



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 09:44 PM UTC

PDB ID : 6CO7 / pdb_00006co7
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)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

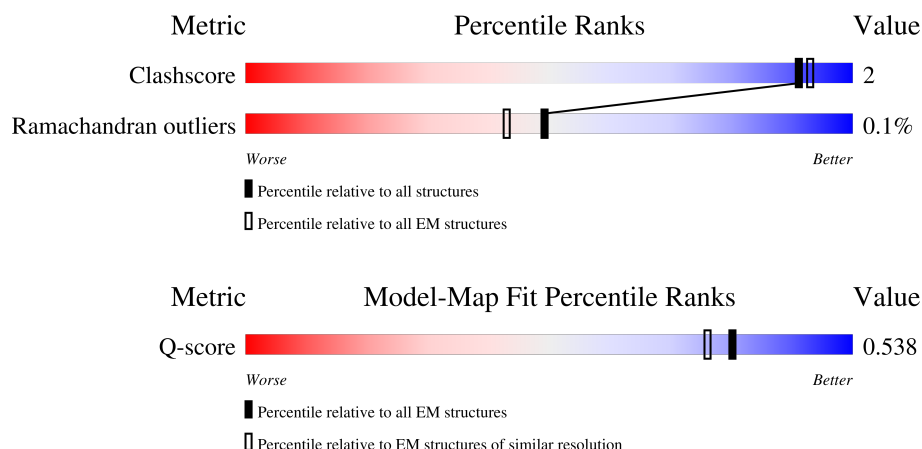
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

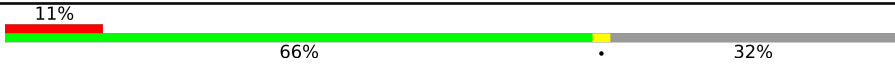
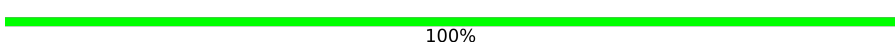
The reported resolution of this entry is 3.07 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

2 Entry composition

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
1	A	1061	Total	C	N	O	S	0	0
			8422	5429	1409	1537	47		
1	B	1061	Total	C	N	O	S	0	0
			8422	5429	1409	1537	47		
1	C	1061	Total	C	N	O	S	0	0
			8422	5429	1409	1537	47		
1	D	1061	Total	C	N	O	S	0	0
			8422	5429	1409	1537	47		

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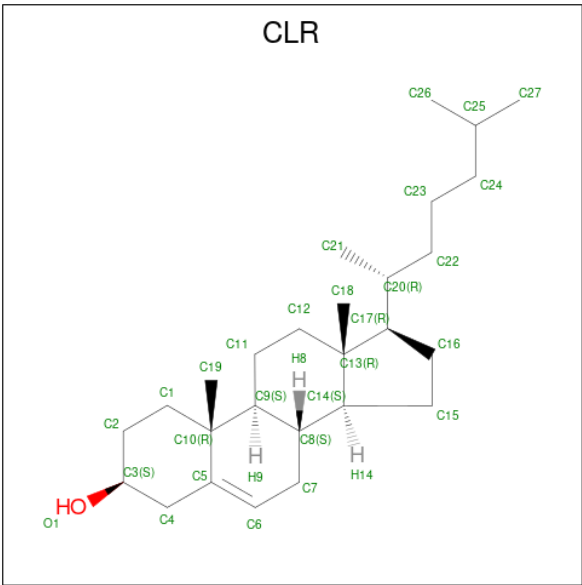
Chain	Residue	Modelled	Actual	Comment	Reference
C	1556	GLU	-	expression tag	UNP A7T1N0
C	1557	VAL	-	expression tag	UNP A7T1N0
C	1558	LEU	-	expression tag	UNP A7T1N0
C	1559	PHE	-	expression tag	UNP A7T1N0
C	1560	GLN	-	expression tag	UNP A7T1N0
D	1552	SER	-	expression tag	UNP A7T1N0
D	1553	ASN	-	expression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



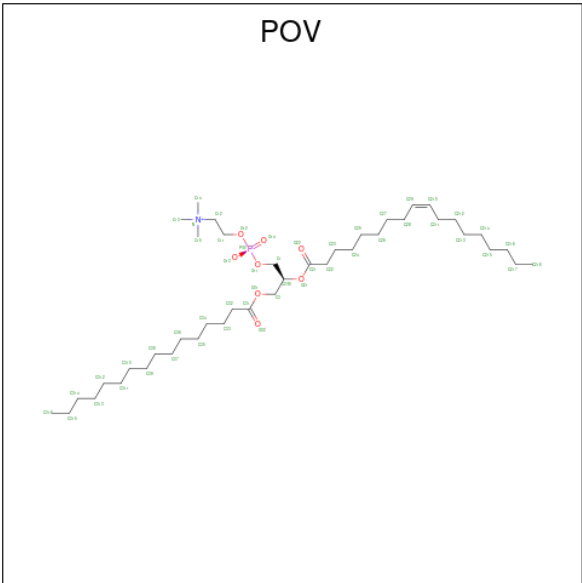
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is CHOLESTEROL (CCD ID: 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 (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O P 42 33 8 1	0
4	A	1	Total C N O P 44 34 1 8 1	0
4	A	1	Total C 16 16	0
4	A	1	Total C O P 38 29 8 1	0
4	A	1	Total C O 33 29 4	0
4	A	1	Total C 16 16	0
4	A	1	Total C 16 16	0
4	A	1	Total C 13 13	0
4	A	1	Total C 12 12	0
4	A	1	Total C O P 31 22 8 1	0
4	A	1	Total C O P 31 22 8 1	0
4	A	1	Total C 16 16	0
4	A	1	Total C 11 11	0
4	A	1	Total C 15 15	0
4	B	1	Total C 15 15	0
4	B	1	Total C O P 42 33 8 1	0
4	B	1	Total C N O P 44 34 1 8 1	0
4	B	1	Total C 16 16	0
4	B	1	Total C O P 38 29 8 1	0
4	B	1	Total C O 33 29 4	0
4	B	1	Total C 16 16	0
4	B	1	Total C 16 16	0

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Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C 13 13	0
4	B	1	Total C 12 12	0
4	B	1	Total C O P 31 22 8 1	0
4	B	1	Total C O P 31 22 8 1	0
4	B	1	Total C 16 16	0
4	B	1	Total C 11 11	0
4	C	1	Total C 15 15	0
4	C	1	Total C O P 42 33 8 1	0
4	C	1	Total C N O P 44 34 1 8 1	0
4	C	1	Total C 16 16	0
4	C	1	Total C O P 38 29 8 1	0
4	C	1	Total C O 33 29 4	0
4	C	1	Total C 16 16	0
4	C	1	Total C 16 16	0
4	C	1	Total C 13 13	0
4	C	1	Total C 12 12	0
4	C	1	Total C O P 31 22 8 1	0
4	C	1	Total C O P 31 22 8 1	0
4	C	1	Total C 16 16	0
4	C	1	Total C 11 11	0
4	D	1	Total C O P 31 22 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C O P 31 22 8 1	0
4	D	1	Total C 16 16	0
4	D	1	Total C 11 11	0
4	D	1	Total C 15 15	0
4	D	1	Total C O P 42 33 8 1	0
4	D	1	Total C N O P 44 34 1 8 1	0
4	D	1	Total C 16 16	0
4	D	1	Total C O P 38 29 8 1	0
4	D	1	Total C O 33 29 4	0
4	D	1	Total C 16 16	0
4	D	1	Total C 16 16	0
4	D	1	Total C 13 13	0
4	D	1	Total C 12 12	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

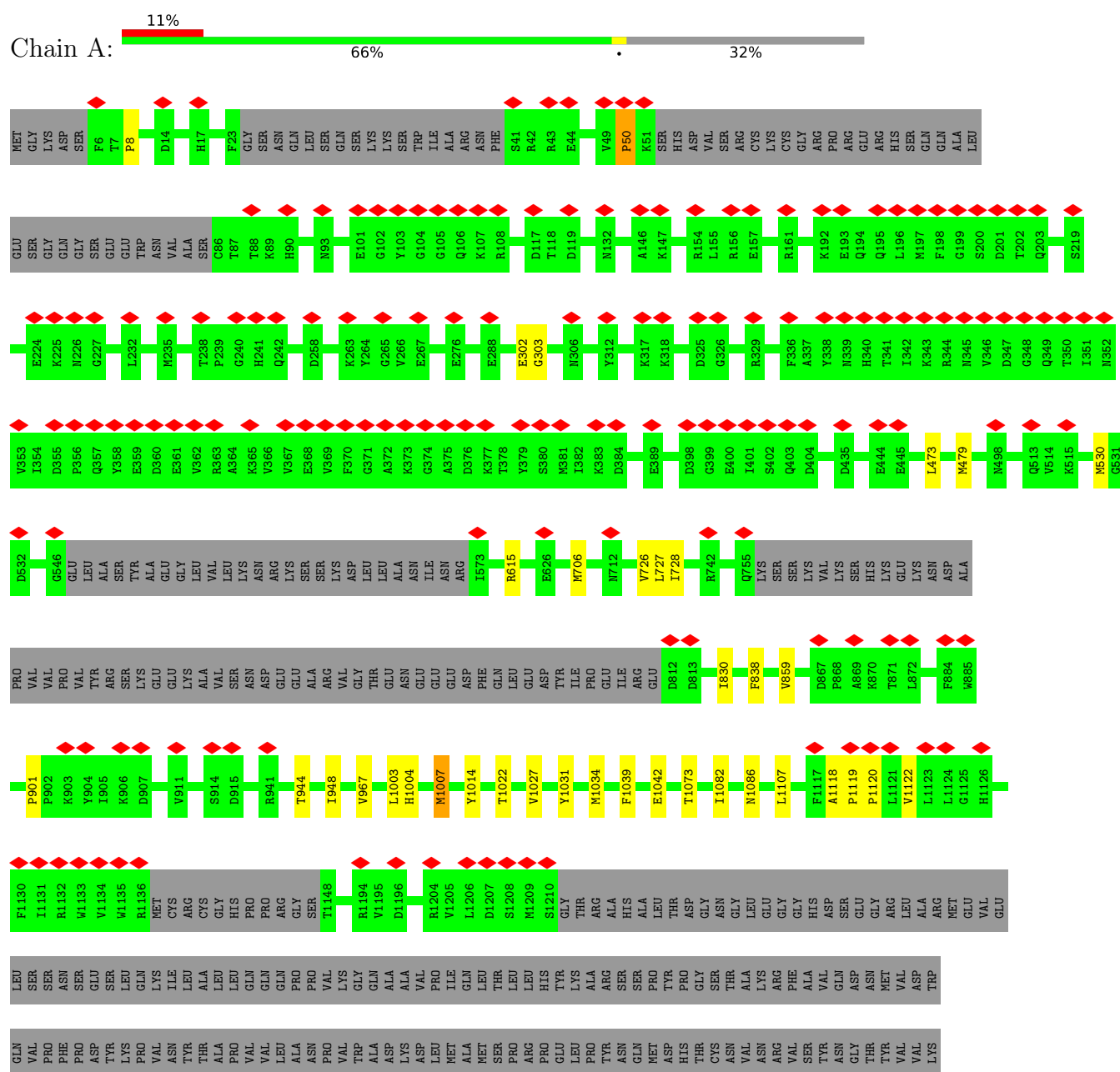
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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.

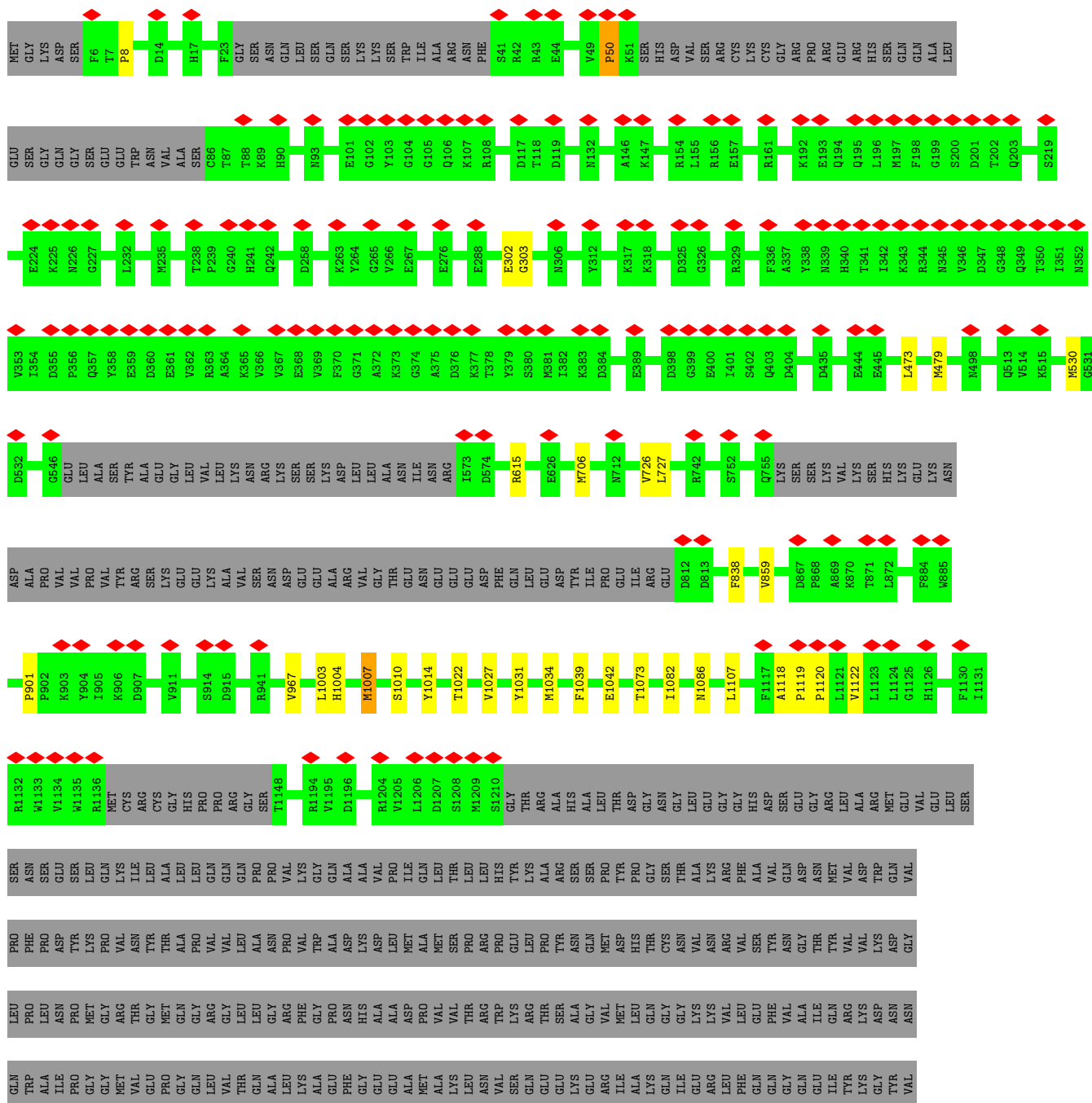
• Molecule 1: Predicted protein



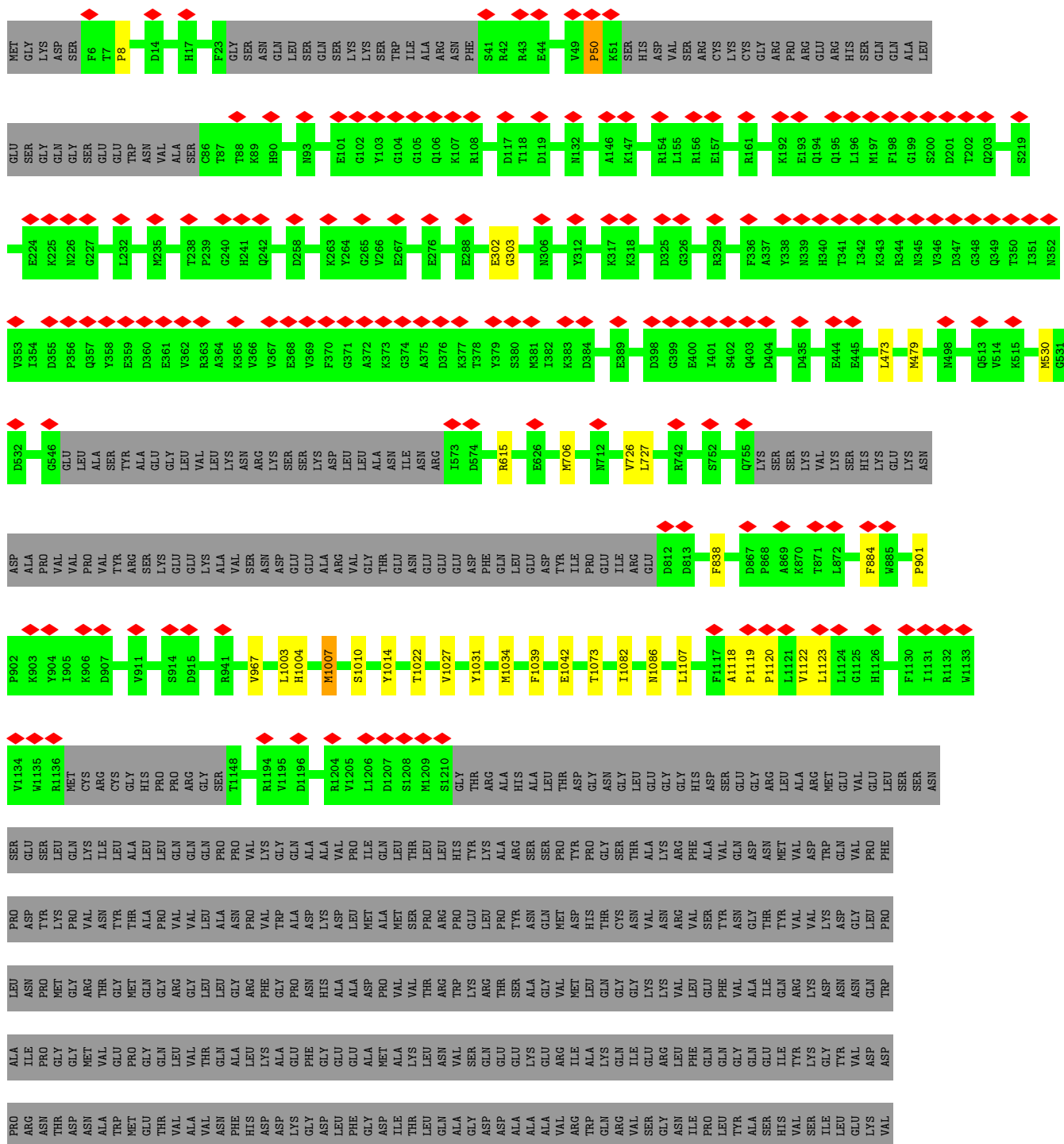
LEU	TYR	ASN	ASP
GLU	VAL	ASN	GLY
LYS	ASP	GLN	LEU
VAL	ASP	TRP	PRO
ALA	PRO	ALA	LEU
LYS	ARG	IIE	ASN
MET	ASN	PRO	PRO
ARG	THR	GLY	MET
ASP	ASP	GLY	GLY
ALA	ASN	MET	ARG
ALA	ALA	VAL	THR
PHE	TRP	GLU	GLY
SER	MET	PRO	MET
ASN	GLU	GLY	GLN
SER	THR	GLN	GLY
LEU	VAL	LEU	ARG
GLU	ALA	VAL	GLY
VAL	VAL	THR	LEU
LEU	ASN	GLN	LEU
PHE	PHE	ALA	GLY
GLN	HIS	LYS	ARG
	ASP	LEV	PHE
	ASP	ALA	GLY
	LYS	GLU	PRO
	GLY	PHE	ASN
	ASP	GLU	HIS
	LEU	GLY	ALA
	PHE	GLU	ALA
	GLY	ALA	ASP
	ASP	MET	PRO
	IIE	ALA	VAL
	THR	LYS	VAL
	LEU	LEU	THR
	GLN	ASN	ARG
	ALA	VAL	TRP
	GLY	SER	LYS
	ASP	GLN	ARG
	ALA	GLU	THR
	ALA	LYS	SER
	ALA	GLY	ALA
	VAL	ARG	GLY
	ARG	IIE	VAL
	GLN	LYS	MET
	ARG	GLN	LEU
	VAL	IIE	GLY
	SER	GLU	LYS
	GLY	ARG	LYS
	ASN	LEU	VAL
	IIE	PHE	LEU
	PRO	GLN	GLU
	LEU	GLN	PHE
	TTR	GLY	VAL
	ALA	GLN	ALA
	SER	GLU	IIE
	HIS	IIE	GLN
	VAL	TTR	ARG
	SER	LYS	LYS
	IIE	GLY	ASN

- Molecule 1: Predicted protein

[illegible]



- Molecule 1: Predicted protein



ALA
LYS
MET
ARG
ASP
ALA
PHE
SER
ASN
SER
LEU
GLU
VAL
LEU
PHE
GLN

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

Chain E:  100%

WAG1
WAG2

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

Chain F:  100%

WAG1
WAG2

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

Chain G:  100%

WAG1
WAG2

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

Chain H:  100%

WAG1
WAG2

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 ($\text{\AA}$)	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 ($\text{\AA}$)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.57	2/8602 (0.0%)	0.81	4/11656 (0.0%)
1	B	0.57	2/8602 (0.0%)	0.82	4/11656 (0.0%)
1	C	0.57	2/8602 (0.0%)	0.81	4/11656 (0.0%)
1	D	0.57	2/8602 (0.0%)	0.82	4/11656 (0.0%)
All	All	0.57	8/34408 (0.0%)	0.82	16/46624 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1007	MET	C-N	12.49	1.48	1.33
1	A	1007	MET	C-N	12.43	1.48	1.33
1	D	1007	MET	C-N	12.43	1.48	1.33
1	B	1007	MET	C-N	12.36	1.48	1.33
1	B	1014	TYR	C-N	-5.53	1.25	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	PRO	N-CA-CB	8.04	110.44	103.36
1	C	8	PRO	N-CA-CB	8.04	110.44	103.36
1	D	8	PRO	N-CA-CB	8.03	110.42	103.36
1	A	8	PRO	N-CA-CB	8.02	110.42	103.36
1	D	50	PRO	N-CA-CB	7.00	110.60	103.25

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	27	0
1	B	8422	0	8382	27	0
1	C	8422	0	8382	26	0
1	D	8422	0	8382	26	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	112	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 2.

The worst 5 of 112 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

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%)	48	76
1	B	1049/1560 (67%)	989 (94%)	59 (6%)	1 (0%)	48	76
1	C	1049/1560 (67%)	990 (94%)	58 (6%)	1 (0%)	48	76
1	D	1049/1560 (67%)	989 (94%)	59 (6%)	1 (0%)	48	76
All	All	4196/6240 (67%)	3957 (94%)	235 (6%)	4 (0%)	49	76

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](#)

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

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 ⓘ

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	0.33	0	17,19,21	0.86	0
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	F	1	1,2	14,14,15	0.32	0	17,19,21	0.87	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.63	0
2	NAG	G	1	1,2	14,14,15	0.32	0	17,19,21	0.87	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	H	1	1,2	14,14,15	0.33	0	17,19,21	0.86	0
2	NAG	H	2	2	14,14,15	0.30	0	17,19,21	0.63	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.

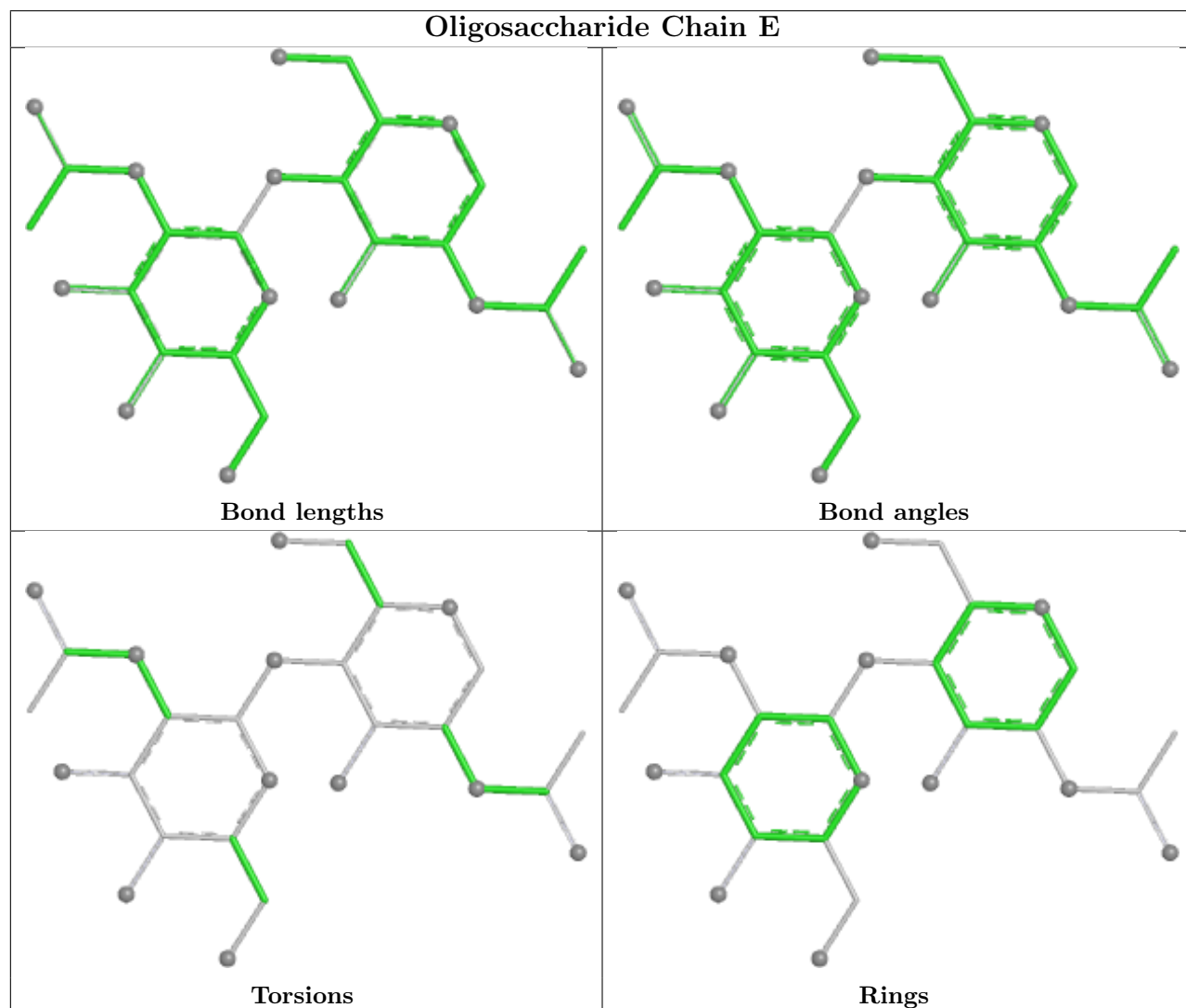
There are no chirality outliers.

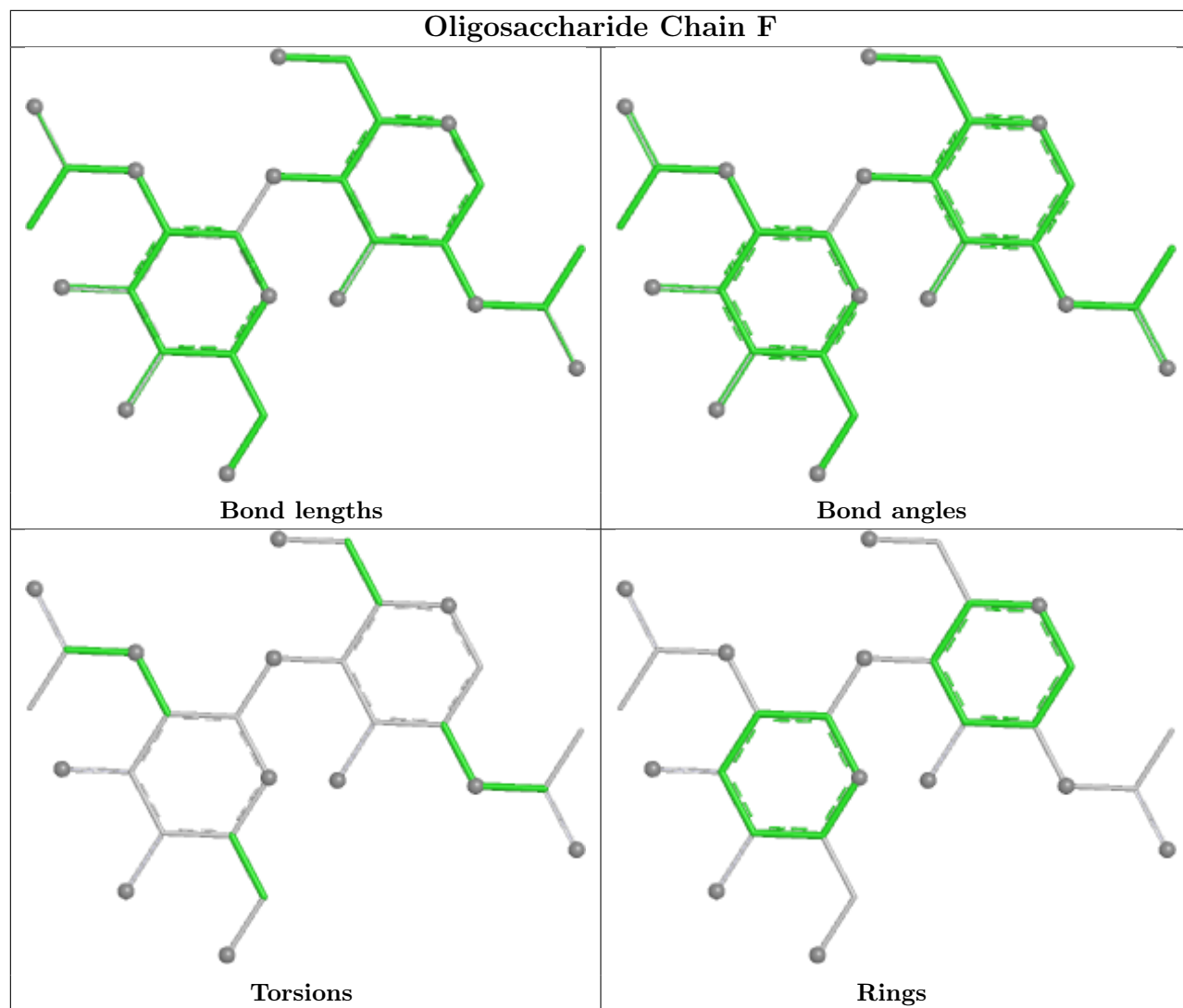
There are no torsion outliers.

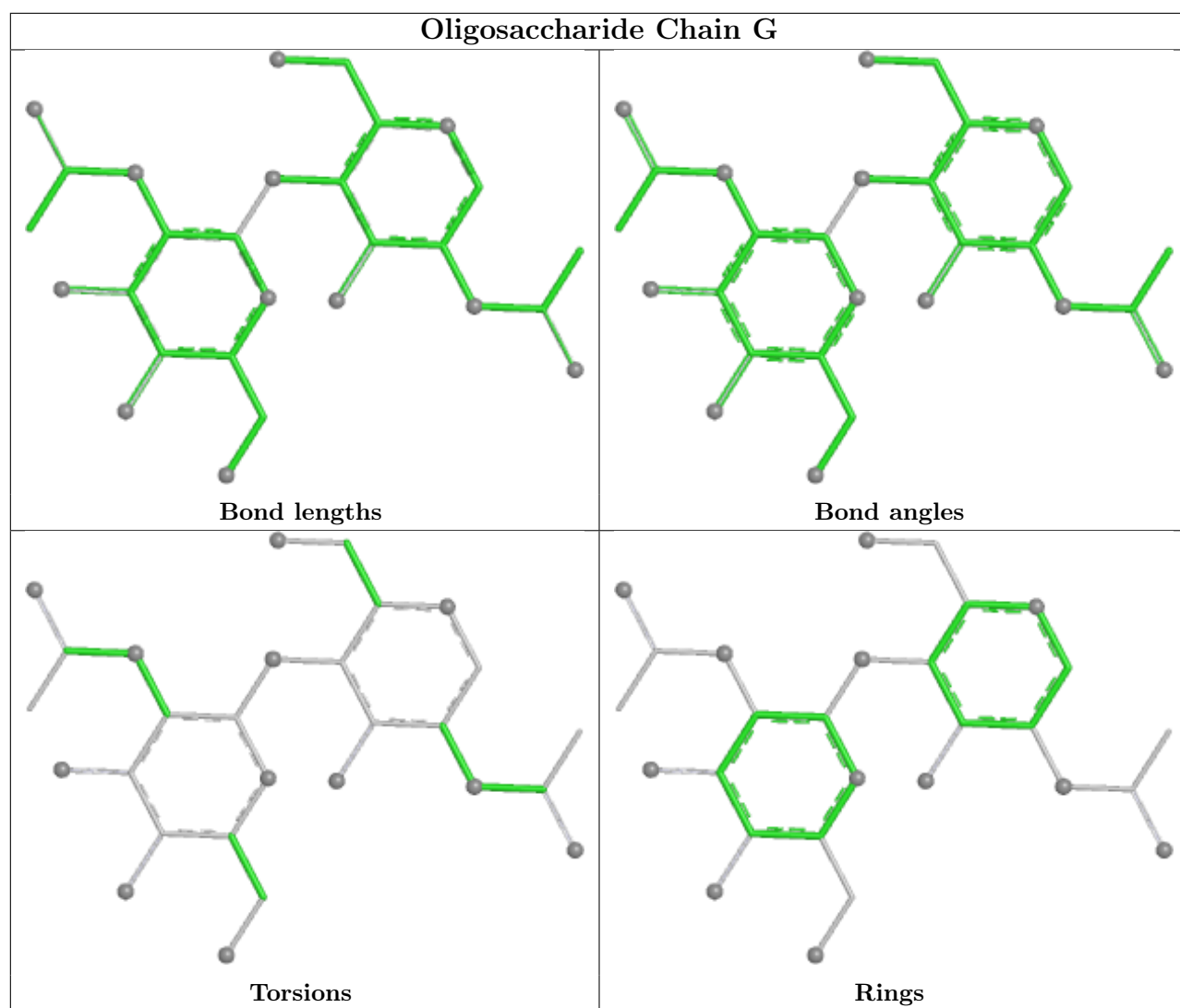
There are no ring outliers.

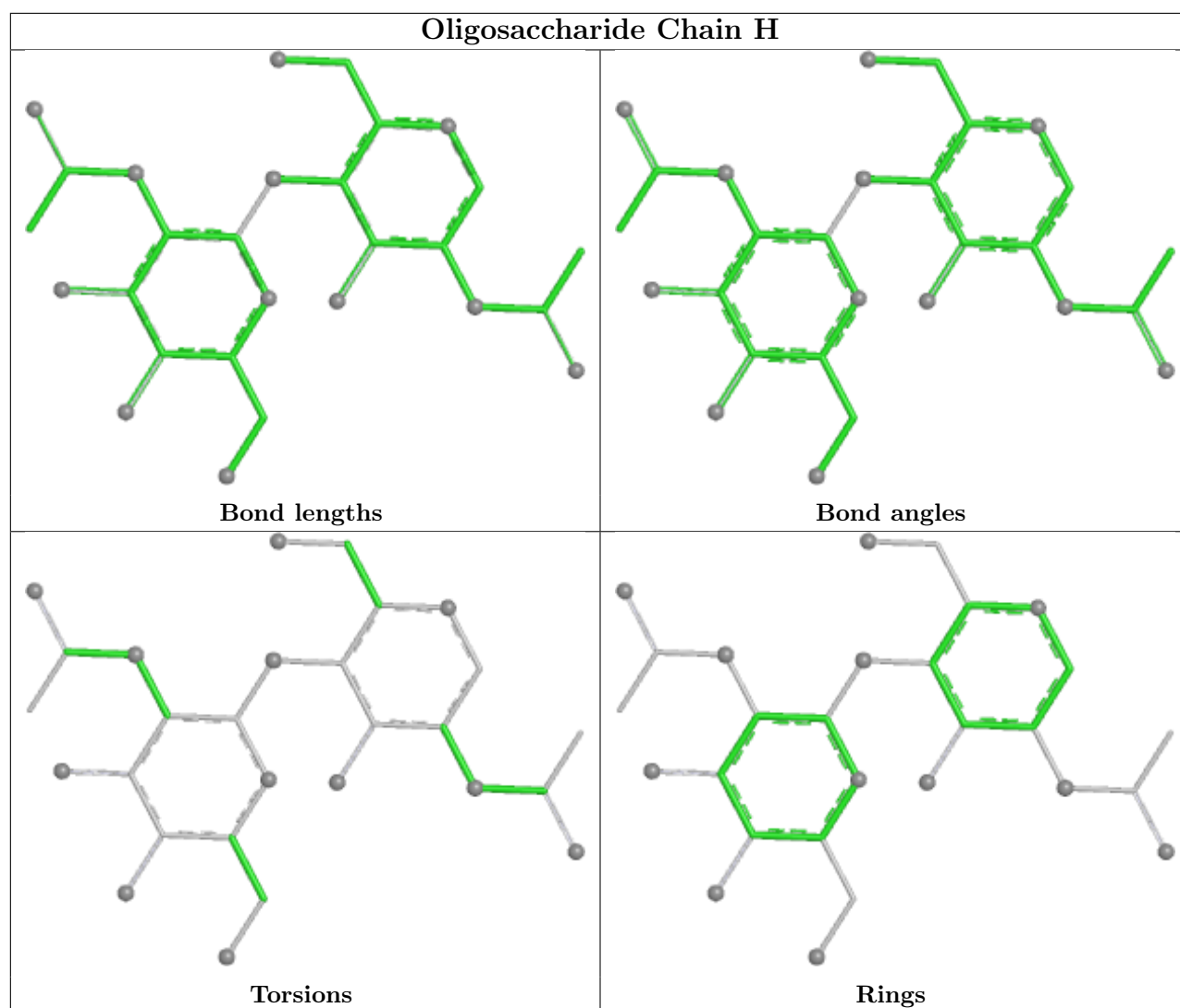
No monomer is involved in short contacts.

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	B	3002	-	43,43,51	1.21	5 (11%)	49,51,59	0.98	2 (4%)
4	POV	C	3010	-	30,30,51	1.33	5 (16%)	31,34,59	1.27	2 (6%)
4	POV	B	3004	-	37,37,51	1.32	6 (16%)	40,42,59	1.14	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	C	3008	-	12,12,51	0.43	0	11,11,59	0.74	0
4	POV	D	3002	-	43,43,51	1.21	5 (11%)	49,51,59	0.98	2 (4%)
4	POV	A	3008	-	12,12,51	0.43	0	11,11,59	0.75	0
4	POV	A	3005	-	32,32,51	1.29	5 (15%)	34,34,59	1.09	2 (5%)
4	POV	B	3011	-	30,30,51	1.33	5 (16%)	31,34,59	1.22	2 (6%)
4	POV	C	3012	-	15,15,51	0.39	0	14,14,59	0.77	0
4	POV	A	3011	-	30,30,51	1.34	5 (16%)	31,34,59	1.22	2 (6%)
4	POV	B	3001	-	41,41,51	1.25	7 (17%)	44,46,59	1.28	3 (6%)
4	POV	D	3001	-	41,41,51	1.25	7 (17%)	44,46,59	1.28	3 (6%)
4	POV	C	3006	-	15,15,51	0.36	0	14,14,59	0.87	0
4	POV	B	3014	-	14,14,51	1.07	1 (7%)	13,13,59	0.86	0
4	POV	C	3007	-	15,15,51	0.40	0	14,14,59	0.76	0
4	POV	D	3011	-	30,30,51	1.34	5 (16%)	31,34,59	1.22	2 (6%)
4	POV	D	3005	-	32,32,51	1.29	5 (15%)	34,34,59	1.09	2 (5%)
4	POV	C	3009	-	11,11,51	0.41	0	10,10,59	0.82	0
4	POV	D	3003	-	15,15,51	1.05	1 (6%)	14,14,59	0.83	0
4	POV	B	3005	-	32,32,51	1.29	5 (15%)	34,34,59	1.09	2 (5%)
4	POV	A	3012	-	15,15,51	0.39	0	14,14,59	0.77	0
4	POV	A	3010	-	30,30,51	1.34	5 (16%)	31,34,59	1.26	2 (6%)
4	POV	C	3001	-	41,41,51	1.25	7 (17%)	44,46,59	1.28	3 (6%)
4	POV	B	3003	-	15,15,51	1.05	1 (6%)	14,14,59	0.84	0
4	POV	B	3012	-	15,15,51	0.39	0	14,14,59	0.76	0
4	POV	D	3014	-	14,14,51	1.07	1 (7%)	13,13,59	0.86	0
4	POV	A	3014	-	14,14,51	1.07	1 (7%)	13,13,59	0.86	0
4	POV	B	3010	-	30,30,51	1.34	5 (16%)	31,34,59	1.27	2 (6%)
3	CLR	C	3000	-	31,31,31	0.79	1 (3%)	48,48,48	1.42	7 (14%)
3	CLR	A	3000	-	31,31,31	0.79	1 (3%)	48,48,48	1.42	7 (14%)
4	POV	A	3003	-	15,15,51	1.05	1 (6%)	14,14,59	0.83	0
4	POV	D	3010	-	30,30,51	1.34	5 (16%)	31,34,59	1.26	2 (6%)
4	POV	C	3002	-	43,43,51	1.21	5 (11%)	49,51,59	0.98	2 (4%)
3	CLR	B	3000	-	31,31,31	0.78	1 (3%)	48,48,48	1.42	7 (14%)
4	POV	A	3007	-	15,15,51	0.40	0	14,14,59	0.76	0
4	POV	B	3009	-	11,11,51	0.40	0	10,10,59	0.82	0
4	POV	C	3003	-	15,15,51	1.05	1 (6%)	14,14,59	0.83	0
4	POV	D	3012	-	15,15,51	0.39	0	14,14,59	0.77	0
4	POV	D	3009	-	11,11,51	0.40	0	10,10,59	0.82	0
4	POV	B	3013	-	10,10,51	0.43	0	9,9,59	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	B	3007	-	15,15,51	0.40	0	14,14,59	0.76	0
4	POV	A	3009	-	11,11,51	0.40	0	10,10,59	0.82	0
4	POV	B	3008	-	12,12,51	0.43	0	11,11,59	0.75	0
4	POV	C	3004	-	37,37,51	1.33	6 (16%)	40,42,59	1.14	3 (7%)
3	CLR	D	3000	-	31,31,31	0.79	0	48,48,48	1.42	7 (14%)
4	POV	A	3006	-	15,15,51	0.36	0	14,14,59	0.87	0
4	POV	A	3013	-	10,10,51	0.43	0	9,9,59	0.80	0
4	POV	C	3011	-	30,30,51	1.34	5 (16%)	31,34,59	1.22	2 (6%)
4	POV	C	3005	-	32,32,51	1.28	5 (15%)	34,34,59	1.09	2 (5%)
4	POV	B	3006	-	15,15,51	0.35	0	14,14,59	0.87	0
4	POV	D	3008	-	12,12,51	0.43	0	11,11,59	0.75	0
4	POV	C	3014	-	14,14,51	1.07	1 (7%)	13,13,59	0.86	0
4	POV	D	3004	-	37,37,51	1.32	6 (16%)	40,42,59	1.14	3 (7%)
4	POV	A	3002	-	43,43,51	1.21	5 (11%)	49,51,59	0.98	2 (4%)
4	POV	C	3013	-	10,10,51	0.43	0	9,9,59	0.80	0
4	POV	A	3001	-	41,41,51	1.25	7 (17%)	44,46,59	1.28	3 (6%)
4	POV	D	3013	-	10,10,51	0.43	0	9,9,59	0.80	0
4	POV	D	3006	-	15,15,51	0.36	0	14,14,59	0.87	0
4	POV	D	3007	-	15,15,51	0.39	0	14,14,59	0.76	0
4	POV	A	3004	-	37,37,51	1.32	6 (16%)	40,42,59	1.14	3 (7%)

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	POV	B	3002	-	-	15/47/47/55	-
4	POV	C	3010	-	-	8/31/31/55	-
4	POV	B	3004	-	-	18/39/39/55	-
4	POV	C	3008	-	-	5/10/10/55	-
4	POV	D	3002	-	-	15/47/47/55	-
4	POV	A	3008	-	-	5/10/10/55	-
4	POV	A	3005	-	-	5/33/33/55	-
4	POV	B	3011	-	-	13/31/31/55	-
4	POV	C	3012	-	-	8/13/13/55	-
4	POV	A	3011	-	-	13/31/31/55	-
4	POV	B	3001	-	-	18/43/43/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	D	3001	-	-	18/43/43/55	-
4	POV	C	3006	-	-	0/13/13/55	-
4	POV	B	3014	-	-	3/12/12/55	-
4	POV	C	3007	-	-	7/13/13/55	-
4	POV	D	3011	-	-	13/31/31/55	-
4	POV	D	3005	-	-	5/33/33/55	-
4	POV	C	3009	-	-	1/9/9/55	-
4	POV	D	3003	-	-	7/13/13/55	-
4	POV	B	3005	-	-	5/33/33/55	-
4	POV	A	3012	-	-	8/13/13/55	-
4	POV	A	3010	-	-	8/31/31/55	-
4	POV	C	3001	-	-	18/43/43/55	-
4	POV	B	3003	-	-	7/13/13/55	-
4	POV	B	3012	-	-	8/13/13/55	-
4	POV	D	3014	-	-	3/12/12/55	-
4	POV	A	3014	-	-	3/12/12/55	-
4	POV	B	3010	-	-	8/31/31/55	-
3	CLR	C	3000	-	-	0/10/68/68	0/4/4/4
3	CLR	A	3000	-	-	0/10/68/68	0/4/4/4
4	POV	A	3003	-	-	7/13/13/55	-
4	POV	D	3010	-	-	8/31/31/55	-
4	POV	C	3002	-	-	15/47/47/55	-
3	CLR	B	3000	-	-	0/10/68/68	0/4/4/4
4	POV	A	3007	-	-	7/13/13/55	-
4	POV	B	3009	-	-	1/9/9/55	-
4	POV	C	3003	-	-	7/13/13/55	-
4	POV	D	3012	-	-	8/13/13/55	-
4	POV	D	3009	-	-	1/9/9/55	-
4	POV	B	3013	-	-	0/8/8/55	-
4	POV	B	3007	-	-	7/13/13/55	-
4	POV	A	3009	-	-	1/9/9/55	-
4	POV	B	3008	-	-	5/10/10/55	-
4	POV	C	3004	-	-	18/39/39/55	-
3	CLR	D	3000	-	-	0/10/68/68	0/4/4/4
4	POV	A	3006	-	-	0/13/13/55	-
4	POV	A	3013	-	-	0/8/8/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	C	3011	-	-	13/31/31/55	-
4	POV	C	3005	-	-	5/33/33/55	-
4	POV	B	3006	-	-	0/13/13/55	-
4	POV	D	3008	-	-	5/10/10/55	-
4	POV	C	3014	-	-	3/12/12/55	-
4	POV	D	3004	-	-	18/39/39/55	-
4	POV	A	3002	-	-	15/47/47/55	-
4	POV	C	3013	-	-	0/8/8/55	-
4	POV	A	3001	-	-	18/43/43/55	-
4	POV	D	3013	-	-	0/8/8/55	-
4	POV	D	3006	-	-	0/13/13/55	-
4	POV	D	3007	-	-	7/13/13/55	-
4	POV	A	3004	-	-	18/39/39/55	-

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3004	POV	C29-C210	3.92	1.54	1.31
4	B	3004	POV	C29-C210	3.92	1.54	1.31
4	C	3004	POV	C29-C210	3.92	1.54	1.31
4	D	3004	POV	C29-C210	3.91	1.53	1.31
4	C	3003	POV	C29-C210	3.90	1.53	1.31

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3000	CLR	C13-C17-C20	-4.54	112.49	119.50
3	A	3000	CLR	C13-C17-C20	-4.48	112.58	119.50
3	C	3000	CLR	C13-C17-C20	-4.47	112.59	119.50
3	D	3000	CLR	C13-C17-C20	-4.46	112.61	119.50
4	B	3001	POV	O21-C21-C22	4.39	120.97	111.48

There are no chirality outliers.

5 of 432 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

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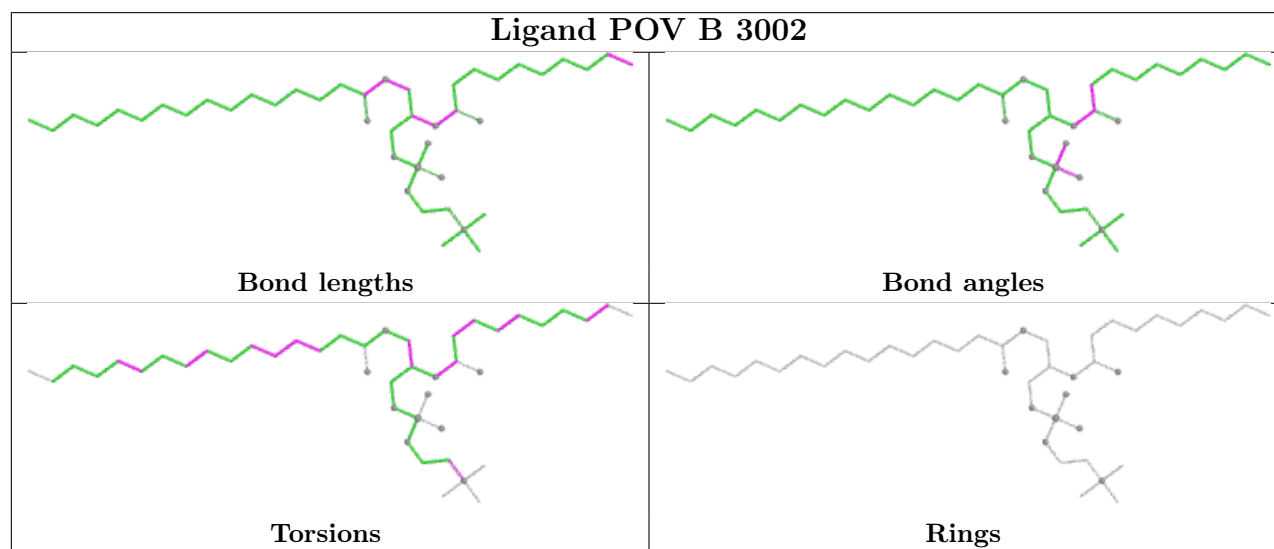
Mol	Chain	Res	Type	Atoms
4	A	3004	POV	O11-C1-C2-O21
4	A	3004	POV	C22-C21-O21-C2

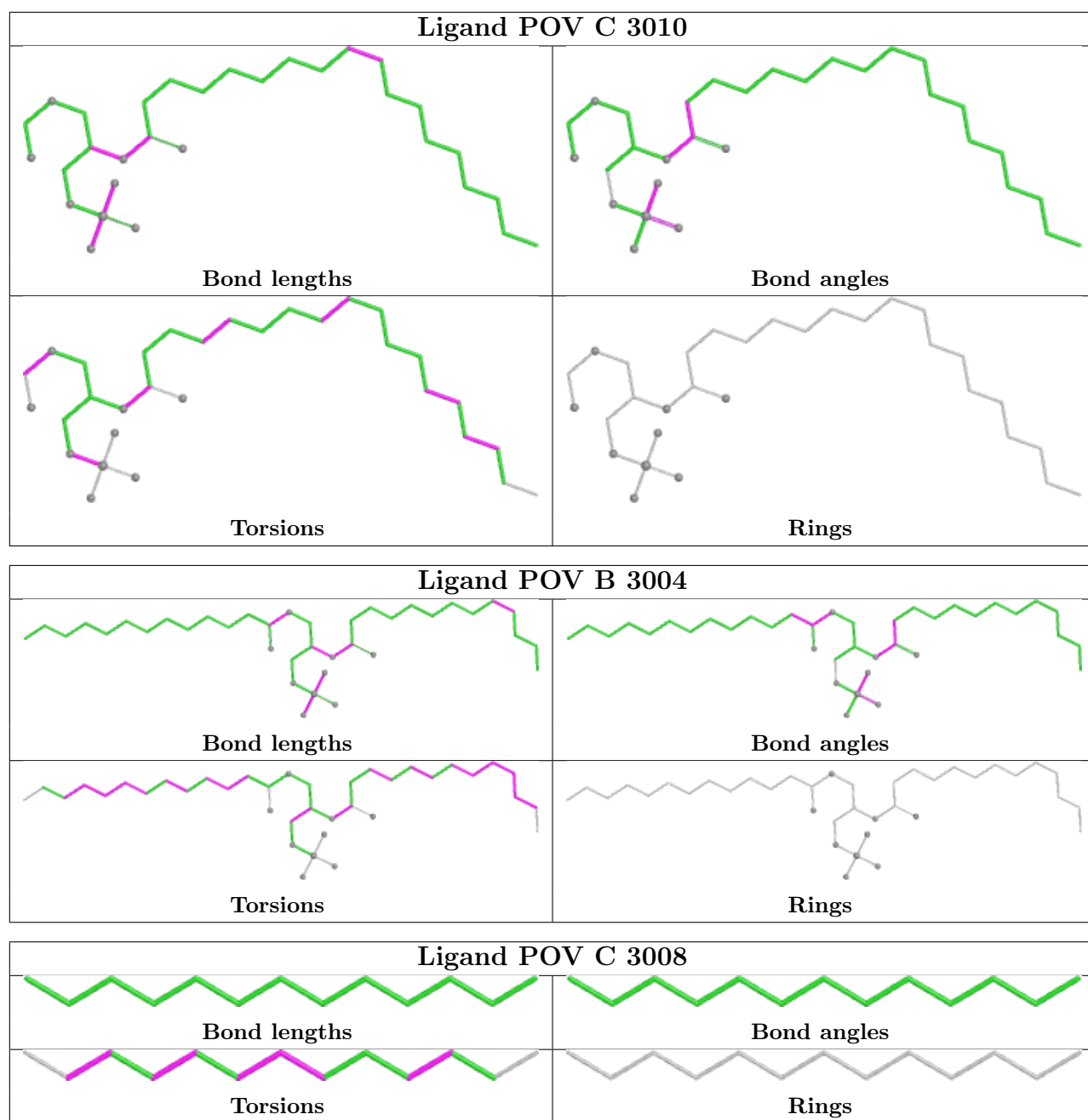
There are no ring outliers.

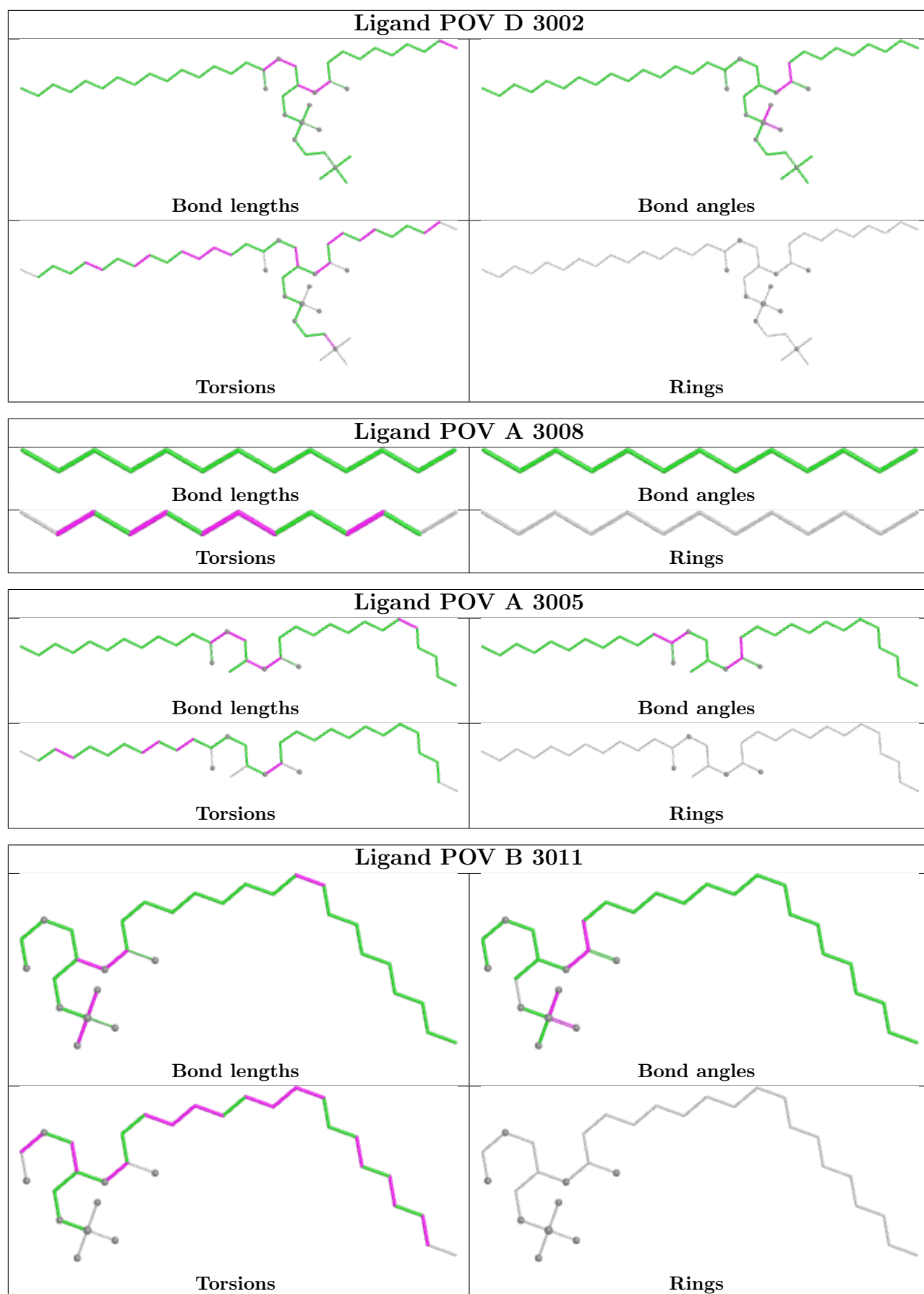
4 monomers are involved in 37 short contacts:

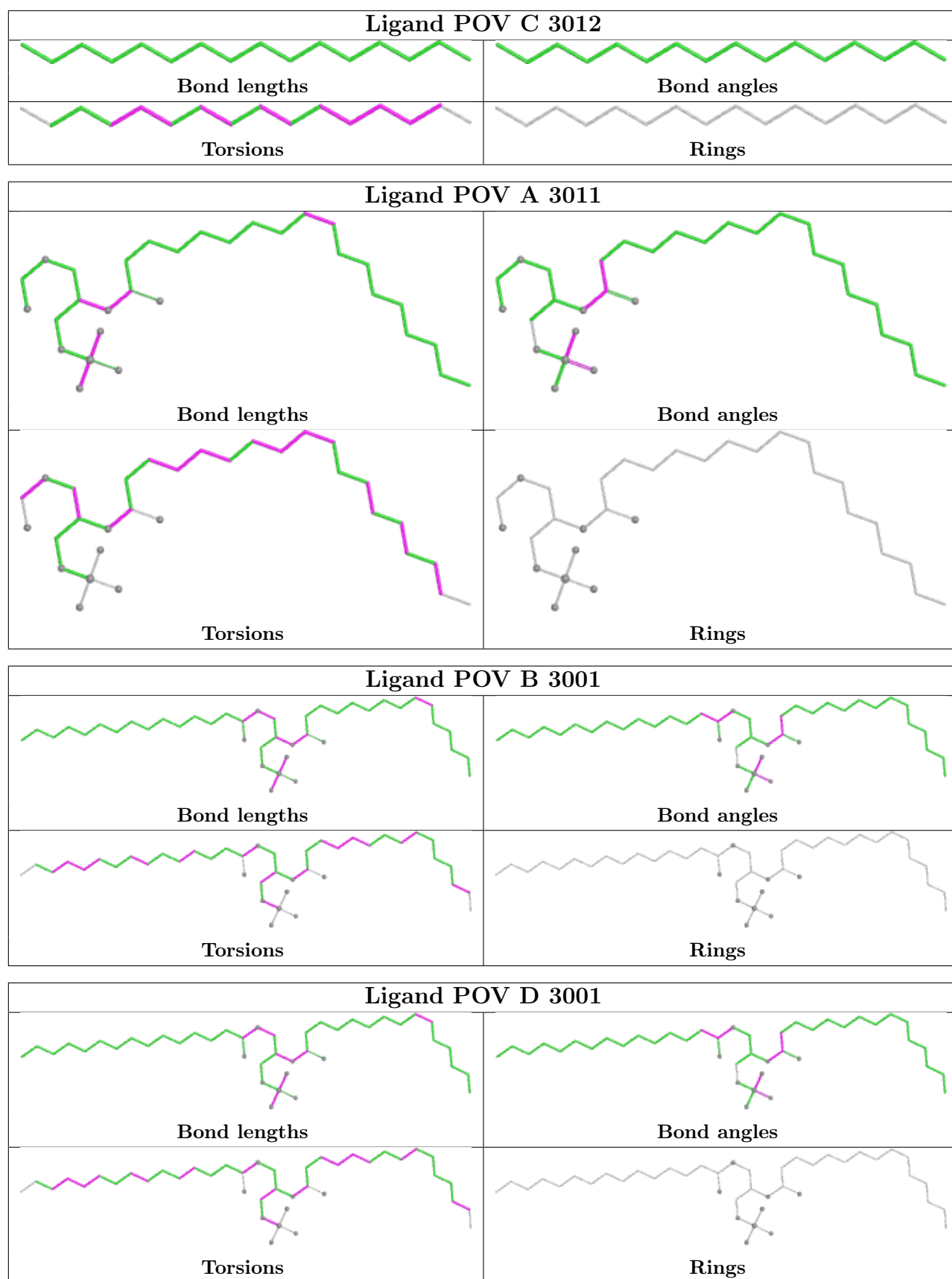
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3000	CLR	9	0
3	A	3000	CLR	9	0
3	B	3000	CLR	10	0
3	D	3000	CLR	9	0

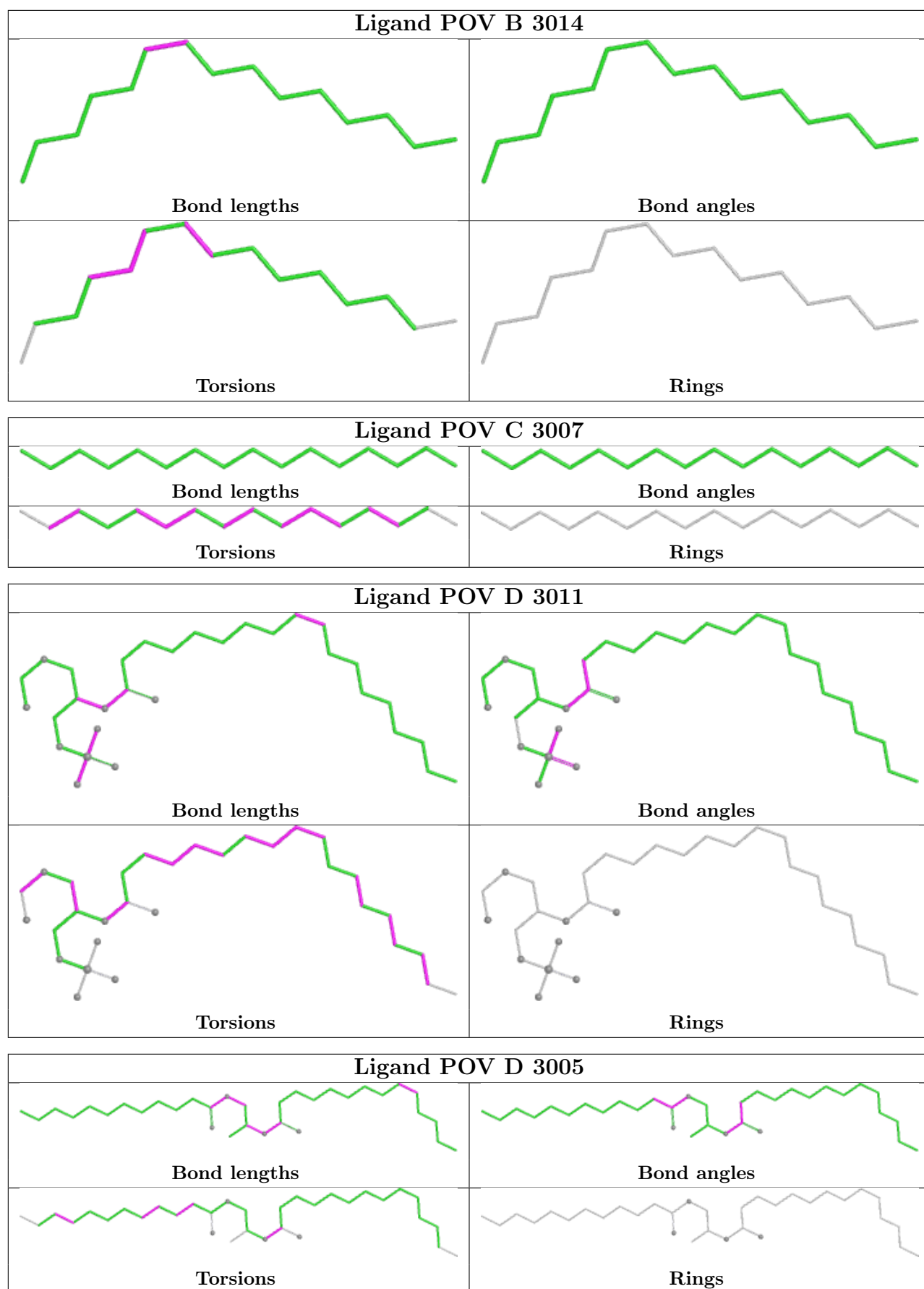
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

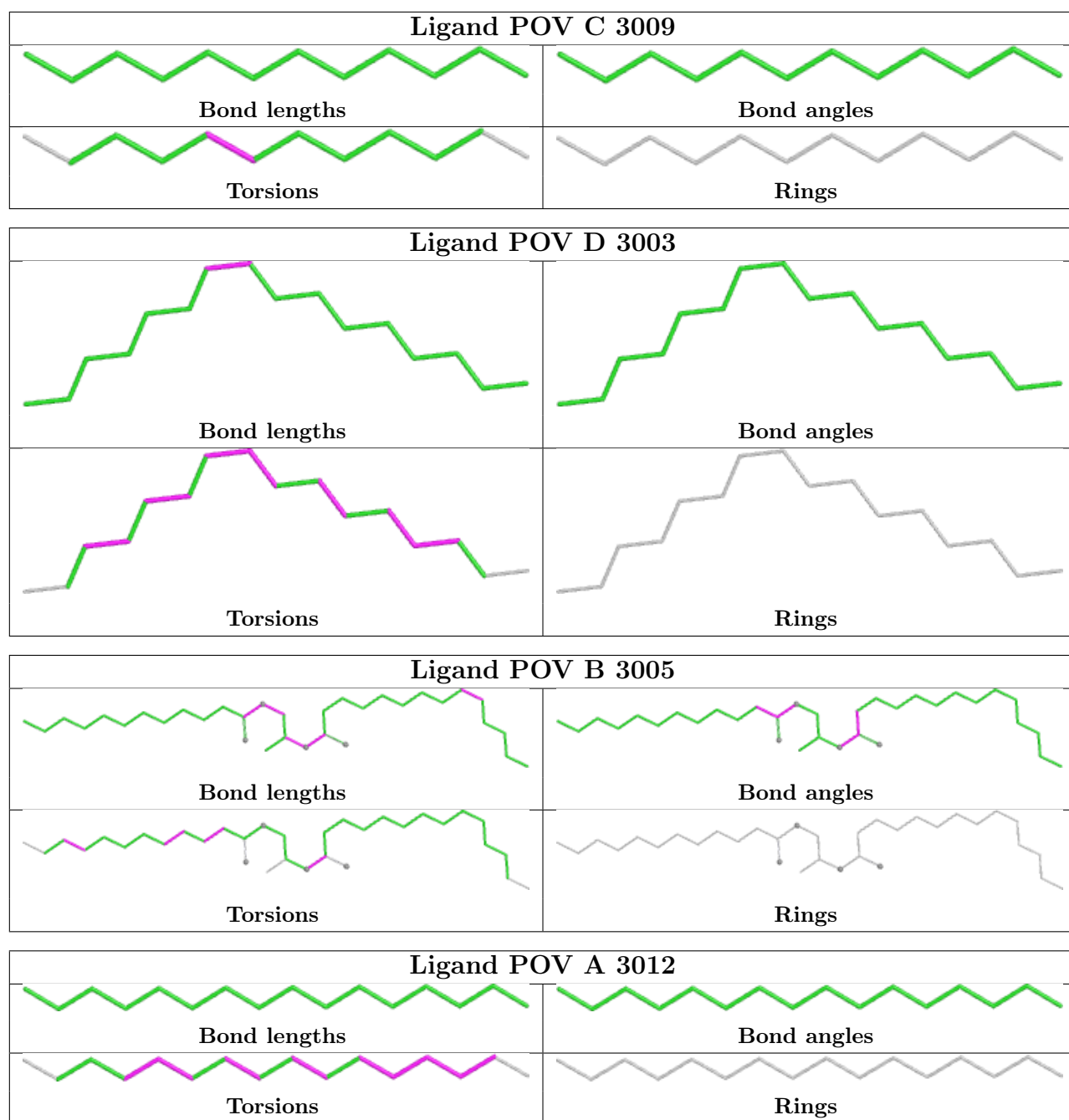


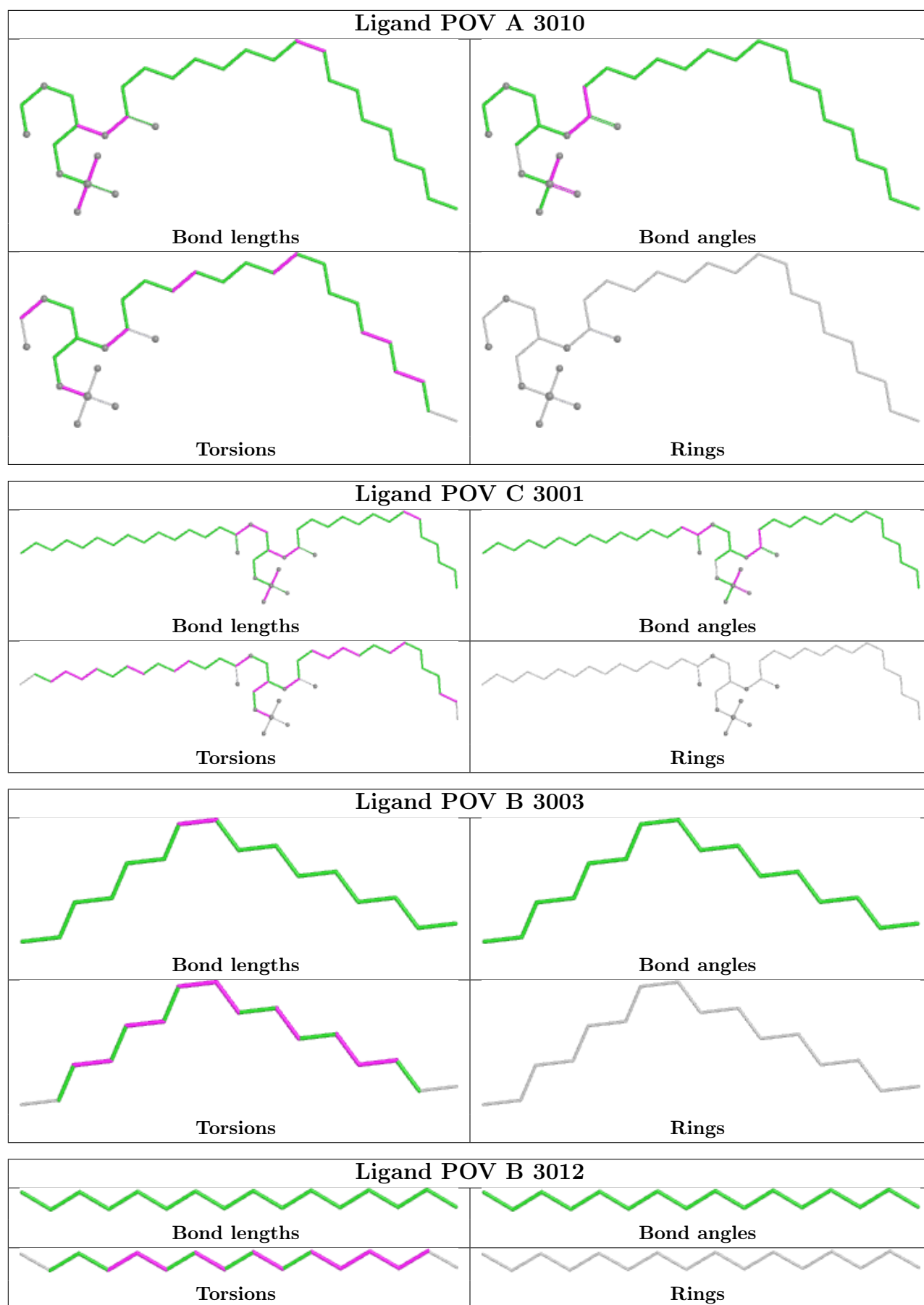


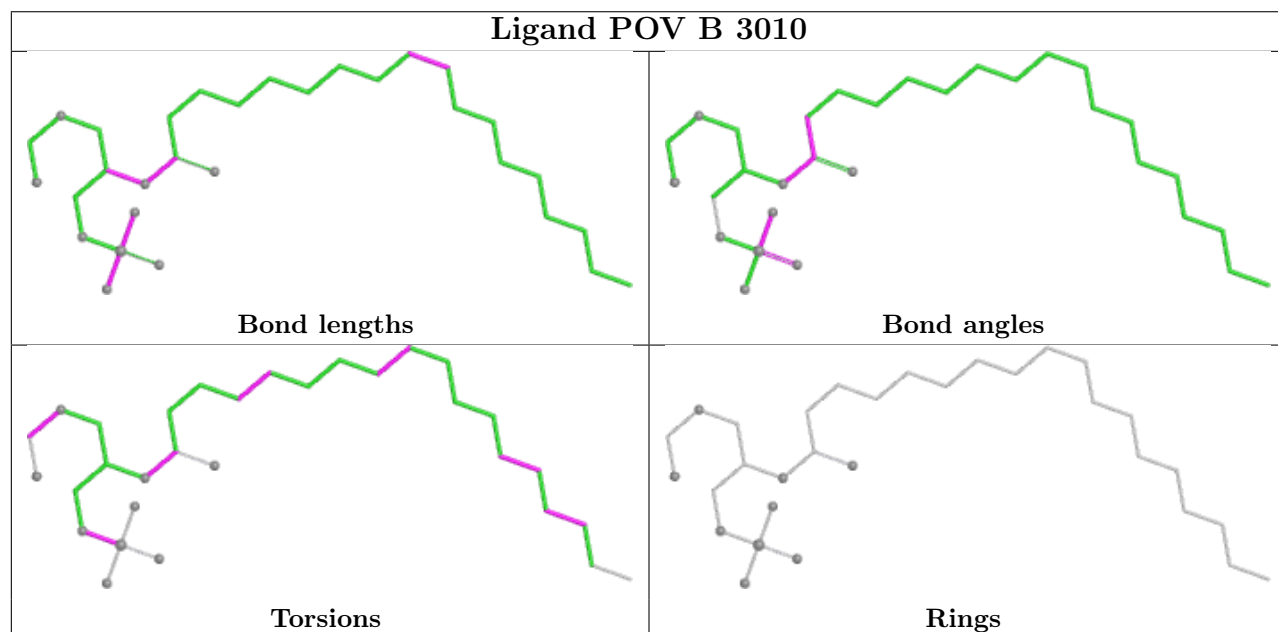
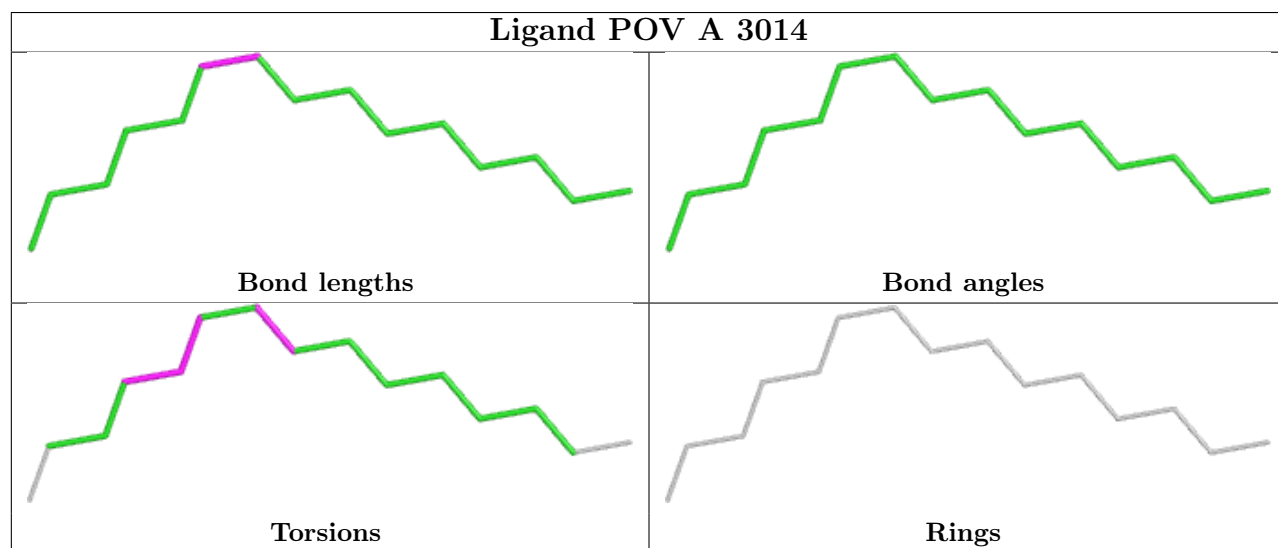
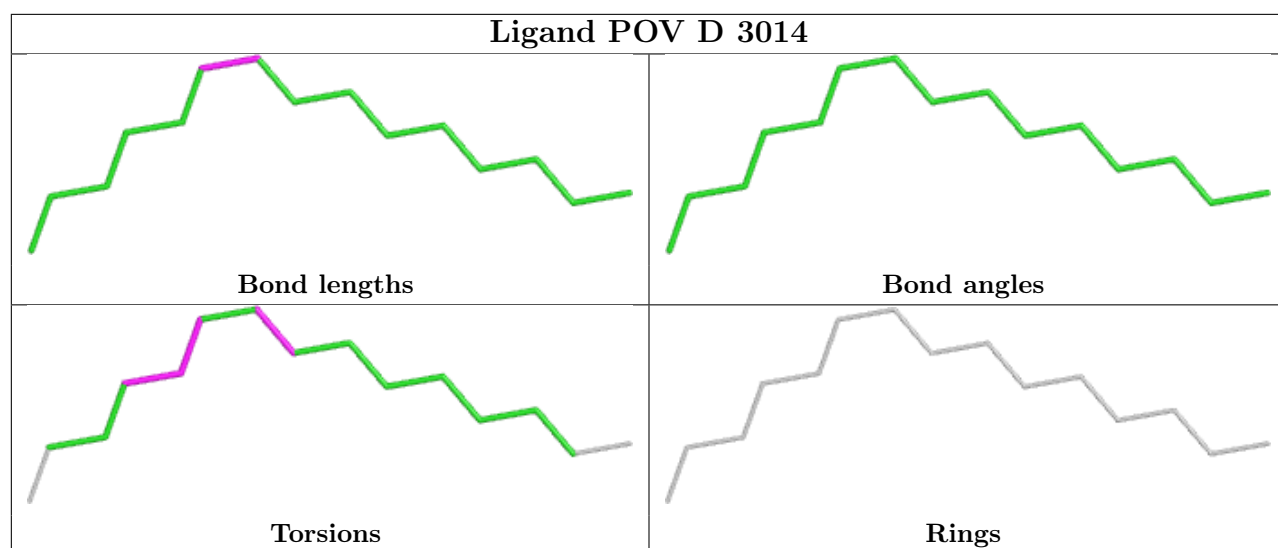


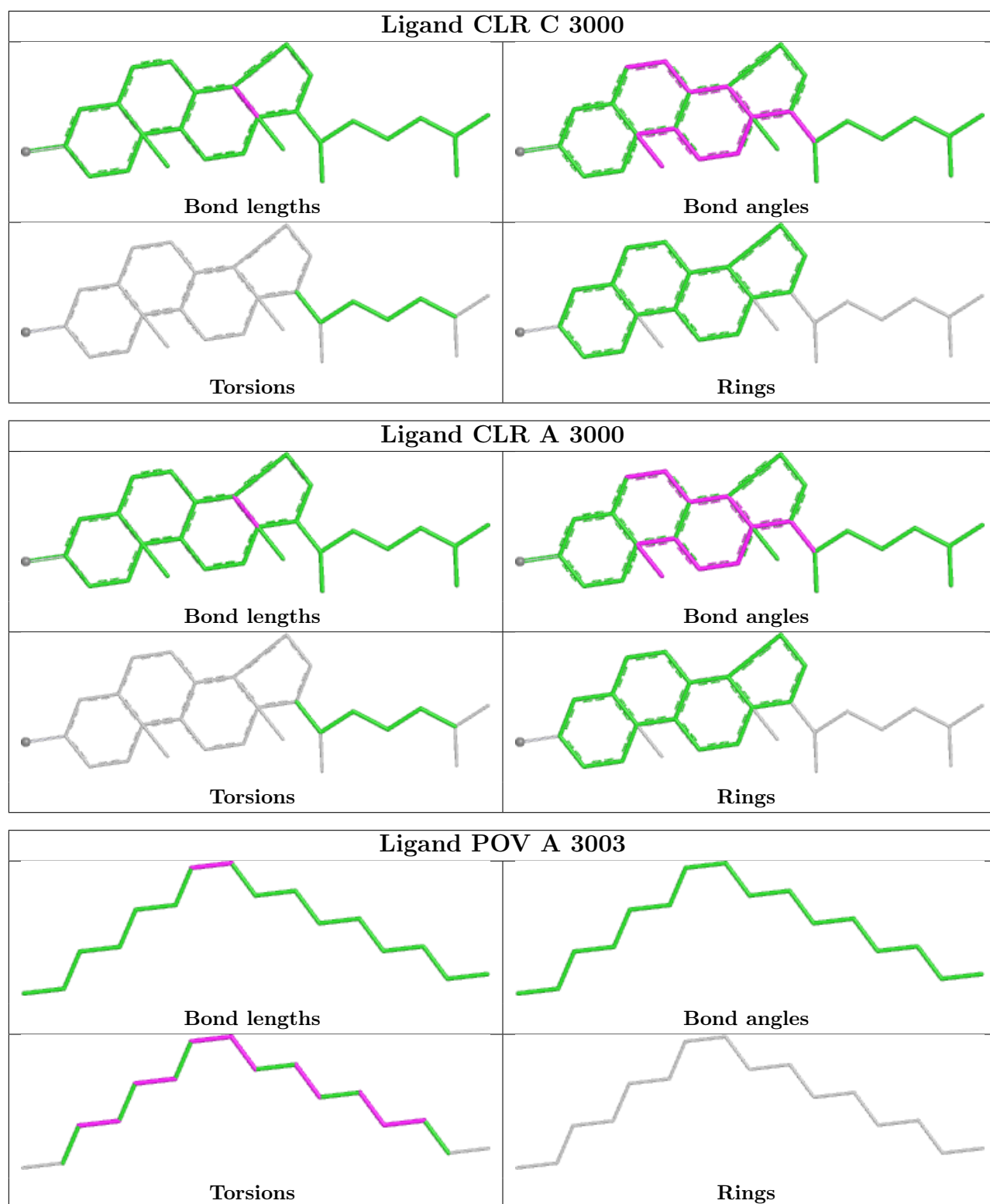


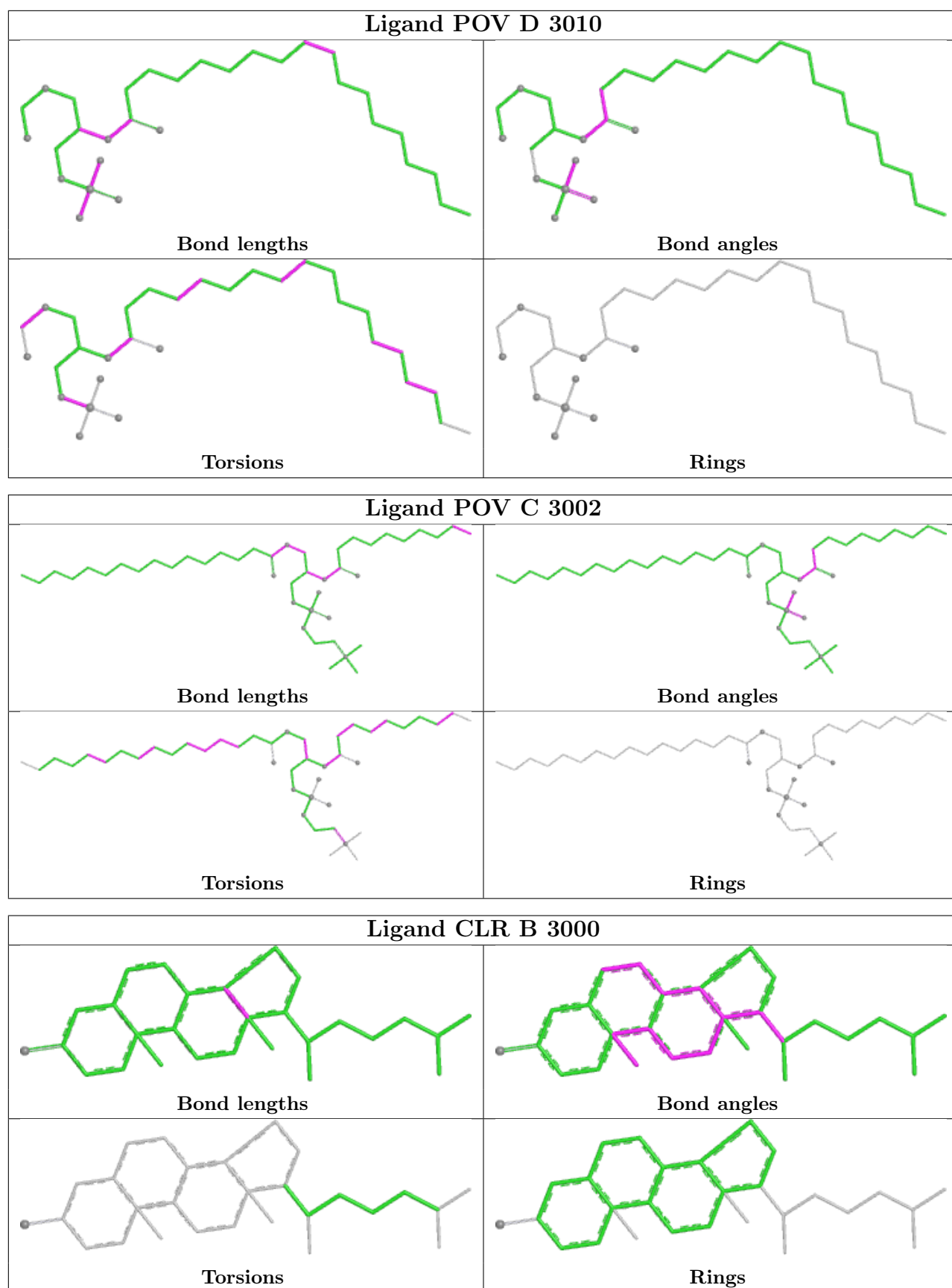


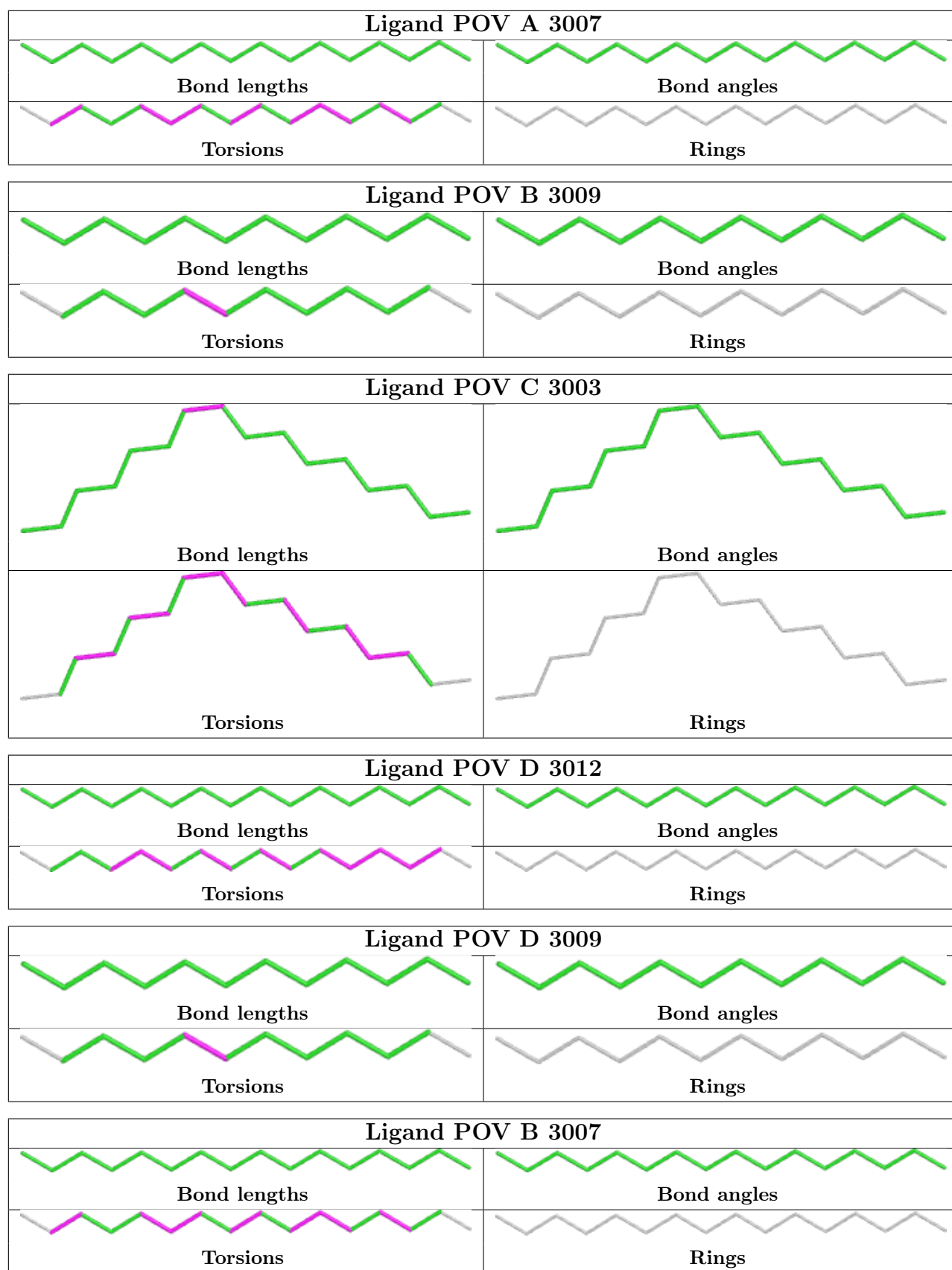


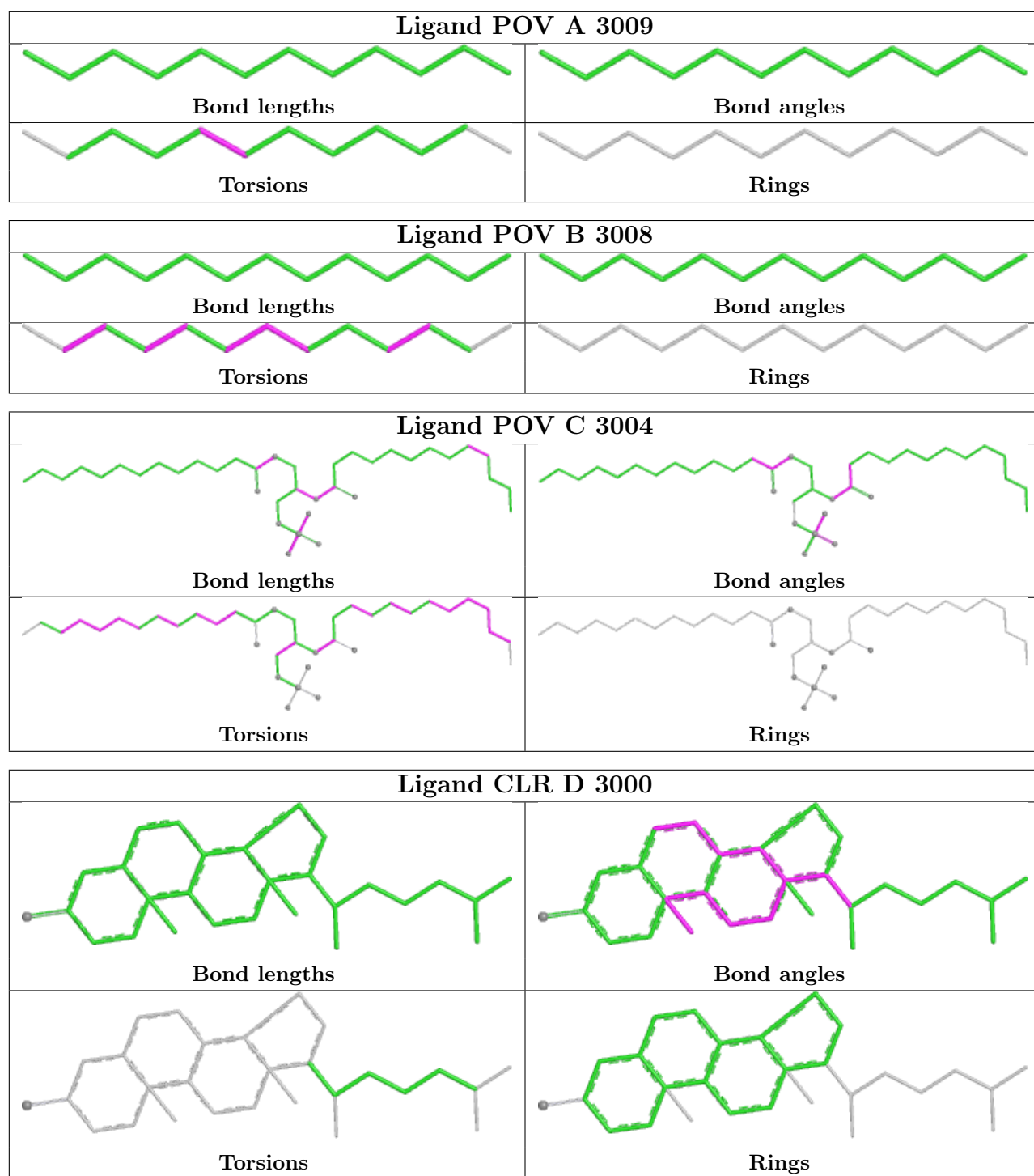


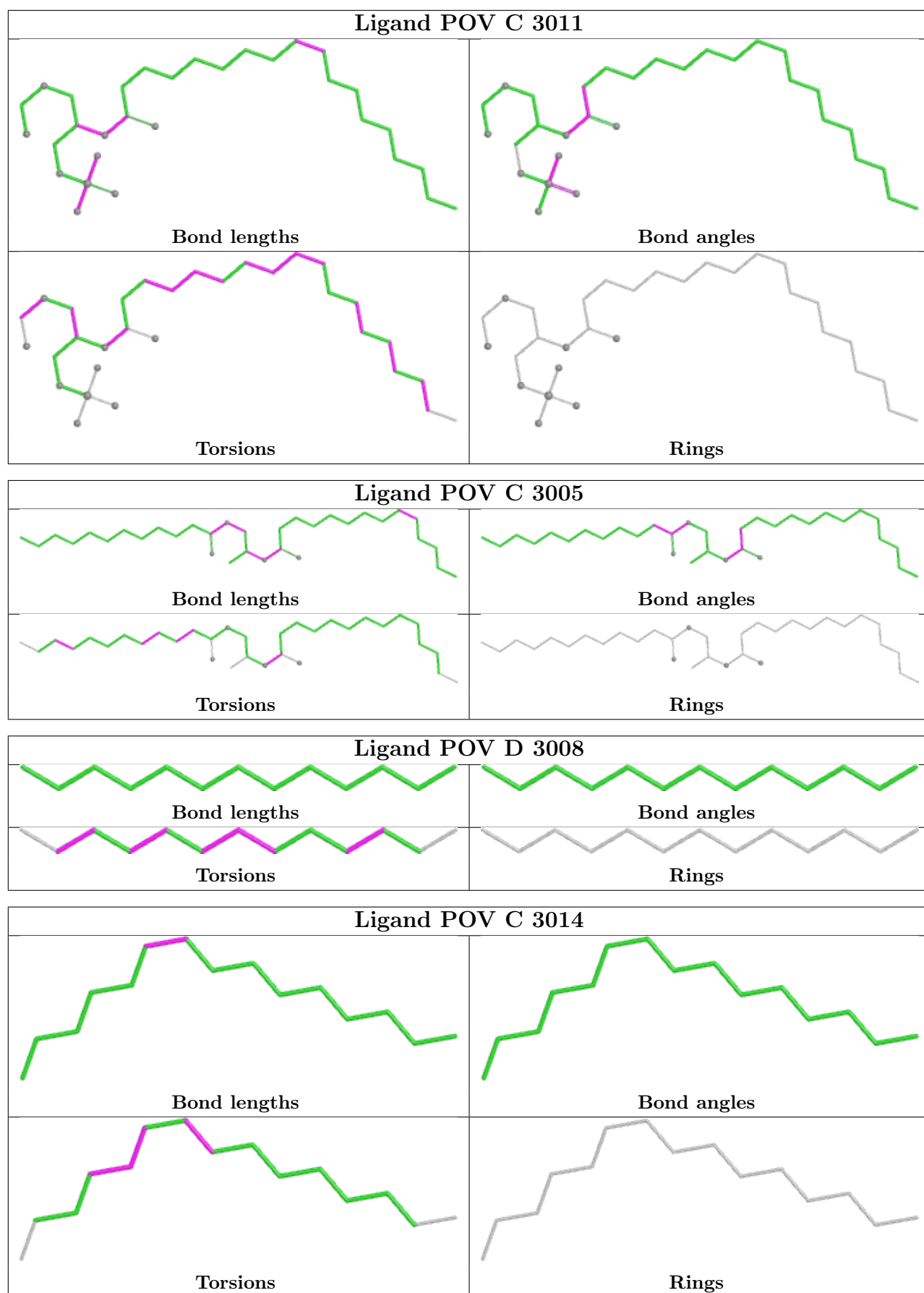


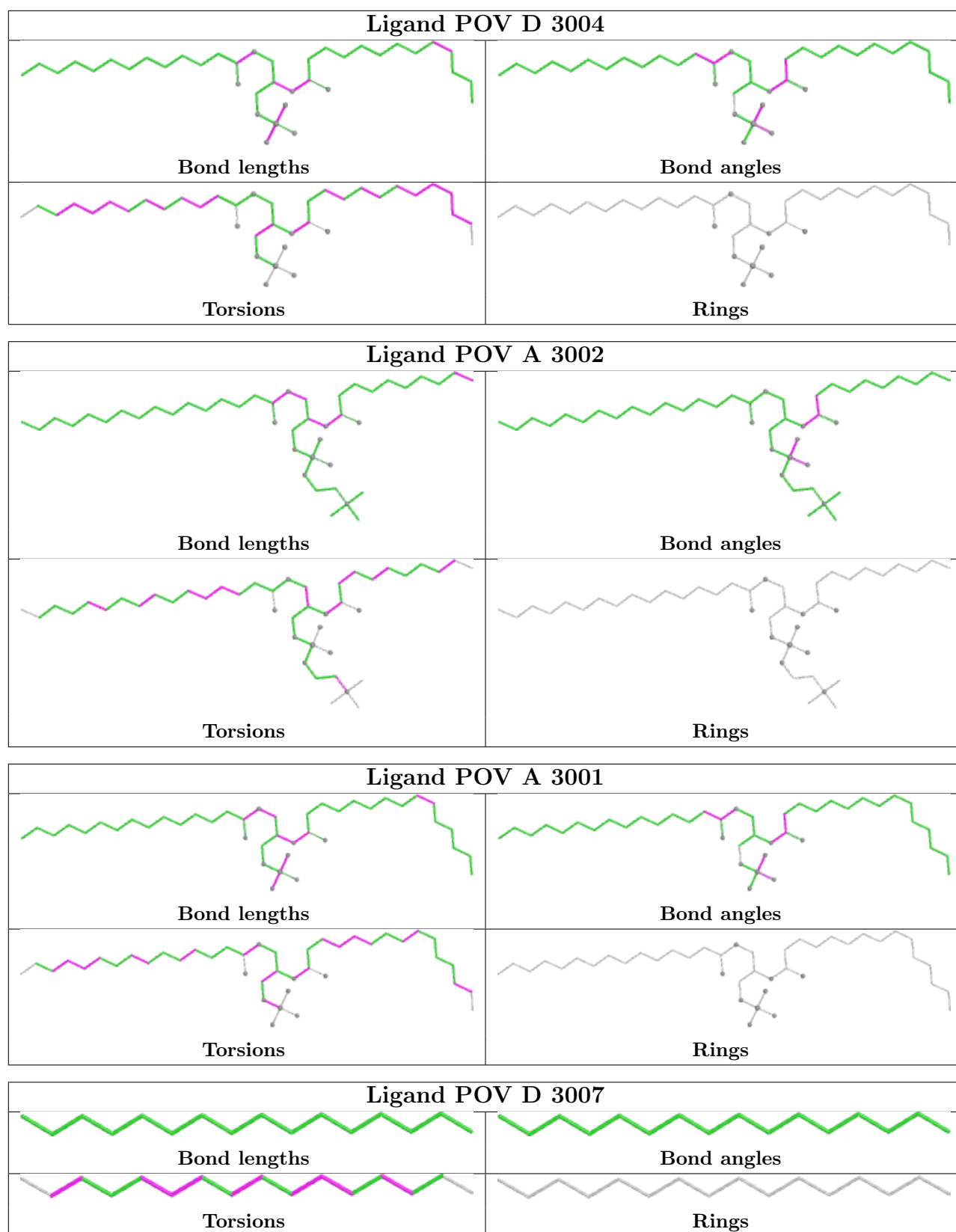


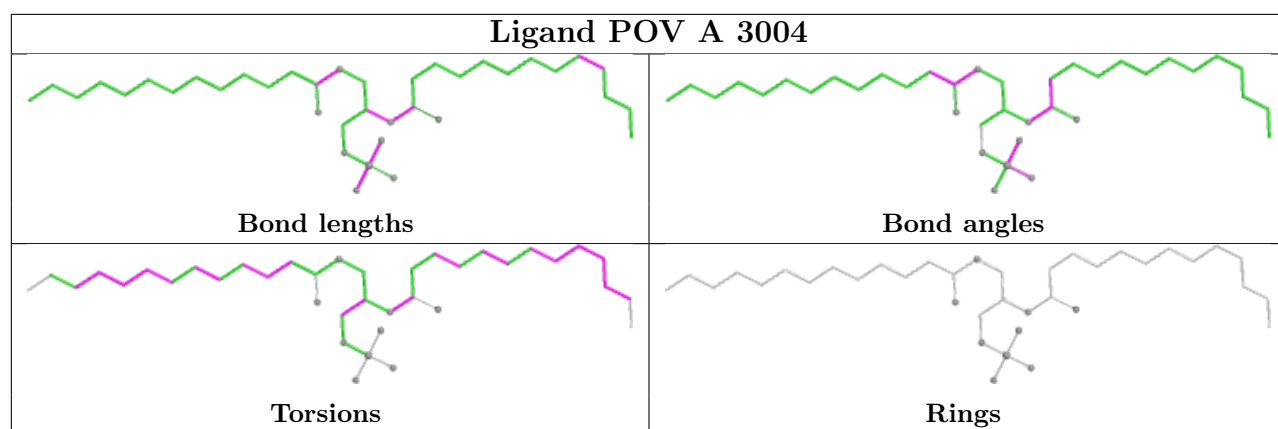












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

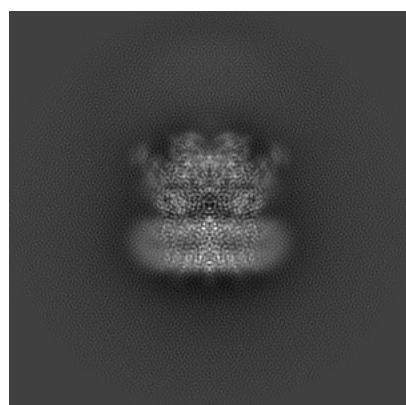
6 Map visualisation [i](#)

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.

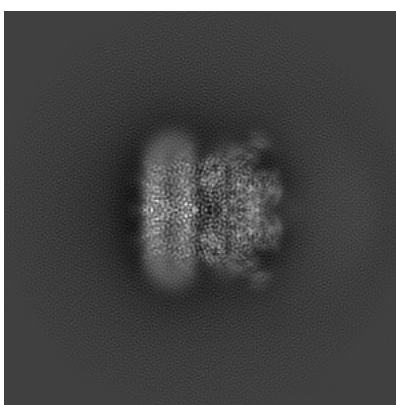
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

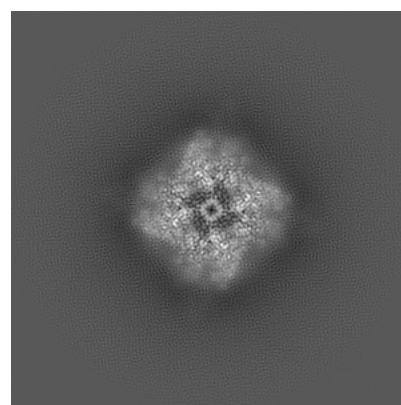
6.1.1 Primary map



X



Y

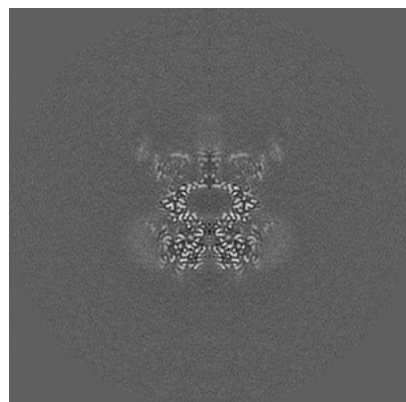


Z

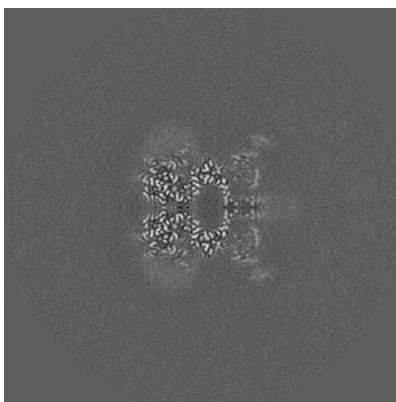
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

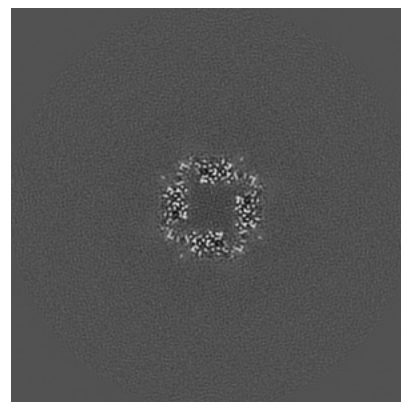
6.2.1 Primary map



X Index: 192



Y Index: 192

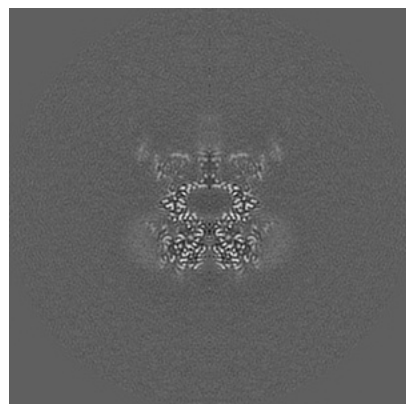


Z Index: 192

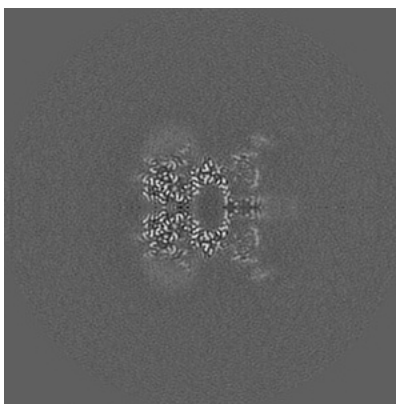
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

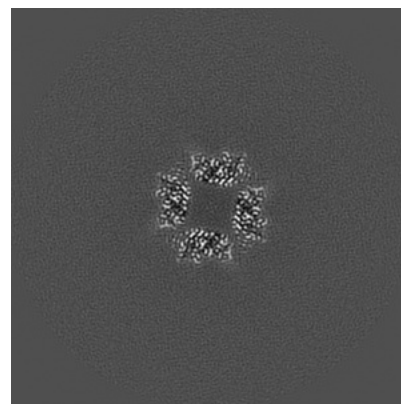
6.3.1 Primary map



X Index: 192



Y Index: 192

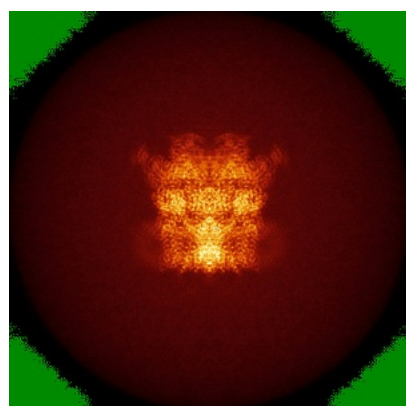


Z Index: 198

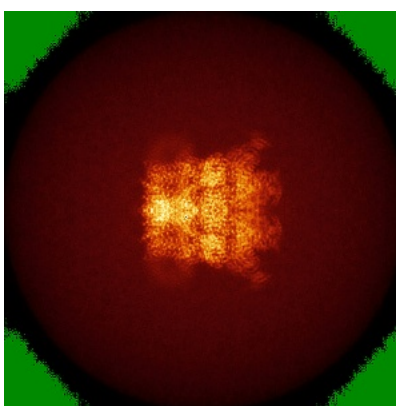
The images above show the largest variance slices of the map in three orthogonal directions.

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

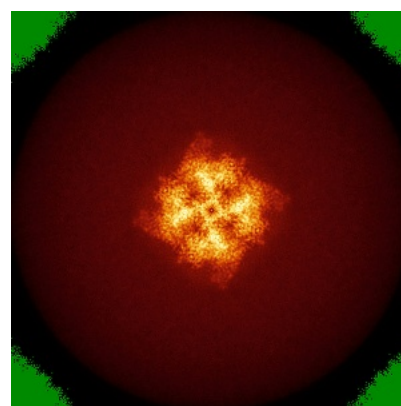
6.4.1 Primary map



X



Y

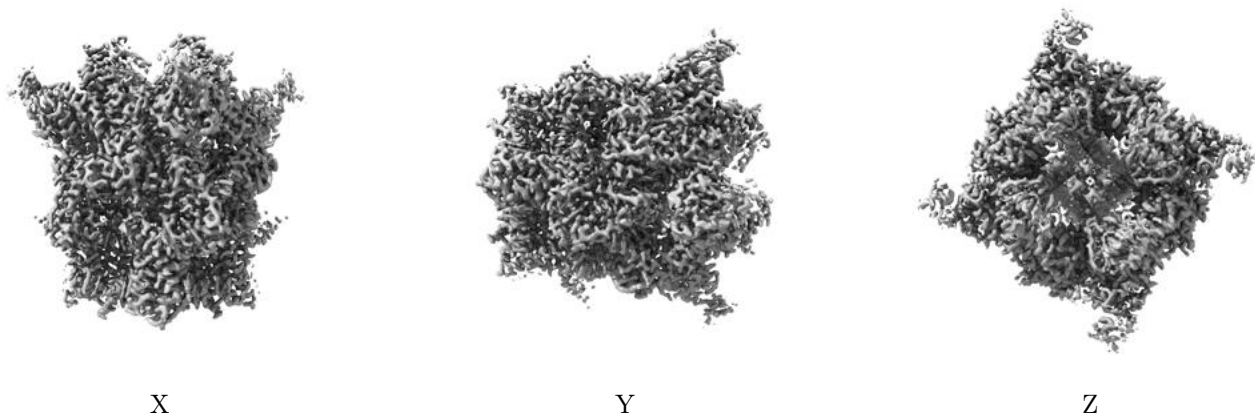


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

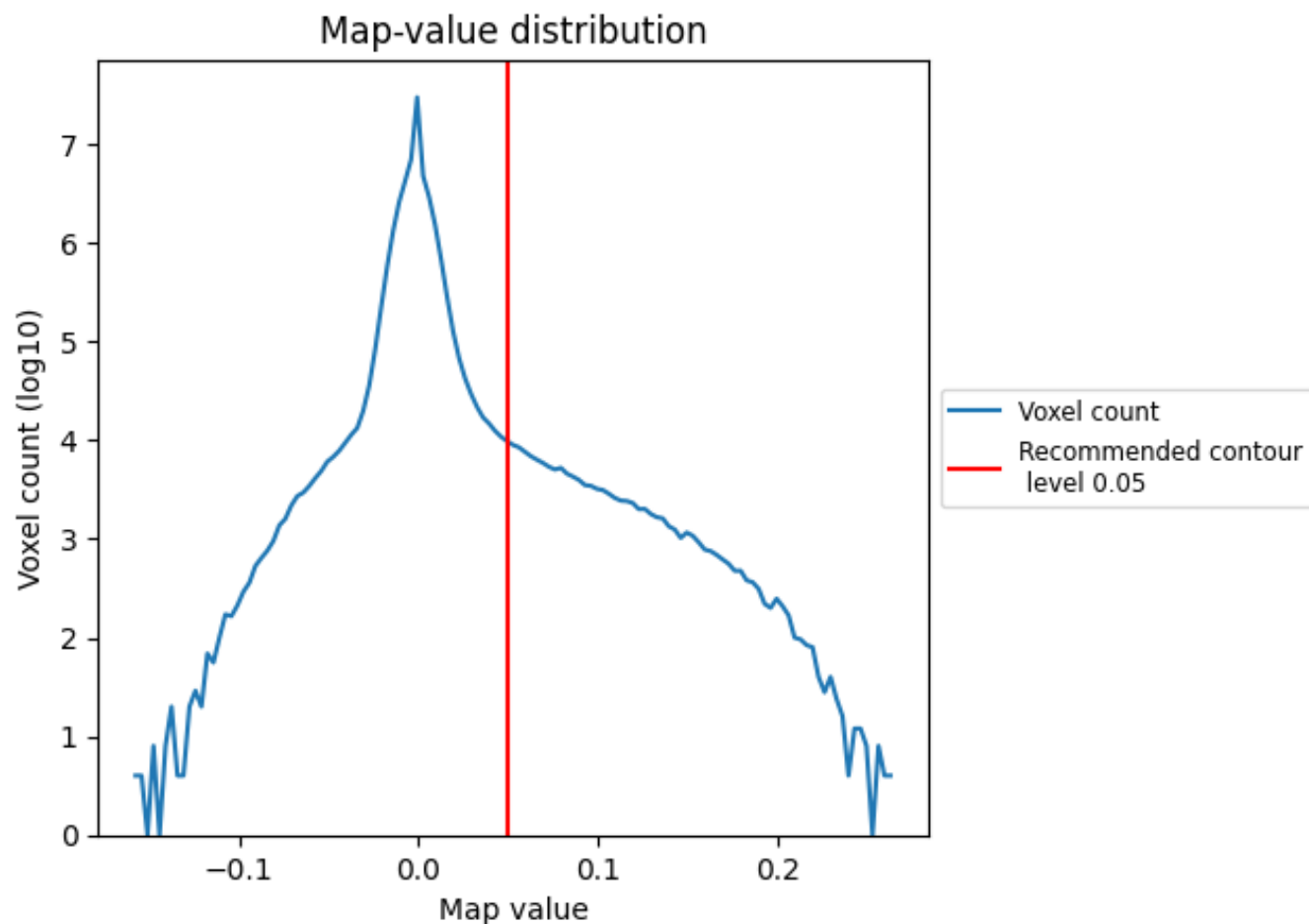
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

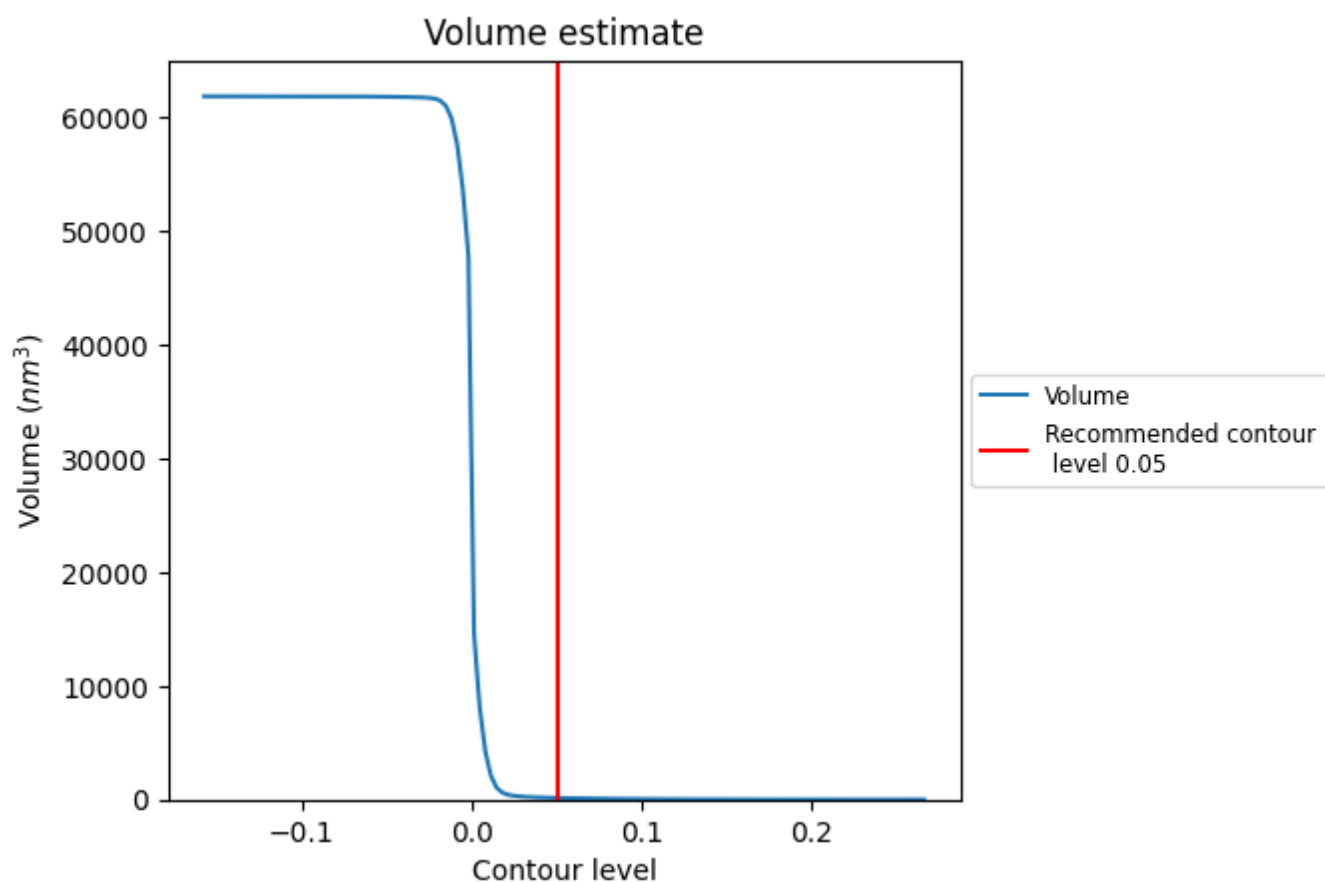
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

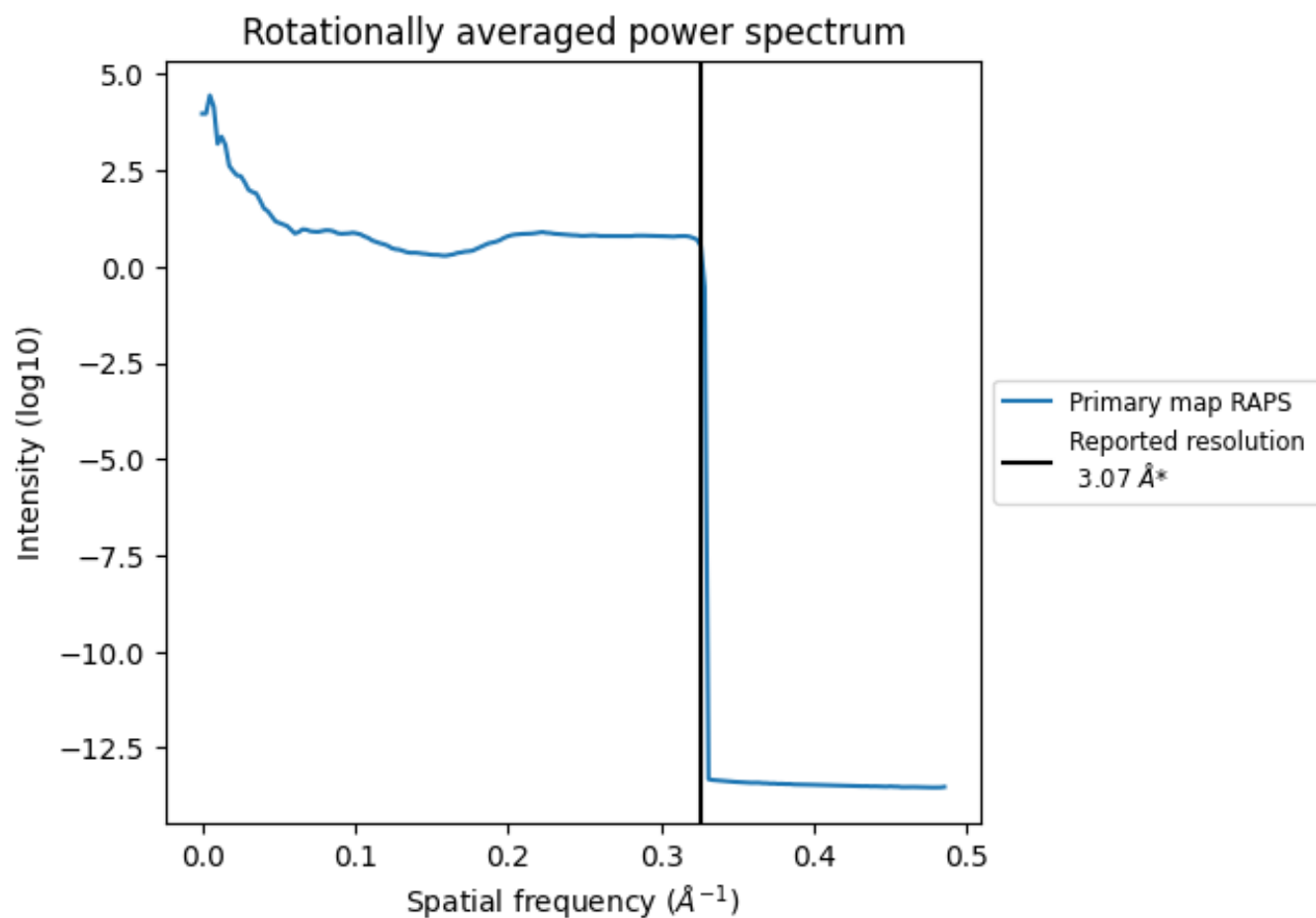
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.326 $\text{\AA}^{-1}$

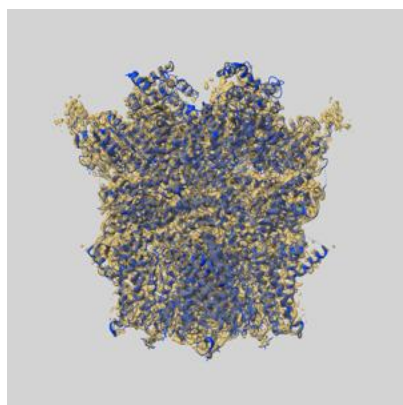
8 Fourier-Shell correlation

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

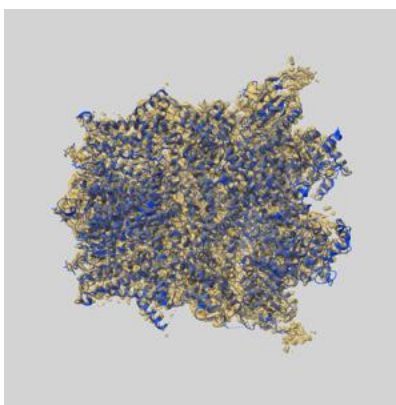
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7542 and PDB model 6CO7. Per-residue inclusion information can be found in section [3](#) on page [11](#).

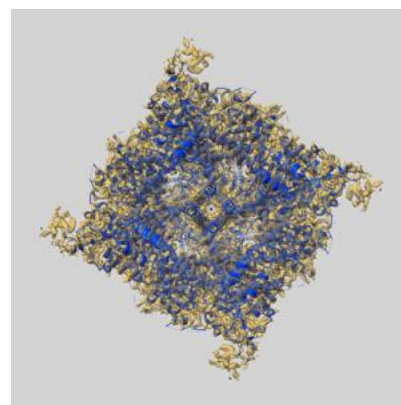
9.1 Map-model overlay [i](#)



X



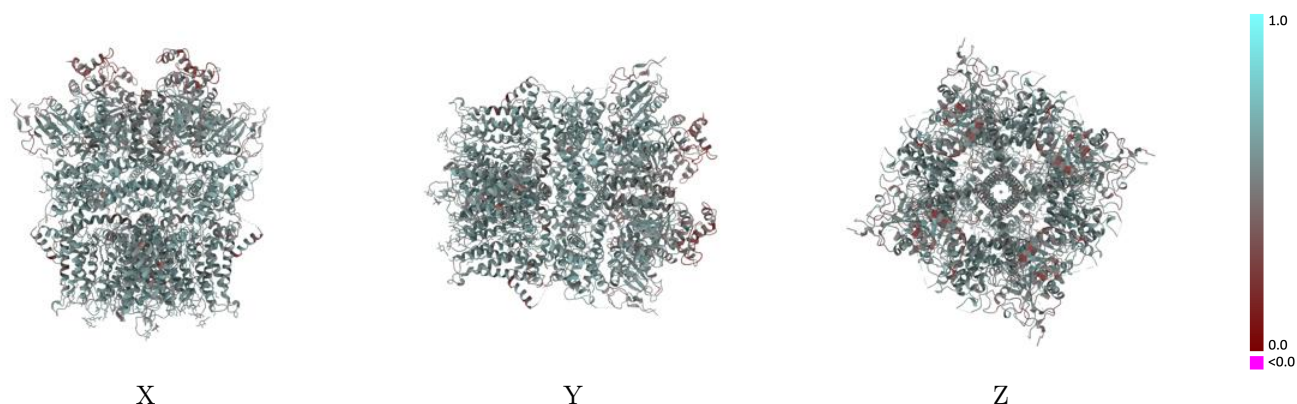
Y



Z

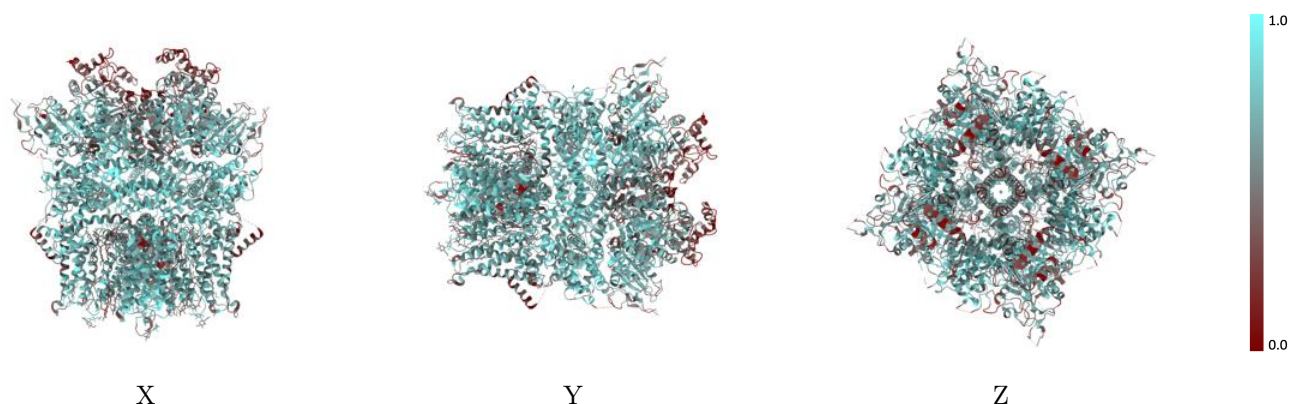
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



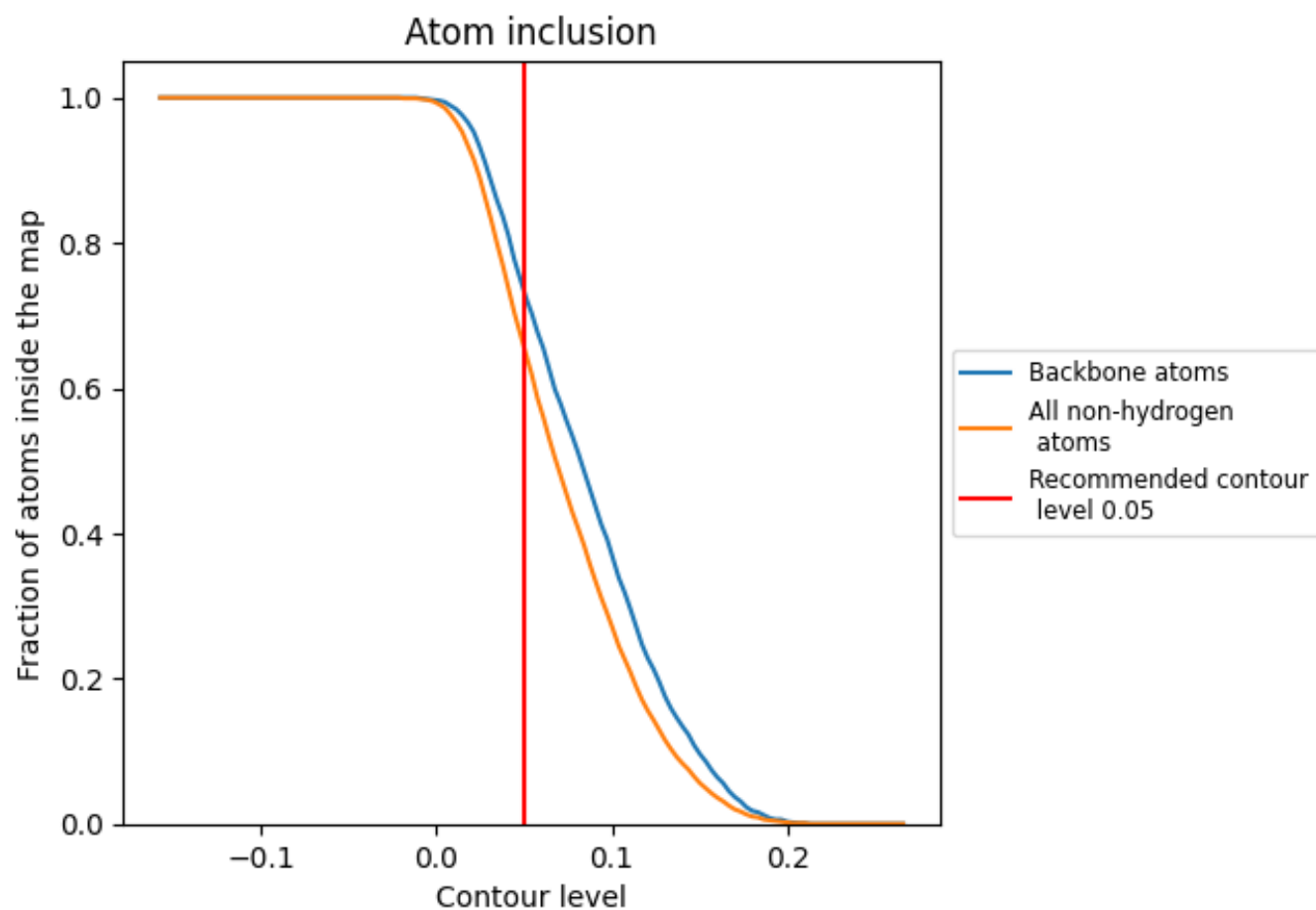
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.6550	0.5380
A	0.6560	0.5390
B	0.6560	0.5380
C	0.6550	0.5380
D	0.6560	0.5390
E	0.5710	0.5350
F	0.5710	0.5350
G	0.5710	0.5290
H	0.5710	0.5300

