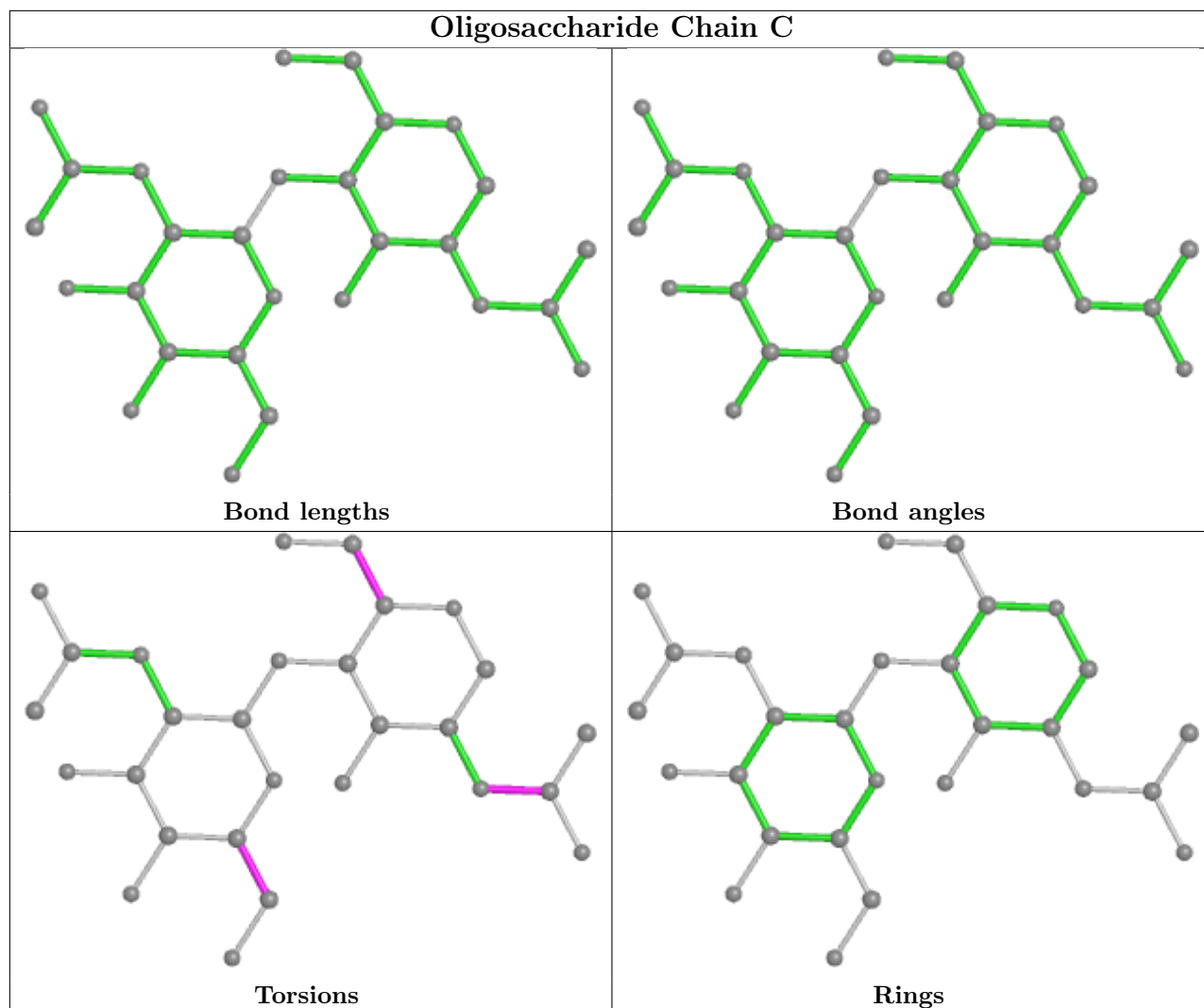
There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

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





5.6 Ligand geometry [i](#)

25 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$
6	PCW	A	2014	-	39,39,53	1.13	3 (7%)	44,47,61	1.71	8 (18%)
5	CLR	A	2005	-	31,31,31	0.88	2 (6%)	48,48,48	1.32	5 (10%)
5	CLR	A	2016	-	31,31,31	1.44	5 (16%)	48,48,48	2.91	21 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PCW	A	2007	-	46,46,53	1.02	2 (4%)	52,54,61	1.17	3 (5%)
7	LPE	A	2015	-	33,33,33	0.58	0	37,39,39	1.15	3 (8%)
7	LPE	A	2019	-	20,20,33	1.08	0	24,26,39	1.18	2 (8%)
4	95T	A	2004	-	23,27,27	1.62	4 (17%)	29,37,37	4.37	10 (34%)
6	PCW	A	2006	-	46,46,53	0.98	2 (4%)	52,54,61	1.15	4 (7%)
7	LPE	A	2008	-	21,21,33	0.57	0	25,27,39	0.53	0
7	LPE	A	2017	-	21,21,33	0.66	0	25,27,39	0.78	1 (4%)
3	NAG	A	2002	1	14,14,15	0.48	0	17,19,21	1.50	3 (17%)
5	CLR	A	2025	-	31,31,31	0.71	0	48,48,48	1.14	5 (10%)
7	LPE	A	2012	-	22,22,33	0.61	0	26,28,39	0.70	0
6	PCW	A	2013	-	40,40,53	1.00	2 (5%)	43,45,61	1.28	4 (9%)
7	LPE	A	2009	-	21,21,33	0.57	0	25,27,39	0.60	0
8	P5S	A	2024	-	47,48,53	1.00	2 (4%)	51,55,60	1.39	5 (9%)
7	LPE	A	2011	-	22,22,33	0.59	0	26,28,39	0.58	0
7	LPE	A	2018	-	21,21,33	0.57	0	25,27,39	0.70	0
8	P5S	A	2023	-	35,36,53	1.13	2 (5%)	39,43,60	1.78	4 (10%)
6	PCW	A	2010	-	31,31,53	1.19	2 (6%)	34,36,61	1.30	3 (8%)
3	NAG	A	2003	1	14,14,15	0.31	0	17,19,21	1.98	3 (17%)
3	NAG	A	2001	1	14,14,15	0.29	0	17,19,21	1.50	3 (17%)
8	P5S	A	2022	-	43,44,53	0.95	3 (6%)	47,51,60	1.48	8 (17%)
7	LPE	A	2020	-	24,24,33	0.52	0	28,30,39	0.61	0
5	CLR	A	2021	-	31,31,31	2.16	10 (32%)	48,48,48	2.53	17 (35%)

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
6	PCW	A	2014	-	-	21/43/43/57	-
5	CLR	A	2005	-	-	7/10/68/68	0/4/4/4
5	CLR	A	2016	-	-	5/10/68/68	0/4/4/4
6	PCW	A	2007	-	-	16/50/50/57	-
7	LPE	A	2015	-	-	21/34/34/34	-
7	LPE	A	2019	-	-	11/21/21/34	-
4	95T	A	2004	-	-	6/11/16/16	0/3/3/3
6	PCW	A	2006	-	-	20/50/50/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LPE	A	2008	-	-	13/22/22/34	-
7	LPE	A	2017	-	-	10/22/22/34	-
3	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
5	CLR	A	2025	-	-	0/10/68/68	0/4/4/4
7	LPE	A	2012	-	-	8/23/23/34	-
6	PCW	A	2013	-	-	14/42/42/57	-
7	LPE	A	2009	-	-	4/22/22/34	-
8	P5S	A	2024	-	-	8/54/54/59	-
7	LPE	A	2011	-	-	10/23/23/34	-
7	LPE	A	2018	-	-	4/22/22/34	-
8	P5S	A	2023	-	-	15/42/42/59	-
6	PCW	A	2010	-	-	7/33/33/57	-
3	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2001	1	-	3/6/23/26	0/1/1/1
8	P5S	A	2022	-	-	13/50/50/59	-
7	LPE	A	2020	-	-	11/25/25/34	-
5	CLR	A	2021	-	-	3/10/68/68	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2021	CLR	C12-C13	-4.86	1.45	1.54
5	A	2021	CLR	C10-C9	-4.55	1.48	1.56
5	A	2021	CLR	C13-C14	-4.49	1.46	1.55
6	A	2007	PCW	O3-C11	4.43	1.46	1.33
8	A	2024	P5S	O37-C38	4.42	1.46	1.34
8	A	2024	P5S	O19-C17	4.40	1.46	1.33
8	A	2023	P5S	O37-C38	4.36	1.46	1.34
6	A	2010	PCW	O2-C31	4.23	1.46	1.34
6	A	2007	PCW	O2-C31	4.22	1.46	1.34
6	A	2010	PCW	O3-C11	4.21	1.45	1.33
6	A	2006	PCW	O2-C31	4.15	1.46	1.34
5	A	2021	CLR	C13-C17	-4.10	1.47	1.55
8	A	2023	P5S	O19-C17	4.05	1.45	1.33
6	A	2013	PCW	O2-C31	3.94	1.45	1.34
6	A	2013	PCW	O3-C11	3.90	1.44	1.33
6	A	2006	PCW	O3-C11	3.81	1.44	1.33
8	A	2022	P5S	O19-C17	3.77	1.44	1.33
8	A	2022	P5S	O37-C38	3.64	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2016	CLR	C13-C14	-3.50	1.48	1.55
6	A	2014	PCW	O2-C31	3.33	1.43	1.34
4	A	2004	95T	C15-C08	-3.22	1.34	1.39
5	A	2021	CLR	C18-C13	-3.15	1.48	1.54
5	A	2021	CLR	C11-C9	-3.14	1.48	1.53
4	A	2004	95T	O05-C13	-3.10	1.17	1.23
5	A	2016	CLR	C8-C14	-2.83	1.48	1.53
6	A	2014	PCW	O3-C11	2.82	1.41	1.33
5	A	2016	CLR	C20-C17	-2.64	1.49	1.54
5	A	2021	CLR	C8-C14	-2.60	1.48	1.53
4	A	2004	95T	C14-C17	-2.53	1.34	1.38
5	A	2016	CLR	C13-C17	-2.53	1.50	1.55
5	A	2021	CLR	C1-C10	-2.50	1.49	1.54
5	A	2021	CLR	C8-C9	-2.45	1.48	1.53
5	A	2005	CLR	C10-C9	-2.40	1.52	1.56
5	A	2021	CLR	C15-C14	-2.31	1.49	1.54
5	A	2016	CLR	C10-C9	-2.16	1.52	1.56
4	A	2004	95T	O03-C24	-2.11	1.36	1.42
5	A	2005	CLR	C13-C14	-2.06	1.51	1.55
8	A	2022	P5S	O37-C2	-2.04	1.41	1.46
6	A	2014	PCW	P-O1P	-2.02	1.45	1.55

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	95T	C09-C13-N06	16.91	139.89	113.89
4	A	2004	95T	C11-C07-C10	-10.46	119.00	128.77
5	A	2021	CLR	C11-C9-C10	-8.69	101.64	113.08
8	A	2023	P5S	OG-CB-CA	8.38	115.36	108.06
4	A	2004	95T	O05-C13-N06	-8.31	104.73	123.71
5	A	2016	CLR	C13-C14-C8	-6.70	104.46	114.38
5	A	2016	CLR	C7-C6-C5	-6.50	113.07	125.06
5	A	2016	CLR	C1-C2-C3	6.15	118.36	110.47
5	A	2016	CLR	C13-C17-C20	-6.14	109.87	119.49
5	A	2016	CLR	C7-C8-C9	6.05	117.05	109.71
6	A	2014	PCW	C3-C2-C1	-6.01	97.57	111.79
4	A	2004	95T	C08-N06-C13	5.94	142.01	126.58
5	A	2021	CLR	C16-C17-C13	-5.85	96.79	103.84
5	A	2021	CLR	C13-C17-C20	-5.78	110.43	119.49
8	A	2024	P5S	OG-CB-CA	5.56	112.91	108.06
5	A	2016	CLR	C4-C5-C10	5.08	123.17	116.42
5	A	2016	CLR	C8-C7-C6	-5.07	105.45	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2022	P5S	OG-CB-CA	5.04	112.45	108.06
5	A	2021	CLR	C15-C14-C13	-4.90	97.94	103.84
6	A	2007	PCW	O2-C31-C32	4.88	122.01	111.50
5	A	2016	CLR	C15-C14-C13	-4.51	98.40	103.84
6	A	2014	PCW	O2-C31-C32	4.33	120.83	111.50
6	A	2010	PCW	O2-C31-C32	4.30	120.78	111.50
3	A	2003	NAG	C2-N2-C7	4.29	129.02	122.90
3	A	2003	NAG	C4-C3-C2	-4.28	104.75	111.02
5	A	2021	CLR	C18-C13-C12	-4.26	103.86	110.59
3	A	2002	NAG	O5-C1-C2	-4.00	104.97	111.29
8	A	2022	P5S	O37-C38-C39	3.97	120.06	111.50
8	A	2023	P5S	O37-C38-C39	3.96	120.04	111.50
6	A	2013	PCW	O2-C31-C32	3.96	120.03	111.50
8	A	2024	P5S	O37-C38-C39	3.92	119.95	111.50
3	A	2001	NAG	C4-C3-C2	-3.89	105.31	111.02
6	A	2014	PCW	C2-O2-C31	3.75	127.03	117.79
5	A	2005	CLR	C13-C17-C20	-3.74	113.63	119.49
6	A	2006	PCW	O2-C31-C32	3.70	119.47	111.50
7	A	2015	LPE	O3-P-O31	-3.49	95.42	109.07
3	A	2003	NAG	O5-C1-C2	3.41	116.67	111.29
5	A	2016	CLR	C15-C14-C8	-3.37	113.52	119.08
5	A	2021	CLR	C17-C13-C14	3.36	104.06	100.07
5	A	2021	CLR	C2-C3-C4	3.31	114.84	110.31
5	A	2016	CLR	C12-C13-C14	3.30	112.39	107.27
5	A	2025	CLR	C13-C17-C20	-3.29	114.33	119.49
6	A	2007	PCW	O3-C11-C12	3.25	122.09	111.91
3	A	2001	NAG	C2-N2-C7	3.23	127.50	122.90
5	A	2021	CLR	C2-C1-C10	-3.21	105.80	112.74
8	A	2022	P5S	O19-C17-C20	3.19	121.91	111.91
6	A	2006	PCW	O3-C11-C12	3.18	121.89	111.91
7	A	2019	LPE	O2H-C2-C3	-3.15	98.49	109.56
5	A	2021	CLR	C11-C12-C13	-3.11	107.45	112.78
5	A	2016	CLR	C9-C10-C5	-3.11	104.78	109.65
5	A	2016	CLR	C10-C5-C6	-3.05	118.24	122.90
5	A	2021	CLR	C23-C22-C20	-2.92	106.65	115.03
8	A	2023	P5S	OXT-C-O	-2.90	117.49	124.09
5	A	2016	CLR	C22-C20-C17	-2.90	104.29	110.28
5	A	2005	CLR	C4-C5-C10	2.89	120.26	116.42
4	A	2004	95T	C24-O03-C16	-2.88	111.25	117.51
5	A	2016	CLR	C21-C20-C22	2.88	114.88	110.36
3	A	2002	NAG	C4-C3-C2	-2.87	106.81	111.02
5	A	2021	CLR	C12-C13-C14	2.84	111.68	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2005	CLR	C8-C7-C6	-2.80	108.71	112.73
8	A	2024	P5S	OXT-C-O	-2.78	117.77	124.09
5	A	2021	CLR	C8-C7-C6	-2.78	108.74	112.73
4	A	2004	95T	O05-C13-C09	-2.77	115.05	121.08
5	A	2016	CLR	C11-C9-C10	-2.74	109.48	113.08
5	A	2016	CLR	C2-C3-C4	2.73	114.05	110.31
6	A	2010	PCW	O3-C11-C12	2.73	120.48	111.91
6	A	2013	PCW	C2-O2-C31	-2.73	111.08	117.79
5	A	2021	CLR	C15-C14-C8	-2.72	114.60	119.08
5	A	2021	CLR	C13-C14-C8	-2.71	110.37	114.38
8	A	2024	P5S	OXT-C-CA	2.68	122.51	113.38
6	A	2014	PCW	C14-C13-C12	-2.61	103.81	113.19
8	A	2022	P5S	OXT-C-O	-2.59	118.21	124.09
8	A	2023	P5S	OXT-C-CA	2.58	122.16	113.38
5	A	2016	CLR	C23-C24-C25	-2.56	103.94	115.98
5	A	2016	CLR	C12-C13-C17	-2.55	112.76	116.57
5	A	2016	CLR	C11-C12-C13	-2.54	108.42	112.78
5	A	2025	CLR	C11-C12-C13	-2.53	108.45	112.78
6	A	2014	PCW	O3-C11-O11	-2.52	117.22	123.59
5	A	2025	CLR	C13-C14-C8	-2.50	110.68	114.38
6	A	2007	PCW	O3-C3-C2	2.49	115.69	108.43
6	A	2006	PCW	C3-C2-C1	-2.49	105.90	111.79
6	A	2014	PCW	O3-C11-C12	2.45	119.60	111.91
6	A	2014	PCW	C34-C33-C32	-2.45	104.40	113.19
4	A	2004	95T	C18-C17-C14	-2.41	117.14	120.98
6	A	2010	PCW	O1P-P-O2P	2.41	120.10	110.68
5	A	2005	CLR	C4-C5-C6	-2.40	117.15	120.61
8	A	2024	P5S	O19-C17-C20	2.39	119.41	111.91
5	A	2025	CLR	C17-C13-C14	2.35	102.85	100.07
5	A	2016	CLR	C10-C9-C8	-2.34	109.22	112.73
6	A	2006	PCW	O3-C11-O11	-2.34	117.70	123.59
6	A	2013	PCW	O3-C11-C12	2.32	119.19	111.91
7	A	2017	LPE	C3-C2-C1	-2.31	105.98	112.79
8	A	2022	P5S	OXT-C-CA	2.30	121.22	113.38
4	A	2004	95T	C20-C10-C07	-2.28	117.54	120.42
7	A	2015	LPE	O32-P-O31	2.27	123.46	112.24
7	A	2015	LPE	C17-C16-C15	-2.26	102.96	114.42
8	A	2022	P5S	O37-C38-O47	-2.25	118.26	123.70
6	A	2013	PCW	O1P-P-O2P	2.25	119.49	110.68
5	A	2005	CLR	C11-C9-C10	-2.23	110.14	113.08
5	A	2025	CLR	C4-C5-C10	2.20	119.35	116.42
5	A	2021	CLR	C21-C20-C22	-2.19	106.94	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2022	P5S	C2-O37-C38	-2.17	112.44	117.79
3	A	2001	NAG	C1-C2-N2	-2.14	106.83	110.49
5	A	2021	CLR	C1-C10-C5	2.13	112.65	108.75
5	A	2016	CLR	C21-C20-C17	-2.10	109.71	112.92
8	A	2022	P5S	O19-C17-O18	-2.07	118.36	123.59
5	A	2021	CLR	C11-C9-C8	-2.07	108.77	111.75
6	A	2014	PCW	C16-C17-C18	-2.07	104.77	113.79
3	A	2002	NAG	C3-C4-C5	-2.02	106.63	110.24
4	A	2004	95T	C14-C08-N06	-2.02	113.59	120.18
4	A	2004	95T	C14-C08-C15	2.01	122.26	119.57
7	A	2019	LPE	O2H-C2-C1	-2.00	102.54	109.56

There are no chirality outliers.

All (233) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	NAG	C3-C2-N2-C7
3	A	2001	NAG	C8-C7-N2-C2
3	A	2001	NAG	O7-C7-N2-C2
3	A	2003	NAG	C3-C2-N2-C7
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
6	A	2006	PCW	O4P-C4-C5-N
6	A	2006	PCW	C4-O4P-P-O2P
6	A	2007	PCW	C1-O3P-P-O1P
6	A	2010	PCW	C39-C40-C41-C42
6	A	2013	PCW	C12-C11-O3-C3
6	A	2013	PCW	O11-C11-O3-C3
6	A	2013	PCW	C19-C20-C21-C22
6	A	2013	PCW	C32-C31-O2-C2
6	A	2013	PCW	C1-O3P-P-O1P
6	A	2013	PCW	C1-O3P-P-O2P
6	A	2013	PCW	C1-O3P-P-O4P
6	A	2014	PCW	C36-C37-C38-C39
6	A	2014	PCW	C1-O3P-P-O1P
6	A	2014	PCW	C4-O4P-P-O1P
6	A	2014	PCW	C4-O4P-P-O2P
6	A	2014	PCW	C4-O4P-P-O3P
7	A	2008	LPE	C3-O3-P-O32
7	A	2008	LPE	C31-O33-P-O3
7	A	2008	LPE	C31-O33-P-O31
7	A	2008	LPE	C31-O33-P-O32

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Mol	Chain	Res	Type	Atoms
7	A	2011	LPE	C31-O33-P-O31
7	A	2011	LPE	C31-O33-P-O32
7	A	2012	LPE	O2H-C2-C3-O3
7	A	2012	LPE	C3-O3-P-O32
7	A	2012	LPE	C31-O33-P-O32
7	A	2015	LPE	C3-O3-P-O33
7	A	2015	LPE	C31-O33-P-O3
7	A	2015	LPE	C31-O33-P-O32
7	A	2015	LPE	O33-C31-C32-N
7	A	2017	LPE	C3-O3-P-O32
7	A	2017	LPE	C31-O33-P-O32
7	A	2018	LPE	O33-C31-C32-N
7	A	2019	LPE	C3-O3-P-O31
7	A	2019	LPE	C3-O3-P-O32
7	A	2019	LPE	C32-C31-O33-P
7	A	2020	LPE	C3-O3-P-O31
7	A	2020	LPE	C3-O3-P-O33
7	A	2020	LPE	C31-O33-P-O32
8	A	2022	P5S	O-C-CA-N
8	A	2022	P5S	O47-C38-O37-C2
8	A	2023	P5S	O-C-CA-N
8	A	2023	P5S	O-C-CA-CB
8	A	2023	P5S	OXT-C-CA-CB
8	A	2023	P5S	C-CA-CB-OG
8	A	2023	P5S	N-CA-CB-OG
8	A	2023	P5S	CB-OG-P12-O16
8	A	2023	P5S	C39-C38-O37-C2
4	A	2004	95T	O05-C13-N06-C08
4	A	2004	95T	C09-C13-N06-C08
5	A	2005	CLR	C13-C17-C20-C21
4	A	2004	95T	C14-C17-O04-C25
4	A	2004	95T	C18-C17-O04-C25
6	A	2007	PCW	O31-C31-O2-C2
6	A	2013	PCW	O31-C31-O2-C2
8	A	2023	P5S	O47-C38-O37-C2
8	A	2022	P5S	C39-C38-O37-C2
5	A	2016	CLR	C21-C20-C22-C23
5	A	2005	CLR	C16-C17-C20-C21
5	A	2005	CLR	C13-C17-C20-C22
6	A	2006	PCW	C12-C11-O3-C3
7	A	2020	LPE	C31-C32-N-C2N
5	A	2005	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
6	A	2007	PCW	C32-C31-O2-C2
5	A	2005	CLR	C21-C20-C22-C23
6	A	2006	PCW	O11-C11-O3-C3
5	A	2005	CLR	C17-C20-C22-C23
8	A	2022	P5S	OXT-C-CA-N
8	A	2023	P5S	OXT-C-CA-N
7	A	2012	LPE	C1-C2-C3-O3
6	A	2014	PCW	C4-C5-N-C6
5	A	2016	CLR	C17-C20-C22-C23
5	A	2021	CLR	C17-C20-C22-C23
4	A	2004	95T	C15-C16-O03-C24
5	A	2021	CLR	C22-C23-C24-C25
4	A	2004	95T	C18-C16-O03-C24
6	A	2006	PCW	C4-C5-N-C7
5	A	2005	CLR	C20-C22-C23-C24
5	A	2021	CLR	C21-C20-C22-C23
6	A	2007	PCW	C1-O3P-P-O4P
6	A	2014	PCW	C1-O3P-P-O4P
7	A	2008	LPE	C3-O3-P-O33
7	A	2011	LPE	C31-O33-P-O3
7	A	2012	LPE	C3-O3-P-O33
7	A	2012	LPE	C31-O33-P-O3
7	A	2017	LPE	C3-O3-P-O33
7	A	2017	LPE	C31-O33-P-O3
7	A	2018	LPE	C31-O33-P-O3
7	A	2019	LPE	C3-O3-P-O33
6	A	2014	PCW	C4-C5-N-C7
6	A	2014	PCW	C4-C5-N-C8
7	A	2011	LPE	C31-C32-N-C1N
7	A	2020	LPE	C31-C32-N-C1N
8	A	2024	P5S	C44-C45-C46-C48
7	A	2015	LPE	C16-C17-C18-C19
8	A	2023	P5S	C1-C2-O37-C38
6	A	2006	PCW	C35-C36-C37-C38
6	A	2014	PCW	C33-C34-C35-C36
7	A	2017	LPE	C2-C3-O3-P
7	A	2015	LPE	O2H-C2-C3-O3
8	A	2024	P5S	C21-C22-C23-C24
7	A	2011	LPE	C31-C32-N-C2N
7	A	2011	LPE	C31-C32-N-C3N
7	A	2020	LPE	C31-C32-N-C3N
6	A	2007	PCW	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	A	2015	LPE	C23-C24-C25-C26
5	A	2016	CLR	C22-C23-C24-C25
7	A	2015	LPE	C18-C19-C20-C21
6	A	2010	PCW	C32-C31-O2-C2
6	A	2014	PCW	C35-C36-C37-C38
7	A	2015	LPE	C24-C25-C26-C27
6	A	2010	PCW	O31-C31-O2-C2
6	A	2006	PCW	C4-C5-N-C6
6	A	2006	PCW	C4-C5-N-C8
7	A	2015	LPE	C19-C20-C21-C22
6	A	2006	PCW	C15-C16-C17-C18
6	A	2014	PCW	C12-C11-O3-C3
7	A	2015	LPE	C12-C13-C14-C15
6	A	2006	PCW	C34-C35-C36-C37
6	A	2014	PCW	C2-C1-O3P-P
8	A	2023	P5S	C22-C23-C24-C25
6	A	2014	PCW	C14-C15-C16-C17
6	A	2013	PCW	C39-C40-C41-C42
6	A	2006	PCW	C40-C41-C42-C43
7	A	2008	LPE	C2-C1-O1-C11
7	A	2011	LPE	C2-C1-O1-C11
6	A	2013	PCW	C2-C1-O3P-P
8	A	2023	P5S	O37-C2-C3-O16
6	A	2014	PCW	O11-C11-O3-C3
7	A	2019	LPE	C12-C13-C14-C15
7	A	2015	LPE	C1-C2-C3-O3
6	A	2013	PCW	O3P-C1-C2-C3
7	A	2015	LPE	C2-C3-O3-P
8	A	2024	P5S	O19-C1-C2-C3
7	A	2015	LPE	C20-C21-C22-C23
7	A	2015	LPE	C25-C26-C27-C28
7	A	2020	LPE	C31-O33-P-O3
8	A	2022	P5S	O37-C2-C3-O16
7	A	2015	LPE	C13-C14-C15-C16
8	A	2023	P5S	C2-C3-O16-P12
8	A	2022	P5S	C28-C29-C30-C31
8	A	2022	P5S	C1-C2-C3-O16
7	A	2011	LPE	C12-C11-O1-C1
6	A	2007	PCW	C3-C2-O2-C31
6	A	2006	PCW	O3P-C1-C2-O2
6	A	2013	PCW	O3P-C1-C2-O2
6	A	2013	PCW	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
8	A	2024	P5S	O19-C1-C2-O37
8	A	2022	P5S	N-CA-CB-OG
8	A	2024	P5S	N-CA-CB-OG
6	A	2006	PCW	C16-C17-C18-C19
6	A	2006	PCW	C4-O4P-P-O3P
7	A	2020	LPE	O1-C11-C12-C13
6	A	2006	PCW	C4-O4P-P-O1P
7	A	2018	LPE	C31-O33-P-O31
7	A	2020	LPE	C31-O33-P-O31
6	A	2010	PCW	C12-C11-O3-C3
8	A	2023	P5S	C1-C2-C3-O16
7	A	2008	LPE	O1-C1-C2-C3
6	A	2014	PCW	C5-C4-O4P-P
7	A	2020	LPE	C32-C31-O33-P
6	A	2010	PCW	O11-C11-O3-C3
6	A	2006	PCW	C32-C33-C34-C35
7	A	2008	LPE	C1-C2-C3-O3
7	A	2018	LPE	C2-C1-O1-C11
7	A	2008	LPE	O2H-C2-C3-O3
6	A	2014	PCW	C12-C13-C14-C15
6	A	2014	PCW	O4P-C4-C5-N
7	A	2012	LPE	O33-C31-C32-N
7	A	2017	LPE	O33-C31-C32-N
7	A	2019	LPE	O33-C31-C32-N
6	A	2014	PCW	C32-C33-C34-C35
6	A	2013	PCW	C31-C32-C33-C34
7	A	2017	LPE	O1-C1-C2-C3
6	A	2010	PCW	C31-C32-C33-C34
7	A	2015	LPE	C11-C12-C13-C14
7	A	2020	LPE	C12-C11-O1-C1
6	A	2006	PCW	O2-C2-C3-O3
6	A	2007	PCW	C4-O4P-P-O3P
7	A	2009	LPE	C3-O3-P-O33
7	A	2011	LPE	C3-O3-P-O33
7	A	2019	LPE	C31-O33-P-O3
8	A	2024	P5S	C3-O16-P12-OG
7	A	2019	LPE	C12-C11-O1-C1
7	A	2015	LPE	C12-C11-O1-C1
5	A	2016	CLR	C13-C17-C20-C21
6	A	2014	PCW	C16-C17-C18-C19
8	A	2022	P5S	C45-C46-C48-C49
5	A	2016	CLR	C13-C17-C20-C22

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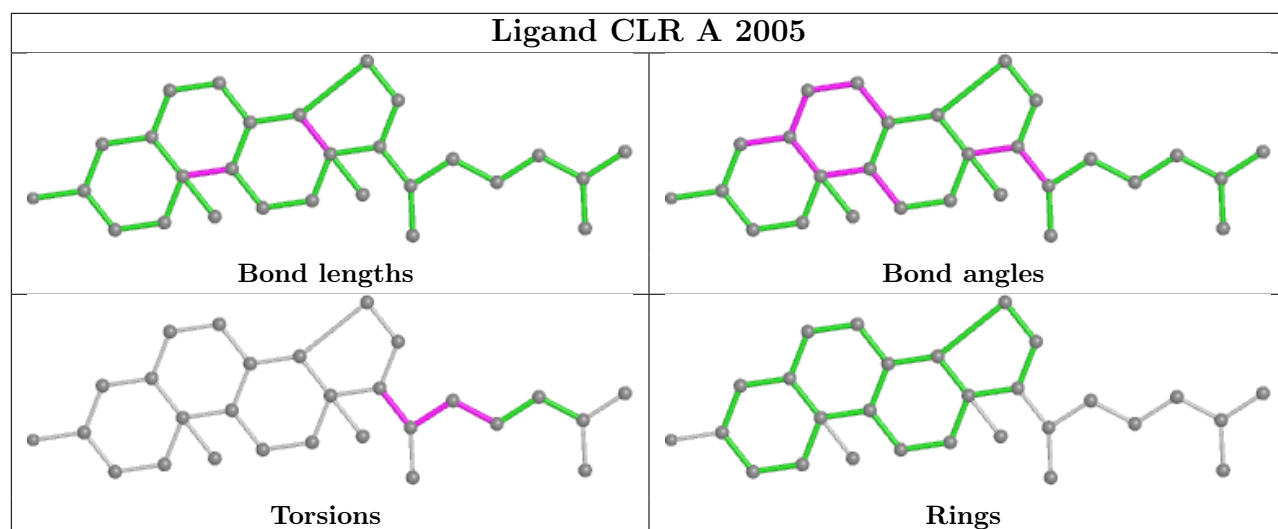
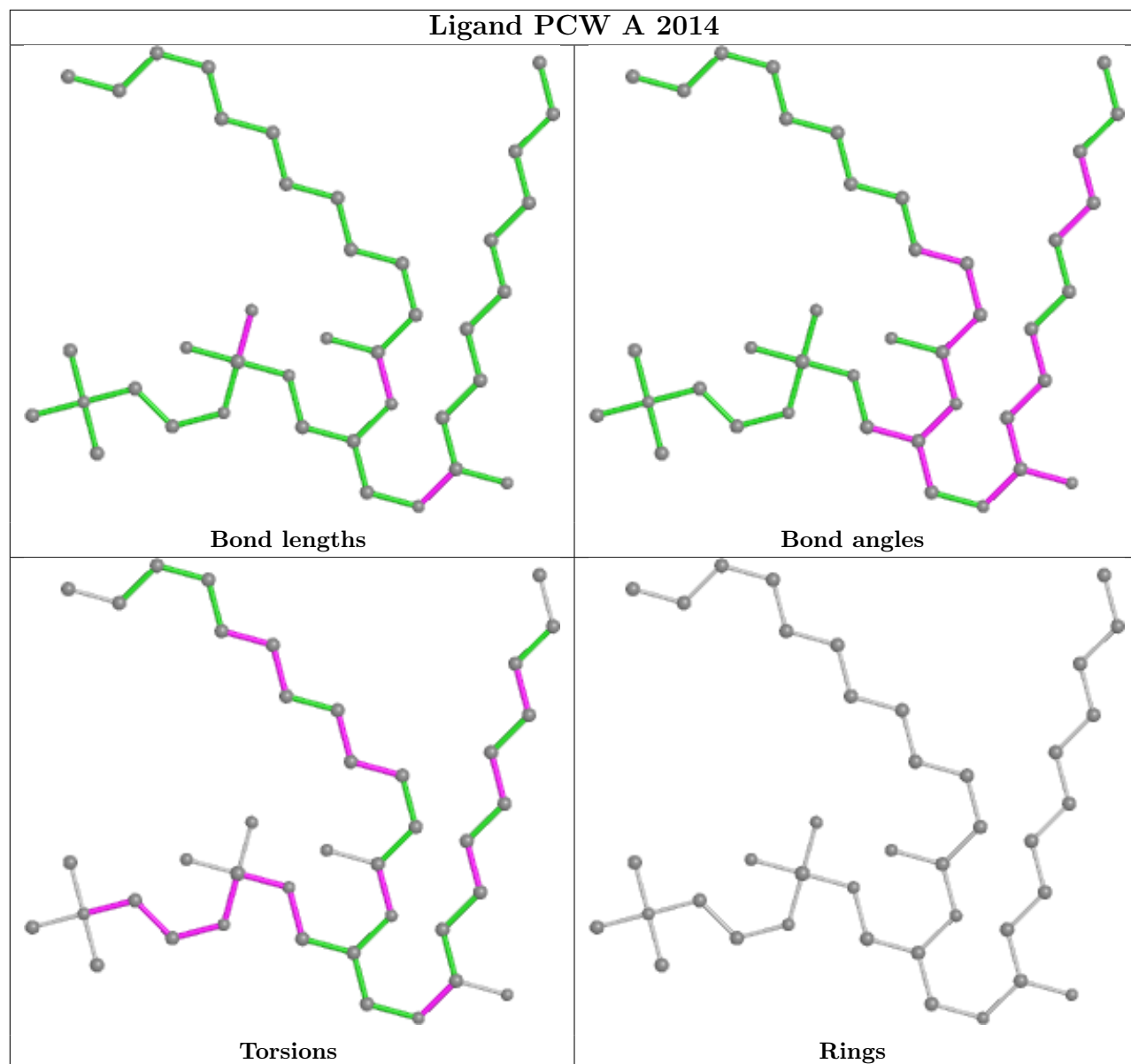
Mol	Chain	Res	Type	Atoms
7	A	2017	LPE	C11-C12-C13-C14
7	A	2009	LPE	C31-C32-N-C2N
6	A	2007	PCW	C39-C40-C41-C42
6	A	2007	PCW	C31-C32-C33-C34
6	A	2006	PCW	O3P-C1-C2-C3
6	A	2010	PCW	C37-C38-C39-C40
7	A	2015	LPE	C31-C32-N-C2N
6	A	2007	PCW	C4-C5-N-C6
7	A	2017	LPE	C12-C13-C14-C15
6	A	2006	PCW	C39-C40-C41-C42
7	A	2008	LPE	C31-C32-N-C3N
6	A	2007	PCW	O2-C2-C3-O3
7	A	2008	LPE	O1-C1-C2-O2H
8	A	2024	P5S	C17-C20-C21-C22
7	A	2009	LPE	C31-C32-N-C1N
7	A	2009	LPE	C31-C32-N-C3N
7	A	2019	LPE	C11-C12-C13-C14
8	A	2022	P5S	O37-C38-C39-C40
6	A	2007	PCW	C4-C5-N-C8
6	A	2006	PCW	C17-C18-C19-C20
8	A	2024	P5S	OXT-C-CA-N
7	A	2012	LPE	C31-C32-N-C2N
6	A	2007	PCW	O3-C11-C12-C13
7	A	2015	LPE	C31-C32-N-C1N
8	A	2022	P5S	C39-C40-C41-C42
6	A	2014	PCW	O31-C31-O2-C2
6	A	2007	PCW	C4-O4P-P-O2P
7	A	2008	LPE	C31-C32-N-C1N
7	A	2015	LPE	C31-C32-N-C3N
7	A	2017	LPE	C31-C32-N-C2N
7	A	2019	LPE	C31-O33-P-O31
8	A	2022	P5S	CB-OG-P12-O13
6	A	2007	PCW	O11-C11-C12-C13
8	A	2022	P5S	O47-C38-C39-C40
7	A	2011	LPE	C12-C13-C14-C15
8	A	2023	P5S	O37-C38-C39-C40
6	A	2007	PCW	C4-C5-N-C7
7	A	2008	LPE	C31-C32-N-C2N
7	A	2019	LPE	O2H-C2-C3-O3

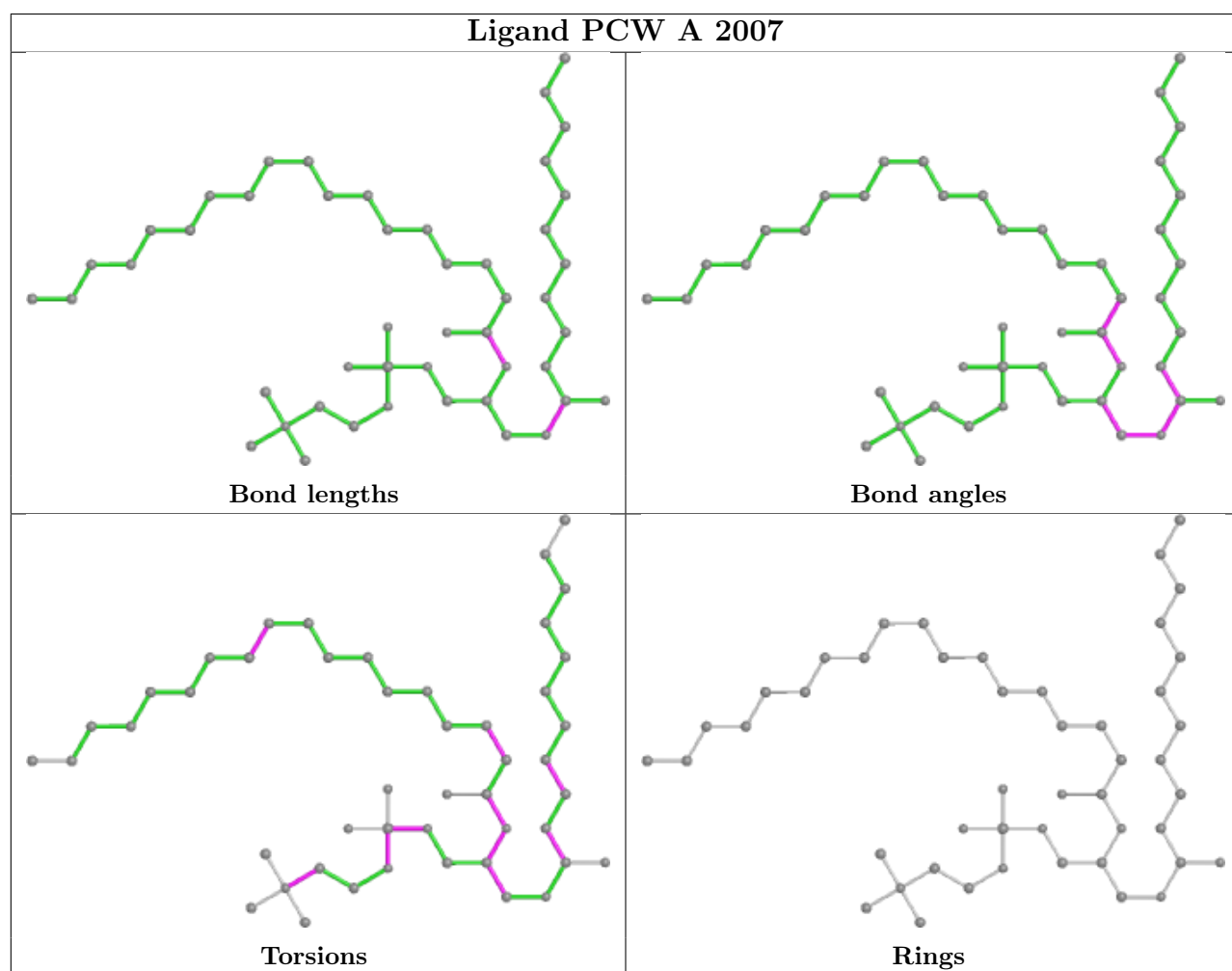
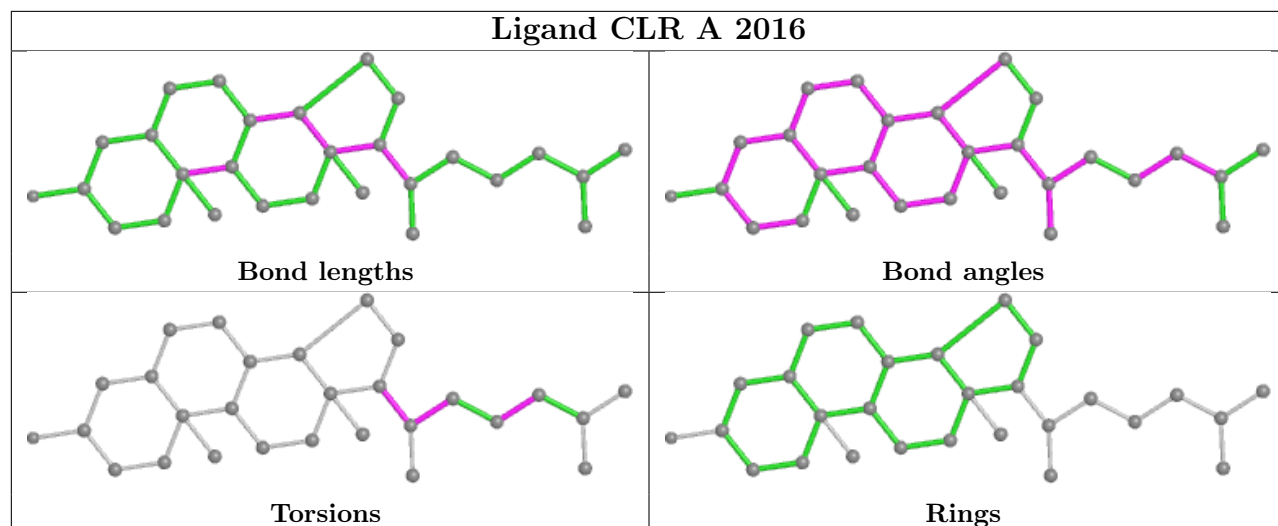
There are no ring outliers.

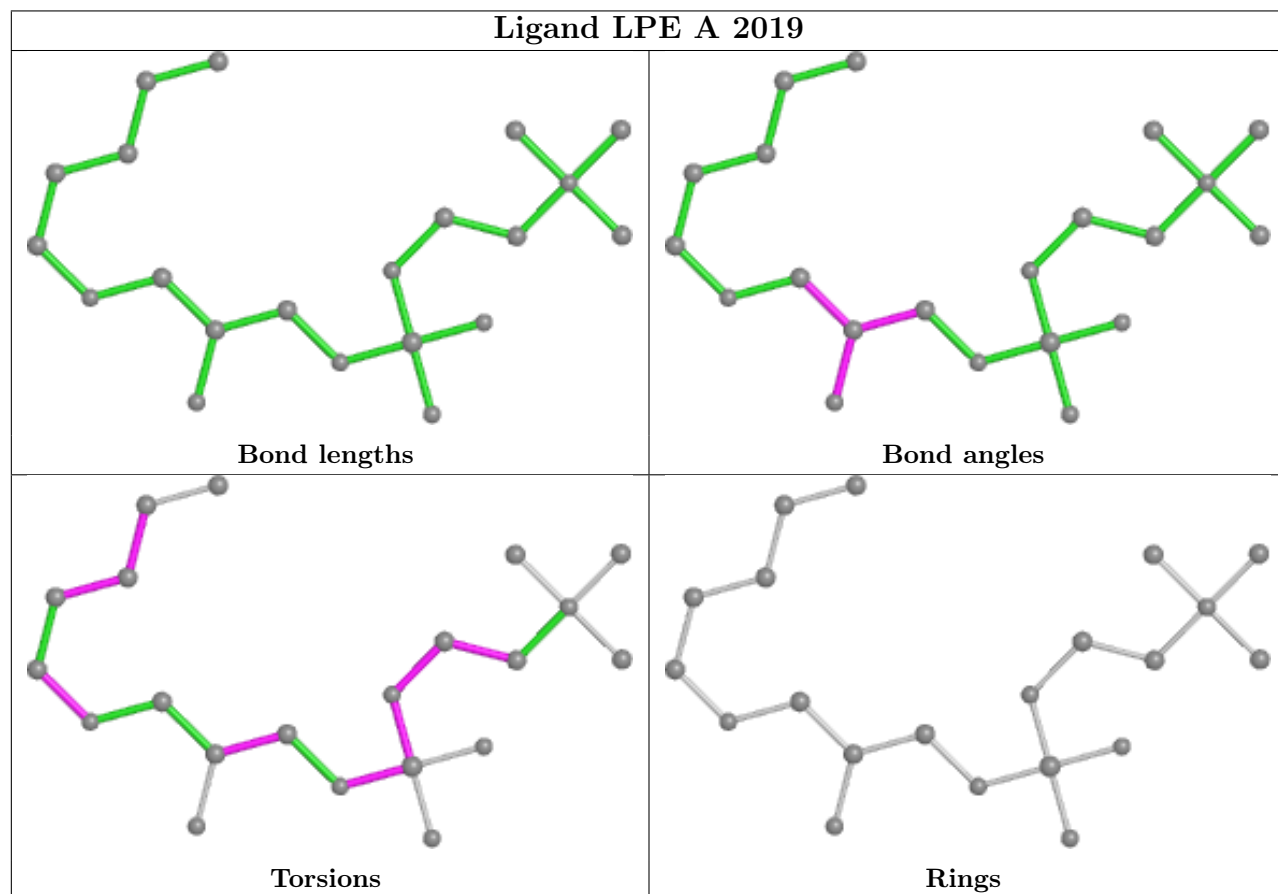
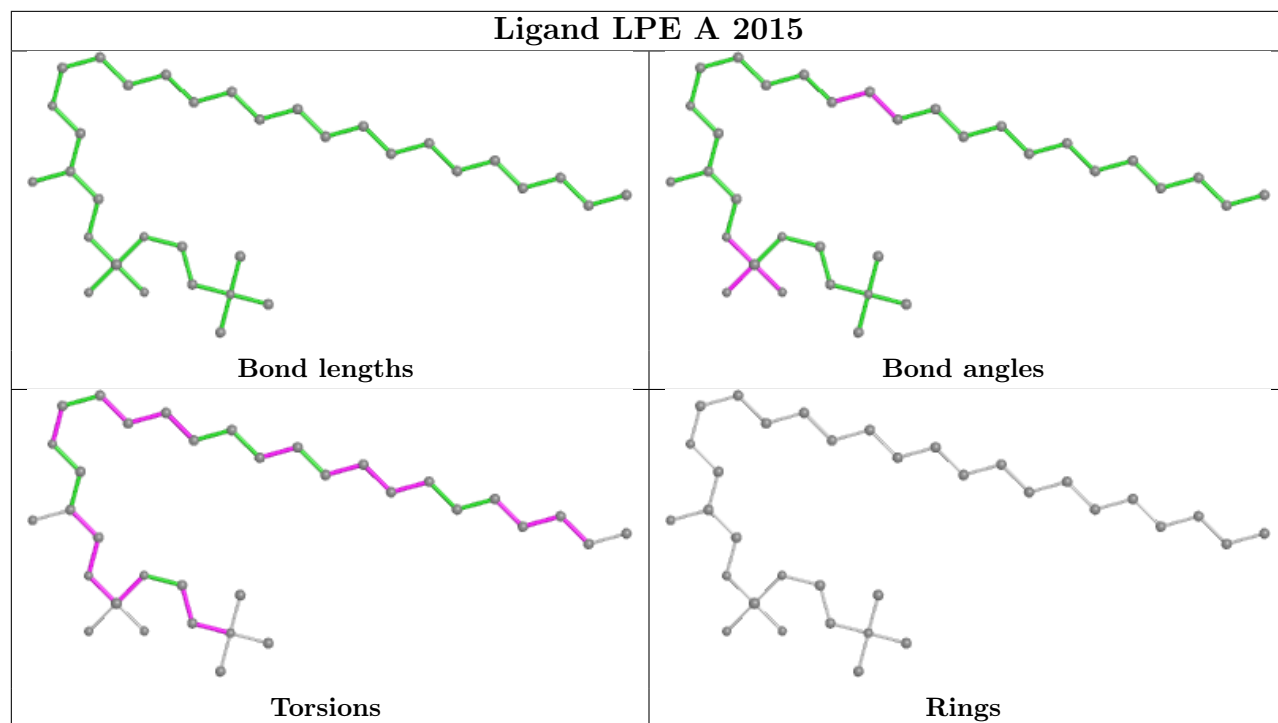
20 monomers are involved in 122 short contacts:

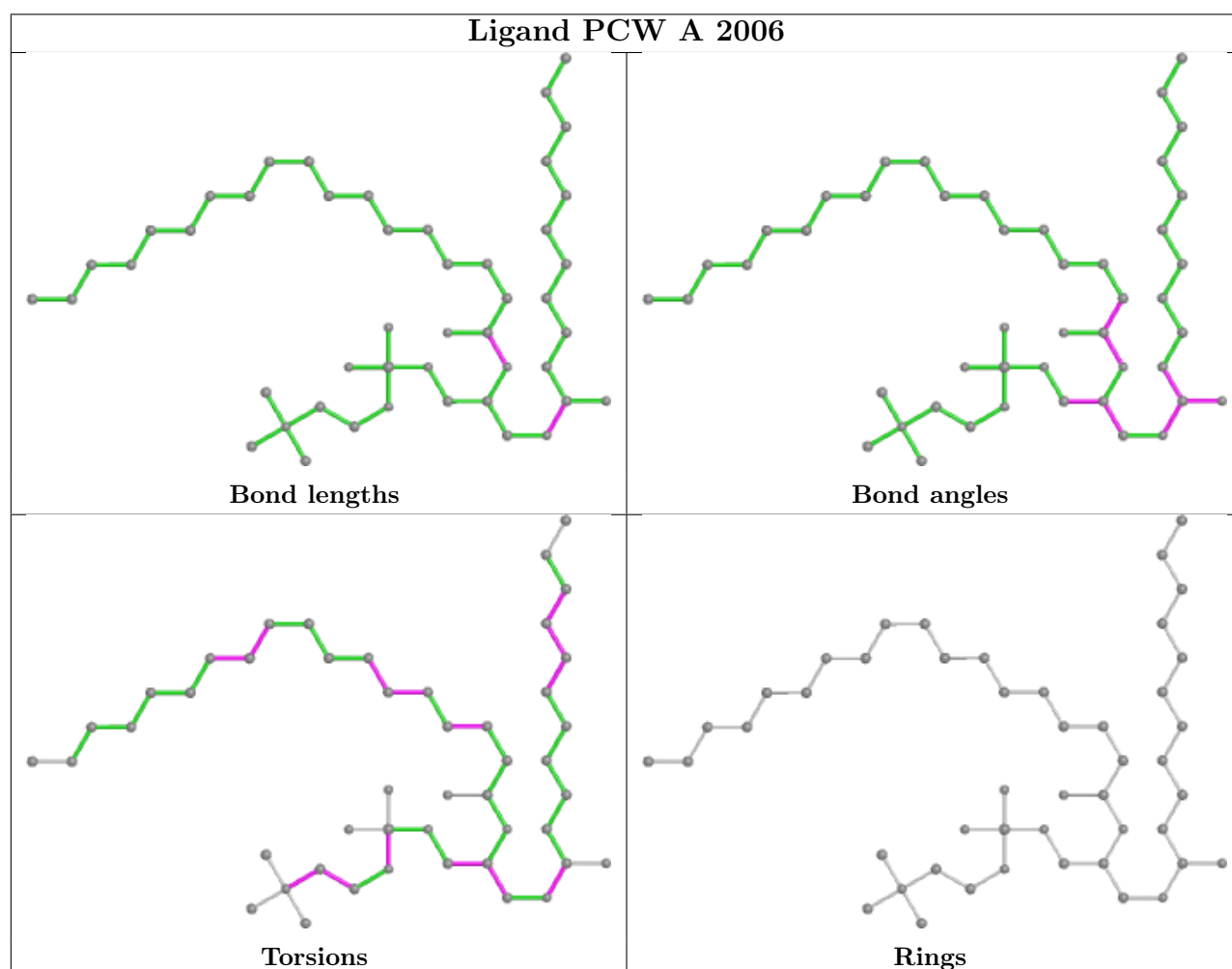
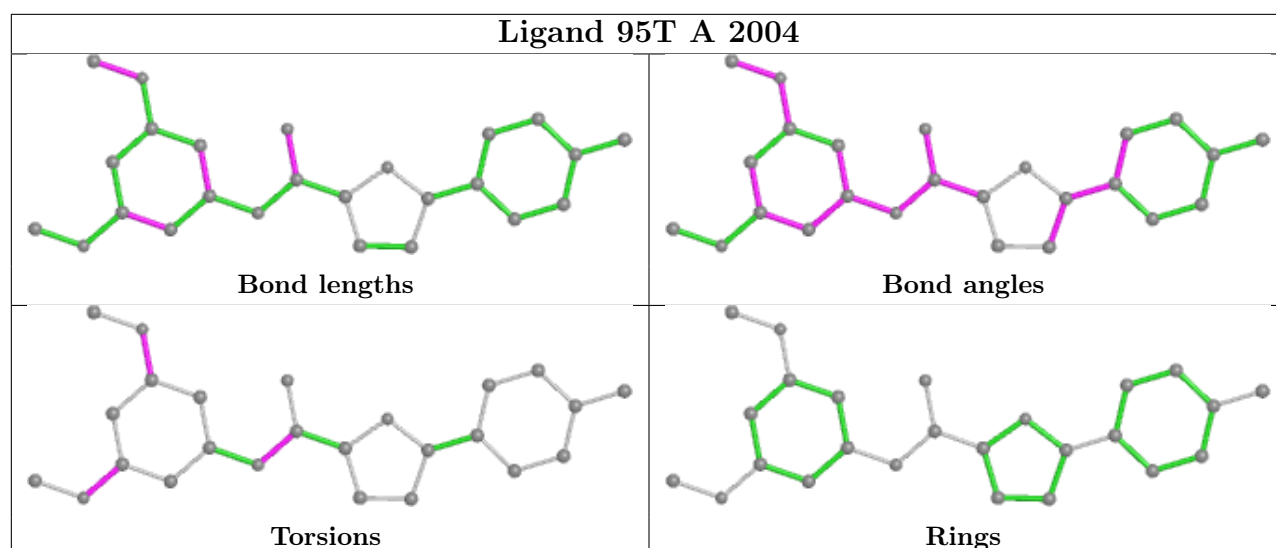
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2014	PCW	3	0
5	A	2005	CLR	5	0
5	A	2016	CLR	6	0
6	A	2007	PCW	6	0
7	A	2015	LPE	7	0
7	A	2019	LPE	1	0
4	A	2004	95T	1	0
6	A	2006	PCW	10	0
7	A	2008	LPE	1	0
7	A	2017	LPE	5	0
5	A	2025	CLR	20	0
7	A	2012	LPE	13	0
6	A	2013	PCW	5	0
7	A	2009	LPE	1	0
8	A	2024	P5S	9	0
7	A	2018	LPE	4	0
8	A	2023	P5S	3	0
8	A	2022	P5S	6	0
7	A	2020	LPE	8	0
5	A	2021	CLR	12	0

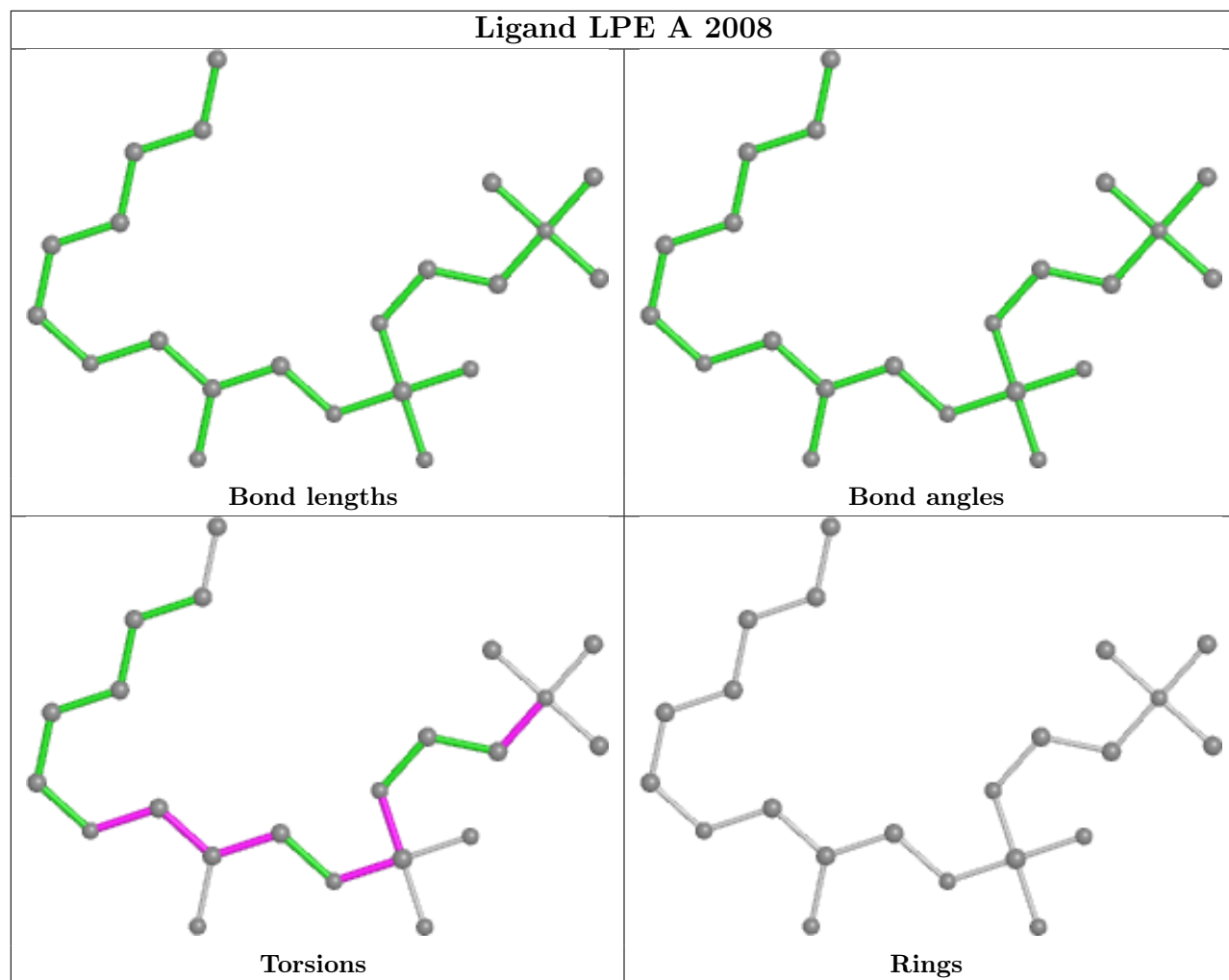
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

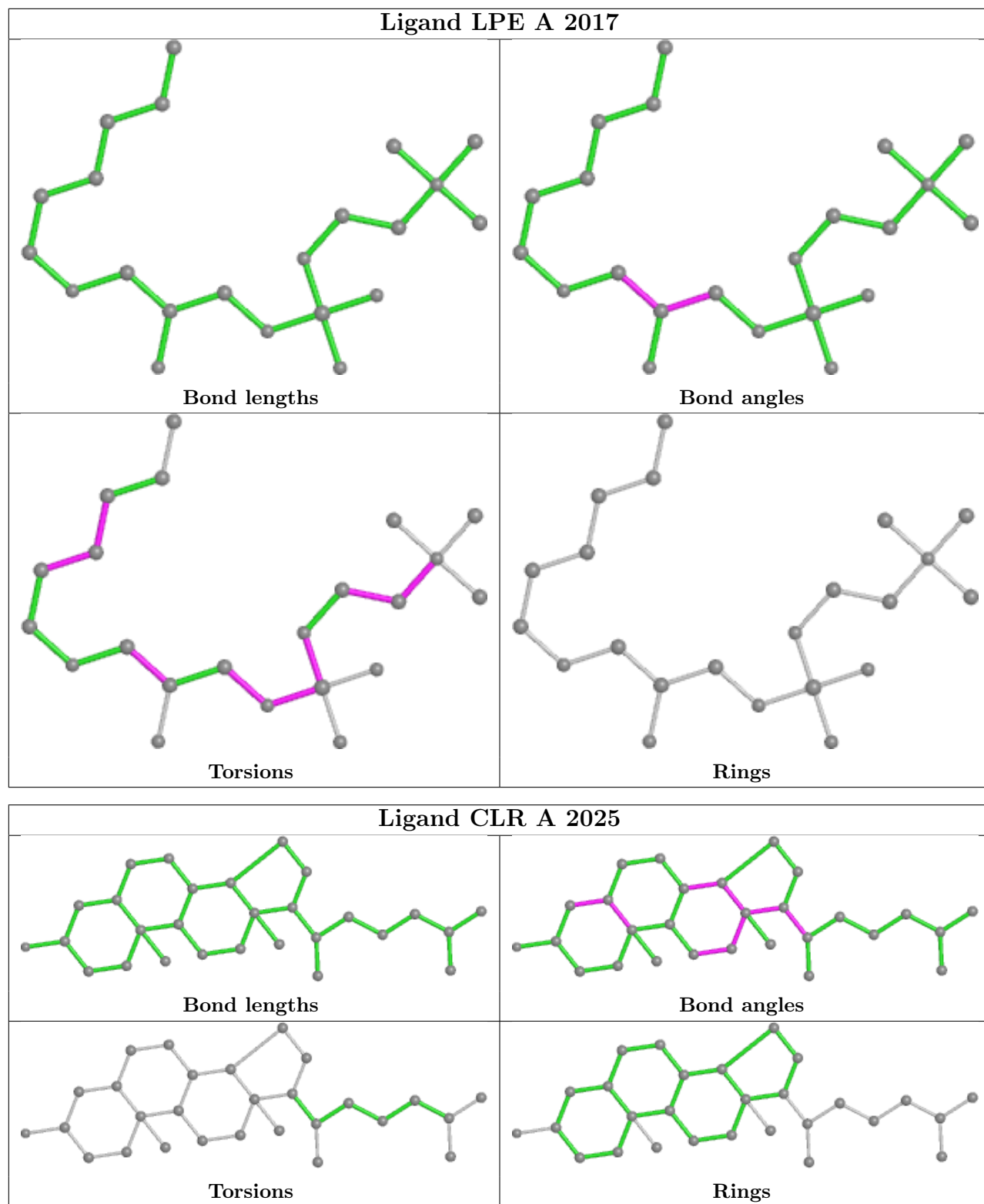


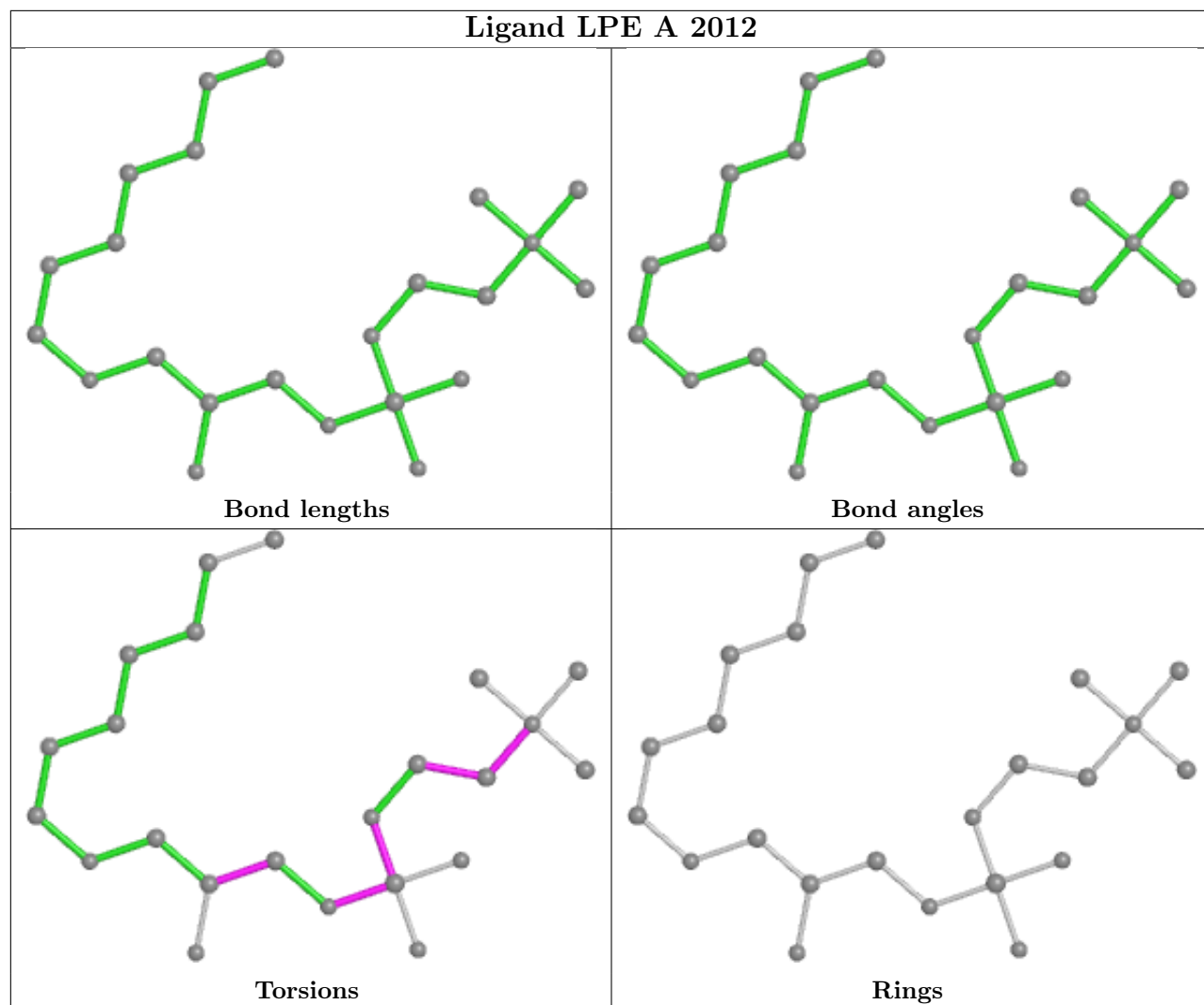


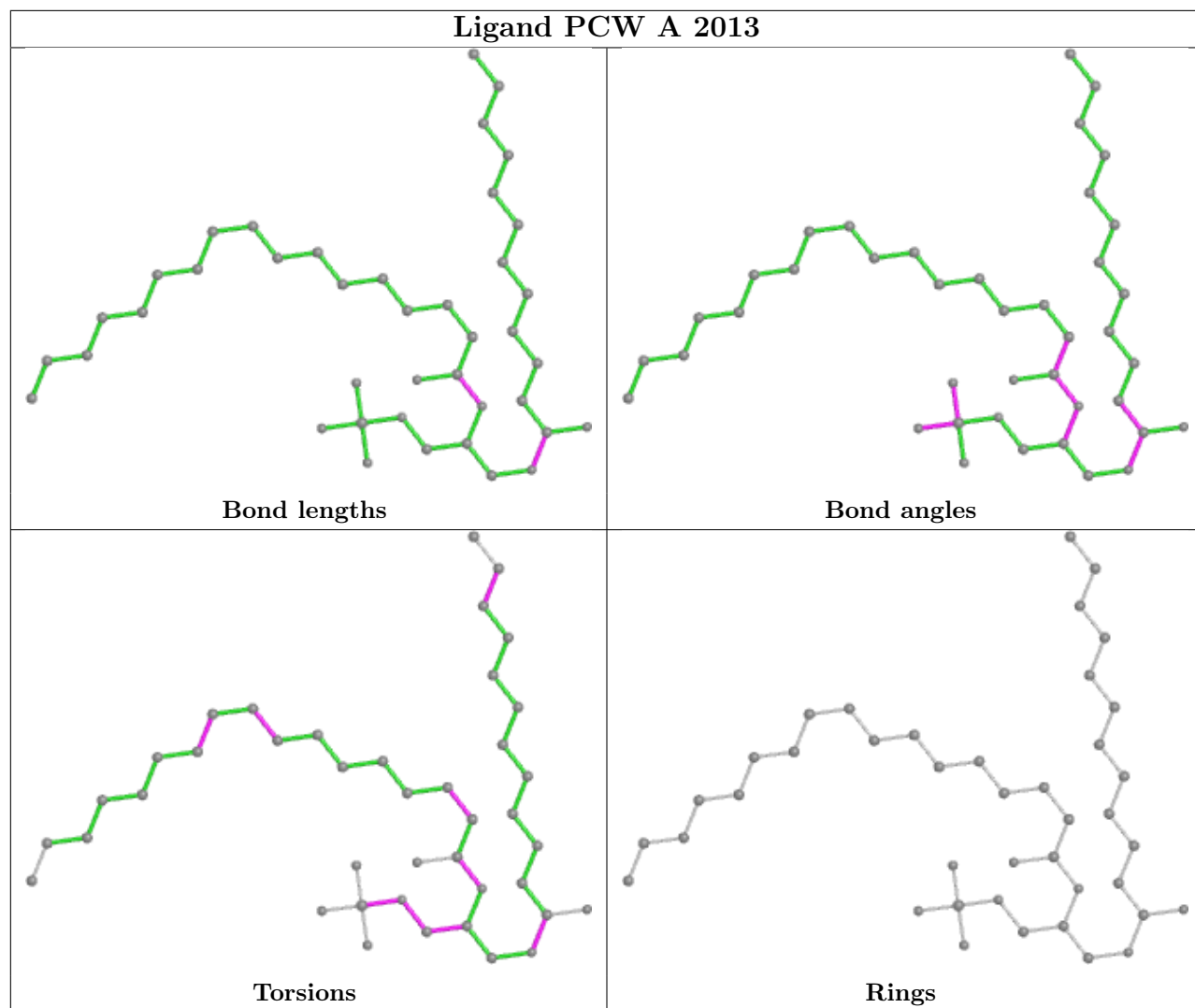


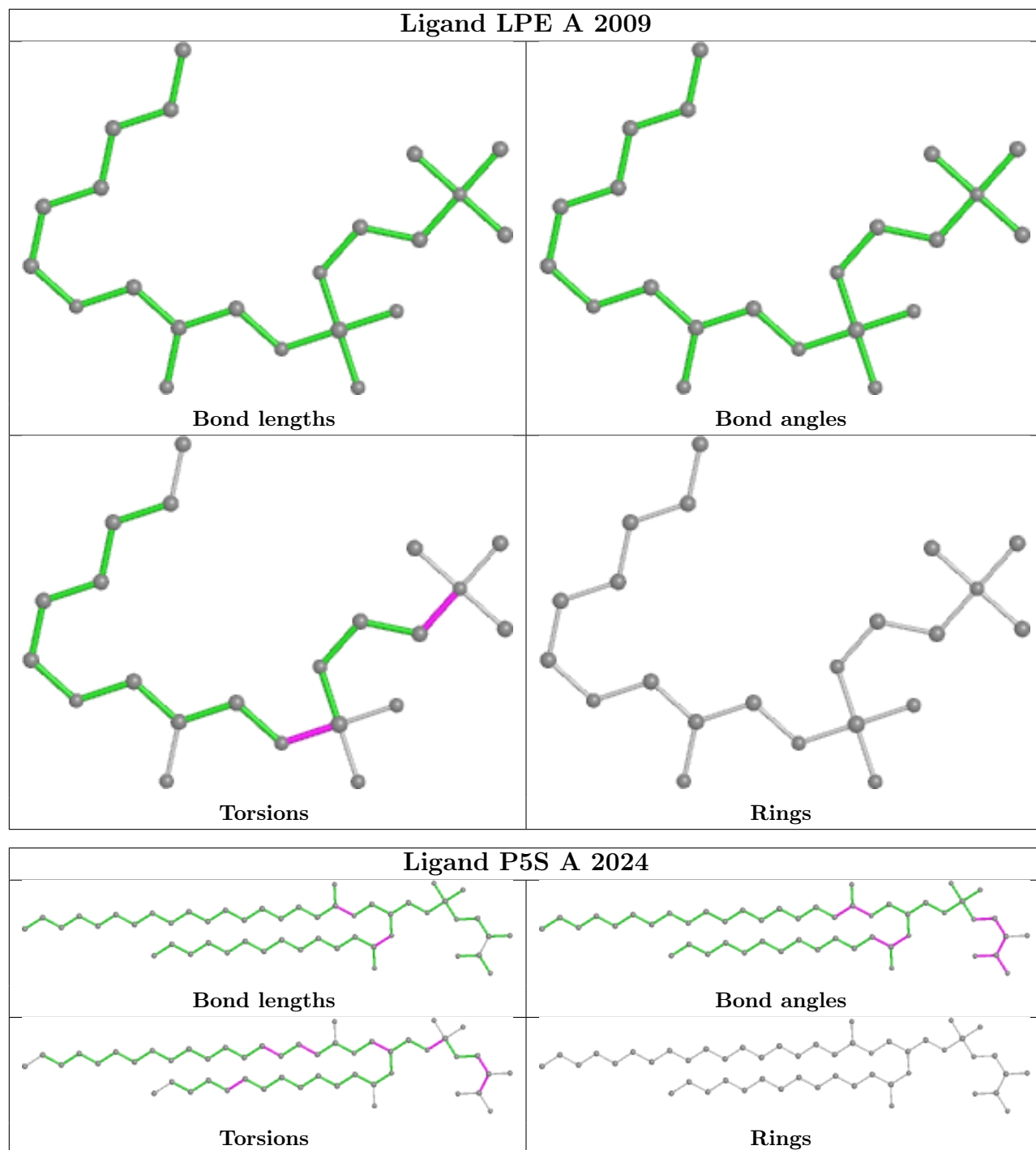


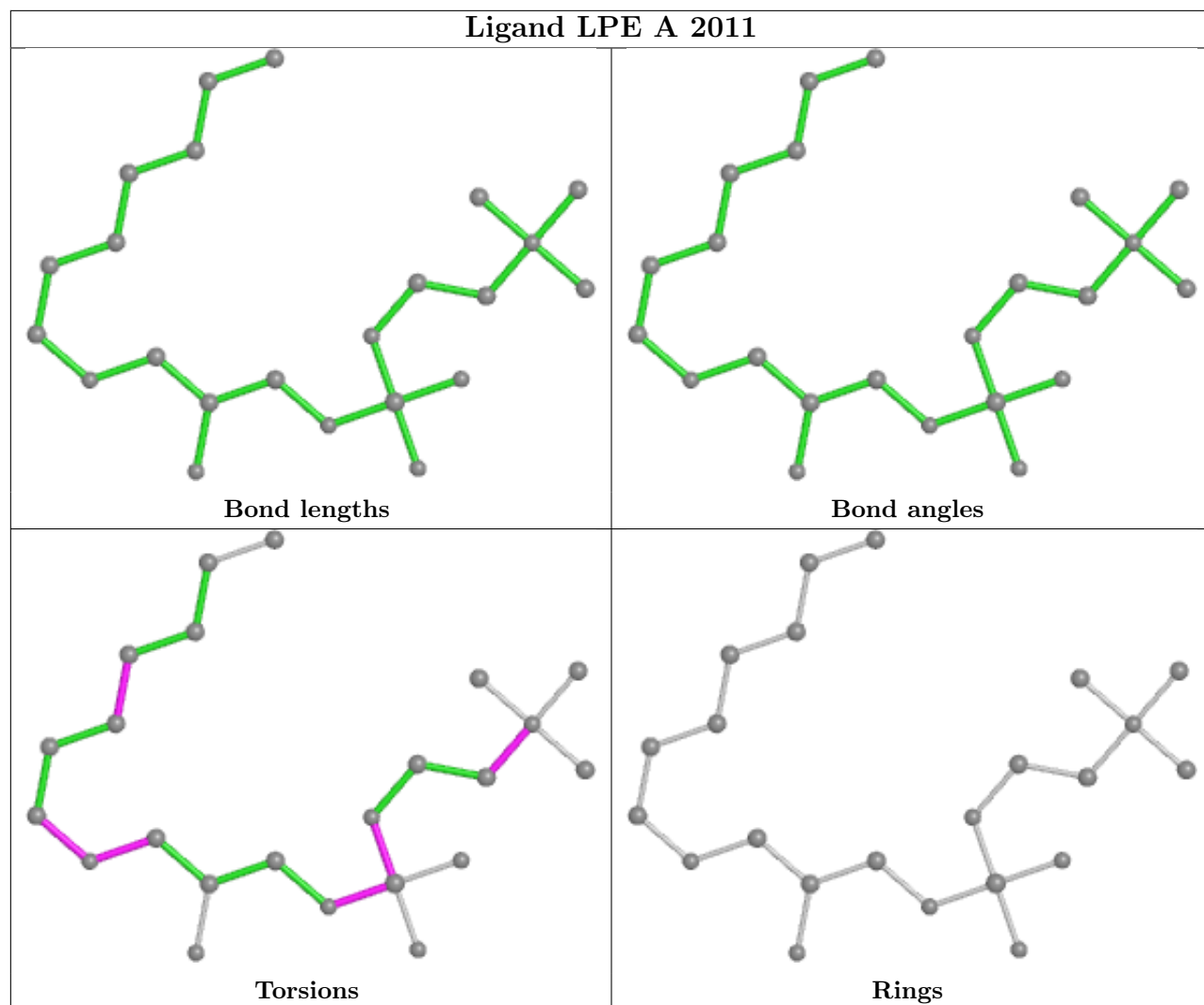


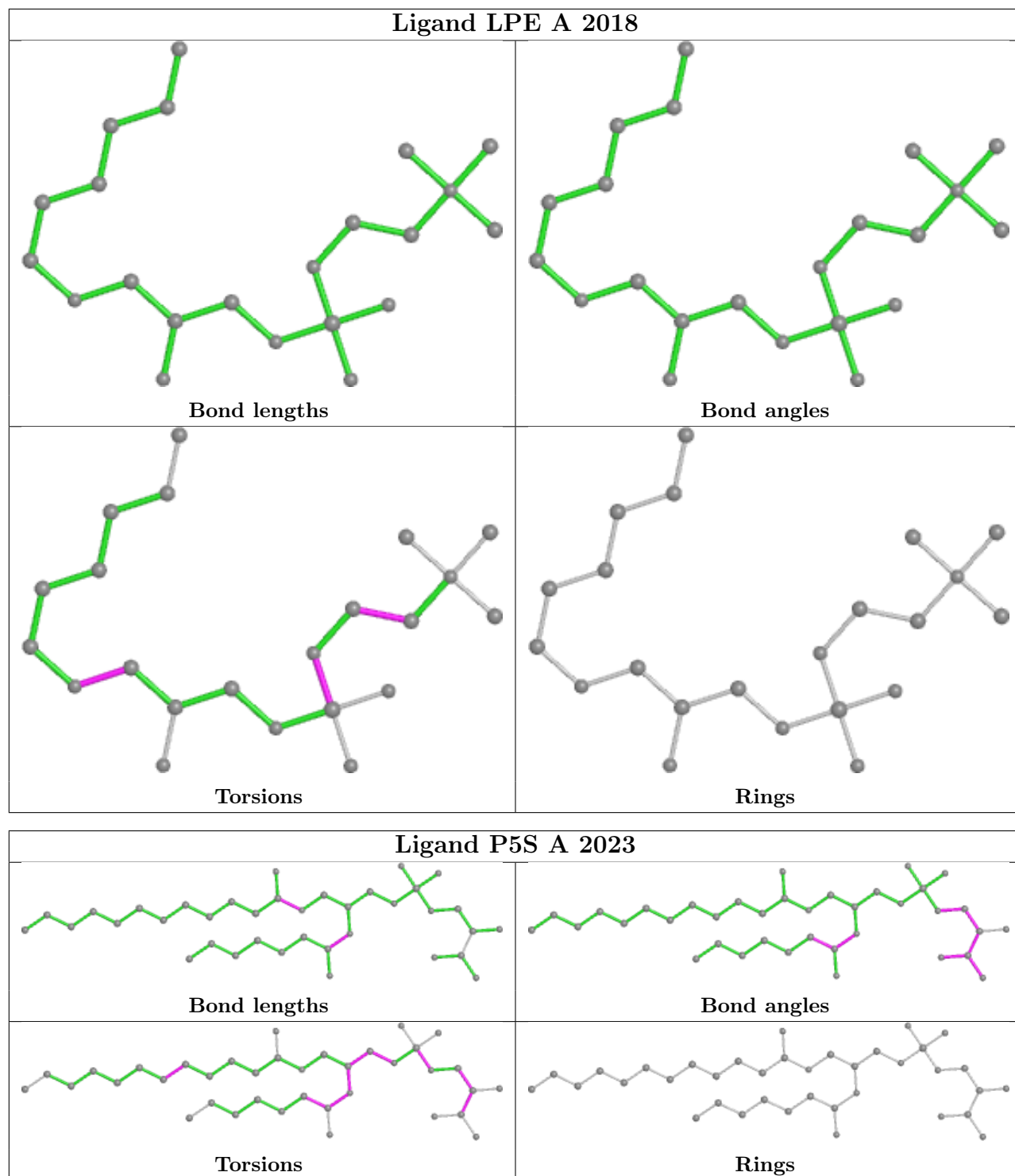


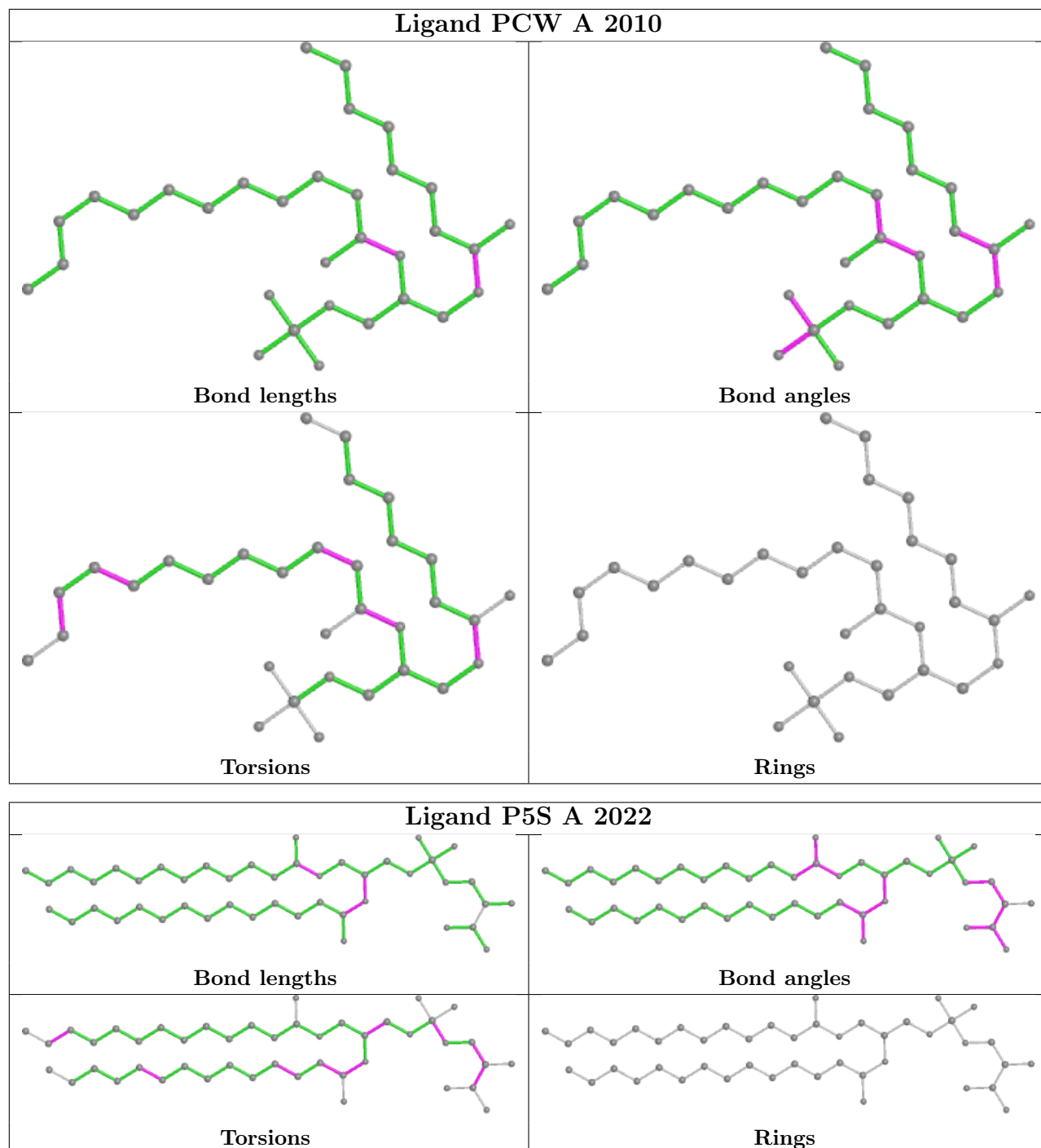


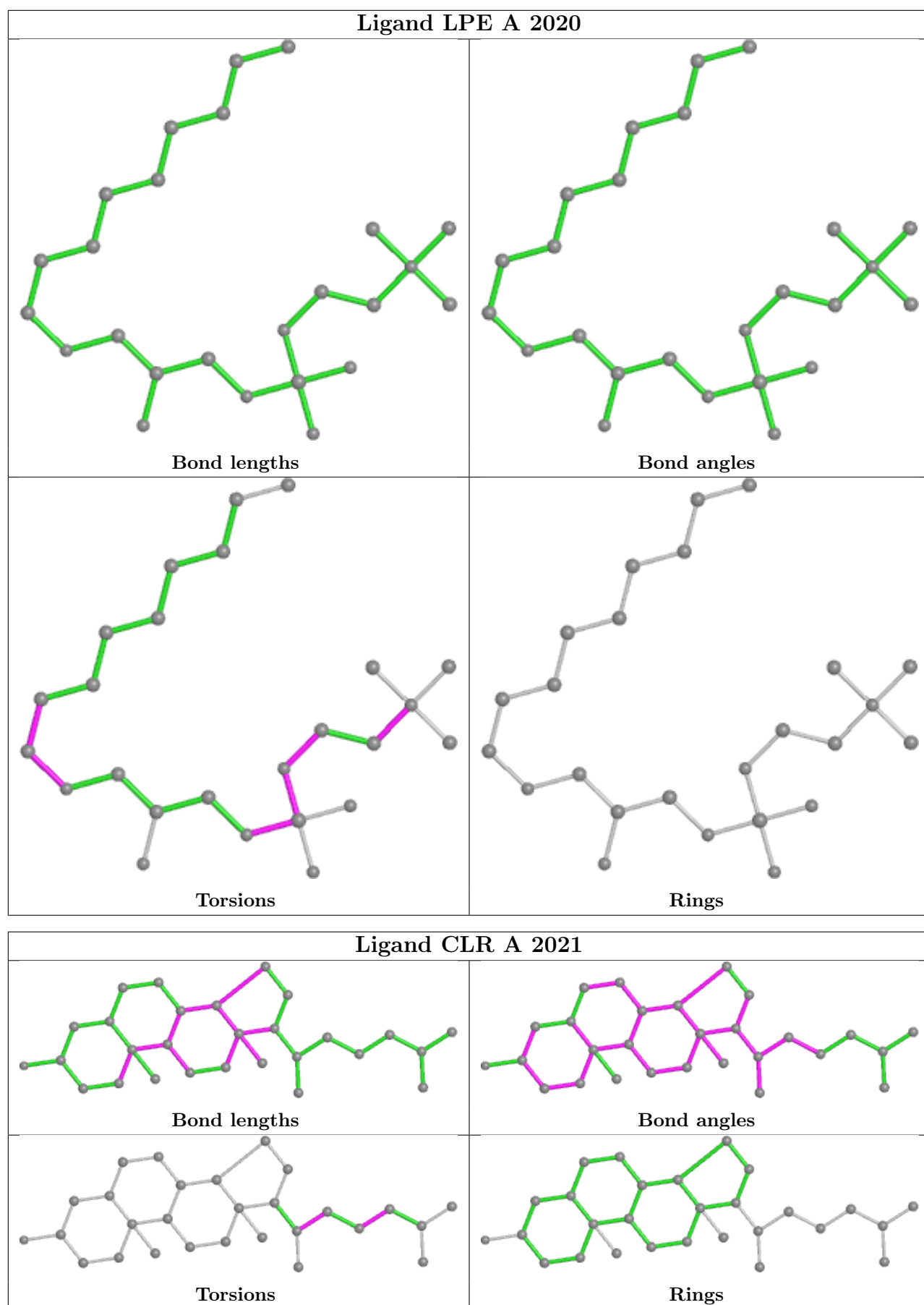












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

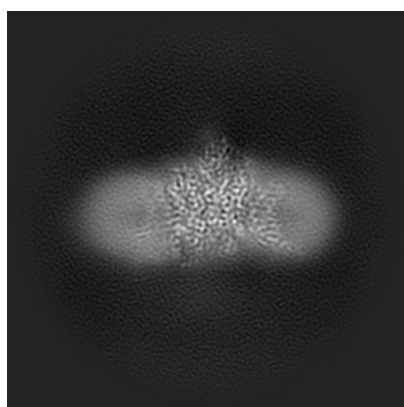
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32439. These allow visual inspection of the internal detail of the map and identification of artifacts.

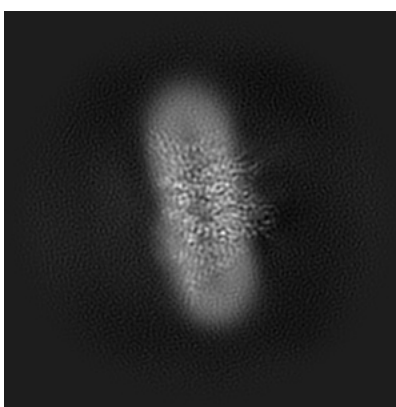
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

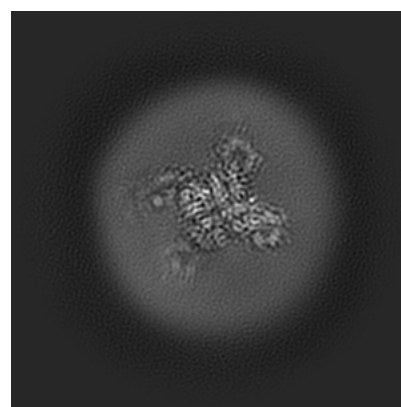
6.1.1 Primary map



X



Y

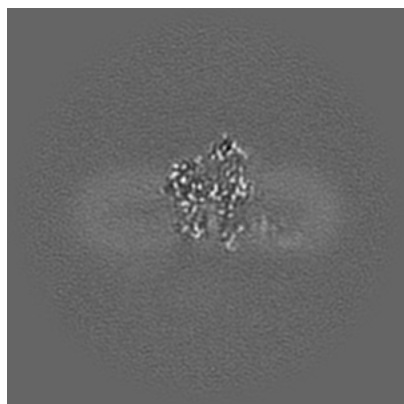


Z

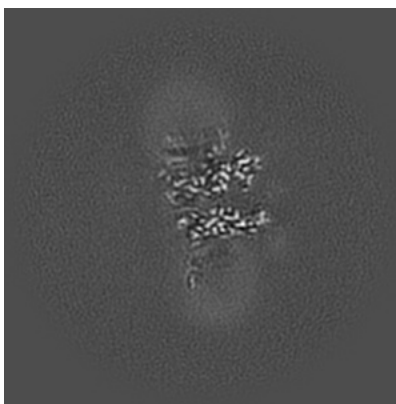
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

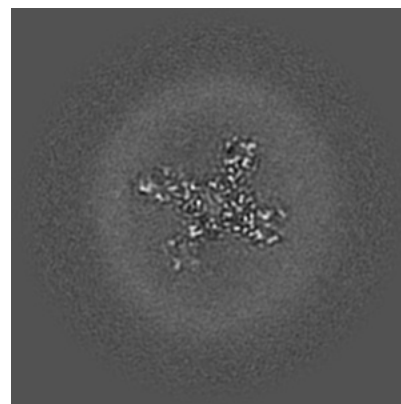
6.2.1 Primary map



X Index: 120



Y Index: 120

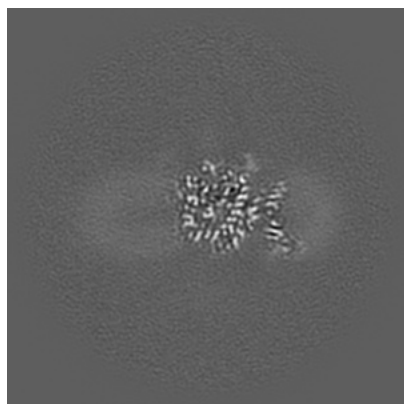


Z Index: 120

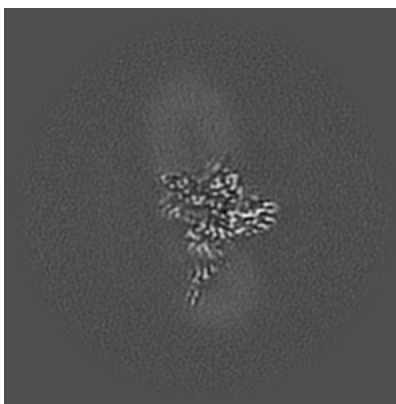
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

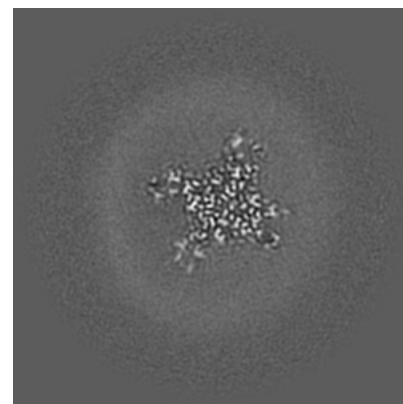
6.3.1 Primary map



X Index: 134



Y Index: 131



Z Index: 126

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 0.565. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

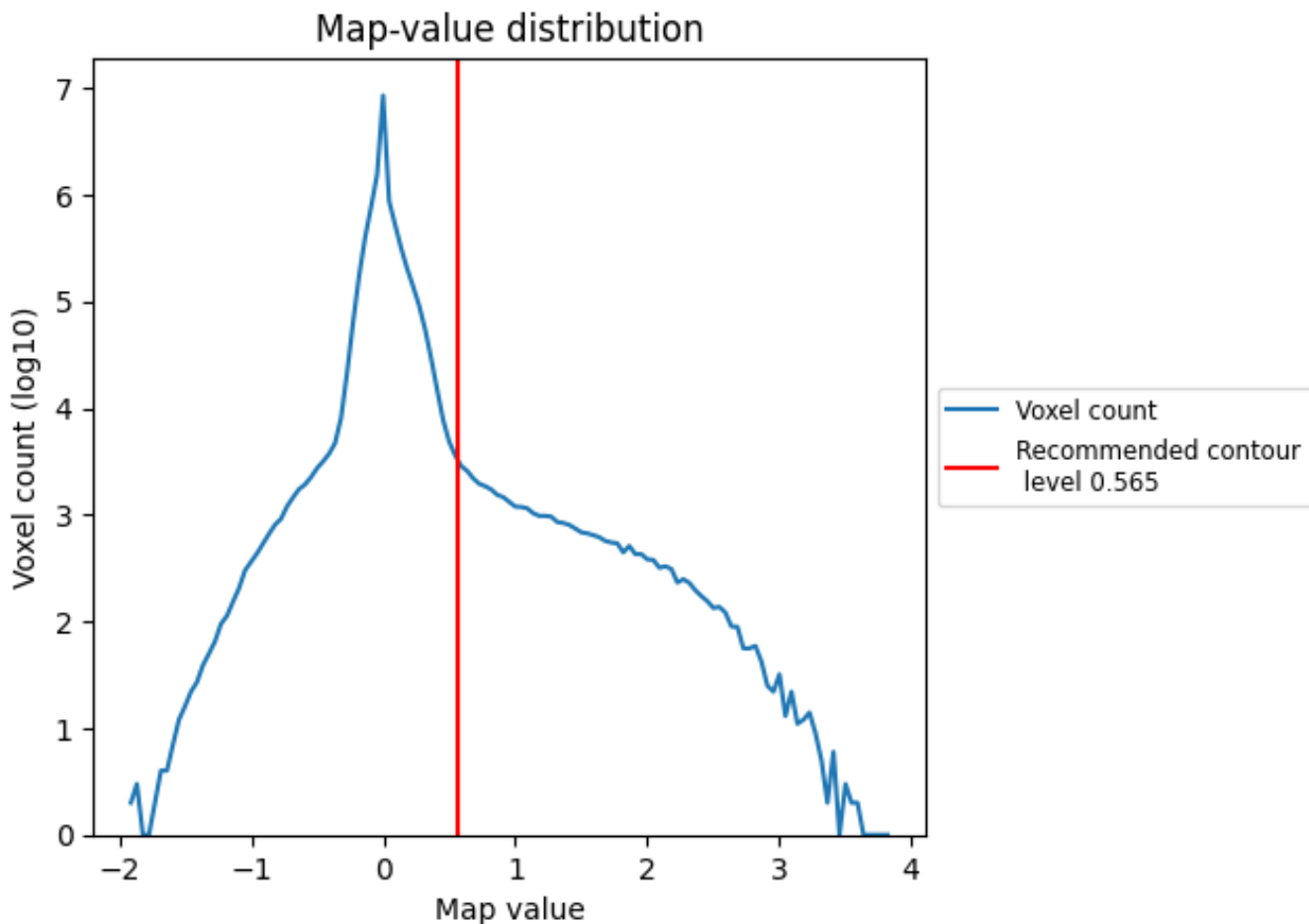
6.5 Mask visualisation

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

7 Map analysis [i](#)

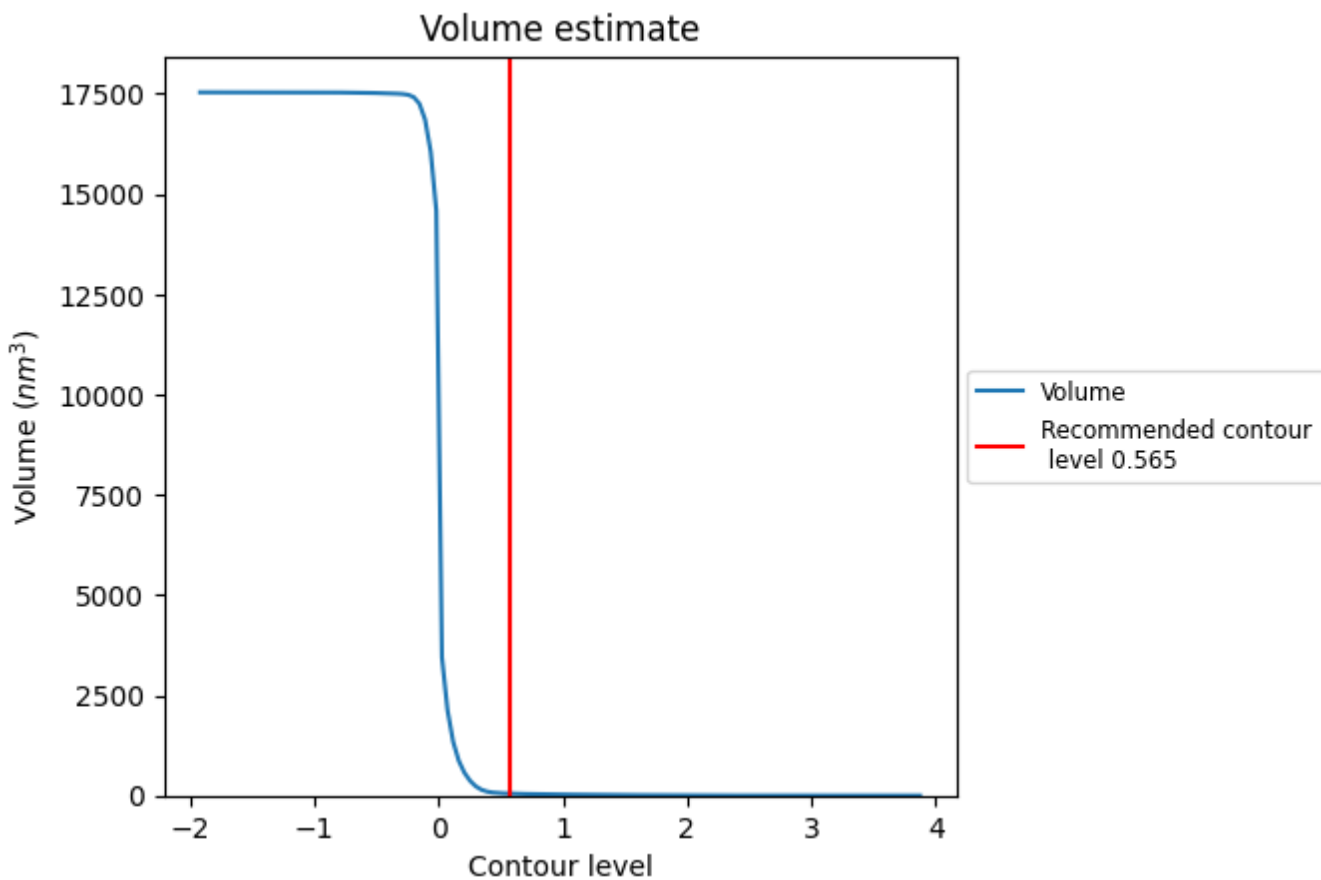
This section contains the results of statistical analysis of the map.

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.

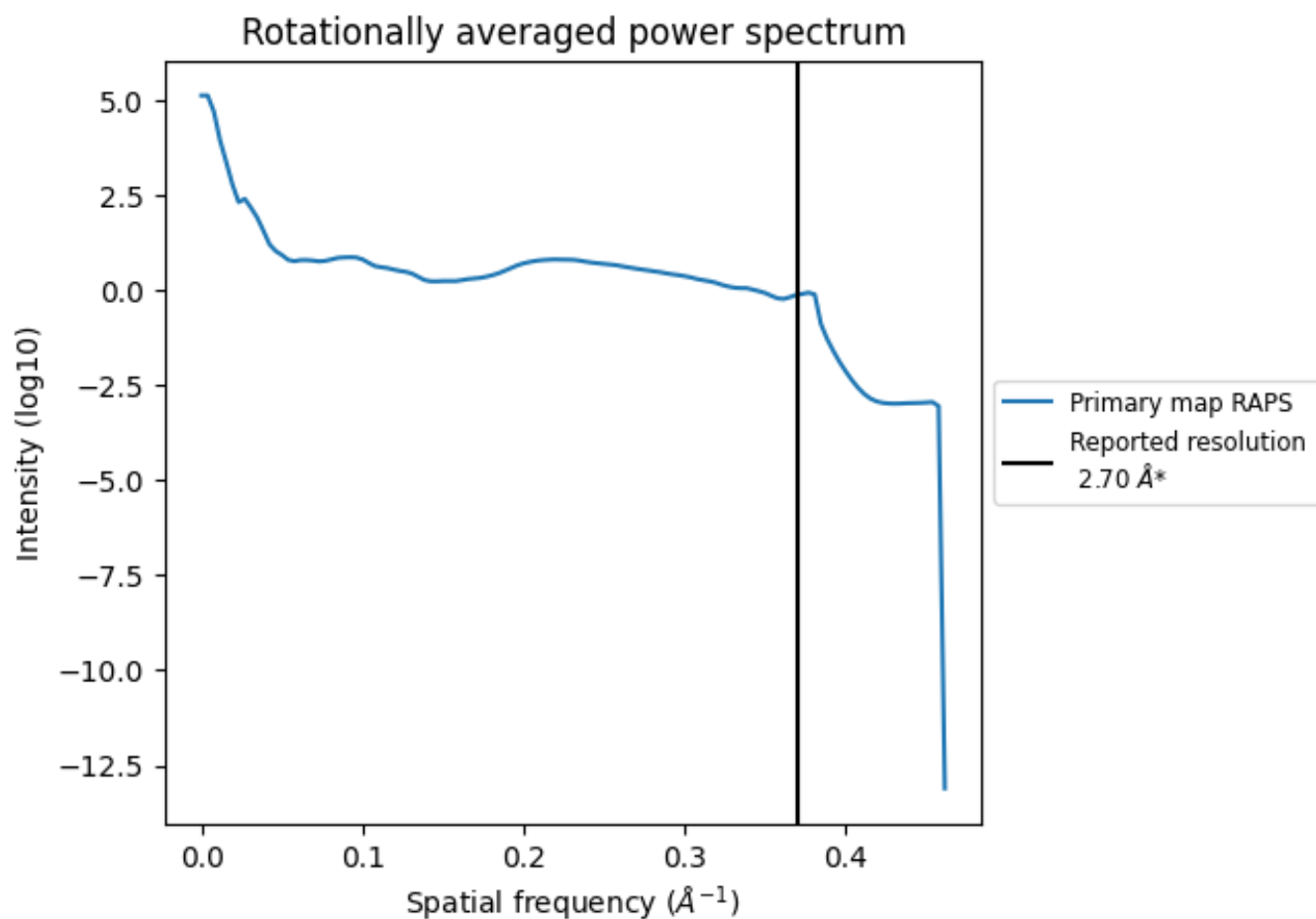
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm³; this corresponds to an approximate mass of 46 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 0.370\AA^{-1}

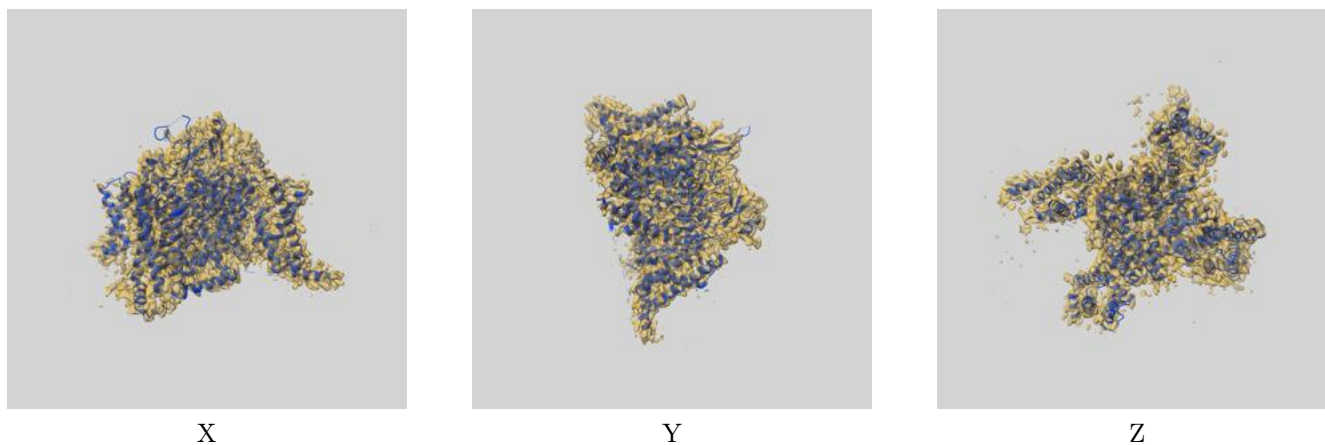
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

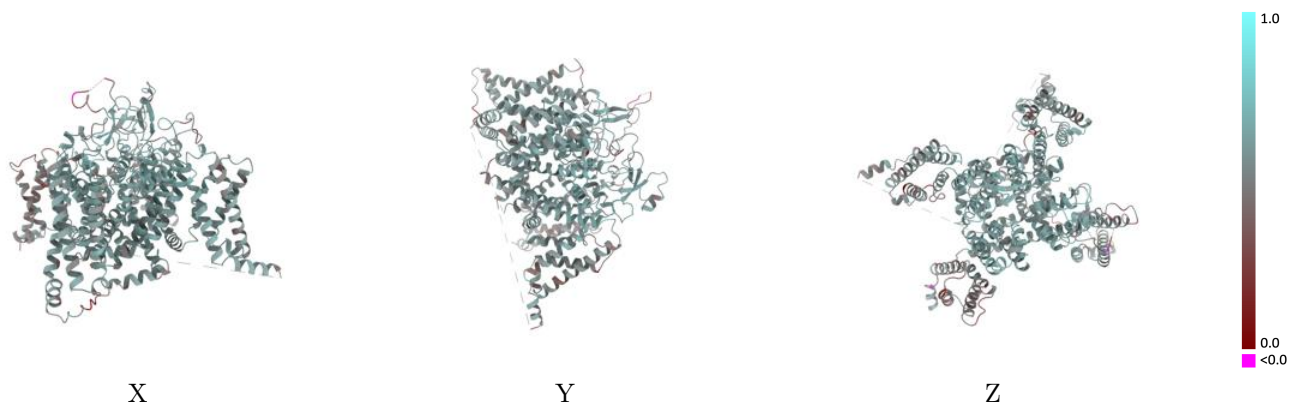
This section contains information regarding the fit between EMDB map EMD-32439 and PDB model 7WE4. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



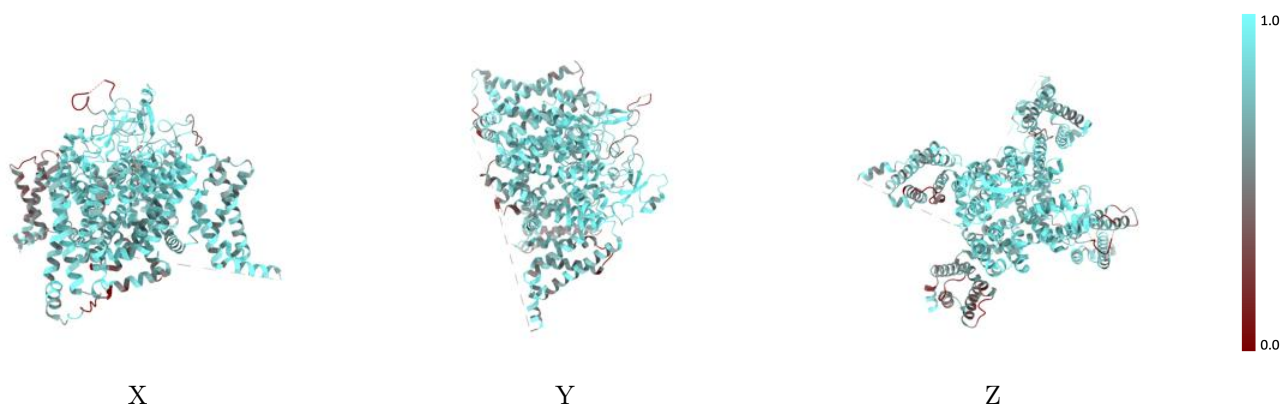
The images above show the 3D surface view of the map at the recommended contour level 0.565 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



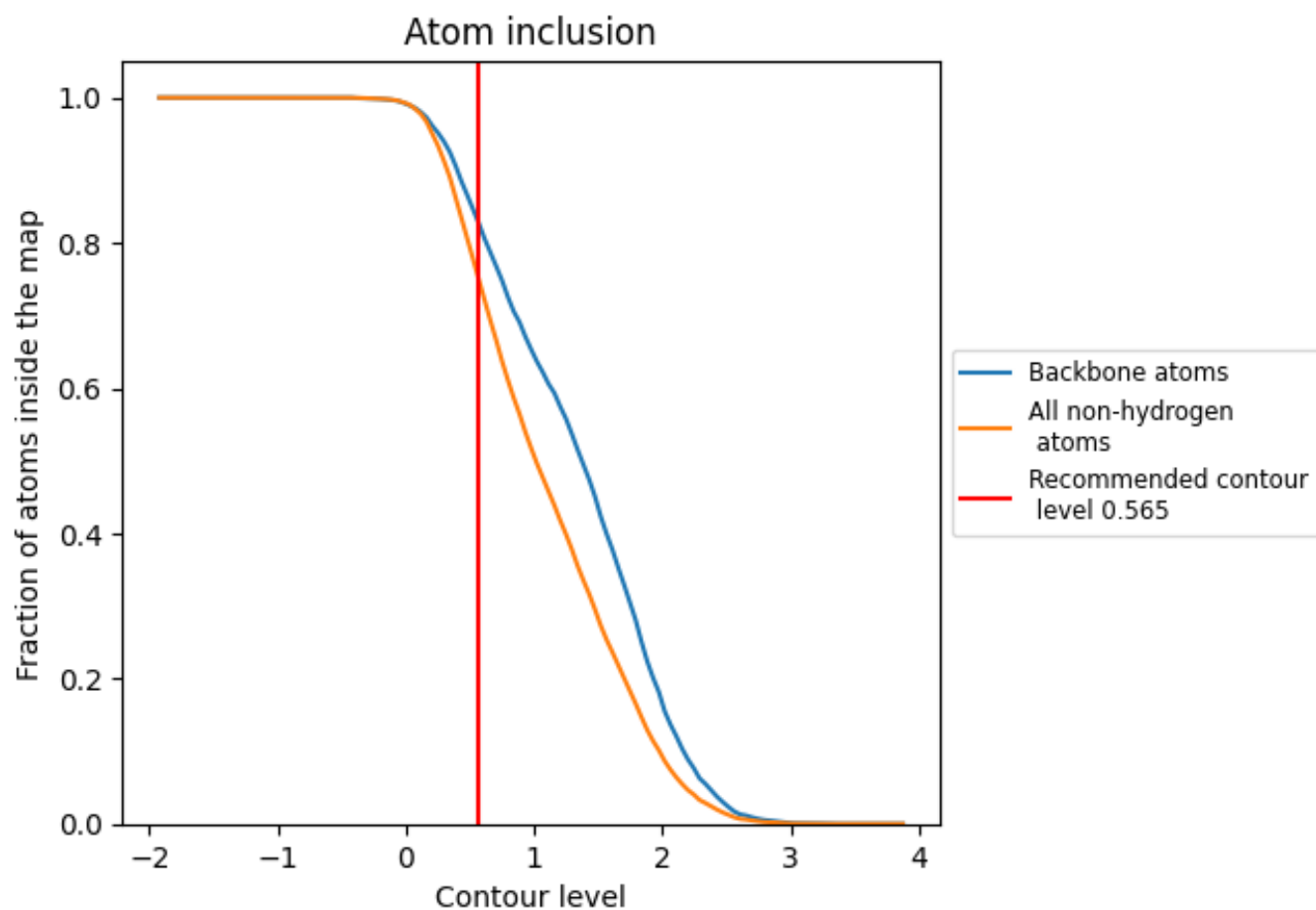
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.565).









9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.565) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7519	 0.5500
A	 0.7523	 0.5500
B	 0.5357	 0.4620
C	 0.8214	 0.5550

