



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 08:52 PM UTC

PDB ID : 21TP / pdb_000021tp
EMDB ID : EMD-67990
Title : Open-state structure of veratridine-activated human Nav1.7
Authors : Fan, X.; Huang, J.; Yan, N.
Deposited on : 2025-12-24
Resolution : 3.00 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:

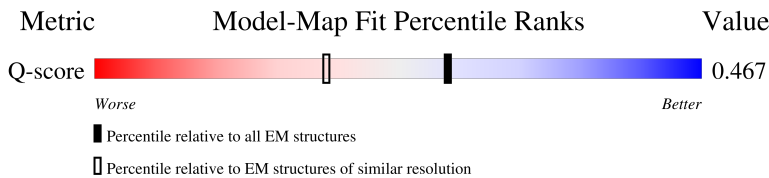
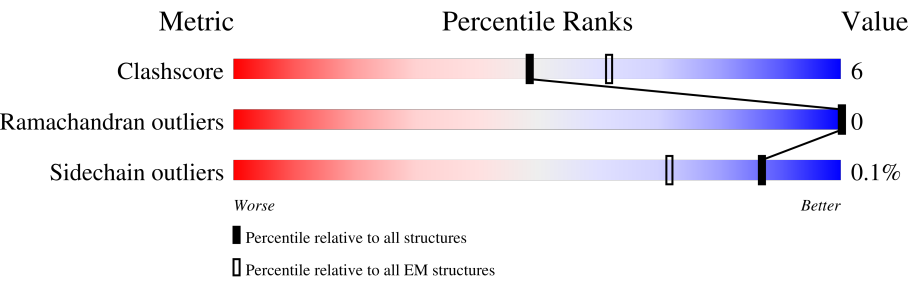
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	1988	<div><div></div><div>52%7%41%</div></div>
2	B	173	<div><div></div><div>88%12%</div></div>
3	C	119	<div><div>61%</div><div>82%18%</div></div>
4	D	2	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
4	E	2	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12524 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 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1180	Total	C	N	O	S	0	0
			9514	6324	1485	1631	74		

- Molecule 2 is a protein called Sodium channel regulatory subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1417	902	232	273	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	0	0
			975	611	172	181	11		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



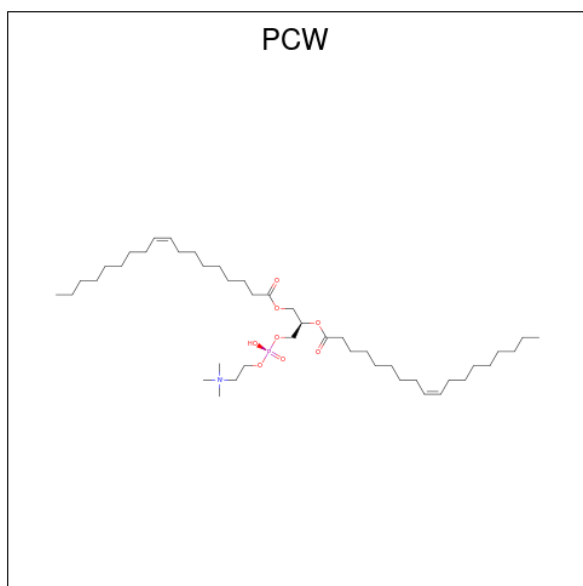
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
7	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
7	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
7	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
7	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
7	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	A	1	Total	C	N	O	P	0
			47	37	1	8	1	

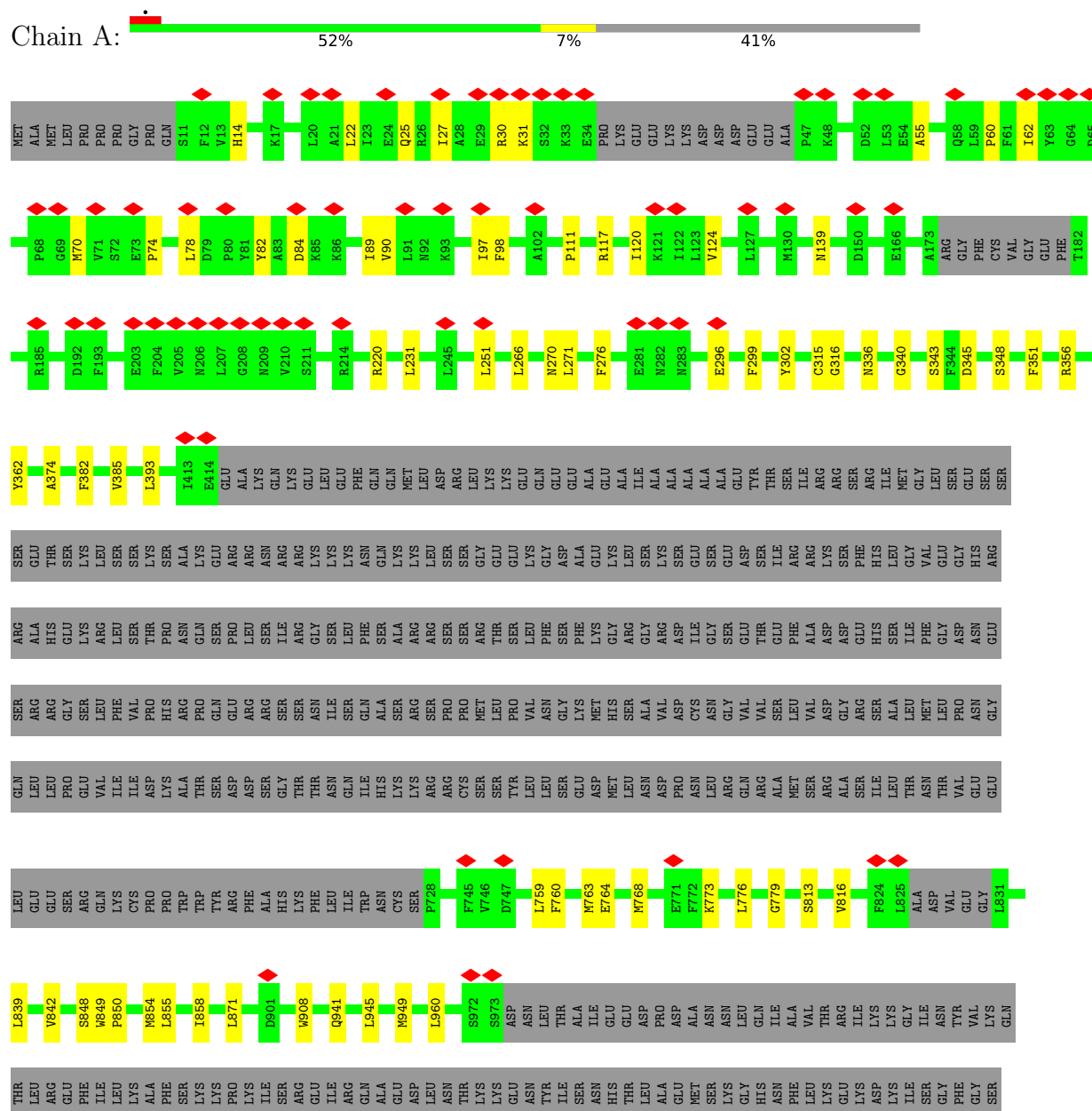
- Molecule 9 is Veratridine (CCD ID: A1E26) (formula: $C_{36}H_{51}NO_{11}$).



3 Residue-property plots

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

- Molecule 1: Sodium channel protein type 9 subunit alpha



MAG1
MAG2

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

Chain E:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	133758, 133758, 133758, 133758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.874	Depositor
Minimum map value	-2.849	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.65	Depositor
Map size (\AA)	356.47998, 356.47998, 356.47998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.114, 1.114, 1.114	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, NAG, PCW, Y01, A1E26

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	0.10	0/9749	0.26	0/13217
2	B	0.09	0/1443	0.28	0/1949
3	C	0.11	0/997	0.31	0/1346
All	All	0.10	0/12189	0.27	0/16512

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	9514	0	9729	109	0
2	B	1417	0	1380	14	0
3	C	975	0	937	11	0
4	D	28	0	25	2	0
4	E	28	0	25	0	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
6	A	140	0	196	26	0
7	A	175	0	242	16	0
7	B	17	0	19	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	98	0	136	14	0
9	A	48	0	0	2	0
All	All	12524	0	12767	146	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 (146) 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:1330:ILE:HD11	6:A:2005:Y01:HAN1	1.37	1.06
1:A:849:TRP:CD1	6:A:2005:Y01:HAD3	1.91	1.05
2:B:178:MET:HE3	7:B:304:LPE:C11	1.86	1.05
1:A:1329:LEU:HD23	6:A:2016:Y01:HAA3	1.47	0.96
2:B:178:MET:CE	7:B:304:LPE:C11	2.51	0.88
1:A:849:TRP:HA	6:A:2005:Y01:CAD	2.04	0.88
1:A:759:LEU:HD22	6:A:2016:Y01:HAC3	1.56	0.87
1:A:1684:PHE:CE2	7:A:2014:LPE:O2H	2.28	0.85
1:A:849:TRP:CD1	6:A:2005:Y01:CAD	2.63	0.81
1:A:1329:LEU:HD23	6:A:2016:Y01:CAA	2.11	0.80
1:A:1330:ILE:CD1	6:A:2005:Y01:HAN1	2.15	0.76
1:A:849:TRP:HA	6:A:2005:Y01:HAD1	1.69	0.74
1:A:1653:LEU:HD13	7:A:2014:LPE:C19	2.18	0.73
1:A:848:SER:O	6:A:2005:Y01:HAR2	1.90	0.71
1:A:941:GLN:NE2	8:A:2012:PCW:H52	2.05	0.71
1:A:336:ASN:HB2	1:A:340:GLY:HA2	1.72	0.71
1:A:949:MET:HB3	8:A:2012:PCW:H232	1.74	0.70
1:A:941:GLN:HE22	8:A:2012:PCW:H52	1.55	0.70
1:A:1330:ILE:HD11	6:A:2005:Y01:CAN	2.20	0.68
1:A:849:TRP:HA	6:A:2005:Y01:HAD2	1.79	0.65
2:B:118:ASP:OD1	2:B:143:HIS:ND1	2.29	0.65
1:A:1210:ALA:CB	7:A:2014:LPE:H11	2.28	0.64
3:C:98:ARG:NH2	3:C:116:ASN:O	2.28	0.64
1:A:759:LEU:CD2	6:A:2016:Y01:HAC3	2.29	0.63
1:A:345:ASP:HB2	1:A:1537:GLU:HB3	1.81	0.62
2:B:92:TRP:O	2:B:96:ARG:NH2	2.32	0.62
1:A:1646:ASN:OD1	1:A:1647:ILE:HD12	1.99	0.62
1:A:1671:LYS:HG2	1:A:1675:ILE:HG22	1.82	0.61
1:A:315:CYS:SG	1:A:316:GLY:N	2.73	0.61
1:A:111:PRO:O	1:A:117:ARG:NH1	2.34	0.60
1:A:1254:PHE:O	1:A:1260:TRP:NE1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:CYS:HB2	1:A:1452:PHE:HZ	1.65	0.60
1:A:1257:ALA:HB1	7:A:2011:LPE:H31	1.83	0.60
1:A:1306:GLY:HA3	1:A:1646:ASN:HB2	1.84	0.59
1:A:1528:ASN:HD21	1:A:1619:ARG:HH21	1.49	0.59
1:A:271:LEU:HD12	1:A:343:SER:HA	1.85	0.59
1:A:764:GLU:OE2	1:A:1341:ASN:ND2	2.36	0.58
1:A:74:PRO:HA	1:A:90:VAL:HG12	1.85	0.58
1:A:759:LEU:HD22	6:A:2016:Y01:CAC	2.30	0.58
3:C:104:ASN:N	3:C:109:ASP:O	2.34	0.58
9:A:2017:A1E26:O9	9:A:2017:A1E26:O11	2.22	0.56
1:A:1312:ASN:OD1	7:A:2011:LPE:H312	2.06	0.56
1:A:1385:LEU:O	1:A:1388:ASN:ND2	2.39	0.56
1:A:78:LEU:HD23	1:A:82:TYR:HB3	1.88	0.56
1:A:1655:MET:CE	7:A:2013:LPE:H172	2.35	0.55
1:A:30:ARG:NH1	1:A:84:ASP:OD1	2.39	0.55
1:A:855:LEU:HD13	1:A:1451:LEU:HD22	1.88	0.55
3:C:72:CYS:SG	3:C:75:CYS:N	2.80	0.55
1:A:139:ASN:HD21	1:A:220:ARG:HE	1.55	0.55
1:A:1328:CYS:HB2	1:A:1452:PHE:CZ	2.42	0.54
1:A:850:PRO:HD2	6:A:2005:Y01:HAD1	1.89	0.54
1:A:1419:VAL:HG12	1:A:1420:ASN:H	1.73	0.53
1:A:960:LEU:HD22	9:A:2017:A1E26:C27	2.39	0.53
1:A:848:SER:O	6:A:2005:Y01:CAR	2.57	0.53
1:A:842:VAL:HG11	1:A:1334:ILE:HD11	1.92	0.52
1:A:251:LEU:HD11	1:A:1633:LEU:HD12	1.90	0.52
1:A:1210:ALA:HB3	7:A:2014:LPE:H11	1.90	0.52
3:C:62:GLN:HG3	3:C:132:PRO:HG2	1.91	0.52
1:A:1658:TYR:CZ	7:A:2010:LPE:O31	2.63	0.51
1:A:949:MET:CB	8:A:2012:PCW:H20	2.40	0.51
1:A:945:LEU:CD2	8:A:2012:PCW:H342	2.42	0.50
1:A:14:HIS:CE1	1:A:70:MET:HG3	2.46	0.50
1:A:120:ILE:O	1:A:124:VAL:HG22	2.12	0.50
1:A:849:TRP:CE3	6:A:2005:Y01:CAE	2.95	0.50
1:A:89:ILE:HG23	1:A:98:PHE:O	2.12	0.49
1:A:849:TRP:CG	6:A:2005:Y01:CAD	2.95	0.49
1:A:1502:ASN:O	1:A:1506:GLY:N	2.34	0.49
1:A:1658:TYR:HE1	7:A:2010:LPE:H1N2	1.78	0.49
1:A:1738:PHE:CD1	7:A:2008:LPE:H161	2.49	0.48
1:A:340:GLY:HA3	8:A:2012:PCW:H61	1.95	0.48
1:A:949:MET:CB	8:A:2012:PCW:H232	2.41	0.48
1:A:768:MET:HE2	1:A:773:LYS:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ARG:HH21	2:B:157:ILE:HD13	1.78	0.48
1:A:1560:GLY:HA2	1:A:1563:VAL:HG22	1.96	0.47
1:A:1739:TYR:HA	7:A:2010:LPE:H1N1	1.96	0.47
1:A:348:SER:HB3	8:A:2012:PCW:H332	1.97	0.47
1:A:1191:HIS:CE1	1:A:1193:TRP:HD1	2.33	0.47
1:A:760:PHE:CZ	1:A:779:GLY:HA3	2.49	0.47
2:B:178:MET:HE1	7:B:304:LPE:C11	2.40	0.47
1:A:1685:GLY:O	1:A:1689:ILE:HG12	2.15	0.46
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.97	0.46
1:A:1658:TYR:CE1	7:A:2010:LPE:H1N2	2.51	0.46
7:A:2010:LPE:H142	7:A:2010:LPE:H112	1.38	0.46
2:B:42:SER:O	2:B:125:ARG:NH2	2.47	0.46
1:A:849:TRP:CA	6:A:2005:Y01:HAD2	2.43	0.46
1:A:849:TRP:CD2	6:A:2005:Y01:HAE1	2.50	0.46
1:A:1443:PHE:CZ	6:A:2006:Y01:CAB	2.99	0.45
1:A:296:GLU:HA	1:A:299:PHE:HB2	1.98	0.45
1:A:760:PHE:CZ	1:A:776:LEU:HA	2.51	0.45
1:A:351:PHE:CD2	8:A:2012:PCW:H412	2.52	0.45
6:A:2016:Y01:HAP1	6:A:2016:Y01:HAO2	1.26	0.45
3:C:30:MET:HB3	3:C:136:HIS:HB3	1.98	0.45
2:B:43:CYS:SG	2:B:102:GLN:NE2	2.89	0.45
4:D:1:NAG:O3	4:D:2:NAG:N2	2.50	0.45
2:B:113:TYR:HA	2:B:146:VAL:HG11	1.98	0.45
1:A:1690:CYS:O	1:A:1694:ILE:HG12	2.17	0.45
3:C:92:LEU:O	3:C:96:GLN:N	2.50	0.45
1:A:356:ARG:NH2	1:A:362:TYR:O	2.49	0.45
1:A:760:PHE:HA	1:A:763:MET:HE2	1.98	0.45
1:A:1419:VAL:HG23	1:A:1425:PRO:HA	1.98	0.44
8:A:2009:PCW:H412	8:A:2009:PCW:H442	1.72	0.44
2:B:93:ASN:O	2:B:105:SER:OG	2.35	0.44
2:B:113:TYR:O	2:B:116:SER:OG	2.27	0.44
1:A:1408:TRP:H	1:A:1408:TRP:CD1	2.35	0.44
1:A:60:PRO:HG2	1:A:62:ILE:HG12	1.98	0.43
8:A:2009:PCW:H352	6:A:2016:Y01:HAK1	2.00	0.43
6:A:2016:Y01:HAC2	6:A:2016:Y01:HAJ1	1.74	0.43
7:A:2014:LPE:H112	7:A:2014:LPE:H141	1.84	0.43
1:A:266:LEU:O	1:A:1610:ARG:NH1	2.50	0.43
1:A:27:ILE:O	1:A:31:LYS:HG2	2.19	0.43
1:A:1452:PHE:O	1:A:1455:VAL:HG22	2.18	0.43
1:A:55:ALA:HA	1:A:97:ILE:HG23	2.00	0.43
3:C:32:VAL:HG12	3:C:34:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:TRP:HB3	3:C:80:PHE:CZ	2.54	0.43
1:A:1581:PHE:HA	1:A:1584:VAL:HG22	2.00	0.43
1:A:1661:PHE:CD2	7:A:2010:LPE:H311	2.53	0.43
1:A:382:PHE:HA	1:A:385:VAL:HG12	2.01	0.43
6:A:2016:Y01:HAE2	6:A:2016:Y01:HBB	1.92	0.42
1:A:854:MET:O	1:A:858:ILE:HG12	2.19	0.42
1:A:1669:VAL:HG23	1:A:1730:CYS:HA	2.00	0.42
1:A:1348:TYR:CE1	1:A:1384:ASN:HB2	2.54	0.42
3:C:45:ASP:HB3	3:C:113:MET:HE1	2.01	0.42
1:A:949:MET:HB2	8:A:2012:PCW:H20	2.00	0.42
1:A:1406:LYS:HE2	1:A:1698:ALA:HA	2.00	0.42
2:B:148:ASP:OD1	2:B:148:ASP:N	2.50	0.42
4:D:1:NAG:H4	4:D:2:NAG:H2	1.77	0.42
1:A:813:SER:HA	1:A:816:VAL:HG12	2.02	0.42
8:A:2012:PCW:H322	8:A:2012:PCW:H122	2.00	0.42
1:A:849:TRP:CG	6:A:2005:Y01:HAD3	2.46	0.41
1:A:908:TRP:NE1	1:A:1413:TYR:OH	2.46	0.41
1:A:1289:LEU:HA	1:A:1292:LEU:HD13	2.02	0.41
8:A:2012:PCW:C43	7:A:2015:LPE:H152	2.50	0.41
3:C:127:CYS:SG	3:C:129:ILE:HD11	2.61	0.41
1:A:1528:ASN:HD21	1:A:1619:ARG:HE	1.69	0.41
2:B:89:ARG:HH11	2:B:110:ASN:HB3	1.85	0.41
1:A:22:LEU:HA	1:A:25:GLN:HG2	2.03	0.41
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	2.01	0.41
2:B:78:LEU:HD22	2:B:92:TRP:HB2	2.02	0.41
1:A:276:PHE:CE1	1:A:302:TYR:HB3	2.56	0.40
1:A:1690:CYS:HB3	1:A:1703:LEU:HD21	2.03	0.40
3:C:34:VAL:HG12	3:C:50:CYS:HA	2.03	0.40
1:A:231:LEU:HD11	1:A:871:LEU:HD23	2.02	0.40
1:A:1585:VAL:HG11	1:A:1622:ARG:HD3	2.03	0.40
1:A:839:LEU:HB3	1:A:1334:ILE:HD12	2.02	0.40
1:A:1310:VAL:O	1:A:1314:LEU:HG	2.22	0.40
1:A:270:ASN:HD22	1:A:374:ALA:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1166/1988 (59%)	1148 (98%)	18 (2%)	0	100	100
2	B	171/173 (99%)	171 (100%)	0	0	100	100
3	C	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
All	All	1454/2280 (64%)	1435 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	1056/1778 (59%)	1055 (100%)	1 (0%)	88	93
2	B	157/157 (100%)	157 (100%)	0	100	100
3	C	112/112 (100%)	112 (100%)	0	100	100
All	All	1325/2047 (65%)	1324 (100%)	1 (0%)	87	93

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

Mol	Chain	Res	Type
1	A	393	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	139	ASN
1	A	336	ASN
1	A	757	ASN
1	A	941	GLN
1	A	1180	ASN
1	A	1528	ASN
1	A	1539	GLN
1	A	1541	GLN
3	C	62	GLN
3	C	66	ASN
3	C	70	GLN
3	C	82	GLN
3	C	118	GLN
3	C	143	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.53	0	17,19,21	0.57	0
4	NAG	E	1	4,2	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.43	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

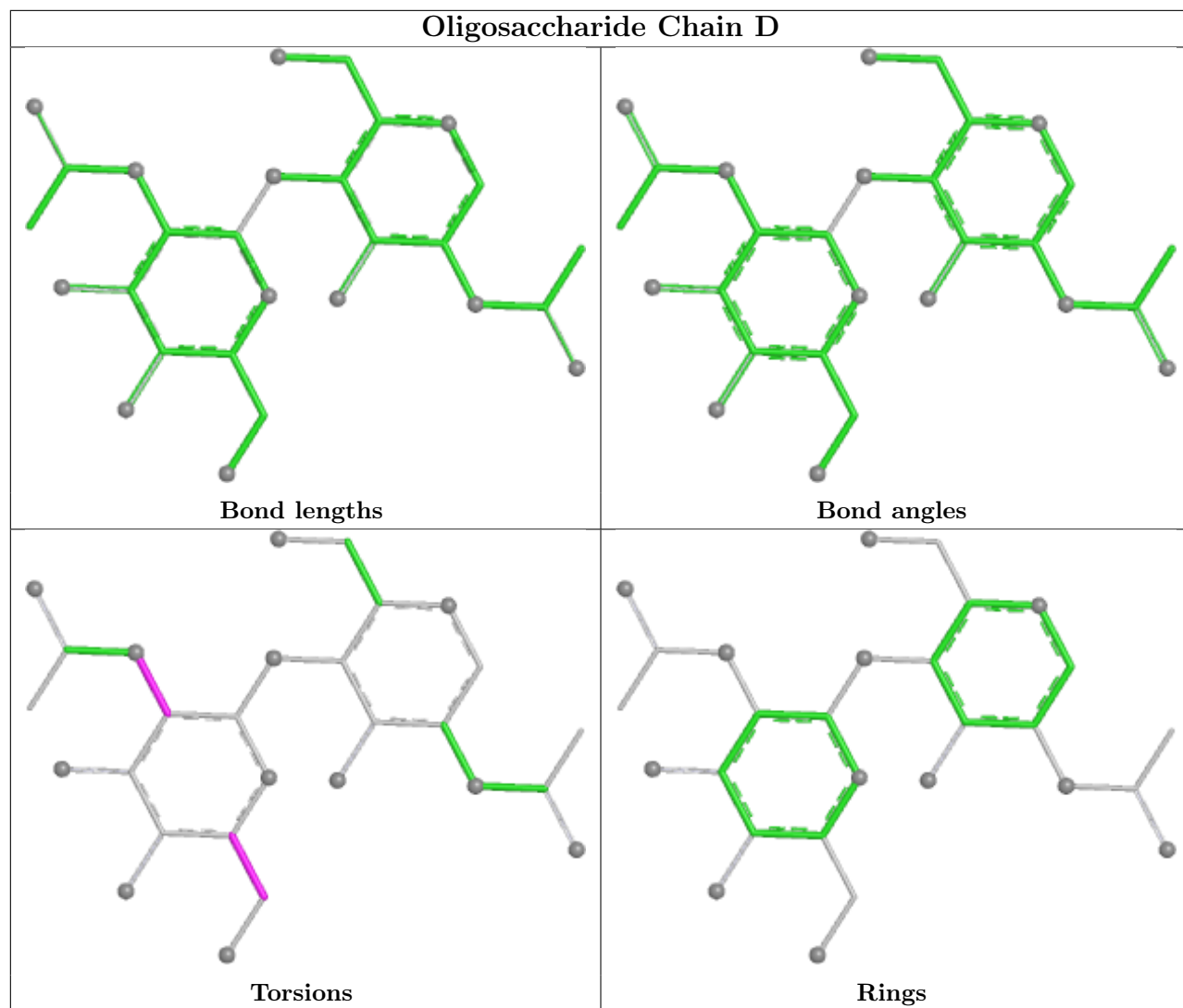
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7

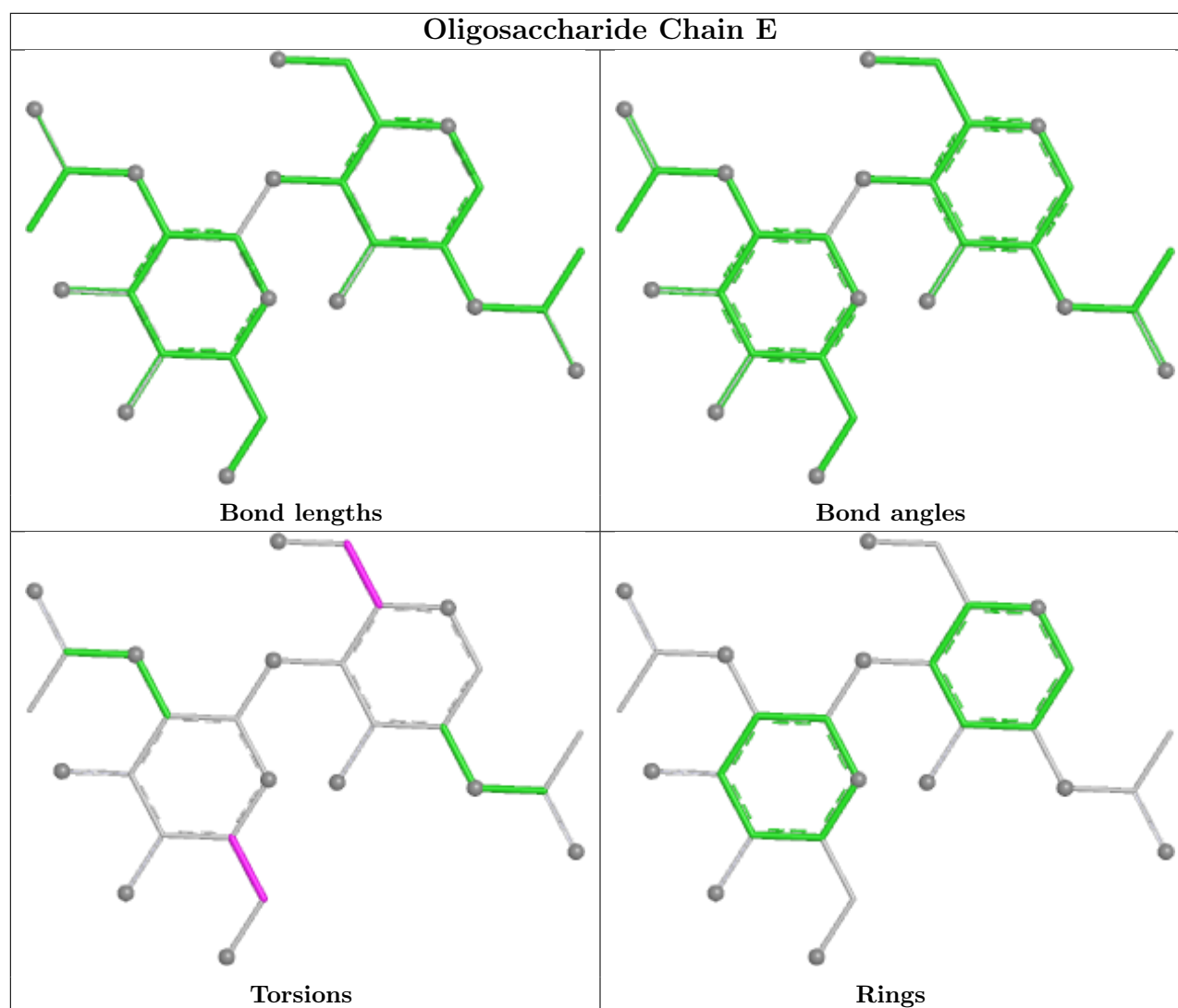
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
4	D	2	NAG	2	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](#)

21 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	$\# Z > 2$
5	NAG	B	302	2	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	A	2001	1	14,14,15	0.27	0	17,19,21	0.45	0
8	PCW	A	2012	-	46,46,53	0.35	0	52,54,61	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LPE	A	2011	-	27,27,33	0.27	0	31,33,39	0.36	0
5	NAG	B	303	2	14,14,15	0.26	0	17,19,21	0.43	0
8	PCW	A	2009	-	50,50,53	0.34	0	56,58,61	0.30	0
7	LPE	A	2013	-	24,24,33	0.30	0	28,30,39	0.47	0
7	LPE	A	2010	-	21,21,33	0.37	0	25,27,39	0.54	0
7	LPE	B	304	-	16,16,33	0.36	0	20,22,39	0.42	0
7	LPE	A	2007	-	24,24,33	0.28	0	28,30,39	0.38	0
7	LPE	A	2015	-	24,24,33	0.29	0	28,30,39	0.39	0
5	NAG	A	2003	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	A	2002	1	14,14,15	0.21	0	17,19,21	0.43	0
6	Y01	A	2004	-	38,38,38	0.46	0	57,57,57	0.50	0
9	A1E26	A	2017	-	51,55,55	1.17	2 (3%)	63,95,95	0.79	2 (3%)
6	Y01	A	2006	-	38,38,38	0.45	0	57,57,57	0.54	0
7	LPE	A	2014	-	24,24,33	0.28	0	28,30,39	0.37	0
5	NAG	B	301	2	14,14,15	0.18	0	17,19,21	0.46	0
6	Y01	A	2005	-	38,38,38	0.45	0	57,57,57	0.64	0
7	LPE	A	2008	-	24,24,33	0.32	0	25,27,39	0.42	0
6	Y01	A	2016	-	38,38,38	0.48	0	57,57,57	0.61	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
5	NAG	B	302	2	-	2/6/23/26	0/1/1/1
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
8	PCW	A	2012	-	-	35/50/50/57	-
7	LPE	A	2011	-	-	4/28/28/34	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
8	PCW	A	2009	-	-	34/54/54/57	-
7	LPE	A	2013	-	-	16/25/25/34	-
7	LPE	A	2010	-	-	14/22/22/34	-
7	LPE	B	304	-	-	13/17/17/34	-
7	LPE	A	2007	-	-	4/25/25/34	-
7	LPE	A	2015	-	-	15/25/25/34	-
5	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
6	Y01	A	2004	-	-	2/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1E26	A	2017	-	-	2/12/138/138	0/1/8/8
6	Y01	A	2006	-	-	9/19/77/77	0/4/4/4
7	LPE	A	2014	-	-	21/25/25/34	-
5	NAG	B	301	2	-	2/6/23/26	0/1/1/1
6	Y01	A	2005	-	-	10/19/77/77	0/4/4/4
7	LPE	A	2008	-	-	4/25/25/34	-
6	Y01	A	2016	-	-	12/19/77/77	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2017	A1E26	C17-C20	-6.30	1.49	1.57
9	A	2017	A1E26	C22-N1	3.85	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2017	A1E26	C26-N1-C22	-2.11	107.19	111.32
9	A	2017	A1E26	C20-C17-C13	2.10	114.52	111.20

There are no chirality outliers.

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2016	Y01	CAO-CBB-CBE-CAP
6	A	2016	Y01	CAC-CBB-CBE-CBI
7	A	2008	LPE	C31-O33-P-O31
7	A	2008	LPE	C32-C31-O33-P
7	A	2010	LPE	O1-C1-C2-O2H
7	A	2010	LPE	O1-C1-C2-C3
7	A	2010	LPE	C1-C2-C3-O3
7	A	2010	LPE	C3-O3-P-O31
7	A	2010	LPE	C3-O3-P-O32
7	A	2010	LPE	C3-O3-P-O33
7	A	2010	LPE	C31-O33-P-O3
7	A	2013	LPE	O1-C1-C2-O2H
7	A	2013	LPE	O1-C1-C2-C3
7	A	2013	LPE	O2H-C2-C3-O3
7	A	2013	LPE	C3-O3-P-O32
7	A	2013	LPE	C3-O3-P-O33

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Mol	Chain	Res	Type	Atoms
7	A	2013	LPE	C31-O33-P-O3
7	A	2013	LPE	C31-O33-P-O31
7	A	2013	LPE	C31-O33-P-O32
7	A	2013	LPE	O33-C31-C32-N
7	A	2014	LPE	O1-C1-C2-O2H
7	A	2014	LPE	C3-O3-P-O32
7	A	2014	LPE	C3-O3-P-O33
7	A	2014	LPE	C31-O33-P-O3
7	A	2015	LPE	O2H-C2-C3-O3
7	A	2015	LPE	C3-O3-P-O31
7	A	2015	LPE	C3-O3-P-O32
7	A	2015	LPE	C3-O3-P-O33
7	A	2015	LPE	O33-C31-C32-N
7	B	304	LPE	O1-C1-C2-O2H
7	B	304	LPE	O1-C1-C2-C3
7	B	304	LPE	C3-O3-P-O31
7	B	304	LPE	C3-O3-P-O33
7	B	304	LPE	C31-O33-P-O3
7	B	304	LPE	O33-C31-C32-N
8	A	2009	PCW	O4P-C4-C5-N
8	A	2009	PCW	C1-O3P-P-O1P
8	A	2009	PCW	C1-O3P-P-O2P
8	A	2009	PCW	C1-O3P-P-O4P
8	A	2009	PCW	C4-O4P-P-O1P
8	A	2009	PCW	C4-O4P-P-O2P
8	A	2009	PCW	C4-O4P-P-O3P
8	A	2012	PCW	C40-C41-C42-C43
8	A	2012	PCW	C1-O3P-P-O2P
8	A	2012	PCW	C4-O4P-P-O1P
8	A	2012	PCW	C4-O4P-P-O2P
8	A	2012	PCW	C4-O4P-P-O3P
6	A	2005	Y01	CAR-CBC-OAW-CAY
6	A	2016	Y01	CAC-CBB-CBE-CAP
6	A	2016	Y01	CAO-CBB-CBE-CBI
7	A	2010	LPE	C11-C12-C13-C14
6	A	2016	Y01	CAJ-CAO-CBB-CAC
8	A	2009	PCW	C4-C5-N-C6
7	A	2010	LPE	O2H-C2-C3-O3
8	A	2012	PCW	C12-C11-O3-C3
5	A	2001	NAG	O5-C5-C6-O6
8	A	2012	PCW	O11-C11-O3-C3
8	A	2009	PCW	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
7	A	2013	LPE	C1-C2-C3-O3
8	A	2009	PCW	C41-C42-C43-C44
5	A	2001	NAG	C4-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
6	A	2016	Y01	CAJ-CAO-CBB-CBE
7	A	2013	LPE	O1-C11-C12-C13
5	B	301	NAG	C4-C5-C6-O6
7	A	2015	LPE	C11-C12-C13-C14
6	A	2005	Y01	CAJ-CAO-CBB-CBE
5	B	302	NAG	C4-C5-C6-O6
8	A	2009	PCW	C4-C5-N-C7
6	A	2005	Y01	CAJ-CAO-CBB-CAC
7	A	2015	LPE	C1-C2-C3-O3
7	A	2015	LPE	C31-C32-N-C1N
8	A	2012	PCW	C38-C39-C40-C41
7	A	2010	LPE	O1-C11-C12-C13
6	A	2005	Y01	CAO-CAJ-CAN-CBA
6	A	2016	Y01	CAM-CAY-OAW-CBC
8	A	2012	PCW	C32-C31-O2-C2
7	A	2015	LPE	C31-C32-N-C2N
7	A	2015	LPE	C31-C32-N-C3N
8	A	2009	PCW	C15-C16-C17-C18
7	A	2013	LPE	C12-C13-C14-C15
8	A	2012	PCW	O31-C31-O2-C2
6	A	2005	Y01	CAM-CAY-OAW-CBC
6	A	2016	Y01	OAG-CAY-OAW-CBC
5	B	302	NAG	O5-C5-C6-O6
8	A	2009	PCW	C4-C5-N-C8
7	A	2014	LPE	C12-C13-C14-C15
7	A	2014	LPE	C14-C15-C16-C17
7	A	2015	LPE	C13-C14-C15-C16
7	A	2014	LPE	O1-C1-C2-C3
8	A	2012	PCW	C35-C36-C37-C38
8	A	2009	PCW	C32-C31-O2-C2
6	A	2005	Y01	OAG-CAY-OAW-CBC
8	A	2009	PCW	O31-C31-O2-C2
8	A	2012	PCW	C34-C35-C36-C37
8	A	2012	PCW	C4-C5-N-C7
8	A	2009	PCW	C34-C35-C36-C37
7	A	2014	LPE	C2-C1-O1-C11
8	A	2009	PCW	C43-C44-C45-C46
7	A	2013	LPE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	A	2010	LPE	C12-C13-C14-C15
6	A	2004	Y01	CAR-CBC-OAW-CAY
8	A	2012	PCW	C39-C40-C41-C42
7	A	2014	LPE	O2H-C2-C3-O3
9	A	2017	A1E26	O12-C28-C29-C34
7	A	2014	LPE	C13-C14-C15-C16
8	A	2012	PCW	C36-C37-C38-C39
5	A	2002	NAG	C4-C5-C6-O6
8	A	2012	PCW	C1-C2-C3-O3
8	A	2009	PCW	C35-C36-C37-C38
8	A	2009	PCW	C16-C17-C18-C19
8	A	2012	PCW	C12-C13-C14-C15
8	A	2012	PCW	C4-C5-N-C6
8	A	2009	PCW	C33-C34-C35-C36
8	A	2009	PCW	C36-C37-C38-C39
8	A	2012	PCW	C18-C19-C20-C21
8	A	2012	PCW	C22-C23-C24-C25
7	A	2010	LPE	C2-C1-O1-C11
7	A	2015	LPE	C12-C13-C14-C15
8	A	2012	PCW	O2-C2-C3-O3
6	A	2016	Y01	CAN-CAJ-CAO-CBB
8	A	2009	PCW	C23-C24-C25-C26
6	A	2004	Y01	CAV-CBC-OAW-CAY
8	A	2009	PCW	C37-C38-C39-C40
8	A	2009	PCW	C32-C33-C34-C35
6	A	2016	Y01	CAJ-CAN-CBA-CAA
6	A	2016	Y01	CAJ-CAN-CBA-CAB
8	A	2009	PCW	O3P-C1-C2-O2
7	A	2014	LPE	C2-C3-O3-P
7	A	2015	LPE	C14-C15-C16-C17
6	A	2005	Y01	CAN-CAJ-CAO-CBB
5	A	2003	NAG	C1-C2-N2-C7
7	A	2013	LPE	C15-C16-C17-C18
8	A	2009	PCW	O3P-C1-C2-C3
7	A	2014	LPE	C15-C16-C17-C18
6	A	2006	Y01	CAJ-CAN-CBA-CAB
8	A	2012	PCW	C33-C34-C35-C36
7	A	2007	LPE	C32-C31-O33-P
7	A	2014	LPE	C32-C31-O33-P
7	B	304	LPE	C32-C31-O33-P
8	A	2012	PCW	C20-C21-C22-C23
6	A	2006	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
8	A	2009	PCW	C42-C43-C44-C45
8	A	2009	PCW	C22-C23-C24-C25
5	A	2002	NAG	O5-C5-C6-O6
7	A	2013	LPE	C13-C14-C15-C16
7	A	2007	LPE	O33-C31-C32-N
7	A	2010	LPE	O33-C31-C32-N
7	A	2014	LPE	O33-C31-C32-N
7	A	2014	LPE	C1-C2-C3-O3
7	A	2014	LPE	C31-C32-N-C2N
7	B	304	LPE	C31-C32-N-C1N
8	A	2012	PCW	C4-C5-N-C8
8	A	2009	PCW	C38-C39-C40-C41
7	A	2007	LPE	C2-C3-O3-P
8	A	2012	PCW	O3P-C1-C2-O2
6	A	2006	Y01	CAC-CBB-CBE-CBI
7	A	2014	LPE	C31-C32-N-C1N
7	B	304	LPE	C31-C32-N-C2N
8	A	2009	PCW	C11-C12-C13-C14
5	A	2003	NAG	C3-C2-N2-C7
7	A	2011	LPE	C3-O3-P-O31
7	A	2011	LPE	C31-O33-P-O31
7	A	2014	LPE	C31-O33-P-O31
7	B	304	LPE	C3-O3-P-O32
7	B	304	LPE	C31-O33-P-O31
9	A	2017	A1E26	O13-C28-C29-C34
6	A	2006	Y01	CAJ-CAN-CBA-CAA
6	A	2006	Y01	CAO-CBB-CBE-CAP
8	A	2012	PCW	C23-C24-C25-C26
7	A	2014	LPE	C16-C17-C18-C19
7	A	2010	LPE	C13-C14-C15-C16
7	A	2015	LPE	C2-C1-O1-C11
8	A	2009	PCW	O3-C11-C12-C13
6	A	2016	Y01	CAO-CAJ-CAN-CBA
7	A	2014	LPE	C31-C32-N-C3N
7	B	304	LPE	C31-C32-N-C3N
8	A	2012	PCW	C37-C38-C39-C40
7	A	2008	LPE	C14-C15-C16-C17
6	A	2006	Y01	CAM-CAL-CAX-OAF
8	A	2012	PCW	C32-C33-C34-C35
7	A	2015	LPE	C2-C3-O3-P
6	A	2006	Y01	CAM-CAL-CAX-OAH
7	B	304	LPE	C2-C1-O1-C11

Continued on next page...

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Mol	Chain	Res	Type	Atoms
7	A	2013	LPE	C11-C12-C13-C14
7	A	2011	LPE	C2-C3-O3-P
7	A	2011	LPE	O1-C1-C2-C3
6	A	2005	Y01	CAM-CAL-CAX-OAH
8	A	2012	PCW	C17-C18-C19-C20
6	A	2006	Y01	CAO-CAJ-CAN-CBA
7	A	2008	LPE	C13-C14-C15-C16
7	A	2014	LPE	C11-C12-C13-C14
6	A	2005	Y01	CAM-CAL-CAX-OAF
8	A	2012	PCW	C19-C20-C21-C22
8	A	2012	PCW	O3P-C1-C2-C3
6	A	2006	Y01	CAC-CBB-CBE-CAP
8	A	2012	PCW	O3-C11-C12-C13
6	A	2005	Y01	CAV-CBC-OAW-CAY
7	A	2007	LPE	C12-C11-O1-C1
8	A	2009	PCW	C39-C40-C41-C42
8	A	2012	PCW	O11-C11-C12-C13
8	A	2009	PCW	O2-C31-C32-C33
8	A	2012	PCW	C14-C15-C16-C17
8	A	2012	PCW	C11-C12-C13-C14
8	A	2009	PCW	O31-C31-C32-C33

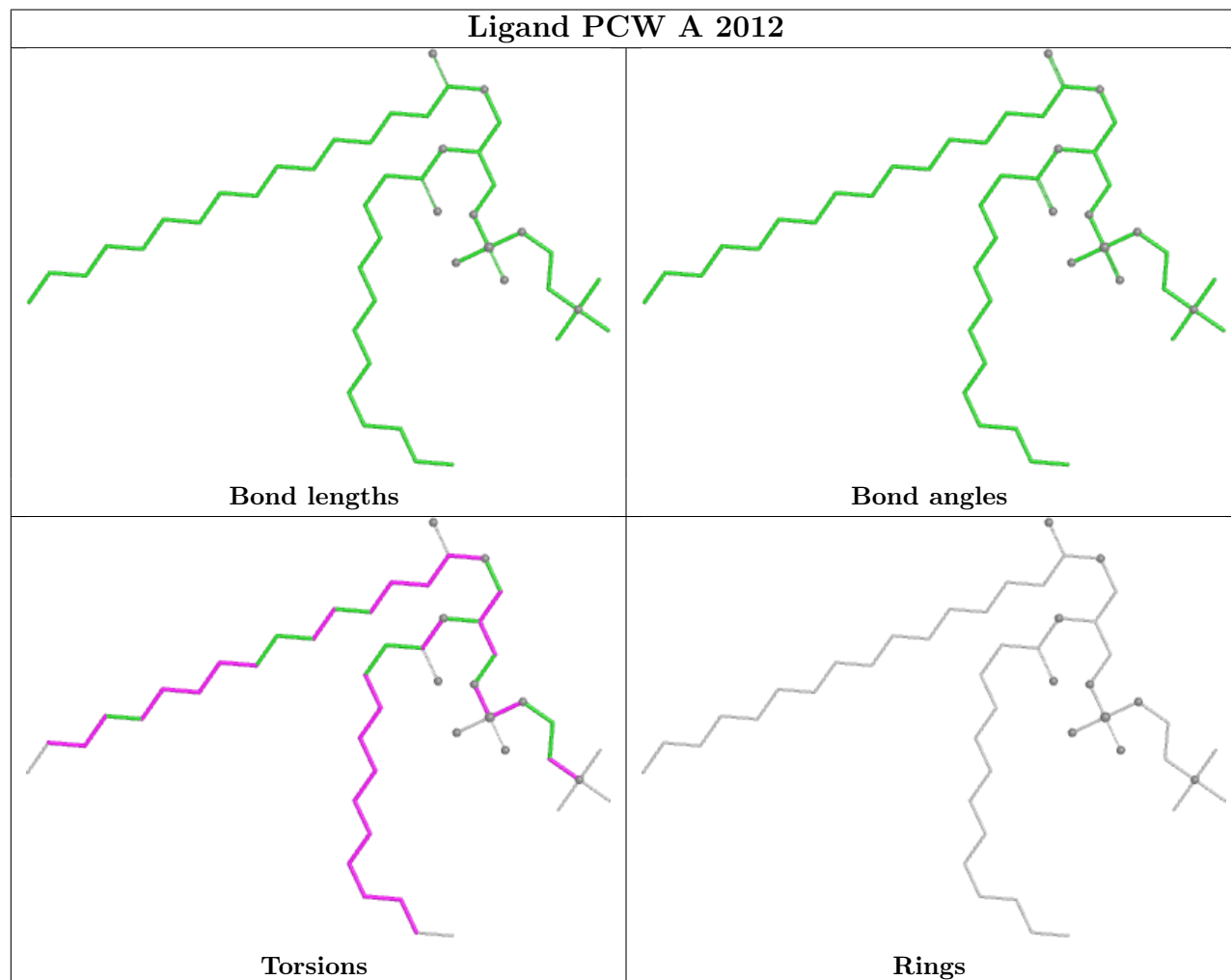
There are no ring outliers.

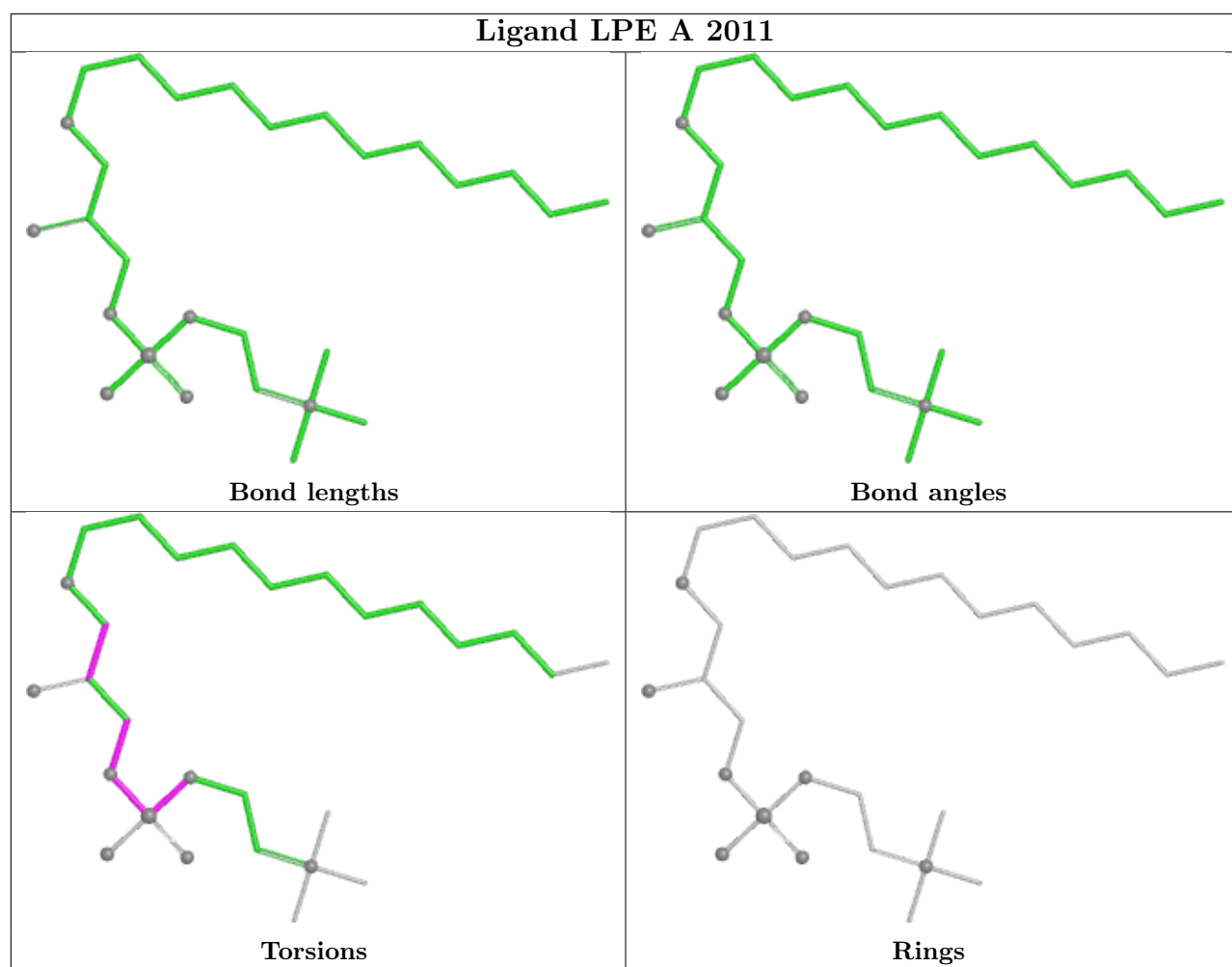
13 monomers are involved in 59 short contacts:

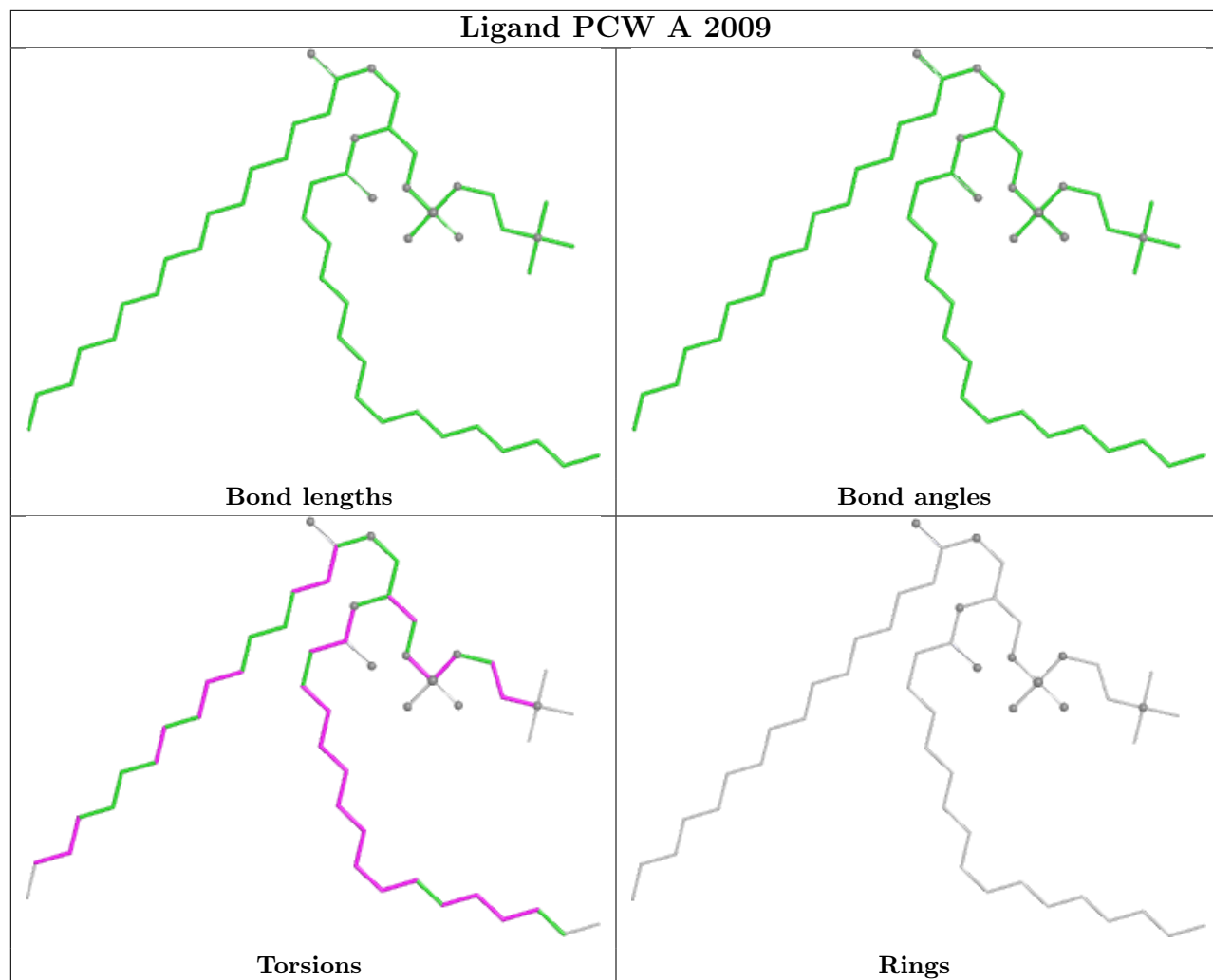
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2012	PCW	12	0
7	A	2011	LPE	2	0
8	A	2009	PCW	2	0
7	A	2013	LPE	1	0
7	A	2010	LPE	6	0
7	B	304	LPE	3	0
7	A	2015	LPE	1	0
9	A	2017	A1E26	2	0
6	A	2006	Y01	1	0
7	A	2014	LPE	5	0
6	A	2005	Y01	16	0
7	A	2008	LPE	1	0
6	A	2016	Y01	9	0

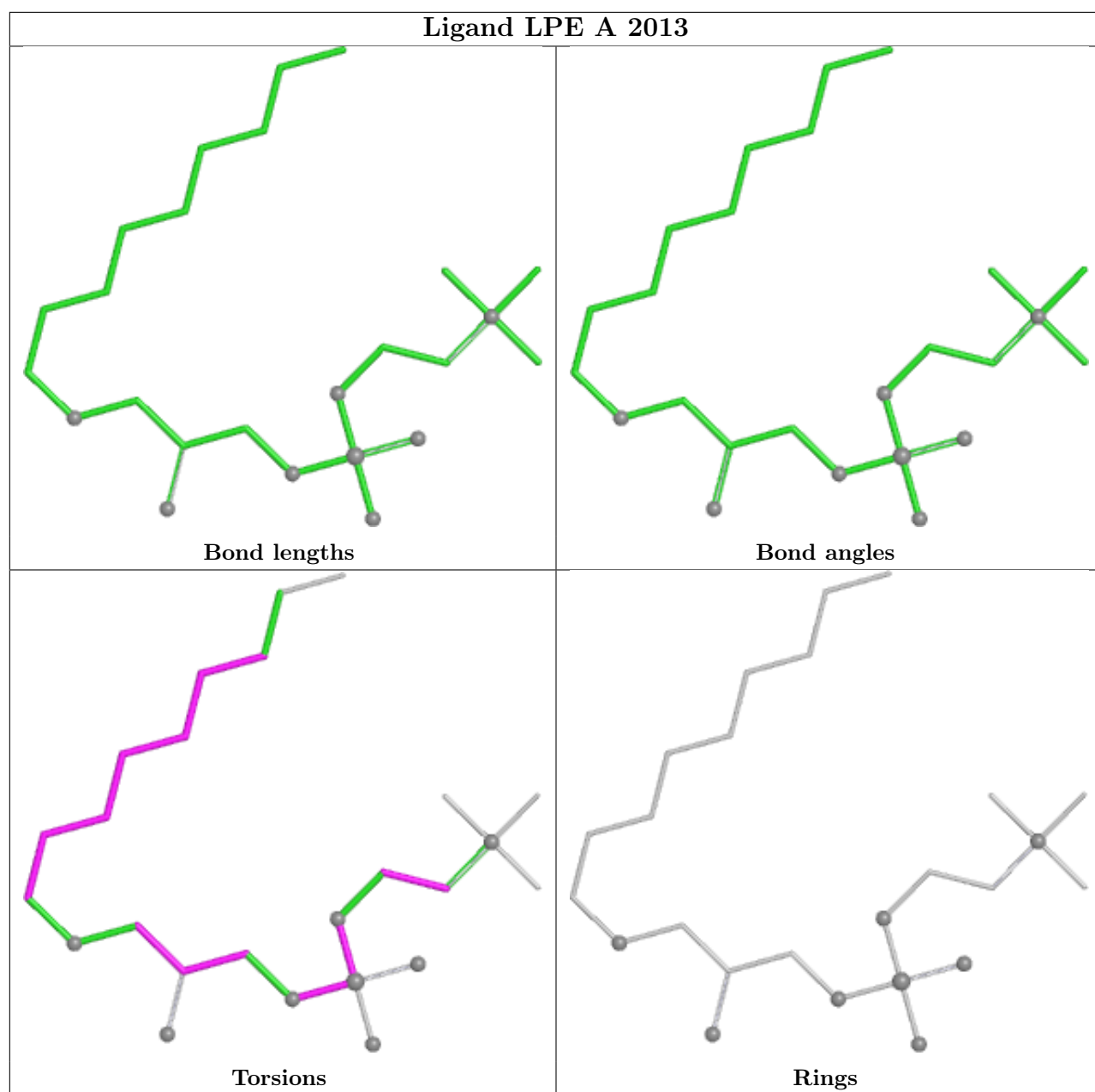
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

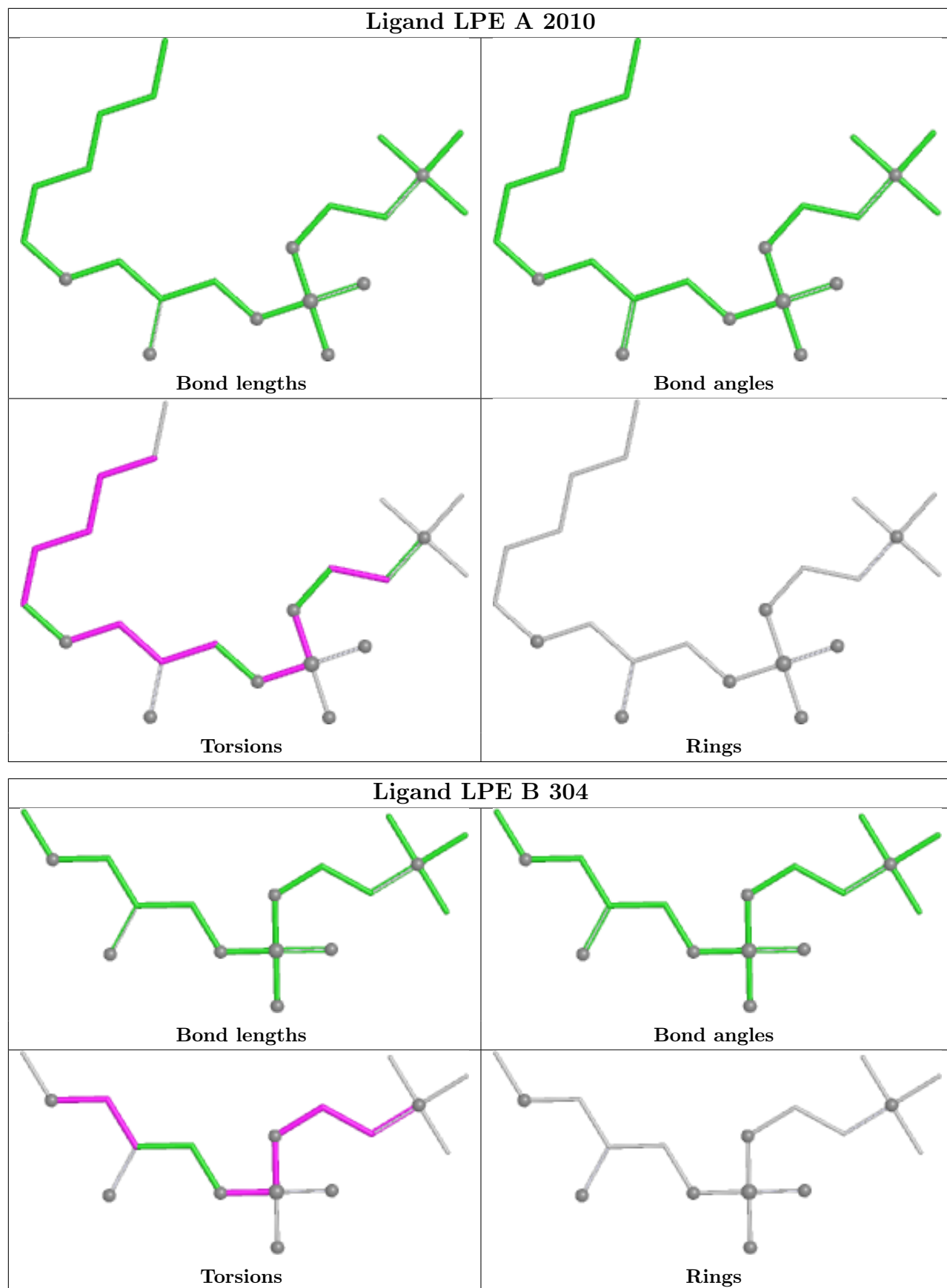
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

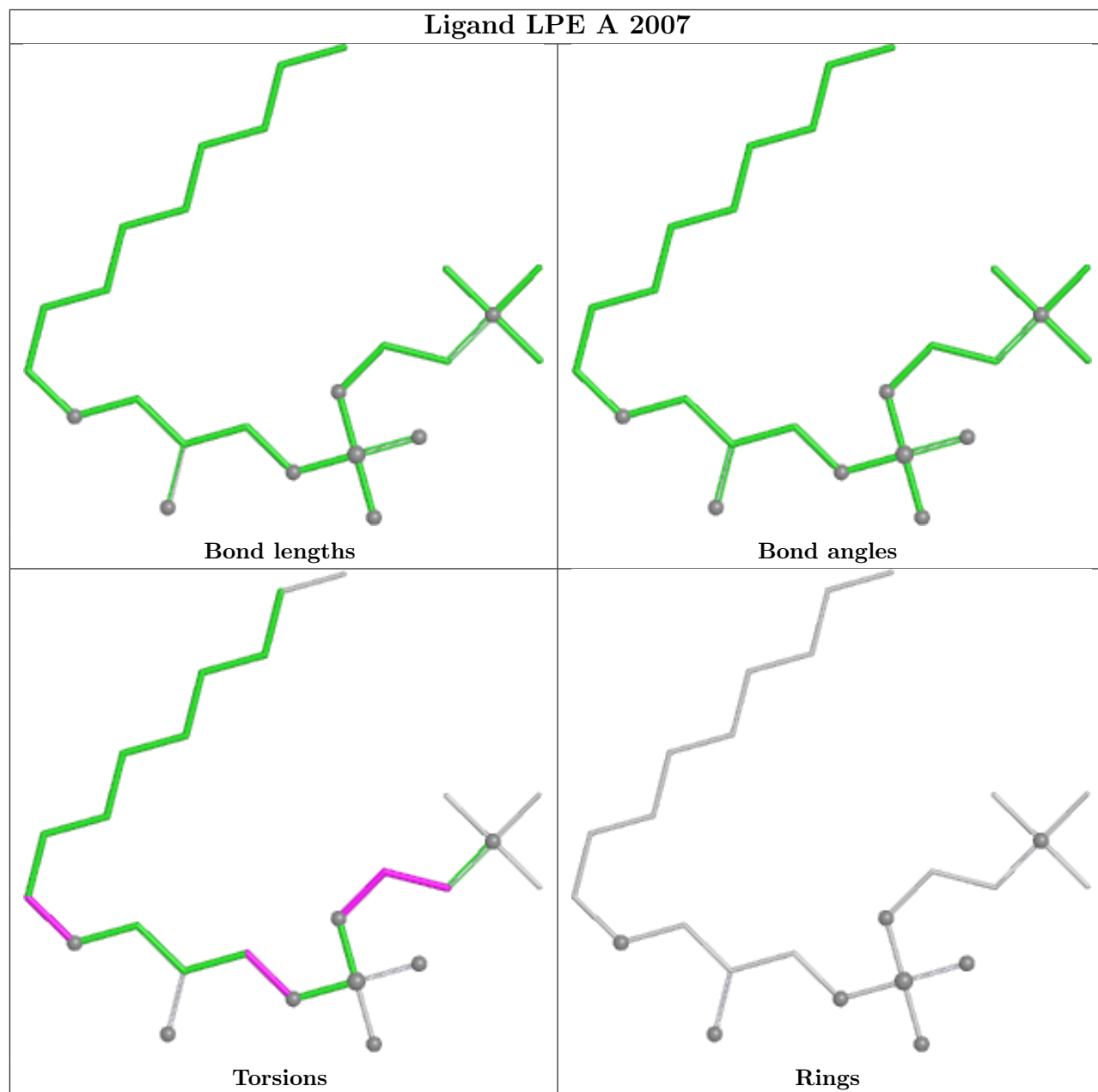


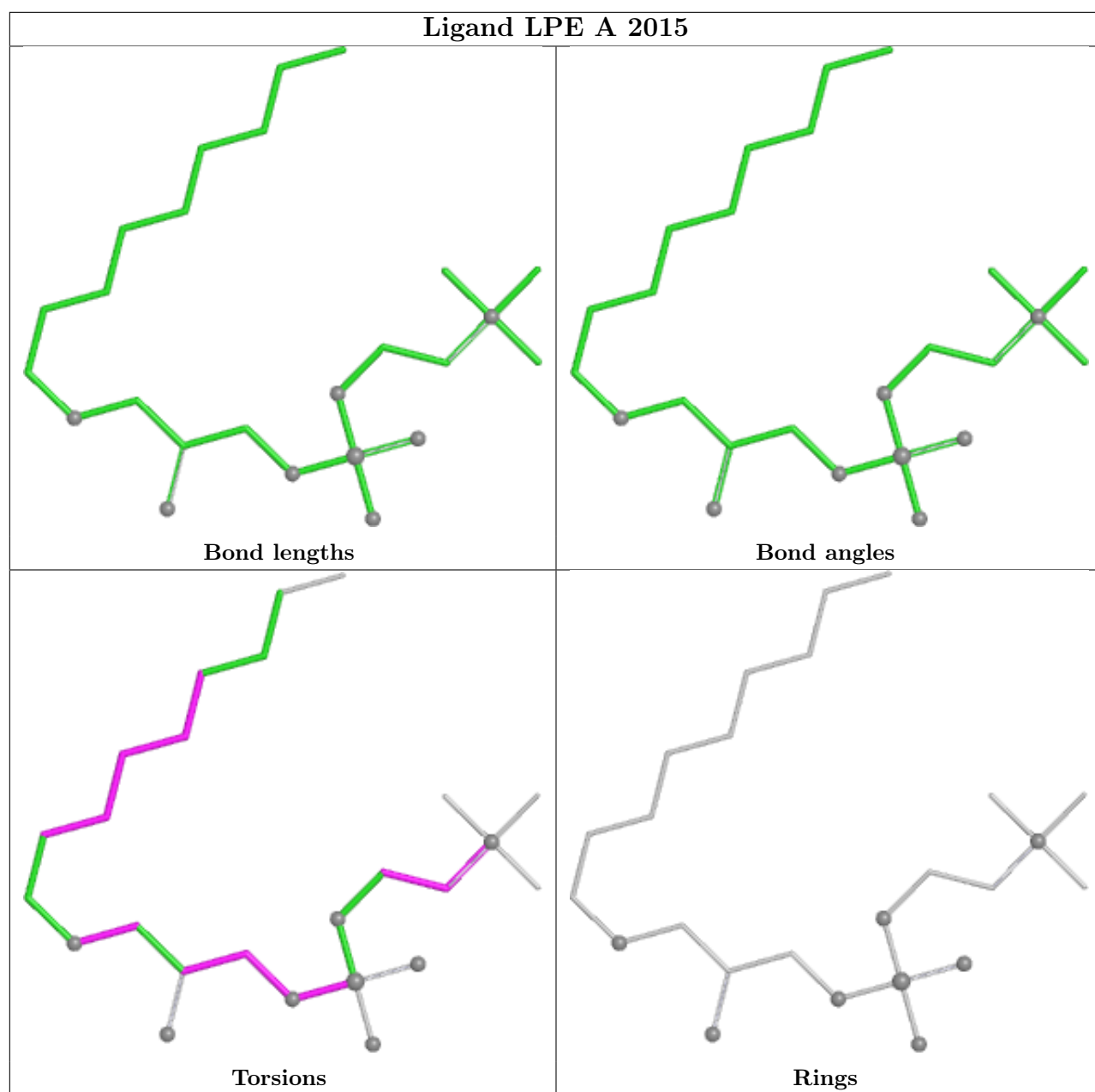


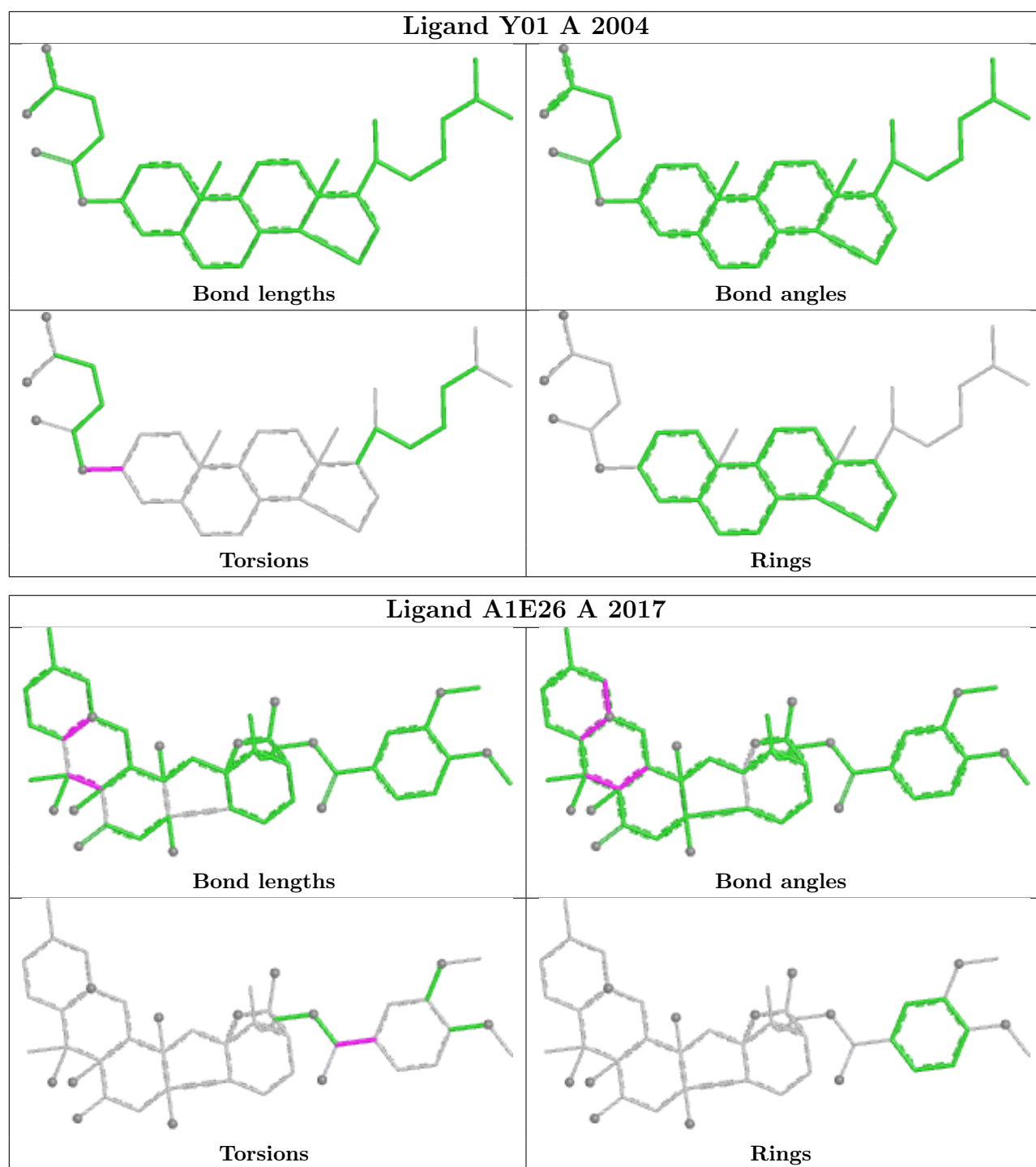


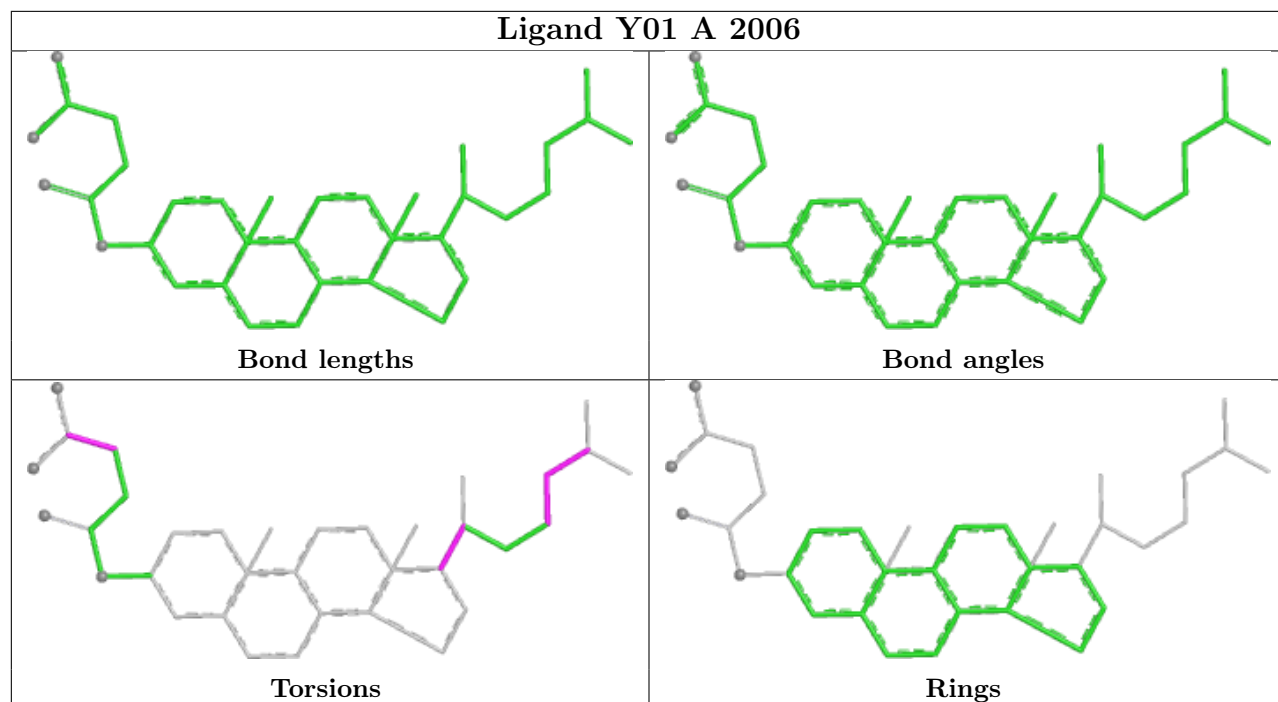


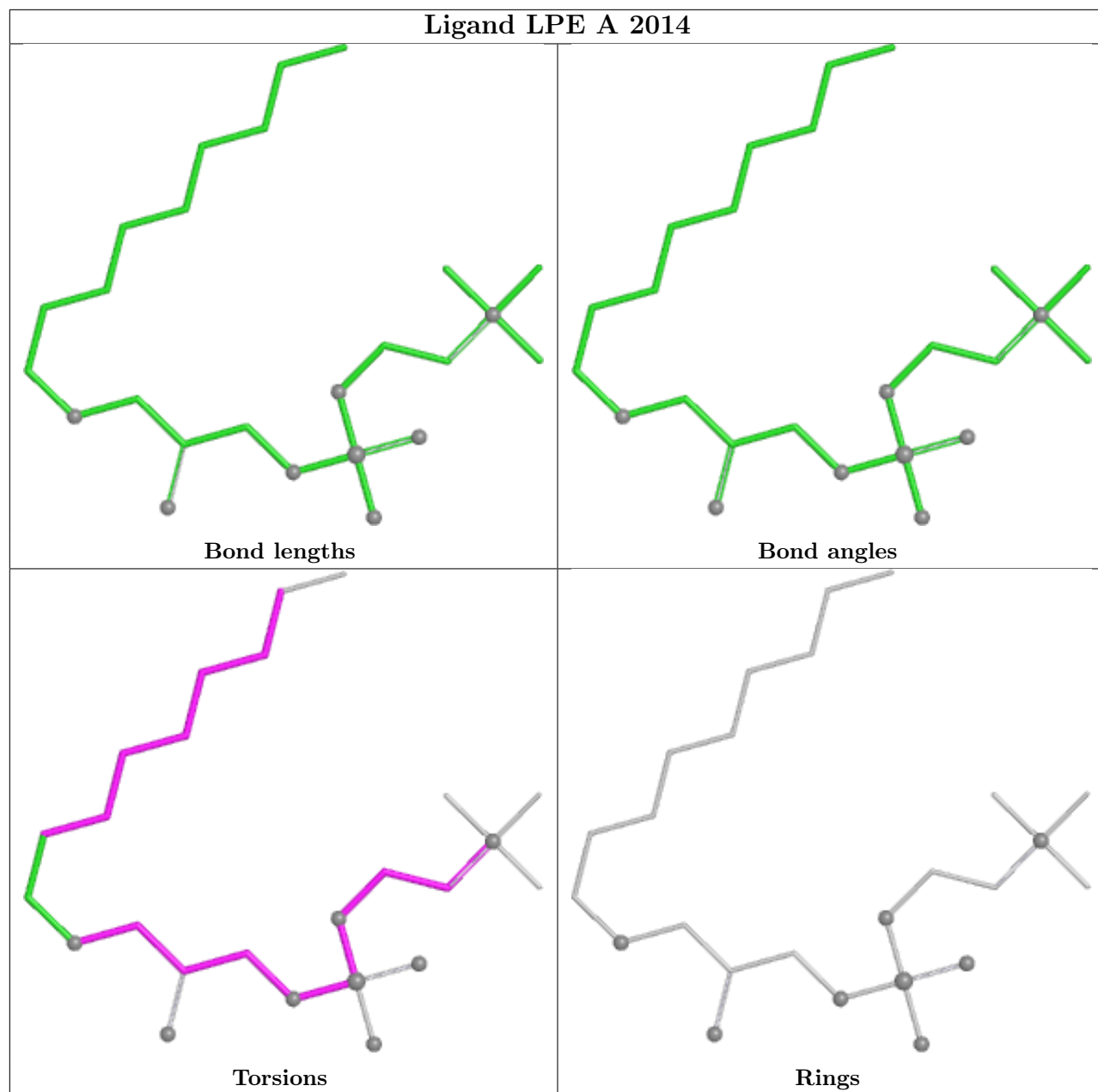


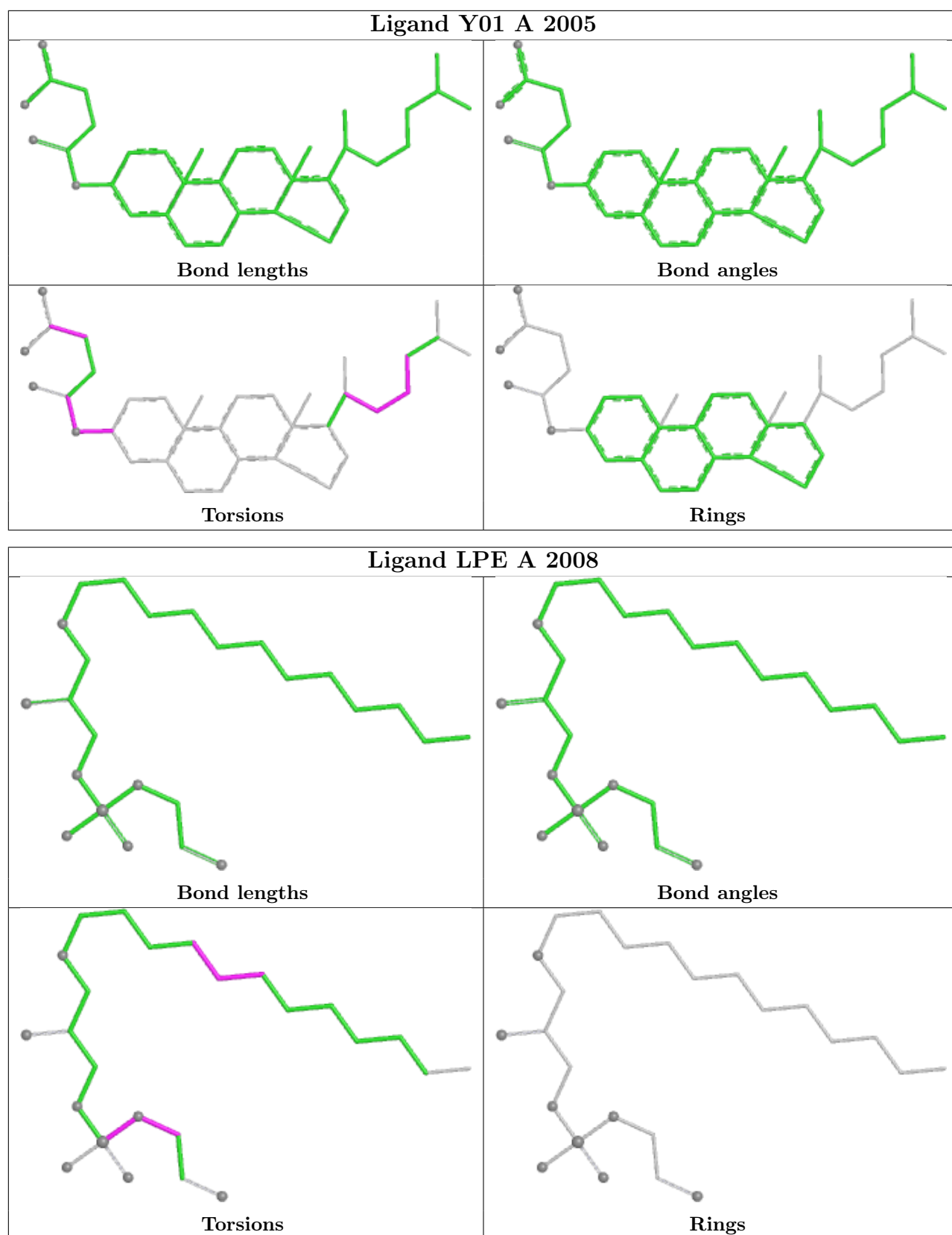


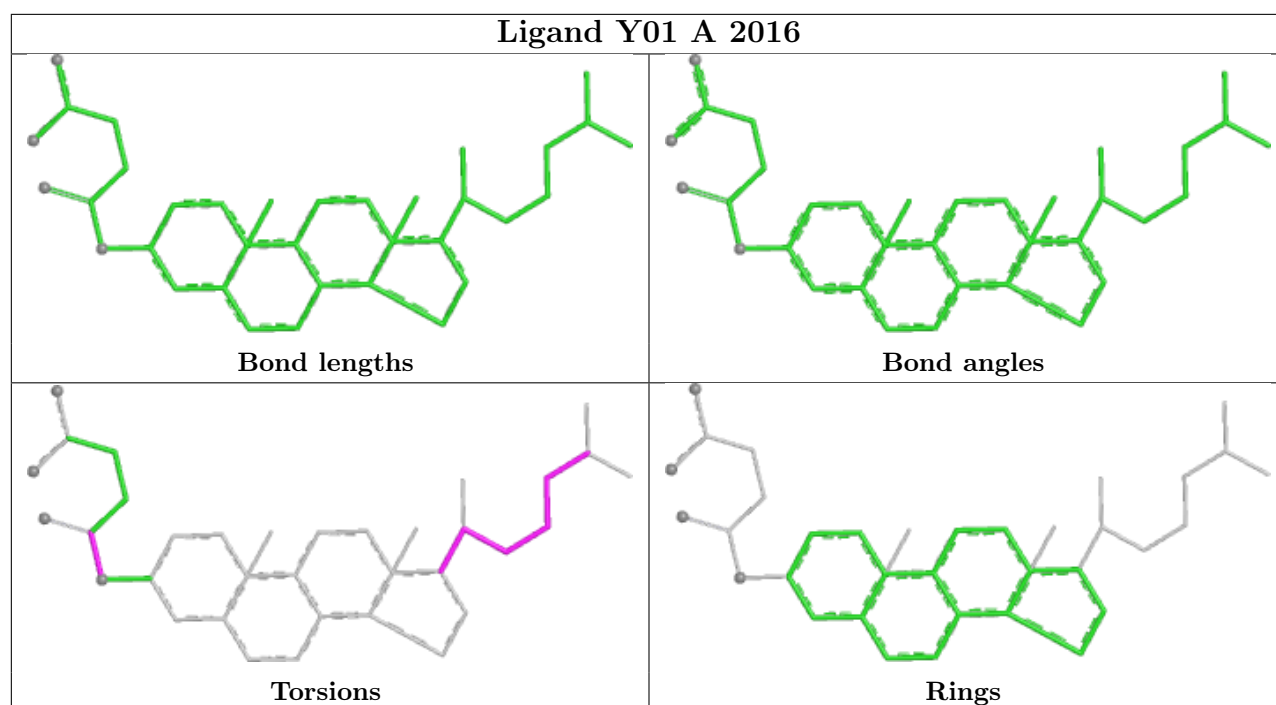












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

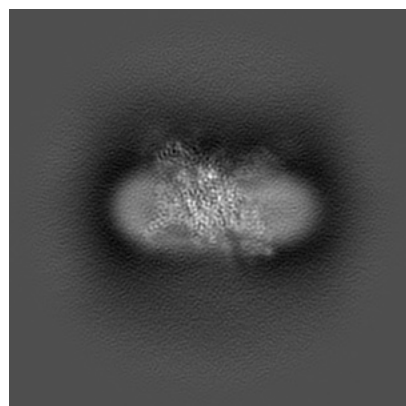
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67990. These allow visual inspection of the internal detail of the map and identification of artifacts.

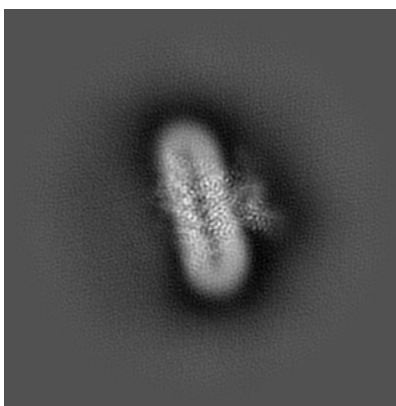
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

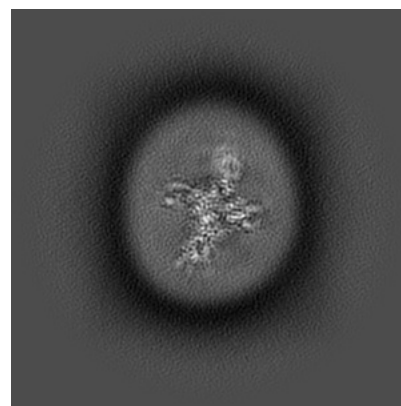
6.1.1 Primary map



X

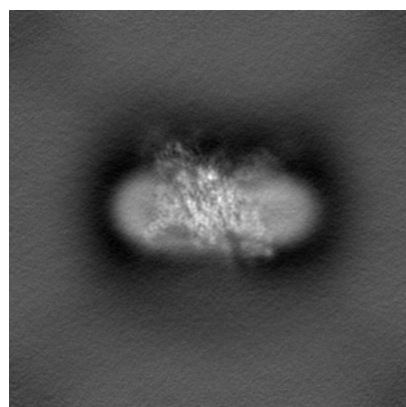


Y

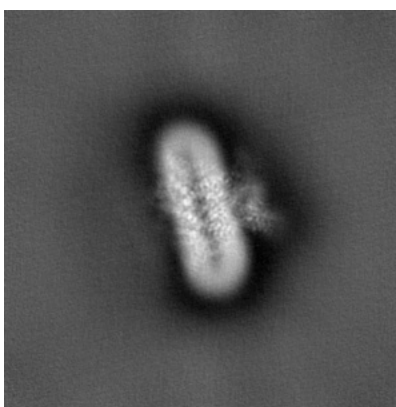


Z

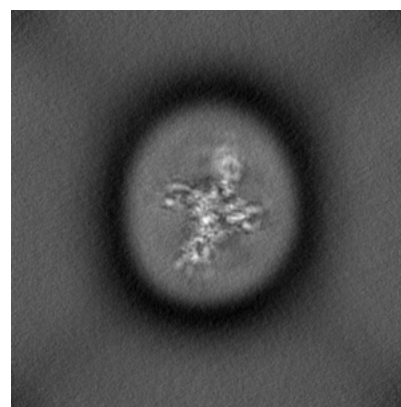
6.1.2 Raw map



X



Y

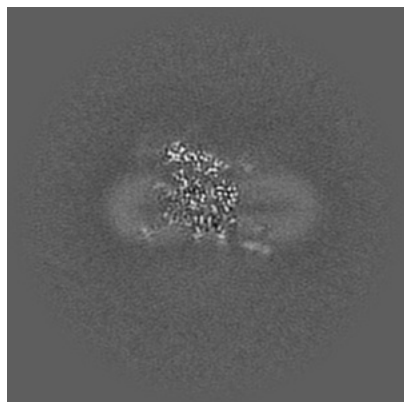


Z

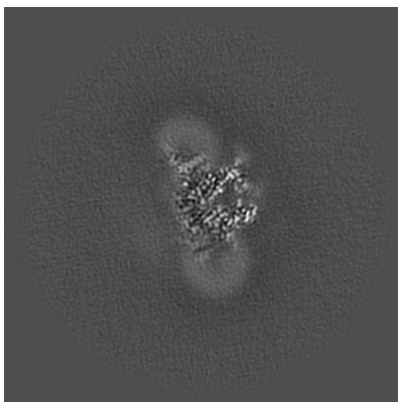
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

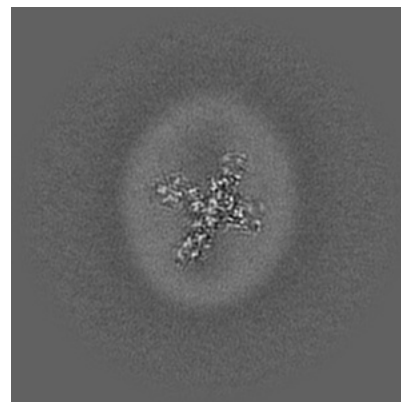
6.2.1 Primary map



X Index: 160

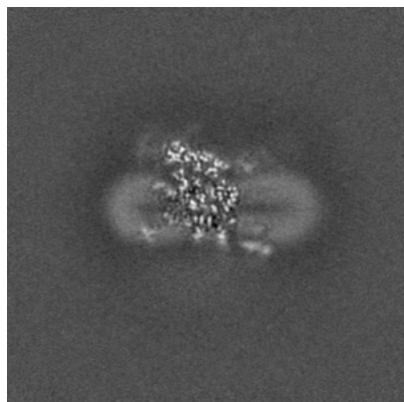


Y Index: 160

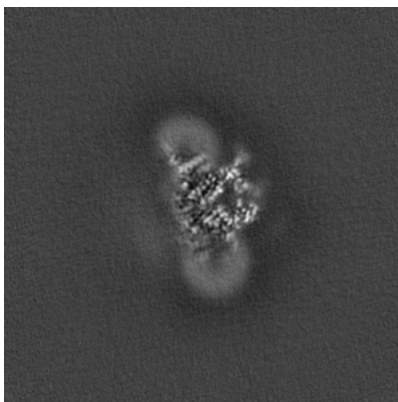


Z Index: 160

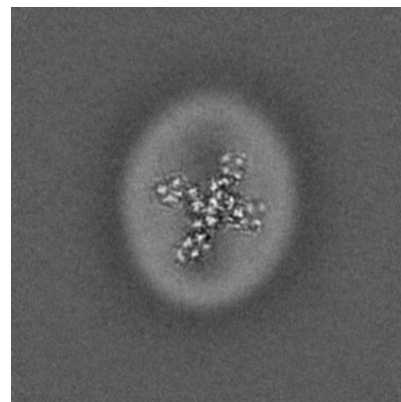
6.2.2 Raw map



X Index: 160



Y Index: 160

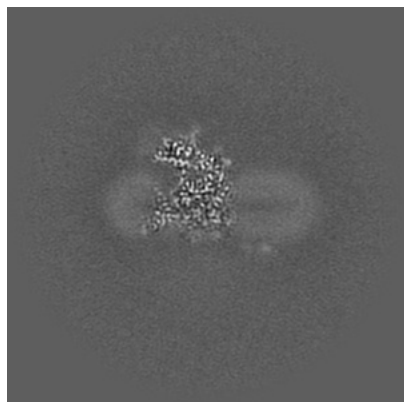


Z Index: 160

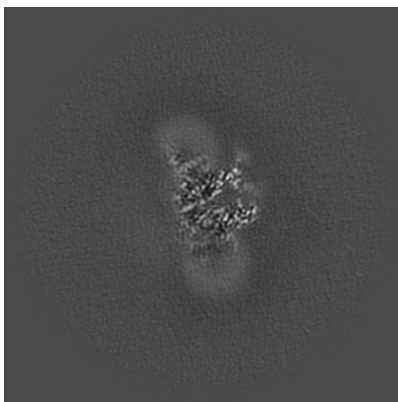
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

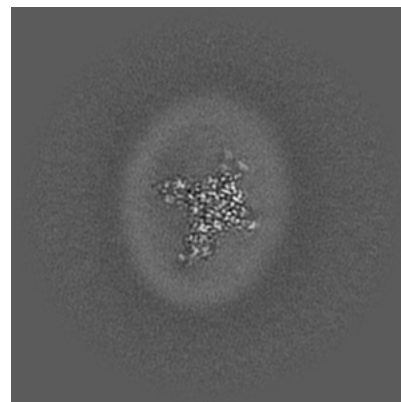
6.3.1 Primary map



X Index: 153

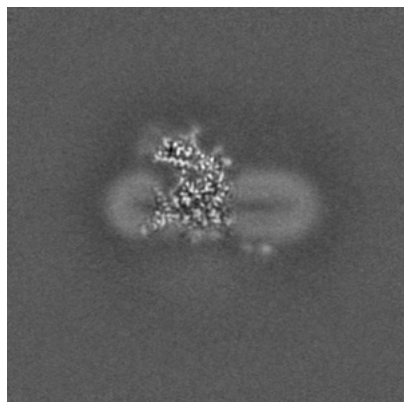


Y Index: 161

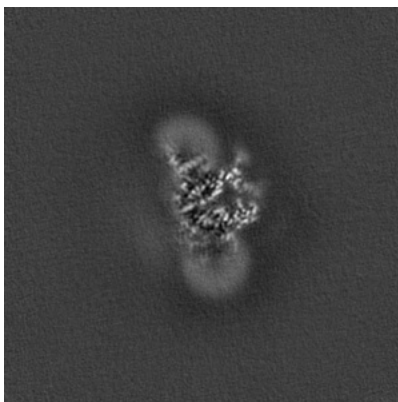


Z Index: 166

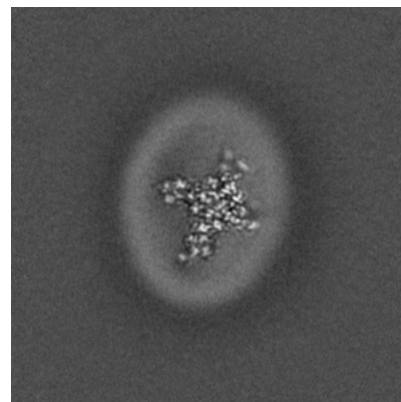
6.3.2 Raw map



X Index: 153



Y Index: 161

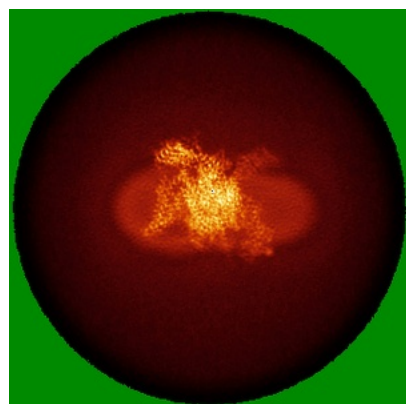


Z Index: 166

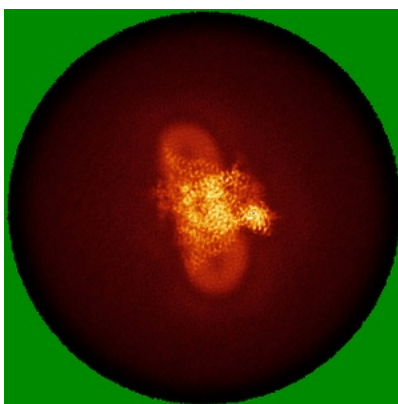
The images above show the largest variance slices of the map in three orthogonal directions.

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

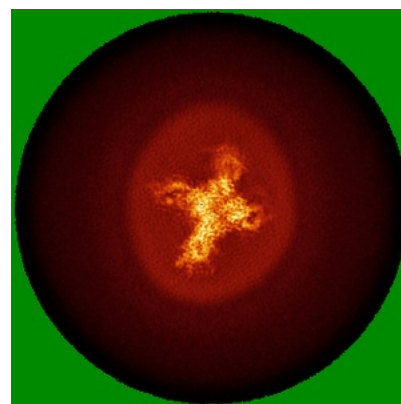
6.4.1 Primary map



X

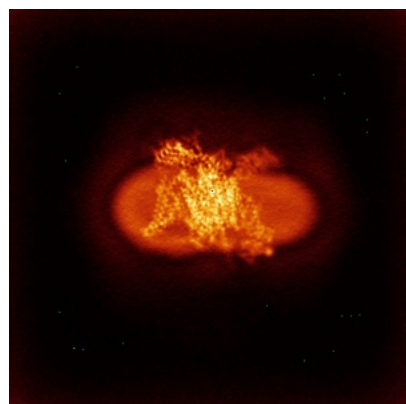


Y

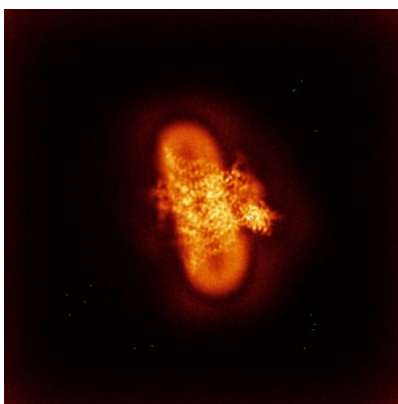


Z

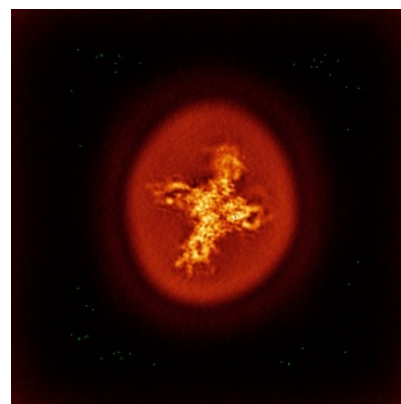
6.4.2 Raw map



X



Y

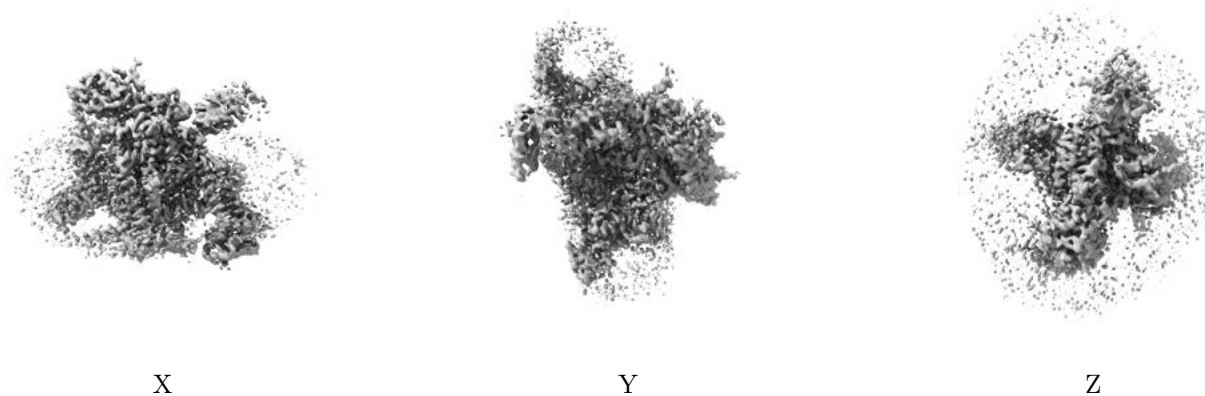


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

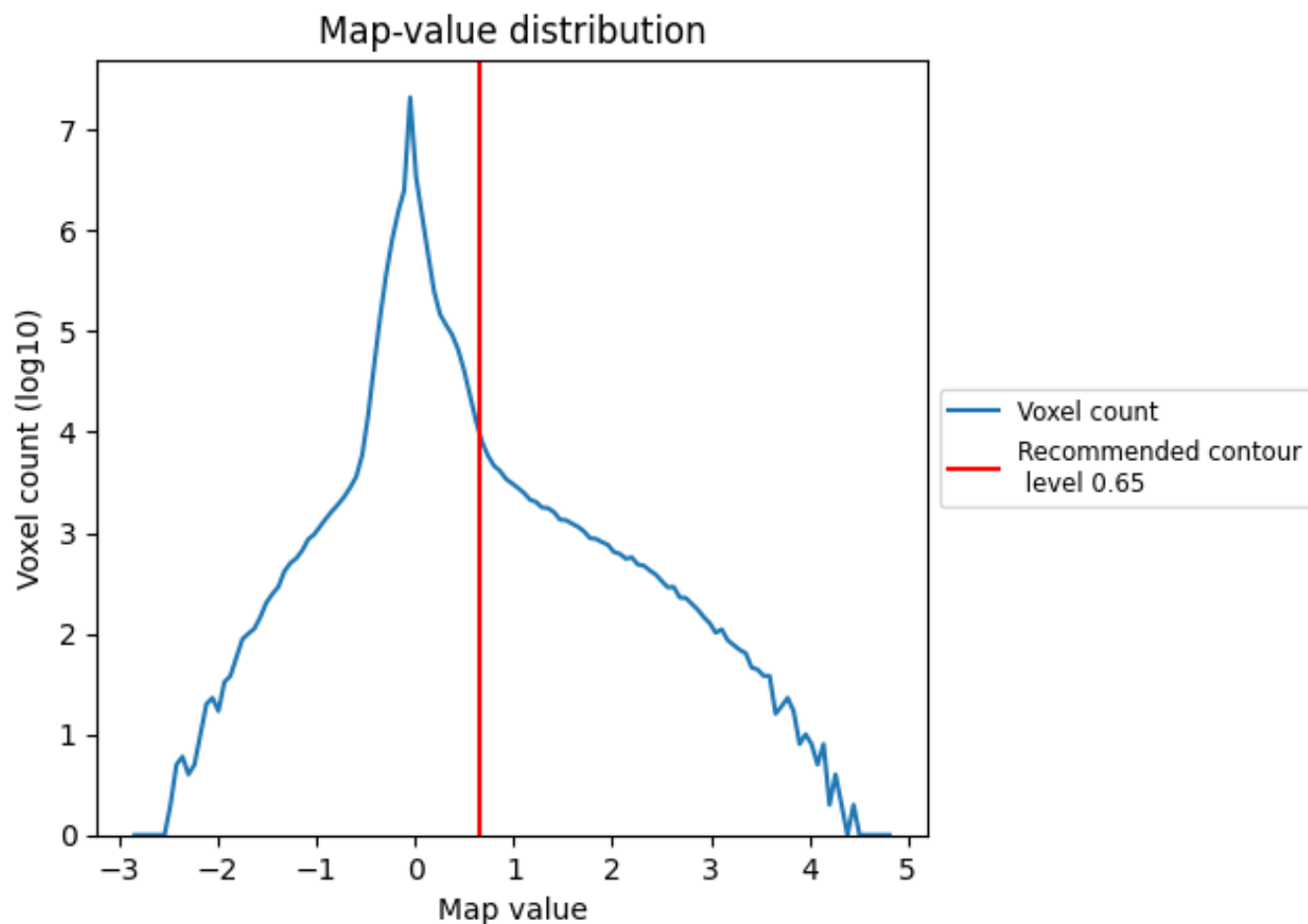
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

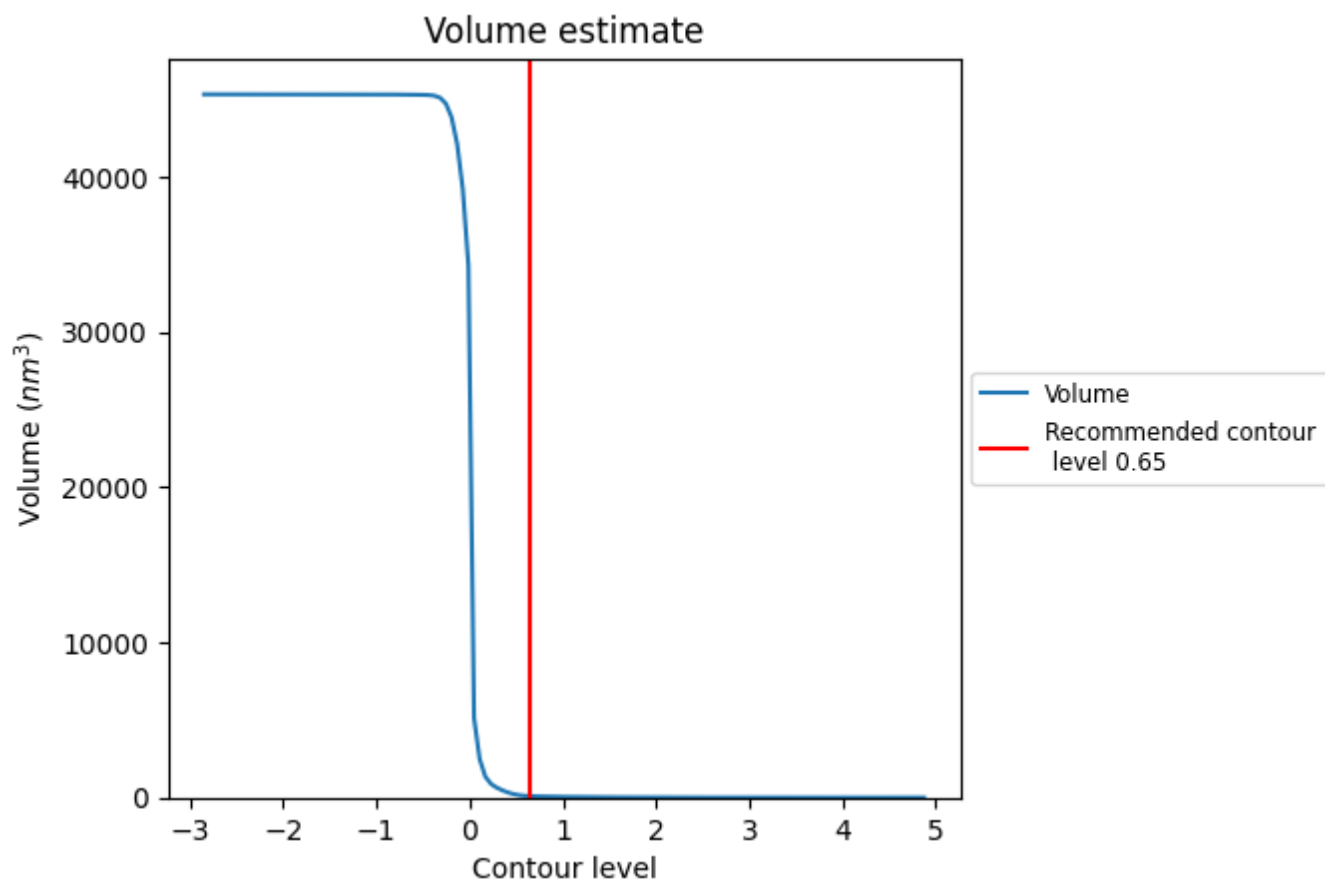
This section contains the results of statistical analysis of the map.

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.

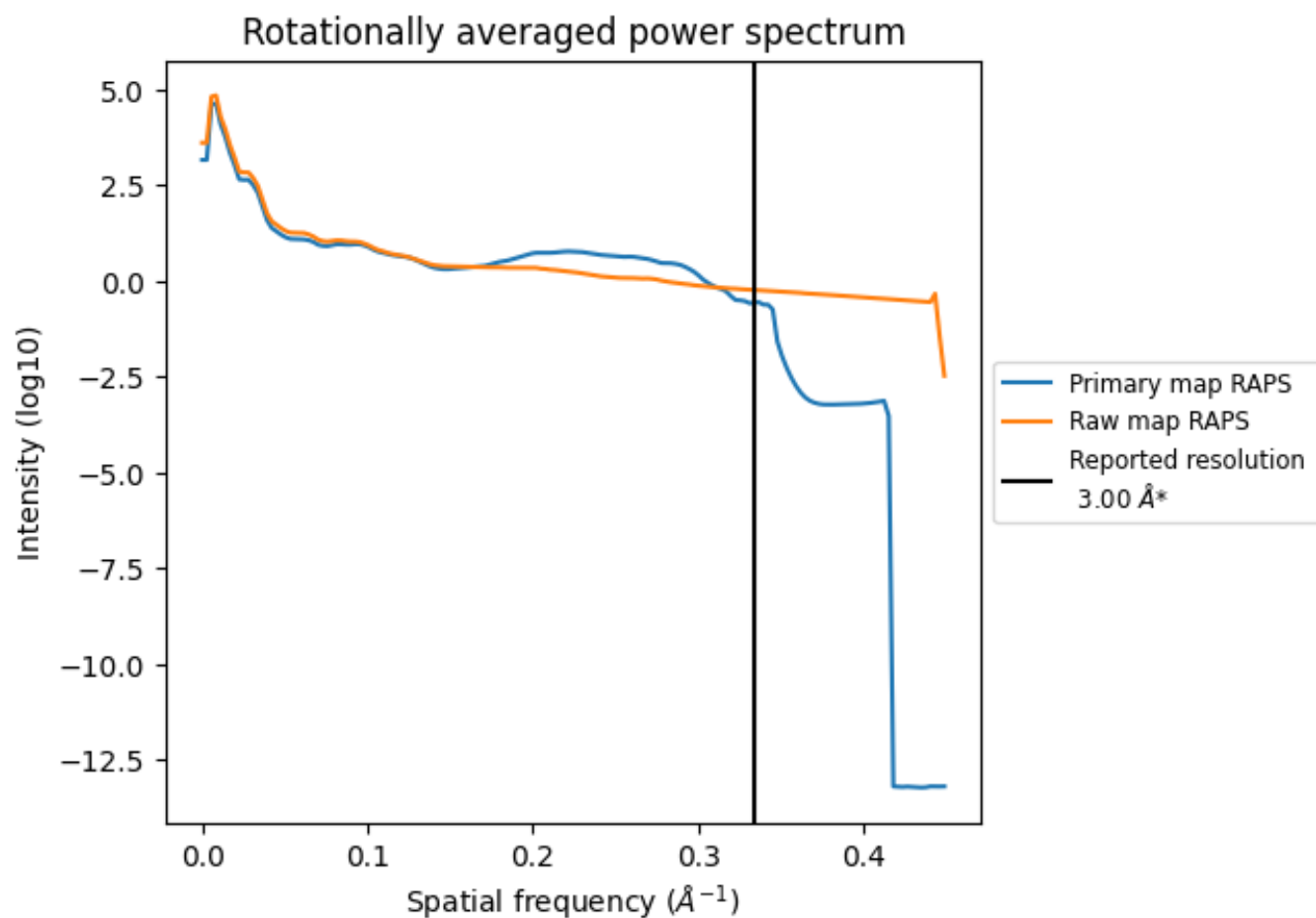
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

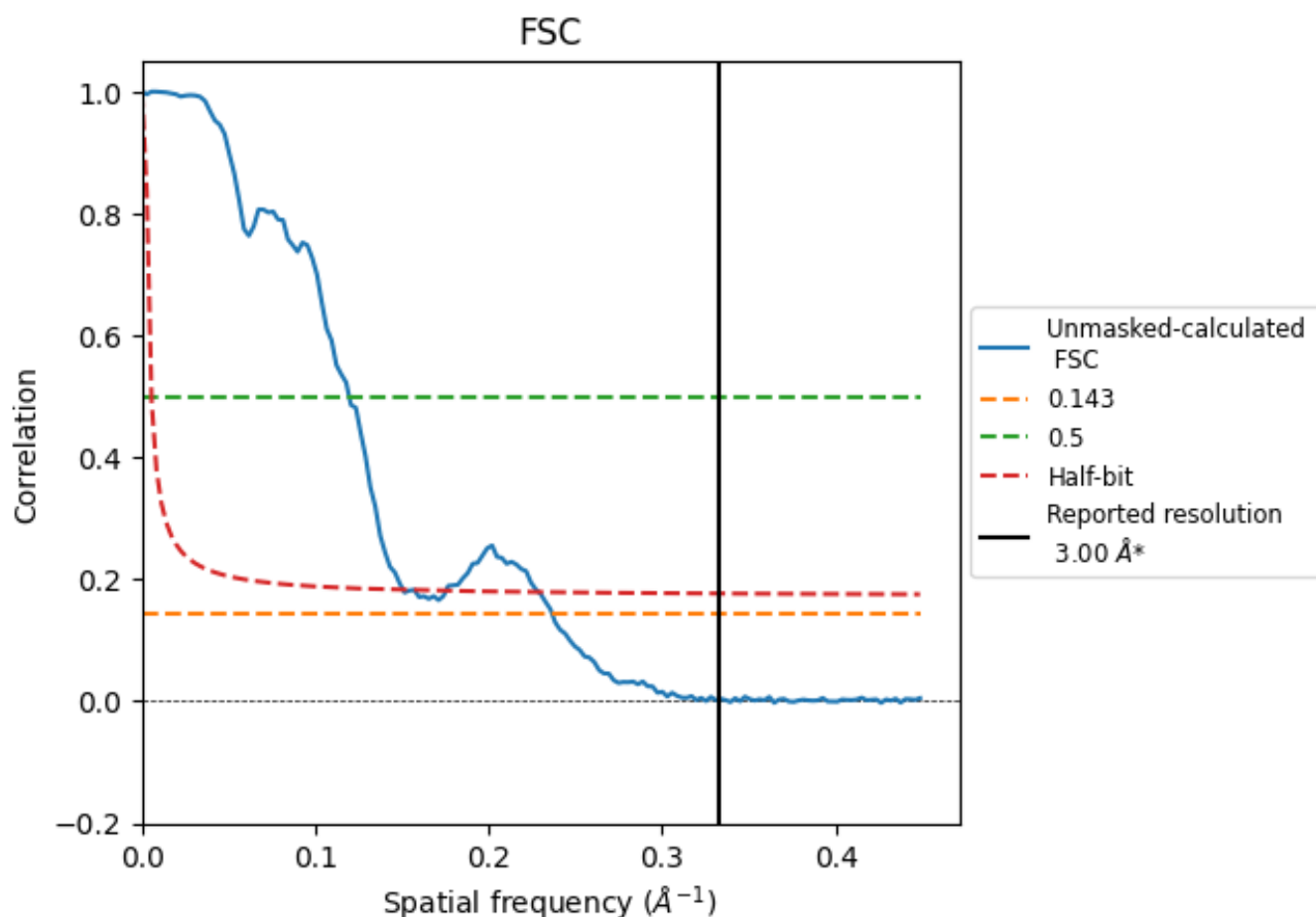


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

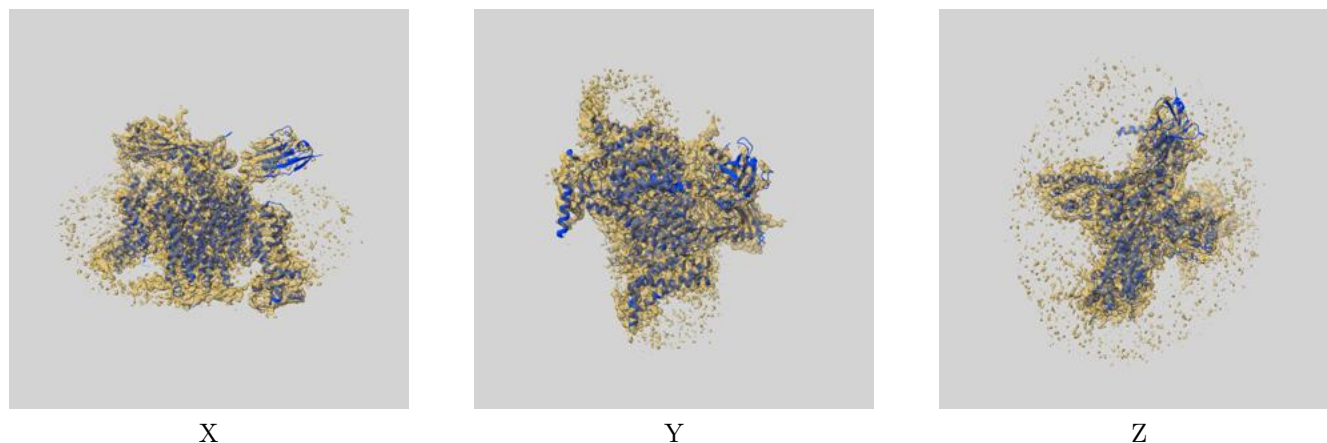
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	8.37	6.64

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

9 Map-model fit [i](#)

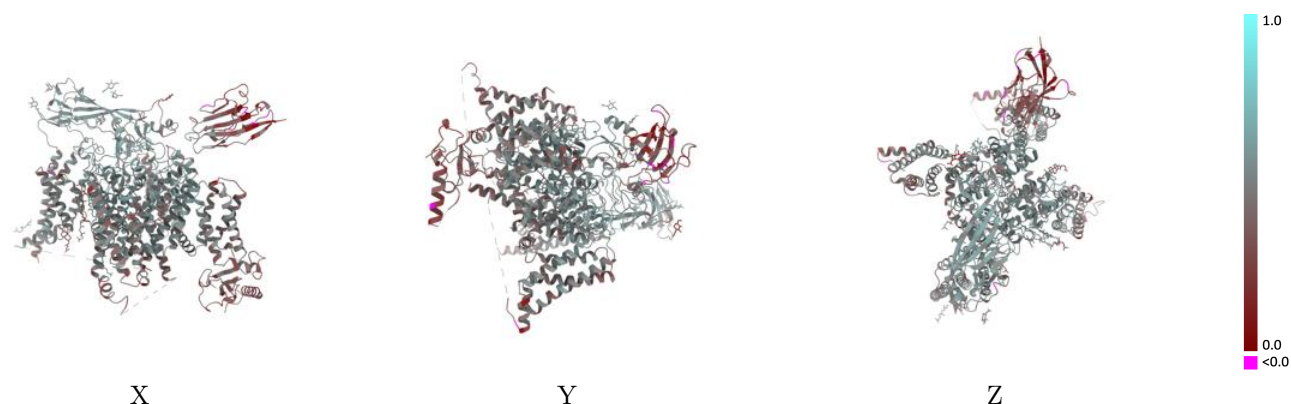
This section contains information regarding the fit between EMDB map EMD-67990 and PDB model 21TP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



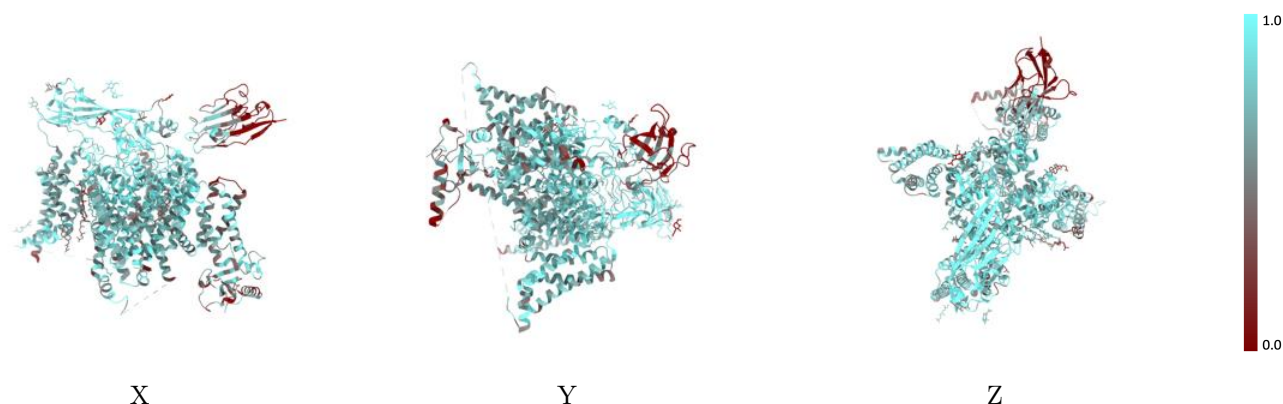
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



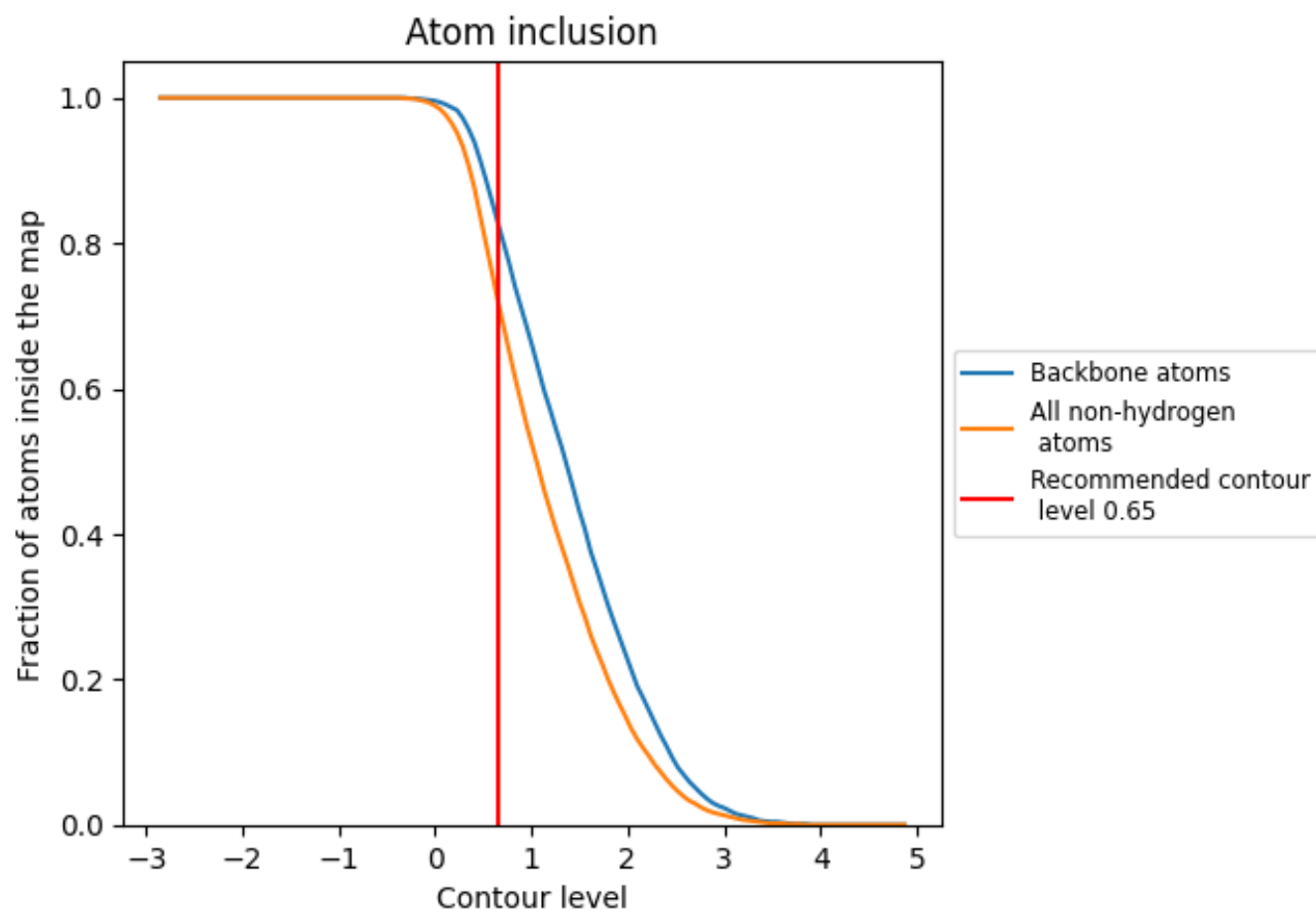
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 72% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7220	<div></div> 0.4670
A	<div></div> 0.7490	<div></div> 0.4750
B	<div></div> 0.8030	<div></div> 0.5160
C	<div></div> 0.3260	<div></div> 0.3020
D	<div></div> 0.6430	<div></div> 0.4600
E	<div></div> 0.8570	<div></div> 0.5430

