



# Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 09:22 PM EST

PDB ID : 7XVF  
EMDB ID : EMD-33485  
Title : Nav1.7 mutant class2  
Authors : Huang, G.; Wu, Q.; Li, Z.; Pan, X.; Yan, N.  
Deposited on : 2022-05-22  
Resolution : 2.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

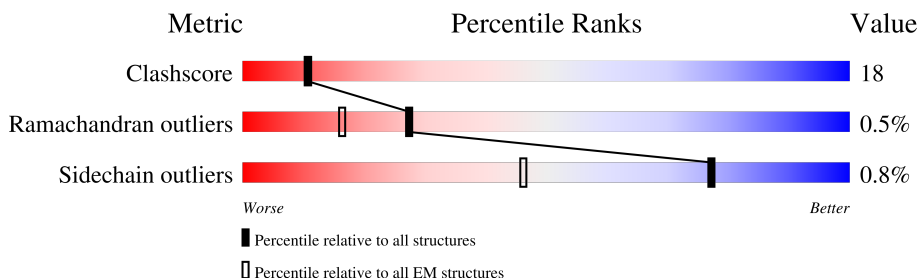
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2022	
2	B	218	
3	C	215	
4	D	2	
4	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	Y01	A	2021	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13625 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	1261	Total	C	N	O	S	0	0
			10100	6703	1587	1731	79		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	156	LYS	GLU	engineered mutation	UNP Q15858
A	779	ARG	GLY	engineered mutation	UNP Q15858
A	866	PHE	LEU	engineered mutation	UNP Q15858
A	870	MET	THR	engineered mutation	UNP Q15858
A	874	PHE	ALA	engineered mutation	UNP Q15858
A	947	PHE	VAL	engineered mutation	UNP Q15858
A	952	PHE	MET	engineered mutation	UNP Q15858
A	953	PHE	VAL	engineered mutation	UNP Q15858
A	1438	ILE	VAL	engineered mutation	UNP Q15858
A	1439	PHE	VAL	engineered mutation	UNP Q15858
A	1454	CYS	GLY	engineered mutation	UNP Q15858

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

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

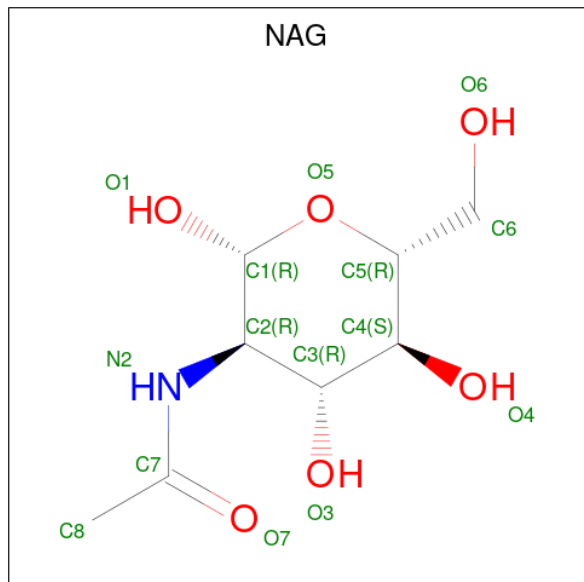
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	120	Total	C	N	O	S	0	0
			980	614	173	182	11		

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



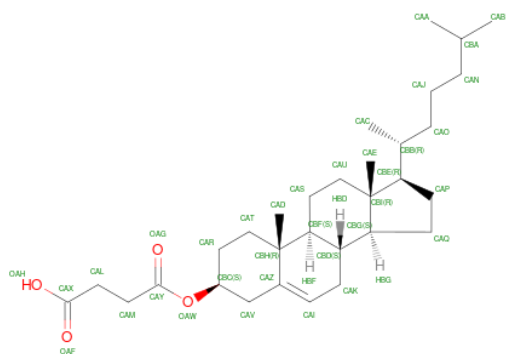
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



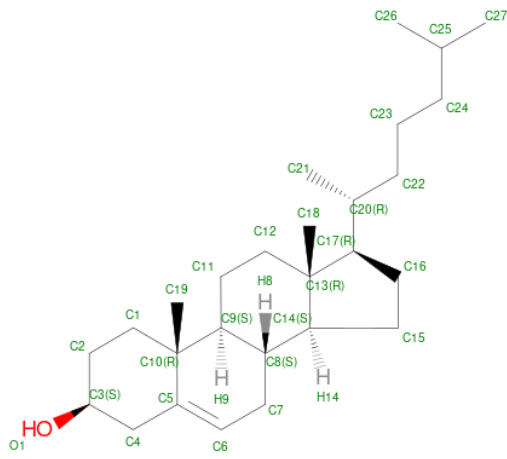
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

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



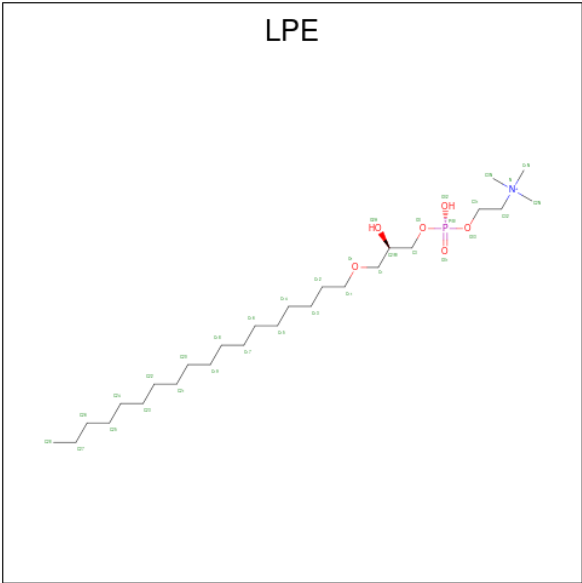
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



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

- Molecule 8 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C<sub>26</sub>H<sub>57</sub>NO<sub>6</sub>P).



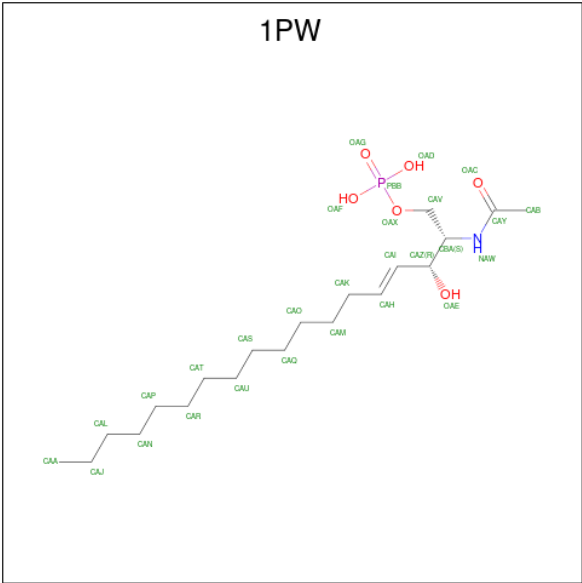
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
8	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
8	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	

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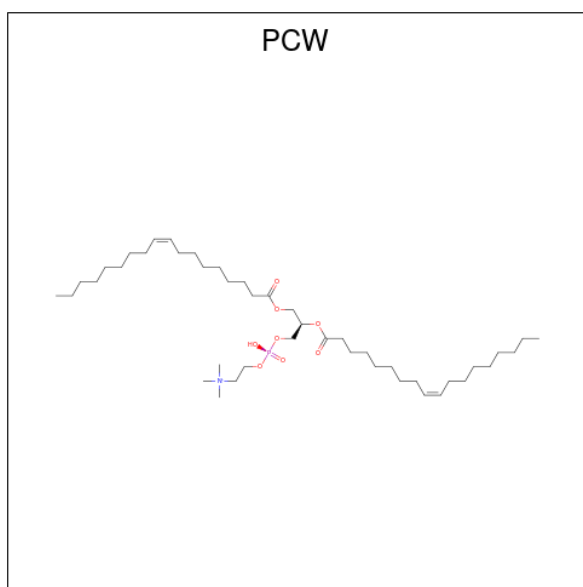
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
8	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
8	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 9 is (2S,3R,4E)-2-(acetylamino)-3-hydroxyoctadec-4-en-1-yl dihydrogen phosphate (three-letter code: 1PW) (formula: C<sub>20</sub>H<sub>40</sub>NO<sub>6</sub>P).



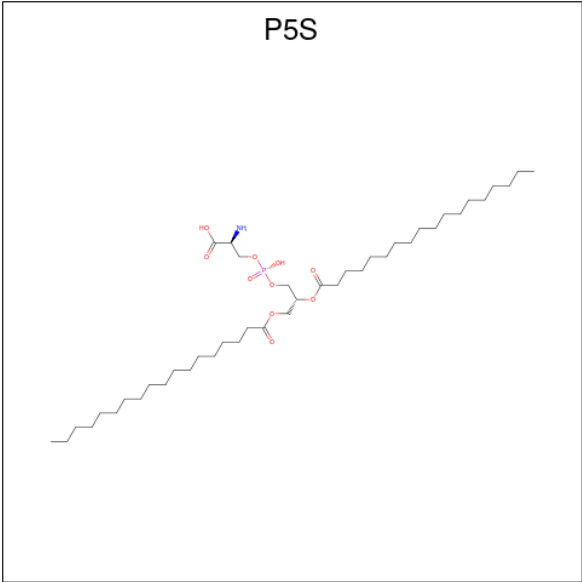
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			24	18	5	1	

- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
10	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
10	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
10	A	1	Total	C	N	O	P	1
			88	68	2	16	2	
10	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
10	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 11 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>10</sub>P).

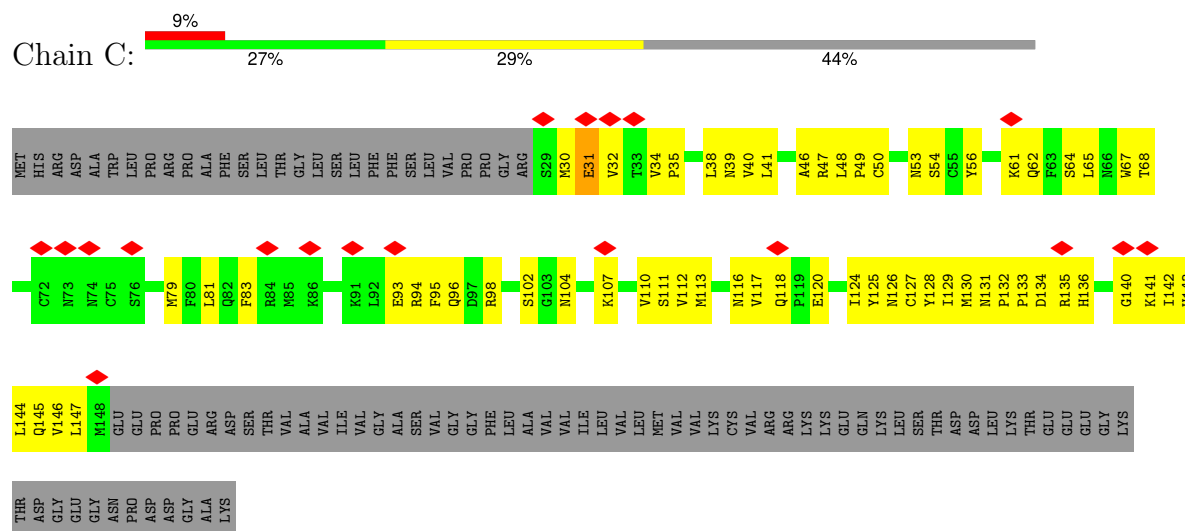


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			34	22	1	10	1	

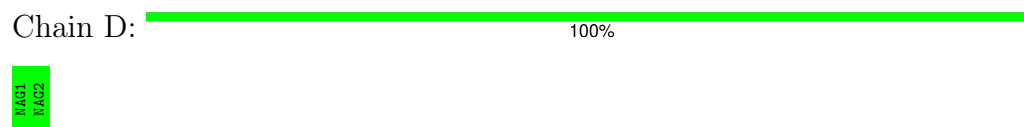




- Molecule 3: Sodium channel subunit beta-2



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	394163	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	5.058	Depositor
Minimum map value	-2.630	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.52	Depositor
Map size (Å)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPE, 1PW, Y01, PCW, CLR, NAG, P5S

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	0.64	0/10350	0.64	0/14021
2	B	0.62	0/1442	0.56	0/1949
3	C	0.34	0/1002	0.66	0/1354
All	All	0.62	0/12794	0.63	0/17324

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10100	0	10231	353	0
2	B	1416	0	1380	33	0
3	C	980	0	941	70	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	28	0	26	0	0
5	B	56	0	52	3	0
5	C	14	0	13	0	0
6	A	175	0	245	69	0
7	A	28	0	46	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	377	0	511	39	0
8	B	17	0	19	1	0
9	A	24	0	33	4	0
10	A	320	0	443	20	0
11	A	34	0	34	0	0
All	All	13625	0	14024	505	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 18.

All (505) 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:191:LEU:HD22	1:A:223:LYS:CE	1.65	1.26
1:A:1433:MET:CE	6:A:2021:Y01:HAR1	1.63	1.26
1:A:1732:ASN:ND2	8:A:2006:LPE:H321	1.53	1.24
1:A:89:ILE:HD11	1:A:99:ARG:NH1	1.60	1.17
6:A:2021:Y01:HAM2	6:A:2021:Y01:HAT2	1.30	1.13
6:A:2021:Y01:HAA1	6:A:2021:Y01:HAO2	1.32	1.10
1:A:749:ALA:HA	1:A:752:ILE:HD12	1.14	1.07
1:A:1433:MET:CE	6:A:2021:Y01:CAR	2.33	1.07
1:A:204:PHE:HD2	1:A:205:VAL:HG23	1.22	1.04
1:A:191:LEU:HD22	1:A:223:LYS:HE3	1.09	1.04
1:A:1433:MET:SD	6:A:2021:Y01:HAR1	1.98	1.02
3:C:62:GLN:HB3	3:C:132:PRO:HB2	1.37	1.02
1:A:1732:ASN:HB3	1:A:1735:VAL:CG1	1.91	1.01
1:A:1433:MET:HE1	6:A:2021:Y01:HAR1	1.37	1.01
1:A:1732:ASN:HB3	1:A:1735:VAL:HG12	1.43	1.00
3:C:64:SER:OG	3:C:130:MET:HB3	1.62	0.98
1:A:204:PHE:CD2	1:A:205:VAL:HG23	1.98	0.98
1:A:100:PHE:HA	1:A:181:PHE:CD2	2.02	0.95
1:A:1703:LEU:O	1:A:1706:PRO:HD2	1.67	0.94
1:A:100:PHE:CD1	1:A:181:PHE:HE2	1.85	0.94
1:A:168:LEU:HD12	1:A:169:VAL:N	1.85	0.92
1:A:1439:PHE:CD2	6:A:2021:Y01:HAJ1	2.05	0.92
6:A:2024:Y01:HAV1	6:A:2024:Y01:HAM2	1.52	0.91
1:A:119:SER:HB2	1:A:172:LEU:HD23	1.50	0.91
1:A:1732:ASN:HD21	8:A:2006:LPE:H321	1.34	0.90
1:A:161:GLY:O	1:A:164:THR:HG22	1.70	0.90
1:A:132:ILE:HG21	1:A:166:GLU:OE2	1.72	0.89
1:A:1732:ASN:HD22	8:A:2006:LPE:H321	1.32	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2022:Y01:HAC2	6:A:2022:Y01:HAE2	1.55	0.88
1:A:810:ILE:HD12	1:A:811:PHE:H	1.37	0.88
2:B:182:TYR:O	2:B:185:ILE:HG22	1.75	0.87
1:A:1183:LYS:HE3	2:B:185:ILE:HD11	1.56	0.87
1:A:823:LEU:C	1:A:823:LEU:HD13	1.95	0.87
1:A:191:LEU:HD22	1:A:223:LYS:HE2	1.57	0.86
3:C:67:TRP:HB2	3:C:81:LEU:HB3	1.57	0.86
1:A:1328:CYS:SG	1:A:1448:THR:HG23	2.16	0.86
1:A:193:PHE:O	1:A:196:ILE:HG12	1.78	0.84
1:A:810:ILE:HD12	1:A:811:PHE:N	1.93	0.84
1:A:191:LEU:CD2	1:A:223:LYS:HE3	2.03	0.83
1:A:105:ALA:HA	1:A:178:VAL:HG21	1.58	0.83
1:A:12:PHE:CE1	1:A:91:LEU:CD1	2.62	0.83
1:A:12:PHE:HE1	1:A:91:LEU:HD11	1.43	0.83
1:A:1732:ASN:ND2	8:A:2006:LPE:C32	2.40	0.82
1:A:165:PHE:O	1:A:168:LEU:HG	1.79	0.82
1:A:895:CYS:HB2	1:A:938:VAL:HG23	1.60	0.82
6:A:2021:Y01:HAM2	6:A:2021:Y01:CAT	2.09	0.81
1:A:1191:HIS:HD2	8:A:2032:LPE:H2N3	1.45	0.80
1:A:192:ASP:O	1:A:196:ILE:HG23	1.80	0.80
1:A:1433:MET:HE2	6:A:2021:Y01:CAR	2.12	0.80
1:A:100:PHE:CD1	1:A:181:PHE:CE2	2.69	0.79
1:A:1433:MET:HE1	6:A:2021:Y01:HBC	1.65	0.79
6:A:2021:Y01:HAT2	6:A:2021:Y01:CAM	2.10	0.79
1:A:100:PHE:HD1	1:A:181:PHE:HE2	1.27	0.79
1:A:1433:MET:CE	6:A:2021:Y01:HBC	2.13	0.79
1:A:12:PHE:CE1	1:A:91:LEU:HD11	2.18	0.78
1:A:1433:MET:HE1	6:A:2021:Y01:CAR	2.08	0.78
1:A:1322:MET:O	1:A:1326:LEU:HD13	1.81	0.78
3:C:68:THR:HG22	3:C:79:MET:HG2	1.66	0.78
1:A:190:TRP:O	1:A:194:VAL:HG23	1.85	0.77
10:A:2013:PCW:H171	10:A:2014[B]:PCW:H352	1.67	0.76
1:A:193:PHE:O	1:A:197:VAL:HG13	1.84	0.76
6:A:2024:Y01:HAR2	6:A:2024:Y01:CAM	2.16	0.76
10:A:2013:PCW:H171	10:A:2014[A]:PCW:H352	1.67	0.76
1:A:922:ARG:HG3	1:A:1408:TRP:HH2	1.48	0.75
1:A:1260:TRP:CG	6:A:2023:Y01:CAE	2.69	0.75
3:C:38:LEU:HD23	3:C:39:ASN:N	2.01	0.75
2:B:93:ASN:OD1	2:B:107:PHE:HB2	1.86	0.75
1:A:197:VAL:O	1:A:201:LEU:HG	1.87	0.74
3:C:125:TYR:HB2	3:C:142:ILE:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HB3	1:A:223:LYS:HE2	1.68	0.74
1:A:196:ILE:O	1:A:200:TYR:HD2	1.70	0.74
3:C:130:MET:HG3	3:C:132:PRO:HD3	1.69	0.74
6:A:2023:Y01:CAP	6:A:2023:Y01:HAJ2	2.16	0.74
6:A:2024:Y01:HAR2	6:A:2024:Y01:HAM1	1.69	0.74
3:C:126:ASN:HB3	3:C:128:TYR:HE1	1.52	0.74
1:A:119:SER:HB2	1:A:172:LEU:CD2	2.17	0.74
1:A:362:TYR:CE2	1:A:365:ASN:ND2	2.56	0.74
6:A:2003:Y01:HAV2	10:A:2009:PCW:H31	1.69	0.74
10:A:2013:PCW:C17	10:A:2014[A]:PCW:H352	2.18	0.74
1:A:104:PRO:HB2	1:A:107:TYR:HA	1.69	0.73
1:A:1433:MET:SD	6:A:2021:Y01:CAR	2.76	0.73
1:A:823:LEU:HD13	1:A:823:LEU:O	1.88	0.73
1:A:1732:ASN:HB3	1:A:1735:VAL:HG11	1.70	0.73
1:A:194:VAL:O	1:A:197:VAL:HG22	1.89	0.73
1:A:1191:HIS:CD2	8:A:2032:LPE:H322	2.24	0.72
1:A:108:MET:C	1:A:109:LEU:HD12	2.09	0.72
1:A:1327:VAL:O	1:A:1331:PHE:HD2	1.73	0.72
6:A:2023:Y01:HAJ2	6:A:2023:Y01:HAP2	1.71	0.72
1:A:1732:ASN:CB	1:A:1735:VAL:HG12	2.18	0.72
1:A:1732:ASN:HD21	8:A:2006:LPE:C32	2.02	0.71
1:A:798:MET:HE1	1:A:803:TYR:HA	1.72	0.71
3:C:64:SER:OG	3:C:130:MET:CB	2.39	0.71
1:A:1685:GLY:N	8:A:2018:LPE:O2H	2.23	0.70
10:A:2013:PCW:C17	10:A:2014[B]:PCW:H352	2.21	0.70
1:A:749:ALA:CA	1:A:752:ILE:HD12	2.07	0.70
6:A:2021:Y01:HAO2	6:A:2021:Y01:CAA	2.16	0.70
3:C:41:LEU:HA	3:C:147:LEU:HB2	1.71	0.70
1:A:91:LEU:HD23	1:A:97:ILE:HA	1.74	0.70
3:C:95:PHE:HA	3:C:98:ARG:HH22	1.57	0.70
1:A:47:PRO:HB2	1:A:81:TYR:CE2	2.27	0.70
1:A:196:ILE:O	1:A:200:TYR:CD2	2.45	0.70
1:A:1207:GLY:O	1:A:1211:PHE:CD2	2.45	0.69
3:C:118:GLN:OE1	3:C:120:GLU:HG3	1.93	0.69
3:C:49:PRO:HA	3:C:111:SER:OG	1.92	0.69
3:C:56:TYR:CD1	3:C:134:ASP:HB2	2.28	0.69
1:A:12:PHE:CE1	1:A:91:LEU:HD12	2.28	0.68
1:A:1575:THR:O	10:A:2014[B]:PCW:H63	1.94	0.68
1:A:1433:MET:CE	6:A:2021:Y01:CBC	2.71	0.68
1:A:199:ALA:O	1:A:202:THR:HG22	1.94	0.68
3:C:54:SER:CB	3:C:131:ASN:HD22	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:ASP:HA	1:A:1287:LYS:HE3	1.74	0.68
1:A:67:PRO:HB2	1:A:70:MET:HG3	1.75	0.67
3:C:50:CYS:HB3	3:C:110:VAL:HG23	1.76	0.67
1:A:1191:HIS:CD2	8:A:2032:LPE:H2N3	2.29	0.67
1:A:1685:GLY:HA3	8:A:2018:LPE:O2H	1.94	0.67
3:C:47:ARG:NH2	3:C:102:SER:O	2.28	0.67
1:A:89:ILE:HD11	1:A:99:ARG:HH11	1.59	0.67
1:A:823:LEU:C	1:A:823:LEU:CD1	2.64	0.66
1:A:105:ALA:HB3	1:A:116:ARG:HH22	1.60	0.66
3:C:104:ASN:HD22	3:C:107:LYS:HE3	1.61	0.66
1:A:1188:ILE:HG12	8:A:2032:LPE:H3N3	1.78	0.66
1:A:798:MET:CE	1:A:803:TYR:HA	2.26	0.66
1:A:1260:TRP:CD1	6:A:2023:Y01:CAE	2.79	0.65
2:B:93:ASN:HD22	5:B:301:NAG:C7	2.09	0.65
3:C:131:ASN:O	3:C:134:ASP:HB3	1.96	0.65
1:A:168:LEU:HD12	1:A:168:LEU:C	2.15	0.65
1:A:762:ALA:CB	6:A:2003:Y01:HAU1	2.26	0.65
1:A:802:GLU:HA	1:A:805:GLN:CD	2.17	0.65
1:A:1183:LYS:HE3	2:B:185:ILE:CD1	2.24	0.65
1:A:1207:GLY:O	1:A:1211:PHE:HD2	1.78	0.65
6:A:2021:Y01:HAA1	6:A:2021:Y01:CAO	2.17	0.65
1:A:30:ARG:NH2	1:A:84:ASP:OD2	2.29	0.65
1:A:1429:TYR:OH	6:A:2022:Y01:HAK2	1.97	0.65
1:A:813:SER:O	1:A:817:THR:HG23	1.97	0.64
3:C:135:ARG:C	3:C:135:ARG:HD2	2.17	0.64
1:A:248:VAL:HG21	1:A:400:VAL:HG21	1.80	0.64
6:A:2022:Y01:HAC2	6:A:2022:Y01:CAE	2.27	0.64
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.78	0.64
1:A:1432:TYR:HB2	6:A:2021:Y01:OAH	1.97	0.63
3:C:49:PRO:HA	3:C:111:SER:CB	2.28	0.63
1:A:1429:TYR:CZ	6:A:2022:Y01:HAK2	2.33	0.63
1:A:191:LEU:CD2	1:A:223:LYS:CE	2.60	0.63
1:A:758:THR:HG21	1:A:839:LEU:HD22	1.78	0.63
1:A:1296:ARG:N	1:A:1297:PRO:CD	2.60	0.63
1:A:132:ILE:HG21	1:A:166:GLU:CD	2.19	0.62
1:A:136:ILE:HD12	1:A:220:ARG:HD3	1.81	0.62
1:A:1245:TRP:HH2	6:A:2024:Y01:HAB2	1.64	0.62
1:A:1720:VAL:HG23	1:A:1722:PRO:HD3	1.81	0.62
1:A:110:SER:HB2	1:A:111:PRO:HD2	1.82	0.62
1:A:874:PHE:CB	7:A:2004:CLR:H261	2.29	0.62
1:A:1183:LYS:CE	2:B:185:ILE:HD11	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1683:THR:HB	8:A:2018:LPE:H32	1.82	0.62
1:A:1733:PRO:HD2	8:A:2006:LPE:C32	2.29	0.62
1:A:1453:ILE:HA	1:A:1753:ASN:HD21	1.64	0.62
1:A:129:SER:HA	1:A:132:ILE:HG12	1.82	0.62
1:A:60:PRO:HB2	1:A:62:ILE:HG12	1.81	0.62
1:A:128:PHE:CE2	1:A:166:GLU:HG3	2.35	0.62
1:A:1260:TRP:CD2	6:A:2023:Y01:HAE3	2.35	0.62
3:C:65:LEU:H	3:C:83:PHE:HB3	1.65	0.61
1:A:1327:VAL:O	1:A:1331:PHE:CD2	2.53	0.61
1:A:936:MET:HG2	1:A:941:GLN:HA	1.81	0.61
1:A:1250:TYR:HE2	8:A:2027:LPE:H172	1.65	0.61
1:A:762:ALA:HB1	6:A:2003:Y01:HAU1	1.83	0.61
1:A:1260:TRP:CG	6:A:2023:Y01:HAE3	2.34	0.61
1:A:1685:GLY:CA	8:A:2018:LPE:O2H	2.48	0.61
3:C:93:GLU:O	3:C:96:GLN:NE2	2.34	0.61
1:A:89:ILE:CD1	1:A:99:ARG:NH1	2.51	0.61
1:A:110:SER:O	1:A:116:ARG:HD2	2.00	0.61
1:A:1250:TYR:CE2	8:A:2027:LPE:H172	2.36	0.61
1:A:1433:MET:HE1	6:A:2021:Y01:CBC	2.29	0.61
1:A:759:LEU:HD11	8:A:2005:LPE:H162	1.82	0.60
1:A:1439:PHE:HD2	6:A:2021:Y01:HAC3	1.66	0.60
3:C:124:ILE:HD12	3:C:141:LYS:HE2	1.82	0.60
1:A:922:ARG:HG3	1:A:1408:TRP:CH2	2.35	0.60
1:A:1296:ARG:N	1:A:1297:PRO:HD2	2.16	0.60
1:A:1322:MET:CE	9:A:2007:1PW:H12	2.32	0.60
1:A:802:GLU:HA	1:A:805:GLN:NE2	2.16	0.59
1:A:1433:MET:HE2	6:A:2021:Y01:CBC	2.31	0.59
1:A:1435:ILE:HG22	6:A:2021:Y01:CAC	2.32	0.59
1:A:348:SER:HB2	10:A:2012:PCW:H342	1.85	0.59
3:C:64:SER:HG	3:C:130:MET:HB3	1.68	0.59
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.37	0.59
2:B:38:ILE:O	2:B:105:SER:HB3	2.02	0.59
1:A:1750:VAL:HG23	1:A:1751:VAL:H	1.67	0.59
1:A:798:MET:HE2	1:A:803:TYR:N	2.18	0.58
3:C:127:CYS:O	3:C:140:GLY:N	2.30	0.58
1:A:1634:LEU:HB3	10:A:2013:PCW:H351	1.86	0.58
1:A:1322:MET:HE1	9:A:2007:1PW:H12	1.84	0.58
1:A:47:PRO:HB2	1:A:81:TYR:CD2	2.39	0.58
1:A:1702:GLY:O	1:A:1706:PRO:HD3	2.03	0.58
1:A:1325:LEU:O	1:A:1329:LEU:HG	2.03	0.58
1:A:1435:ILE:HG22	6:A:2021:Y01:HAC3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:ASN:O	1:A:1503:LYS:C	2.43	0.57
1:A:231:LEU:HD21	1:A:871:LEU:HD23	1.85	0.57
1:A:1746:ILE:O	1:A:1750:VAL:HG22	2.05	0.57
1:A:1250:TYR:HD2	8:A:2027:LPE:H131	1.69	0.57
1:A:362:TYR:CZ	1:A:365:ASN:CG	2.78	0.57
3:C:145:GLN:NE2	3:C:146:VAL:O	2.37	0.57
1:A:89:ILE:HG12	1:A:99:ARG:HG3	1.86	0.56
1:A:1708:LEU:O	1:A:1733:PRO:HG3	2.05	0.56
3:C:62:GLN:HB3	3:C:132:PRO:CB	2.23	0.56
1:A:1694:ILE:HD12	1:A:1700:TRP:HA	1.86	0.56
1:A:1733:PRO:HD2	8:A:2006:LPE:H321	1.87	0.56
1:A:100:PHE:HA	1:A:181:PHE:CE2	2.40	0.56
1:A:106:LEU:HD12	1:A:106:LEU:N	2.21	0.56
1:A:1180:ASN:HA	1:A:1183:LYS:HE2	1.87	0.56
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.87	0.56
1:A:161:GLY:O	1:A:164:THR:CG2	2.49	0.56
1:A:320:ASP:HB3	8:A:2017:LPE:H321	1.87	0.56
3:C:95:PHE:HA	3:C:98:ARG:NH2	2.20	0.56
1:A:1433:MET:HG2	6:A:2021:Y01:HAR2	1.87	0.55
1:A:211:SER:HB3	1:A:887:LEU:HD23	1.87	0.55
10:A:2014[B]:PCW:H31	10:A:2029:PCW:H42	1.89	0.55
1:A:1694:ILE:HD11	1:A:1703:LEU:HD12	1.89	0.55
1:A:215:THR:O	1:A:218:VAL:HG12	2.07	0.55
1:A:348:SER:HB2	10:A:2012:PCW:C34	2.37	0.55
1:A:1191:HIS:CG	8:A:2032:LPE:H322	2.42	0.55
1:A:1260:TRP:CD1	6:A:2023:Y01:HAE3	2.42	0.55
1:A:1439:PHE:CD2	6:A:2021:Y01:HAC3	2.42	0.55
1:A:798:MET:CE	1:A:802:GLU:C	2.75	0.55
1:A:12:PHE:HE1	1:A:91:LEU:CD1	2.05	0.55
1:A:116:ARG:O	1:A:120:ILE:HG12	2.07	0.55
1:A:1575:THR:HG22	10:A:2014[B]:PCW:H61	1.89	0.55
6:A:2023:Y01:CAP	6:A:2023:Y01:CAJ	2.85	0.55
1:A:749:ALA:HA	1:A:752:ILE:CD1	2.09	0.54
2:B:56:GLU:OE2	2:B:72:ARG:HD2	2.07	0.54
1:A:1250:TYR:HD2	8:A:2027:LPE:C13	2.19	0.54
1:A:1406:LYS:HG3	1:A:1697:SER:O	2.07	0.54
3:C:40:VAL:HG12	3:C:117:VAL:HG21	1.88	0.54
1:A:9:PRO:HA	1:A:63:TYR:HA	1.89	0.54
3:C:50:CYS:O	3:C:110:VAL:HG22	2.08	0.54
1:A:132:ILE:CG2	1:A:166:GLU:CD	2.76	0.54
3:C:94:ARG:NH2	3:C:120:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ALA:HA	1:A:1392:VAL:HG21	1.89	0.54
1:A:874:PHE:HB2	7:A:2004:CLR:H261	1.89	0.53
1:A:1183:LYS:HE3	2:B:185:ILE:CG1	2.39	0.53
3:C:125:TYR:HB2	3:C:142:ILE:CG2	2.38	0.53
5:B:304:NAG:O7	5:B:304:NAG:O3	2.19	0.53
3:C:38:LEU:HD22	3:C:40:VAL:HG23	1.89	0.53
1:A:120:ILE:O	1:A:124:VAL:HG22	2.08	0.53
1:A:213:LEU:HD12	1:A:213:LEU:N	2.24	0.53
1:A:284:GLU:HB3	1:A:289:ILE:HD11	1.89	0.53
3:C:132:PRO:HA	3:C:133:PRO:C	2.27	0.53
1:A:362:TYR:CE2	1:A:365:ASN:CB	2.91	0.53
1:A:183:PHE:CZ	1:A:193:PHE:HB2	2.44	0.53
1:A:1245:TRP:O	8:A:2027:LPE:H162	2.09	0.53
1:A:132:ILE:HG22	1:A:166:GLU:OE1	2.09	0.53
3:C:35:PRO:O	3:C:142:ILE:HG13	2.08	0.53
1:A:897:CYS:HB2	3:C:56:TYR:CE2	2.43	0.53
1:A:1276:ASN:ND2	1:A:1290:ARG:HH21	2.07	0.53
1:A:1745:ILE:HD12	8:A:2006:LPE:H212	1.91	0.53
1:A:1260:TRP:CD1	6:A:2023:Y01:HAE1	2.44	0.53
1:A:1666:PHE:HE2	1:A:1739:TYR:CD2	2.27	0.53
1:A:91:LEU:CD2	1:A:97:ILE:HA	2.38	0.52
1:A:166:GLU:HG2	1:A:170:LYS:HE2	1.92	0.52
1:A:1683:THR:CB	8:A:2018:LPE:H32	2.39	0.52
3:C:127:CYS:SG	3:C:140:GLY:HA3	2.50	0.52
1:A:54:GLU:HB3	1:A:57:LYS:HD3	1.89	0.52
1:A:183:PHE:HZ	1:A:193:PHE:HB2	1.74	0.52
1:A:953:PHE:HD1	1:A:957:LEU:HD22	1.74	0.52
6:A:2021:Y01:CAR	6:A:2021:Y01:CAM	2.88	0.52
1:A:183:PHE:CE1	1:A:189:ASN:HB3	2.44	0.52
1:A:89:ILE:HD11	1:A:99:ARG:HH12	1.67	0.52
1:A:1717:PRO:O	1:A:1728:GLY:HA3	2.09	0.52
2:B:58:THR:OG1	2:B:120:GLU:HB2	2.08	0.52
3:C:31:GLU:HG3	3:C:53:ASN:HB3	1.91	0.52
3:C:40:VAL:HG11	3:C:46:ALA:HB2	1.91	0.52
10:A:2014[A]:PCW:H31	10:A:2029:PCW:H42	1.92	0.51
3:C:38:LEU:HD23	3:C:39:ASN:H	1.70	0.51
1:A:816:VAL:O	1:A:820:LEU:HD23	2.11	0.51
2:B:51:ALA:HB2	2:B:127:LEU:HD23	1.92	0.51
1:A:1733:PRO:HD2	8:A:2006:LPE:H322	1.92	0.51
1:A:874:PHE:CG	7:A:2004:CLR:H261	2.46	0.51
1:A:1260:TRP:CE2	6:A:2023:Y01:HAE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:PRO:HA	3:C:111:SER:HB3	1.92	0.51
3:C:61:LYS:HG3	3:C:62:GLN:OE1	2.11	0.51
1:A:119:SER:CB	1:A:172:LEU:HD23	2.33	0.51
1:A:293:LEU:HD22	1:A:298:ASP:HB3	1.93	0.51
1:A:357:LEU:HD23	1:A:363:TRP:HB2	1.93	0.51
1:A:191:LEU:CD2	1:A:223:LYS:HE2	2.32	0.51
6:A:2024:Y01:HAM2	6:A:2024:Y01:HAR2	1.93	0.50
1:A:1690:CYS:O	1:A:1694:ILE:HG12	2.10	0.50
1:A:326:GLU:HG3	2:B:45:ARG:HG3	1.91	0.50
1:A:1276:ASN:HD21	1:A:1290:ARG:HH21	1.58	0.50
1:A:748:LEU:O	1:A:752:ILE:HG13	2.12	0.50
2:B:65:GLU:O	2:B:65:GLU:HG2	2.12	0.50
1:A:762:ALA:HB3	6:A:2003:Y01:HAU1	1.93	0.50
1:A:1314:LEU:HD11	1:A:1750:VAL:HG12	1.93	0.50
1:A:92:ASN:C	1:A:94:GLY:H	2.15	0.50
1:A:398:LEU:HD11	1:A:964:LEU:HD23	1.93	0.50
1:A:109:LEU:HD12	1:A:109:LEU:N	2.27	0.49
1:A:362:TYR:CE2	1:A:365:ASN:HB2	2.46	0.49
6:A:2022:Y01:HAE2	6:A:2022:Y01:CAC	2.36	0.49
2:B:71:LEU:HB3	2:B:80:LEU:HD23	1.93	0.49
1:A:362:TYR:CZ	1:A:365:ASN:HB2	2.47	0.49
6:A:2022:Y01:OAG	6:A:2022:Y01:HAR1	2.11	0.49
1:A:846:ALA:C	1:A:848:SER:H	2.16	0.49
1:A:106:LEU:N	1:A:106:LEU:CD1	2.76	0.49
1:A:331:VAL:HG13	1:A:333:ILE:HG22	1.93	0.49
2:B:103:ASP:C	2:B:104:LEU:HD12	2.33	0.49
3:C:124:ILE:HD13	3:C:143:HIS:ND1	2.28	0.49
1:A:136:ILE:CD1	1:A:163:TYR:HE1	2.25	0.49
1:A:815:ILE:HG21	1:A:838:ARG:HG2	1.95	0.49
1:A:240:GLN:OE1	1:A:243:LYS:NZ	2.37	0.49
1:A:362:TYR:CE2	1:A:365:ASN:CG	2.86	0.49
1:A:177:CYS:HA	1:A:182:THR:HG21	1.94	0.49
1:A:759:LEU:HD23	1:A:759:LEU:O	2.13	0.49
1:A:1325:LEU:HD22	9:A:2007:1PW:H17	1.94	0.49
1:A:868:ASN:O	1:A:872:VAL:HG23	2.12	0.49
1:A:132:ILE:O	1:A:136:ILE:HG12	2.13	0.48
1:A:1502:ASN:O	1:A:1504:ILE:N	2.46	0.48
1:A:144:THR:HG22	1:A:913:PHE:CD1	2.48	0.48
1:A:1392:VAL:HG12	1:A:1392:VAL:O	2.13	0.48
6:A:2022:Y01:CAE	6:A:2022:Y01:CAC	2.91	0.48
1:A:1433:MET:HE2	6:A:2021:Y01:HBC	1.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:TYR:HA	2:B:185:ILE:HG22	1.94	0.48
1:A:1188:ILE:HG12	8:A:2032:LPE:C3N	2.42	0.48
1:A:1348:TYR:CE2	1:A:1384:ASN:HB2	2.48	0.48
2:B:125:ARG:HB3	2:B:136:THR:HB	1.95	0.48
3:C:131:ASN:O	3:C:134:ASP:N	2.47	0.48
1:A:1408:TRP:CE3	1:A:1412:MET:SD	3.07	0.48
2:B:126:LEU:HD12	2:B:134:HIS:O	2.13	0.48
1:A:759:LEU:CD1	8:A:2005:LPE:H162	2.44	0.47
1:A:857:LYS:HE3	1:A:857:LYS:HB2	1.56	0.47
1:A:132:ILE:HG13	1:A:133:MET:HE2	1.96	0.47
3:C:62:GLN:CB	3:C:132:PRO:HB2	2.27	0.47
1:A:161:GLY:C	1:A:164:THR:HG22	2.32	0.47
1:A:202:THR:HB	1:A:213:LEU:HD23	1.96	0.47
1:A:136:ILE:CD1	1:A:163:TYR:CE1	2.97	0.47
1:A:1486:LYS:O	1:A:1487:LYS:C	2.52	0.47
1:A:798:MET:CE	1:A:803:TYR:N	2.78	0.47
10:A:2009:PCW:H431	10:A:2009:PCW:H461	1.47	0.47
6:A:2024:Y01:HAM2	6:A:2024:Y01:CAV	2.29	0.47
1:A:132:ILE:O	1:A:135:THR:OG1	2.24	0.47
1:A:194:VAL:O	1:A:198:PHE:HD2	1.98	0.47
1:A:1178:TRP:CZ3	1:A:1182:ARG:HD2	2.50	0.47
6:A:2021:Y01:HAC1	6:A:2021:Y01:HAU2	1.96	0.47
2:B:182:TYR:C	2:B:185:ILE:HG22	2.35	0.47
1:A:131:LEU:O	1:A:135:THR:HG23	2.15	0.47
1:A:832:SER:O	1:A:835:ARG:HG2	2.15	0.47
3:C:32:VAL:HG12	3:C:129:ILE:HD12	1.97	0.47
3:C:34:VAL:HG21	3:C:141:LYS:H	1.80	0.47
10:A:2009:PCW:H40	10:A:2009:PCW:H432	1.62	0.47
1:A:191:LEU:O	1:A:195:VAL:HG23	2.14	0.46
1:A:1731:GLY:O	1:A:1733:PRO:HD3	2.15	0.46
1:A:1732:ASN:O	1:A:1735:VAL:HG12	2.15	0.46
2:B:92:TRP:CZ2	2:B:94:GLY:HA3	2.50	0.46
1:A:1435:ILE:CG2	6:A:2021:Y01:HAC1	2.45	0.46
3:C:30:MET:HB2	3:C:136:HIS:HD2	1.81	0.46
1:A:168:LEU:HD12	1:A:169:VAL:CA	2.45	0.46
6:A:2023:Y01:HAC1	6:A:2023:Y01:HAU2	1.97	0.46
1:A:127:LEU:HD12	1:A:128:PHE:N	2.31	0.46
1:A:1258:TRP:CZ3	8:A:2011:LPE:H21	2.50	0.46
1:A:798:MET:CE	1:A:803:TYR:CA	2.93	0.46
1:A:1575:THR:HG22	10:A:2014[B]:PCW:C6	2.46	0.46
6:A:2024:Y01:HAV1	6:A:2024:Y01:CAM	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD13	1:A:163:TYR:OH	2.16	0.46
1:A:362:TYR:HE2	1:A:365:ASN:ND2	2.09	0.46
1:A:762:ALA:HB1	6:A:2003:Y01:HBE	1.98	0.46
7:A:2004:CLR:H162	7:A:2004:CLR:H221	1.71	0.46
3:C:104:ASN:HB3	3:C:107:LYS:HE3	1.97	0.46
1:A:191:LEU:CB	1:A:223:LYS:HE2	2.41	0.46
1:A:202:THR:HG23	1:A:203:GLU:N	2.29	0.46
1:A:1461:ASN:HA	1:A:1464:LYS:HE3	1.98	0.46
2:B:182:TYR:O	2:B:185:ILE:CG2	2.54	0.46
1:A:139:ASN:O	1:A:143:MET:HG3	2.16	0.46
8:A:2027:LPE:H312	8:A:2027:LPE:H2N2	1.60	0.46
1:A:798:MET:HE1	1:A:803:TYR:CA	2.45	0.46
1:A:1322:MET:O	1:A:1326:LEU:CD1	2.59	0.45
2:B:91:VAL:HG23	2:B:107:PHE:HB3	1.98	0.45
1:A:132:ILE:HG13	1:A:133:MET:N	2.31	0.45
1:A:1230:ASP:OD2	1:A:1296:ARG:NH2	2.50	0.45
8:A:2016:LPE:H2N2	8:A:2016:LPE:H312	1.76	0.45
3:C:102:SER:HB3	3:C:113:MET:HB2	1.99	0.45
1:A:1666:PHE:HE2	1:A:1739:TYR:CG	2.34	0.45
1:A:364:GLU:HG2	1:A:365:ASN:N	2.32	0.45
1:A:379:MET:O	1:A:383:VAL:HG23	2.16	0.45
1:A:398:LEU:HD23	1:A:398:LEU:C	2.36	0.45
2:B:40:CYS:HB3	2:B:104:LEU:O	2.17	0.45
2:B:93:ASN:ND2	5:B:301:NAG:C7	2.79	0.45
3:C:38:LEU:O	3:C:144:LEU:HD12	2.17	0.45
3:C:48:LEU:O	3:C:111:SER:HB3	2.17	0.45
3:C:54:SER:OG	3:C:131:ASN:ND2	2.37	0.45
1:A:138:THR:HA	1:A:141:ILE:HD12	1.97	0.45
1:A:1694:ILE:HD11	1:A:1703:LEU:CD1	2.47	0.45
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.86	0.45
10:A:2012:PCW:H211	10:A:2012:PCW:H181	1.74	0.45
8:A:2028:LPE:H1N2	8:A:2028:LPE:H311	1.66	0.45
1:A:164:THR:HG23	1:A:165:PHE:N	2.31	0.45
10:A:2013:PCW:H181	10:A:2014[B]:PCW:H372	1.99	0.45
2:B:22:VAL:HG12	2:B:24:VAL:HG23	1.98	0.45
2:B:121:CYS:HB3	2:B:140:LYS:HB2	1.99	0.45
3:C:39:ASN:OD1	3:C:145:GLN:HB3	2.17	0.45
2:B:54:PHE:CE2	2:B:124:TYR:HD1	2.35	0.45
1:A:1408:TRP:HE3	1:A:1412:MET:SD	2.39	0.44
6:A:2021:Y01:CAA	6:A:2021:Y01:CAO	2.86	0.44
1:A:161:GLY:HA2	1:A:164:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2019:LPE:H312	8:A:2019:LPE:H2N2	1.59	0.44
8:A:2020:LPE:H2N3	8:A:2020:LPE:H312	1.59	0.44
3:C:50:CYS:HB3	3:C:110:VAL:CG2	2.45	0.44
1:A:953:PHE:CD1	1:A:957:LEU:HD22	2.52	0.44
1:A:1604:VAL:HG12	1:A:1604:VAL:O	2.17	0.44
9:A:2007:1PW:H13	9:A:2007:1PW:H6	1.69	0.44
6:A:2024:Y01:HAU2	6:A:2024:Y01:HAC1	1.99	0.44
2:B:54:PHE:CZ	2:B:124:TYR:HD1	2.35	0.44
3:C:48:LEU:HB2	3:C:112:VAL:CG1	2.48	0.44
2:B:175:VAL:HG13	8:B:305:LPE:C11	2.47	0.44
3:C:39:ASN:HB3	3:C:147:LEU:HD11	1.98	0.44
3:C:141:LYS:NZ	3:C:143:HIS:HB2	2.33	0.44
1:A:136:ILE:HD13	1:A:163:TYR:CE1	2.52	0.44
1:A:1311:VAL:O	1:A:1315:ILE:HG12	2.18	0.44
1:A:1409:THR:HA	1:A:1412:MET:HE2	2.00	0.44
1:A:1515:GLN:O	1:A:1519:ILE:HG12	2.18	0.44
6:A:2021:Y01:CAT	6:A:2021:Y01:CAM	2.84	0.44
2:B:65:GLU:N	2:B:65:GLU:OE1	2.50	0.44
1:A:89:ILE:CG1	1:A:99:ARG:HG3	2.48	0.43
1:A:144:THR:HG22	1:A:913:PHE:CE1	2.54	0.43
1:A:168:LEU:C	1:A:168:LEU:CD1	2.85	0.43
1:A:1717:PRO:O	1:A:1728:GLY:CA	2.66	0.43
1:A:128:PHE:CZ	1:A:166:GLU:HG3	2.53	0.43
1:A:106:LEU:HD11	1:A:176:PHE:HB3	2.00	0.43
1:A:209:ASN:HB3	1:A:213:LEU:HD11	2.00	0.43
1:A:1359:PHE:HD1	1:A:1363:GLN:NE2	2.17	0.43
3:C:65:LEU:HD22	3:C:110:VAL:HB	1.99	0.43
1:A:1401:GLN:HG2	1:A:1700:TRP:CZ2	2.53	0.43
10:A:2029:PCW:H63	10:A:2029:PCW:H41	1.58	0.43
1:A:293:LEU:HD13	1:A:299:PHE:HA	2.00	0.43
2:B:58:THR:HA	2:B:69:LYS:HA	2.01	0.43
1:A:300:ARG:HD2	1:A:305:TYR:CG	2.54	0.43
3:C:96:GLN:N	3:C:98:ARG:HH12	2.16	0.43
1:A:1694:ILE:HG23	1:A:1700:TRP:HB3	2.01	0.43
10:A:2014[B]:PCW:H182	10:A:2014[B]:PCW:H211	1.75	0.43
1:A:213:LEU:N	1:A:213:LEU:CD1	2.82	0.43
1:A:1298:LEU:O	1:A:1301:LEU:HB3	2.19	0.43
1:A:1721:HIS:HE2	1:A:1728:GLY:C	2.22	0.43
1:A:202:THR:HB	1:A:213:LEU:CD2	2.49	0.43
1:A:1251:LYS:HE2	8:A:2026:LPE:H321	2.00	0.43
1:A:1367:ARG:NH2	1:A:1371:PHE:CZ	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:ASN:O	1:A:1505:GLN:N	2.48	0.43
8:A:2010:LPE:H3N2	8:A:2010:LPE:H312	1.76	0.43
1:A:798:MET:HE1	1:A:802:GLU:O	2.19	0.42
3:C:32:VAL:CG1	3:C:129:ILE:HD12	2.49	0.42
1:A:23:ILE:HG23	1:A:84:ASP:O	2.19	0.42
1:A:957:LEU:N	1:A:957:LEU:HD12	2.34	0.42
1:A:1296:ARG:HB2	1:A:1297:PRO:HD3	2.00	0.42
1:A:383:VAL:HA	1:A:1692:PHE:CZ	2.55	0.42
1:A:814:LEU:O	1:A:817:THR:OG1	2.30	0.42
1:A:857:LYS:O	1:A:858:ILE:C	2.55	0.42
1:A:1335:PHE:CZ	6:A:2021:Y01:HAB2	2.54	0.42
8:A:2015:LPE:H312	8:A:2015:LPE:H1N2	1.64	0.42
1:A:1435:ILE:HB	6:A:2021:Y01:HAU2	2.01	0.42
1:A:1429:TYR:CE1	6:A:2022:Y01:HAK2	2.53	0.42
6:A:2024:Y01:CAM	6:A:2024:Y01:CAR	2.85	0.42
1:A:16:THR:O	1:A:17:LYS:C	2.57	0.42
1:A:91:LEU:HD21	1:A:97:ILE:HG12	2.01	0.42
1:A:109:LEU:N	1:A:109:LEU:CD1	2.82	0.42
1:A:1716:ASP:HA	1:A:1717:PRO:HD2	1.76	0.42
1:A:1751:VAL:O	1:A:1755:TYR:HB2	2.19	0.42
1:A:364:GLU:O	1:A:368:GLN:HG3	2.20	0.42
6:A:2023:Y01:HAJ2	6:A:2023:Y01:HAP1	1.97	0.42
8:A:2025:LPE:H172	8:A:2025:LPE:H142	1.75	0.42
3:C:129:ILE:CG2	3:C:130:MET:N	2.83	0.42
10:A:2013:PCW:H181	10:A:2014[A]:PCW:H372	2.02	0.41
3:C:54:SER:HB3	3:C:131:ASN:HD22	1.82	0.41
1:A:53:LEU:O	1:A:99:ARG:NH2	2.53	0.41
1:A:210:VAL:HG13	1:A:211:SER:N	2.35	0.41
1:A:957:LEU:H	1:A:957:LEU:CD1	2.33	0.41
1:A:1318:ILE:O	1:A:1319:PRO:C	2.56	0.41
1:A:1429:TYR:O	6:A:2022:Y01:HAT1	2.20	0.41
2:B:80:LEU:HD23	2:B:80:LEU:HA	1.90	0.41
1:A:85:LYS:HE2	1:A:85:LYS:HB2	1.87	0.41
1:A:264:LEU:O	1:A:268:MET:HB2	2.20	0.41
2:B:116:SER:HB2	2:B:146:VAL:HG23	2.02	0.41
1:A:52:ASP:C	1:A:54:GLU:H	2.24	0.41
3:C:56:TYR:HD1	3:C:134:ASP:HB2	1.84	0.41
1:A:72:SER:HB3	1:A:121:LYS:HG2	2.01	0.41
3:C:98:ARG:HD2	3:C:116:ASN:HB2	2.03	0.41
1:A:79:ASP:HA	1:A:80:PRO:HD3	1.91	0.41
1:A:92:ASN:ND2	1:A:124:VAL:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:LEU:HA	1:A:1239:LEU:HD23	1.80	0.41
6:A:2003:Y01:HAE2	6:A:2003:Y01:HBB	1.69	0.41
1:A:132:ILE:CG2	1:A:166:GLU:OE1	2.69	0.41
1:A:1710:SER:HB2	1:A:1733:PRO:HD3	2.01	0.41
1:A:314:LEU:HD22	1:A:373:ALA:HB2	2.03	0.41
1:A:315:CYS:SG	1:A:316:GLY:N	2.93	0.41
1:A:810:ILE:O	1:A:811:PHE:C	2.60	0.41
1:A:957:LEU:N	1:A:957:LEU:CD1	2.84	0.41
1:A:1515:GLN:H	1:A:1515:GLN:HG3	1.77	0.41
1:A:1718:LYS:HA	1:A:1727:GLU:HG2	2.02	0.41
8:A:2008:LPE:H311	8:A:2008:LPE:H1N2	1.66	0.41
1:A:907:ARG:HG2	1:A:1427:TYR:OH	2.21	0.41
1:A:1410:ILE:H	1:A:1410:ILE:HG13	1.70	0.41
1:A:90:VAL:HG11	1:A:120:ILE:HG21	2.01	0.40
1:A:137:LEU:O	1:A:141:ILE:HD12	2.20	0.40
1:A:895:CYS:HB2	1:A:938:VAL:CG2	2.42	0.40
1:A:161:GLY:CA	1:A:164:THR:HG22	2.52	0.40
1:A:798:MET:HE2	1:A:802:GLU:C	2.41	0.40
1:A:820:LEU:N	1:A:820:LEU:HD22	2.36	0.40
3:C:35:PRO:HD3	3:C:49:PRO:HG2	2.04	0.40
1:A:1694:ILE:HD12	1:A:1694:ILE:HG23	1.87	0.40
3:C:135:ARG:C	3:C:135:ARG:CD	2.85	0.40
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.89	0.40
1:A:730:TRP:O	1:A:734:LYS:HG3	2.22	0.40
1:A:1324:VAL:CG2	1:A:1455:VAL:HG21	2.52	0.40
3:C:40:VAL:O	3:C:147:LEU:N	2.34	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	1247/2022 (62%)	1172 (94%)	68 (6%)	7 (1%)	22	51
2	B	171/218 (78%)	162 (95%)	9 (5%)	0	100	100
3	C	118/215 (55%)	111 (94%)	7 (6%)	0	100	100
All	All	1536/2455 (63%)	1445 (94%)	84 (6%)	7 (0%)	27	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	210	VAL
1	A	1442	ILE
1	A	93	LYS
1	A	797	ALA
1	A	1360	PRO
1	A	1503	LYS

### 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	1101/1804 (61%)	1091 (99%)	10 (1%)	75	92
2	B	157/190 (83%)	157 (100%)	0	100	100
3	C	113/193 (58%)	112 (99%)	1 (1%)	75	92
All	All	1371/2187 (63%)	1360 (99%)	11 (1%)	77	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	315	CYS
1	A	330	CYS
1	A	747	ASP
1	A	966	LEU
1	A	1230	ASP

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Mol	Chain	Res	Type
1	A	1280	TYR
1	A	1283	LEU
1	A	1528	ASN
1	A	1747	SER
3	C	31	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	A	365	ASN
1	A	412	ASN
1	A	805	GLN
1	A	809	ASN
1	A	1180	ASN
1	A	1191	HIS
1	A	1276	ASN
1	A	1363	GLN
1	A	1470	GLN
1	A	1514	ASN
1	A	1665	ASN
1	A	1732	ASN
1	A	1753	ASN
2	B	75	ASN
2	B	131	ASN
3	C	73	ASN
3	C	82	GLN
3	C	131	ASN
3	C	136	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	0.52	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.18	0	17,19,21	0.57	0
4	NAG	E	1	4,1	14,14,15	0.34	0	17,19,21	1.09	2 (11%)
4	NAG	E	2	4	14,14,15	0.35	0	17,19,21	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
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	E	1	NAG	C2-N2-C7	3.00	126.92	122.90
4	E	1	NAG	C1-C2-N2	2.24	113.96	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
4	E	1	NAG	C8-C7-N2-C2

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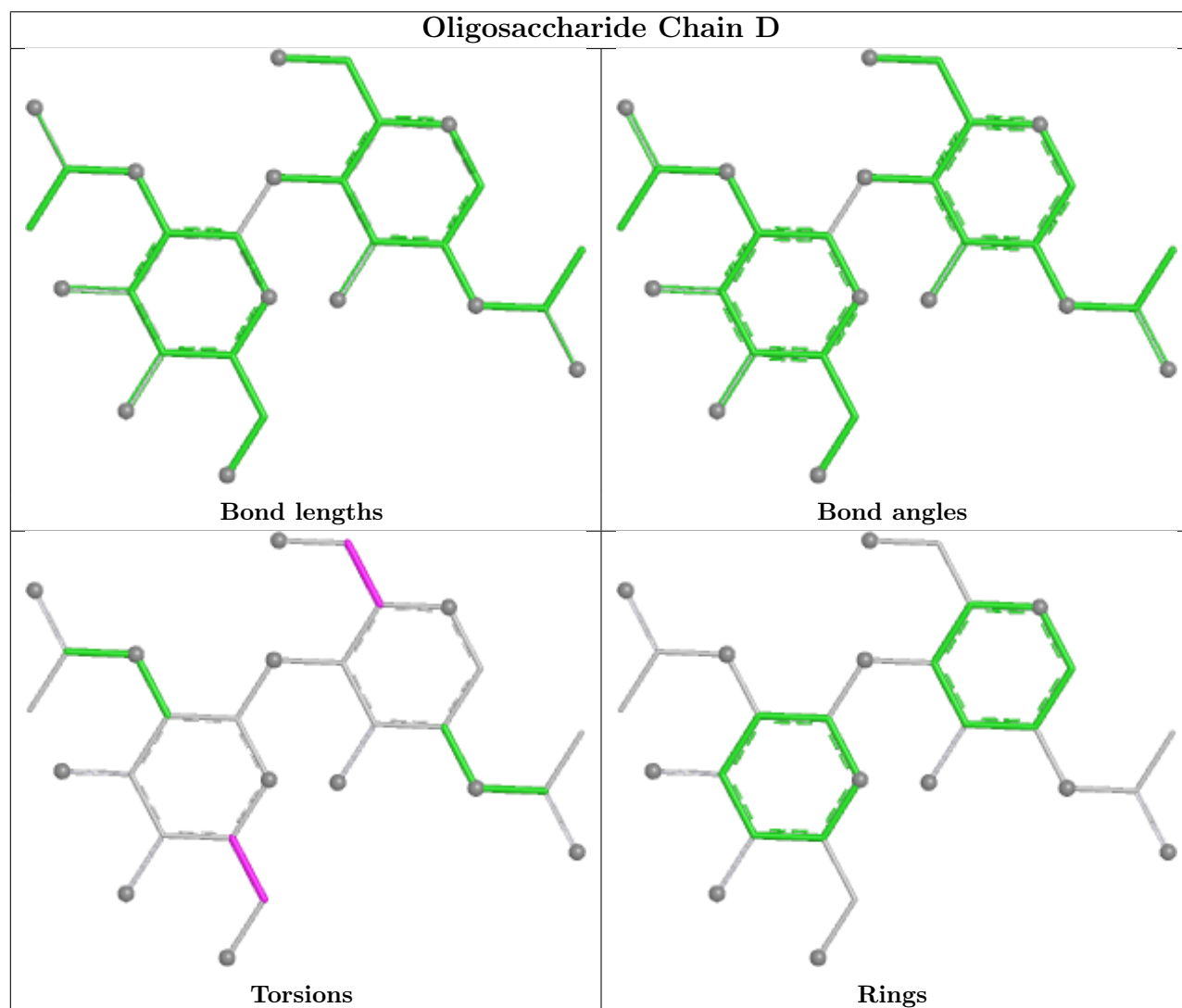
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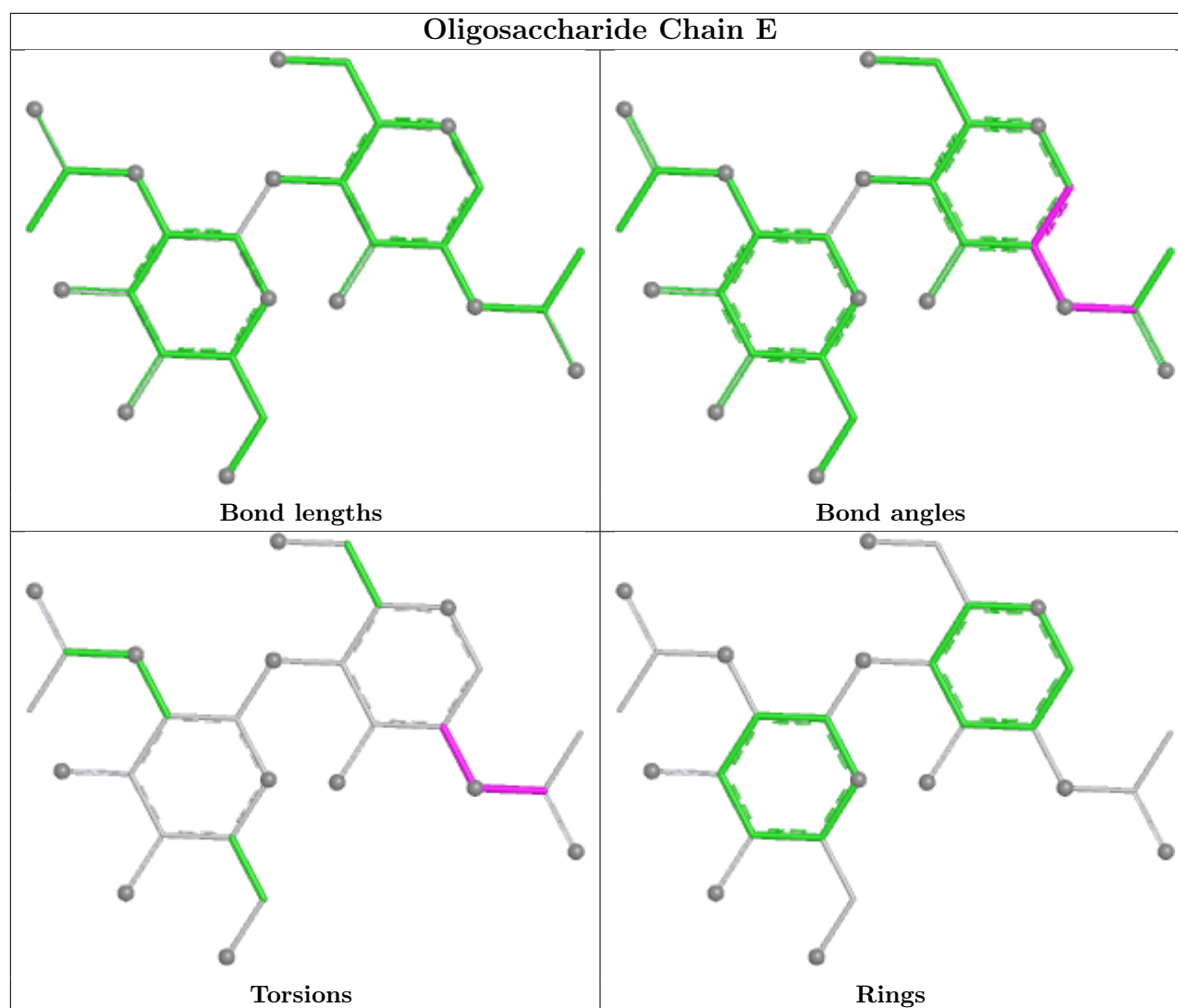
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

39 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	304	2	14,14,15	1.00	1 (7%)	17,19,21	0.69	0
10	PCW	A	2009	-	52,52,53	0.93	2 (3%)	58,60,61	1.02	3 (5%)
5	NAG	B	303	2	14,14,15	0.36	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	301	3	14,14,15	0.20	0	17,19,21	0.53	0
5	NAG	A	2002	1	14,14,15	0.21	0	17,19,21	0.54	0
6	Y01	A	2021	-	38,38,38	0.47	0	57,57,57	0.86	1 (1%)
8	LPE	A	2019	-	24,24,33	0.58	0	28,30,39	0.66	1 (3%)
8	LPE	A	2006	-	24,24,33	0.41	0	25,27,39	0.49	0
8	LPE	A	2028	-	16,16,33	0.63	0	20,22,39	0.57	0
8	LPE	A	2026	-	16,16,33	0.63	0	20,22,39	0.45	0
8	LPE	A	2005	-	24,24,33	0.54	0	28,30,39	0.66	0
8	LPE	A	2015	-	24,24,33	0.55	0	28,30,39	0.64	0
8	LPE	A	2010	-	27,27,33	0.53	0	31,33,39	0.66	0
10	PCW	A	2014[B]	-	43,43,53	1.06	2 (4%)	49,51,61	1.17	2 (4%)
11	P5S	A	2031	-	32,33,53	1.14	2 (6%)	34,40,60	1.53	5 (14%)
5	NAG	B	302	2	14,14,15	0.29	0	17,19,21	0.42	0
9	1PW	A	2007	-	23,23,27	0.42	0	24,26,32	0.41	0
6	Y01	A	2022	-	38,38,38	0.44	0	57,57,57	0.47	0
10	PCW	A	2029	-	43,43,53	1.02	2 (4%)	49,51,61	1.06	3 (6%)
8	LPE	A	2027	-	24,24,33	0.57	0	28,30,39	0.60	0
10	PCW	A	2030	-	43,43,53	1.03	2 (4%)	49,51,61	1.05	2 (4%)
10	PCW	A	2013	-	43,43,53	1.04	2 (4%)	49,51,61	0.98	3 (6%)
7	CLR	A	2004	-	31,31,31	0.80	1 (3%)	48,48,48	1.18	5 (10%)
8	LPE	B	305	-	16,16,33	0.67	0	20,22,39	0.64	0
10	PCW	A	2014[A]	-	43,43,53	1.10	2 (4%)	49,51,61	1.31	3 (6%)
8	LPE	A	2016	-	24,24,33	0.55	0	28,30,39	0.61	0
6	Y01	A	2023	-	38,38,38	0.47	0	57,57,57	0.73	1 (1%)
8	LPE	A	2025	-	24,24,33	0.69	0	28,30,39	0.85	0
10	PCW	A	2012	-	46,46,53	0.97	2 (4%)	52,54,61	1.07	3 (5%)
6	Y01	A	2003	-	38,38,38	4.05	17 (44%)	57,57,57	2.32	15 (26%)
8	LPE	A	2032	-	16,16,33	0.74	0	20,22,39	0.68	0
5	NAG	A	2001	1	14,14,15	0.43	0	17,19,21	0.53	0
6	Y01	A	2024	-	38,38,38	0.48	0	57,57,57	0.53	0
8	LPE	A	2008	-	19,19,33	0.63	0	23,25,39	0.59	0
8	LPE	A	2011	-	27,27,33	0.56	0	31,33,39	0.64	0
8	LPE	A	2020	-	24,24,33	0.54	0	28,30,39	0.55	0
5	NAG	B	301	2	14,14,15	0.51	0	17,19,21	0.38	0
8	LPE	A	2017	-	24,24,33	0.55	0	28,30,39	0.53	0
8	LPE	A	2018	-	24,24,33	0.58	0	28,30,39	0.68	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	304	2	-	1/6/23/26	0/1/1/1
10	PCW	A	2009	-	-	29/56/56/57	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
5	NAG	C	301	3	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
6	Y01	A	2021	-	-	5/19/77/77	0/4/4/4
8	LPE	A	2019	-	-	12/25/25/34	-
8	LPE	A	2006	-	-	20/25/25/34	-
8	LPE	A	2028	-	-	7/17/17/34	-
8	LPE	A	2026	-	-	12/17/17/34	-
8	LPE	A	2005	-	-	12/25/25/34	-
8	LPE	A	2015	-	-	12/25/25/34	-
8	LPE	A	2010	-	-	13/28/28/34	-
10	PCW	A	2014[B]	-	-	22/47/47/57	-
11	P5S	A	2031	-	-	16/39/39/59	-
5	NAG	B	302	2	-	1/6/23/26	0/1/1/1
9	1PW	A	2007	-	-	17/22/22/29	-
6	Y01	A	2022	-	-	8/19/77/77	0/4/4/4
10	PCW	A	2029	-	-	21/47/47/57	-
8	LPE	A	2027	-	-	16/25/25/34	-
10	PCW	A	2030	-	-	30/47/47/57	-
10	PCW	A	2013	-	-	13/47/47/57	-
7	CLR	A	2004	-	-	7/10/68/68	0/4/4/4
8	LPE	B	305	-	-	10/17/17/34	-
10	PCW	A	2014[A]	-	-	22/47/47/57	-
8	LPE	A	2016	-	-	12/25/25/34	-
6	Y01	A	2023	-	-	5/19/77/77	0/4/4/4
8	LPE	A	2025	-	-	13/25/25/34	-
10	PCW	A	2012	-	-	21/50/50/57	-
6	Y01	A	2003	-	-	11/19/77/77	0/4/4/4
8	LPE	A	2032	-	-	11/17/17/34	-
5	NAG	A	2001	1	-	4/6/23/26	0/1/1/1
6	Y01	A	2024	-	-	5/19/77/77	0/4/4/4
8	LPE	A	2008	-	-	8/20/20/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LPE	A	2011	-	-	15/28/28/34	-
8	LPE	A	2020	-	-	14/25/25/34	-
5	NAG	B	301	2	-	2/6/23/26	0/1/1/1
8	LPE	A	2017	-	-	17/25/25/34	-
8	LPE	A	2018	-	-	13/25/25/34	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2003	Y01	CBI-CBE	-11.32	1.34	1.55
6	A	2003	Y01	CAQ-CBG	-10.08	1.33	1.54
6	A	2003	Y01	CAS-CBF	9.43	1.69	1.53
6	A	2003	Y01	CAI-CAZ	9.07	1.51	1.33
6	A	2003	Y01	CBI-CBG	9.06	1.71	1.55
6	A	2003	Y01	CAP-CBE	5.67	1.66	1.54
10	A	2014[A]	PCW	O2-C31	4.73	1.47	1.34
10	A	2014[B]	PCW	O2-C31	4.38	1.46	1.34
10	A	2013	PCW	O3-C11	4.28	1.45	1.33
10	A	2029	PCW	O3-C11	4.27	1.45	1.33
10	A	2009	PCW	O3-C11	4.24	1.45	1.33
10	A	2030	PCW	O3-C11	4.20	1.45	1.33
10	A	2013	PCW	O2-C31	4.18	1.46	1.34
11	A	2031	P5S	O19-C17	4.13	1.45	1.33
10	A	2012	PCW	O3-C11	4.13	1.45	1.33
10	A	2030	PCW	O2-C31	4.12	1.45	1.34
11	A	2031	P5S	O37-C38	4.04	1.45	1.34
10	A	2009	PCW	O2-C31	4.00	1.45	1.34
10	A	2029	PCW	O2-C31	3.95	1.45	1.34
10	A	2014[B]	PCW	O3-C11	3.94	1.44	1.33
10	A	2012	PCW	O2-C31	3.78	1.45	1.34
10	A	2014[A]	PCW	O3-C11	3.77	1.44	1.33
5	B	304	NAG	O5-C1	-3.66	1.37	1.43
6	A	2003	Y01	CAU-CAS	3.55	1.60	1.53
6	A	2003	Y01	CAT-CAR	3.19	1.59	1.53
6	A	2003	Y01	CAK-CBD	3.11	1.58	1.53
6	A	2003	Y01	CBH-CAZ	3.10	1.58	1.52
6	A	2003	Y01	OAW-CBC	-3.01	1.39	1.46
6	A	2003	Y01	CAK-CAI	2.80	1.55	1.50
6	A	2003	Y01	CAQ-CAP	2.67	1.61	1.54
7	A	2004	CLR	C10-C9	-2.46	1.52	1.56
6	A	2003	Y01	CAV-CBC	2.43	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2003	Y01	CBD-CBG	2.25	1.57	1.53
6	A	2003	Y01	CAV-CAZ	2.25	1.56	1.51
6	A	2003	Y01	CAR-CBC	2.21	1.57	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2003	Y01	CAK-CAI-CAZ	-8.19	111.19	125.02
6	A	2003	Y01	CBH-CAZ-CAI	-7.17	112.46	122.93
6	A	2003	Y01	CAV-CAZ-CAI	-6.62	111.60	120.57
10	A	2014[A]	PCW	O2-C31-C32	5.51	123.41	111.48
11	A	2031	P5S	OG-CB-CA	5.07	112.48	108.06
10	A	2014[B]	PCW	O2-C31-C32	4.76	121.78	111.48
6	A	2021	Y01	CAR-CBC-CAV	4.43	117.13	110.97
6	A	2003	Y01	CAU-CBI-CBE	-4.24	110.36	116.60
6	A	2023	Y01	CAR-CBC-CAV	4.11	116.69	110.97
10	A	2029	PCW	O2-C31-C32	4.08	120.32	111.48
10	A	2030	PCW	O2-C31-C32	4.06	120.27	111.48
11	A	2031	P5S	O37-C38-C39	4.02	120.18	111.48
10	A	2012	PCW	O2-C31-C32	3.88	119.86	111.48
10	A	2009	PCW	O2-C31-C32	3.87	119.85	111.48
10	A	2013	PCW	O2-C31-C32	3.69	119.47	111.48
6	A	2003	Y01	OAW-CAY-CAM	3.66	119.41	111.48
6	A	2003	Y01	CAV-CAZ-CBH	-3.64	111.76	116.42
6	A	2003	Y01	CAD-CBH-CBF	-3.21	108.06	111.66
6	A	2003	Y01	CAC-CBB-CAO	-3.10	105.54	110.34
10	A	2014[A]	PCW	O3-C11-C12	3.10	121.29	111.83
10	A	2009	PCW	C2-O2-C31	-3.08	110.43	117.80
6	A	2003	Y01	CAT-CBH-CAZ	2.91	113.77	108.74
10	A	2014[B]	PCW	O3-C11-C12	2.88	120.62	111.83
10	A	2030	PCW	O3-C11-C12	2.82	120.42	111.83
10	A	2012	PCW	O3-C11-C12	2.78	120.30	111.83
6	A	2003	Y01	CAK-CBD-CBF	2.72	112.86	109.72
6	A	2003	Y01	CAP-CAQ-CBG	-2.71	99.83	105.14
6	A	2003	Y01	CAK-CBD-CBG	-2.71	107.10	110.93
11	A	2031	P5S	OXT-C-O	-2.70	117.95	124.08
6	A	2003	Y01	CAP-CBE-CBB	-2.68	108.12	112.18
10	A	2029	PCW	O3-C11-C12	2.65	119.92	111.83
11	A	2031	P5S	O19-C17-C20	2.56	119.64	111.83
7	A	2004	CLR	C13-C17-C20	-2.56	115.55	119.50
7	A	2004	CLR	C4-C5-C10	2.44	119.55	116.42
6	A	2003	Y01	CBI-CBE-CBB	-2.42	115.76	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2013	PCW	O3-C11-C12	2.38	119.10	111.83
11	A	2031	P5S	C2-O37-C38	-2.33	112.22	117.80
10	A	2009	PCW	O3-C11-C12	2.28	118.80	111.83
10	A	2029	PCW	C2-O2-C31	-2.25	112.40	117.80
7	A	2004	CLR	C11-C9-C10	-2.19	110.39	113.08
10	A	2012	PCW	C2-O2-C31	-2.10	112.78	117.80
7	A	2004	CLR	C7-C8-C9	2.09	112.14	109.72
6	A	2003	Y01	CBF-CBD-CBG	-2.08	106.37	109.09
10	A	2014[A]	PCW	O31-C31-C32	-2.08	115.65	123.78
7	A	2004	CLR	C13-C14-C8	-2.04	111.52	114.41
8	A	2019	LPE	C31-C32-N	-2.03	109.32	115.82
10	A	2013	PCW	C2-O2-C31	-2.02	112.95	117.80

There are no chirality outliers.

All (461) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2021	Y01	OAG-CAY-OAW-CBC
6	A	2021	Y01	CAM-CAY-OAW-CBC
6	A	2024	Y01	OAG-CAY-OAW-CBC
6	A	2024	Y01	CAM-CAY-OAW-CBC
8	A	2005	LPE	C3-O3-P-O32
8	A	2005	LPE	C3-O3-P-O33
8	A	2005	LPE	O33-C31-C32-N
8	A	2006	LPE	C3-O3-P-O32
8	A	2006	LPE	C3-O3-P-O33
8	A	2006	LPE	C31-O33-P-O3
8	A	2006	LPE	C31-O33-P-O32
8	A	2006	LPE	O33-C31-C32-N
8	A	2008	LPE	C3-O3-P-O32
8	A	2010	LPE	C31-O33-P-O3
8	A	2010	LPE	C31-O33-P-O31
8	A	2010	LPE	O33-C31-C32-N
8	A	2011	LPE	C3-O3-P-O32
8	A	2011	LPE	C3-O3-P-O33
8	A	2011	LPE	O33-C31-C32-N
8	A	2015	LPE	C3-O3-P-O31
8	A	2015	LPE	C3-O3-P-O32
8	A	2015	LPE	C3-O3-P-O33
8	A	2015	LPE	C31-O33-P-O3
8	A	2015	LPE	C31-O33-P-O31
8	A	2015	LPE	O33-C31-C32-N

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Mol	Chain	Res	Type	Atoms
8	A	2016	LPE	O1-C1-C2-C3
8	A	2016	LPE	O2H-C2-C3-O3
8	A	2016	LPE	C31-O33-P-O31
8	A	2016	LPE	O33-C31-C32-N
8	A	2017	LPE	C3-O3-P-O32
8	A	2017	LPE	C3-O3-P-O33
8	A	2017	LPE	C31-O33-P-O3
8	A	2018	LPE	C31-O33-P-O3
8	A	2018	LPE	O33-C31-C32-N
8	A	2019	LPE	C3-O3-P-O32
8	A	2019	LPE	C3-O3-P-O33
8	A	2019	LPE	C31-O33-P-O3
8	A	2019	LPE	O33-C31-C32-N
8	A	2020	LPE	O1-C1-C2-C3
8	A	2020	LPE	C3-O3-P-O33
8	A	2020	LPE	O33-C31-C32-N
8	A	2025	LPE	O1-C1-C2-C3
8	A	2025	LPE	C31-O33-P-O3
8	A	2025	LPE	C31-O33-P-O31
8	A	2025	LPE	O33-C31-C32-N
8	A	2026	LPE	C31-O33-P-O3
8	A	2026	LPE	C31-O33-P-O32
8	A	2026	LPE	O33-C31-C32-N
8	A	2027	LPE	O1-C1-C2-O2H
8	A	2027	LPE	C3-O3-P-O31
8	A	2027	LPE	C3-O3-P-O32
8	A	2027	LPE	C3-O3-P-O33
8	A	2027	LPE	O33-C31-C32-N
8	A	2028	LPE	O1-C1-C2-C3
8	A	2028	LPE	C3-O3-P-O32
8	A	2032	LPE	O1-C1-C2-C3
8	A	2032	LPE	C3-O3-P-O32
8	A	2032	LPE	C3-O3-P-O33
8	A	2032	LPE	C31-O33-P-O3
8	A	2032	LPE	C32-C31-O33-P
8	A	2032	LPE	O33-C31-C32-N
8	B	305	LPE	O1-C1-C2-C3
8	B	305	LPE	C3-O3-P-O31
8	B	305	LPE	C3-O3-P-O32
8	B	305	LPE	C3-O3-P-O33
8	B	305	LPE	C31-O33-P-O3
8	B	305	LPE	C31-O33-P-O31

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Mol	Chain	Res	Type	Atoms
8	B	305	LPE	C31-O33-P-O32
8	B	305	LPE	O33-C31-C32-N
9	A	2007	1PW	CAI-CAZ-CBA-CAV
9	A	2007	1PW	OAE-CAZ-CBA-CAV
9	A	2007	1PW	OAX-CAV-CBA-CAZ
9	A	2007	1PW	CAV-OAX-PBB-OAF
9	A	2007	1PW	CAV-OAX-PBB-OAG
10	A	2009	PCW	O4P-C4-C5-N
10	A	2009	PCW	C4-O4P-P-O2P
10	A	2012	PCW	O4P-C4-C5-N
10	A	2012	PCW	C1-O3P-P-O1P
10	A	2012	PCW	C1-O3P-P-O4P
10	A	2013	PCW	C4-O4P-P-O1P
10	A	2013	PCW	C4-O4P-P-O2P
10	A	2013	PCW	C4-O4P-P-O3P
10	A	2014[A]	PCW	C5-C4-O4P-P
10	A	2014[B]	PCW	O4P-C4-C5-N
10	A	2014[B]	PCW	C4-O4P-P-O2P
10	A	2014[B]	PCW	C4-O4P-P-O3P
10	A	2029	PCW	O4P-C4-C5-N
10	A	2029	PCW	C32-C31-O2-C2
10	A	2029	PCW	O31-C31-O2-C2
10	A	2029	PCW	C4-O4P-P-O3P
10	A	2030	PCW	C32-C31-O2-C2
10	A	2030	PCW	O31-C31-O2-C2
10	A	2030	PCW	C1-O3P-P-O1P
10	A	2030	PCW	C1-O3P-P-O2P
10	A	2030	PCW	C1-O3P-P-O4P
10	A	2030	PCW	C4-O4P-P-O2P
11	A	2031	P5S	C-CA-CB-OG
11	A	2031	P5S	N-CA-CB-OG
11	A	2031	P5S	CA-CB-OG-P12
11	A	2031	P5S	CB-OG-P12-O13
11	A	2031	P5S	CB-OG-P12-O16
10	A	2030	PCW	O11-C11-O3-C3
11	A	2031	P5S	O18-C17-O19-C1
6	A	2021	Y01	CAV-CBC-OAW-CAY
6	A	2022	Y01	CAR-CBC-OAW-CAY
6	A	2024	Y01	CAV-CBC-OAW-CAY
11	A	2031	P5S	C20-C17-O19-C1
10	A	2029	PCW	O11-C11-O3-C3
6	A	2003	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
7	A	2004	CLR	C13-C17-C20-C22
10	A	2014[A]	PCW	O31-C31-O2-C2
10	A	2030	PCW	C12-C11-O3-C3
7	A	2004	CLR	C21-C20-C22-C23
7	A	2004	CLR	C13-C17-C20-C21
10	A	2029	PCW	C12-C11-O3-C3
8	A	2028	LPE	C2-C1-O1-C11
5	B	301	NAG	C4-C5-C6-O6
8	A	2010	LPE	O2H-C2-C3-O3
8	A	2017	LPE	O2H-C2-C3-O3
8	A	2028	LPE	O2H-C2-C3-O3
8	A	2032	LPE	O2H-C2-C3-O3
10	A	2014[A]	PCW	C12-C11-O3-C3
10	A	2014[B]	PCW	C12-C11-O3-C3
5	C	301	NAG	O5-C5-C6-O6
8	A	2016	LPE	O1-C1-C2-O2H
8	A	2020	LPE	O1-C1-C2-O2H
8	A	2025	LPE	O1-C1-C2-O2H
8	A	2028	LPE	O1-C1-C2-O2H
8	A	2032	LPE	O1-C1-C2-O2H
8	B	305	LPE	O1-C1-C2-O2H
10	A	2014[A]	PCW	C32-C31-O2-C2
10	A	2014[B]	PCW	C32-C31-O2-C2
6	A	2023	Y01	CAV-CBC-OAW-CAY
5	A	2002	NAG	O5-C5-C6-O6
6	A	2003	Y01	CAJ-CAO-CBB-CBE
5	A	2001	NAG	C4-C5-C6-O6
8	A	2026	LPE	C2-C1-O1-C11
10	A	2014[A]	PCW	O11-C11-O3-C3
10	A	2014[B]	PCW	O31-C31-O2-C2
6	A	2003	Y01	CAJ-CAO-CBB-CAC
10	A	2014[B]	PCW	O11-C11-O3-C3
5	A	2001	NAG	O5-C5-C6-O6
7	A	2004	CLR	C16-C17-C20-C21
5	B	301	NAG	O5-C5-C6-O6
8	A	2010	LPE	C1-C2-C3-O3
8	A	2016	LPE	C1-C2-C3-O3
8	A	2026	LPE	C1-C2-C3-O3
8	A	2028	LPE	C1-C2-C3-O3
10	A	2013	PCW	C12-C11-O3-C3
8	A	2026	LPE	C31-C32-N-C2N
10	A	2014[A]	PCW	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
10	A	2029	PCW	C4-C5-N-C6
8	A	2005	LPE	O2H-C2-C3-O3
8	A	2026	LPE	O2H-C2-C3-O3
10	A	2013	PCW	O11-C11-O3-C3
9	A	2007	1PW	CAL-CAN-CAP-CAR
10	A	2012	PCW	C11-C12-C13-C14
10	A	2029	PCW	C11-C12-C13-C14
10	A	2030	PCW	C11-C12-C13-C14
7	A	2004	CLR	C17-C20-C22-C23
6	A	2003	Y01	CAO-CAJ-CAN-CBA
8	A	2006	LPE	O1-C11-C12-C13
8	A	2026	LPE	C31-C32-N-C3N
8	A	2027	LPE	C31-C32-N-C2N
8	A	2027	LPE	C31-C32-N-C3N
10	A	2014[A]	PCW	C4-C5-N-C6
10	A	2029	PCW	C4-C5-N-C8
10	A	2030	PCW	C31-C32-C33-C34
5	C	301	NAG	C4-C5-C6-O6
10	A	2014[A]	PCW	C11-C12-C13-C14
10	A	2014[B]	PCW	C11-C12-C13-C14
10	A	2014[B]	PCW	C31-C32-C33-C34
8	A	2010	LPE	O1-C11-C12-C13
10	A	2012	PCW	C31-C32-C33-C34
10	A	2014[A]	PCW	C31-C32-C33-C34
5	A	2002	NAG	C4-C5-C6-O6
8	A	2020	LPE	O1-C11-C12-C13
7	A	2004	CLR	C16-C17-C20-C22
6	A	2003	Y01	CAC-CBB-CBE-CAP
10	A	2009	PCW	C4-C5-N-C6
10	A	2009	PCW	C4-C5-N-C7
10	A	2009	PCW	C4-C5-N-C8
8	A	2016	LPE	O1-C11-C12-C13
7	A	2004	CLR	C20-C22-C23-C24
10	A	2009	PCW	C32-C31-O2-C2
11	A	2031	P5S	C39-C38-O37-C2
8	A	2027	LPE	O1-C1-C2-C3
10	A	2009	PCW	O31-C31-O2-C2
11	A	2031	P5S	O47-C38-O37-C2
6	A	2003	Y01	CAO-CBB-CBE-CBI
8	A	2008	LPE	O2H-C2-C3-O3
10	A	2012	PCW	C40-C41-C42-C43
8	A	2011	LPE	O1-C1-C2-O2H

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Mol	Chain	Res	Type	Atoms
10	A	2009	PCW	C43-C44-C45-C46
8	A	2026	LPE	C31-C32-N-C1N
10	A	2029	PCW	C4-C5-N-C7
10	A	2009	PCW	C32-C33-C34-C35
6	A	2022	Y01	CAO-CBB-CBE-CAP
6	A	2022	Y01	CAO-CBB-CBE-CBI
8	A	2005	LPE	C12-C13-C14-C15
8	A	2005	LPE	C13-C14-C15-C16
8	A	2020	LPE	C14-C15-C16-C17
8	A	2027	LPE	C12-C13-C14-C15
10	A	2014[A]	PCW	C23-C24-C25-C26
10	A	2030	PCW	C15-C16-C17-C18
10	A	2030	PCW	C32-C33-C34-C35
10	A	2029	PCW	C12-C13-C14-C15
8	A	2025	LPE	C13-C14-C15-C16
10	A	2012	PCW	C34-C35-C36-C37
10	A	2009	PCW	C11-C12-C13-C14
8	A	2027	LPE	C11-C12-C13-C14
10	A	2012	PCW	C12-C13-C14-C15
10	A	2014[B]	PCW	C23-C24-C25-C26
10	A	2009	PCW	C12-C13-C14-C15
8	A	2017	LPE	C1-C2-C3-O3
8	A	2019	LPE	C14-C15-C16-C17
8	A	2020	LPE	C13-C14-C15-C16
10	A	2012	PCW	C21-C22-C23-C24
8	A	2011	LPE	C17-C18-C19-C20
8	A	2010	LPE	C14-C15-C16-C17
8	A	2019	LPE	C13-C14-C15-C16
10	A	2014[B]	PCW	C14-C15-C16-C17
8	A	2016	LPE	C11-C12-C13-C14
8	A	2027	LPE	C31-C32-N-C1N
10	A	2014[A]	PCW	C4-C5-N-C8
10	A	2012	PCW	C33-C34-C35-C36
8	A	2011	LPE	C11-C12-C13-C14
10	A	2029	PCW	C21-C22-C23-C24
8	A	2011	LPE	O1-C1-C2-C3
8	A	2020	LPE	C12-C13-C14-C15
10	A	2009	PCW	C34-C35-C36-C37
10	A	2012	PCW	C13-C14-C15-C16
10	A	2029	PCW	C15-C16-C17-C18
8	A	2006	LPE	C14-C15-C16-C17
8	A	2015	LPE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	A	2007	1PW	CAN-CAP-CAR-CAT
10	A	2030	PCW	C13-C14-C15-C16
10	A	2009	PCW	C20-C21-C22-C23
8	A	2010	LPE	C15-C16-C17-C18
8	A	2010	LPE	C13-C14-C15-C16
10	A	2029	PCW	C34-C35-C36-C37
8	A	2018	LPE	O1-C11-C12-C13
10	A	2014[A]	PCW	C14-C15-C16-C17
8	A	2027	LPE	C14-C15-C16-C17
10	A	2013	PCW	C32-C31-O2-C2
8	A	2019	LPE	C11-C12-C13-C14
10	A	2014[A]	PCW	C16-C17-C18-C19
10	A	2014[B]	PCW	C16-C17-C18-C19
9	A	2007	1PW	CAR-CAT-CAU-CAS
8	A	2019	LPE	C12-C13-C14-C15
10	A	2014[A]	PCW	C15-C16-C17-C18
10	A	2014[B]	PCW	C15-C16-C17-C18
10	A	2030	PCW	C23-C24-C25-C26
8	A	2011	LPE	C2-C3-O3-P
6	A	2022	Y01	CAC-CBB-CBE-CAP
8	A	2027	LPE	C1-C2-C3-O3
8	A	2032	LPE	C1-C2-C3-O3
10	A	2029	PCW	C22-C23-C24-C25
10	A	2029	PCW	C33-C34-C35-C36
8	A	2008	LPE	C11-C12-C13-C14
8	A	2010	LPE	C16-C17-C18-C19
10	A	2012	PCW	C36-C37-C38-C39
11	A	2031	P5S	C1-C2-C3-O16
10	A	2009	PCW	C15-C16-C17-C18
10	A	2012	PCW	C32-C31-O2-C2
5	B	302	NAG	O5-C5-C6-O6
10	A	2014[A]	PCW	C1-C2-C3-O3
10	A	2014[B]	PCW	C1-C2-C3-O3
9	A	2007	1PW	CAH-CAK-CAM-CAO
8	A	2027	LPE	C15-C16-C17-C18
8	A	2017	LPE	O1-C11-C12-C13
10	A	2012	PCW	C20-C21-C22-C23
10	A	2012	PCW	C15-C16-C17-C18
8	A	2017	LPE	C2-C1-O1-C11
8	A	2011	LPE	C13-C14-C15-C16
6	A	2003	Y01	CAM-CAY-OAW-CBC
8	A	2019	LPE	O1-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	A	2030	PCW	C12-C13-C14-C15
8	A	2006	LPE	C12-C13-C14-C15
9	A	2007	1PW	CAJ-CAL-CAN-CAP
8	A	2011	LPE	C14-C15-C16-C17
10	A	2029	PCW	C20-C21-C22-C23
11	A	2031	P5S	C42-C43-C44-C45
8	A	2006	LPE	C13-C14-C15-C16
9	A	2007	1PW	CAP-CAR-CAT-CAU
10	A	2009	PCW	C35-C36-C37-C38
8	A	2015	LPE	C12-C13-C14-C15
10	A	2014[A]	PCW	C33-C34-C35-C36
8	A	2027	LPE	O2H-C2-C3-O3
8	A	2020	LPE	C16-C17-C18-C19
9	A	2007	1PW	CAA-CAJ-CAL-CAN
10	A	2009	PCW	C44-C45-C46-C47
8	A	2016	LPE	C16-C17-C18-C19
8	A	2011	LPE	C12-C13-C14-C15
8	A	2010	LPE	C12-C13-C14-C15
8	A	2018	LPE	C16-C17-C18-C19
6	A	2022	Y01	CAV-CBC-OAW-CAY
10	A	2029	PCW	C32-C33-C34-C35
10	A	2030	PCW	C35-C36-C37-C38
10	A	2013	PCW	O31-C31-O2-C2
10	A	2030	PCW	O3P-C1-C2-O2
8	A	2008	LPE	O1-C11-C12-C13
10	A	2009	PCW	C42-C43-C44-C45
8	A	2025	LPE	C14-C15-C16-C17
8	A	2005	LPE	C14-C15-C16-C17
10	A	2009	PCW	C33-C34-C35-C36
8	A	2006	LPE	O1-C1-C2-C3
8	A	2026	LPE	O1-C1-C2-C3
10	A	2012	PCW	C32-C33-C34-C35
5	A	2001	NAG	C1-C2-N2-C7
8	A	2015	LPE	C13-C14-C15-C16
8	A	2011	LPE	C18-C19-C20-C21
10	A	2009	PCW	C41-C42-C43-C44
6	A	2003	Y01	OAG-CAY-OAW-CBC
10	A	2012	PCW	O31-C31-O2-C2
10	A	2030	PCW	C21-C22-C23-C24
8	A	2026	LPE	O1-C1-C2-O2H
10	A	2012	PCW	C16-C17-C18-C19
8	A	2019	LPE	C12-C11-O1-C1

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Mol	Chain	Res	Type	Atoms
8	A	2006	LPE	C32-C31-O33-P
8	A	2017	LPE	C32-C31-O33-P
8	A	2018	LPE	C32-C31-O33-P
8	A	2019	LPE	C32-C31-O33-P
8	A	2020	LPE	C32-C31-O33-P
8	A	2025	LPE	C32-C31-O33-P
8	A	2026	LPE	C32-C31-O33-P
10	A	2013	PCW	C5-C4-O4P-P
8	A	2017	LPE	O1-C1-C2-C3
8	A	2017	LPE	C31-C32-N-C1N
8	A	2006	LPE	C18-C19-C20-C21
8	A	2025	LPE	C2-C3-O3-P
8	A	2016	LPE	C12-C11-O1-C1
8	A	2008	LPE	O33-C31-C32-N
10	A	2030	PCW	O4P-C4-C5-N
8	A	2017	LPE	C12-C11-O1-C1
8	A	2017	LPE	C31-C32-N-C2N
8	A	2005	LPE	C16-C17-C18-C19
10	A	2030	PCW	O3P-C1-C2-C3
8	A	2020	LPE	C11-C12-C13-C14
8	A	2006	LPE	C19-C20-C21-C22
8	A	2011	LPE	C2-C1-O1-C11
8	A	2018	LPE	C2-C1-O1-C11
10	A	2009	PCW	C36-C37-C38-C39
6	A	2003	Y01	CAJ-CAN-CBA-CAB
6	A	2003	Y01	CAO-CBB-CBE-CAP
8	A	2027	LPE	C12-C11-O1-C1
9	A	2007	1PW	CAQ-CAS-CAU-CAT
5	B	304	NAG	C3-C2-N2-C7
8	A	2006	LPE	C3-O3-P-O31
8	A	2008	LPE	C3-O3-P-O31
8	A	2008	LPE	C3-O3-P-O33
8	A	2008	LPE	C31-O33-P-O31
8	A	2010	LPE	C31-O33-P-O32
8	A	2011	LPE	C31-O33-P-O31
8	A	2017	LPE	C31-O33-P-O31
8	A	2018	LPE	C3-O3-P-O31
8	A	2018	LPE	C3-O3-P-O32
8	A	2018	LPE	C3-O3-P-O33
8	A	2018	LPE	C31-O33-P-O31
8	A	2019	LPE	C31-O33-P-O31
8	A	2020	LPE	C3-O3-P-O31

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Mol	Chain	Res	Type	Atoms
8	A	2025	LPE	C31-O33-P-O32
8	A	2032	LPE	C3-O3-P-O31
8	A	2032	LPE	C31-O33-P-O31
10	A	2012	PCW	C1-O3P-P-O2P
10	A	2014[B]	PCW	C4-O4P-P-O1P
10	A	2029	PCW	C4-O4P-P-O2P
11	A	2031	P5S	CB-OG-P12-O15
8	A	2020	LPE	C2-C1-O1-C11
8	A	2006	LPE	C2-C3-O3-P
8	A	2015	LPE	C2-C3-O3-P
6	A	2022	Y01	CAJ-CAO-CBB-CAC
6	A	2003	Y01	CAJ-CAN-CBA-CAA
10	A	2014[A]	PCW	C36-C37-C38-C39
10	A	2030	PCW	C36-C37-C38-C39
6	A	2023	Y01	CAJ-CAO-CBB-CAC
8	A	2005	LPE	C1-C2-C3-O3
11	A	2031	P5S	O37-C2-C3-O16
6	A	2023	Y01	CAR-CBC-OAW-CAY
10	A	2014[A]	PCW	O2-C2-C3-O3
10	A	2014[B]	PCW	O2-C2-C3-O3
10	A	2014[A]	PCW	C21-C22-C23-C24
8	A	2017	LPE	C31-C32-N-C3N
10	A	2009	PCW	C19-C20-C21-C22
8	A	2011	LPE	O1-C11-C12-C13
10	A	2013	PCW	C13-C14-C15-C16
10	A	2009	PCW	C40-C41-C42-C43
8	A	2016	LPE	C2-C1-O1-C11
8	A	2018	LPE	C13-C14-C15-C16
10	A	2030	PCW	O2-C2-C3-O3
9	A	2007	1PW	CAK-CAM-CAO-CAQ
8	A	2020	LPE	C2-C3-O3-P
8	A	2005	LPE	O1-C11-C12-C13
10	A	2009	PCW	C1-C2-C3-O3
10	A	2014[B]	PCW	C12-C13-C14-C15
6	A	2024	Y01	CAM-CAL-CAX-OAF
10	A	2014[B]	PCW	C36-C37-C38-C39
10	A	2013	PCW	C4-C5-N-C7
6	A	2021	Y01	CAM-CAL-CAX-OAF
11	A	2031	P5S	C43-C44-C45-C46
8	A	2028	LPE	C2-C3-O3-P
6	A	2022	Y01	CAM-CAL-CAX-OAF
10	A	2012	PCW	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
10	A	2013	PCW	C4-C5-N-C8
8	A	2025	LPE	C1-C2-C3-O3
9	A	2007	1PW	CAK-CAH-CAI-CAZ
8	A	2025	LPE	C2-C1-O1-C11
8	A	2015	LPE	C16-C17-C18-C19
10	A	2014[A]	PCW	C20-C21-C22-C23
8	A	2006	LPE	O1-C1-C2-O2H
6	A	2021	Y01	CAM-CAL-CAX-OAH
11	A	2031	P5S	C2-C3-O16-P12
10	A	2009	PCW	C14-C15-C16-C17
10	A	2009	PCW	O3P-C1-C2-O2
8	A	2018	LPE	C12-C11-O1-C1
10	A	2013	PCW	C17-C18-C19-C20
5	A	2001	NAG	C3-C2-N2-C7
10	A	2009	PCW	O3P-C1-C2-C3
8	A	2006	LPE	C12-C11-O1-C1
10	A	2009	PCW	C37-C38-C39-C40
10	A	2029	PCW	C17-C18-C19-C20
6	A	2022	Y01	CAM-CAL-CAX-OAH
8	A	2018	LPE	C14-C15-C16-C17
9	A	2007	1PW	CAV-OAX-PBB-OAD
6	A	2024	Y01	CAM-CAL-CAX-OAH
8	A	2010	LPE	C12-C11-O1-C1
6	A	2023	Y01	CAM-CAL-CAX-OAH
10	A	2014[B]	PCW	C20-C21-C22-C23
10	A	2030	PCW	C14-C15-C16-C17
10	A	2009	PCW	C39-C40-C41-C42
6	A	2023	Y01	CAM-CAL-CAX-OAF
8	A	2017	LPE	C12-C13-C14-C15
10	A	2029	PCW	C23-C24-C25-C26
10	A	2012	PCW	C37-C38-C39-C40
10	A	2030	PCW	C17-C18-C19-C20
10	A	2013	PCW	C4-C5-N-C6
10	A	2014[B]	PCW	C21-C22-C23-C24
10	A	2014[B]	PCW	C33-C34-C35-C36
10	A	2030	PCW	O2-C31-C32-C33
8	A	2017	LPE	O1-C1-C2-O2H
9	A	2007	1PW	CAM-CAO-CAQ-CAS
8	A	2005	LPE	C2-C3-O3-P
8	A	2015	LPE	C15-C16-C17-C18
8	A	2006	LPE	C15-C16-C17-C18
8	A	2017	LPE	C13-C14-C15-C16

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
8	A	2006	LPE	C16-C17-C18-C19
10	A	2030	PCW	C2-C1-O3P-P
8	A	2005	LPE	O1-C1-C2-C3
8	A	2025	LPE	O2H-C2-C3-O3
8	A	2016	LPE	C12-C13-C14-C15
10	A	2014[A]	PCW	C12-C13-C14-C15
10	A	2030	PCW	C1-C2-C3-O3
10	A	2014[B]	PCW	O2-C31-C32-C33
11	A	2031	P5S	O37-C38-C39-C40
10	A	2030	PCW	C24-C25-C26-C27
8	B	305	LPE	C2-C1-O1-C11
10	A	2009	PCW	O3-C11-C12-C13
10	A	2030	PCW	C33-C34-C35-C36
10	A	2030	PCW	O31-C31-C32-C33
10	A	2014[A]	PCW	O2-C31-C32-C33
8	A	2006	LPE	C11-C12-C13-C14

There are no ring outliers.

32 monomers are involved in 139 short contacts:

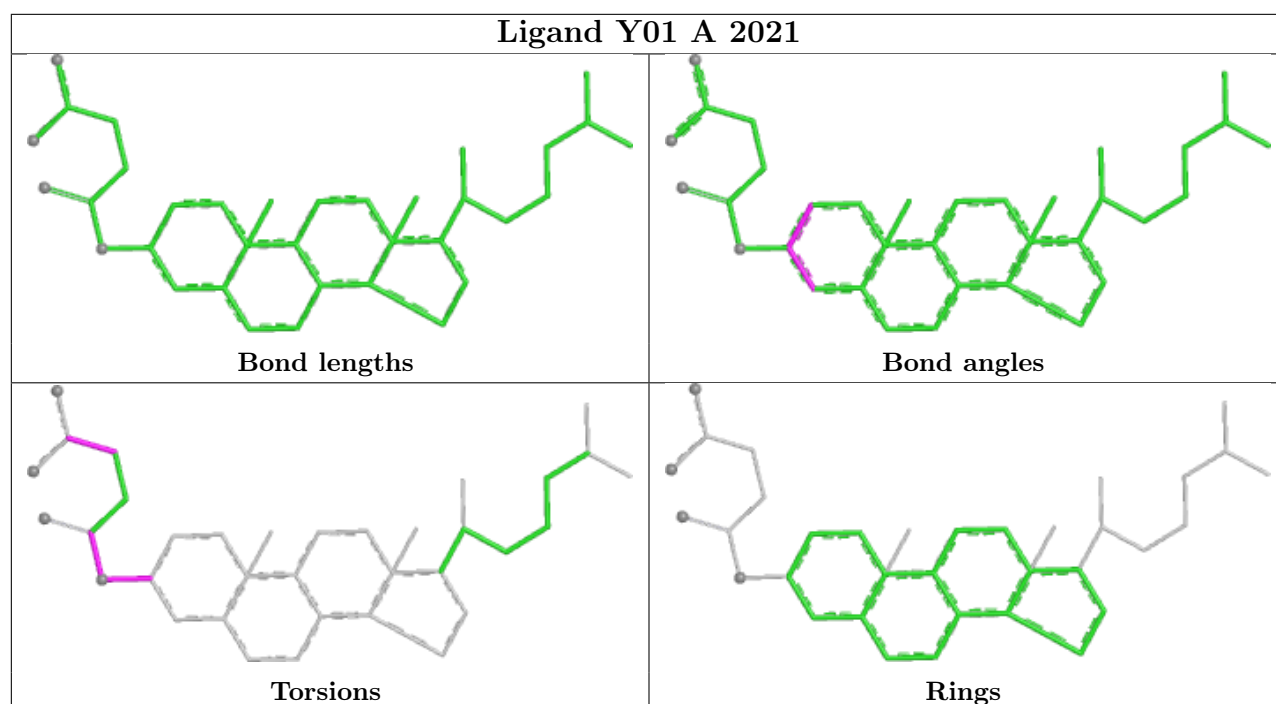
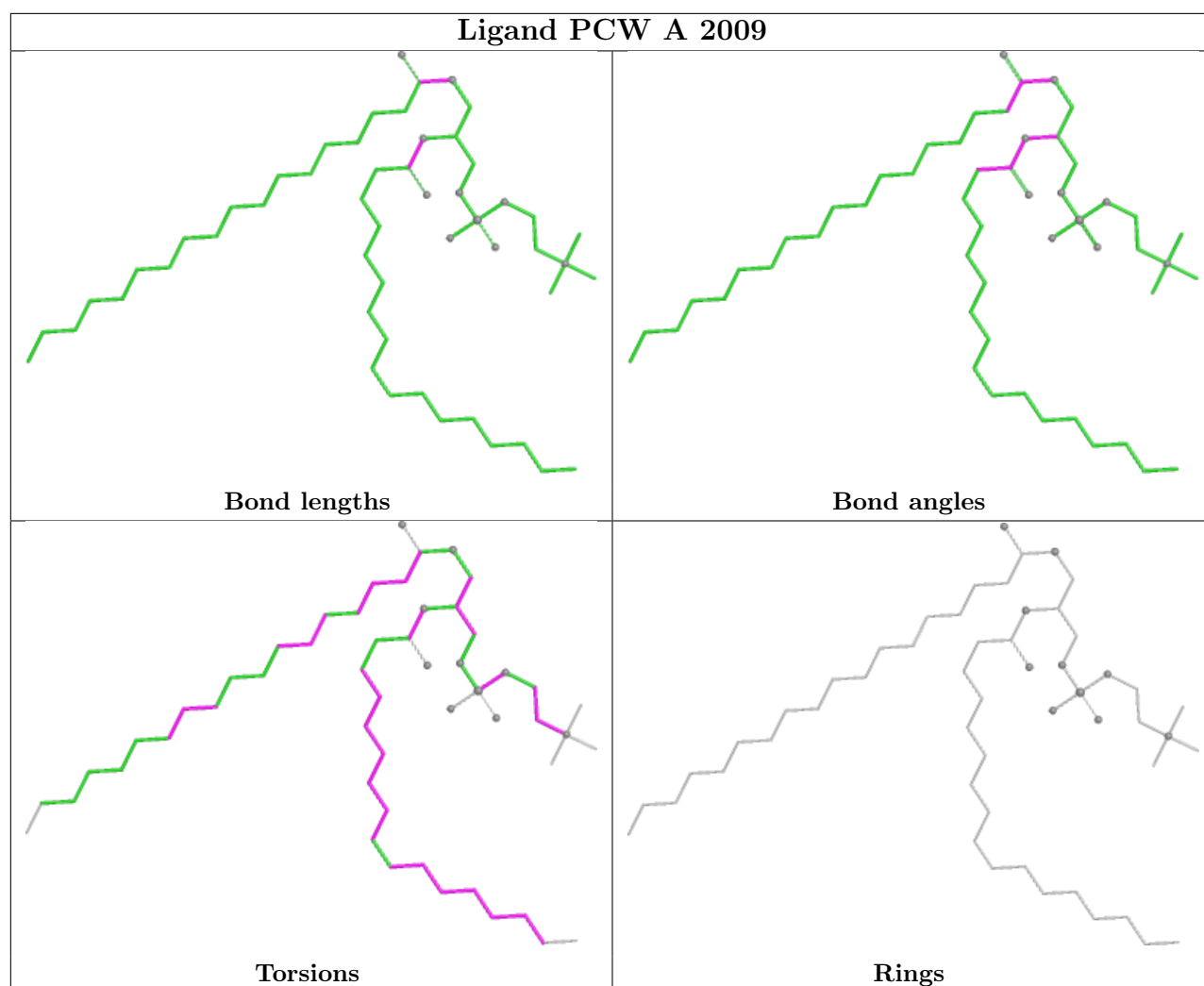
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	NAG	1	0
10	A	2009	PCW	3	0
6	A	2021	Y01	33	0
8	A	2019	LPE	1	0
8	A	2006	LPE	9	0
8	A	2028	LPE	1	0
8	A	2026	LPE	1	0
8	A	2005	LPE	2	0
8	A	2015	LPE	1	0
8	A	2010	LPE	1	0
10	A	2014[B]	PCW	8	0
9	A	2007	1PW	4	0
6	A	2022	Y01	9	0
10	A	2029	PCW	3	0
8	A	2027	LPE	6	0
10	A	2013	PCW	7	0
7	A	2004	CLR	4	0
8	B	305	LPE	1	0
10	A	2014[A]	PCW	4	0
8	A	2016	LPE	1	0
6	A	2023	Y01	12	0

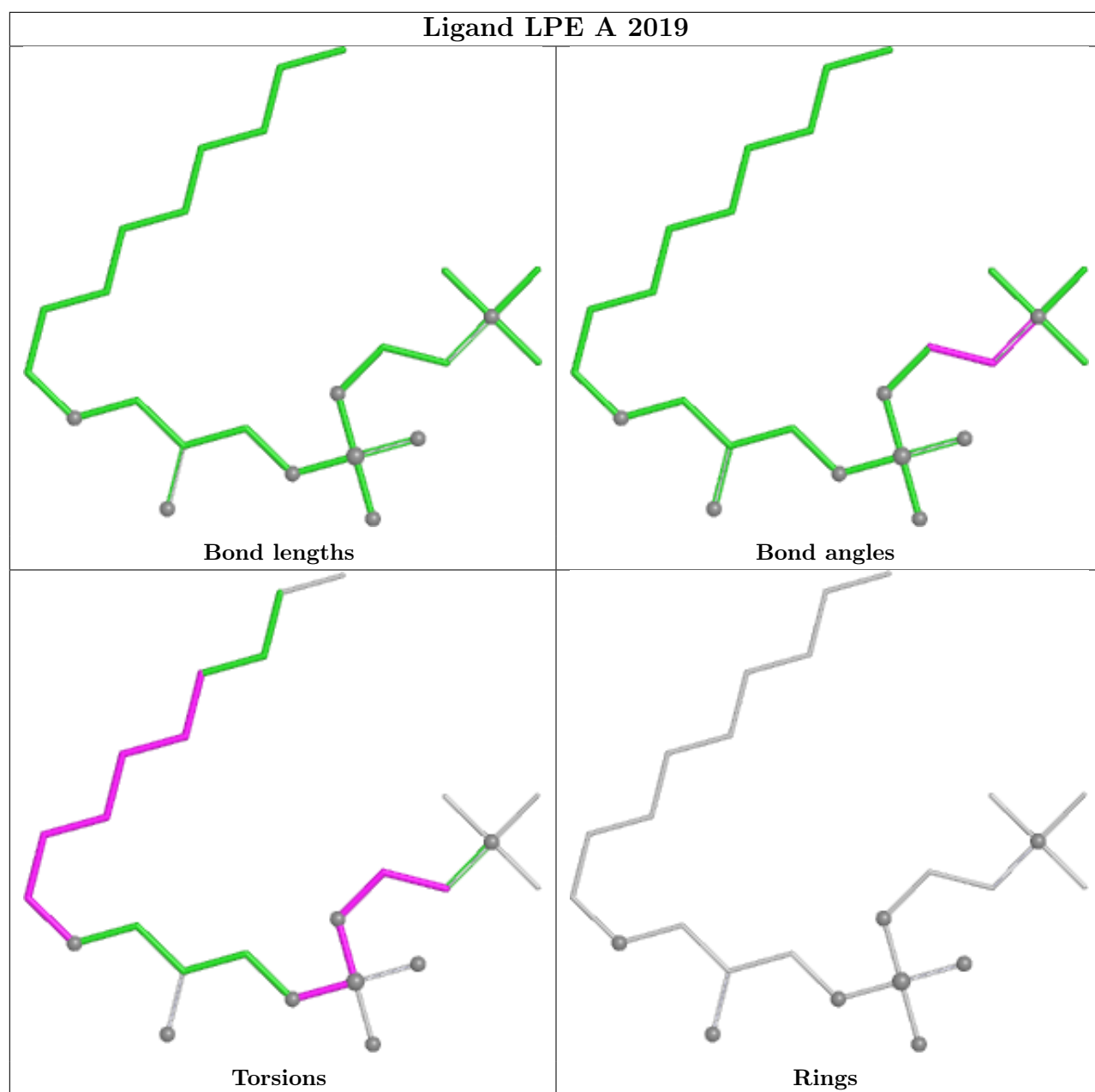
*Continued on next page...*

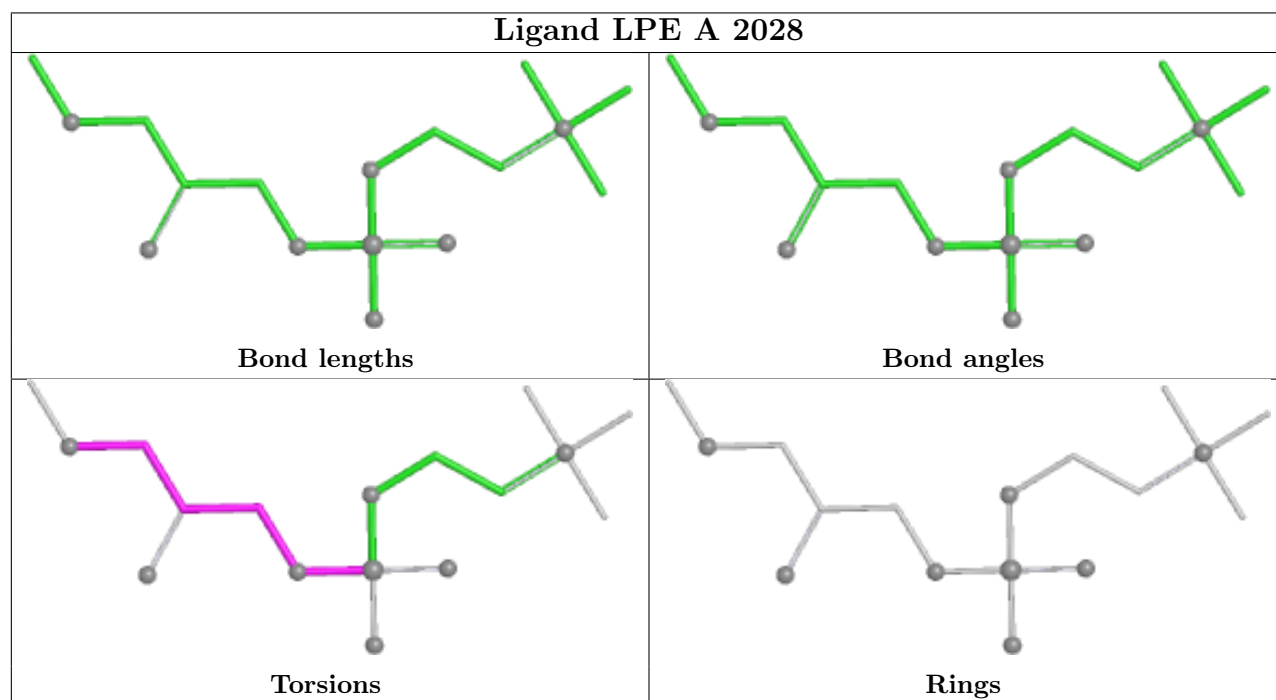
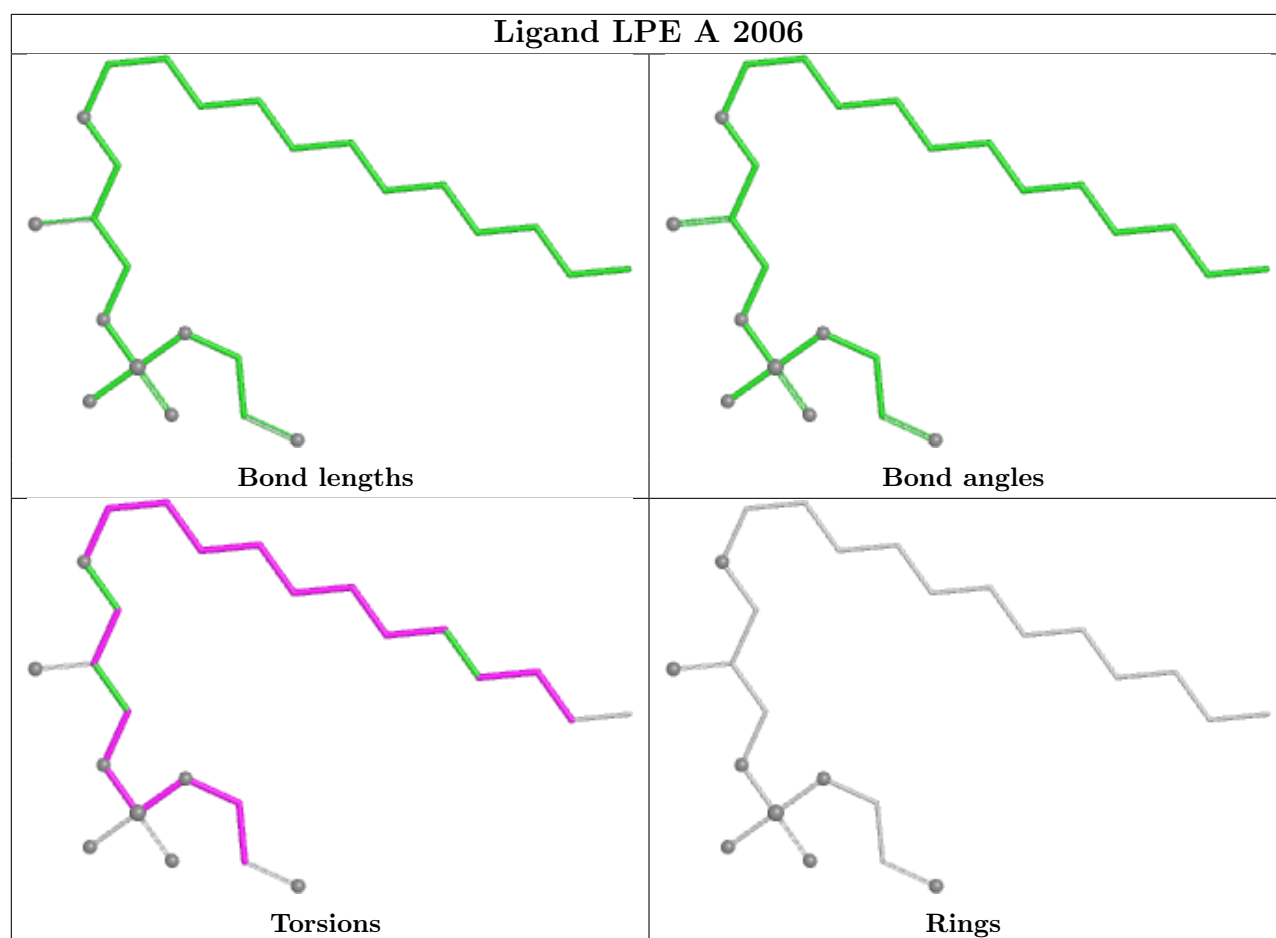
*Continued from previous page...*

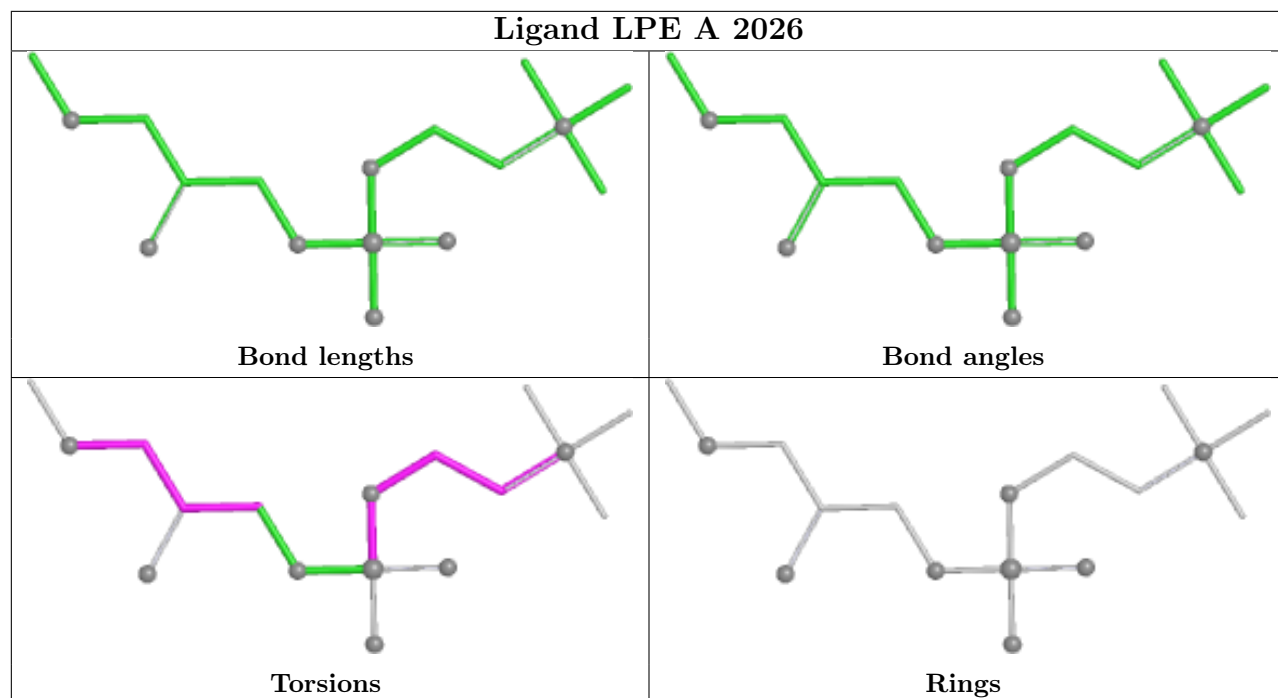
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2025	LPE	1	0
10	A	2012	PCW	3	0
6	A	2003	Y01	6	0
8	A	2032	LPE	6	0
6	A	2024	Y01	9	0
8	A	2008	LPE	1	0
8	A	2011	LPE	1	0
8	A	2020	LPE	1	0
5	B	301	NAG	2	0
8	A	2017	LPE	1	0
8	A	2018	LPE	5	0

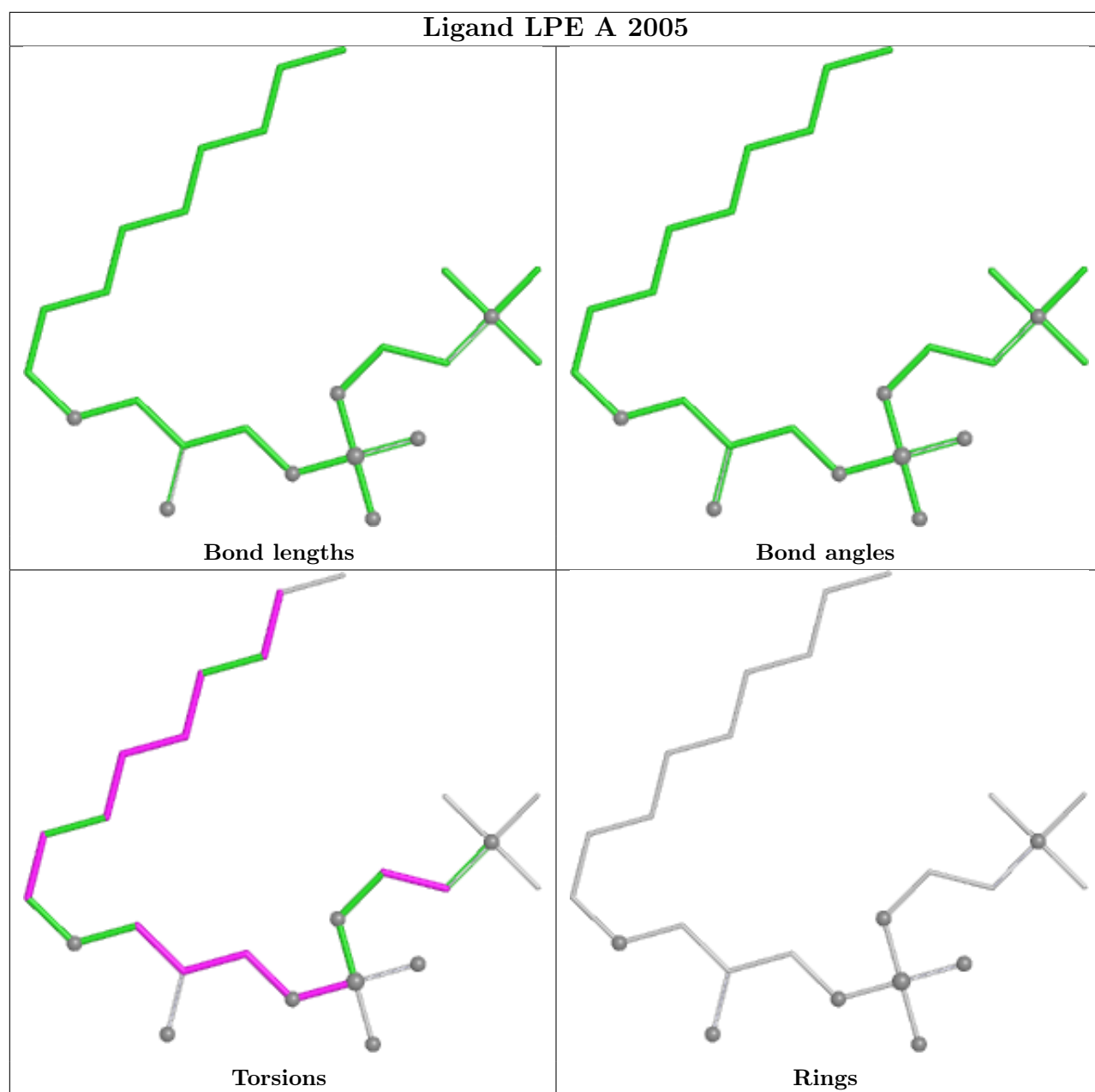
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

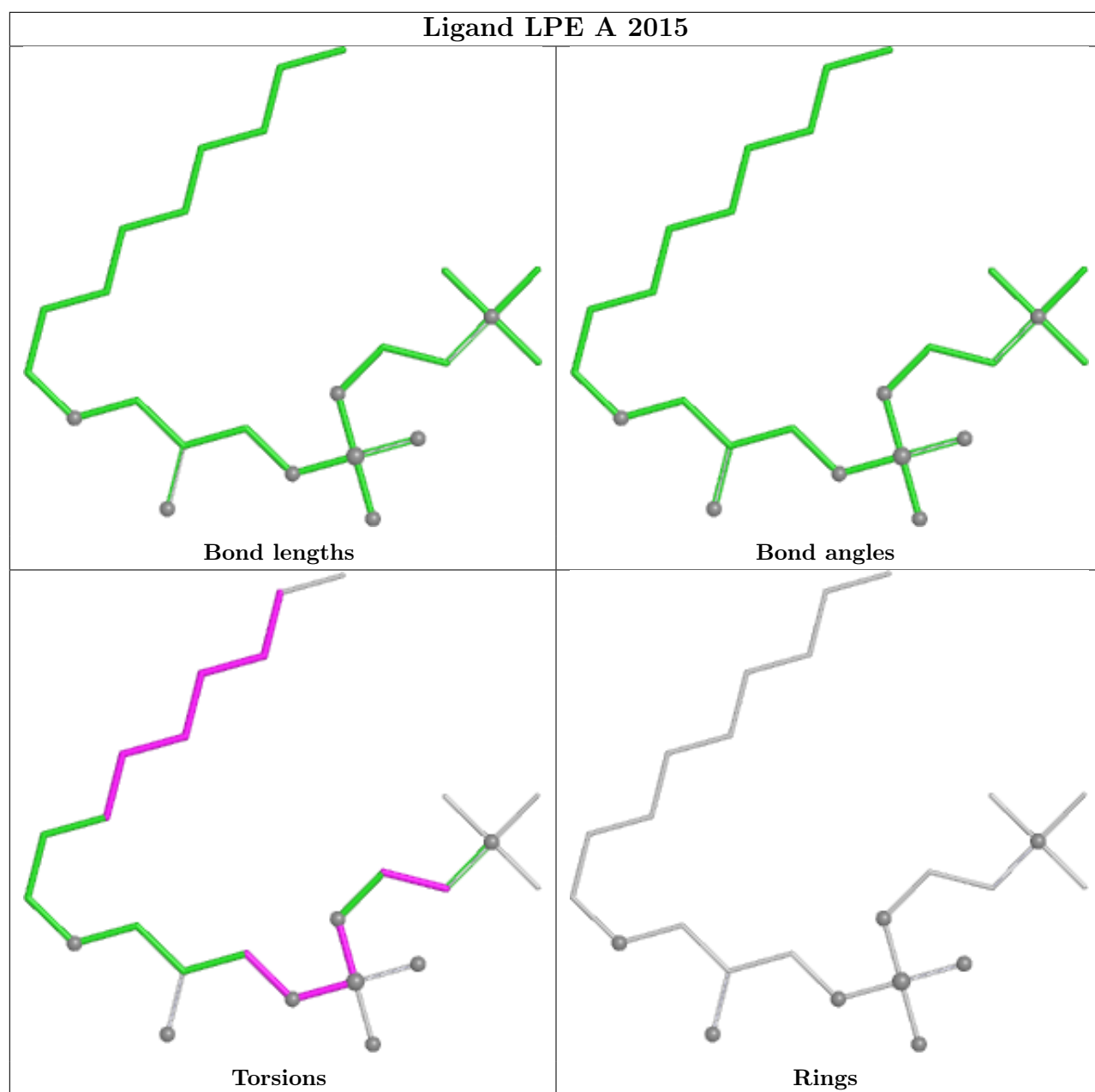


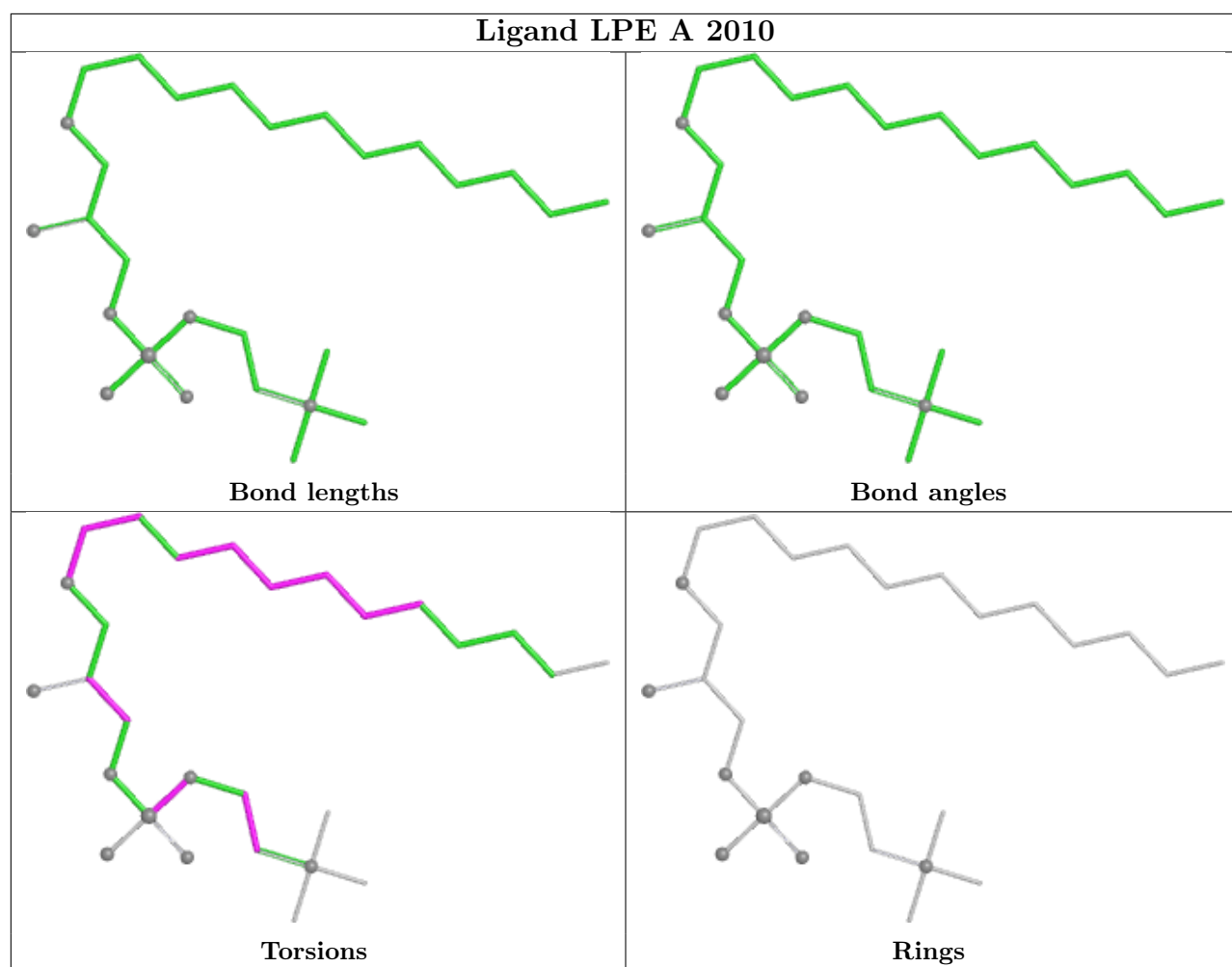


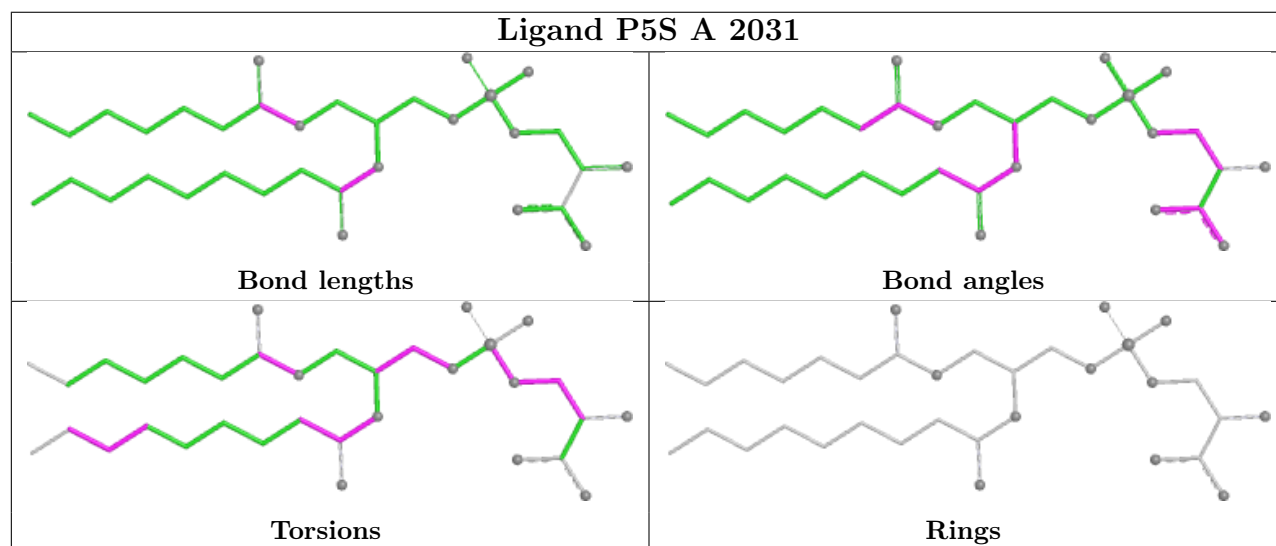
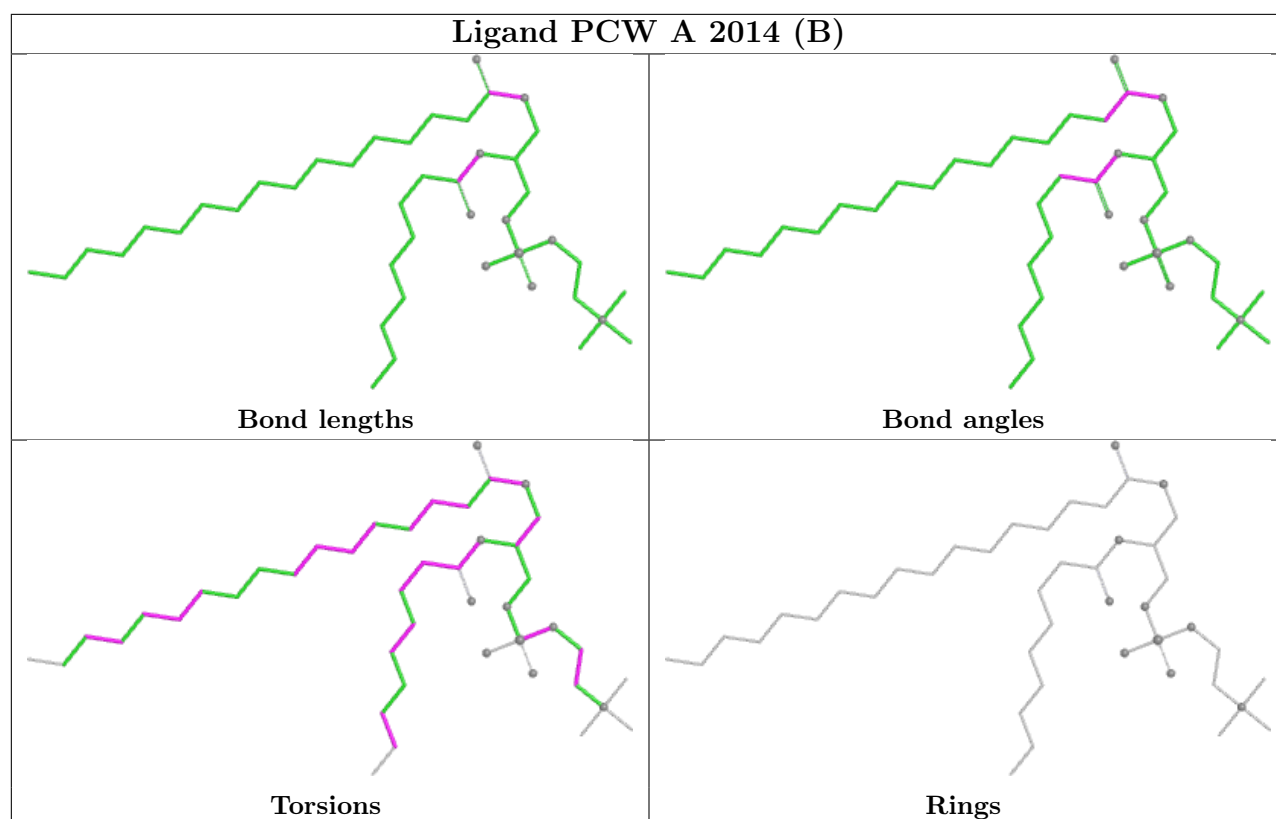


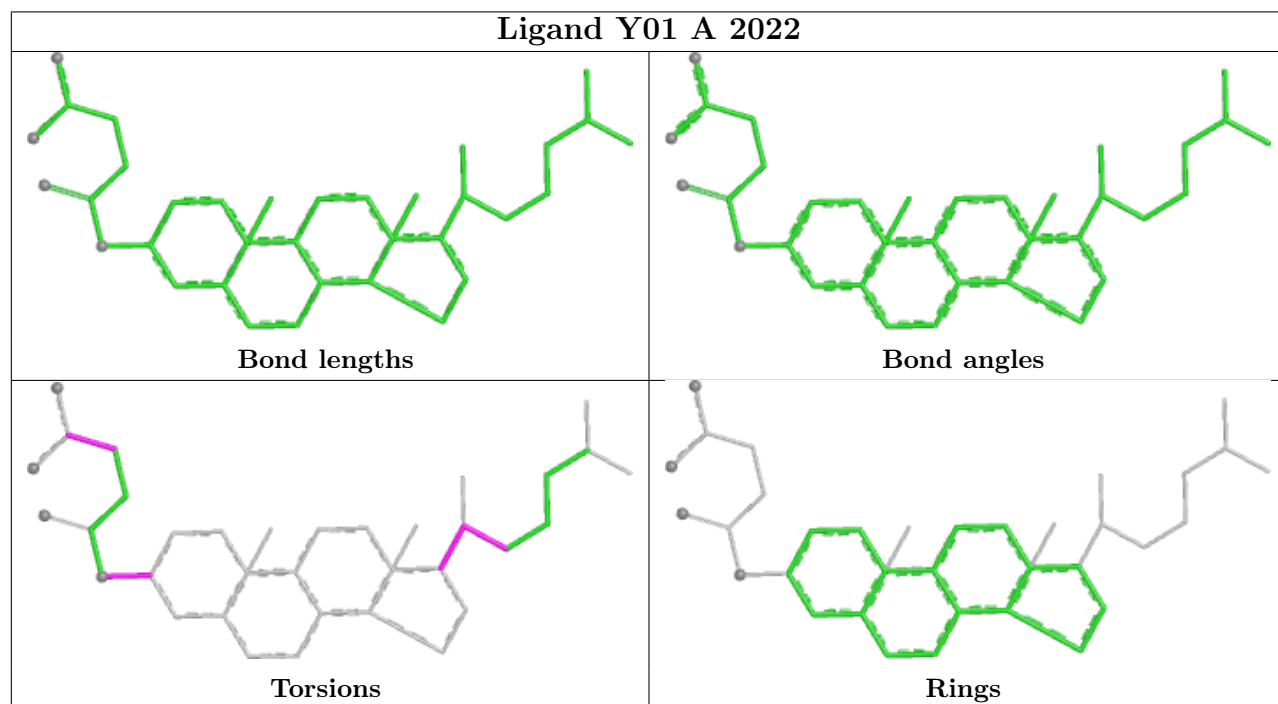
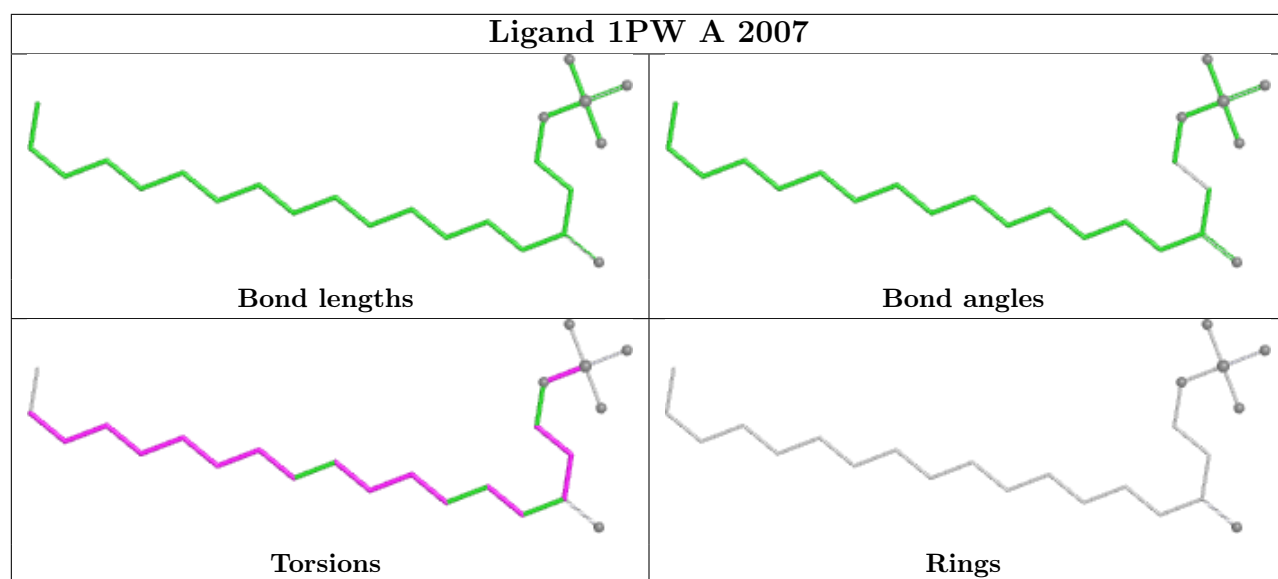


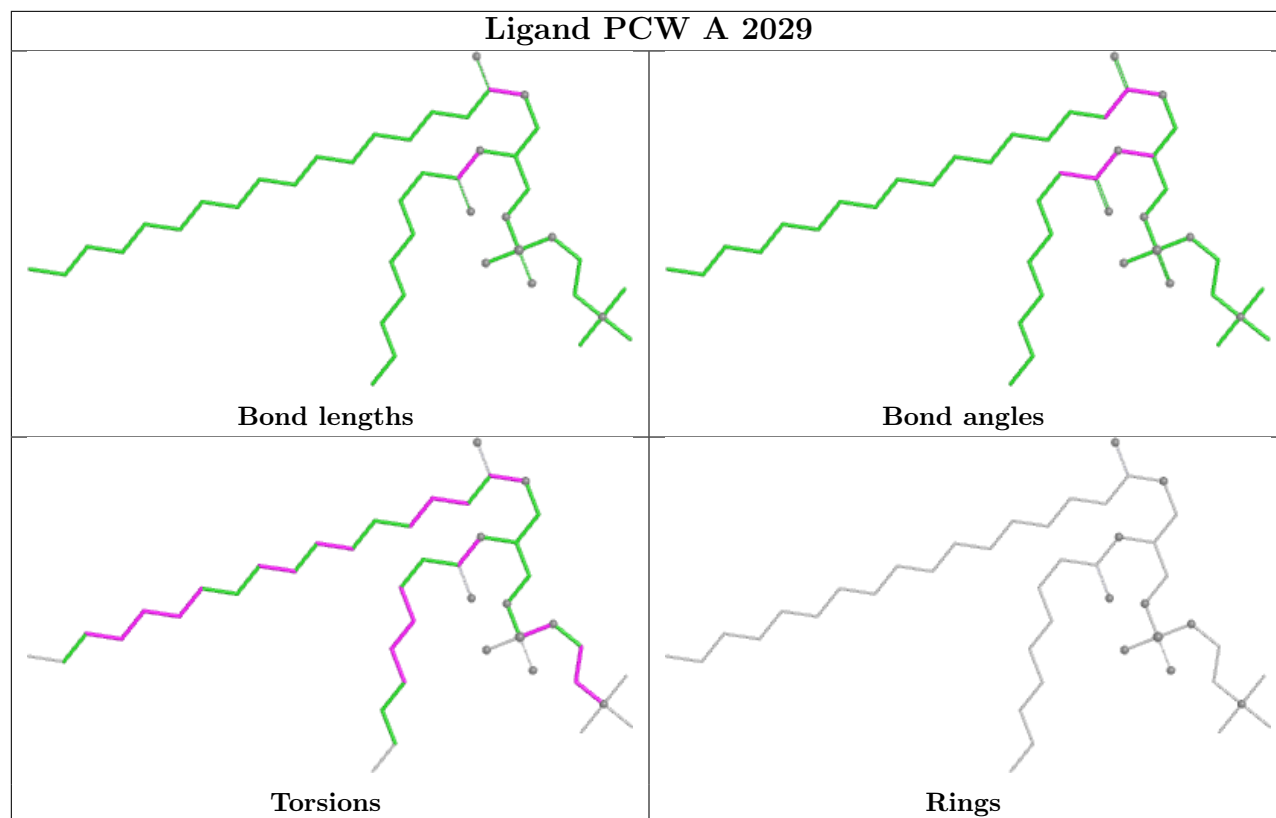


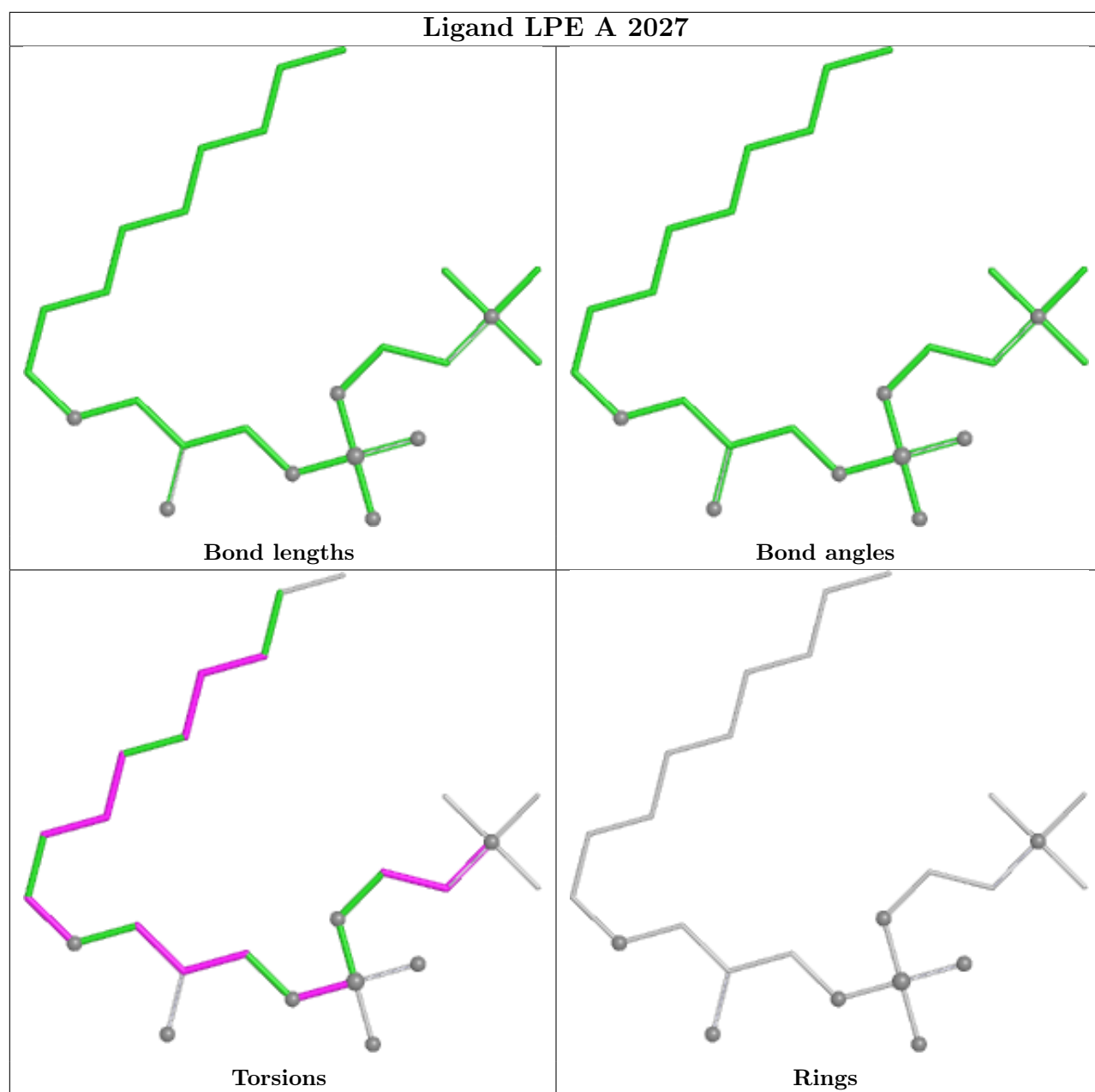


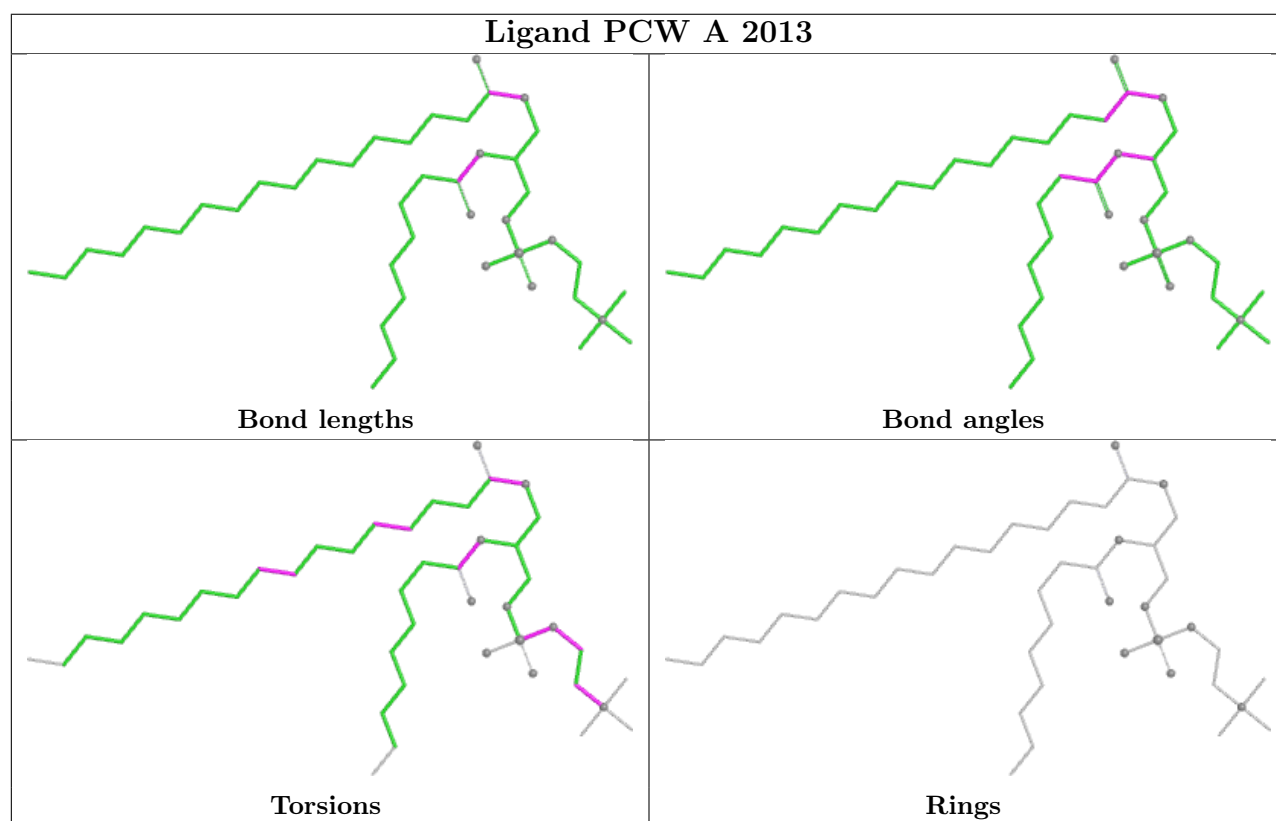
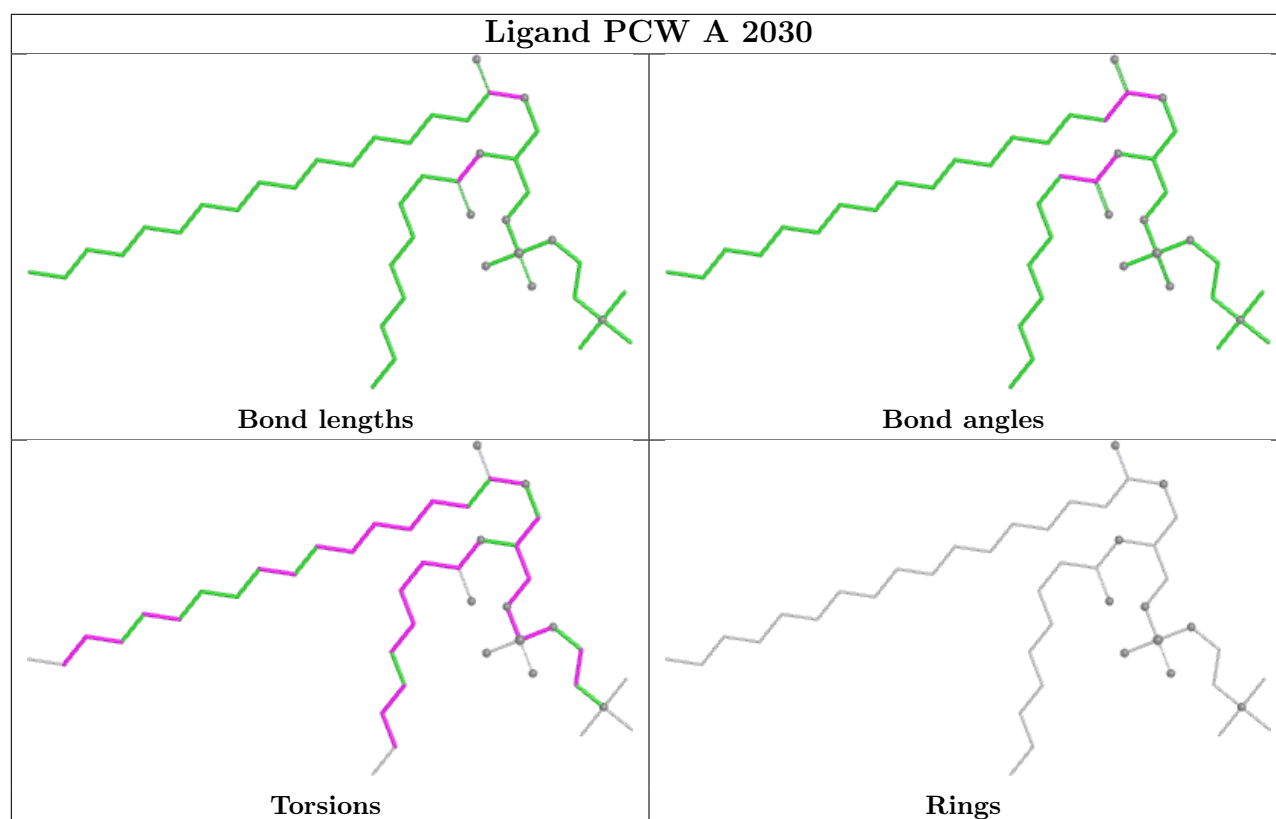


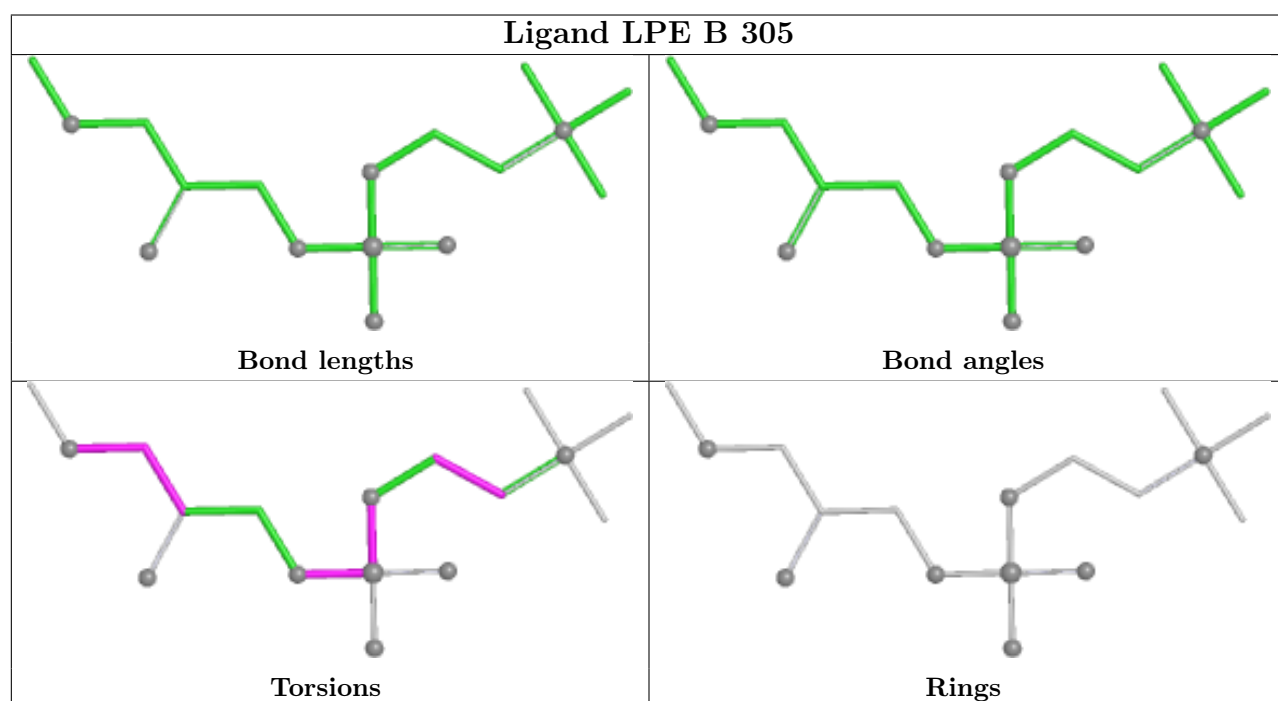
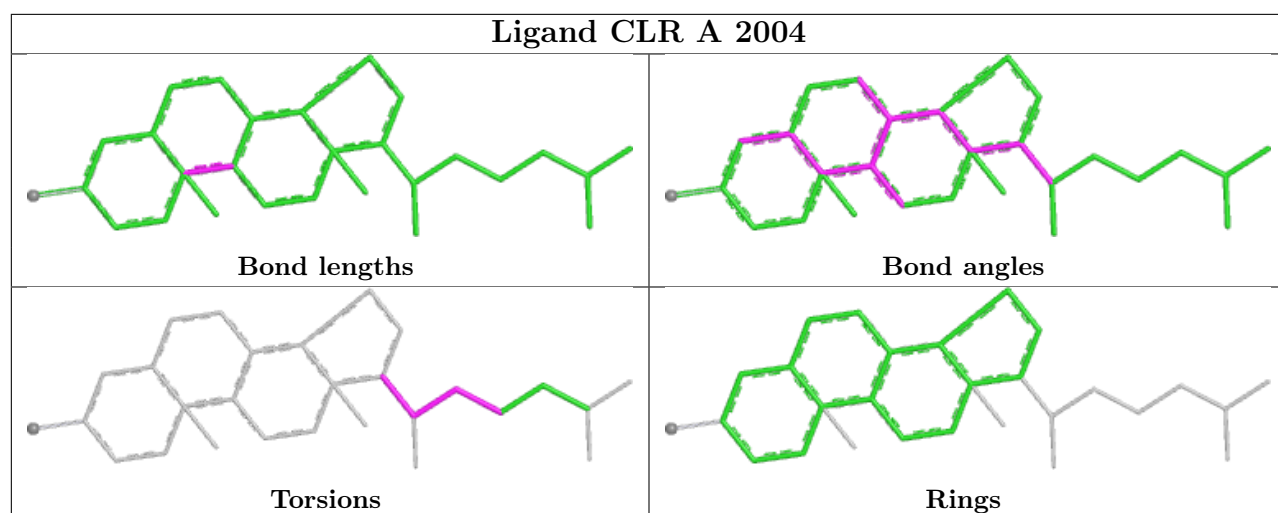


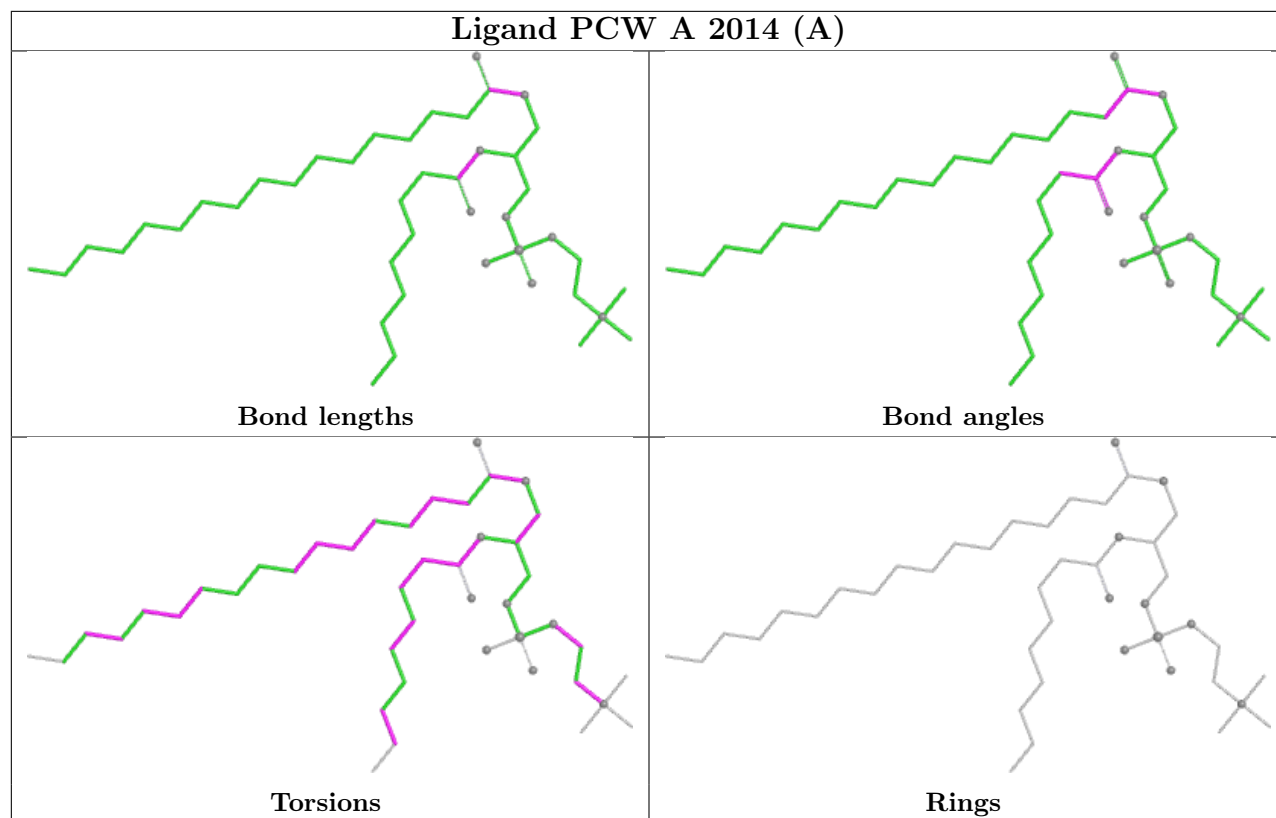


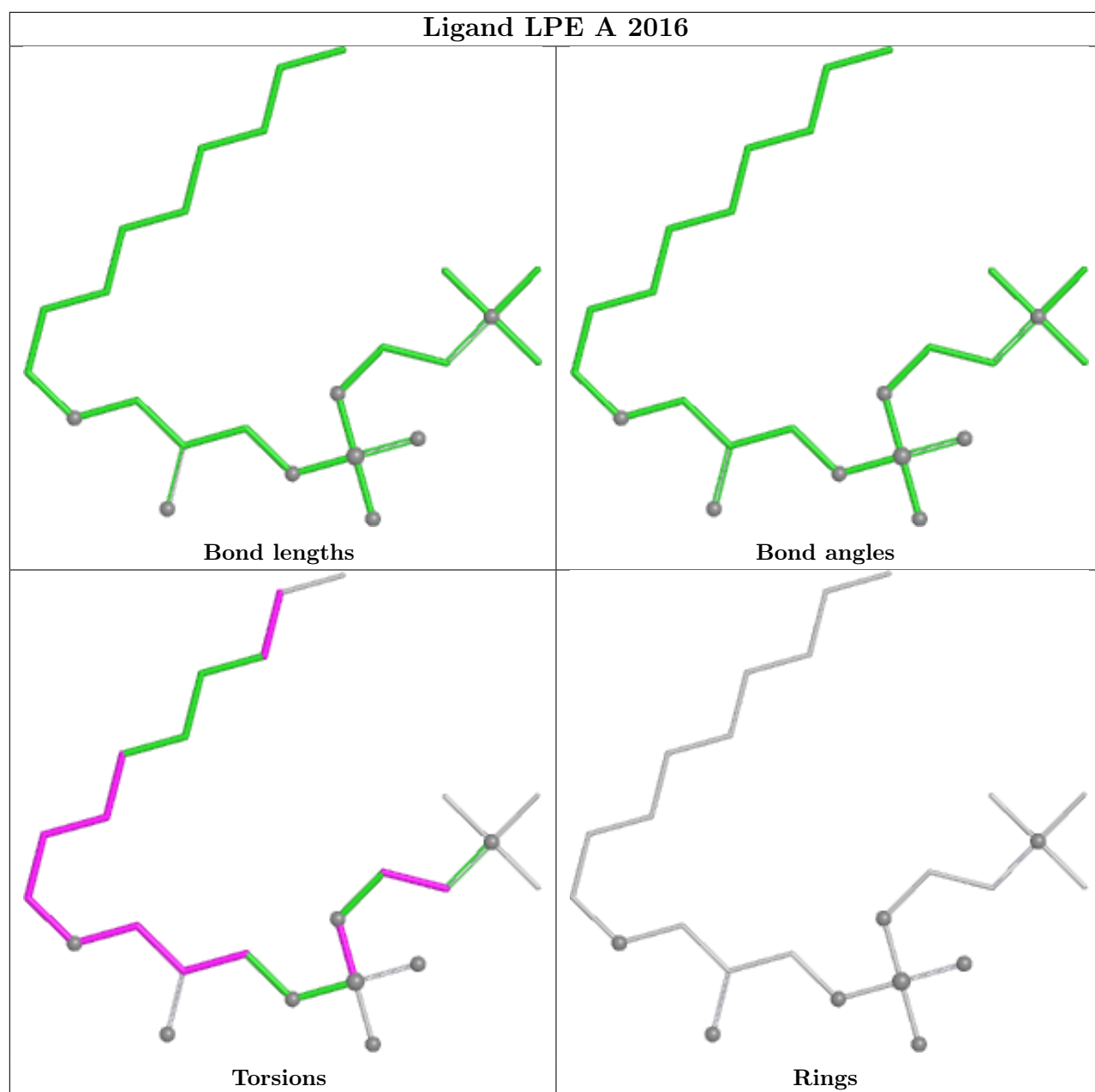


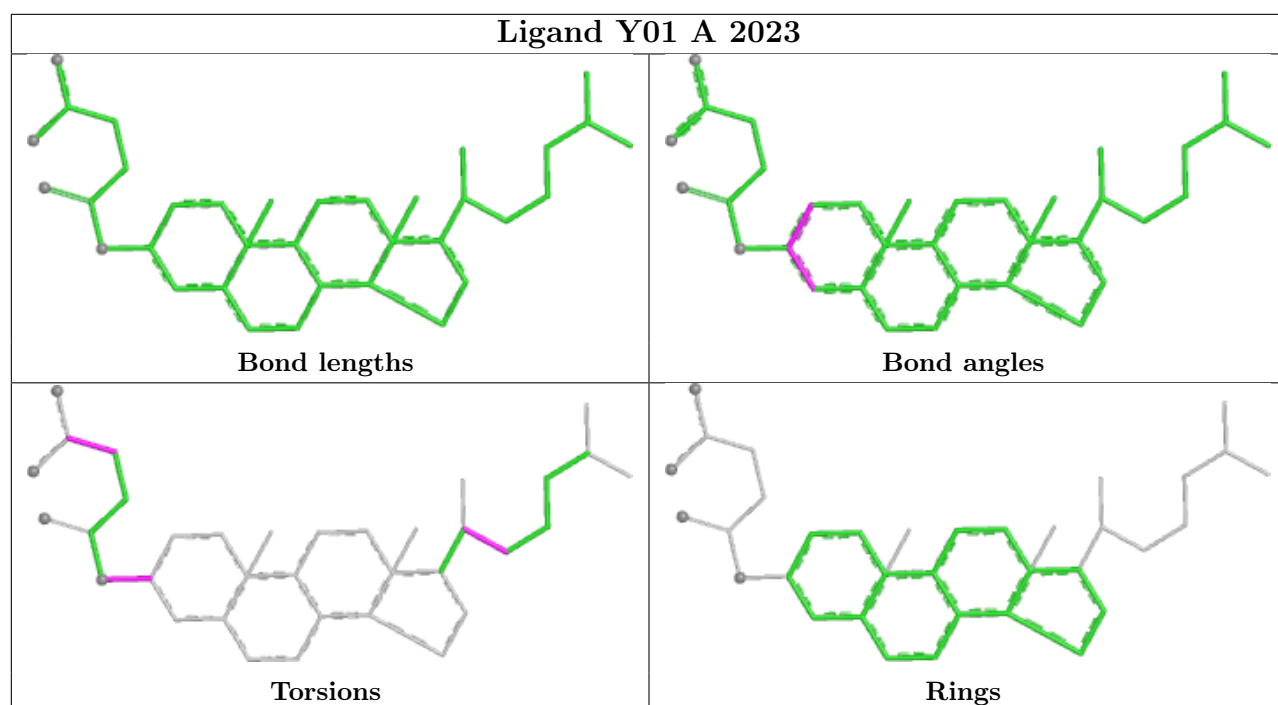


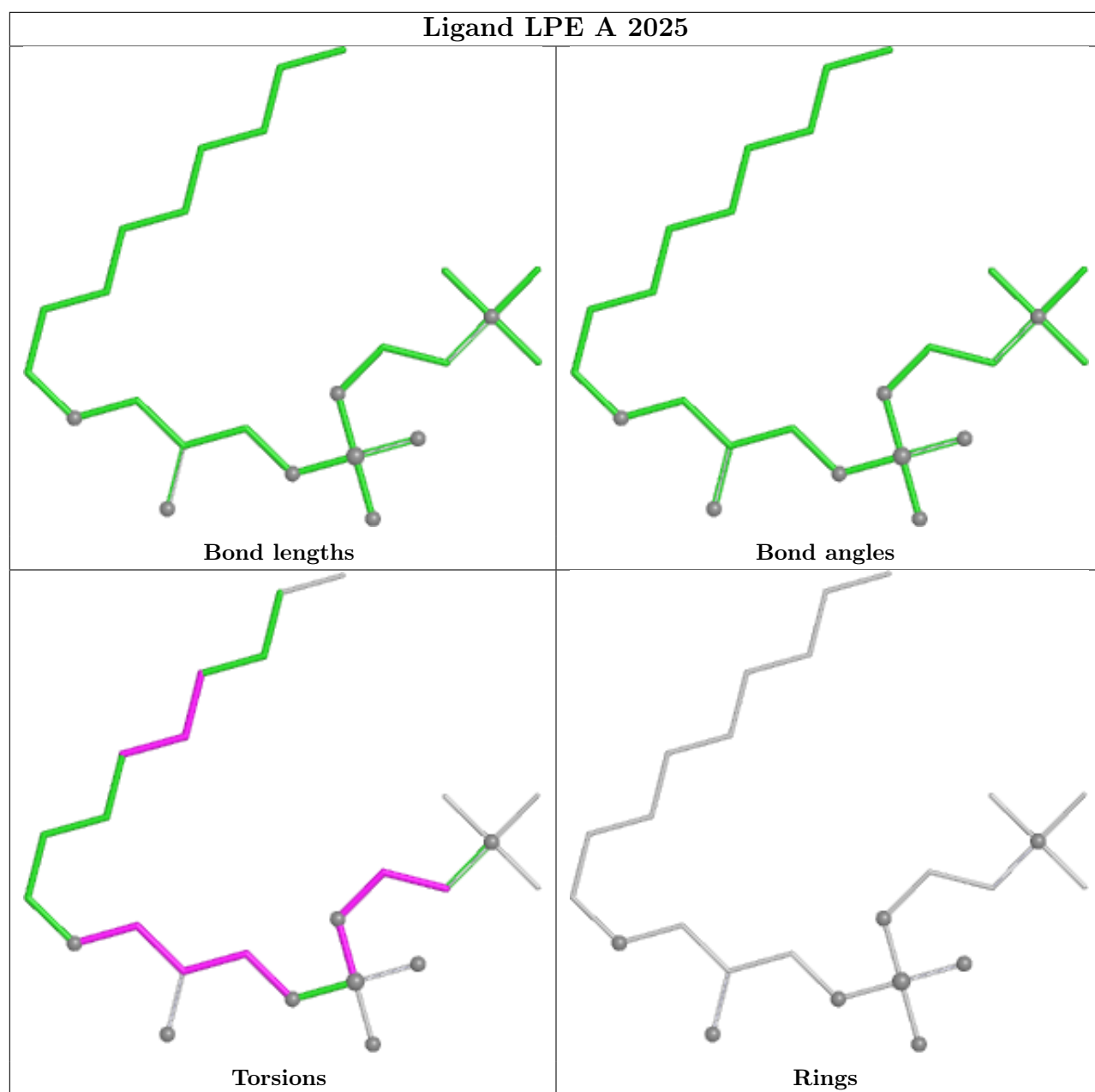


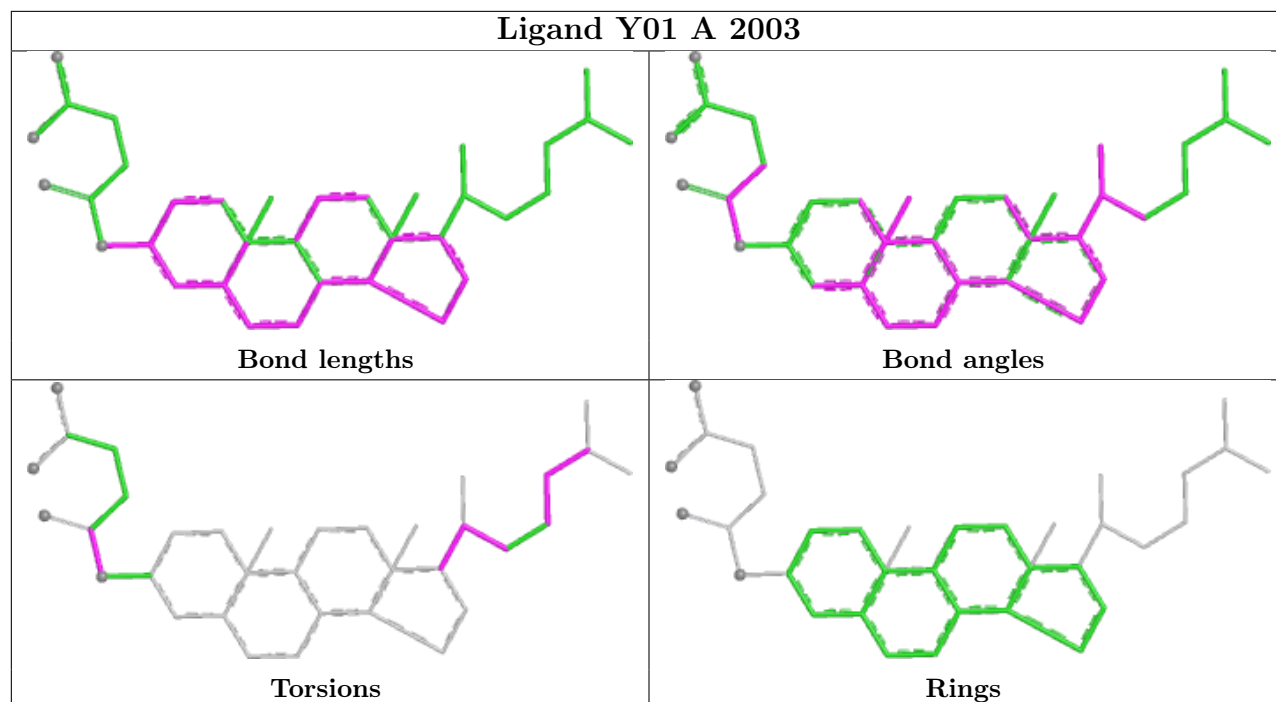
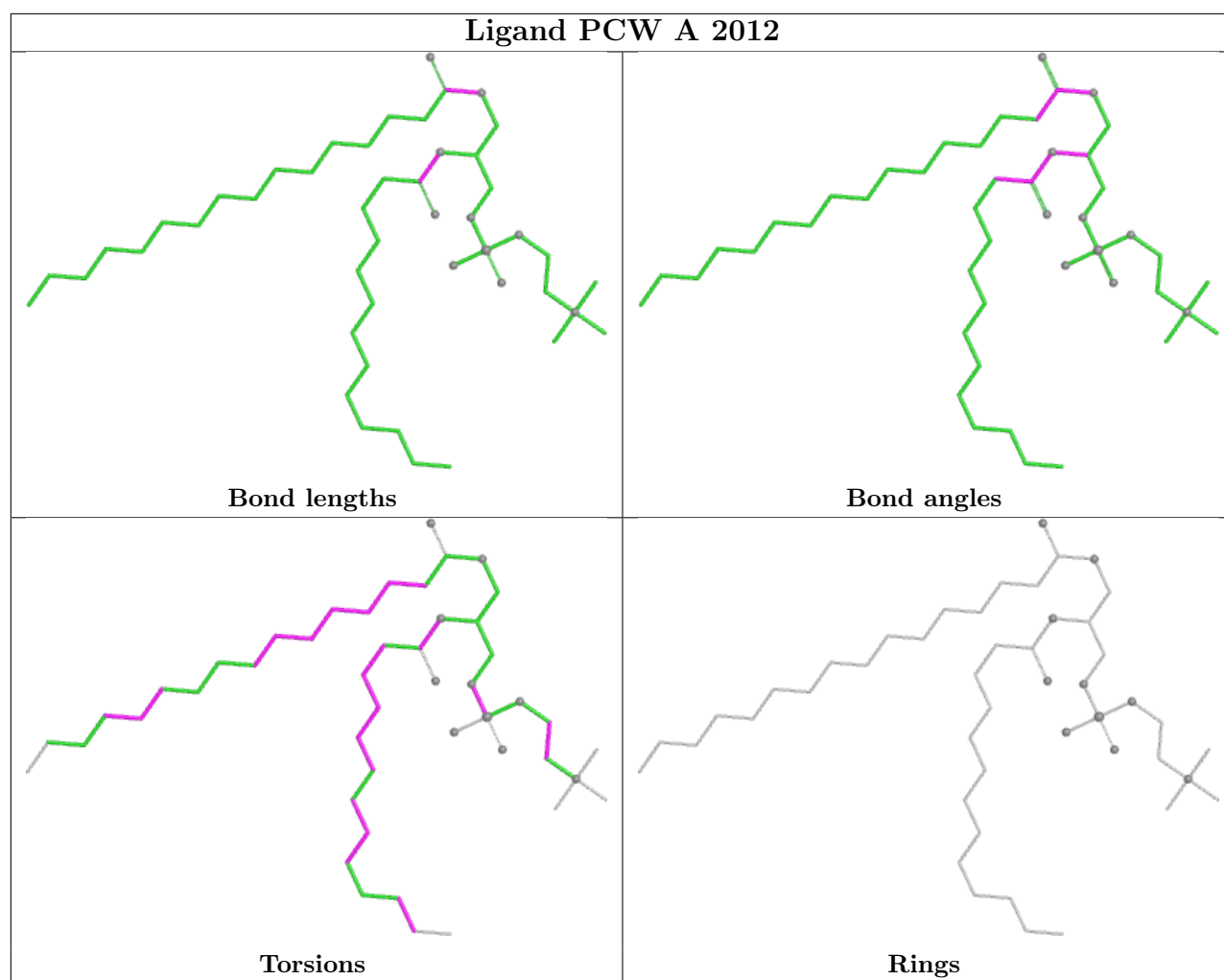


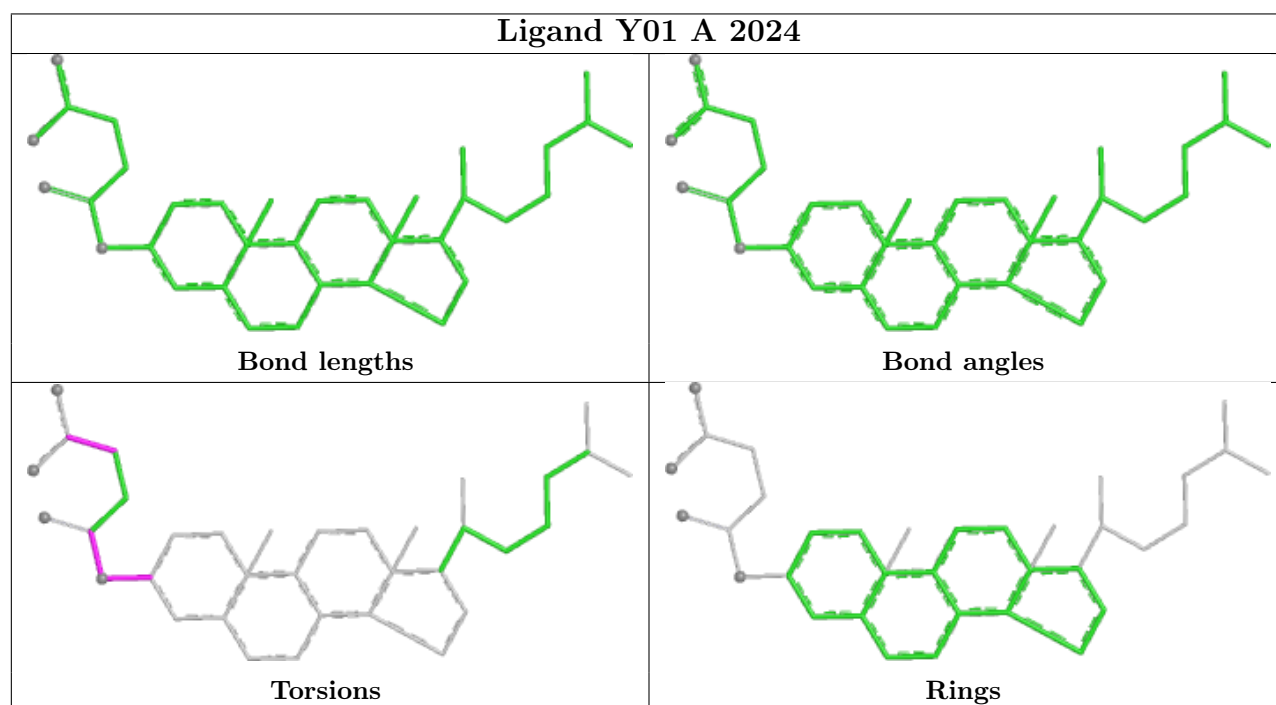
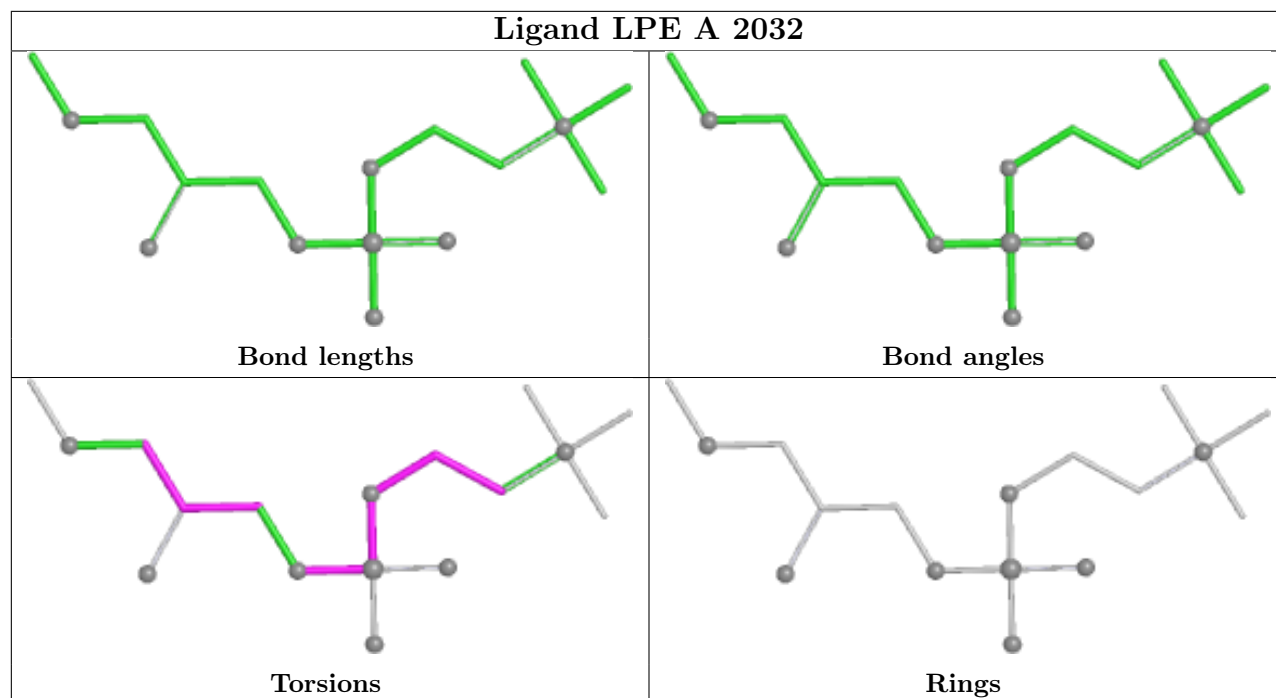


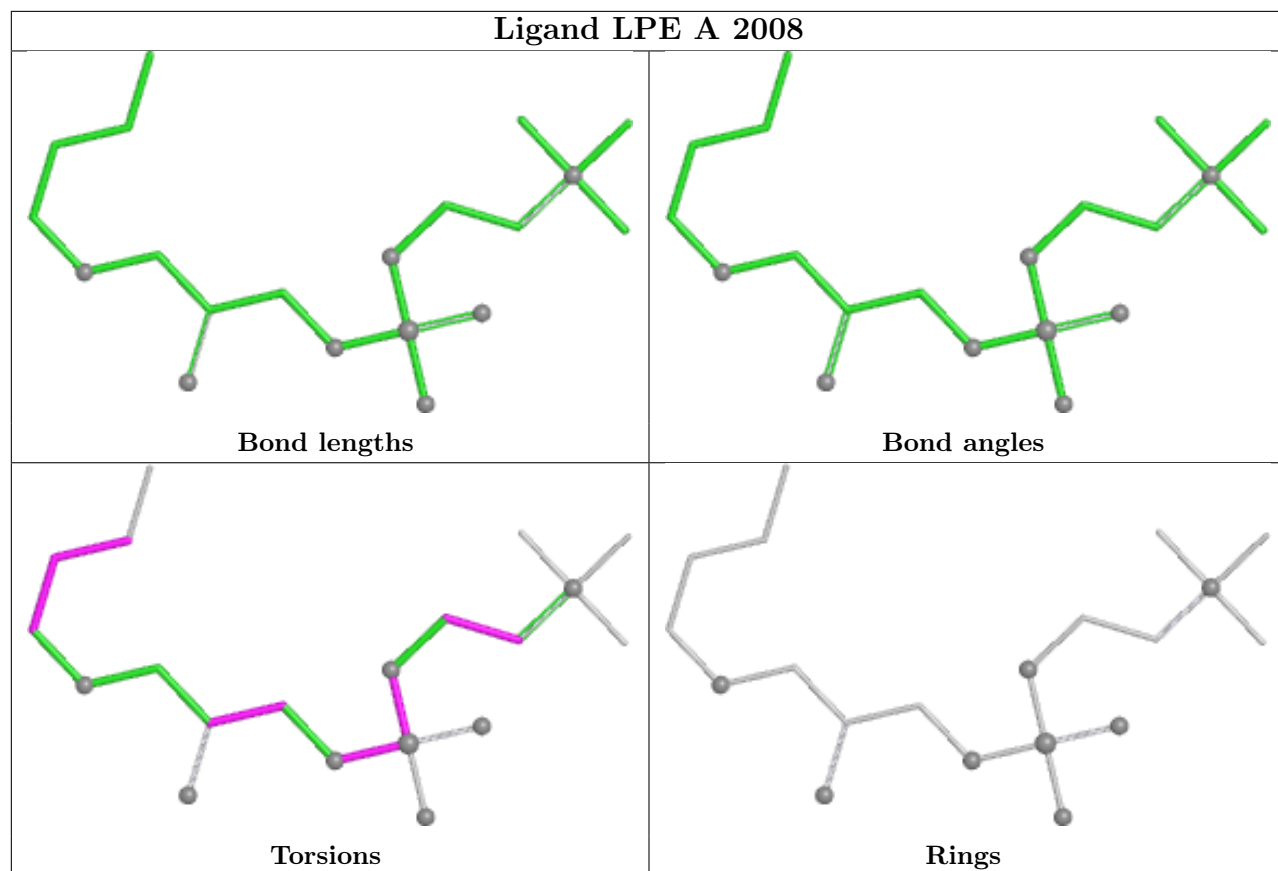


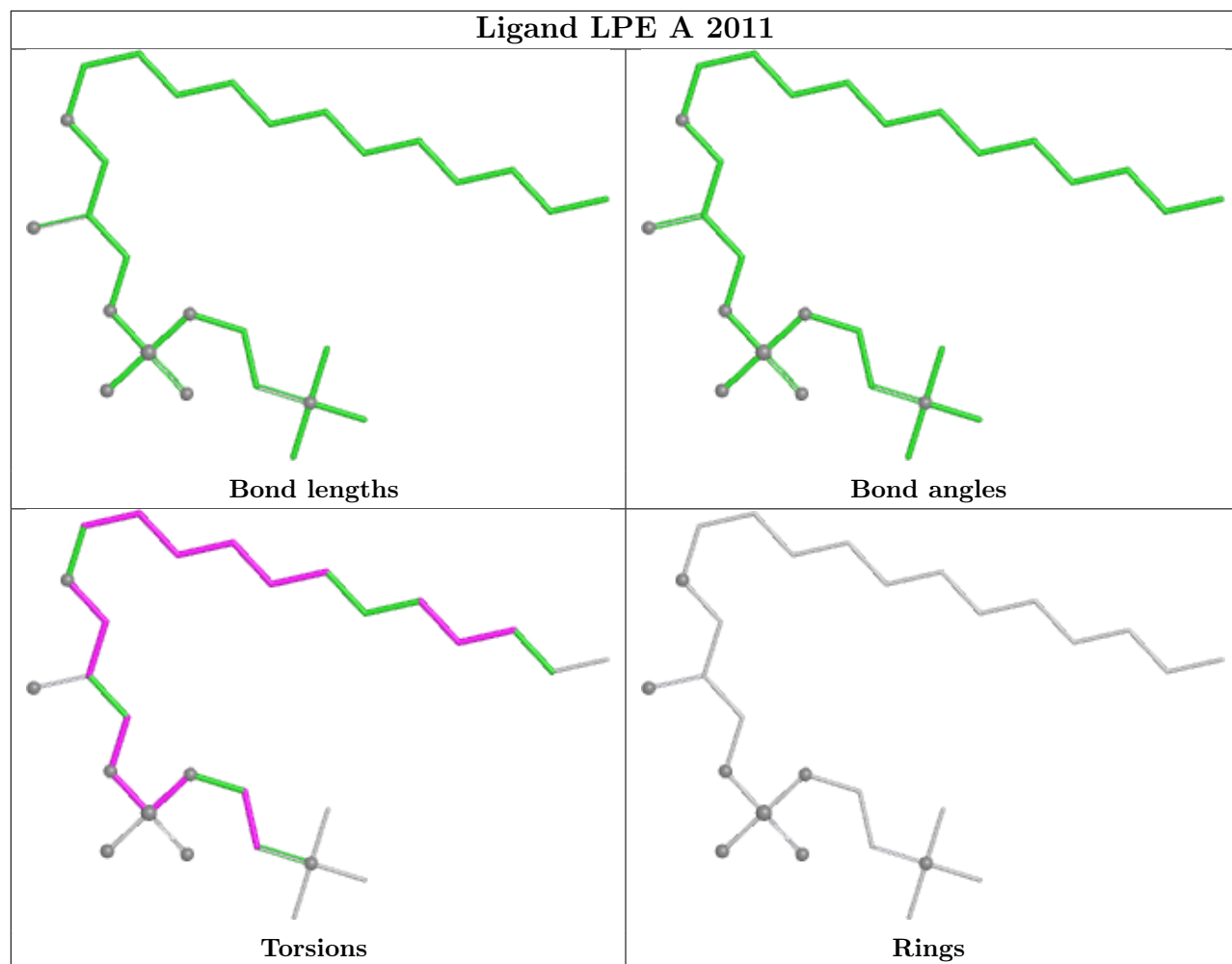


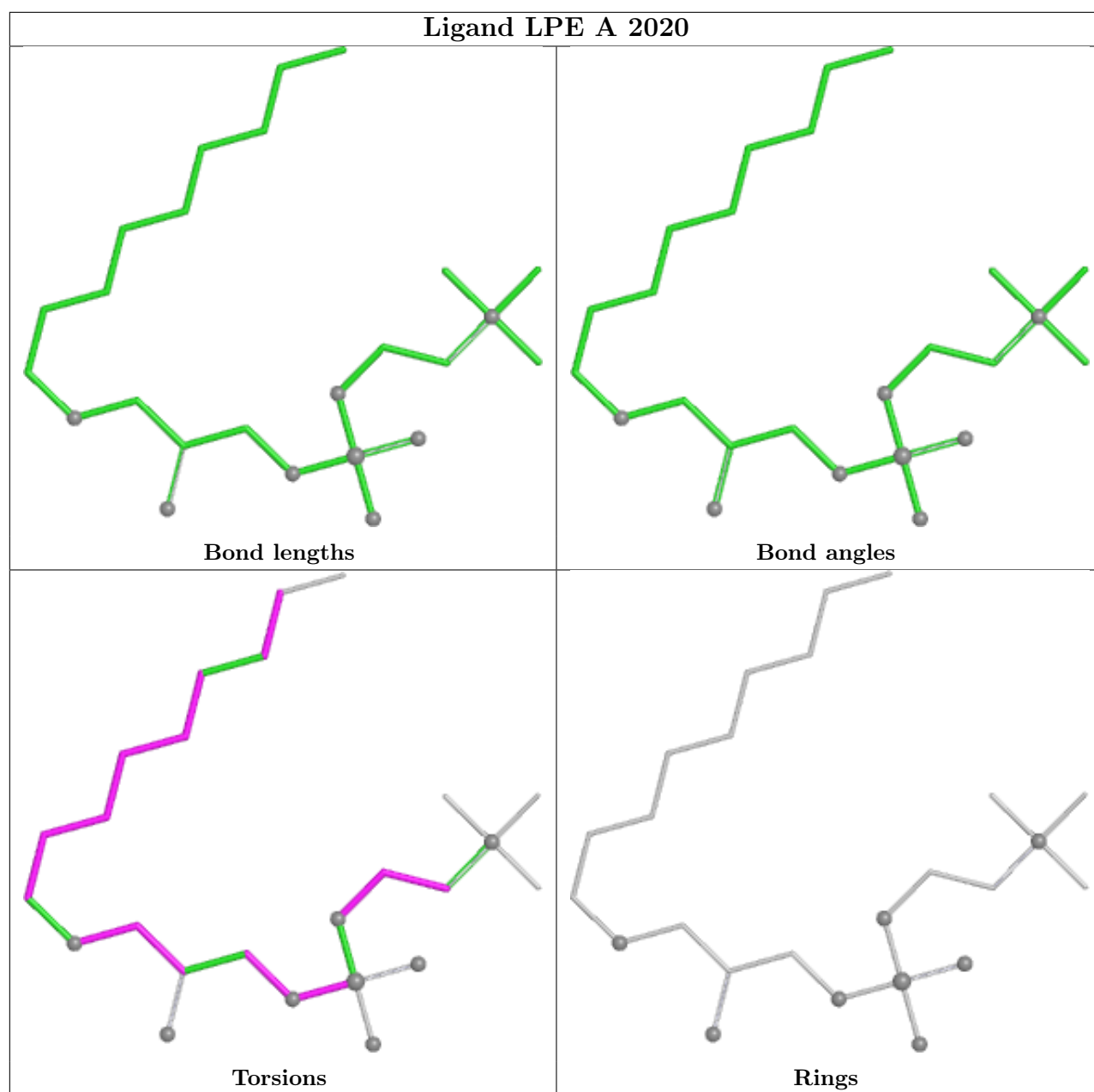


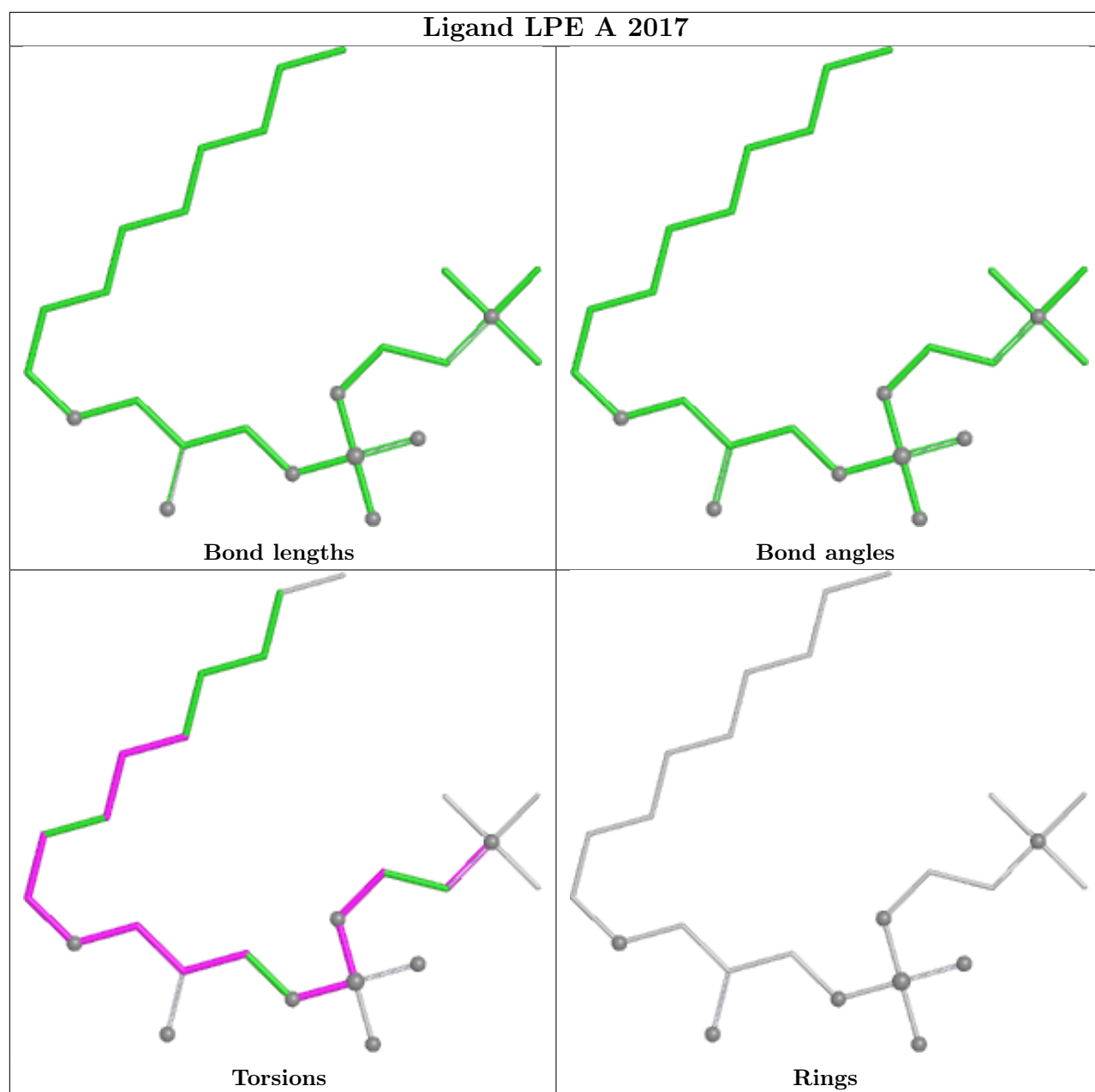


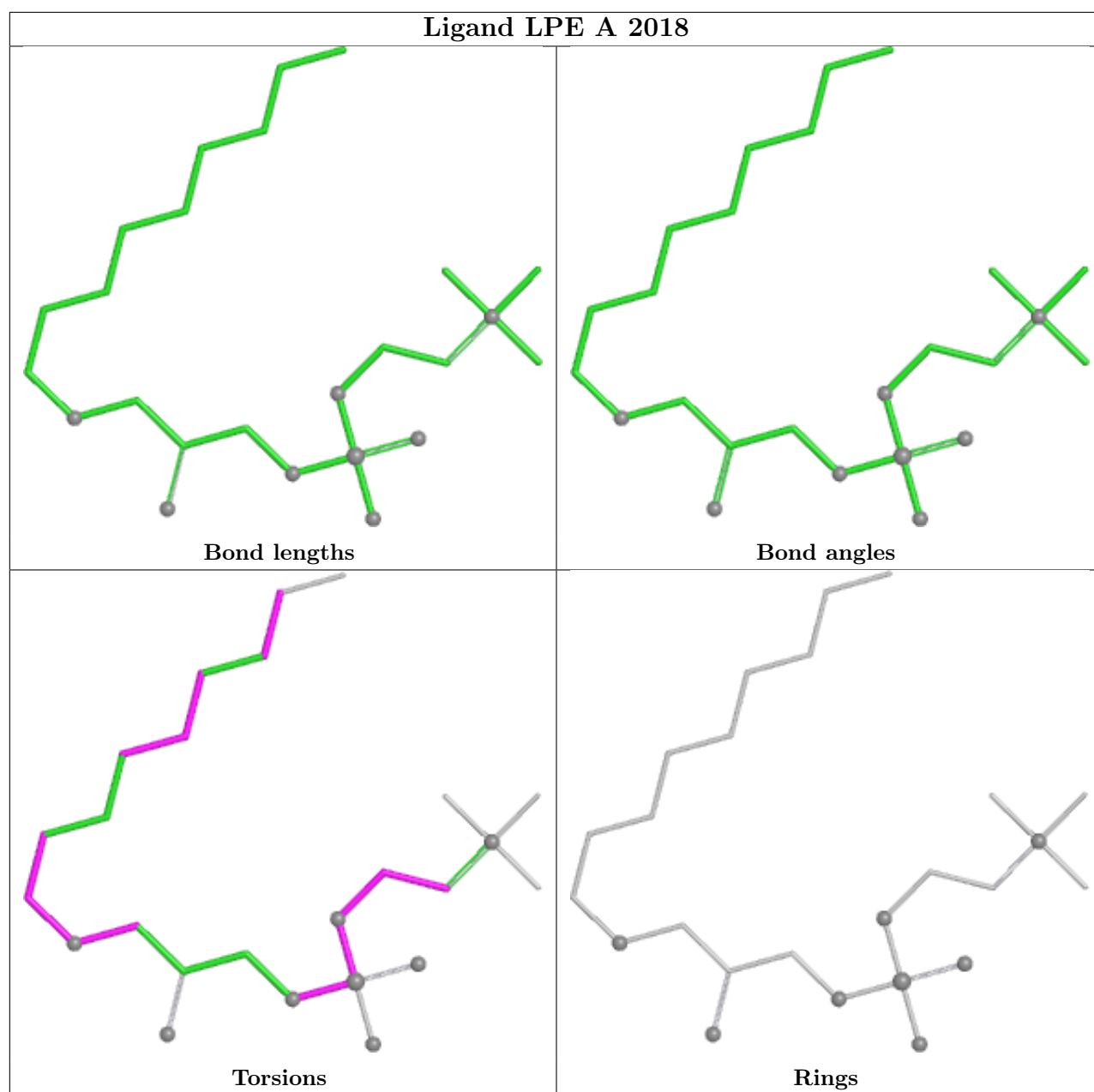












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

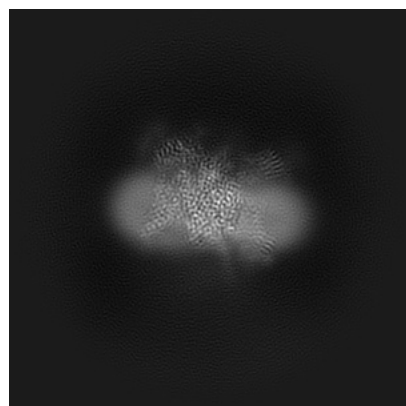
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33485. These allow visual inspection of the internal detail of the map and identification of artifacts.

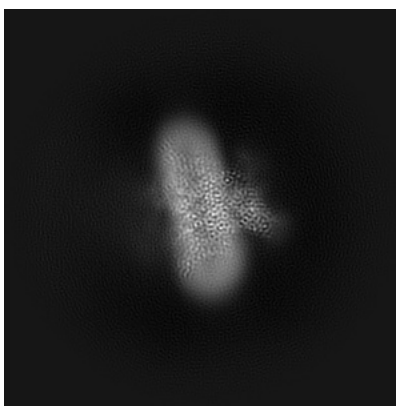
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

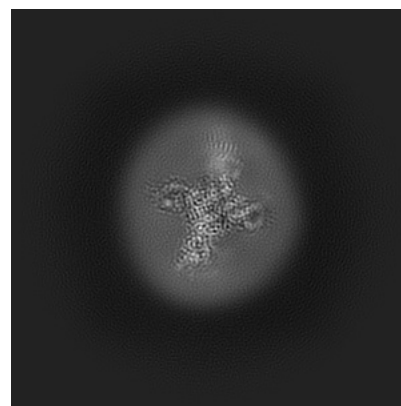
#### 6.1.1 Primary map



X

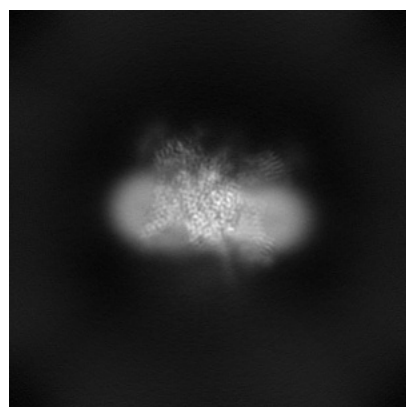


Y

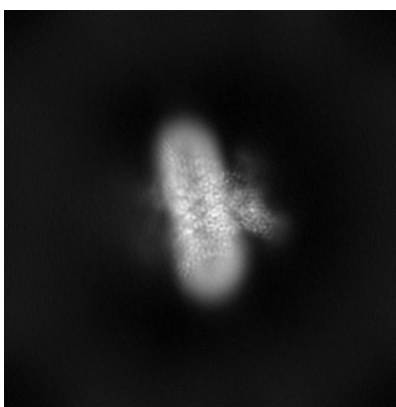


Z

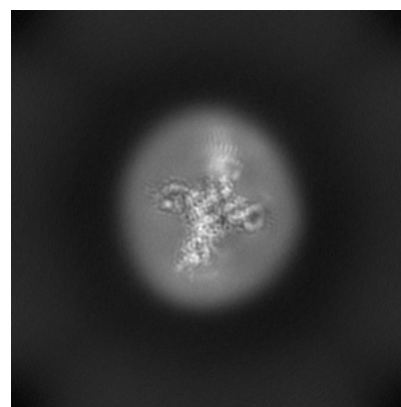
#### 6.1.2 Raw map



X



Y

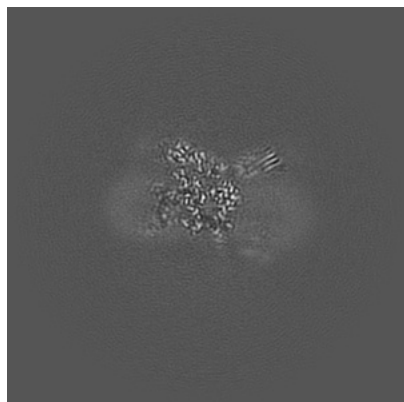


Z

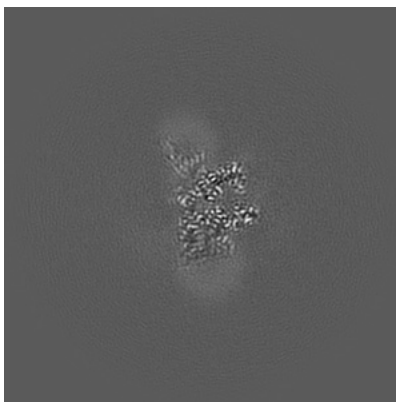
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

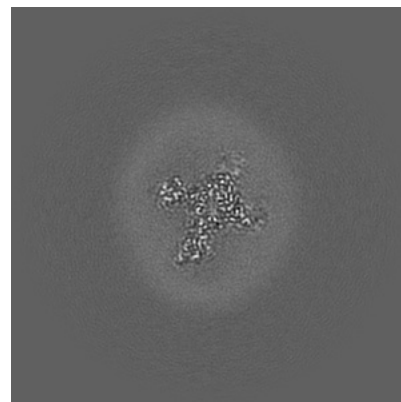
### 6.2.1 Primary map



X Index: 160

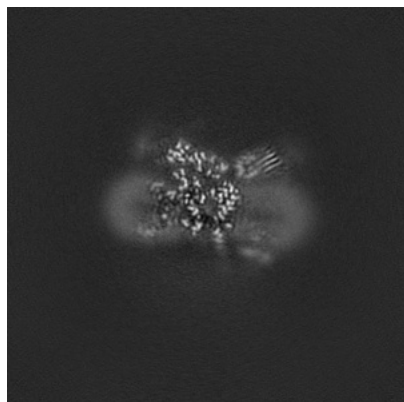


Y Index: 160

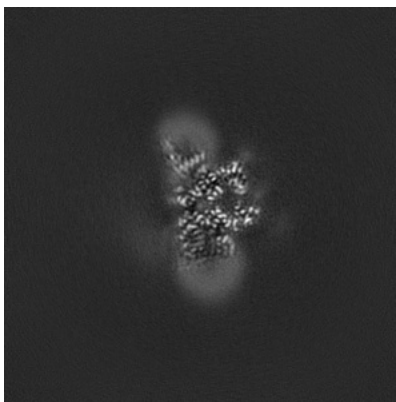


Z Index: 160

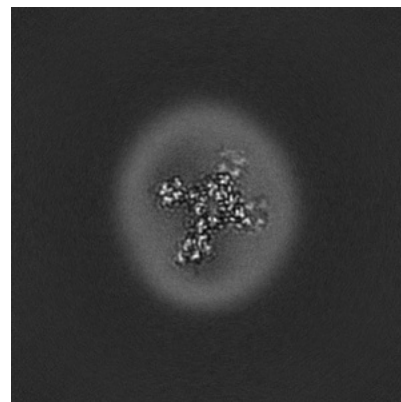
### 6.2.2 Raw map



X Index: 160



Y Index: 160

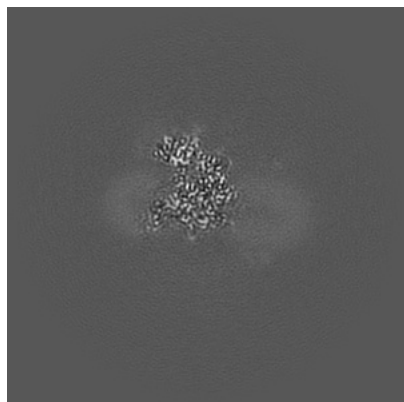


Z Index: 160

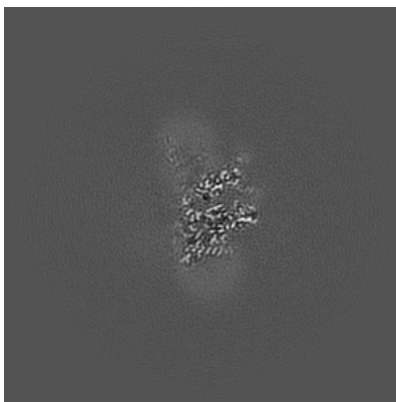
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

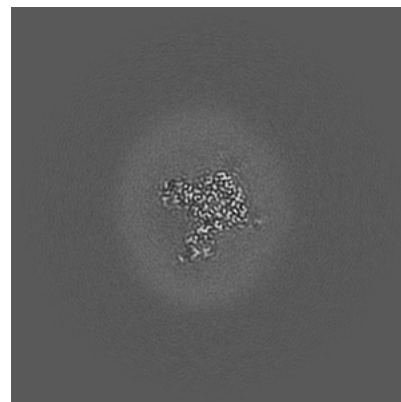
### 6.3.1 Primary map



X Index: 151

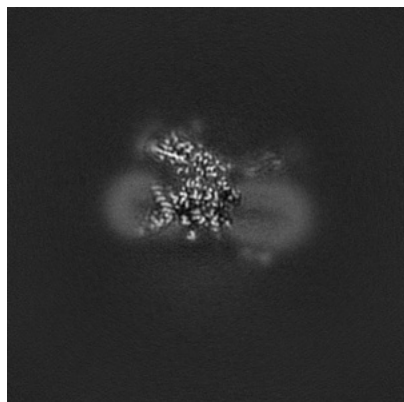


Y Index: 164

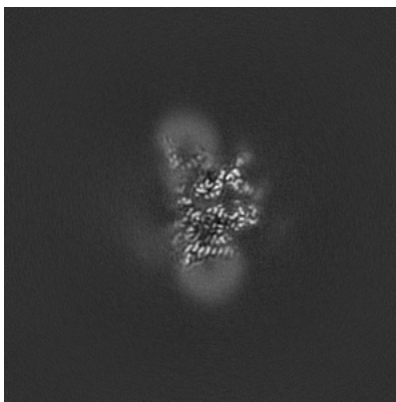


Z Index: 166

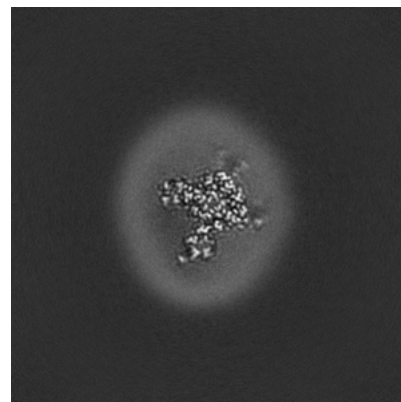
### 6.3.2 Raw map



X Index: 155



Y Index: 163

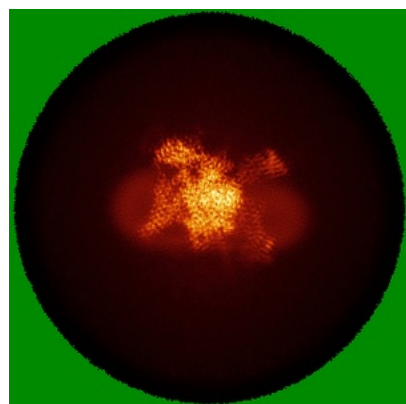


Z Index: 166

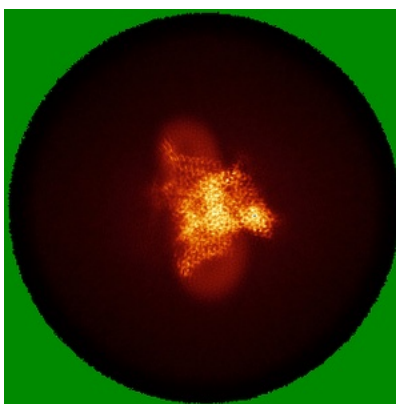
The images above show the largest variance slices of the map in three orthogonal directions.

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

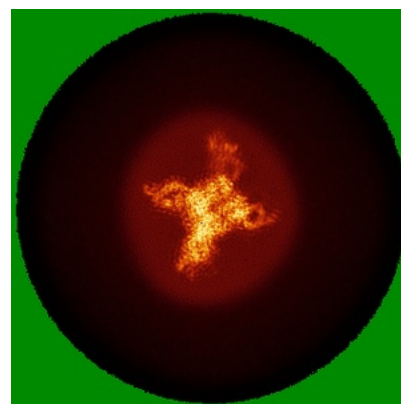
### 6.4.1 Primary map



X

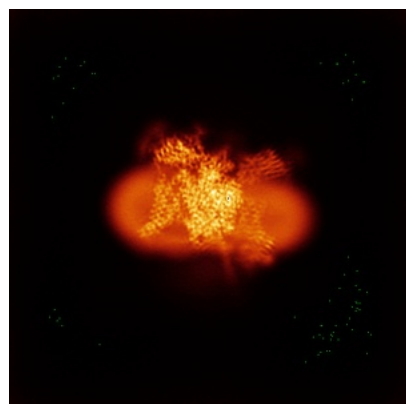


Y

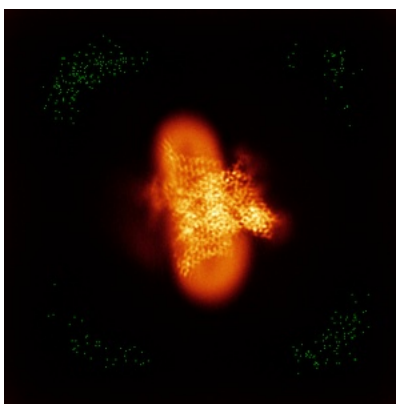


Z

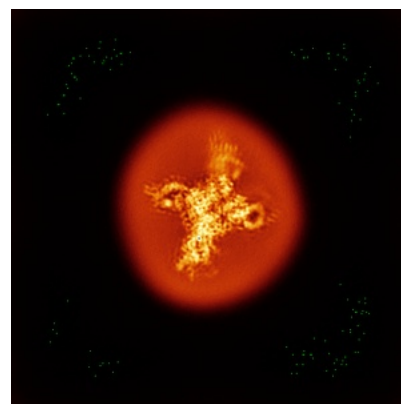
### 6.4.2 Raw map



X



Y

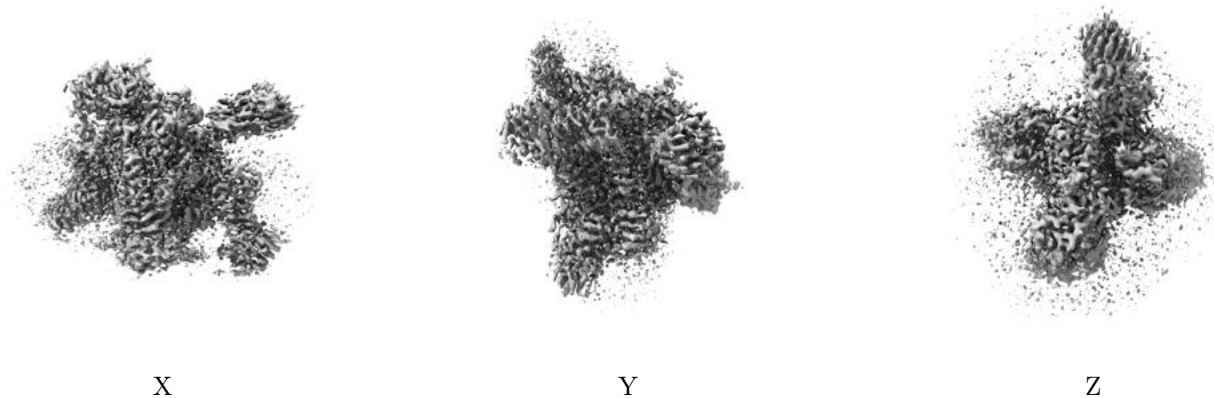


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.52. 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.

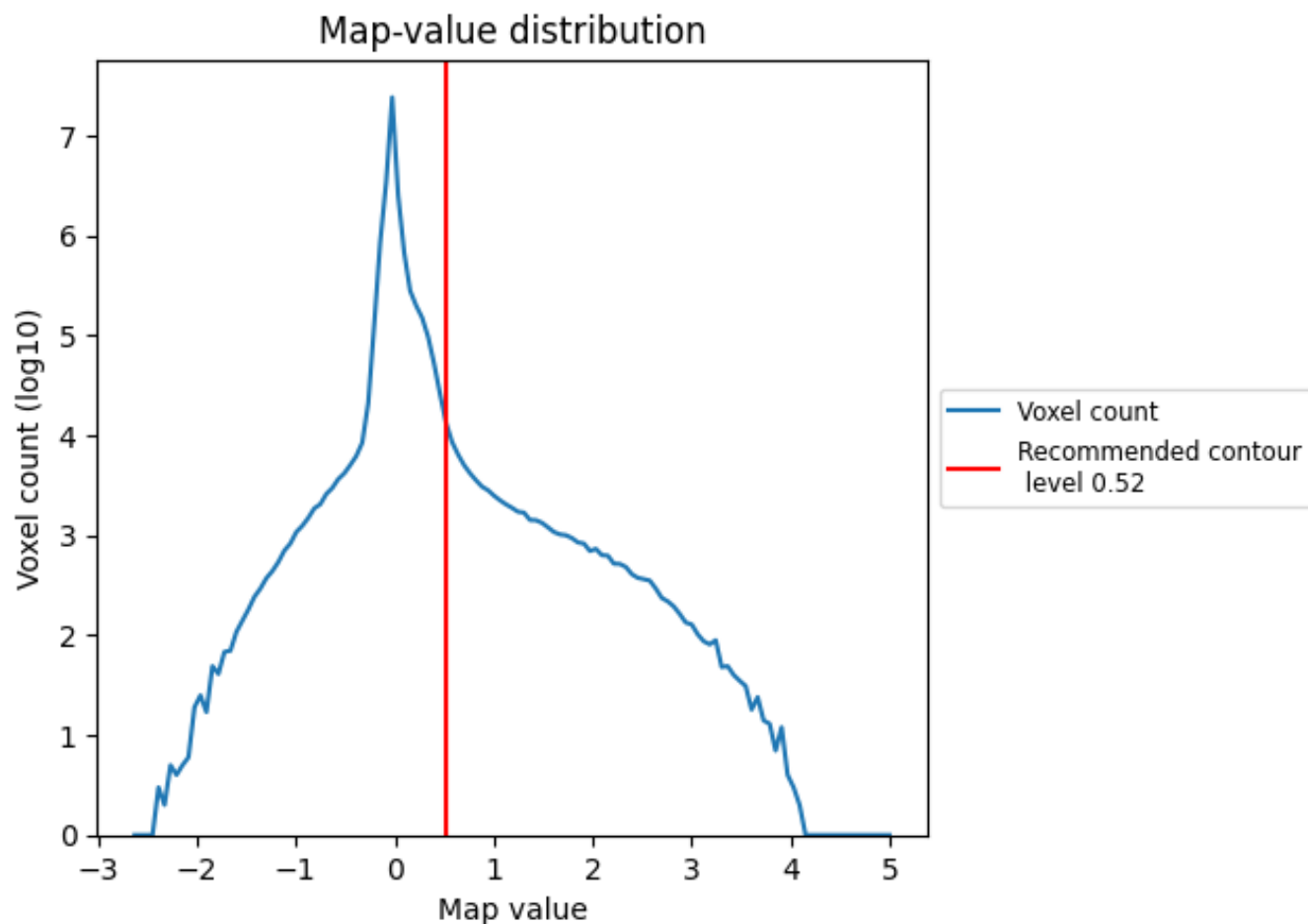
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

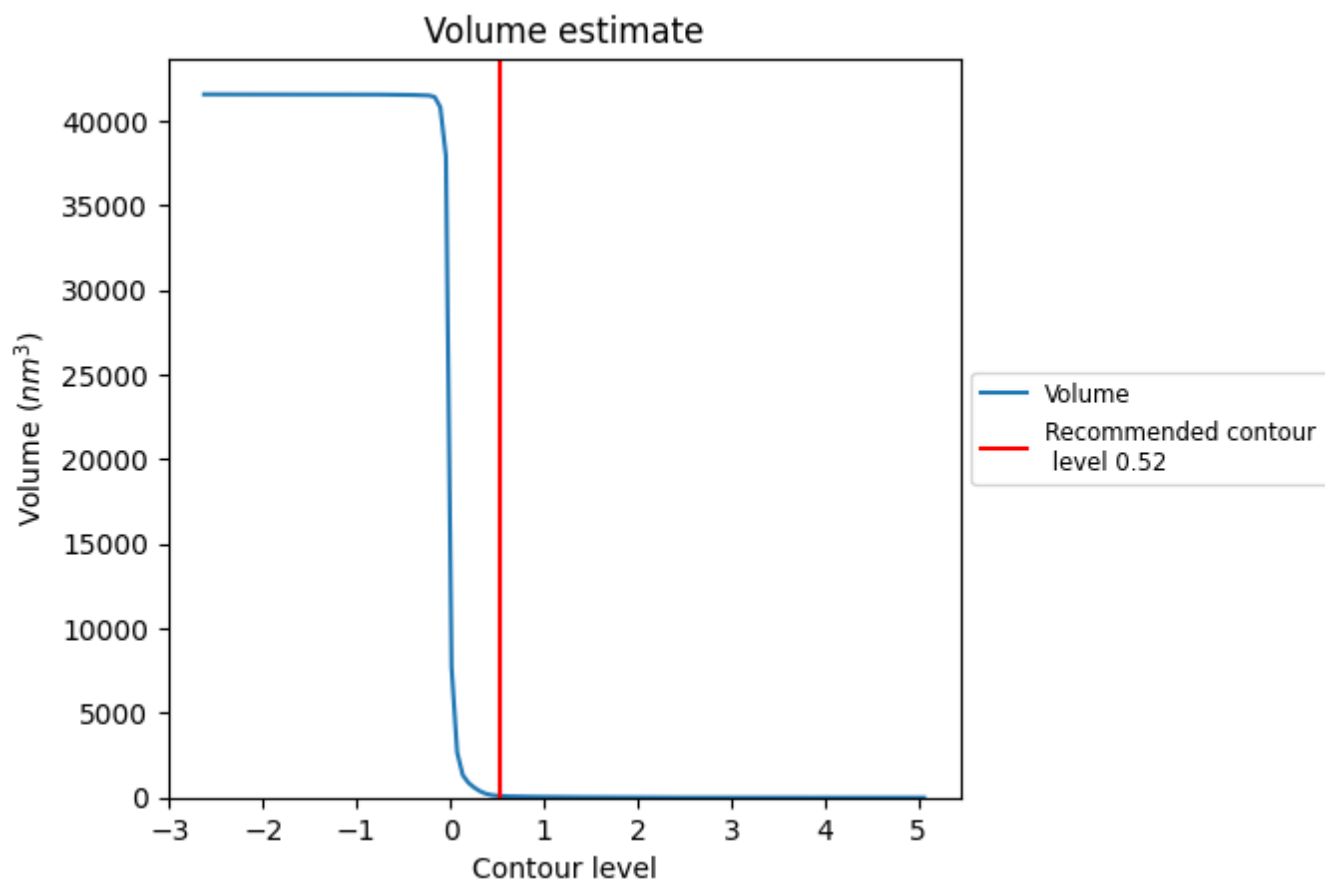
This section contains the results of statistical analysis of the map.

### 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.

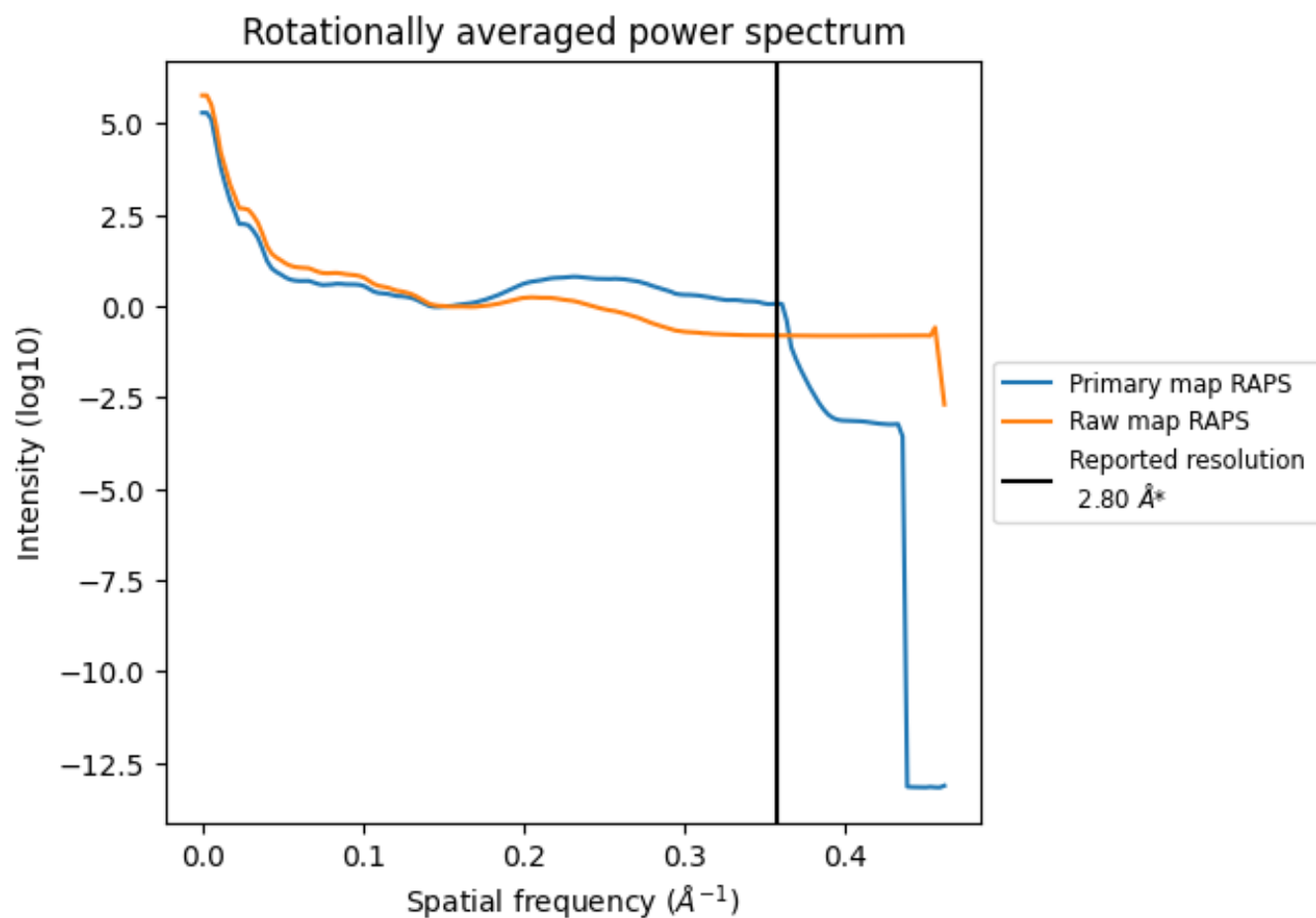
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100  $\text{nm}^3$ ; this corresponds to an approximate mass of 90 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 ⓘ

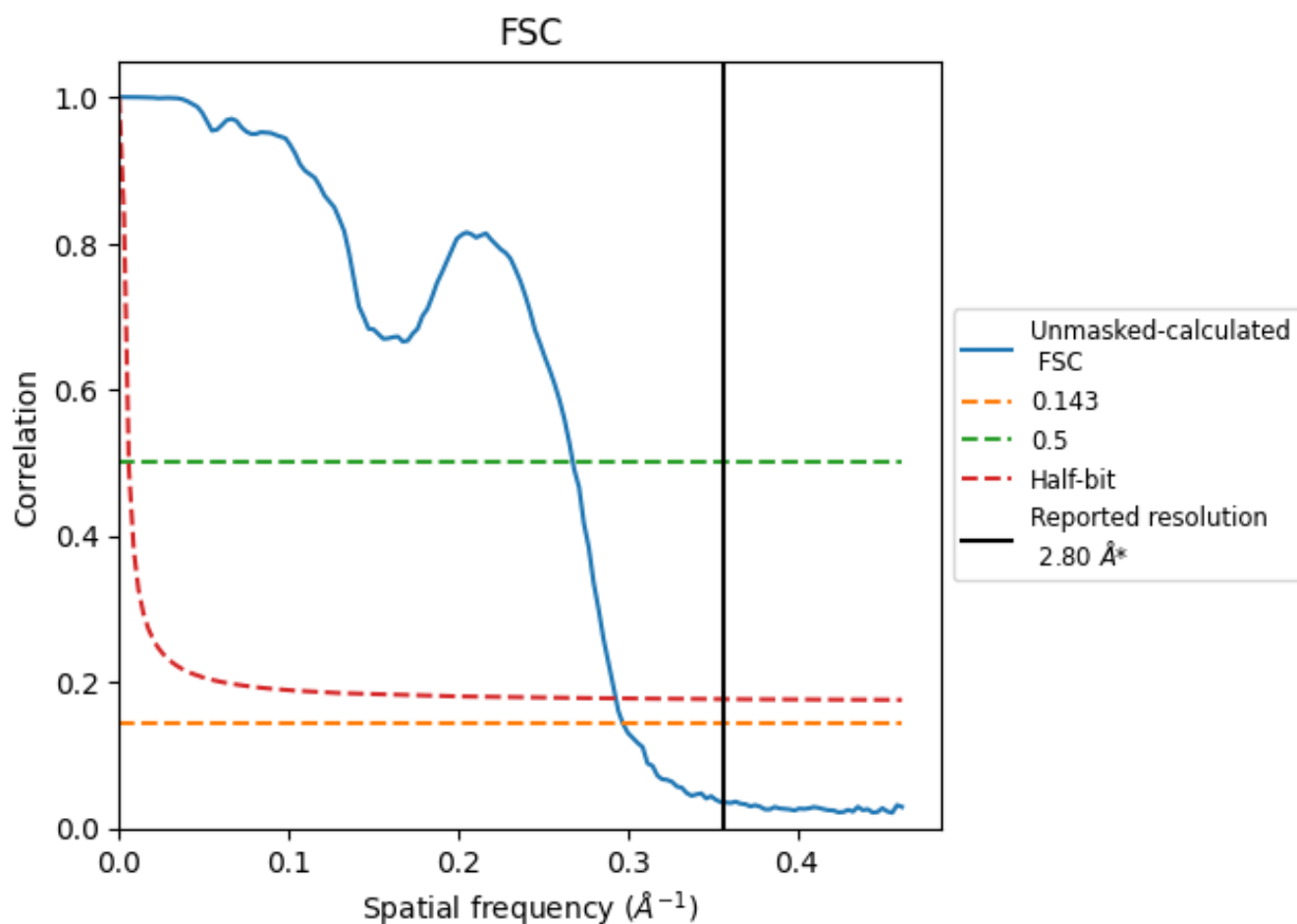


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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  $0.357 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

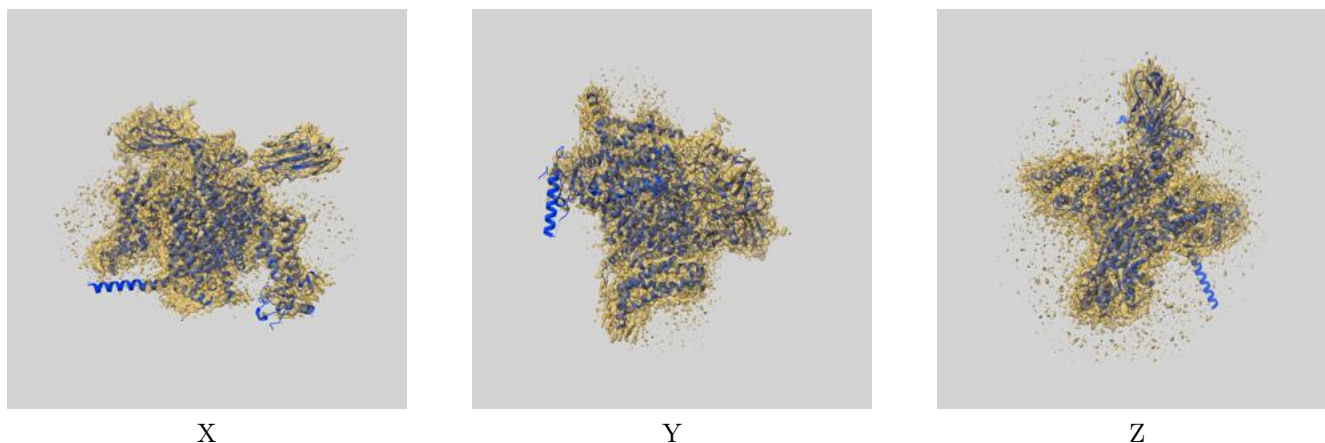
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.74	3.41

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

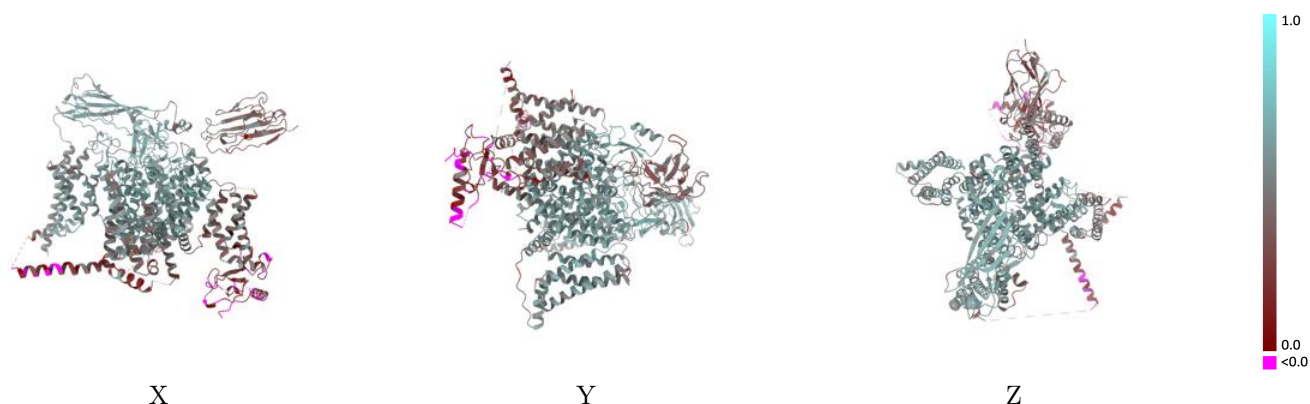
This section contains information regarding the fit between EMDB map EMD-33485 and PDB model 7XVF. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay [i](#)



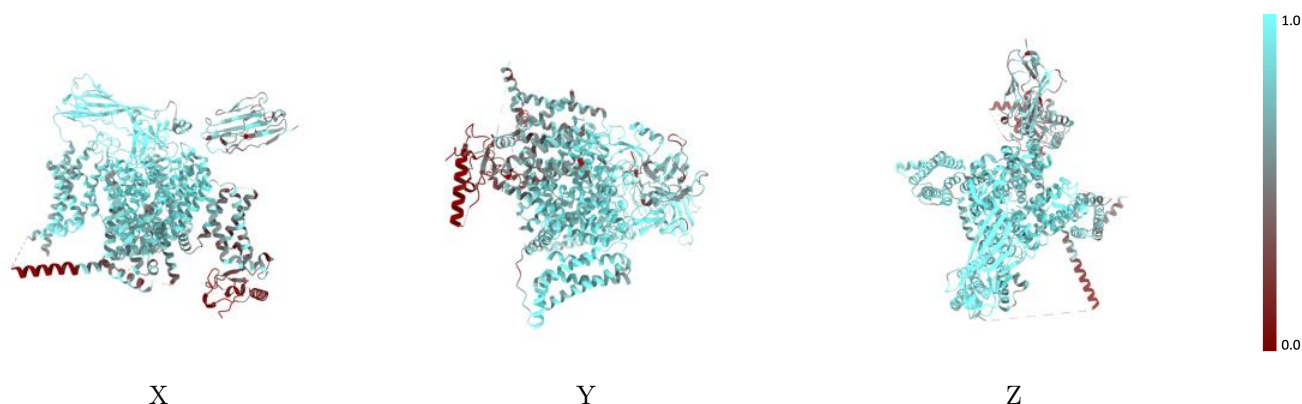
The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



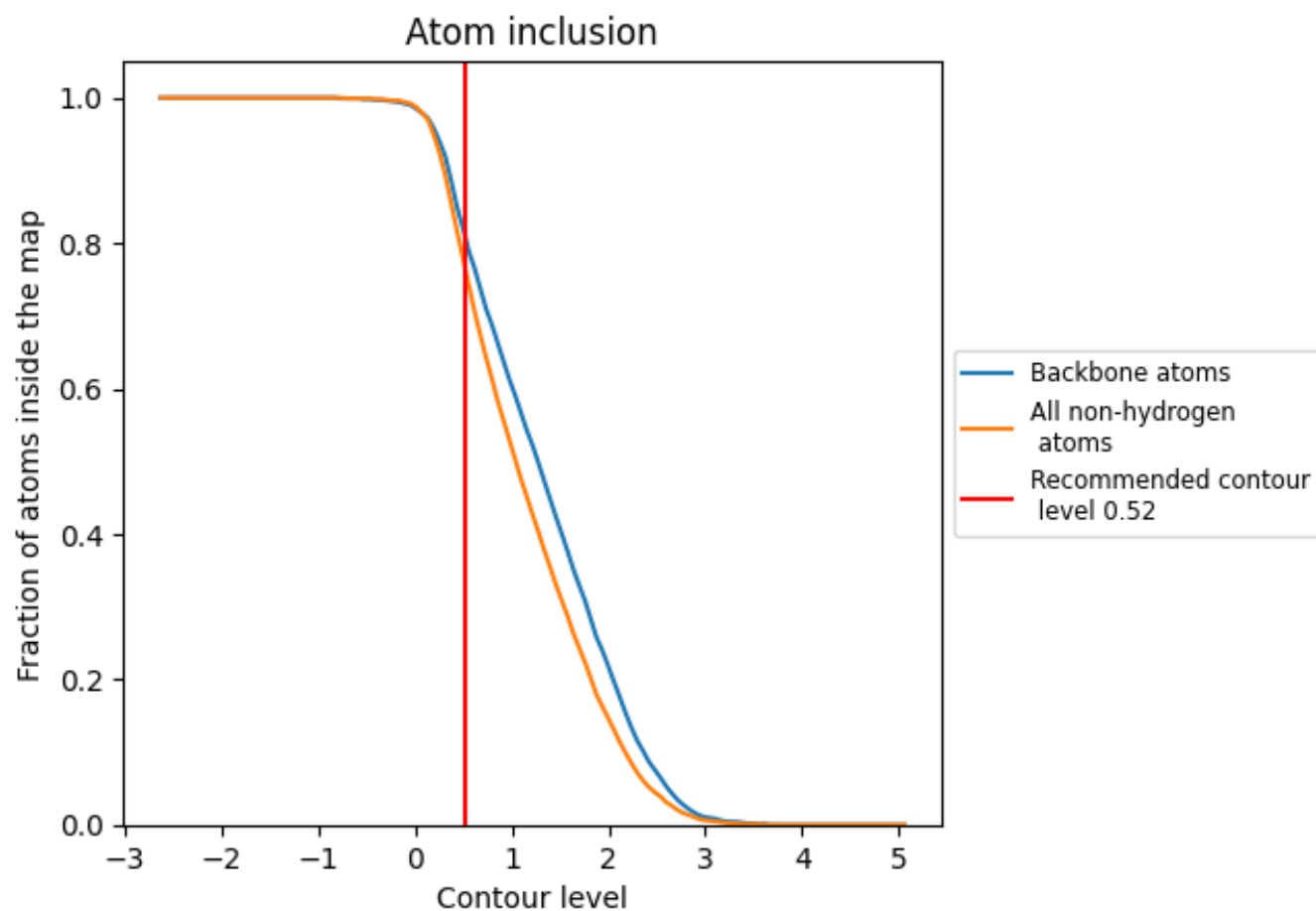
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.52).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7640	<div></div> 0.4910
A	<div></div> 0.7630	<div></div> 0.4940
B	<div></div> 0.8750	<div></div> 0.5470
C	<div></div> 0.6030	<div></div> 0.3770
D	<div></div> 0.7140	<div></div> 0.4570
E	<div></div> 0.8210	<div></div> 0.5160

