



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 07:58 PM EST

PDB ID : 6CO7
EMDB ID : EMD-7542
Title : Structure of the nvTRPM2 channel in complex with Ca²⁺
Authors : Zhang, Z.; Toth, B.; Szollosi, A.; Chen, J.; Csanady, L.
Deposited on : 2018-03-12
Resolution : 3.07 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

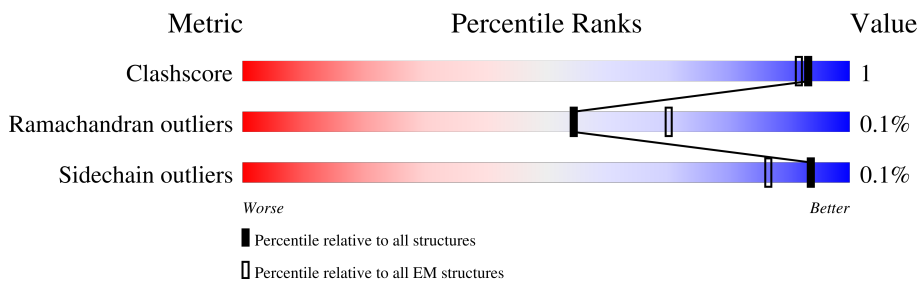
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1560	
1	B	1560	
1	C	1560	
1	D	1560	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 35255 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 Predicted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1061	8422	5429	1409	1537	47	0	0
1	B	1061	8422	5429	1409	1537	47	0	0
1	C	1061	8422	5429	1409	1537	47	0	0
1	D	1061	8422	5429	1409	1537	47	0	0

There are 36 discrepancies between the modelled and reference sequences:

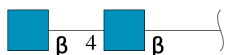
Chain	Residue	Modelled	Actual	Comment	Reference
A	1552	SER	-	expression tag	UNP A7T1N0
A	1553	ASN	-	expression tag	UNP A7T1N0
A	1554	SER	-	expression tag	UNP A7T1N0
A	1555	LEU	-	expression tag	UNP A7T1N0
A	1556	GLU	-	expression tag	UNP A7T1N0
A	1557	VAL	-	expression tag	UNP A7T1N0
A	1558	LEU	-	expression tag	UNP A7T1N0
A	1559	PHE	-	expression tag	UNP A7T1N0
A	1560	GLN	-	expression tag	UNP A7T1N0
B	1552	SER	-	expression tag	UNP A7T1N0
B	1553	ASN	-	expression tag	UNP A7T1N0
B	1554	SER	-	expression tag	UNP A7T1N0
B	1555	LEU	-	expression tag	UNP A7T1N0
B	1556	GLU	-	expression tag	UNP A7T1N0
B	1557	VAL	-	expression tag	UNP A7T1N0
B	1558	LEU	-	expression tag	UNP A7T1N0
B	1559	PHE	-	expression tag	UNP A7T1N0
B	1560	GLN	-	expression tag	UNP A7T1N0
C	1552	SER	-	expression tag	UNP A7T1N0
C	1553	ASN	-	expression tag	UNP A7T1N0
C	1554	SER	-	expression tag	UNP A7T1N0
C	1555	LEU	-	expression tag	UNP A7T1N0

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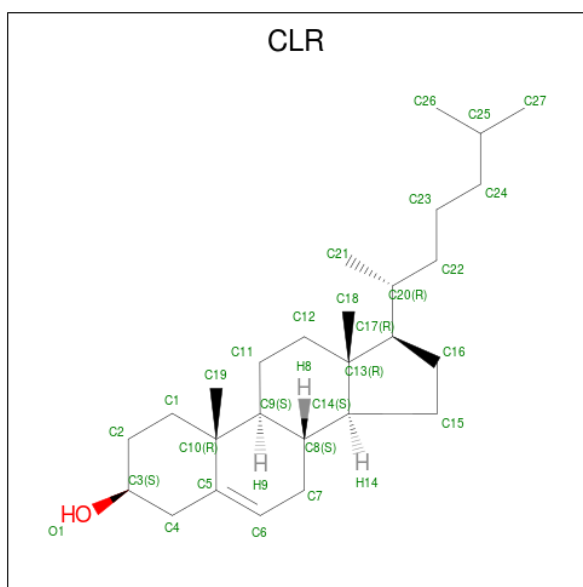
Chain	Residue	Modelled	Actual	Comment	Reference
C	1556	GLU	-	expression tag	UNP A7T1N0
C	1557	VAL	-	expression tag	UNP A7T1N0
C	1558	LEU	-	expression tag	UNP A7T1N0
C	1559	PHE	-	expression tag	UNP A7T1N0
C	1560	GLN	-	expression tag	UNP A7T1N0
D	1552	SER	-	expression tag	UNP A7T1N0
D	1553	ASN	-	expression tag	UNP A7T1N0
D	1554	SER	-	expression tag	UNP A7T1N0
D	1555	LEU	-	expression tag	UNP A7T1N0
D	1556	GLU	-	expression tag	UNP A7T1N0
D	1557	VAL	-	expression tag	UNP A7T1N0
D	1558	LEU	-	expression tag	UNP A7T1N0
D	1559	PHE	-	expression tag	UNP A7T1N0
D	1560	GLN	-	expression tag	UNP A7T1N0

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



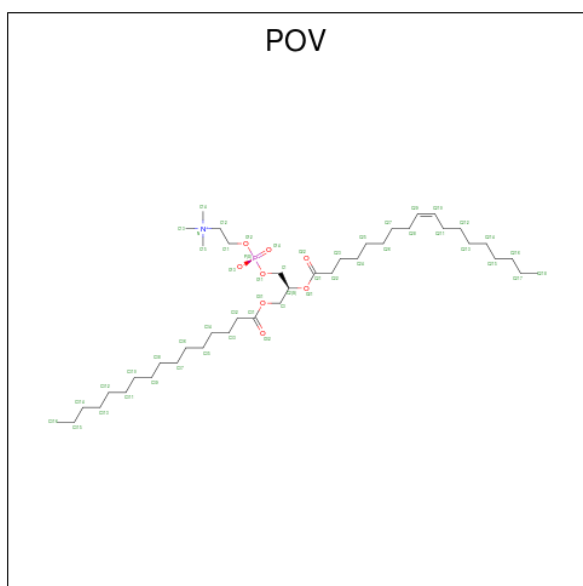
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	B	1	334	284	1	44	5	0
4	B	1	334	284	1	44	5	0
4	B	1	334	284	1	44	5	0
4	B	1	334	284	1	44	5	0
4	B	1	334	284	1	44	5	0
4	B	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	C	1	334	284	1	44	5	0
4	D	1	334	284	1	44	5	0

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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	
4	D	1	Total	C	N	O	P	0
			334	284	1	44	5	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

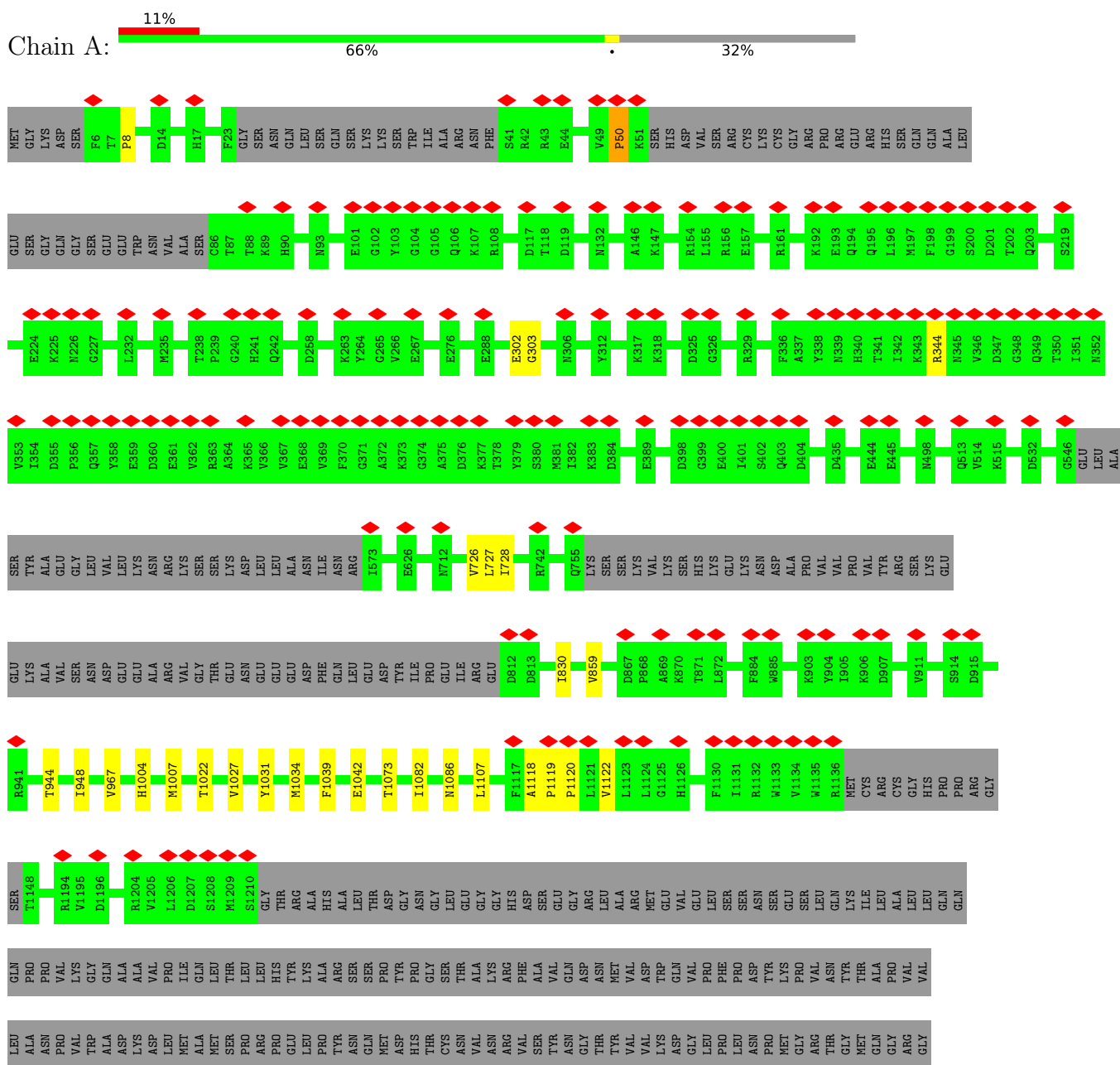
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	A	3	Total 3	Na 3	0

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: Predicted protein



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

Chain E:  100%

MAGE
MAGZ

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

Chain F:  100%

MAGE
MAGZ

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

Chain G:  100%

MAGE
MAGZ

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

Chain H:  100%

MAGE
MAGZ

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.03, 1.03, 1.03	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: NA, CLR, CA, POV, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	1/8602 (0.0%)	0.54	2/11656 (0.0%)
1	B	0.39	1/8602 (0.0%)	0.54	2/11656 (0.0%)
1	C	0.39	1/8602 (0.0%)	0.54	2/11656 (0.0%)
1	D	0.39	1/8602 (0.0%)	0.54	2/11656 (0.0%)
All	All	0.39	4/34408 (0.0%)	0.54	8/46624 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1007	MET	C-N	6.32	1.48	1.34
1	A	1007	MET	C-N	6.29	1.48	1.34
1	D	1007	MET	C-N	6.29	1.48	1.34
1	B	1007	MET	C-N	6.25	1.48	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	PRO	N-CA-CB	6.08	110.60	103.30
1	B	50	PRO	N-CA-CB	6.03	110.53	103.30
1	A	50	PRO	N-CA-CB	6.01	110.51	103.30
1	C	50	PRO	N-CA-CB	6.01	110.51	103.30
1	B	8	PRO	N-CA-CB	5.95	110.44	103.30
1	C	8	PRO	N-CA-CB	5.95	110.44	103.30
1	D	8	PRO	N-CA-CB	5.94	110.42	103.30
1	A	8	PRO	N-CA-CB	5.93	110.42	103.30

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	8422	0	8382	22	0
1	B	8422	0	8382	22	0
1	C	8422	0	8382	21	0
1	D	8422	0	8382	21	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	28	0	46	9	0
3	B	28	0	46	10	0
3	C	28	0	46	9	0
3	D	28	0	46	9	0
4	A	334	0	496	0	0
4	B	334	0	496	0	0
4	C	334	0	496	0	0
4	D	334	0	496	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	3	0	0	0	0
All	All	35255	0	35796	92	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 1.

All (92) 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:C:302:GLU:HG2	1:C:303:GLY:H	1.22	1.03
1:D:302:GLU:HG2	1:D:303:GLY:H	1.22	1.03
1:A:302:GLU:HG2	1:A:303:GLY:H	1.22	1.01
1:B:302:GLU:HG2	1:B:303:GLY:H	1.22	0.99
1:C:302:GLU:HG2	1:C:303:GLY:N	1.97	0.80
1:B:302:GLU:HG2	1:B:303:GLY:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:GLU:HG2	1:D:303:GLY:N	1.97	0.79
1:A:302:GLU:HG2	1:A:303:GLY:N	1.97	0.78
3:A:3000:CLR:O1	3:A:3000:CLR:H192	1.86	0.76
3:B:3000:CLR:O1	3:B:3000:CLR:H192	1.86	0.75
3:D:3000:CLR:O1	3:D:3000:CLR:H192	1.86	0.75
3:C:3000:CLR:H192	3:C:3000:CLR:O1	1.86	0.74
1:A:1027:VAL:CG1	3:A:3000:CLR:H231	2.19	0.72
1:B:1027:VAL:CG1	3:B:3000:CLR:H231	2.19	0.72
1:C:1027:VAL:CG1	3:C:3000:CLR:H231	2.19	0.71
1:C:967:VAL:HG12	1:C:1107:LEU:HD11	1.73	0.71
1:D:1027:VAL:CG1	3:D:3000:CLR:H231	2.19	0.71
1:B:967:VAL:HG12	1:B:1107:LEU:HD11	1.73	0.71
1:A:967:VAL:HG12	1:A:1107:LEU:HD11	1.73	0.71
1:C:302:GLU:CG	1:C:303:GLY:H	2.02	0.71
1:D:967:VAL:HG12	1:D:1107:LEU:HD11	1.73	0.71
1:A:302:GLU:CG	1:A:303:GLY:H	2.02	0.70
1:B:302:GLU:CG	1:B:303:GLY:H	2.01	0.70
1:D:302:GLU:CG	1:D:303:GLY:H	2.02	0.70
1:B:1031:TYR:CD1	3:B:3000:CLR:C26	2.81	0.64
1:D:1031:TYR:CD1	3:D:3000:CLR:C26	2.81	0.64
1:A:1031:TYR:CD1	3:A:3000:CLR:C26	2.81	0.63
1:C:1031:TYR:CD1	3:C:3000:CLR:C26	2.81	0.63
1:D:1031:TYR:CD1	3:D:3000:CLR:H263	2.34	0.63
1:A:1031:TYR:CD1	3:A:3000:CLR:H263	2.34	0.63
1:C:1031:TYR:CD1	3:C:3000:CLR:H263	2.34	0.62
1:D:1027:VAL:HG13	3:D:3000:CLR:H273	1.82	0.62
1:B:1031:TYR:CD1	3:B:3000:CLR:H263	2.34	0.62
1:A:1027:VAL:HG13	3:A:3000:CLR:H273	1.82	0.61
1:C:1027:VAL:HG13	3:C:3000:CLR:H273	1.82	0.61
1:B:1027:VAL:HG13	3:B:3000:CLR:H273	1.82	0.61
1:B:1027:VAL:HG12	3:B:3000:CLR:H231	1.89	0.55
1:C:1027:VAL:HG12	3:C:3000:CLR:H231	1.89	0.55
1:D:1027:VAL:HG12	3:D:3000:CLR:H231	1.89	0.53
1:A:1027:VAL:HG12	3:A:3000:CLR:H231	1.89	0.52
1:C:1118:ALA:O	1:C:1122:VAL:N	2.44	0.51
1:C:1119:PRO:HG2	1:C:1120:PRO:HD3	1.93	0.50
1:A:1118:ALA:O	1:A:1122:VAL:N	2.44	0.50
1:A:1119:PRO:HG2	1:A:1120:PRO:HD3	1.93	0.50
1:D:1118:ALA:O	1:D:1122:VAL:N	2.44	0.50
1:D:1119:PRO:HG2	1:D:1120:PRO:HD3	1.93	0.50
1:B:1118:ALA:O	1:B:1122:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:PRO:HG2	1:B:1120:PRO:HD3	1.93	0.49
3:C:3000:CLR:H212	3:C:3000:CLR:H121	1.95	0.49
3:B:3000:CLR:H212	3:B:3000:CLR:H121	1.95	0.48
1:C:1118:ALA:HB1	1:C:1119:PRO:HD2	1.95	0.48
1:B:1118:ALA:HB1	1:B:1119:PRO:HD2	1.95	0.48
1:A:1118:ALA:HB1	1:A:1119:PRO:HD2	1.95	0.48
1:D:1118:ALA:HB1	1:D:1119:PRO:HD2	1.95	0.47
3:D:3000:CLR:H121	3:D:3000:CLR:H212	1.95	0.47
3:A:3000:CLR:H212	3:A:3000:CLR:H121	1.95	0.47
1:D:1031:TYR:CD1	3:D:3000:CLR:H262	2.50	0.47
1:B:1031:TYR:HD1	3:B:3000:CLR:C26	2.29	0.46
1:B:1031:TYR:CD1	3:B:3000:CLR:H262	2.50	0.46
1:A:1031:TYR:HD1	3:A:3000:CLR:C26	2.29	0.45
1:C:1031:TYR:CD1	3:C:3000:CLR:H262	2.50	0.45
1:A:1031:TYR:CD1	3:A:3000:CLR:H262	2.50	0.45
1:C:1031:TYR:HD1	3:C:3000:CLR:C26	2.29	0.44
1:D:1031:TYR:HD1	3:D:3000:CLR:C26	2.29	0.43
1:D:1082:ILE:O	1:D:1086:ASN:ND2	2.51	0.43
1:B:726:VAL:HG13	1:B:727:LEU:HD12	2.01	0.43
1:D:726:VAL:HG13	1:D:727:LEU:HD12	2.01	0.43
1:B:1082:ILE:O	1:B:1086:ASN:ND2	2.51	0.42
1:C:726:VAL:HG13	1:C:727:LEU:HD12	2.01	0.42
1:A:1082:ILE:O	1:A:1086:ASN:ND2	2.51	0.42
1:A:726:VAL:HG13	1:A:727:LEU:HD12	2.01	0.42
1:C:1082:ILE:O	1:C:1086:ASN:ND2	2.51	0.42
1:C:1034:MET:HG2	1:C:1073:THR:HG21	2.02	0.41
1:B:859:VAL:O	1:C:1010:SER:OG	2.38	0.41
1:A:1004:HIS:CE1	1:A:1022:THR:HG23	2.55	0.41
1:B:1034:MET:HG2	1:B:1073:THR:HG21	2.02	0.41
1:A:728:ILE:HG21	1:A:830:ILE:HG12	2.03	0.41
1:A:859:VAL:O	1:B:1010:SER:OG	2.38	0.41
1:A:1034:MET:HG2	1:A:1073:THR:HG21	2.02	0.41
1:B:728:ILE:HG21	1:B:830:ILE:HG12	2.03	0.41
1:B:1039:PHE:HB3	1:B:1042:GLU:HB2	2.02	0.41
1:C:1004:HIS:CE1	1:C:1022:THR:HG23	2.55	0.41
1:C:859:VAL:O	1:D:1010:SER:OG	2.39	0.41
1:D:1039:PHE:HB3	1:D:1042:GLU:HB2	2.02	0.41
3:B:3000:CLR:H182	3:B:3000:CLR:H8	1.83	0.41
1:C:1039:PHE:HB3	1:C:1042:GLU:HB2	2.02	0.41
1:B:1004:HIS:CE1	1:B:1022:THR:HG23	2.55	0.40
1:A:1039:PHE:HB3	1:A:1042:GLU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:PHE:CE1	1:D:1123:LEU:HD23	2.57	0.40
1:D:1004:HIS:CE1	1:D:1022:THR:HG23	2.55	0.40
1:D:1034:MET:HG2	1:D:1073:THR:HG21	2.02	0.40
1:A:944:THR:HG22	1:A:948:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1049/1560 (67%)	989 (94%)	59 (6%)	1 (0%)	51	82
1	B	1049/1560 (67%)	989 (94%)	59 (6%)	1 (0%)	51	82
1	C	1049/1560 (67%)	990 (94%)	58 (6%)	1 (0%)	51	82
1	D	1049/1560 (67%)	989 (94%)	59 (6%)	1 (0%)	51	82
All	All	4196/6240 (67%)	3957 (94%)	235 (6%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	B	50	PRO
1	C	50	PRO
1	D	50	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	900/1346 (67%)	899 (100%)	1 (0%)	93	97
1	B	900/1346 (67%)	899 (100%)	1 (0%)	93	97
1	C	900/1346 (67%)	899 (100%)	1 (0%)	93	97
1	D	900/1346 (67%)	899 (100%)	1 (0%)	93	97
All	All	3600/5384 (67%)	3596 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	B	344	ARG
1	C	344	ARG
1	D	344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.32	0	17,19,21	0.88	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	F	1	1,2	14,14,15	0.32	0	17,19,21	0.89	0
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.65	0
2	NAG	G	1	1,2	14,14,15	0.32	0	17,19,21	0.89	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	H	1	1,2	14,14,15	0.32	0	17,19,21	0.88	0
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

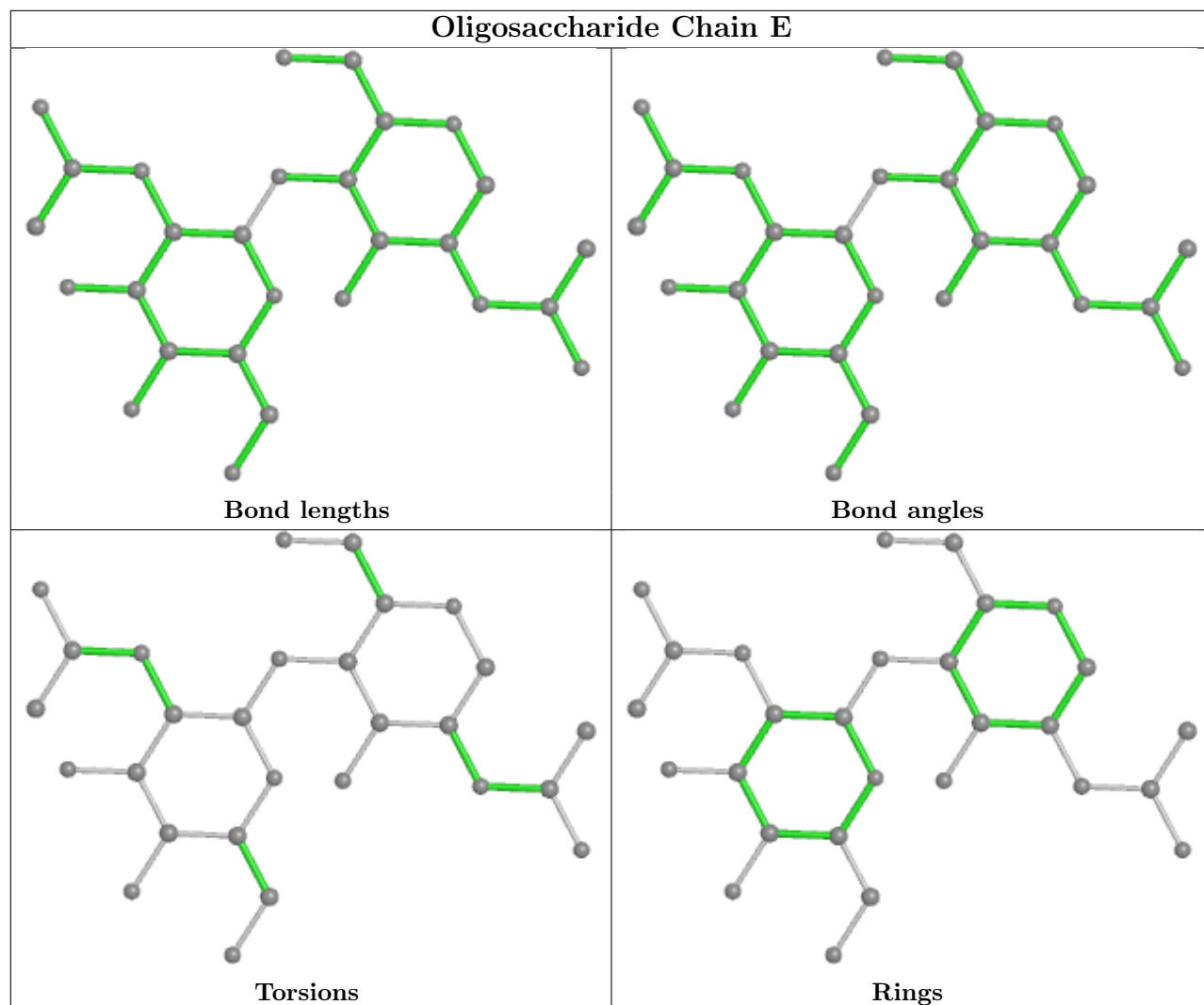
There are no chirality outliers.

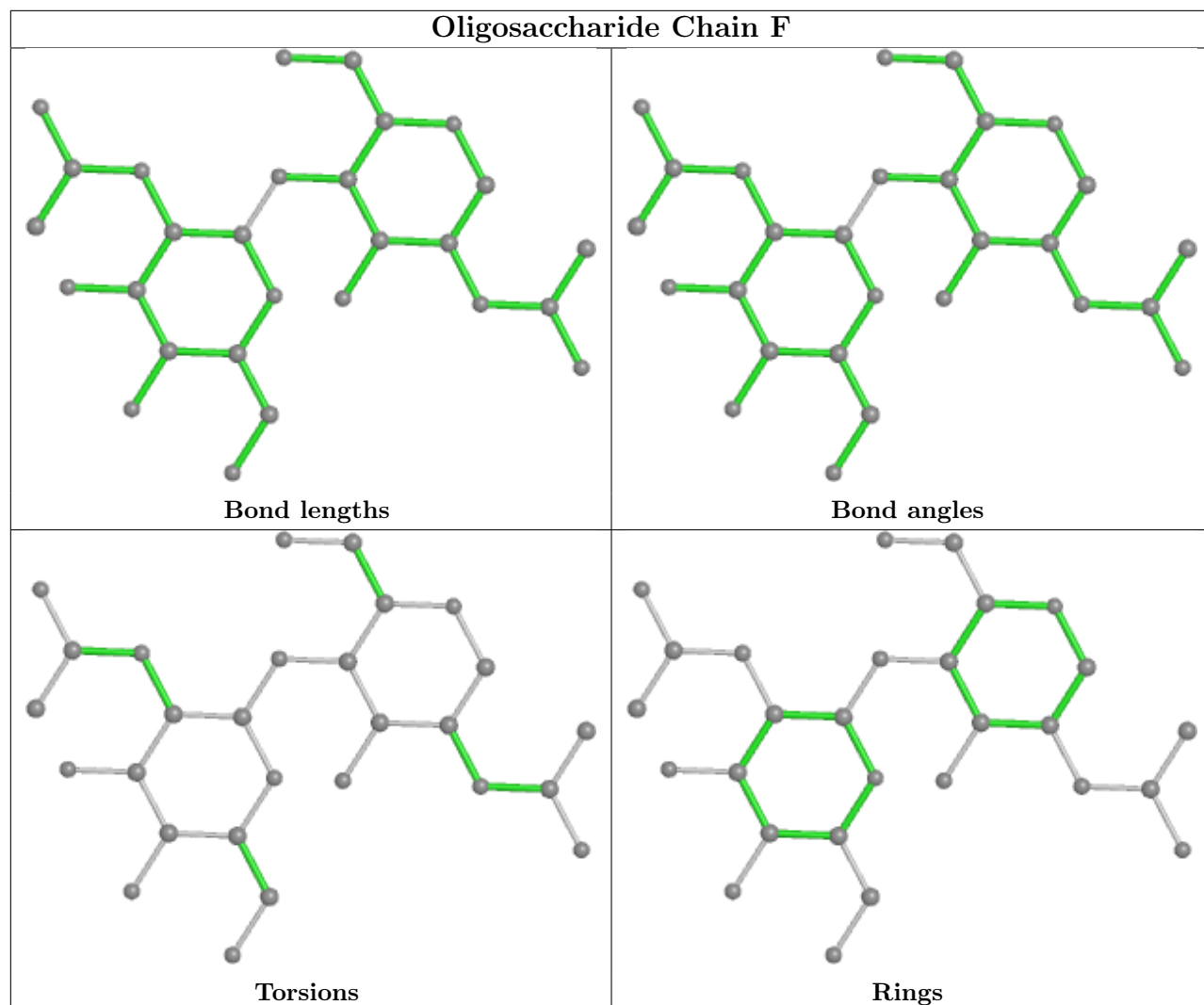
There are no torsion outliers.

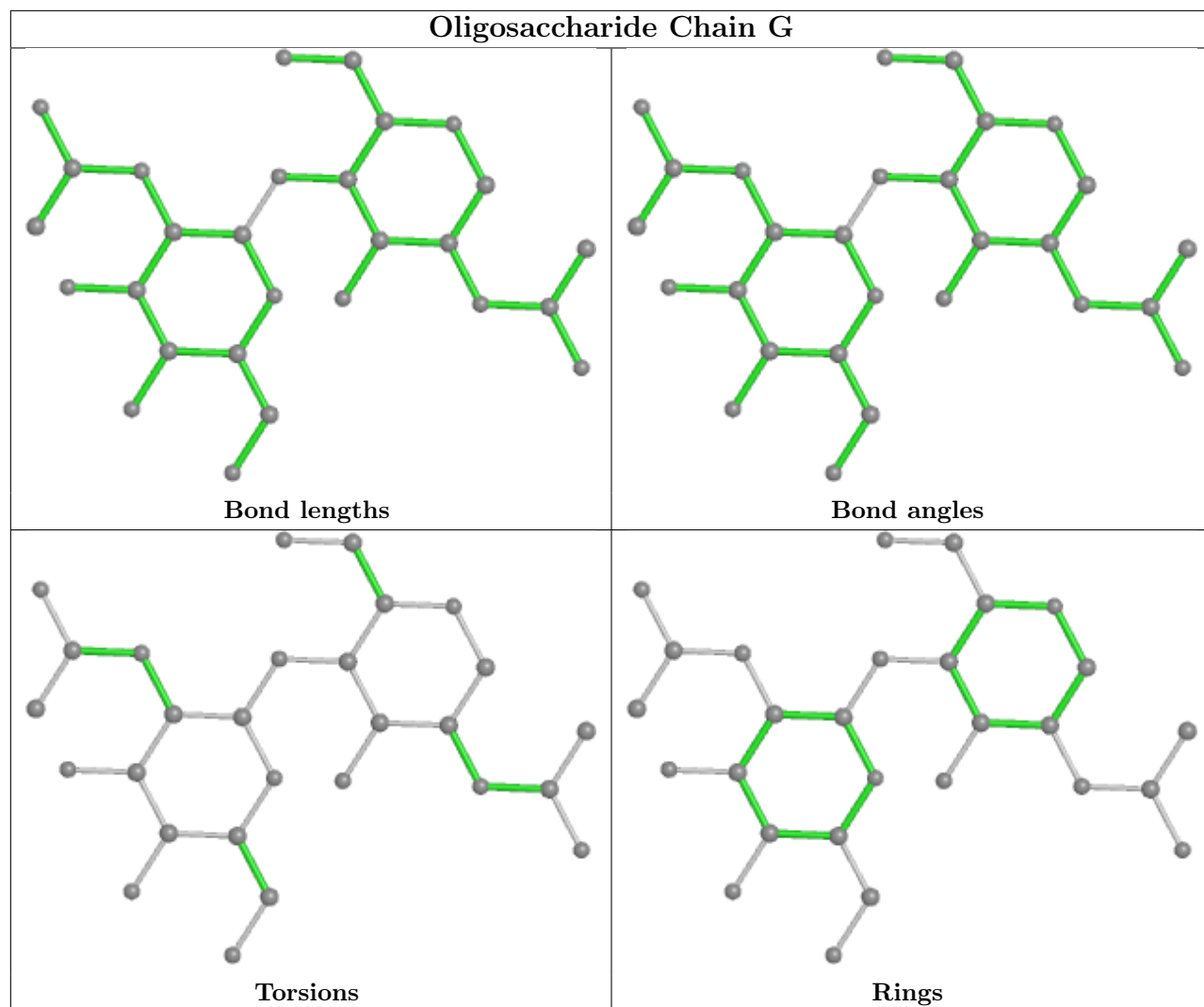
There are no ring outliers.

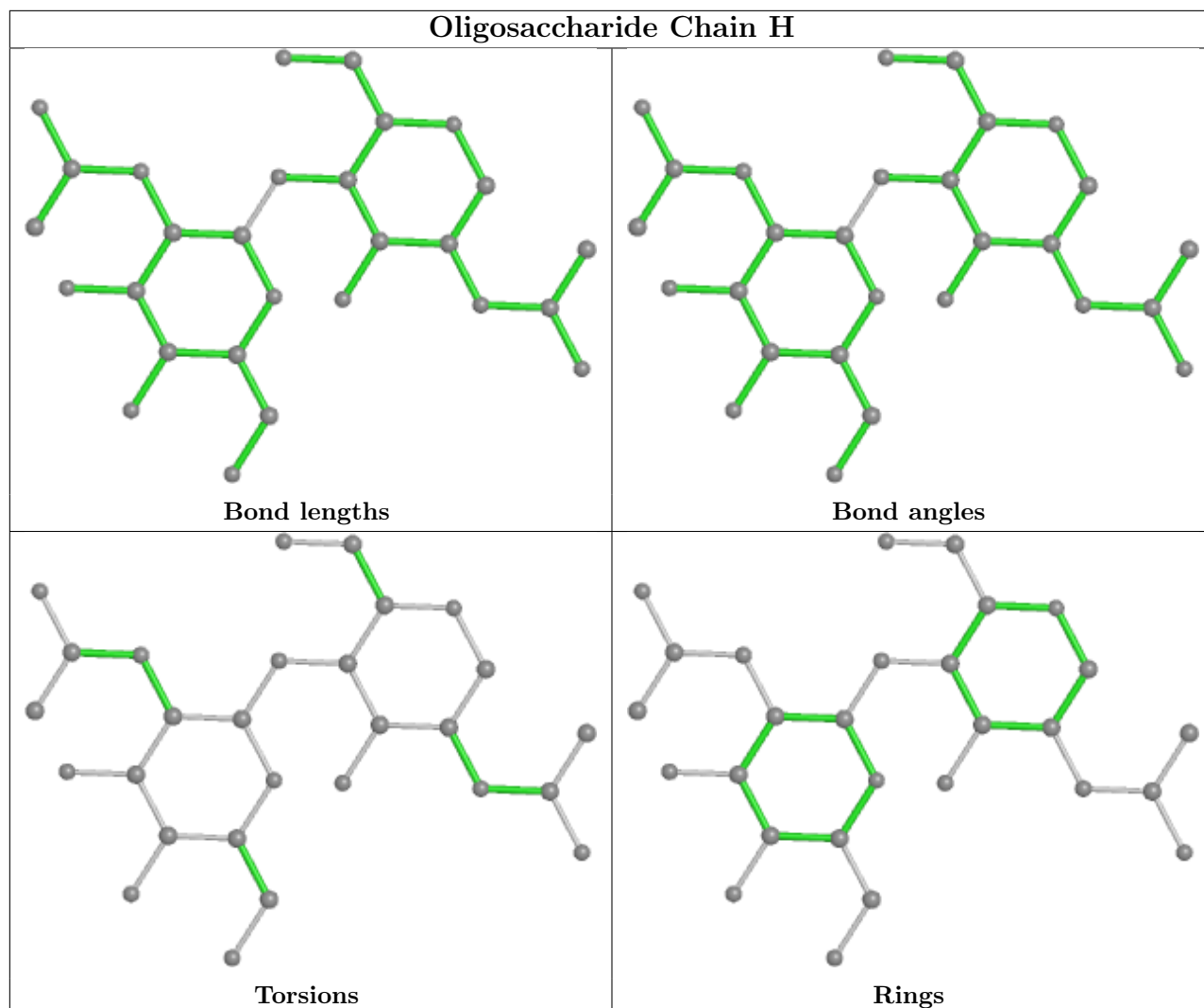
No monomer is involved in short contacts.

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](#)

Of 67 ligands modelled in this entry, 7 are monoatomic - leaving 60 for Mogul analysis.

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	POV	D	3003	-	15,15,51	1.03	1 (6%)	14,14,59	0.82	0
4	POV	B	3005	-	32,32,51	1.27	5 (15%)	34,34,59	1.08	2 (5%)
4	POV	A	3002	-	43,43,51	1.19	4 (9%)	49,51,59	0.98	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	C	3002	-	43,43,51	1.19	4 (9%)	49,51,59	0.98	3 (6%)
4	POV	C	3014	-	14,14,51	1.05	1 (7%)	13,13,59	0.85	0
4	POV	D	3009	-	11,11,51	0.39	0	10,10,59	0.81	0
4	POV	A	3008	-	12,12,51	0.41	0	11,11,59	0.74	0
4	POV	C	3003	-	15,15,51	1.03	1 (6%)	14,14,59	0.83	0
4	POV	C	3008	-	12,12,51	0.41	0	11,11,59	0.74	0
4	POV	C	3013	-	10,10,51	0.41	0	9,9,59	0.79	0
4	POV	D	3002	-	43,43,51	1.20	5 (11%)	49,51,59	0.98	3 (6%)
4	POV	D	3008	-	12,12,51	0.41	0	11,11,59	0.74	0
4	POV	A	3013	-	10,10,51	0.41	0	9,9,59	0.79	0
4	POV	C	3006	-	15,15,51	0.35	0	14,14,59	0.87	0
4	POV	B	3009	-	11,11,51	0.39	0	10,10,59	0.81	0
4	POV	C	3004	-	37,37,51	1.30	6 (16%)	41,42,59	1.11	3 (7%)
4	POV	A	3007	-	15,15,51	0.38	0	14,14,59	0.76	0
4	POV	D	3011	-	30,30,51	1.31	5 (16%)	32,34,59	1.19	2 (6%)
4	POV	C	3009	-	11,11,51	0.39	0	10,10,59	0.81	0
4	POV	C	3011	-	30,30,51	1.31	5 (16%)	32,34,59	1.19	2 (6%)
4	POV	B	3012	-	15,15,51	0.37	0	14,14,59	0.76	0
4	POV	B	3004	-	37,37,51	1.30	6 (16%)	41,42,59	1.12	3 (7%)
4	POV	C	3010	-	30,30,51	1.31	5 (16%)	32,34,59	1.23	2 (6%)
4	POV	B	3010	-	30,30,51	1.31	5 (16%)	32,34,59	1.23	2 (6%)
4	POV	D	3006	-	15,15,51	0.35	0	14,14,59	0.87	0
4	POV	B	3001	-	41,41,51	1.23	7 (17%)	45,46,59	1.25	3 (6%)
4	POV	D	3004	-	37,37,51	1.30	6 (16%)	41,42,59	1.11	3 (7%)
4	POV	A	3005	-	32,32,51	1.27	5 (15%)	34,34,59	1.08	2 (5%)
4	POV	A	3012	-	15,15,51	0.38	0	14,14,59	0.77	0
3	CLR	A	3000	-	31,31,31	0.76	0	48,48,48	1.37	7 (14%)
4	POV	A	3010	-	30,30,51	1.31	5 (16%)	32,34,59	1.23	2 (6%)
4	POV	A	3001	-	41,41,51	1.23	7 (17%)	45,46,59	1.25	3 (6%)
4	POV	B	3002	-	43,43,51	1.20	5 (11%)	49,51,59	0.98	3 (6%)
4	POV	C	3005	-	32,32,51	1.27	5 (15%)	34,34,59	1.08	2 (5%)
4	POV	B	3014	-	14,14,51	1.05	1 (7%)	13,13,59	0.85	0
4	POV	B	3006	-	15,15,51	0.34	0	14,14,59	0.87	0
4	POV	C	3012	-	15,15,51	0.38	0	14,14,59	0.76	0
3	CLR	C	3000	-	31,31,31	0.76	0	48,48,48	1.38	7 (14%)
4	POV	C	3001	-	41,41,51	1.23	7 (17%)	45,46,59	1.25	3 (6%)
4	POV	D	3001	-	41,41,51	1.23	7 (17%)	45,46,59	1.25	3 (6%)
3	CLR	B	3000	-	31,31,31	0.76	0	48,48,48	1.38	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	D	3005	-	32,32,51	1.28	5 (15%)	34,34,59	1.08	2 (5%)
4	POV	A	3006	-	15,15,51	0.35	0	14,14,59	0.87	0
4	POV	B	3013	-	10,10,51	0.41	0	9,9,59	0.79	0
4	POV	D	3013	-	10,10,51	0.41	0	9,9,59	0.79	0
4	POV	A	3014	-	14,14,51	1.04	1 (7%)	13,13,59	0.85	0
4	POV	D	3012	-	15,15,51	0.38	0	14,14,59	0.76	0
4	POV	D	3014	-	14,14,51	1.05	1 (7%)	13,13,59	0.85	0
4	POV	D	3007	-	15,15,51	0.38	0	14,14,59	0.76	0
3	CLR	D	3000	-	31,31,31	0.76	0	48,48,48	1.37	7 (14%)
4	POV	B	3011	-	30,30,51	1.31	5 (16%)	32,34,59	1.19	2 (6%)
4	POV	B	3003	-	15,15,51	1.03	1 (6%)	14,14,59	0.83	0
4	POV	A	3011	-	30,30,51	1.31	5 (16%)	32,34,59	1.19	2 (6%)
4	POV	D	3010	-	30,30,51	1.31	5 (16%)	32,34,59	1.23	2 (6%)
4	POV	A	3009	-	11,11,51	0.39	0	10,10,59	0.81	0
4	POV	C	3007	-	15,15,51	0.39	0	14,14,59	0.76	0
4	POV	A	3003	-	15,15,51	1.03	1 (6%)	14,14,59	0.82	0
4	POV	B	3007	-	15,15,51	0.38	0	14,14,59	0.75	0
4	POV	A	3004	-	37,37,51	1.30	6 (16%)	41,42,59	1.11	3 (7%)
4	POV	B	3008	-	12,12,51	0.41	0	11,11,59	0.74	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	D	3003	-	-	7/13/13/55	-
4	POV	B	3005	-	-	5/33/33/55	-
4	POV	A	3002	-	-	17/47/47/55	-
4	POV	C	3002	-	-	17/47/47/55	-
4	POV	C	3014	-	-	4/12/12/55	-
4	POV	D	3009	-	-	1/9/9/55	-
4	POV	A	3008	-	-	5/10/10/55	-
4	POV	C	3003	-	-	7/13/13/55	-
4	POV	C	3008	-	-	5/10/10/55	-
4	POV	C	3013	-	-	0/8/8/55	-
4	POV	D	3002	-	-	17/47/47/55	-
4	POV	D	3008	-	-	5/10/10/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	A	3013	-	-	0/8/8/55	-
4	POV	C	3006	-	-	0/13/13/55	-
4	POV	B	3009	-	-	1/9/9/55	-
4	POV	C	3004	-	-	18/39/39/55	-
4	POV	A	3007	-	-	7/13/13/55	-
4	POV	D	3011	-	-	13/31/31/55	-
4	POV	C	3009	-	-	1/9/9/55	-
4	POV	C	3011	-	-	13/31/31/55	-
4	POV	B	3012	-	-	8/13/13/55	-
4	POV	B	3004	-	-	18/39/39/55	-
4	POV	C	3010	-	-	8/31/31/55	-
4	POV	B	3010	-	-	8/31/31/55	-
4	POV	D	3006	-	-	0/13/13/55	-
4	POV	B	3001	-	-	18/43/43/55	-
4	POV	D	3004	-	-	18/39/39/55	-
4	POV	A	3005	-	-	5/33/33/55	-
4	POV	A	3012	-	-	8/13/13/55	-
3	CLR	A	3000	-	-	0/10/68/68	0/4/4/4
4	POV	A	3010	-	-	8/31/31/55	-
4	POV	A	3001	-	-	18/43/43/55	-
4	POV	B	3002	-	-	17/47/47/55	-
4	POV	C	3005	-	-	5/33/33/55	-
4	POV	B	3014	-	-	4/12/12/55	-
4	POV	B	3006	-	-	0/13/13/55	-
4	POV	C	3012	-	-	8/13/13/55	-
3	CLR	C	3000	-	-	0/10/68/68	0/4/4/4
4	POV	C	3001	-	-	18/43/43/55	-
4	POV	D	3001	-	-	18/43/43/55	-
3	CLR	B	3000	-	-	0/10/68/68	0/4/4/4
4	POV	D	3005	-	-	5/33/33/55	-
4	POV	A	3006	-	-	0/13/13/55	-
4	POV	B	3013	-	-	0/8/8/55	-
4	POV	D	3013	-	-	0/8/8/55	-
4	POV	A	3014	-	-	4/12/12/55	-
4	POV	D	3012	-	-	8/13/13/55	-
4	POV	D	3014	-	-	4/12/12/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	D	3007	-	-	7/13/13/55	-
3	CLR	D	3000	-	-	0/10/68/68	0/4/4/4
4	POV	B	3011	-	-	13/31/31/55	-
4	POV	B	3003	-	-	7/13/13/55	-
4	POV	A	3011	-	-	13/31/31/55	-
4	POV	D	3010	-	-	8/31/31/55	-
4	POV	A	3009	-	-	1/9/9/55	-
4	POV	C	3007	-	-	7/13/13/55	-
4	POV	A	3003	-	-	7/13/13/55	-
4	POV	B	3007	-	-	7/13/13/55	-
4	POV	A	3004	-	-	18/39/39/55	-
4	POV	B	3008	-	-	5/10/10/55	-

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3004	POV	C29-C210	3.83	1.54	1.31
4	B	3004	POV	C29-C210	3.83	1.54	1.31
4	C	3004	POV	C29-C210	3.83	1.54	1.31
4	D	3004	POV	C29-C210	3.82	1.53	1.31
4	C	3003	POV	C29-C210	3.81	1.53	1.31
4	B	3003	POV	C29-C210	3.81	1.53	1.31
4	D	3003	POV	C29-C210	3.81	1.53	1.31
4	A	3003	POV	C29-C210	3.79	1.53	1.31
4	D	3011	POV	C29-C210	3.79	1.53	1.31
4	C	3011	POV	C29-C210	3.78	1.53	1.31
4	A	3011	POV	C29-C210	3.76	1.53	1.31
4	B	3011	POV	C29-C210	3.76	1.53	1.31
4	C	3014	POV	C29-C210	3.76	1.53	1.31
4	D	3005	POV	C29-C210	3.76	1.53	1.31
4	A	3010	POV	C29-C210	3.75	1.53	1.31
4	D	3010	POV	C29-C210	3.75	1.53	1.31
4	A	3005	POV	C29-C210	3.75	1.53	1.31
4	B	3005	POV	C29-C210	3.75	1.53	1.31
4	A	3001	POV	C29-C210	3.75	1.53	1.31
4	D	3001	POV	C29-C210	3.75	1.53	1.31
4	B	3010	POV	C29-C210	3.74	1.53	1.31
4	B	3014	POV	C29-C210	3.74	1.53	1.31
4	D	3014	POV	C29-C210	3.74	1.53	1.31
4	C	3001	POV	C29-C210	3.74	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3005	POV	C29-C210	3.74	1.53	1.31
4	B	3001	POV	C29-C210	3.74	1.53	1.31
4	C	3010	POV	C29-C210	3.74	1.53	1.31
4	A	3014	POV	C29-C210	3.73	1.53	1.31
4	B	3002	POV	C210-C29	3.71	1.53	1.28
4	A	3002	POV	C210-C29	3.69	1.53	1.28
4	D	3002	POV	C210-C29	3.68	1.53	1.28
4	C	3002	POV	C210-C29	3.68	1.53	1.28
4	D	3005	POV	O21-C2	-3.38	1.41	1.47
4	A	3005	POV	O21-C2	-3.36	1.41	1.47
4	B	3005	POV	O21-C2	-3.36	1.41	1.47
4	C	3005	POV	O21-C2	-3.33	1.41	1.47
4	C	3001	POV	P-O12	2.76	1.65	1.54
4	D	3004	POV	P-O12	2.75	1.65	1.54
4	B	3004	POV	P-O12	2.75	1.65	1.54
4	A	3004	POV	P-O12	2.75	1.65	1.54
4	C	3004	POV	P-O12	2.75	1.65	1.54
4	B	3011	POV	P-O12	2.74	1.65	1.54
4	D	3011	POV	P-O12	2.74	1.65	1.54
4	A	3011	POV	P-O12	2.74	1.65	1.54
4	C	3011	POV	P-O12	2.74	1.65	1.54
4	A	3001	POV	P-O12	2.74	1.65	1.54
4	B	3001	POV	P-O12	2.74	1.65	1.54
4	A	3010	POV	P-O12	2.73	1.65	1.54
4	B	3010	POV	P-O12	2.73	1.65	1.54
4	C	3010	POV	P-O12	2.73	1.65	1.54
4	D	3010	POV	P-O12	2.73	1.65	1.54
4	D	3001	POV	P-O12	2.73	1.65	1.54
4	A	3004	POV	O31-C31	2.69	1.41	1.33
4	D	3004	POV	O31-C31	2.69	1.41	1.33
4	C	3004	POV	O31-C31	2.69	1.41	1.33
4	B	3004	POV	O31-C31	2.68	1.41	1.33
4	C	3002	POV	O31-C31	2.64	1.41	1.33
4	A	3002	POV	O31-C31	2.62	1.41	1.33
4	B	3002	POV	O31-C31	2.62	1.41	1.33
4	D	3002	POV	O31-C31	2.62	1.41	1.33
4	D	3005	POV	O31-C31	2.57	1.40	1.33
4	C	3005	POV	O31-C31	2.57	1.40	1.33
4	A	3005	POV	O31-C31	2.57	1.40	1.33
4	B	3005	POV	O31-C31	2.57	1.40	1.33
4	C	3005	POV	O21-C21	2.41	1.41	1.34
4	A	3005	POV	O21-C21	2.40	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3005	POV	O21-C21	2.40	1.41	1.34
4	D	3005	POV	O21-C21	2.39	1.41	1.34
4	A	3002	POV	O21-C21	2.38	1.41	1.34
4	B	3002	POV	O21-C21	2.38	1.41	1.34
4	C	3002	POV	O21-C21	2.38	1.41	1.34
4	D	3002	POV	O21-C21	2.38	1.41	1.34
4	A	3001	POV	O31-C31	2.36	1.40	1.33
4	D	3001	POV	O31-C31	2.36	1.40	1.33
4	C	3001	POV	O31-C31	2.34	1.40	1.33
4	B	3001	POV	O31-C31	2.34	1.40	1.33
4	C	3001	POV	O31-C3	-2.25	1.40	1.45
4	B	3001	POV	O21-C21	2.24	1.40	1.34
4	C	3001	POV	O21-C21	2.24	1.40	1.34
4	D	3001	POV	O21-C21	2.24	1.40	1.34
4	A	3001	POV	O21-C21	2.23	1.40	1.34
4	A	3001	POV	O31-C3	-2.21	1.40	1.45
4	B	3001	POV	O31-C3	-2.21	1.40	1.45
4	D	3001	POV	O31-C3	-2.20	1.40	1.45
4	A	3010	POV	O21-C21	2.18	1.40	1.34
4	B	3010	POV	O21-C21	2.18	1.40	1.34
4	A	3004	POV	O21-C21	2.18	1.40	1.34
4	C	3010	POV	O21-C21	2.18	1.40	1.34
4	D	3010	POV	O21-C21	2.18	1.40	1.34
4	B	3004	POV	O21-C21	2.18	1.40	1.34
4	C	3004	POV	O21-C21	2.18	1.40	1.34
4	D	3004	POV	O21-C21	2.18	1.40	1.34
4	D	3001	POV	O21-C2	-2.18	1.41	1.46
4	C	3004	POV	P-O13	-2.17	1.46	1.54
4	A	3010	POV	P-O13	-2.16	1.46	1.54
4	D	3010	POV	P-O13	-2.16	1.46	1.54
4	A	3011	POV	O21-C2	-2.16	1.41	1.46
4	B	3011	POV	O21-C2	-2.16	1.41	1.46
4	C	3011	POV	O21-C2	-2.16	1.41	1.46
4	B	3010	POV	P-O13	-2.16	1.46	1.54
4	A	3010	POV	O21-C2	-2.16	1.41	1.46
4	B	3010	POV	O21-C2	-2.16	1.41	1.46
4	C	3010	POV	O21-C2	-2.16	1.41	1.46
4	D	3010	POV	O21-C2	-2.16	1.41	1.46
4	D	3011	POV	O21-C2	-2.15	1.41	1.46
4	A	3004	POV	P-O13	-2.15	1.46	1.54
4	A	3011	POV	O21-C21	2.15	1.40	1.34
4	B	3011	POV	O21-C21	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3011	POV	O21-C21	2.15	1.40	1.34
4	D	3011	POV	O21-C21	2.15	1.40	1.34
4	C	3010	POV	P-O13	-2.14	1.46	1.54
4	A	3001	POV	O21-C2	-2.14	1.41	1.46
4	B	3001	POV	O21-C2	-2.14	1.41	1.46
4	C	3001	POV	O21-C2	-2.14	1.41	1.46
4	C	3011	POV	P-O13	-2.14	1.46	1.54
4	D	3011	POV	P-O13	-2.14	1.46	1.54
4	B	3004	POV	P-O13	-2.14	1.46	1.54
4	D	3004	POV	P-O13	-2.14	1.46	1.54
4	A	3001	POV	P-O13	-2.14	1.46	1.54
4	B	3001	POV	P-O13	-2.14	1.46	1.54
4	C	3001	POV	P-O13	-2.14	1.46	1.54
4	D	3001	POV	P-O13	-2.14	1.46	1.54
4	A	3011	POV	P-O13	-2.13	1.46	1.54
4	B	3011	POV	P-O13	-2.13	1.46	1.54
4	C	3004	POV	O21-C2	-2.09	1.41	1.46
4	D	3004	POV	O21-C2	-2.09	1.41	1.46
4	B	3004	POV	O21-C2	-2.09	1.41	1.46
4	D	3005	POV	O31-C3	-2.09	1.40	1.45
4	B	3005	POV	O31-C3	-2.07	1.40	1.45
4	A	3005	POV	O31-C3	-2.07	1.40	1.45
4	A	3004	POV	O21-C2	-2.04	1.41	1.46
4	C	3002	POV	O31-C3	-2.03	1.40	1.45
4	D	3002	POV	O31-C3	-2.03	1.40	1.45
4	C	3005	POV	O31-C3	-2.03	1.40	1.45
4	D	3002	POV	O21-C2	-2.02	1.41	1.46
4	B	3002	POV	O21-C2	-2.02	1.41	1.46
4	A	3002	POV	O31-C3	-2.01	1.40	1.45
4	B	3002	POV	O31-C3	-2.01	1.40	1.45

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3000	CLR	C13-C17-C20	-4.47	112.49	119.49
3	A	3000	CLR	C13-C17-C20	-4.41	112.58	119.49
3	C	3000	CLR	C13-C17-C20	-4.40	112.59	119.49
4	B	3001	POV	O21-C21-C22	4.39	120.97	111.50
3	D	3000	CLR	C13-C17-C20	-4.39	112.61	119.49
4	A	3001	POV	O21-C21-C22	4.39	120.95	111.50
4	C	3001	POV	O21-C21-C22	4.38	120.95	111.50
4	D	3001	POV	O21-C21-C22	4.38	120.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3010	POV	O21-C21-C22	3.97	120.05	111.50
4	D	3010	POV	O21-C21-C22	3.97	120.05	111.50
4	A	3010	POV	O21-C21-C22	3.96	120.03	111.50
4	B	3010	POV	O21-C21-C22	3.96	120.03	111.50
4	B	3011	POV	O21-C21-C22	3.88	119.87	111.50
4	D	3011	POV	O21-C21-C22	3.88	119.87	111.50
4	A	3011	POV	O21-C21-C22	3.87	119.84	111.50
4	C	3011	POV	O21-C21-C22	3.87	119.84	111.50
4	A	3002	POV	O21-C21-C22	3.66	119.38	111.50
4	B	3002	POV	O21-C21-C22	3.66	119.38	111.50
4	C	3002	POV	O21-C21-C22	3.66	119.38	111.50
4	D	3002	POV	O21-C21-C22	3.66	119.38	111.50
4	B	3004	POV	O21-C21-C22	3.47	118.98	111.50
4	D	3004	POV	O21-C21-C22	3.47	118.98	111.50
4	C	3004	POV	O21-C21-C22	3.46	118.95	111.50
4	A	3004	POV	O21-C21-C22	3.46	118.95	111.50
3	C	3000	CLR	C13-C14-C8	-3.41	109.33	114.38
3	A	3000	CLR	C13-C14-C8	-3.38	109.37	114.38
3	B	3000	CLR	C13-C14-C8	-3.37	109.38	114.38
3	D	3000	CLR	C13-C14-C8	-3.36	109.40	114.38
4	B	3005	POV	O21-C21-C22	3.31	118.64	111.50
4	D	3005	POV	O21-C21-C22	3.31	118.64	111.50
4	A	3005	POV	O21-C21-C22	3.30	118.61	111.50
4	C	3005	POV	O21-C21-C22	3.30	118.60	111.50
3	D	3000	CLR	C17-C13-C14	3.16	103.82	100.07
3	A	3000	CLR	C17-C13-C14	3.13	103.79	100.07
3	C	3000	CLR	C17-C13-C14	3.13	103.79	100.07
3	B	3000	CLR	C17-C13-C14	3.10	103.75	100.07
3	C	3000	CLR	C11-C12-C13	-2.88	107.84	112.78
3	A	3000	CLR	C11-C12-C13	-2.87	107.86	112.78
3	D	3000	CLR	C11-C12-C13	-2.87	107.86	112.78
3	B	3000	CLR	C11-C12-C13	-2.86	107.88	112.78
3	D	3000	CLR	C8-C7-C6	-2.68	108.88	112.73
3	A	3000	CLR	C8-C7-C6	-2.67	108.90	112.73
3	B	3000	CLR	C8-C7-C6	-2.66	108.90	112.73
3	C	3000	CLR	C8-C7-C6	-2.66	108.91	112.73
4	B	3010	POV	O13-P-O14	-2.53	100.79	110.68
4	C	3010	POV	O13-P-O14	-2.53	100.80	110.68
4	C	3001	POV	O31-C31-C32	2.53	119.83	111.91
4	D	3001	POV	O31-C31-C32	2.52	119.81	111.91
4	D	3010	POV	O13-P-O14	-2.51	100.83	110.68
4	A	3001	POV	O31-C31-C32	2.51	119.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3001	POV	O31-C31-C32	2.51	119.78	111.91
4	A	3010	POV	O13-P-O14	-2.51	100.87	110.68
4	B	3004	POV	O13-P-O14	-2.49	100.94	110.68
4	D	3004	POV	O13-P-O14	-2.48	100.97	110.68
4	C	3004	POV	O13-P-O14	-2.48	100.98	110.68
4	A	3004	POV	O13-P-O14	-2.48	100.98	110.68
4	A	3001	POV	O13-P-O14	-2.46	101.05	110.68
4	B	3001	POV	O13-P-O14	-2.46	101.05	110.68
4	C	3001	POV	O13-P-O14	-2.46	101.06	110.68
4	D	3001	POV	O13-P-O14	-2.46	101.06	110.68
4	A	3011	POV	O13-P-O14	-2.43	101.17	110.68
4	C	3011	POV	O13-P-O14	-2.43	101.17	110.68
4	D	3011	POV	O13-P-O14	-2.42	101.19	110.68
4	B	3011	POV	O13-P-O14	-2.42	101.20	110.68
4	D	3005	POV	O31-C31-C32	2.42	119.50	111.91
4	B	3005	POV	O31-C31-C32	2.41	119.47	111.91
4	A	3005	POV	O31-C31-C32	2.41	119.46	111.91
4	C	3005	POV	O31-C31-C32	2.41	119.46	111.91
4	B	3002	POV	O13-P-O14	-2.28	100.99	112.24
4	A	3002	POV	O13-P-O14	-2.27	101.01	112.24
4	D	3002	POV	O13-P-O14	-2.27	101.01	112.24
4	C	3002	POV	O13-P-O14	-2.26	101.05	112.24
4	C	3004	POV	O31-C31-C32	2.11	118.54	111.91
3	D	3000	CLR	C19-C10-C9	-2.11	109.17	111.68
3	A	3000	CLR	C19-C10-C9	-2.11	109.17	111.68
3	B	3000	CLR	C19-C10-C9	-2.11	109.17	111.68
3	C	3000	CLR	C19-C10-C9	-2.10	109.17	111.68
4	B	3004	POV	O31-C31-C32	2.10	118.51	111.91
4	D	3004	POV	O31-C31-C32	2.10	118.49	111.91
4	A	3004	POV	O31-C31-C32	2.09	118.48	111.91
3	C	3000	CLR	C11-C9-C10	-2.09	110.33	113.08
4	B	3002	POV	C28-C29-C210	-2.07	112.75	126.84
4	A	3002	POV	C28-C29-C210	-2.07	112.78	126.84
4	D	3002	POV	C28-C29-C210	-2.07	112.79	126.84
3	D	3000	CLR	C11-C9-C10	-2.06	110.36	113.08
3	A	3000	CLR	C11-C9-C10	-2.06	110.36	113.08
3	B	3000	CLR	C11-C9-C10	-2.06	110.36	113.08
4	C	3002	POV	C28-C29-C210	-2.06	112.83	126.84

There are no chirality outliers.

All (444) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3001	POV	C1-O11-P-O12
4	A	3001	POV	C1-O11-P-O13
4	A	3001	POV	C22-C21-O21-C2
4	A	3004	POV	O11-C1-C2-O21
4	A	3004	POV	C22-C21-O21-C2
4	A	3010	POV	C22-C21-O21-C2
4	A	3010	POV	O32-C31-O31-C3
4	A	3011	POV	C22-C21-O21-C2
4	A	3011	POV	O32-C31-O31-C3
4	B	3001	POV	C1-O11-P-O12
4	B	3001	POV	C1-O11-P-O13
4	B	3001	POV	C22-C21-O21-C2
4	B	3004	POV	O11-C1-C2-O21
4	B	3004	POV	C22-C21-O21-C2
4	B	3010	POV	C22-C21-O21-C2
4	B	3010	POV	O32-C31-O31-C3
4	B	3011	POV	C22-C21-O21-C2
4	B	3011	POV	O32-C31-O31-C3
4	C	3001	POV	C1-O11-P-O12
4	C	3001	POV	C1-O11-P-O13
4	C	3001	POV	C22-C21-O21-C2
4	C	3004	POV	O11-C1-C2-O21
4	C	3004	POV	C22-C21-O21-C2
4	C	3010	POV	C22-C21-O21-C2
4	C	3010	POV	O32-C31-O31-C3
4	C	3011	POV	C22-C21-O21-C2
4	C	3011	POV	O32-C31-O31-C3
4	D	3010	POV	C22-C21-O21-C2
4	D	3010	POV	O32-C31-O31-C3
4	D	3011	POV	C22-C21-O21-C2
4	D	3011	POV	O32-C31-O31-C3
4	D	3001	POV	C1-O11-P-O12
4	D	3001	POV	C1-O11-P-O13
4	D	3001	POV	C22-C21-O21-C2
4	D	3004	POV	O11-C1-C2-O21
4	D	3004	POV	C22-C21-O21-C2
4	A	3001	POV	O22-C21-O21-C2
4	A	3004	POV	O22-C21-O21-C2
4	A	3010	POV	O22-C21-O21-C2
4	A	3011	POV	O22-C21-O21-C2
4	B	3001	POV	O22-C21-O21-C2
4	B	3004	POV	O22-C21-O21-C2
4	B	3010	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
4	B	3011	POV	O22-C21-O21-C2
4	C	3001	POV	O22-C21-O21-C2
4	C	3004	POV	O22-C21-O21-C2
4	C	3010	POV	O22-C21-O21-C2
4	C	3011	POV	O22-C21-O21-C2
4	D	3010	POV	O22-C21-O21-C2
4	D	3011	POV	O22-C21-O21-C2
4	D	3001	POV	O22-C21-O21-C2
4	D	3004	POV	O22-C21-O21-C2
4	A	3004	POV	C211-C210-C29-C28
4	A	3011	POV	C211-C210-C29-C28
4	B	3004	POV	C211-C210-C29-C28
4	B	3011	POV	C211-C210-C29-C28
4	C	3004	POV	C211-C210-C29-C28
4	C	3011	POV	C211-C210-C29-C28
4	D	3011	POV	C211-C210-C29-C28
4	D	3004	POV	C211-C210-C29-C28
4	A	3001	POV	C32-C31-O31-C3
4	B	3001	POV	C32-C31-O31-C3
4	C	3001	POV	C32-C31-O31-C3
4	D	3001	POV	C32-C31-O31-C3
4	A	3001	POV	O32-C31-O31-C3
4	B	3001	POV	O32-C31-O31-C3
4	C	3001	POV	O32-C31-O31-C3
4	D	3001	POV	O32-C31-O31-C3
4	A	3004	POV	C31-C32-C33-C34
4	B	3004	POV	C31-C32-C33-C34
4	C	3004	POV	C31-C32-C33-C34
4	D	3004	POV	C31-C32-C33-C34
4	A	3002	POV	C32-C33-C34-C35
4	B	3002	POV	C32-C33-C34-C35
4	C	3002	POV	C32-C33-C34-C35
4	D	3002	POV	C32-C33-C34-C35
4	A	3002	POV	C37-C38-C39-C310
4	B	3002	POV	C37-C38-C39-C310
4	D	3002	POV	C37-C38-C39-C310
4	C	3002	POV	C37-C38-C39-C310
4	A	3011	POV	C211-C212-C213-C214
4	B	3011	POV	C211-C212-C213-C214
4	C	3011	POV	C211-C212-C213-C214
4	D	3011	POV	C211-C212-C213-C214
4	A	3001	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
4	B	3001	POV	C24-C25-C26-C27
4	C	3001	POV	C24-C25-C26-C27
4	D	3001	POV	C24-C25-C26-C27
4	A	3001	POV	C23-C24-C25-C26
4	B	3001	POV	C23-C24-C25-C26
4	C	3001	POV	C23-C24-C25-C26
4	D	3001	POV	C23-C24-C25-C26
4	A	3002	POV	C33-C34-C35-C36
4	B	3002	POV	C33-C34-C35-C36
4	C	3002	POV	C33-C34-C35-C36
4	D	3002	POV	C33-C34-C35-C36
4	A	3004	POV	C26-C27-C28-C29
4	B	3004	POV	C26-C27-C28-C29
4	C	3004	POV	C26-C27-C28-C29
4	D	3004	POV	C26-C27-C28-C29
4	A	3008	POV	C39-C310-C311-C312
4	B	3008	POV	C39-C310-C311-C312
4	C	3008	POV	C39-C310-C311-C312
4	D	3008	POV	C39-C310-C311-C312
4	A	3001	POV	C36-C37-C38-C39
4	B	3001	POV	C36-C37-C38-C39
4	C	3001	POV	C36-C37-C38-C39
4	D	3001	POV	C36-C37-C38-C39
4	A	3002	POV	C21-C22-C23-C24
4	B	3002	POV	C21-C22-C23-C24
4	C	3002	POV	C21-C22-C23-C24
4	D	3002	POV	C21-C22-C23-C24
4	A	3004	POV	C34-C35-C36-C37
4	B	3004	POV	C34-C35-C36-C37
4	C	3004	POV	C34-C35-C36-C37
4	D	3004	POV	C34-C35-C36-C37
4	A	3011	POV	C26-C27-C28-C29
4	B	3011	POV	C26-C27-C28-C29
4	C	3011	POV	C26-C27-C28-C29
4	D	3011	POV	C26-C27-C28-C29
4	A	3002	POV	O22-C21-O21-C2
4	B	3002	POV	O22-C21-O21-C2
4	C	3002	POV	O22-C21-O21-C2
4	D	3002	POV	O22-C21-O21-C2
4	A	3008	POV	C33-C34-C35-C36
4	B	3008	POV	C33-C34-C35-C36
4	B	3010	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	C	3008	POV	C33-C34-C35-C36
4	D	3010	POV	C23-C24-C25-C26
4	D	3008	POV	C33-C34-C35-C36
4	A	3002	POV	C22-C21-O21-C2
4	B	3002	POV	C22-C21-O21-C2
4	C	3002	POV	C22-C21-O21-C2
4	D	3002	POV	C22-C21-O21-C2
4	A	3010	POV	C23-C24-C25-C26
4	C	3010	POV	C23-C24-C25-C26
4	A	3004	POV	C32-C33-C34-C35
4	B	3004	POV	C32-C33-C34-C35
4	C	3004	POV	C32-C33-C34-C35
4	D	3004	POV	C32-C33-C34-C35
4	A	3004	POV	C24-C25-C26-C27
4	A	3005	POV	C22-C21-O21-C2
4	B	3005	POV	C22-C21-O21-C2
4	C	3005	POV	C22-C21-O21-C2
4	D	3005	POV	C22-C21-O21-C2
4	B	3004	POV	C24-C25-C26-C27
4	C	3004	POV	C24-C25-C26-C27
4	D	3004	POV	C24-C25-C26-C27
4	A	3004	POV	O11-C1-C2-C3
4	B	3004	POV	O11-C1-C2-C3
4	C	3004	POV	O11-C1-C2-C3
4	D	3004	POV	O11-C1-C2-C3
4	A	3002	POV	C1-C2-C3-O31
4	B	3002	POV	C1-C2-C3-O31
4	C	3002	POV	C1-C2-C3-O31
4	D	3002	POV	C1-C2-C3-O31
4	A	3001	POV	C1-O11-P-O14
4	B	3001	POV	C1-O11-P-O14
4	C	3001	POV	C1-O11-P-O14
4	D	3001	POV	C1-O11-P-O14
4	A	3012	POV	C33-C34-C35-C36
4	B	3012	POV	C33-C34-C35-C36
4	A	3003	POV	C211-C210-C29-C28
4	B	3003	POV	C211-C210-C29-C28
4	C	3003	POV	C211-C210-C29-C28
4	D	3003	POV	C211-C210-C29-C28
4	C	3012	POV	C33-C34-C35-C36
4	D	3012	POV	C33-C34-C35-C36
4	A	3005	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
4	B	3005	POV	O22-C21-O21-C2
4	C	3005	POV	O22-C21-O21-C2
4	D	3005	POV	O22-C21-O21-C2
4	C	3007	POV	C32-C33-C34-C35
4	D	3007	POV	C32-C33-C34-C35
4	A	3007	POV	C32-C33-C34-C35
4	B	3007	POV	C32-C33-C34-C35
4	A	3001	POV	C33-C34-C35-C36
4	C	3001	POV	C33-C34-C35-C36
4	D	3001	POV	C33-C34-C35-C36
4	B	3001	POV	C33-C34-C35-C36
4	A	3007	POV	C37-C38-C39-C310
4	C	3007	POV	C37-C38-C39-C310
4	D	3007	POV	C37-C38-C39-C310
4	B	3007	POV	C35-C36-C37-C38
4	B	3007	POV	C37-C38-C39-C310
4	D	3007	POV	C35-C36-C37-C38
4	A	3007	POV	C35-C36-C37-C38
4	C	3007	POV	C35-C36-C37-C38
4	A	3014	POV	C26-C27-C28-C29
4	B	3014	POV	C26-C27-C28-C29
4	C	3014	POV	C26-C27-C28-C29
4	D	3014	POV	C26-C27-C28-C29
4	A	3010	POV	C212-C213-C214-C215
4	D	3010	POV	C212-C213-C214-C215
4	B	3010	POV	C212-C213-C214-C215
4	C	3010	POV	C212-C213-C214-C215
4	A	3002	POV	O21-C2-C3-O31
4	B	3002	POV	O21-C2-C3-O31
4	C	3002	POV	O21-C2-C3-O31
4	D	3002	POV	O21-C2-C3-O31
4	C	3008	POV	C35-C36-C37-C38
4	A	3008	POV	C35-C36-C37-C38
4	B	3008	POV	C35-C36-C37-C38
4	D	3008	POV	C35-C36-C37-C38
4	B	3011	POV	C22-C23-C24-C25
4	C	3011	POV	C22-C23-C24-C25
4	C	3012	POV	C310-C311-C312-C313
4	D	3011	POV	C22-C23-C24-C25
4	D	3012	POV	C310-C311-C312-C313
4	A	3011	POV	C22-C23-C24-C25
4	A	3012	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
4	B	3012	POV	C310-C311-C312-C313
4	A	3007	POV	C313-C314-C315-C316
4	B	3007	POV	C313-C314-C315-C316
4	C	3007	POV	C313-C314-C315-C316
4	D	3007	POV	C313-C314-C315-C316
4	D	3007	POV	C39-C310-C311-C312
4	A	3007	POV	C39-C310-C311-C312
4	B	3007	POV	C39-C310-C311-C312
4	C	3007	POV	C39-C310-C311-C312
4	B	3011	POV	C215-C216-C217-C218
4	C	3011	POV	C215-C216-C217-C218
4	A	3011	POV	C215-C216-C217-C218
4	C	3012	POV	C34-C35-C36-C37
4	D	3011	POV	C215-C216-C217-C218
4	D	3012	POV	C34-C35-C36-C37
4	A	3012	POV	C34-C35-C36-C37
4	B	3012	POV	C34-C35-C36-C37
4	A	3004	POV	C29-C210-C211-C212
4	B	3004	POV	C29-C210-C211-C212
4	C	3004	POV	C29-C210-C211-C212
4	D	3004	POV	C29-C210-C211-C212
4	A	3003	POV	C26-C27-C28-C29
4	B	3003	POV	C26-C27-C28-C29
4	C	3003	POV	C26-C27-C28-C29
4	D	3003	POV	C26-C27-C28-C29
4	B	3003	POV	C214-C215-C216-C217
4	A	3003	POV	C214-C215-C216-C217
4	A	3003	POV	C211-C212-C213-C214
4	B	3003	POV	C211-C212-C213-C214
4	C	3003	POV	C214-C215-C216-C217
4	D	3003	POV	C211-C212-C213-C214
4	D	3003	POV	C214-C215-C216-C217
4	A	3005	POV	C33-C34-C35-C36
4	B	3005	POV	C33-C34-C35-C36
4	C	3003	POV	C211-C212-C213-C214
4	C	3005	POV	C33-C34-C35-C36
4	D	3005	POV	C33-C34-C35-C36
4	A	3007	POV	C34-C35-C36-C37
4	B	3007	POV	C34-C35-C36-C37
4	C	3007	POV	C34-C35-C36-C37
4	D	3002	POV	C23-C24-C25-C26
4	D	3007	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
4	A	3002	POV	C23-C24-C25-C26
4	B	3002	POV	C23-C24-C25-C26
4	C	3002	POV	C23-C24-C25-C26
4	D	3004	POV	C311-C310-C39-C38
4	C	3004	POV	C311-C310-C39-C38
4	A	3004	POV	C311-C310-C39-C38
4	B	3004	POV	C311-C310-C39-C38
4	A	3012	POV	C32-C33-C34-C35
4	C	3012	POV	C32-C33-C34-C35
4	B	3012	POV	C32-C33-C34-C35
4	D	3012	POV	C32-C33-C34-C35
4	A	3004	POV	C210-C211-C212-C213
4	B	3004	POV	C210-C211-C212-C213
4	C	3004	POV	C210-C211-C212-C213
4	D	3004	POV	C210-C211-C212-C213
4	A	3012	POV	C31-C32-C33-C34
4	B	3012	POV	C31-C32-C33-C34
4	C	3012	POV	C31-C32-C33-C34
4	D	3012	POV	C31-C32-C33-C34
4	A	3002	POV	C34-C35-C36-C37
4	B	3002	POV	C34-C35-C36-C37
4	C	3002	POV	C34-C35-C36-C37
4	D	3002	POV	C34-C35-C36-C37
4	B	3002	POV	C310-C311-C312-C313
4	C	3002	POV	C310-C311-C312-C313
4	A	3002	POV	C310-C311-C312-C313
4	D	3002	POV	C310-C311-C312-C313
4	B	3001	POV	C311-C312-C313-C314
4	A	3001	POV	C311-C312-C313-C314
4	C	3001	POV	C311-C312-C313-C314
4	D	3001	POV	C311-C312-C313-C314
4	A	3002	POV	C11-C12-N-C13
4	B	3002	POV	C11-C12-N-C13
4	C	3002	POV	C11-C12-N-C13
4	D	3002	POV	C11-C12-N-C13
4	B	3001	POV	C212-C213-C214-C215
4	D	3001	POV	C212-C213-C214-C215
4	A	3001	POV	C212-C213-C214-C215
4	C	3001	POV	C212-C213-C214-C215
4	B	3004	POV	C39-C310-C311-C312
4	C	3004	POV	C39-C310-C311-C312
4	A	3004	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
4	D	3004	POV	C39-C310-C311-C312
4	A	3011	POV	C213-C214-C215-C216
4	B	3011	POV	C213-C214-C215-C216
4	C	3011	POV	C213-C214-C215-C216
4	D	3011	POV	C213-C214-C215-C216
4	A	3010	POV	C1-O11-P-O14
4	B	3010	POV	C1-O11-P-O14
4	C	3010	POV	C1-O11-P-O14
4	D	3010	POV	C1-O11-P-O14
4	D	3004	POV	C27-C28-C29-C210
4	A	3002	POV	C1-O11-P-O12
4	A	3002	POV	C11-O12-P-O11
4	B	3002	POV	C1-O11-P-O12
4	B	3002	POV	C11-O12-P-O11
4	C	3002	POV	C1-O11-P-O12
4	C	3002	POV	C11-O12-P-O11
4	D	3002	POV	C1-O11-P-O12
4	D	3002	POV	C11-O12-P-O11
4	B	3003	POV	C213-C214-C215-C216
4	D	3003	POV	C213-C214-C215-C216
4	A	3003	POV	C213-C214-C215-C216
4	C	3003	POV	C213-C214-C215-C216
4	D	3011	POV	C23-C24-C25-C26
4	A	3004	POV	C27-C28-C29-C210
4	B	3004	POV	C27-C28-C29-C210
4	C	3004	POV	C27-C28-C29-C210
4	B	3011	POV	C23-C24-C25-C26
4	C	3011	POV	C23-C24-C25-C26
4	A	3011	POV	C23-C24-C25-C26
4	A	3010	POV	C214-C215-C216-C217
4	B	3010	POV	C214-C215-C216-C217
4	D	3010	POV	C214-C215-C216-C217
4	C	3010	POV	C214-C215-C216-C217
4	A	3011	POV	C27-C28-C29-C210
4	A	3014	POV	C27-C28-C29-C210
4	B	3014	POV	C27-C28-C29-C210
4	B	3011	POV	C27-C28-C29-C210
4	C	3014	POV	C27-C28-C29-C210
4	C	3011	POV	C27-C28-C29-C210
4	D	3011	POV	C27-C28-C29-C210
4	D	3014	POV	C27-C28-C29-C210
4	A	3002	POV	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
4	B	3002	POV	C11-C12-N-C14
4	D	3002	POV	C11-C12-N-C14
4	A	3008	POV	C31-C32-C33-C34
4	B	3008	POV	C31-C32-C33-C34
4	D	3008	POV	C31-C32-C33-C34
4	C	3008	POV	C31-C32-C33-C34
4	D	3007	POV	C310-C311-C312-C313
4	A	3007	POV	C310-C311-C312-C313
4	B	3007	POV	C310-C311-C312-C313
4	C	3007	POV	C310-C311-C312-C313
4	C	3002	POV	C11-C12-N-C14
4	A	3002	POV	C27-C28-C29-C210
4	B	3002	POV	C27-C28-C29-C210
4	C	3002	POV	C27-C28-C29-C210
4	D	3002	POV	C27-C28-C29-C210
4	A	3005	POV	C31-C32-C33-C34
4	B	3005	POV	C31-C32-C33-C34
4	C	3005	POV	C31-C32-C33-C34
4	D	3005	POV	C31-C32-C33-C34
4	A	3001	POV	C310-C311-C312-C313
4	B	3001	POV	C310-C311-C312-C313
4	C	3001	POV	C310-C311-C312-C313
4	D	3001	POV	C310-C311-C312-C313
4	B	3012	POV	C311-C312-C313-C314
4	C	3012	POV	C311-C312-C313-C314
4	D	3012	POV	C311-C312-C313-C314
4	A	3012	POV	C311-C312-C313-C314
4	A	3002	POV	C11-C12-N-C15
4	B	3002	POV	C11-C12-N-C15
4	C	3002	POV	C11-C12-N-C15
4	D	3002	POV	C11-C12-N-C15
4	A	3009	POV	C36-C37-C38-C39
4	B	3009	POV	C36-C37-C38-C39
4	C	3009	POV	C36-C37-C38-C39
4	D	3009	POV	C36-C37-C38-C39
4	A	3011	POV	C24-C25-C26-C27
4	B	3011	POV	C24-C25-C26-C27
4	C	3011	POV	C24-C25-C26-C27
4	D	3011	POV	C24-C25-C26-C27
4	A	3004	POV	C37-C38-C39-C310
4	B	3004	POV	C37-C38-C39-C310
4	D	3004	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
4	C	3004	POV	C37-C38-C39-C310
4	A	3004	POV	C22-C23-C24-C25
4	B	3004	POV	C22-C23-C24-C25
4	C	3004	POV	C22-C23-C24-C25
4	D	3004	POV	C22-C23-C24-C25
4	A	3001	POV	C39-C310-C311-C312
4	B	3001	POV	C39-C310-C311-C312
4	C	3001	POV	C39-C310-C311-C312
4	D	3001	POV	C39-C310-C311-C312
4	A	3014	POV	C29-C210-C211-C212
4	B	3014	POV	C29-C210-C211-C212
4	C	3014	POV	C29-C210-C211-C212
4	D	3014	POV	C29-C210-C211-C212
4	C	3012	POV	C311-C310-C39-C38
4	A	3012	POV	C311-C310-C39-C38
4	B	3012	POV	C311-C310-C39-C38
4	D	3012	POV	C311-C310-C39-C38
4	A	3010	POV	C27-C28-C29-C210
4	B	3010	POV	C27-C28-C29-C210
4	C	3010	POV	C27-C28-C29-C210
4	D	3010	POV	C27-C28-C29-C210
4	A	3003	POV	C29-C210-C211-C212
4	C	3003	POV	C29-C210-C211-C212
4	B	3003	POV	C29-C210-C211-C212
4	D	3003	POV	C29-C210-C211-C212
4	B	3003	POV	C24-C25-C26-C27
4	A	3003	POV	C24-C25-C26-C27
4	C	3003	POV	C24-C25-C26-C27
4	D	3003	POV	C24-C25-C26-C27
4	A	3001	POV	O11-C1-C2-O21
4	B	3001	POV	O11-C1-C2-O21
4	C	3001	POV	O11-C1-C2-O21
4	D	3001	POV	O11-C1-C2-O21
4	A	3001	POV	C22-C23-C24-C25
4	B	3001	POV	C22-C23-C24-C25
4	C	3001	POV	C22-C23-C24-C25
4	D	3001	POV	C22-C23-C24-C25
4	A	3011	POV	O21-C2-C3-O31
4	B	3011	POV	O21-C2-C3-O31
4	C	3011	POV	O21-C2-C3-O31
4	D	3011	POV	O21-C2-C3-O31
4	A	3004	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
4	B	3004	POV	C36-C37-C38-C39
4	C	3004	POV	C36-C37-C38-C39
4	D	3004	POV	C36-C37-C38-C39
4	A	3001	POV	C27-C28-C29-C210
4	B	3001	POV	C27-C28-C29-C210
4	D	3001	POV	C27-C28-C29-C210
4	C	3001	POV	C27-C28-C29-C210
4	D	3012	POV	C36-C37-C38-C39
4	B	3012	POV	C36-C37-C38-C39
4	C	3012	POV	C36-C37-C38-C39
4	A	3012	POV	C36-C37-C38-C39
4	A	3014	POV	C211-C210-C29-C28
4	B	3014	POV	C211-C210-C29-C28
4	C	3014	POV	C211-C210-C29-C28
4	D	3014	POV	C211-C210-C29-C28
4	C	3008	POV	C36-C37-C38-C39
4	B	3008	POV	C36-C37-C38-C39
4	A	3008	POV	C36-C37-C38-C39
4	D	3008	POV	C36-C37-C38-C39
4	B	3005	POV	C311-C310-C39-C38
4	C	3005	POV	C311-C310-C39-C38
4	D	3005	POV	C311-C310-C39-C38
4	A	3005	POV	C311-C310-C39-C38

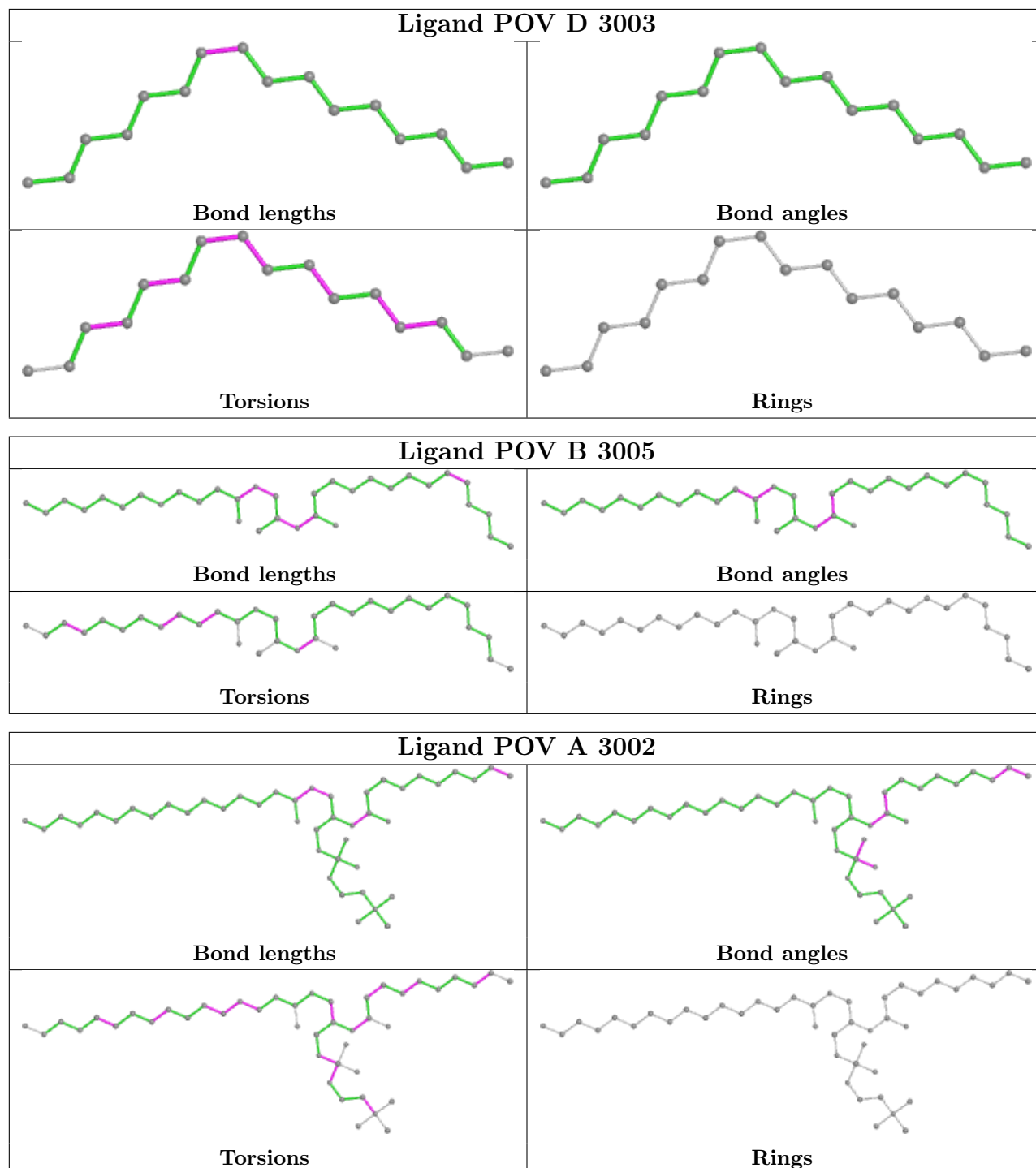
There are no ring outliers.

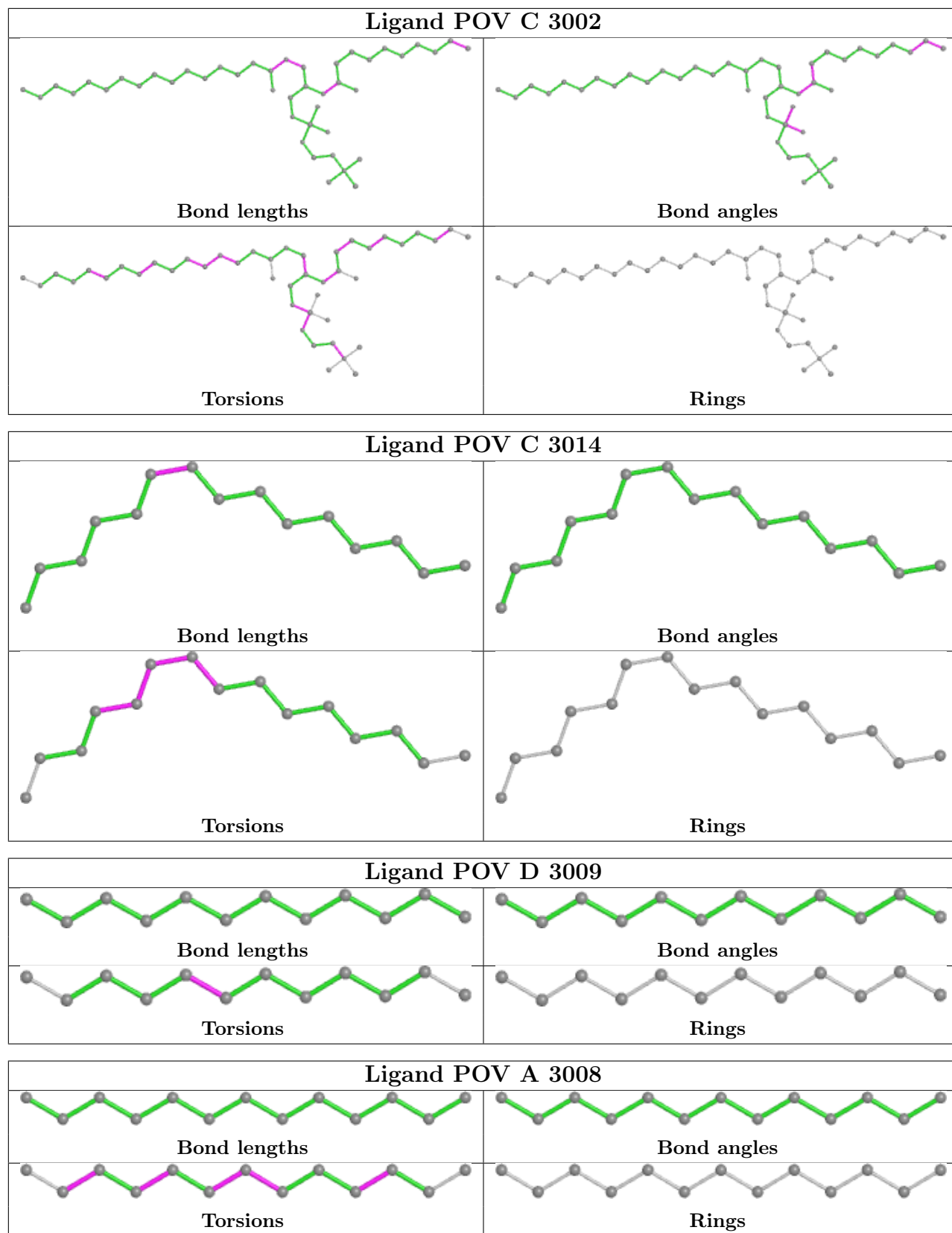
4 monomers are involved in 37 short contacts:

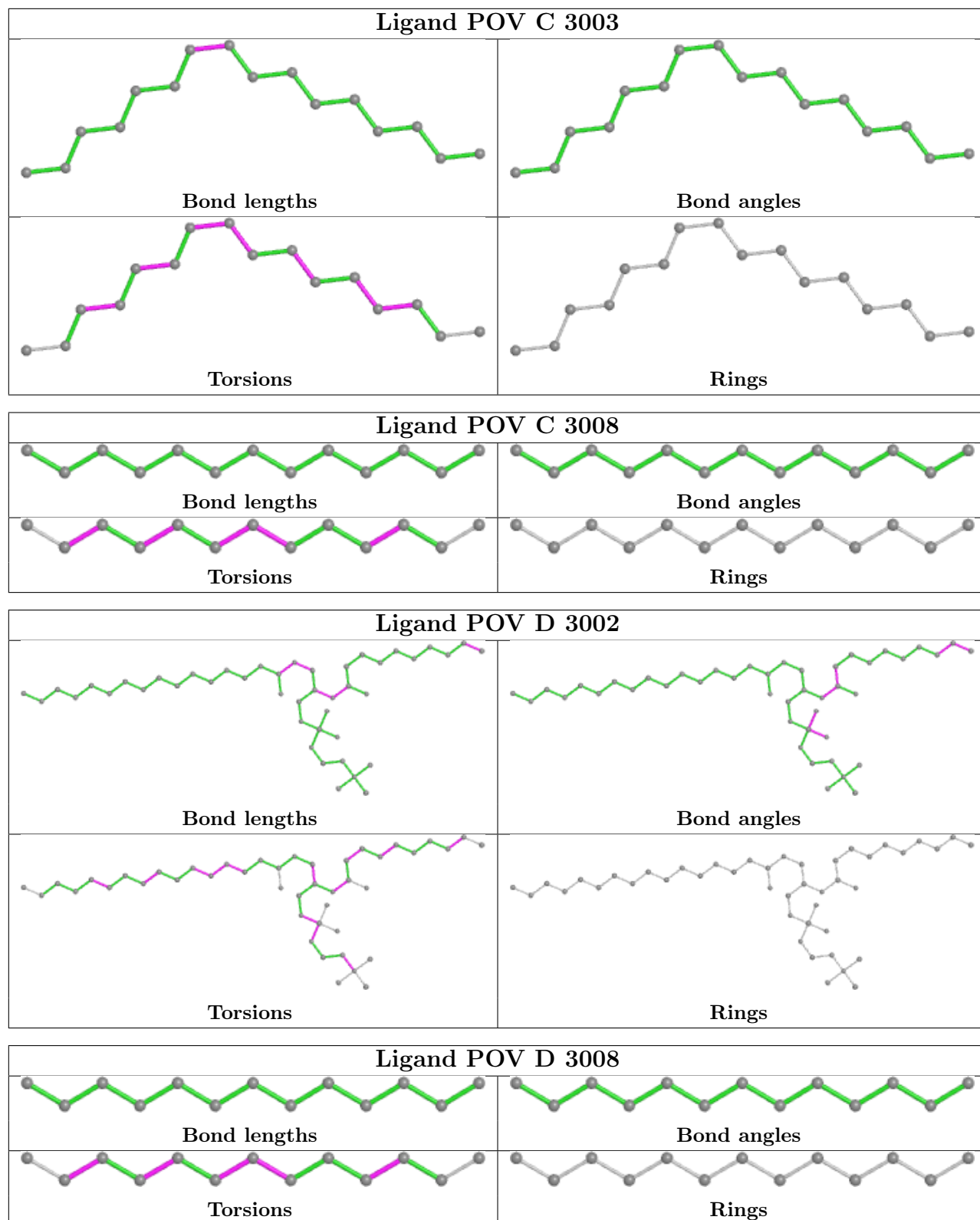
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3000	CLR	9	0
3	C	3000	CLR	9	0
3	B	3000	CLR	10	0
3	D	3000	CLR	9	0

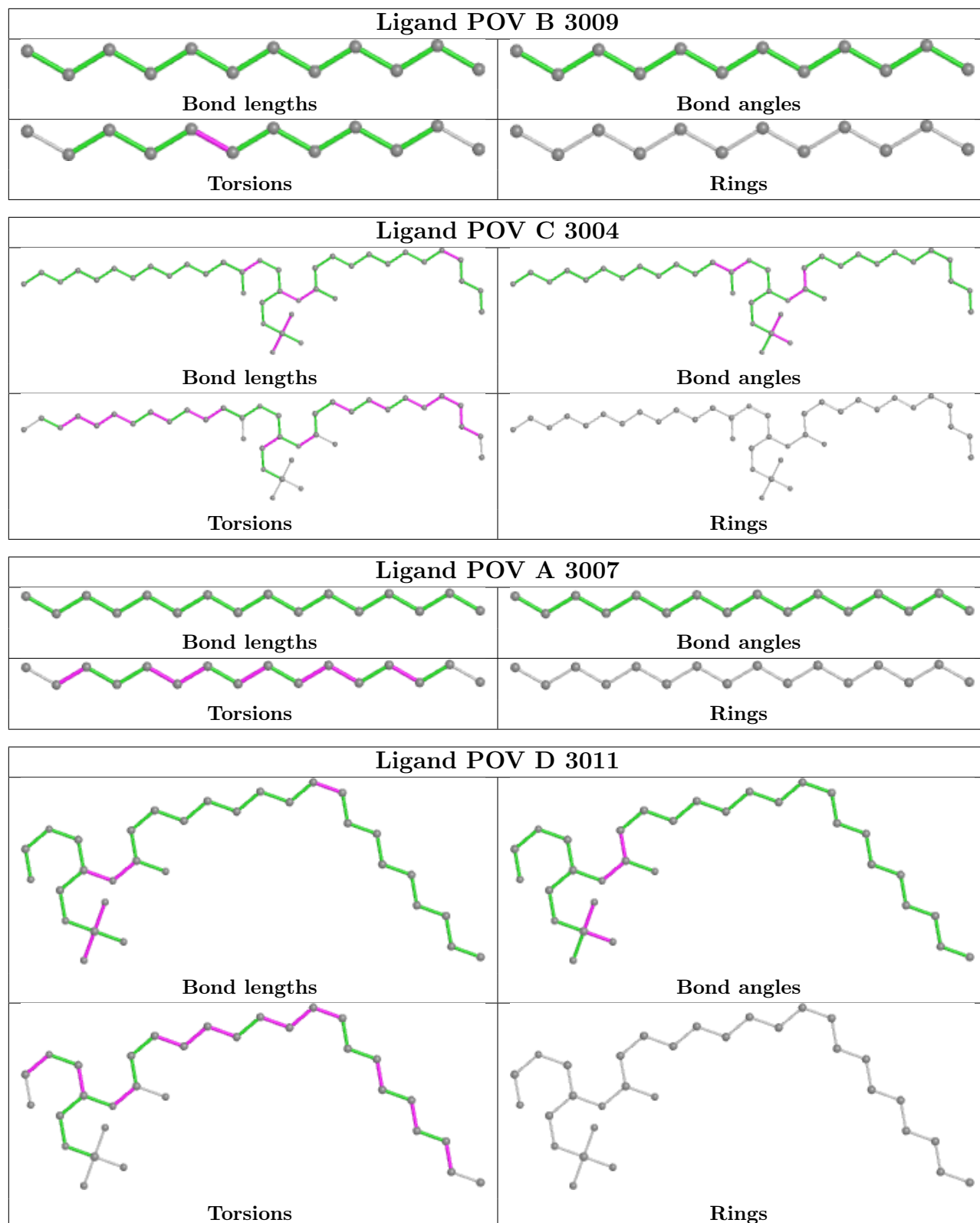
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

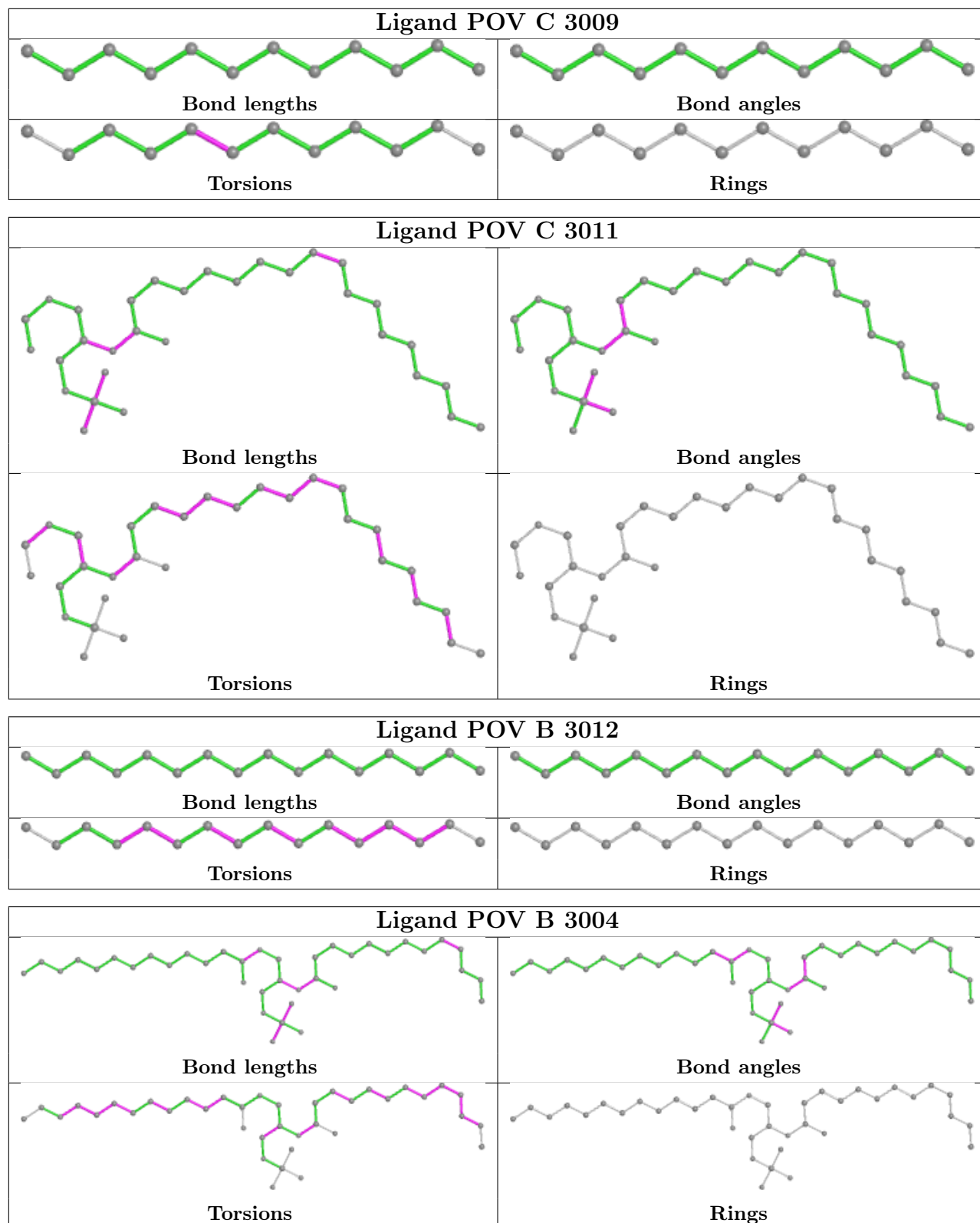
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

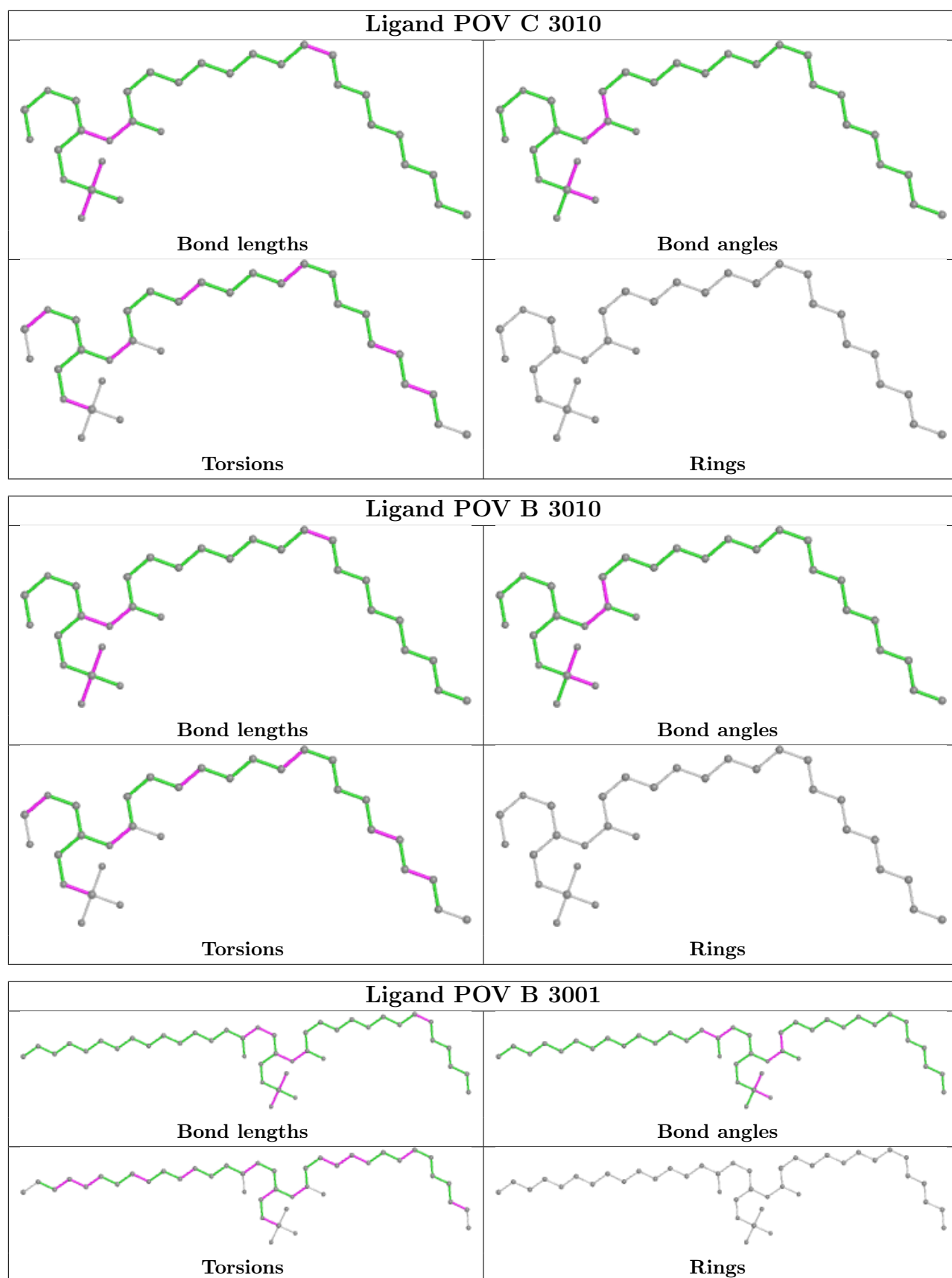


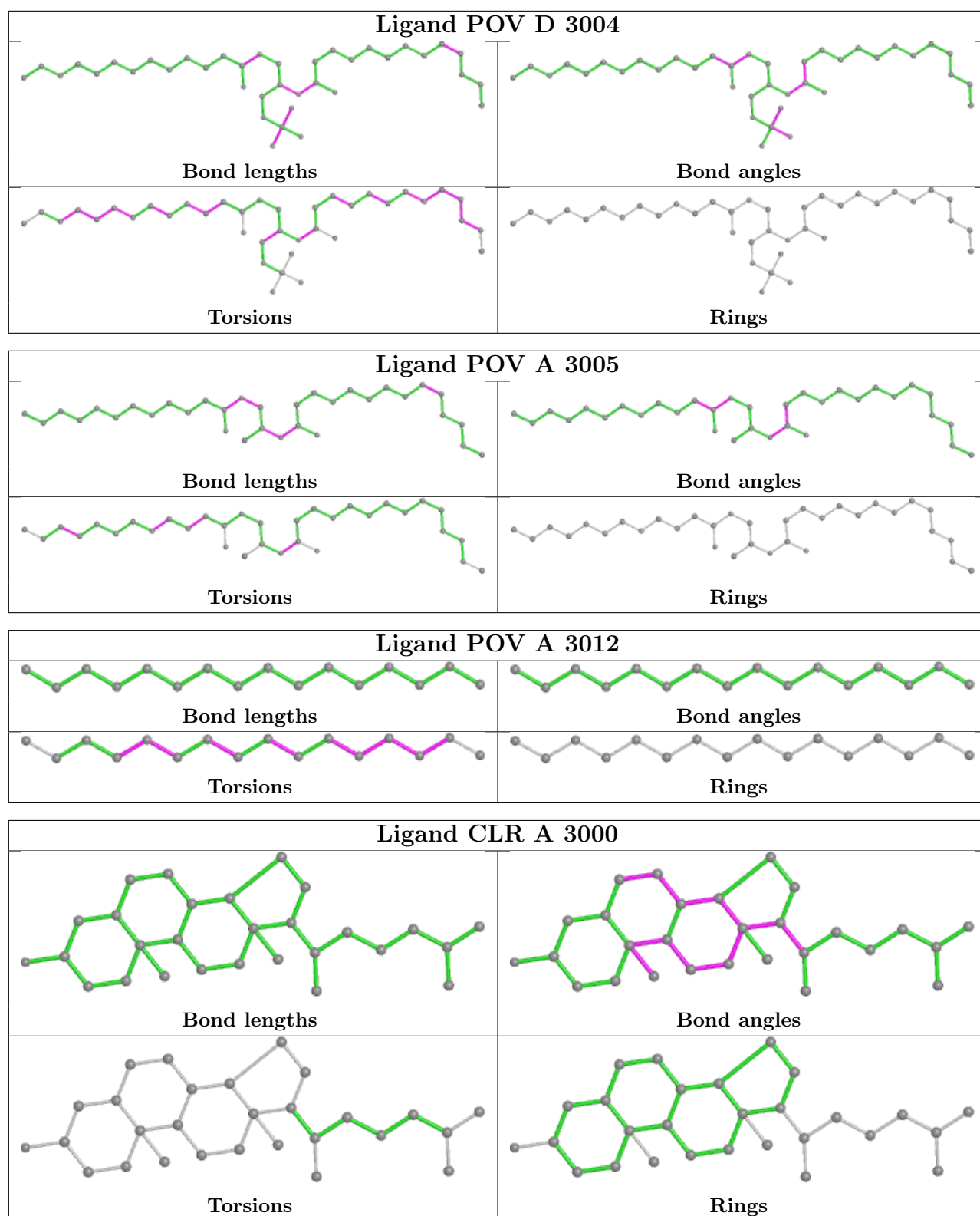


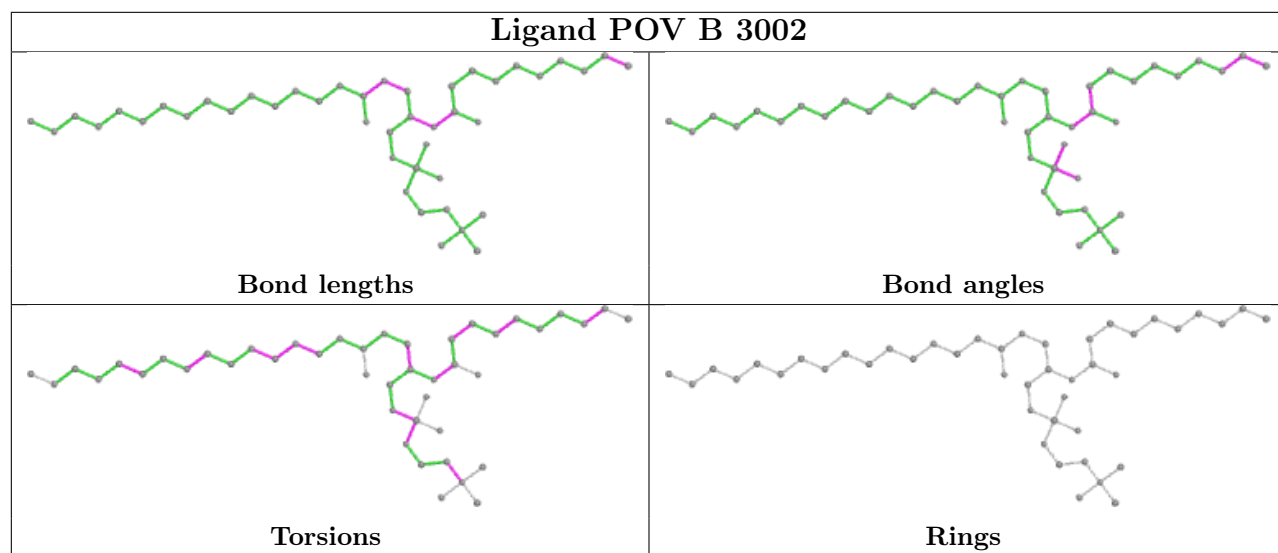
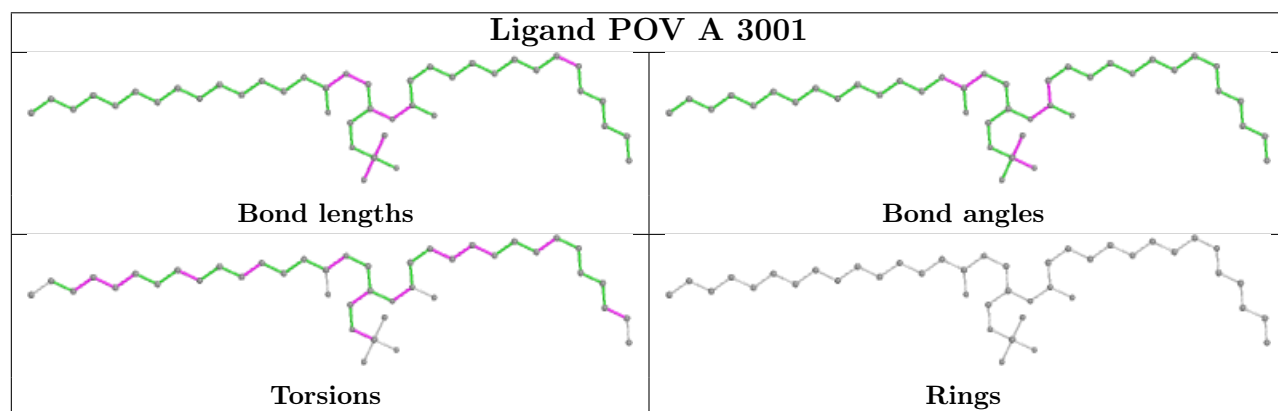
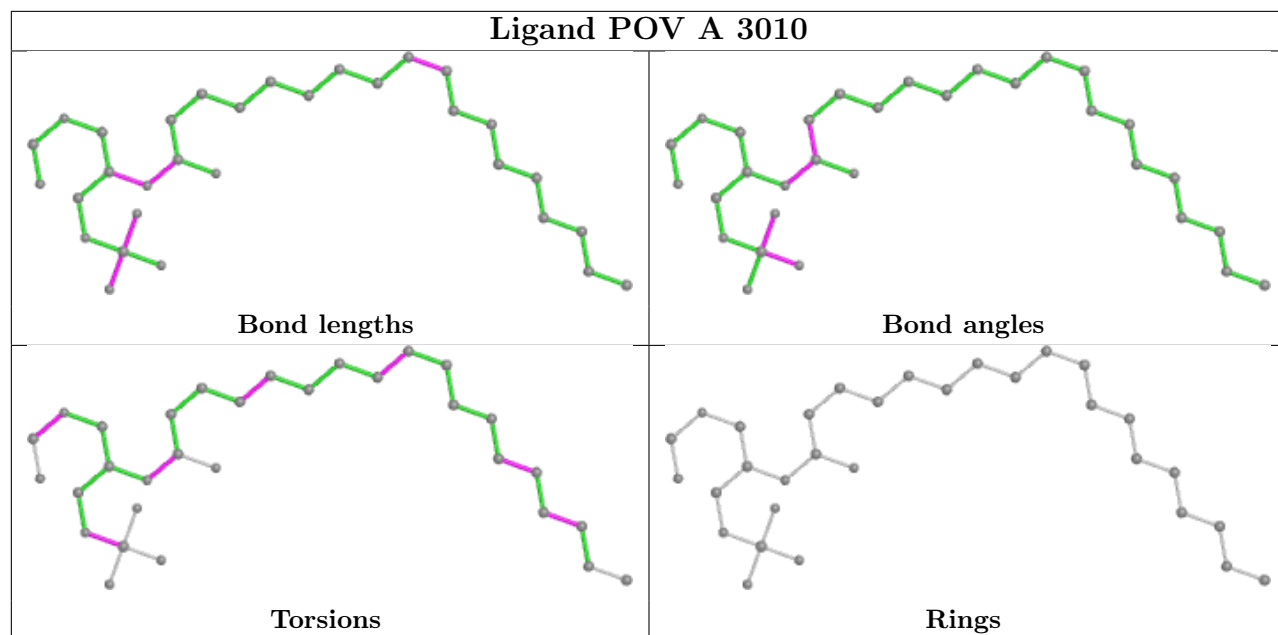


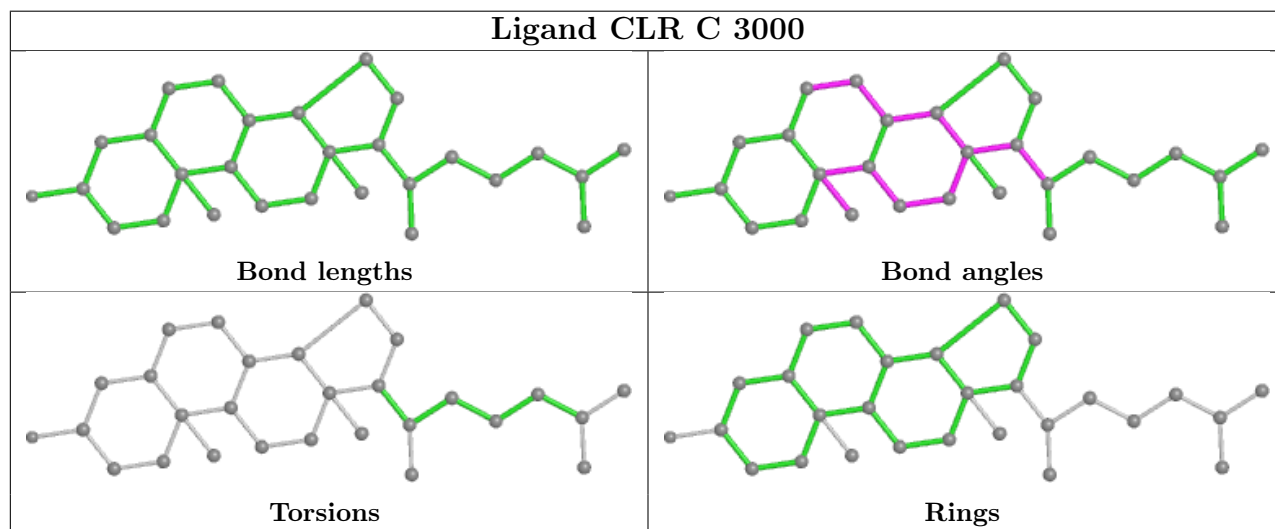
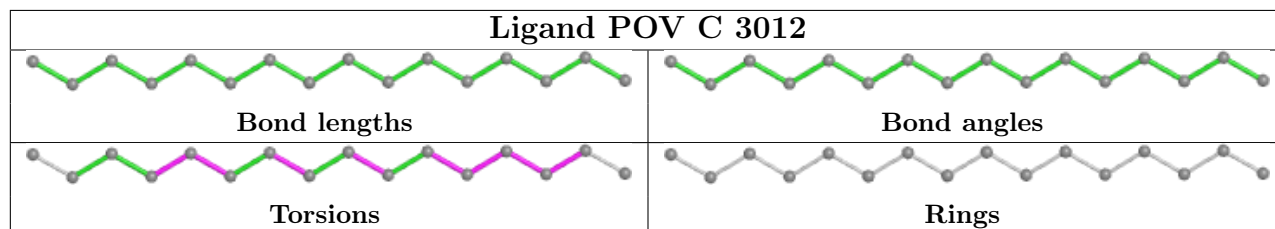
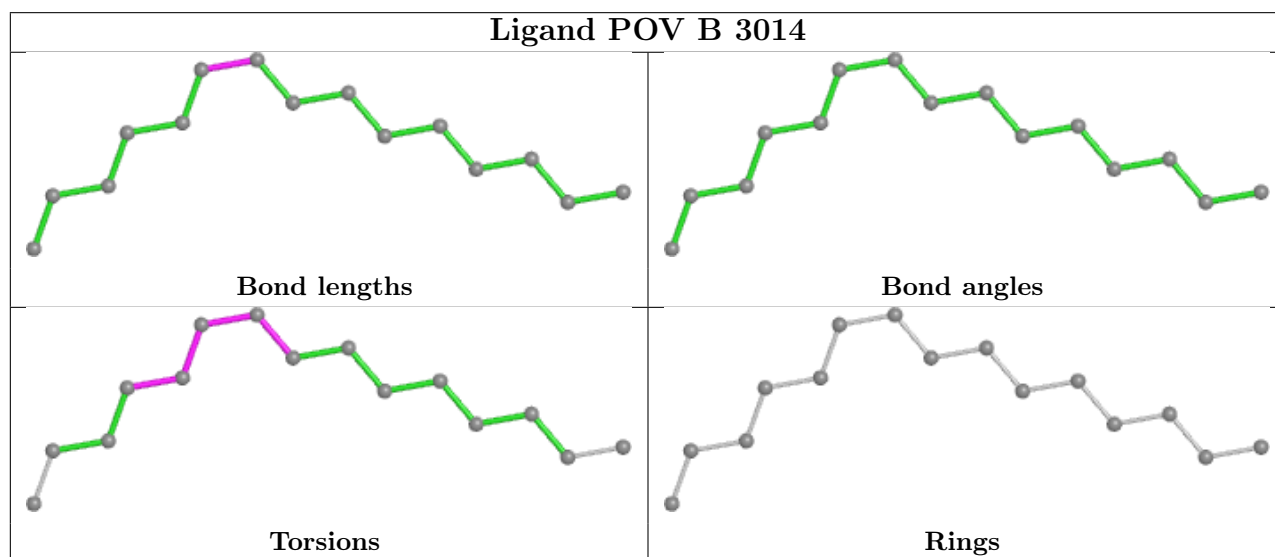
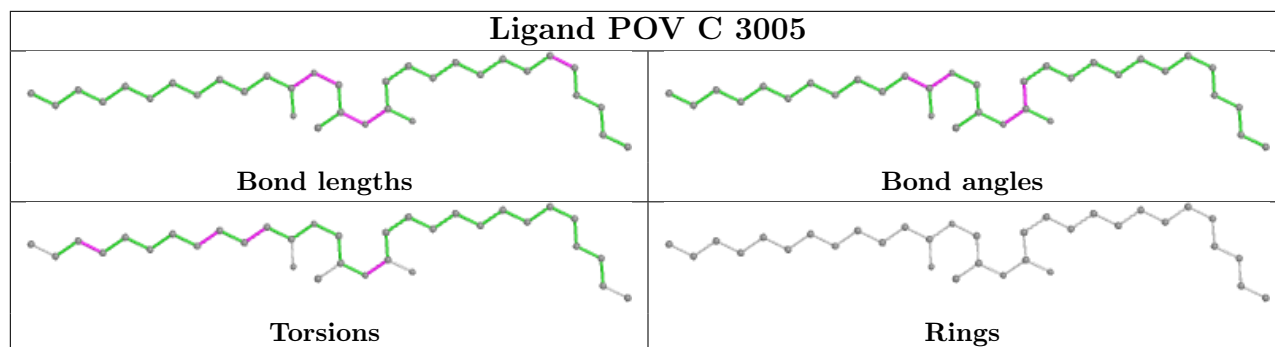


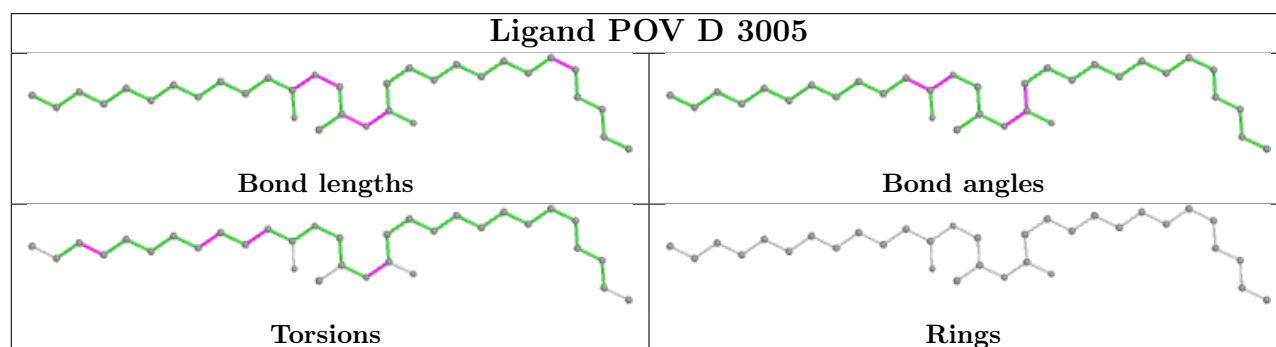
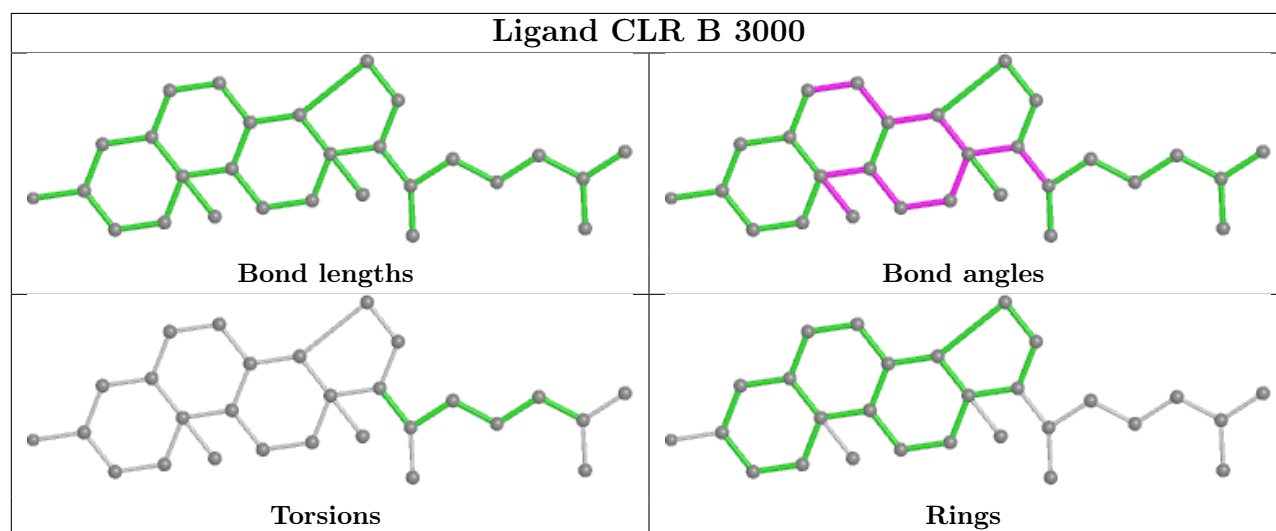
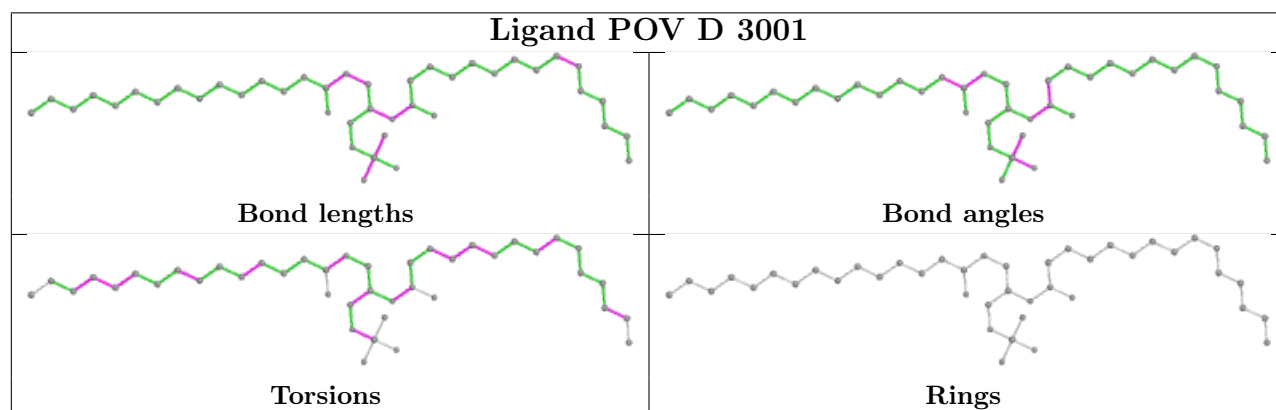
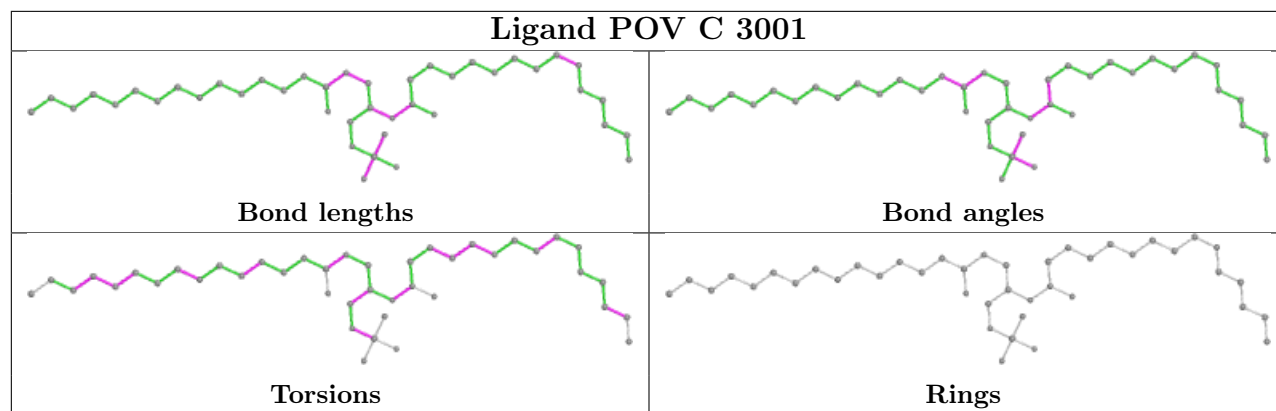


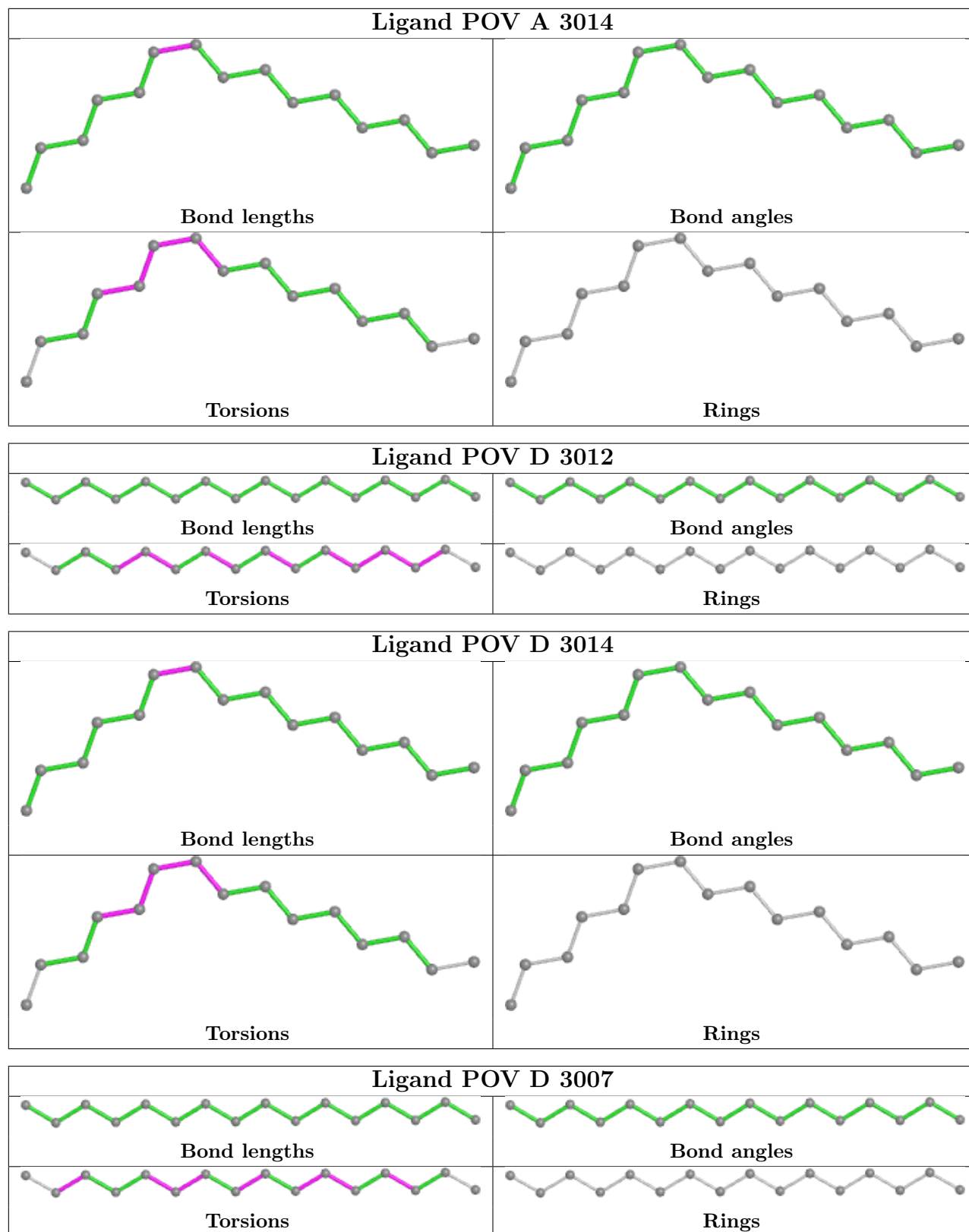


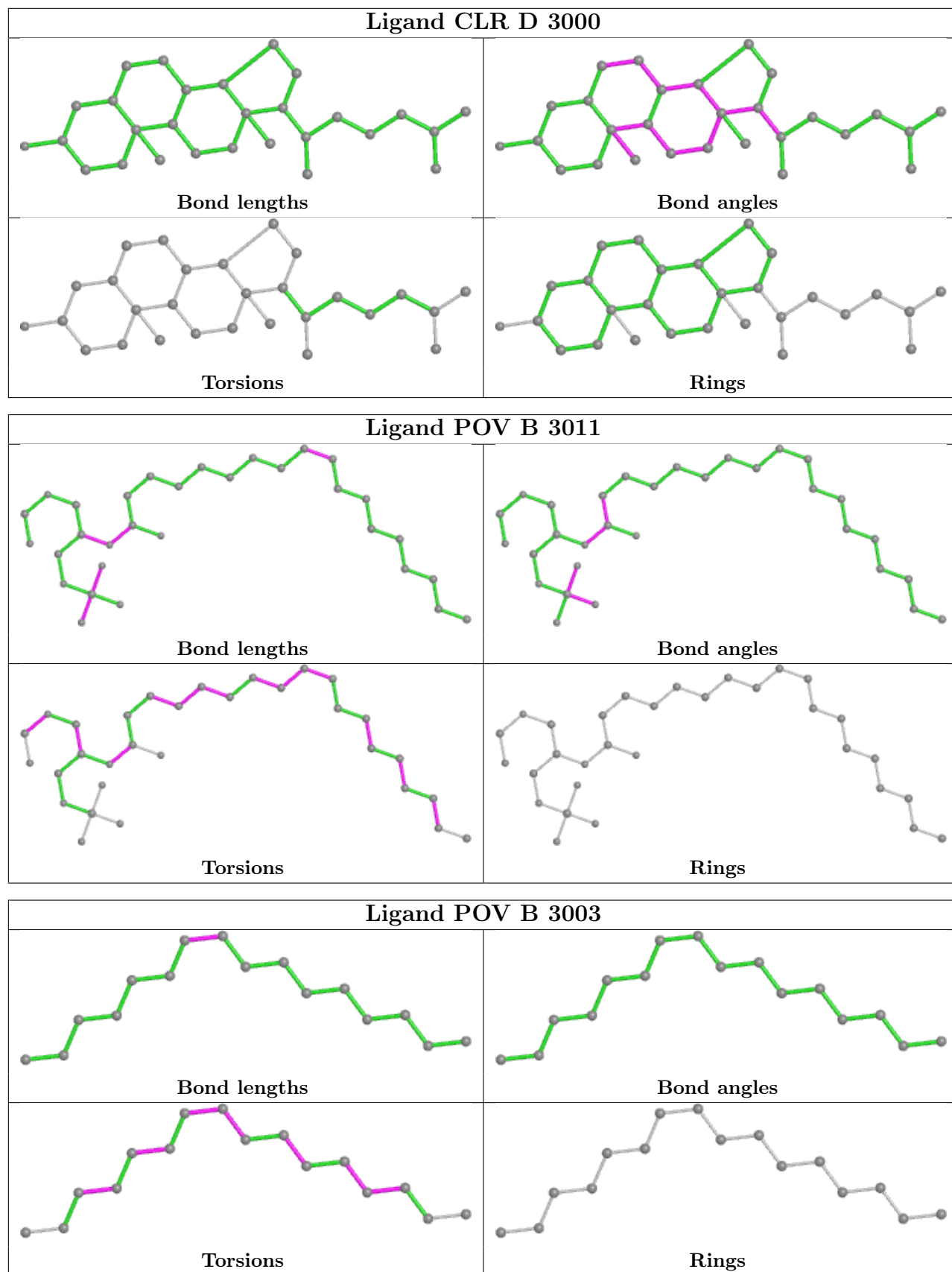


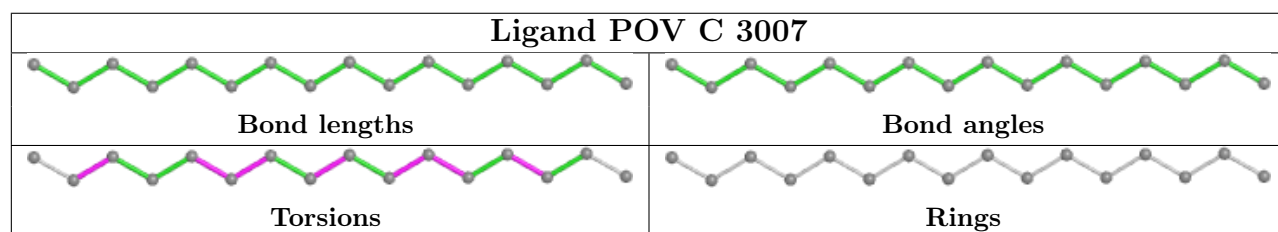
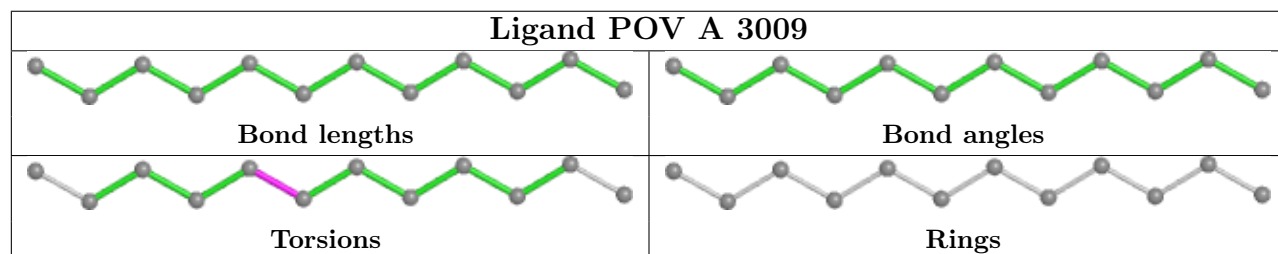
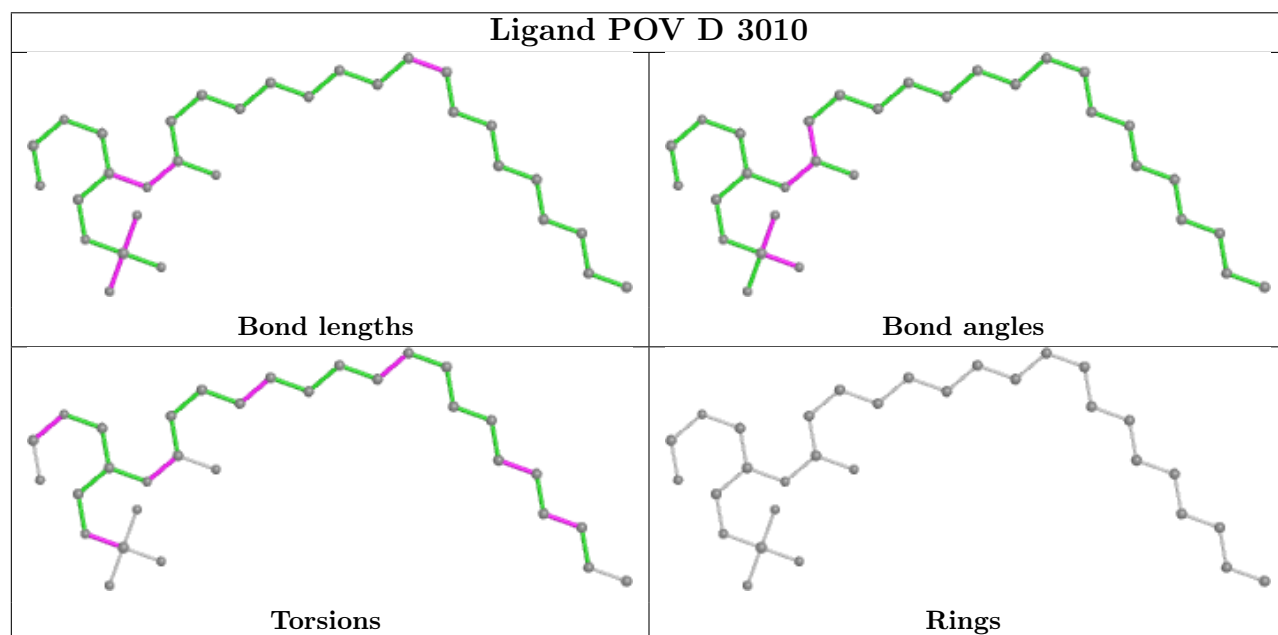
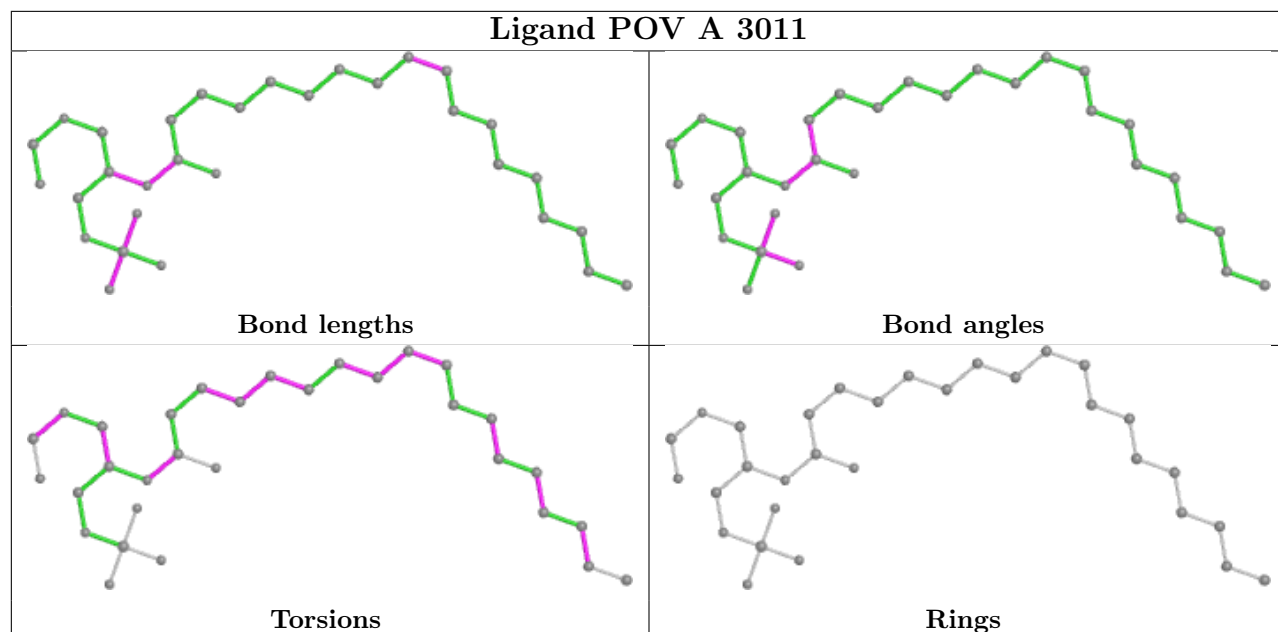


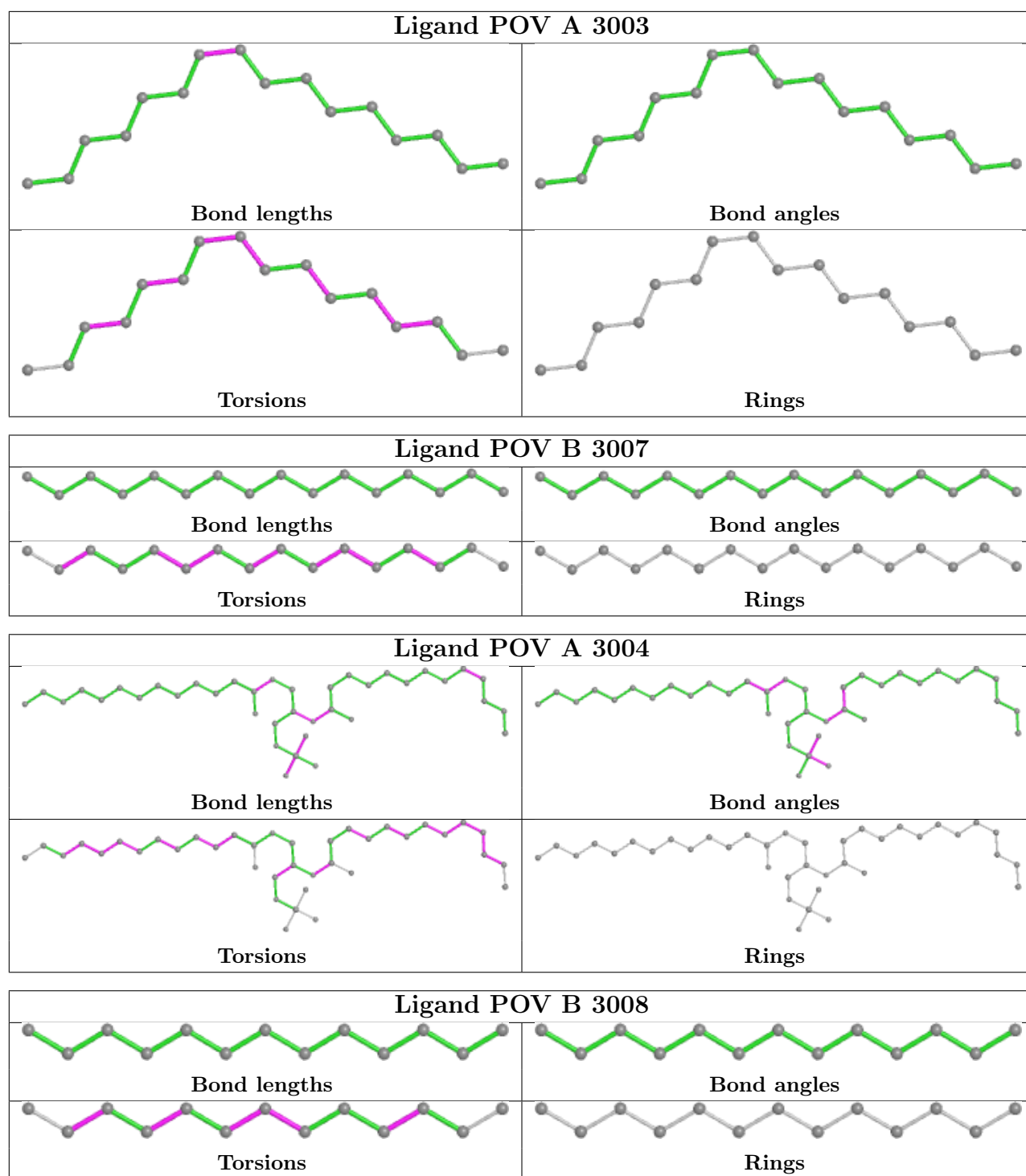












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

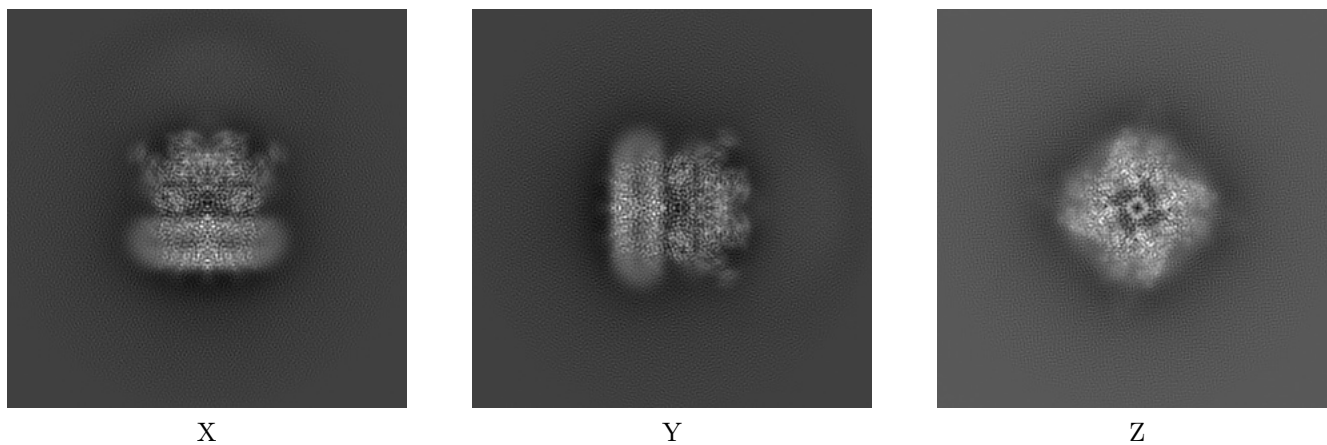
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7542. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

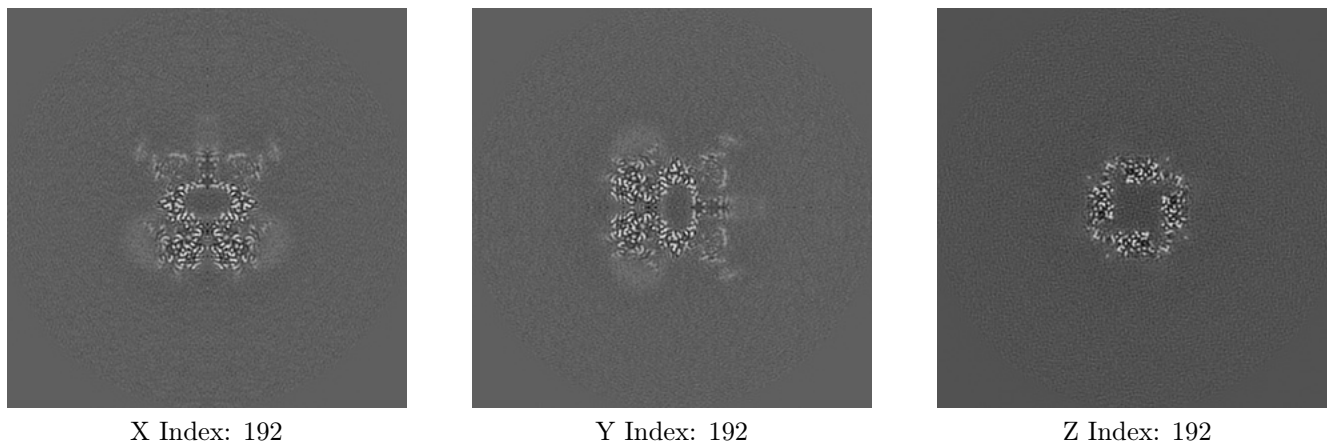
6.1.1 Primary map



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

6.2 Central slices [i](#)

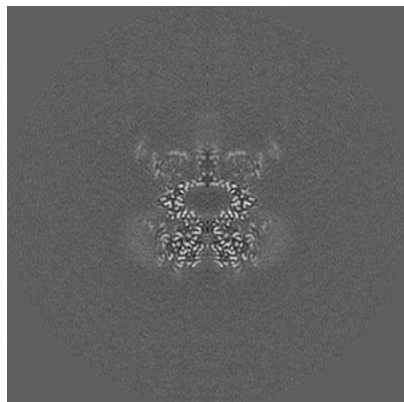
6.2.1 Primary map



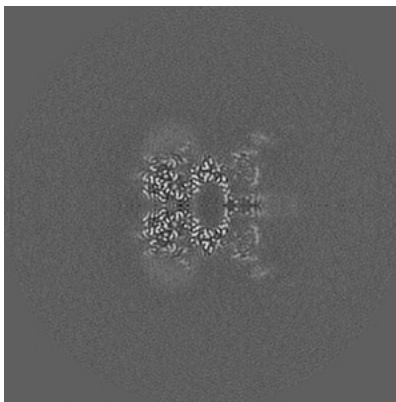
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

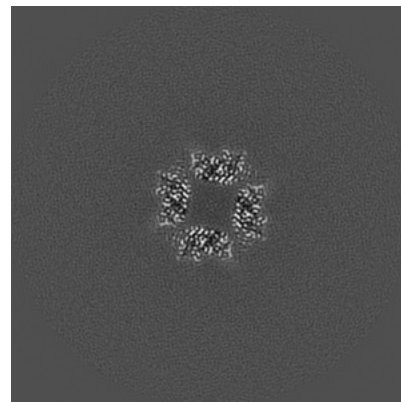
6.3.1 Primary map



X Index: 192



Y Index: 192

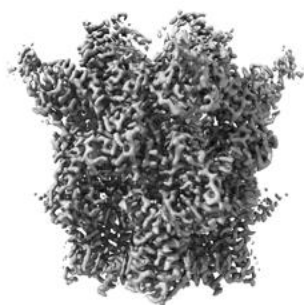


Z Index: 198

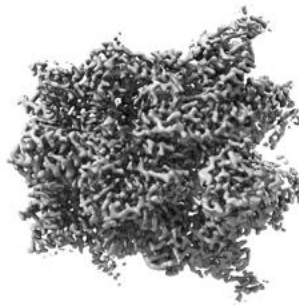
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

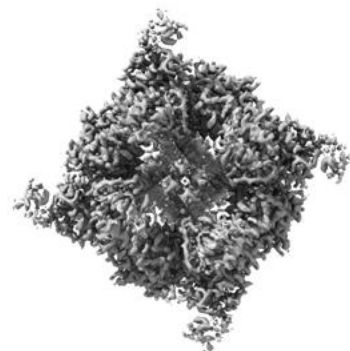
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

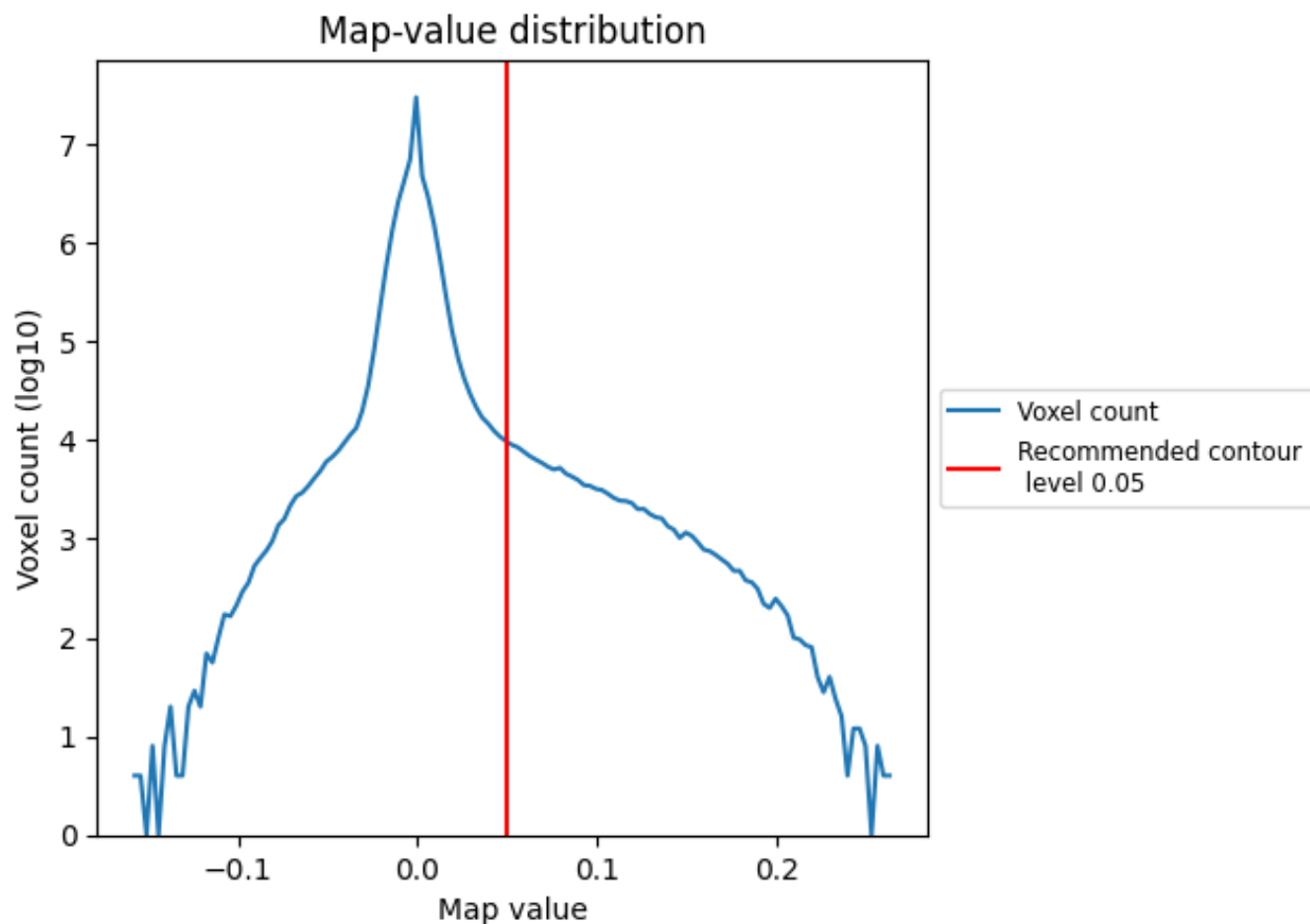
6.5 Mask visualisation

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

7 Map analysis [i](#)

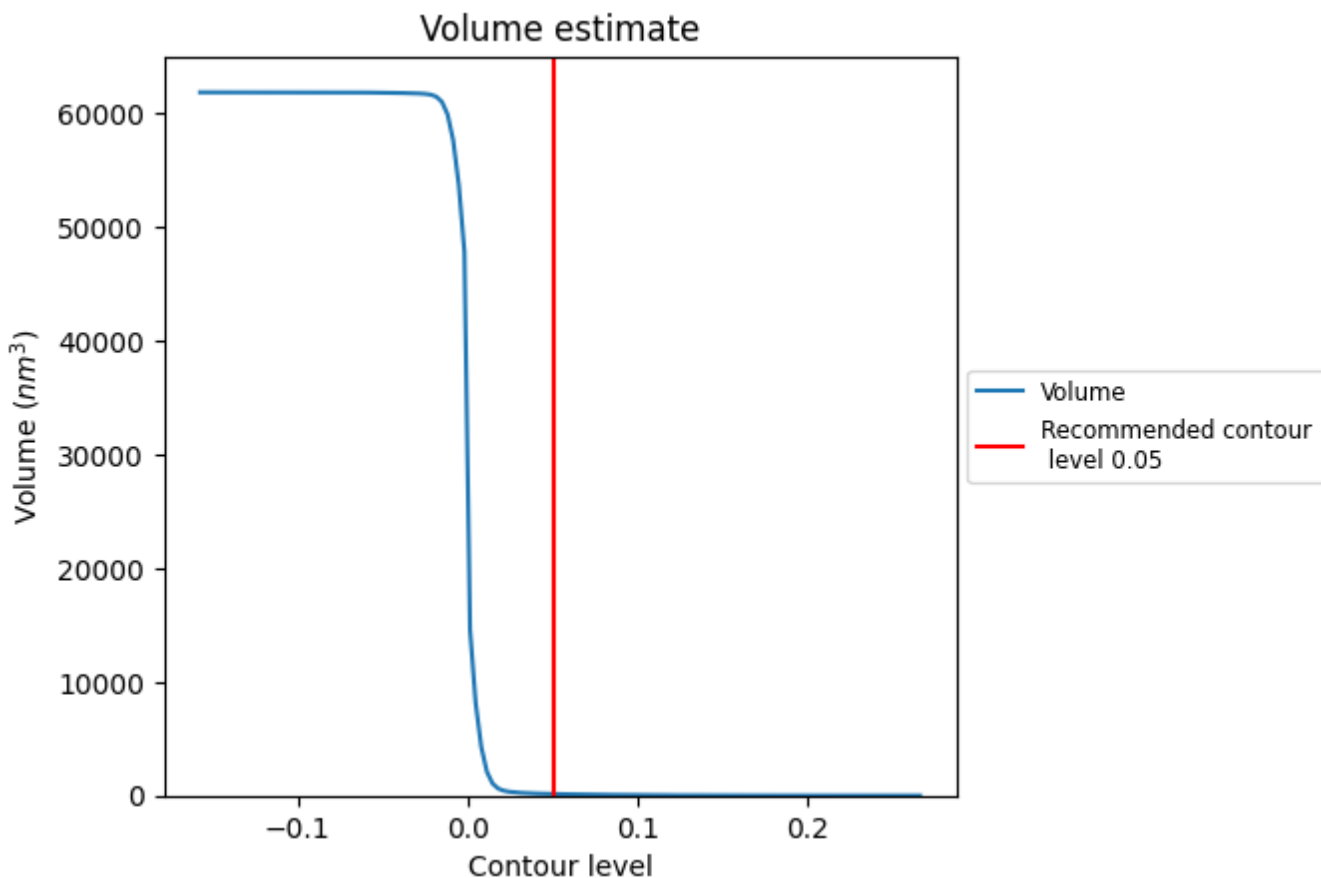
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

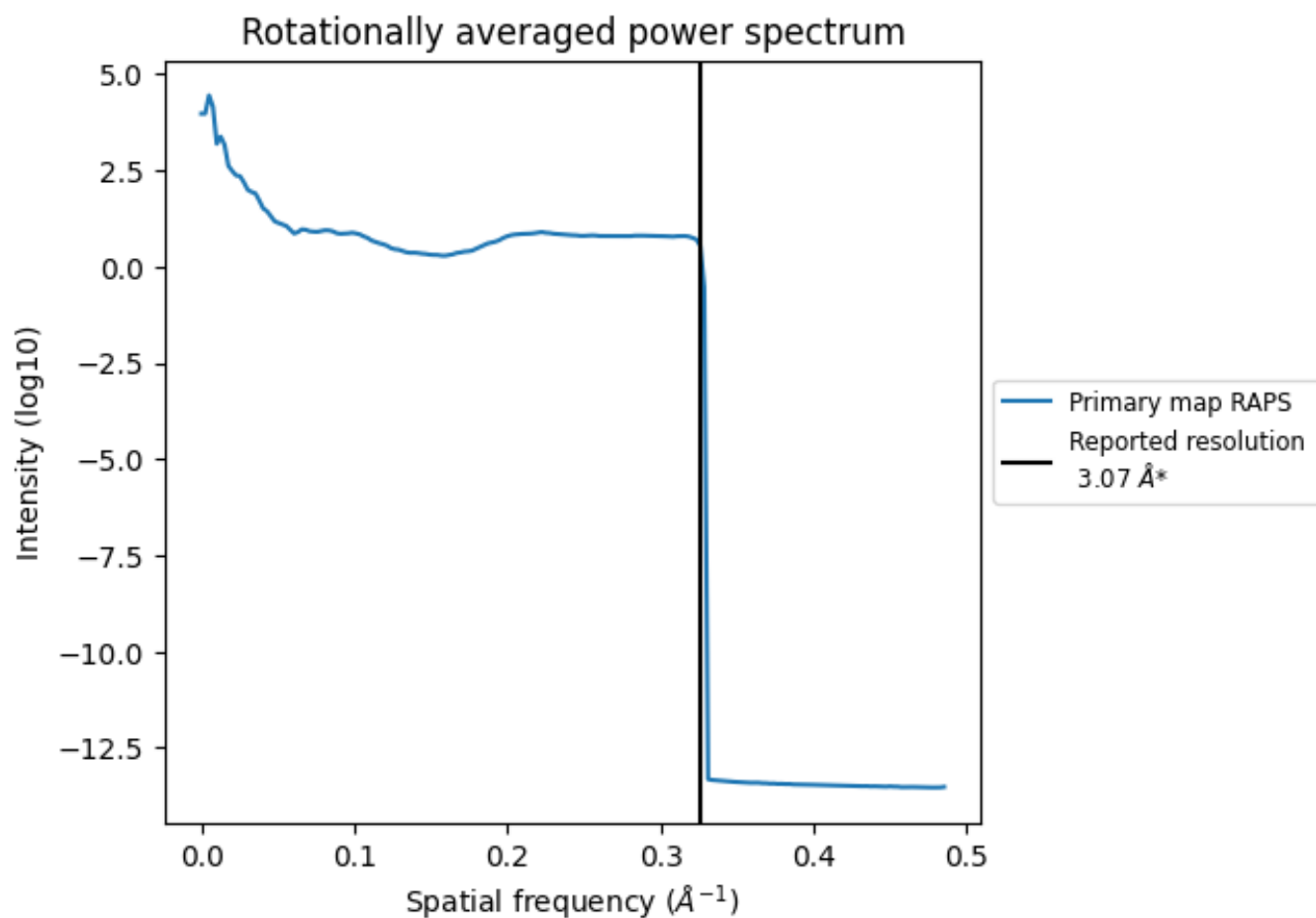
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

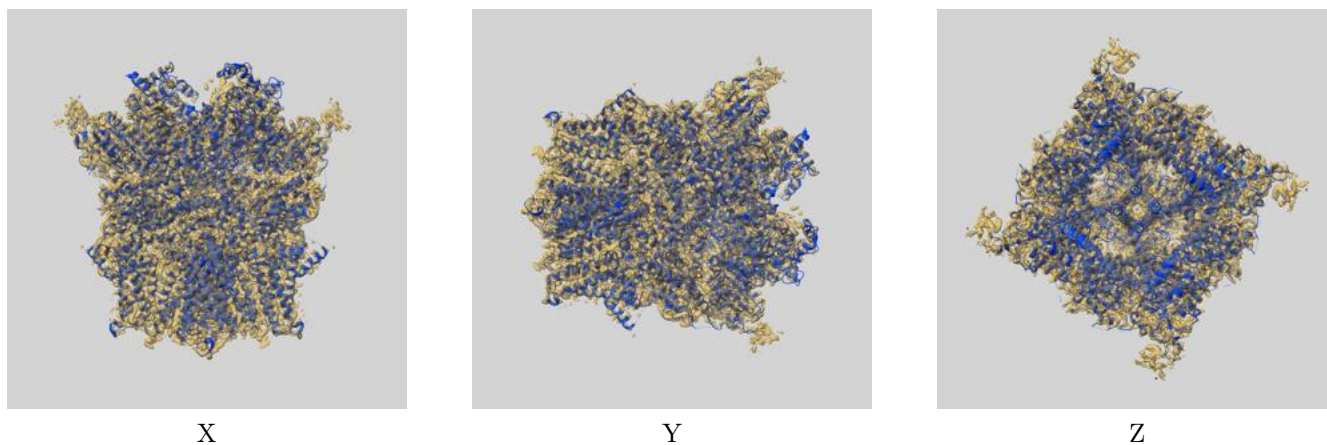
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

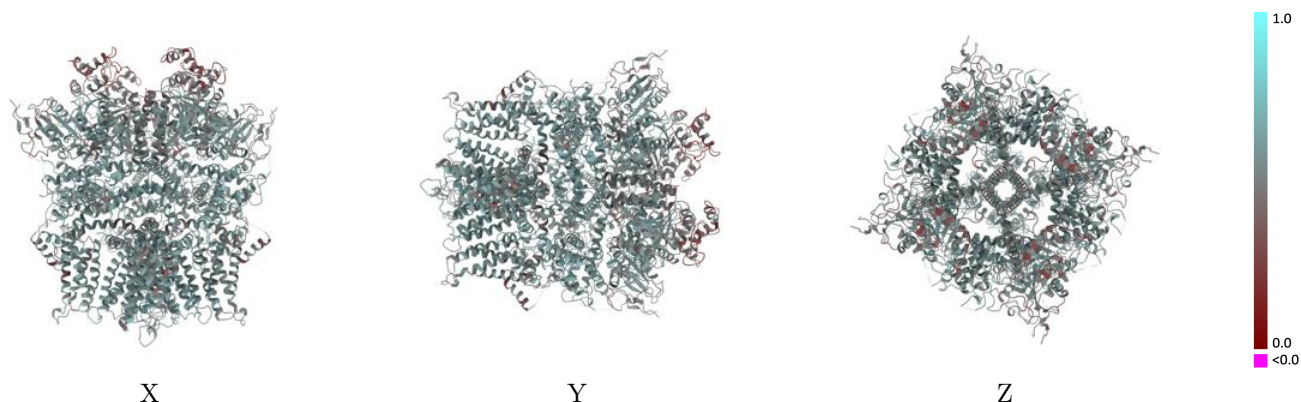
This section contains information regarding the fit between EMDB map EMD-7542 and PDB model 6CO7. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



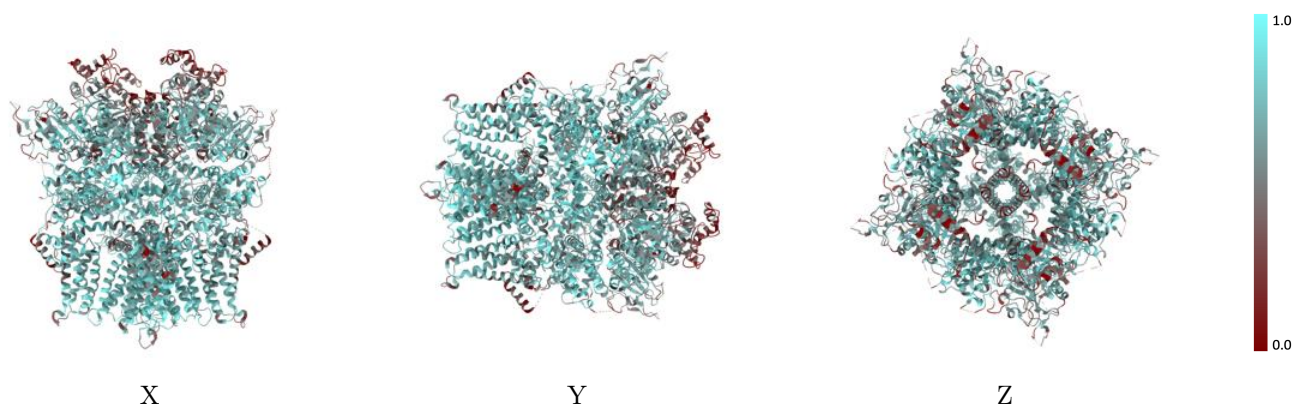
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



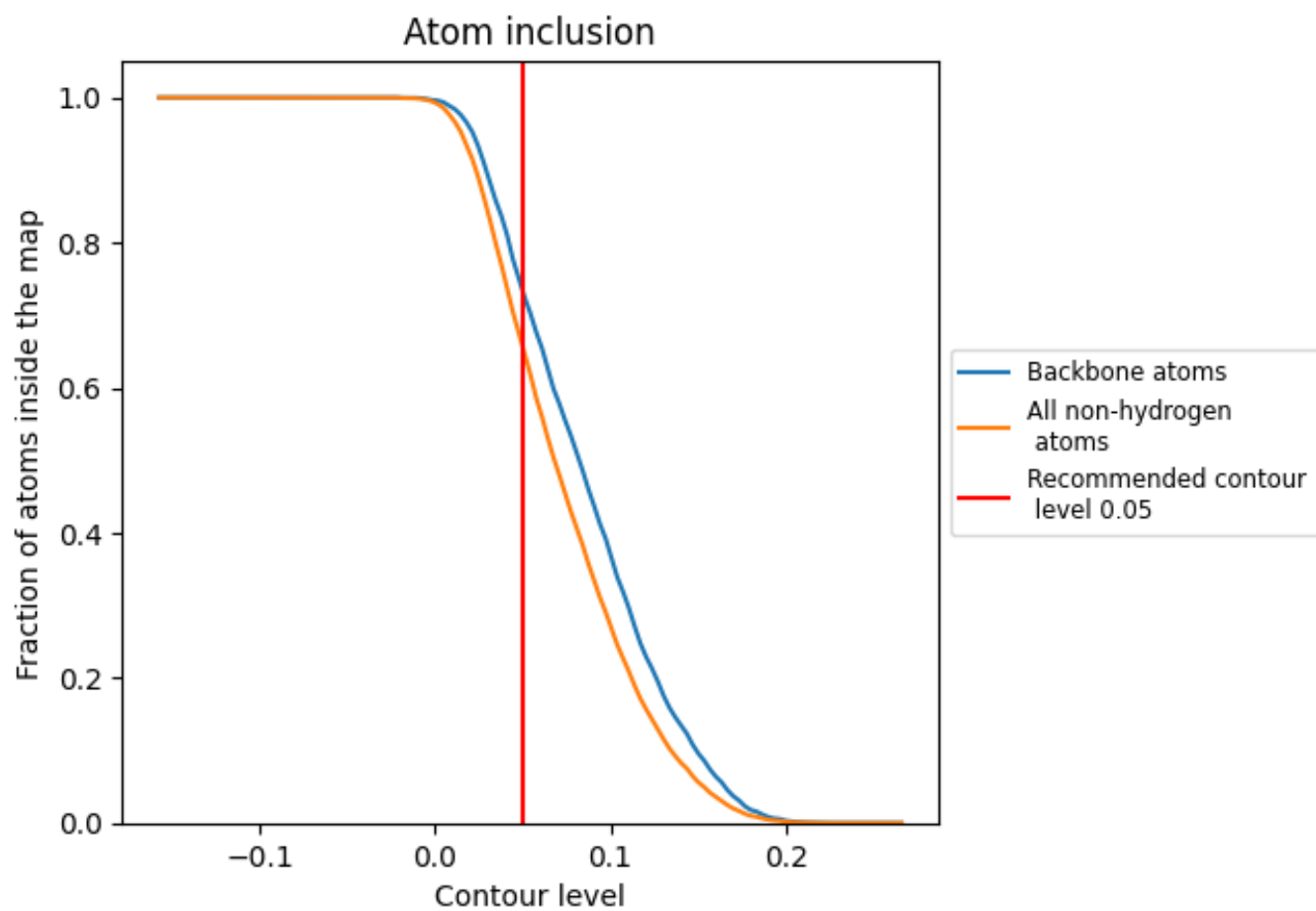
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6552	 0.5380
A	 0.6556	 0.5390
B	 0.6556	 0.5380
C	 0.6550	 0.5380
D	 0.6557	 0.5390
E	 0.5714	 0.5350
F	 0.5714	 0.5350
G	 0.5714	 0.5290
H	 0.5714	 0.5300

