



Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 11:41 PM EST

PDB ID : 6V22
EMDB ID : EMD-21025
Title : Cryo-EM structure of Ca²⁺-bound hsSlo1-beta4 channel complex
Authors : Tao, X.; MacKinnon, R.
Deposited on : 2019-11-22
Resolution : 3.20 Å (reported)
Based on initial models : ?, 3MT5, 5TJ6

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 (i) 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 \(1\)](#)) were used in the production of this report:

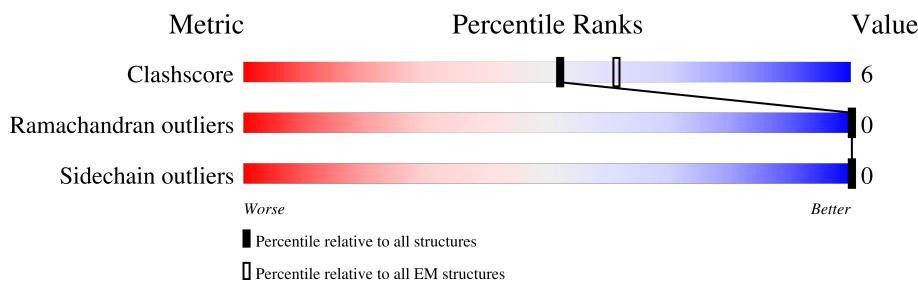
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.20 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 <=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.



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 37004 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	896	Total	C	N	O	S	0	0
			7137	4634	1165	1290	48		
1	B	896	Total	C	N	O	S	0	0
			7137	4634	1165	1290	48		
1	C	896	Total	C	N	O	S	0	0
			7137	4634	1165	1290	48		
1	D	896	Total	C	N	O	S	0	0
			7137	4634	1165	1290	48		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1057	SER	-	expression tag	UNP Q12791
A	1058	ASN	-	expression tag	UNP Q12791
A	1059	SER	-	expression tag	UNP Q12791
A	1060	LEU	-	expression tag	UNP Q12791
A	1061	GLU	-	expression tag	UNP Q12791
A	1062	VAL	-	expression tag	UNP Q12791
A	1063	LEU	-	expression tag	UNP Q12791
A	1064	PHE	-	expression tag	UNP Q12791
A	1065	GLN	-	expression tag	UNP Q12791
B	1057	SER	-	expression tag	UNP Q12791
B	1058	ASN	-	expression tag	UNP Q12791
B	1059	SER	-	expression tag	UNP Q12791
B	1060	LEU	-	expression tag	UNP Q12791
B	1061	GLU	-	expression tag	UNP Q12791
B	1062	VAL	-	expression tag	UNP Q12791
B	1063	LEU	-	expression tag	UNP Q12791
B	1064	PHE	-	expression tag	UNP Q12791
B	1065	GLN	-	expression tag	UNP Q12791
C	1057	SER	-	expression tag	UNP Q12791
C	1058	ASN	-	expression tag	UNP Q12791
C	1059	SER	-	expression tag	UNP Q12791
C	1060	LEU	-	expression tag	UNP Q12791

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1061	GLU	-	expression tag	UNP Q12791
C	1062	VAL	-	expression tag	UNP Q12791
C	1063	LEU	-	expression tag	UNP Q12791
C	1064	PHE	-	expression tag	UNP Q12791
C	1065	GLN	-	expression tag	UNP Q12791
D	1057	SER	-	expression tag	UNP Q12791
D	1058	ASN	-	expression tag	UNP Q12791
D	1059	SER	-	expression tag	UNP Q12791
D	1060	LEU	-	expression tag	UNP Q12791
D	1061	GLU	-	expression tag	UNP Q12791
D	1062	VAL	-	expression tag	UNP Q12791
D	1063	LEU	-	expression tag	UNP Q12791
D	1064	PHE	-	expression tag	UNP Q12791
D	1065	GLN	-	expression tag	UNP Q12791

- Molecule 2 is a protein called Calcium-activated potassium channel subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	199	Total	C	N	O	S		
			1586	1015	263	295	13	0	0
2	F	199	Total	C	N	O	S		
			1586	1015	263	295	13	0	0
2	G	199	Total	C	N	O	S		
			1586	1015	263	295	13	0	0
2	H	199	Total	C	N	O	S		
			1586	1015	263	295	13	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2211	SER	-	expression tag	UNP Q86W47
E	2212	ASN	-	expression tag	UNP Q86W47
E	2213	SER	-	expression tag	UNP Q86W47
E	2214	LEU	-	expression tag	UNP Q86W47
E	2215	GLU	-	expression tag	UNP Q86W47
E	2216	VAL	-	expression tag	UNP Q86W47
E	2217	LEU	-	expression tag	UNP Q86W47
E	2218	PHE	-	expression tag	UNP Q86W47
E	2219	GLN	-	expression tag	UNP Q86W47
F	2211	SER	-	expression tag	UNP Q86W47
F	2212	ASN	-	expression tag	UNP Q86W47
F	2213	SER	-	expression tag	UNP Q86W47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2214	LEU	-	expression tag	UNP Q86W47
F	2215	GLU	-	expression tag	UNP Q86W47
F	2216	VAL	-	expression tag	UNP Q86W47
F	2217	LEU	-	expression tag	UNP Q86W47
F	2218	PHE	-	expression tag	UNP Q86W47
F	2219	GLN	-	expression tag	UNP Q86W47
G	2211	SER	-	expression tag	UNP Q86W47
G	2212	ASN	-	expression tag	UNP Q86W47
G	2213	SER	-	expression tag	UNP Q86W47
G	2214	LEU	-	expression tag	UNP Q86W47
G	2215	GLU	-	expression tag	UNP Q86W47
G	2216	VAL	-	expression tag	UNP Q86W47
G	2217	LEU	-	expression tag	UNP Q86W47
G	2218	PHE	-	expression tag	UNP Q86W47
G	2219	GLN	-	expression tag	UNP Q86W47
H	2211	SER	-	expression tag	UNP Q86W47
H	2212	ASN	-	expression tag	UNP Q86W47
H	2213	SER	-	expression tag	UNP Q86W47
H	2214	LEU	-	expression tag	UNP Q86W47
H	2215	GLU	-	expression tag	UNP Q86W47
H	2216	VAL	-	expression tag	UNP Q86W47
H	2217	LEU	-	expression tag	UNP Q86W47
H	2218	PHE	-	expression tag	UNP Q86W47
H	2219	GLN	-	expression tag	UNP Q86W47

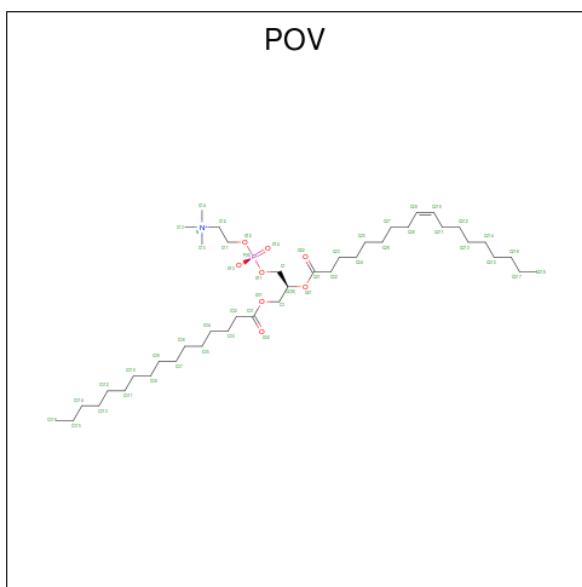
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	D	1	Total Mg 1 1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	

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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	A	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	E	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	E	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	E	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	E	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	B	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	F	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	F	1	Total	C	N	O	P	0
			84	67	1	14	2	

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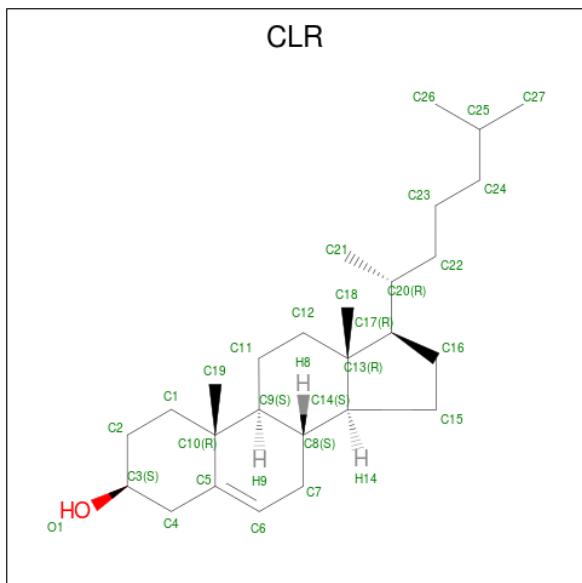
Mol	Chain	Residues	Atoms					AltConf
5	F	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	F	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	C	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	G	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	G	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	G	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	G	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	

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Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	D	1	Total	C	N	O	P	0
			300	224	6	62	8	
5	H	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	H	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	H	1	Total	C	N	O	P	0
			84	67	1	14	2	
5	H	1	Total	C	N	O	P	0
			84	67	1	14	2	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).

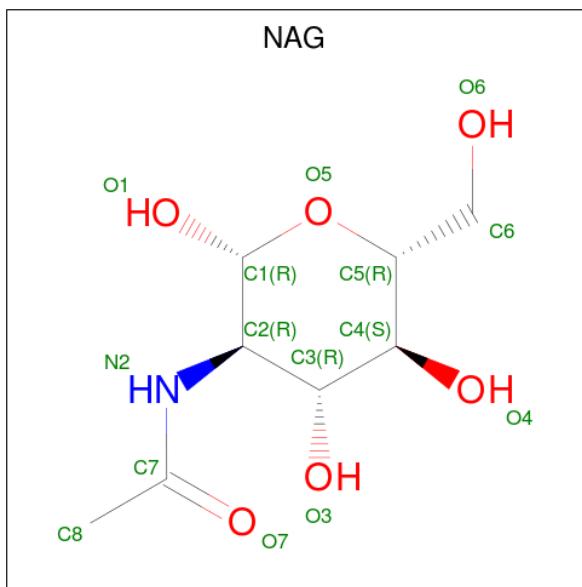


Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 112 108 4	0
6	A	1	Total C O 112 108 4	0
6	A	1	Total C O 112 108 4	0
6	A	1	Total C O 112 108 4	0
6	B	1	Total C O 112 108 4	0
6	B	1	Total C O 112 108 4	0
6	B	1	Total C O 112 108 4	0
6	B	1	Total C O 112 108 4	0
6	C	1	Total C O 112 108 4	0
6	C	1	Total C O 112 108 4	0
6	C	1	Total C O 112 108 4	0
6	C	1	Total C O 112 108 4	0
6	D	1	Total C O 112 108 4	0
6	D	1	Total C O 112 108 4	0
6	D	1	Total C O 112 108 4	0
6	D	1	Total C O 112 108 4	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
7	A	4	Total K 4 4	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

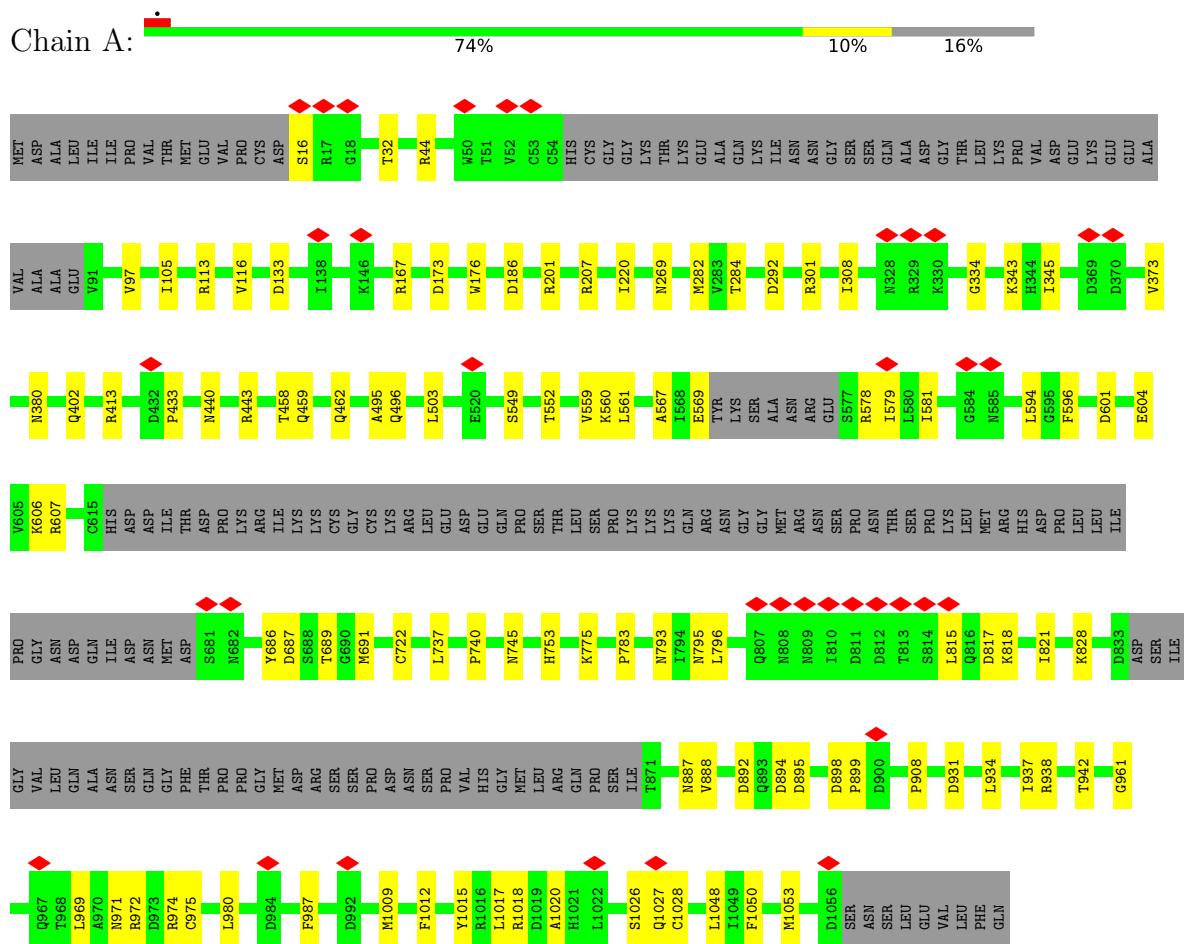


Mol	Chain	Residues	Atoms				AltConf
8	E	1	Total 28	C 16	N 2	O 10	0
8	E	1	Total 28	C 16	N 2	O 10	0
8	F	1	Total 28	C 16	N 2	O 10	0
8	F	1	Total 28	C 16	N 2	O 10	0
8	G	1	Total 28	C 16	N 2	O 10	0
8	G	1	Total 28	C 16	N 2	O 10	0
8	H	1	Total 28	C 16	N 2	O 10	0
8	H	1	Total 28	C 16	N 2	O 10	0

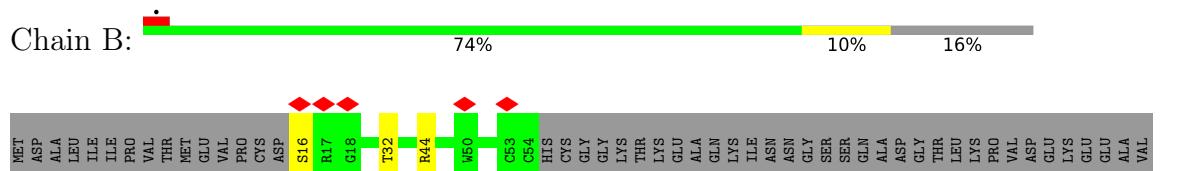
3 Residue-property plots

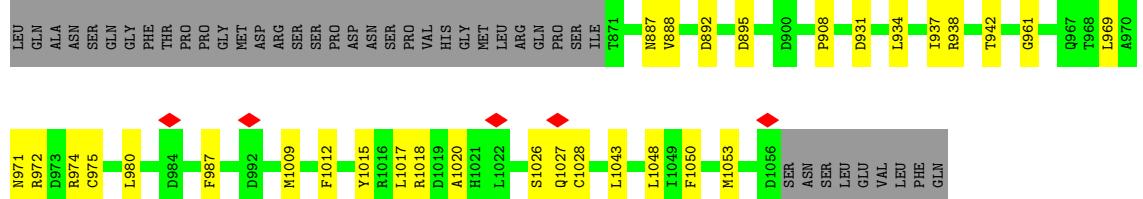
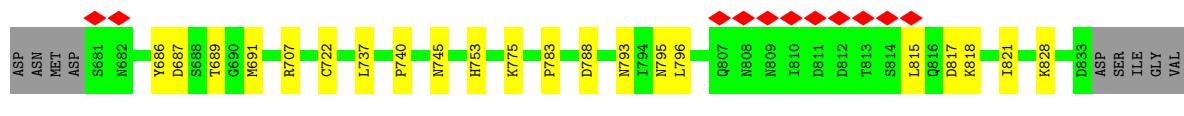
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Calcium-activated potassium channel subunit alpha-1



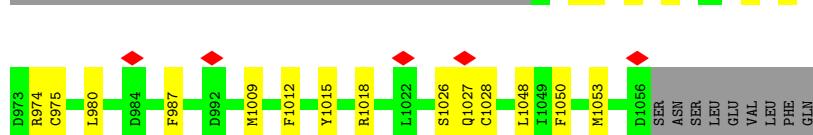
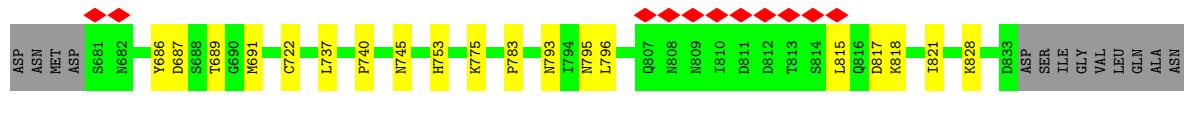
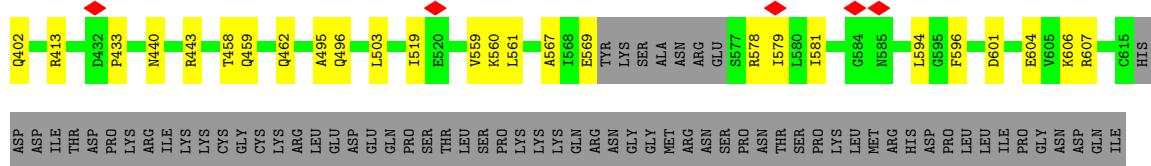
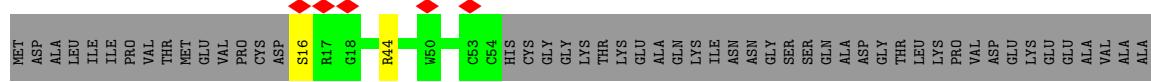
- Molecule 1: Calcium-activated potassium channel subunit alpha-1





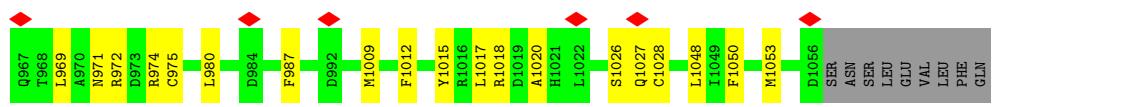
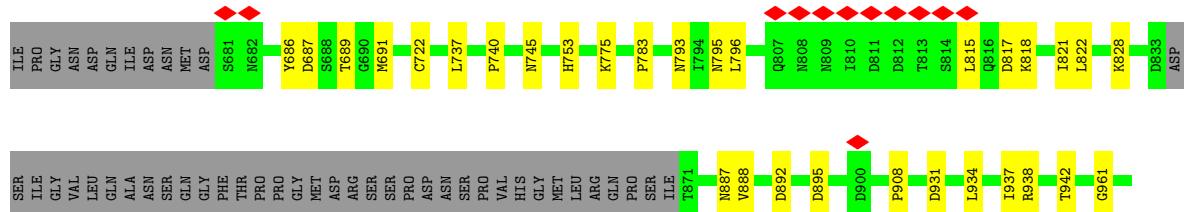
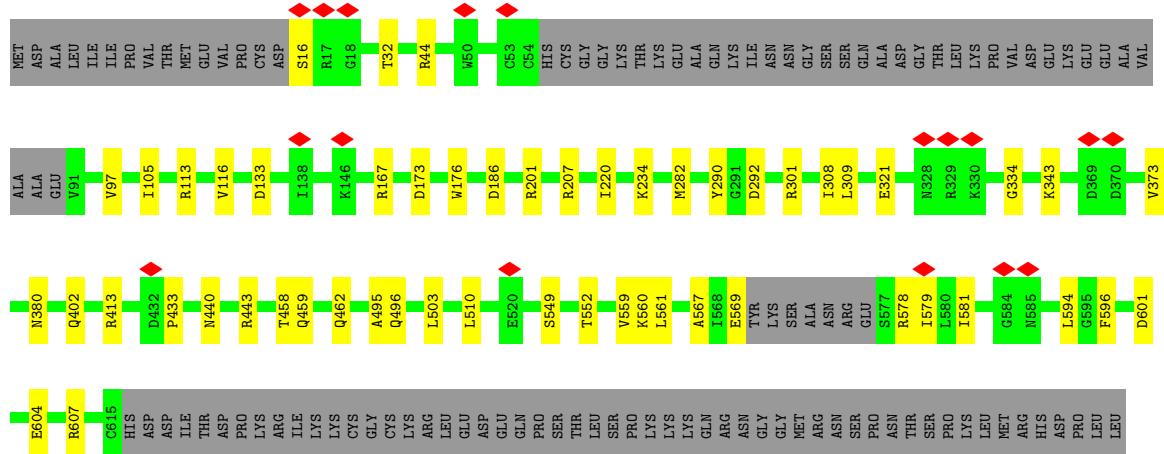
- Molecule 1: Calcium-activated potassium channel subunit alpha-1

Chain C: 75% 9% 16%



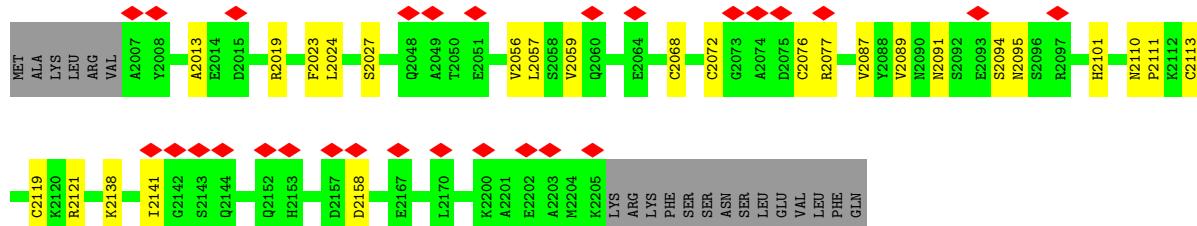
- Molecule 1: Calcium-activated potassium channel subunit alpha-1

Chain D: • 74% 10% 16%



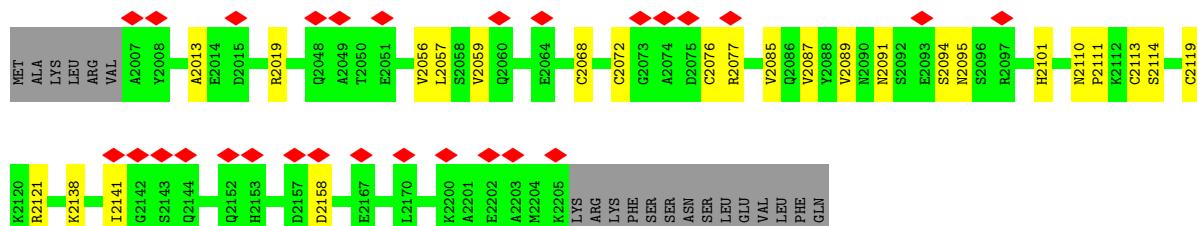
- Molecule 2: Calcium-activated potassium channel subunit beta-4

Chain E: 13% 79% 12% 9%

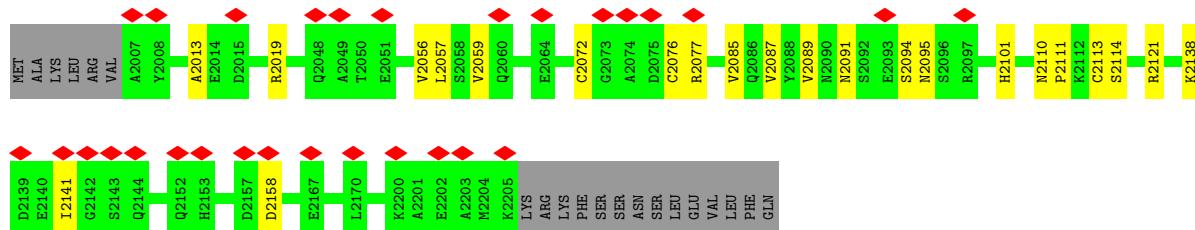


- Molecule 2: Calcium-activated potassium channel subunit beta-4

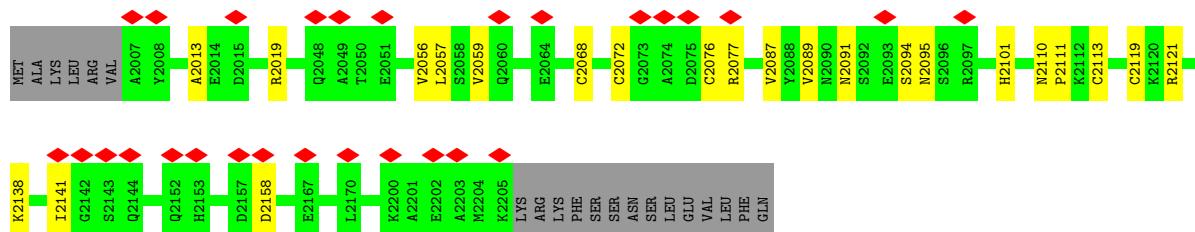
Chain F: 13% 79% 11% 9%



- Molecule 2: Calcium-activated potassium channel subunit beta-4



- Molecule 2: Calcium-activated potassium channel subunit beta-4



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	117791	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 ($e^-/\text{\AA}^2$)	74	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.675	Depositor
Minimum map value	-12.814	Depositor
Average map value	-0.319	Depositor
Map value standard deviation	0.838	Depositor
Recommended contour level	6.19	Depositor
Map size (\AA)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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: CLR, NAG, K, MG, POV, 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	0.40	0/7302	0.50	0/9911
1	B	0.40	0/7302	0.50	0/9911
1	C	0.40	0/7302	0.50	0/9911
1	D	0.40	0/7302	0.50	0/9911
2	E	0.33	0/1624	0.49	0/2211
2	F	0.33	0/1624	0.49	0/2211
2	G	0.33	0/1624	0.49	0/2211
2	H	0.33	0/1624	0.49	0/2211
All	All	0.39	0/35704	0.50	0/48488

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7137	0	7131	69	0
1	B	7137	0	7131	67	0
1	C	7137	0	7131	64	0
1	D	7137	0	7131	67	0
2	E	1586	0	1543	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1586	0	1543	18	0
2	G	1586	0	1543	16	0
2	H	1586	0	1543	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	300	0	378	8	0
5	B	300	0	378	9	0
5	C	300	0	378	8	0
5	D	300	0	378	10	0
5	E	84	0	116	0	0
5	F	84	0	116	0	0
5	G	84	0	116	0	0
5	H	84	0	116	0	0
6	A	112	0	173	24	0
6	B	112	0	173	23	0
6	C	112	0	173	22	0
6	D	112	0	173	24	0
7	A	4	0	0	0	0
8	E	28	0	26	0	0
8	F	28	0	26	0	0
8	G	28	0	26	0	0
8	H	28	0	26	0	0
All	All	37004	0	37468	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (426) 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)
6:C:1115:CLR:C16	6:C:1115:CLR:C17	1.75	1.57
6:D:1115:CLR:C17	6:D:1115:CLR:C16	1.75	1.56
6:A:1111:CLR:C17	6:A:1111:CLR:C16	1.74	1.56
6:B:1118:CLR:C16	6:B:1118:CLR:C17	1.75	1.56
6:B:1115:CLR:C16	6:B:1115:CLR:C17	1.75	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1110:CLR:C16	6:A:1110:CLR:C17	1.75	1.54
6:A:1113:CLR:C16	6:A:1113:CLR:C17	1.75	1.54
6:B:1117:CLR:C17	6:B:1117:CLR:C16	1.75	1.54
6:A:1112:CLR:C16	6:A:1112:CLR:C17	1.75	1.53
6:D:1118:CLR:C16	6:D:1118:CLR:C17	1.75	1.53
6:C:1116:CLR:C17	6:C:1116:CLR:C16	1.74	1.52
6:B:1116:CLR:C16	6:B:1116:CLR:C17	1.74	1.51
6:C:1117:CLR:C16	6:C:1117:CLR:C17	1.75	1.50
6:D:1116:CLR:C16	6:D:1116:CLR:C17	1.74	1.47
6:C:1118:CLR:C16	6:C:1118:CLR:C17	1.75	1.46
6:D:1117:CLR:C16	6:D:1117:CLR:C17	1.75	1.45
6:A:1113:CLR:H221	6:A:1113:CLR:H162	1.59	0.84
6:B:1118:CLR:H221	6:B:1118:CLR:H162	1.60	0.83
6:C:1118:CLR:H221	6:C:1118:CLR:H162	1.60	0.81
6:D:1118:CLR:H162	6:D:1118:CLR:H221	1.60	0.81
6:D:1117:CLR:C16	6:D:1117:CLR:C20	2.60	0.78
6:A:1110:CLR:C16	6:A:1110:CLR:C20	2.60	0.78
6:B:1117:CLR:C16	6:B:1117:CLR:C20	2.60	0.77
6:C:1118:CLR:C16	6:C:1118:CLR:C20	2.61	0.77
6:B:1115:CLR:C16	6:B:1115:CLR:C20	2.60	0.77
6:C:1115:CLR:C16	6:C:1115:CLR:C20	2.60	0.77
6:D:1118:CLR:C16	6:D:1118:CLR:C20	2.61	0.77
6:B:1118:CLR:C16	6:B:1118:CLR:C20	2.61	0.76
6:D:1115:CLR:C16	6:D:1115:CLR:C20	2.60	0.76
6:C:1117:CLR:C16	6:C:1117:CLR:C20	2.60	0.76
6:A:1113:CLR:C16	6:A:1113:CLR:C20	2.61	0.76
6:A:1112:CLR:C16	6:A:1112:CLR:C20	2.60	0.75
6:A:1111:CLR:C16	6:A:1111:CLR:C20	2.64	0.73
6:C:1116:CLR:C16	6:C:1116:CLR:C20	2.64	0.72
6:D:1116:CLR:C16	6:D:1116:CLR:C20	2.64	0.70
2:E:2072:CYS:H	2:E:2076:CYS:HB2	1.59	0.68
2:H:2072:CYS:H	2:H:2076:CYS:HB2	1.59	0.68
2:F:2072:CYS:H	2:F:2076:CYS:HB2	1.59	0.67
2:G:2072:CYS:H	2:G:2076:CYS:HB2	1.59	0.66
6:B:1116:CLR:C16	6:B:1116:CLR:C20	2.64	0.65
6:D:1118:CLR:C16	6:D:1118:CLR:H221	2.25	0.65
6:C:1118:CLR:C16	6:C:1118:CLR:H221	2.25	0.65
6:A:1113:CLR:C16	6:A:1113:CLR:H221	2.25	0.64
6:B:1118:CLR:C16	6:B:1118:CLR:H221	2.25	0.64
6:A:1110:CLR:C16	6:A:1110:CLR:H222	2.28	0.64
6:D:1115:CLR:C16	6:D:1115:CLR:H222	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1115:CLR:C16	6:C:1115:CLR:H222	2.28	0.64
6:B:1115:CLR:C16	6:B:1115:CLR:H222	2.28	0.63
6:D:1115:CLR:H222	6:D:1115:CLR:H162	1.82	0.62
6:B:1115:CLR:H222	6:B:1115:CLR:H162	1.82	0.62
6:A:1110:CLR:H222	6:A:1110:CLR:H162	1.82	0.61
1:A:402:GLN:O	1:A:413:ARG:NH2	2.33	0.61
1:B:308:ILE:HD11	1:C:282:MET:HG3	1.82	0.61
1:C:308:ILE:HD11	1:D:282:MET:HG3	1.82	0.61
6:C:1115:CLR:H222	6:C:1115:CLR:H162	1.82	0.61
6:D:1117:CLR:H162	6:D:1117:CLR:H222	1.83	0.61
1:C:402:GLN:O	1:C:413:ARG:NH2	2.33	0.60
1:A:282:MET:HG3	1:D:308:ILE:HD11	1.82	0.60
2:F:2110:ASN:ND2	2:F:2113:CYS:SG	2.75	0.60
2:E:2110:ASN:ND2	2:E:2113:CYS:SG	2.75	0.60
6:A:1112:CLR:H222	6:A:1112:CLR:H162	1.83	0.60
2:G:2110:ASN:ND2	2:G:2113:CYS:SG	2.75	0.60
1:D:402:GLN:O	1:D:413:ARG:NH2	2.33	0.59
2:H:2110:ASN:ND2	2:H:2113:CYS:SG	2.75	0.59
1:A:308:ILE:HD11	1:B:282:MET:HG3	1.83	0.59
6:C:1117:CLR:H222	6:C:1117:CLR:H162	1.83	0.59
6:B:1117:CLR:H222	6:B:1117:CLR:H162	1.83	0.59
1:B:402:GLN:O	1:B:413:ARG:NH2	2.33	0.59
1:B:745:ASN:ND2	1:B:975:CYS:O	2.37	0.58
1:D:16:SER:O	1:D:201:ARG:NH2	2.37	0.58
1:C:578:ARG:HH21	1:C:579:ILE:HG22	1.69	0.57
1:C:745:ASN:ND2	1:C:975:CYS:O	2.37	0.57
1:A:745:ASN:ND2	1:A:975:CYS:O	2.37	0.57
1:A:931:ASP:OD2	1:A:931:ASP:N	2.38	0.57
6:A:1112:CLR:C16	6:A:1112:CLR:C22	2.83	0.57
1:D:578:ARG:HH21	1:D:579:ILE:HG22	1.69	0.57
1:D:745:ASN:ND2	1:D:975:CYS:O	2.37	0.57
6:C:1117:CLR:C16	6:C:1117:CLR:C22	2.83	0.57
1:A:578:ARG:HH21	1:A:579:ILE:HG22	1.70	0.57
1:A:691:MET:SD	1:A:974:ARG:NE	2.78	0.57
1:B:578:ARG:HH21	1:B:579:ILE:HG22	1.69	0.57
6:B:1115:CLR:C16	6:B:1115:CLR:C22	2.83	0.57
6:D:1115:CLR:C16	6:D:1115:CLR:C22	2.83	0.57
6:B:1117:CLR:C16	6:B:1117:CLR:C22	2.83	0.57
1:A:16:SER:O	1:A:201:ARG:NH2	2.37	0.56
1:B:691:MET:SD	1:B:974:ARG:NE	2.78	0.56
1:D:691:MET:SD	1:D:974:ARG:NE	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:SER:O	1:C:201:ARG:NH2	2.37	0.56
6:C:1118:CLR:C16	6:C:1118:CLR:C22	2.84	0.56
6:D:1117:CLR:C16	6:D:1117:CLR:C22	2.83	0.56
6:A:1110:CLR:C16	6:A:1110:CLR:C22	2.83	0.56
1:C:691:MET:SD	1:C:974:ARG:NE	2.78	0.56
6:D:1118:CLR:C16	6:D:1118:CLR:C22	2.84	0.56
6:C:1115:CLR:C16	6:C:1115:CLR:C22	2.83	0.56
6:A:1111:CLR:C16	6:A:1111:CLR:C22	2.84	0.56
6:A:1113:CLR:C16	6:A:1113:CLR:C22	2.84	0.56
6:B:1116:CLR:C16	6:B:1116:CLR:C22	2.84	0.55
1:C:931:ASP:N	1:C:931:ASP:OD2	2.38	0.55
6:C:1116:CLR:C16	6:C:1116:CLR:C22	2.84	0.55
1:C:817:ASP:OD1	1:C:887:ASN:ND2	2.39	0.55
1:A:561:LEU:O	1:A:607:ARG:NH2	2.40	0.55
5:D:1104:POV:H15A	5:D:1105:POV:H1	1.87	0.55
6:D:1116:CLR:C16	6:D:1116:CLR:C22	2.84	0.55
1:B:16:SER:O	1:B:201:ARG:NH2	2.37	0.55
6:B:1118:CLR:C16	6:B:1118:CLR:C22	2.84	0.55
5:C:1104:POV:H15A	5:C:1105:POV:H1	1.87	0.55
1:D:1009:MET:HG2	1:D:1053:MET:HA	1.89	0.55
5:A:1121:POV:H15A	5:A:1122:POV:H1	1.87	0.54
1:B:561:LEU:O	1:B:607:ARG:NH2	2.40	0.54
1:A:1009:MET:HG2	1:A:1053:MET:HA	1.89	0.54
1:D:561:LEU:O	1:D:607:ARG:NH2	2.40	0.54
5:B:1104:POV:H15A	5:B:1105:POV:H1	1.87	0.54
1:C:561:LEU:O	1:C:607:ARG:NH2	2.40	0.54
1:A:689:THR:O	1:A:971:ASN:ND2	2.41	0.54
1:A:938:ARG:O	1:A:942:THR:OG1	2.26	0.54
1:C:1009:MET:HG2	1:C:1053:MET:HA	1.89	0.54
1:D:689:THR:O	1:D:971:ASN:ND2	2.41	0.54
1:B:689:THR:O	1:B:971:ASN:ND2	2.41	0.54
1:B:817:ASP:OD1	1:B:887:ASN:ND2	2.40	0.54
1:D:938:ARG:O	1:D:942:THR:OG1	2.26	0.54
1:B:284:THR:HG1	1:C:290:TYR:HH	1.56	0.54
2:E:2091:ASN:O	2:E:2095:ASN:ND2	2.41	0.54
1:B:931:ASP:OD2	1:B:931:ASP:N	2.38	0.54
1:B:1009:MET:HG2	1:B:1053:MET:HA	1.89	0.53
1:A:1015:TYR:HB3	1:A:1048:LEU:HB2	1.91	0.53
2:F:2091:ASN:O	2:F:2095:ASN:ND2	2.41	0.53
1:A:817:ASP:OD1	1:A:887:ASN:ND2	2.39	0.53
1:D:1015:TYR:HB3	1:D:1048:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2091:ASN:O	2:G:2095:ASN:ND2	2.41	0.53
1:D:292:ASP:N	1:D:292:ASP:OD1	2.42	0.53
1:D:753:HIS:HD1	1:D:775:LYS:HB3	1.74	0.53
1:B:938:ARG:O	1:B:942:THR:OG1	2.26	0.53
1:B:1015:TYR:HB3	1:B:1048:LEU:HB2	1.91	0.53
1:C:689:THR:O	1:C:971:ASN:ND2	2.41	0.53
1:D:817:ASP:OD1	1:D:887:ASN:ND2	2.40	0.53
2:H:2091:ASN:O	2:H:2095:ASN:ND2	2.41	0.53
1:D:1026:SER:OG	1:D:1027:GLN:N	2.42	0.52
1:B:1026:SER:OG	1:B:1027:GLN:N	2.42	0.52
1:C:828:LYS:NZ	1:C:892:ASP:OD1	2.43	0.52
1:A:686:TYR:OH	1:A:972:ARG:NH1	2.43	0.52
1:B:828:LYS:NZ	1:B:892:ASP:OD1	2.43	0.52
1:C:753:HIS:HD1	1:C:775:LYS:HB3	1.74	0.52
1:C:97:VAL:HG23	6:C:1115:CLR:H183	1.91	0.52
1:C:567:ALA:HB3	1:C:596:PHE:HD2	1.75	0.52
1:A:753:HIS:HD1	1:A:775:LYS:HB3	1.74	0.52
1:C:1015:TYR:HB3	1:C:1048:LEU:HB2	1.91	0.52
1:D:97:VAL:HG23	6:D:1115:CLR:H183	1.90	0.52
1:D:686:TYR:OH	1:D:972:ARG:NH1	2.43	0.52
1:B:686:TYR:OH	1:B:972:ARG:NH1	2.43	0.52
1:C:567:ALA:HB2	1:C:581:ILE:HG23	1.92	0.52
1:C:938:ARG:O	1:C:942:THR:OG1	2.26	0.52
1:A:97:VAL:HG23	6:A:1110:CLR:H183	1.91	0.52
1:A:292:ASP:OD1	1:A:292:ASP:N	2.42	0.52
1:C:292:ASP:OD1	1:C:292:ASP:N	2.42	0.52
1:C:686:TYR:OH	1:C:972:ARG:NH1	2.43	0.52
1:A:691:MET:O	1:A:974:ARG:NH2	2.44	0.51
1:A:1026:SER:OG	1:A:1027:GLN:N	2.42	0.51
1:C:1026:SER:OG	1:C:1027:GLN:N	2.42	0.51
1:D:691:MET:O	1:D:974:ARG:NH2	2.44	0.51
1:A:334:GLY:O	1:A:413:ARG:NH1	2.42	0.51
1:B:567:ALA:HB3	1:B:596:PHE:HD2	1.75	0.51
1:D:567:ALA:HB2	1:D:581:ILE:HG23	1.92	0.51
1:B:753:HIS:HD1	1:B:775:LYS:HB3	1.74	0.51
1:D:334:GLY:O	1:D:413:ARG:NH1	2.42	0.51
1:B:133:ASP:OD2	1:B:207:ARG:NH1	2.44	0.51
1:D:828:LYS:NZ	1:D:892:ASP:OD1	2.43	0.51
1:A:567:ALA:HB2	1:A:581:ILE:HG23	1.92	0.51
1:A:567:ALA:HB3	1:A:596:PHE:HD2	1.75	0.51
1:B:97:VAL:HG23	6:B:1115:CLR:H183	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:CYS:HB3	1:C:783:PRO:HB3	1.93	0.51
1:C:133:ASP:OD2	1:C:207:ARG:NH1	2.44	0.51
1:D:722:CYS:HB3	1:D:783:PRO:HB3	1.93	0.51
1:D:567:ALA:HB3	1:D:596:PHE:HD2	1.75	0.51
1:D:795:ASN:N	1:D:795:ASN:OD1	2.44	0.51
1:A:722:CYS:HB3	1:A:783:PRO:HB3	1.93	0.50
1:A:828:LYS:NZ	1:A:892:ASP:OD1	2.43	0.50
6:A:1113:CLR:H162	6:A:1113:CLR:C22	2.39	0.50
1:B:292:ASP:OD1	1:B:292:ASP:N	2.42	0.50
1:C:691:MET:O	1:C:974:ARG:NH2	2.44	0.50
1:C:795:ASN:OD1	1:C:795:ASN:N	2.44	0.50
1:A:895:ASP:OD1	1:A:895:ASP:N	2.44	0.50
2:E:2019:ARG:NH2	5:B:1104:POV:O13	2.41	0.50
1:B:691:MET:O	1:B:974:ARG:NH2	2.44	0.50
1:A:1018:ARG:NH2	1:A:1028:CYS:SG	2.85	0.50
1:D:133:ASP:OD2	1:D:207:ARG:NH1	2.44	0.50
1:B:1018:ARG:NH2	1:B:1028:CYS:SG	2.85	0.50
1:A:44:ARG:HH21	6:A:1111:CLR:H193	1.77	0.50
1:C:334:GLY:O	1:C:413:ARG:NH1	2.42	0.50
1:B:567:ALA:HB2	1:B:581:ILE:HG23	1.92	0.49
1:B:722:CYS:HB3	1:B:783:PRO:HB3	1.93	0.49
1:B:969:LEU:HD13	1:B:972:ARG:HD3	1.94	0.49
6:B:1115:CLR:H162	6:B:1115:CLR:C22	2.43	0.49
1:B:334:GLY:O	1:B:413:ARG:NH1	2.42	0.49
1:C:969:LEU:HD13	1:C:972:ARG:HD3	1.94	0.49
1:A:133:ASP:OD2	1:A:207:ARG:NH1	2.44	0.49
1:C:1018:ARG:NH2	1:C:1028:CYS:SG	2.85	0.49
2:G:2019:ARG:NH2	5:D:1104:POV:O13	2.41	0.49
1:C:895:ASP:OD1	1:C:895:ASP:N	2.44	0.49
1:A:687:ASP:HA	1:A:961:GLY:HA2	1.94	0.49
1:C:687:ASP:HA	1:C:961:GLY:HA2	1.94	0.49
1:D:44:ARG:HH21	6:D:1116:CLR:H193	1.77	0.49
1:D:1018:ARG:NH2	1:D:1028:CYS:SG	2.85	0.49
6:C:1115:CLR:H162	6:C:1115:CLR:C22	2.43	0.49
2:H:2091:ASN:HB3	2:H:2095:ASN:H	1.77	0.49
1:A:969:LEU:HD13	1:A:972:ARG:HD3	1.94	0.49
6:A:1110:CLR:H162	6:A:1110:CLR:C22	2.42	0.49
1:C:44:ARG:HH21	6:C:1116:CLR:H193	1.77	0.49
2:G:2091:ASN:HB3	2:G:2095:ASN:H	1.77	0.49
1:D:687:ASP:HA	1:D:961:GLY:HA2	1.94	0.49
1:A:569:GLU:HB3	1:A:594:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:NH2	1:B:173:ASP:OD1	2.34	0.48
1:B:44:ARG:HH21	6:B:1116:CLR:H193	1.77	0.48
1:D:931:ASP:OD2	1:D:931:ASP:N	2.38	0.48
1:D:969:LEU:HD13	1:D:972:ARG:HD3	1.94	0.48
2:G:2057:LEU:H	2:G:2089:VAL:HA	1.79	0.48
6:D:1115:CLR:H162	6:D:1115:CLR:C22	2.43	0.48
2:F:2057:LEU:H	2:F:2089:VAL:HA	1.79	0.48
1:A:821:ILE:HD11	1:A:887:ASN:HB3	1.96	0.47
1:B:687:ASP:HA	1:B:961:GLY:HA2	1.94	0.47
1:D:569:GLU:HB3	1:D:594:LEU:HB2	1.95	0.47
1:B:821:ILE:HD11	1:B:887:ASN:HB3	1.96	0.47
1:A:980:LEU:HD13	1:A:987:PHE:HZ	1.79	0.47
1:C:173:ASP:HB3	1:C:176:TRP:HB3	1.96	0.47
2:H:2057:LEU:H	2:H:2089:VAL:HA	1.79	0.47
1:C:821:ILE:HD11	1:C:887:ASN:HB3	1.96	0.47
1:D:821:ILE:HD11	1:D:887:ASN:HB3	1.96	0.47
1:A:894:ASP:OD1	1:A:894:ASP:N	2.41	0.47
1:C:980:LEU:HD13	1:C:987:PHE:HZ	1.79	0.47
2:E:2091:ASN:HB3	2:E:2095:ASN:H	1.77	0.47
1:A:173:ASP:HB3	1:A:176:TRP:HB3	1.96	0.47
1:A:815:LEU:HB2	1:A:818:LYS:HB2	1.97	0.47
2:F:2068:CYS:HB2	2:F:2119:CYS:HB2	1.79	0.47
2:F:2091:ASN:HB3	2:F:2095:ASN:H	1.77	0.47
1:C:569:GLU:HB3	1:C:594:LEU:HB2	1.95	0.47
1:D:173:ASP:HB3	1:D:176:TRP:HB3	1.96	0.47
1:D:815:LEU:HB2	1:D:818:LYS:HB2	1.97	0.47
1:B:980:LEU:HD13	1:B:987:PHE:HZ	1.79	0.47
1:C:496:GLN:HB3	1:C:503:LEU:HD23	1.96	0.47
2:G:2091:ASN:HD22	2:G:2094:SER:H	1.63	0.47
1:D:895:ASP:N	1:D:895:ASP:OD1	2.44	0.47
2:E:2091:ASN:HD22	2:E:2094:SER:H	1.63	0.47
1:B:173:ASP:HB3	1:B:176:TRP:HB3	1.96	0.47
2:F:2111:PRO:O	2:G:2121:ARG:NH2	2.48	0.47
2:G:2101:HIS:NE2	2:G:2158:ASP:OD1	2.48	0.47
2:E:2057:LEU:H	2:E:2089:VAL:HA	1.79	0.47
1:B:895:ASP:N	1:B:895:ASP:OD1	2.44	0.47
2:E:2059:VAL:HG22	2:E:2087:VAL:HG22	1.97	0.46
2:H:2059:VAL:HG22	2:H:2087:VAL:HG22	1.97	0.46
1:A:496:GLN:HB3	1:A:503:LEU:HD23	1.96	0.46
1:B:495:ALA:HB2	1:B:737:LEU:HD12	1.97	0.46
2:G:2059:VAL:HG22	2:G:2087:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2091:ASN:HD22	2:H:2094:SER:H	1.63	0.46
2:F:2059:VAL:HG22	2:F:2087:VAL:HG22	1.97	0.46
2:F:2091:ASN:HD22	2:F:2094:SER:H	1.63	0.46
1:C:495:ALA:HB2	1:C:737:LEU:HD12	1.97	0.46
1:D:496:GLN:HB3	1:D:503:LEU:HD23	1.96	0.46
1:B:496:GLN:HB3	1:B:503:LEU:HD23	1.96	0.46
2:F:2019:ARG:NH2	5:C:1104:POV:O13	2.41	0.46
1:D:380:ASN:N	1:D:380:ASN:OD1	2.49	0.46
1:B:569:GLU:HB3	1:B:594:LEU:HB2	1.95	0.46
2:G:2111:PRO:O	2:H:2121:ARG:NH2	2.48	0.46
1:D:980:LEU:HD13	1:D:987:PHE:HZ	1.79	0.46
1:A:795:ASN:OD1	1:A:795:ASN:N	2.44	0.46
2:E:2111:PRO:O	2:F:2121:ARG:NH2	2.49	0.46
2:E:2121:ARG:NH2	2:H:2111:PRO:O	2.48	0.46
2:F:2085:VAL:O	2:F:2114:SER:OG	2.32	0.46
1:D:495:ALA:HB2	1:D:737:LEU:HD12	1.97	0.46
2:H:2101:HIS:NE2	2:H:2158:ASP:OD1	2.48	0.46
1:B:815:LEU:HB2	1:B:818:LYS:HB2	1.97	0.46
1:D:44:ARG:NH2	1:D:173:ASP:OD1	2.34	0.46
1:A:495:ALA:HB2	1:A:737:LEU:HD12	1.97	0.46
2:E:2101:HIS:NE2	2:E:2158:ASP:OD1	2.48	0.46
1:B:433:PRO:HB2	1:B:462:GLN:HE22	1.81	0.45
2:F:2101:HIS:NE2	2:F:2158:ASP:OD1	2.48	0.45
1:B:380:ASN:OD1	1:B:380:ASN:N	2.49	0.45
1:C:815:LEU:HB2	1:C:818:LYS:HB2	1.97	0.45
1:A:440:ASN:OD1	1:A:443:ARG:NH1	2.50	0.45
5:A:1121:POV:O13	2:H:2019:ARG:NH2	2.41	0.45
1:D:433:PRO:HB2	1:D:462:GLN:HE22	1.81	0.45
5:D:1111:POV:HG2A	5:D:1111:POV:H3	1.81	0.45
1:A:888:VAL:HG22	1:A:908:PRO:HG2	1.99	0.45
1:C:440:ASN:OD1	1:C:443:ARG:NH1	2.50	0.45
1:B:440:ASN:OD1	1:B:443:ARG:NH1	2.50	0.44
1:B:888:VAL:HG22	1:B:908:PRO:HG2	1.99	0.44
1:C:433:PRO:HB2	1:C:462:GLN:HE22	1.81	0.44
2:G:2085:VAL:O	2:G:2114:SER:OG	2.32	0.44
1:D:888:VAL:HG22	1:D:908:PRO:HG2	1.99	0.44
1:B:795:ASN:N	1:B:795:ASN:OD1	2.44	0.44
2:H:2138:LYS:HA	2:H:2138:LYS:HD2	1.77	0.44
5:C:1109:POV:H34	5:C:1109:POV:H37	1.81	0.44
1:C:380:ASN:OD1	1:C:380:ASN:N	2.49	0.44
1:C:888:VAL:HG22	1:C:908:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HB2	1:A:462:GLN:HE22	1.81	0.44
1:D:440:ASN:OD1	1:D:443:ARG:NH1	2.50	0.44
1:A:301:ARG:HD2	5:B:1101:POV:H33	2.00	0.44
1:A:559:VAL:HG23	1:A:560:LYS:HG2	2.00	0.44
1:A:606:LYS:HA	1:A:606:LYS:HD3	1.79	0.44
1:A:740:PRO:HG3	1:A:942:THR:HA	2.00	0.44
5:A:1118:POV:H33	1:D:301:ARG:HD2	2.00	0.44
1:D:176:TRP:HB2	2:H:2013:ALA:HB2	2.00	0.44
1:C:284:THR:OG1	1:D:290:TYR:OH	2.29	0.44
5:C:1111:POV:H32A	5:C:1111:POV:H3	1.81	0.44
1:D:740:PRO:HG3	1:D:942:THR:HA	2.00	0.44
1:B:559:VAL:HG23	1:B:560:LYS:HG2	2.00	0.44
1:C:301:ARG:HD2	5:D:1101:POV:H33	2.00	0.44
1:A:176:TRP:HB2	2:E:2013:ALA:HB2	1.99	0.44
6:B:1118:CLR:H162	6:B:1118:CLR:C22	2.39	0.44
1:A:601:ASP:HB3	1:A:604:GLU:HG2	2.00	0.43
1:B:301:ARG:HD2	5:C:1101:POV:H33	2.00	0.43
1:B:116:VAL:HG13	1:B:220:ILE:HB	2.01	0.43
1:B:707:ARG:NE	1:B:788:ASP:OD1	2.43	0.43
1:B:740:PRO:HG3	1:B:942:THR:HA	2.00	0.43
2:G:2056:VAL:HG13	2:G:2141:ILE:HD12	2.00	0.43
1:D:601:ASP:HB3	1:D:604:GLU:HG2	2.00	0.43
2:H:2056:VAL:HG13	2:H:2141:ILE:HD12	2.00	0.43
1:B:176:TRP:HB2	2:F:2013:ALA:HB2	2.00	0.43
1:D:234:LYS:NZ	1:D:321:GLU:OE2	2.41	0.43
1:A:32:THR:HA	6:A:1112:CLR:H262	1.96	0.43
1:A:116:VAL:HG13	1:A:220:ILE:HB	2.01	0.43
1:A:818:LYS:HE3	1:A:818:LYS:HB3	1.85	0.43
1:B:32:THR:HA	6:B:1117:CLR:H262	1.96	0.43
1:D:559:VAL:HG23	1:D:560:LYS:HG2	2.00	0.43
2:H:2068:CYS:HB2	2:H:2119:CYS:HB2	1.79	0.43
1:A:934:LEU:HA	1:A:937:ILE:HD12	2.00	0.43
1:C:559:VAL:HG23	1:C:560:LYS:HG2	2.00	0.43
1:C:740:PRO:HG3	1:C:942:THR:HA	2.00	0.43
1:A:380:ASN:OD1	1:A:380:ASN:N	2.49	0.43
1:C:176:TRP:HB2	2:G:2013:ALA:HB2	1.99	0.43
1:D:113:ARG:HH11	5:D:1110:POV:H32	1.84	0.43
1:D:116:VAL:HG13	1:D:220:ILE:HB	2.01	0.43
2:E:2056:VAL:HG13	2:E:2141:ILE:HD12	2.00	0.43
2:F:2056:VAL:HG13	2:F:2141:ILE:HD12	2.00	0.43
1:C:601:ASP:HB3	1:C:604:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:934:LEU:HA	1:C:937:ILE:HD12	2.00	0.43
5:D:1109:POV:H34	5:D:1109:POV:H37	1.81	0.43
1:B:1012:PHE:HD2	1:B:1050:PHE:HB3	1.84	0.42
1:C:116:VAL:HG13	1:C:220:ILE:HB	2.01	0.42
1:A:113:ARG:HH11	5:A:1105:POV:H32	1.84	0.42
1:A:458:THR:OG1	1:A:459:GLN:N	2.52	0.42
1:B:601:ASP:HB3	1:B:604:GLU:HG2	2.00	0.42
5:B:1109:POV:H37	5:B:1109:POV:H34	1.81	0.42
6:C:1115:CLR:H272	6:C:1115:CLR:H232	1.87	0.42
5:D:1103:POV:H32	5:D:1103:POV:H3A	1.92	0.42
2:H:2076:CYS:O	2:H:2077:ARG:NE	2.52	0.42
1:A:793:ASN:HB3	1:A:796:LEU:HD12	2.01	0.42
1:B:269:ASN:OD1	1:B:269:ASN:N	2.51	0.42
1:B:793:ASN:HB3	1:B:796:LEU:HD12	2.00	0.42
1:B:934:LEU:HA	1:B:937:ILE:HD12	2.01	0.42
5:B:1101:POV:H14A	5:B:1101:POV:H11A	1.87	0.42
6:D:1117:CLR:H211	6:D:1117:CLR:H232	1.89	0.42
1:C:113:ARG:HH11	5:C:1110:POV:H32	1.84	0.42
6:A:1110:CLR:H272	6:A:1110:CLR:H232	1.87	0.42
2:E:2138:LYS:HD2	2:E:2138:LYS:HA	1.77	0.42
2:G:2076:CYS:O	2:G:2077:ARG:NE	2.52	0.42
1:D:549:SER:OG	1:D:552:THR:OG1	2.28	0.42
1:D:934:LEU:HA	1:D:937:ILE:HD12	2.01	0.42
5:D:1109:POV:H35A	5:D:1109:POV:H32A	1.87	0.42
6:D:1117:CLR:H162	6:D:1117:CLR:C22	2.47	0.42
2:H:2059:VAL:HB	2:H:2138:LYS:HD3	2.01	0.42
1:B:519:ILE:HD13	1:B:519:ILE:HA	1.95	0.42
1:A:44:ARG:NH2	1:A:173:ASP:OD1	2.34	0.42
1:B:1043:LEU:HD12	1:B:1043:LEU:HA	1.92	0.42
1:C:269:ASN:OD1	1:C:269:ASN:N	2.51	0.42
1:D:793:ASN:HB3	1:D:796:LEU:HD12	2.00	0.42
1:A:1012:PHE:HD2	1:A:1050:PHE:HB3	1.84	0.42
2:F:2059:VAL:HB	2:F:2138:LYS:HD3	2.01	0.42
1:C:1012:PHE:HD2	1:C:1050:PHE:HB3	1.84	0.42
2:E:2076:CYS:O	2:E:2077:ARG:NE	2.52	0.42
2:G:2059:VAL:HB	2:G:2138:LYS:HD3	2.01	0.42
1:D:458:THR:OG1	1:D:459:GLN:N	2.52	0.42
5:D:1101:POV:H11A	5:D:1101:POV:H14A	1.87	0.42
1:B:113:ARG:HH11	5:B:1110:POV:H32	1.84	0.42
1:B:458:THR:OG1	1:B:459:GLN:N	2.52	0.42
1:C:458:THR:OG1	1:C:459:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH2	1:A:186:ASP:OD2	2.53	0.41
1:A:1017:LEU:HB2	1:A:1020:ALA:HB2	2.02	0.41
1:C:793:ASN:HB3	1:C:796:LEU:HD12	2.01	0.41
1:A:345:ILE:HD13	1:A:345:ILE:HA	1.92	0.41
5:A:1118:POV:H11A	5:A:1118:POV:H14A	1.87	0.41
1:C:167:ARG:NH2	1:C:186:ASP:OD2	2.53	0.41
1:D:32:THR:HA	6:D:1117:CLR:H262	1.96	0.41
1:D:594:LEU:HD23	1:D:594:LEU:HA	1.88	0.41
1:D:822:LEU:HD23	1:D:822:LEU:HA	1.92	0.41
5:C:1109:POV:H32A	5:C:1109:POV:H35A	1.87	0.41
5:B:1111:POV:H3	5:B:1111:POV:H32A	1.81	0.41
1:A:105:ILE:HD13	1:A:105:ILE:HA	1.91	0.41
1:A:284:THR:OG1	1:B:290:TYR:OH	2.29	0.41
2:F:2076:CYS:O	2:F:2077:ARG:NE	2.52	0.41
1:D:510:LEU:HD23	1:D:510:LEU:HA	1.89	0.41
1:B:606:LYS:HA	1:B:606:LYS:HD3	1.79	0.41
1:D:1017:LEU:HB2	1:D:1020:ALA:HB2	2.02	0.41
5:A:1104:POV:H35A	5:A:1104:POV:H32A	1.87	0.41
2:E:2059:VAL:HB	2:E:2138:LYS:HD3	2.01	0.41
2:F:2138:LYS:HD2	2:F:2138:LYS:HA	1.77	0.41
1:D:1012:PHE:HD2	1:D:1050:PHE:HB3	1.84	0.41
5:A:1120:POV:H13A	5:A:1120:POV:H11	1.88	0.41
2:E:2023:PHE:O	2:E:2027:SER:OG	2.32	0.41
1:B:167:ARG:NH2	1:B:186:ASP:OD2	2.53	0.41
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.90	0.41
1:D:309:LEU:HD23	1:D:309:LEU:HA	1.93	0.41
5:B:1111:POV:H13A	5:B:1111:POV:H11	1.89	0.41
1:C:923:LEU:HA	1:C:923:LEU:HD23	1.89	0.41
1:D:105:ILE:HD13	1:D:105:ILE:HA	1.91	0.41
5:D:1103:POV:H11	5:D:1103:POV:H13A	1.88	0.41
6:D:1118:CLR:H162	6:D:1118:CLR:C22	2.39	0.41
1:A:898:ASP:HA	1:A:899:PRO:HD3	1.97	0.40
5:A:1106:POV:H11	5:A:1106:POV:H13A	1.89	0.40
5:B:1112:POV:H25	5:B:1112:POV:H22	1.86	0.40
1:C:519:ILE:HD13	1:C:519:ILE:HA	1.95	0.40
6:C:1118:CLR:H162	6:C:1118:CLR:C22	2.39	0.40
1:D:167:ARG:NH2	1:D:186:ASP:OD2	2.53	0.40
2:E:2024:LEU:HD23	2:E:2024:LEU:HA	1.94	0.40
1:B:1017:LEU:HB2	1:B:1020:ALA:HB2	2.02	0.40
1:A:269:ASN:OD1	1:A:269:ASN:N	2.51	0.40
1:A:343:LYS:HG3	1:A:373:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:OG	1:A:552:THR:OG1	2.28	0.40
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.88	0.40
1:B:284:THR:OG1	1:C:290:TYR:OH	2.29	0.40
6:A:1111:CLR:H162	6:A:1111:CLR:H222	2.03	0.40
2:E:2068:CYS:HB2	2:E:2119:CYS:HB2	1.79	0.40
6:B:1116:CLR:H222	6:B:1116:CLR:H162	2.03	0.40
5:C:1101:POV:H11A	5:C:1101:POV:H14A	1.87	0.40
1:B:343:LYS:HG3	1:B:373:VAL:HG12	2.04	0.40
1:C:343:LYS:HG3	1:C:373:VAL:HG12	2.04	0.40
1:C:606:LYS:HD3	1:C:606:LYS:HA	1.79	0.40
1:D:343:LYS:HG3	1:D:373:VAL:HG12	2.04	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	886/1065 (83%)	847 (96%)	39 (4%)	0	100 100
1	B	886/1065 (83%)	847 (96%)	39 (4%)	0	100 100
1	C	886/1065 (83%)	846 (96%)	40 (4%)	0	100 100
1	D	886/1065 (83%)	847 (96%)	39 (4%)	0	100 100
2	E	197/219 (90%)	190 (96%)	7 (4%)	0	100 100
2	F	197/219 (90%)	190 (96%)	7 (4%)	0	100 100
2	G	197/219 (90%)	190 (96%)	7 (4%)	0	100 100
2	H	197/219 (90%)	190 (96%)	7 (4%)	0	100 100
All	All	4332/5136 (84%)	4147 (96%)	185 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	788/937 (84%)	788 (100%)	0	100 100
1	B	788/937 (84%)	788 (100%)	0	100 100
1	C	788/937 (84%)	788 (100%)	0	100 100
1	D	788/937 (84%)	788 (100%)	0	100 100
2	E	180/199 (90%)	180 (100%)	0	100 100
2	F	180/199 (90%)	180 (100%)	0	100 100
2	G	180/199 (90%)	180 (100%)	0	100 100
2	H	180/199 (90%)	180 (100%)	0	100 100
All	All	3872/4544 (85%)	3872 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	143	ASN
1	A	200	ASN
1	A	471	ASN
1	A	534	ASN
1	A	793	ASN
1	A	884	ASN
1	A	1054	GLN
2	E	2095	ASN
2	E	2144	GLN
1	B	142	GLN
1	B	143	ASN
1	B	200	ASN
1	B	471	ASN
1	B	534	ASN
1	B	793	ASN
1	B	884	ASN

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Mol	Chain	Res	Type
1	B	1054	GLN
2	F	2095	ASN
2	F	2144	GLN
1	C	142	GLN
1	C	143	ASN
1	C	200	ASN
1	C	471	ASN
1	C	534	ASN
1	C	793	ASN
1	C	884	ASN
1	C	1054	GLN
2	G	2095	ASN
1	D	142	GLN
1	D	143	ASN
1	D	200	ASN
1	D	471	ASN
1	D	534	ASN
1	D	793	ASN
1	D	884	ASN
1	D	1054	GLN
2	H	2091	ASN
2	H	2095	ASN
2	H	2144	GLN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 100 ligands modelled in this entry, 16 are monoatomic - leaving 84 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
6	CLR	C	1116	-	31,31,31	4.25	14 (45%)	48,48,48	2.52	17 (35%)
5	POV	D	1112	-	23,23,51	1.44	1 (4%)	28,30,59	1.40	3 (10%)
8	NAG	F	2305	2	14,14,15	0.53	0	17,19,21	1.54	2 (11%)
5	POV	C	1103	-	34,34,51	1.36	5 (14%)	39,42,59	1.19	3 (7%)
5	POV	B	1109	-	30,30,51	1.37	7 (23%)	34,35,59	1.42	4 (11%)
5	POV	A	1105	-	12,12,51	0.94	1 (8%)	12,12,59	1.17	1 (8%)
5	POV	H	2303	-	8,8,51	0.30	0	7,7,59	0.78	0
8	NAG	F	2306	2	14,14,15	0.56	0	17,19,21	1.04	1 (5%)
5	POV	E	2302	-	7,7,51	0.27	0	6,6,59	0.74	0
5	POV	A	1107	-	23,23,51	1.44	1 (4%)	28,30,59	1.40	3 (10%)
5	POV	C	1105	-	39,39,51	1.14	4 (10%)	45,47,59	1.18	3 (6%)
6	CLR	C	1115	-	31,31,31	4.23	14 (45%)	48,48,48	2.49	16 (33%)
5	POV	A	1118	-	44,44,51	1.17	5 (11%)	50,52,59	1.22	4 (8%)
5	POV	G	2303	-	8,8,51	0.30	0	7,7,59	0.78	0
5	POV	E	2301	-	51,51,51	1.12	5 (9%)	57,59,59	1.14	3 (5%)
6	CLR	B	1116	-	31,31,31	4.25	14 (45%)	48,48,48	2.52	17 (35%)
8	NAG	H	2305	2	14,14,15	0.53	0	17,19,21	1.54	2 (11%)
5	POV	B	1101	-	44,44,51	1.17	5 (11%)	50,52,59	1.22	4 (8%)
6	CLR	D	1115	-	31,31,31	4.23	14 (45%)	48,48,48	2.49	16 (33%)
6	CLR	B	1118	-	31,31,31	4.26	14 (45%)	48,48,48	2.48	14 (29%)
5	POV	D	1111	-	35,35,51	1.33	5 (14%)	41,43,59	1.26	3 (7%)
5	POV	C	1114	-	12,12,51	0.27	0	11,11,59	0.76	0
5	POV	D	1109	-	30,30,51	1.37	7 (23%)	34,35,59	1.42	4 (11%)
5	POV	F	2302	-	7,7,51	0.27	0	6,6,59	0.75	0
5	POV	F	2304	-	14,14,51	1.46	3 (21%)	17,17,59	1.27	2 (11%)
5	POV	B	1110	-	12,12,51	0.93	1 (8%)	12,12,59	1.18	0
6	CLR	B	1115	-	31,31,31	4.23	14 (45%)	48,48,48	2.49	16 (33%)
5	POV	D	1110	-	12,12,51	0.93	1 (8%)	12,12,59	1.18	0
5	POV	C	1101	-	44,44,51	1.17	5 (11%)	50,52,59	1.22	4 (8%)
6	CLR	B	1117	-	31,31,31	4.18	14 (45%)	48,48,48	2.54	18 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	POV	A	1120	-	34,34,51	1.36	5 (14%)	39,42,59	1.19	3 (7%)
5	POV	C	1111	-	35,35,51	1.33	4 (11%)	41,43,59	1.26	3 (7%)
8	NAG	G	2305	2	14,14,15	0.53	0	17,19,21	1.55	2 (11%)
5	POV	B	1105	-	39,39,51	1.14	4 (10%)	45,47,59	1.18	3 (6%)
8	NAG	H	2306	2	14,14,15	0.56	0	17,19,21	1.04	1 (5%)
5	POV	H	2302	-	7,7,51	0.27	0	6,6,59	0.75	0
6	CLR	D	1117	-	31,31,31	4.18	14 (45%)	48,48,48	2.54	18 (37%)
5	POV	D	1102	-	22,22,51	1.38	4 (18%)	25,25,59	1.30	2 (8%)
5	POV	C	1104	-	31,31,51	1.23	4 (12%)	37,39,59	1.15	3 (8%)
5	POV	B	1112	-	23,23,51	1.44	1 (4%)	28,30,59	1.40	3 (10%)
5	POV	E	2303	-	8,8,51	0.30	0	7,7,59	0.78	0
6	CLR	A	1110	-	31,31,31	4.22	14 (45%)	48,48,48	2.49	16 (33%)
6	CLR	D	1116	-	31,31,31	4.25	14 (45%)	48,48,48	2.52	17 (35%)
5	POV	G	2302	-	7,7,51	0.27	0	6,6,59	0.74	0
5	POV	A	1119	-	22,22,51	1.38	4 (18%)	25,25,59	1.30	2 (8%)
5	POV	C	1113	-	7,7,51	0.27	0	6,6,59	0.76	0
5	POV	H	2304	-	14,14,51	1.46	3 (21%)	17,17,59	1.27	2 (11%)
5	POV	D	1105	-	39,39,51	1.14	5 (12%)	45,47,59	1.18	3 (6%)
8	NAG	E	2305	2	14,14,15	0.52	0	17,19,21	1.55	2 (11%)
6	CLR	A	1111	-	31,31,31	4.25	14 (45%)	48,48,48	2.52	17 (35%)
5	POV	B	1114	-	12,12,51	0.27	0	11,11,59	0.76	0
5	POV	D	1113	-	7,7,51	0.26	0	6,6,59	0.76	0
6	CLR	D	1118	-	31,31,31	4.26	14 (45%)	48,48,48	2.48	14 (29%)
5	POV	A	1121	-	31,31,51	1.23	4 (12%)	37,39,59	1.15	3 (8%)
8	NAG	G	2306	2	14,14,15	0.56	0	17,19,21	1.04	1 (5%)
5	POV	A	1109	-	12,12,51	0.27	0	11,11,59	0.76	0
5	POV	A	1106	-	35,35,51	1.33	4 (11%)	41,43,59	1.26	3 (7%)
5	POV	F	2301	-	51,51,51	1.12	5 (9%)	57,59,59	1.14	3 (5%)
5	POV	B	1104	-	31,31,51	1.23	4 (12%)	37,39,59	1.16	3 (8%)
6	CLR	C	1118	-	31,31,31	4.25	14 (45%)	48,48,48	2.48	14 (29%)
5	POV	C	1110	-	12,12,51	0.94	1 (8%)	12,12,59	1.18	1 (8%)
5	POV	D	1114	-	12,12,51	0.27	0	11,11,59	0.76	0
5	POV	A	1104	-	30,30,51	1.37	7 (23%)	34,35,59	1.42	4 (11%)
5	POV	B	1111	-	35,35,51	1.33	5 (14%)	41,43,59	1.26	3 (7%)
5	POV	B	1103	-	34,34,51	1.36	5 (14%)	39,42,59	1.19	3 (7%)
8	NAG	E	2306	2	14,14,15	0.56	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	POV	H	2301	-	51,51,51	1.12	5 (9%)	57,59,59	1.14	3 (5%)
5	POV	A	1108	-	7,7,51	0.27	0	6,6,59	0.76	0
5	POV	B	1102	-	22,22,51	1.38	4 (18%)	25,25,59	1.30	2 (8%)
5	POV	G	2301	-	51,51,51	1.12	5 (9%)	57,59,59	1.14	3 (5%)
5	POV	B	1113	-	7,7,51	0.26	0	6,6,59	0.76	0
5	POV	A	1122	-	39,39,51	1.14	4 (10%)	45,47,59	1.18	3 (6%)
5	POV	D	1101	-	44,44,51	1.17	4 (9%)	50,52,59	1.22	4 (8%)
5	POV	F	2303	-	8,8,51	0.30	0	7,7,59	0.78	0
6	CLR	C	1117	-	31,31,31	4.18	14 (45%)	48,48,48	2.53	18 (37%)
6	CLR	A	1113	-	31,31,31	4.25	14 (45%)	48,48,48	2.48	14 (29%)
5	POV	C	1109	-	30,30,51	1.37	7 (23%)	34,35,59	1.42	4 (11%)
6	CLR	A	1112	-	31,31,31	4.18	14 (45%)	48,48,48	2.54	18 (37%)
5	POV	C	1112	-	23,23,51	1.44	1 (4%)	28,30,59	1.40	3 (10%)
5	POV	C	1102	-	22,22,51	1.38	4 (18%)	25,25,59	1.30	2 (8%)
5	POV	D	1104	-	31,31,51	1.23	4 (12%)	37,39,59	1.16	3 (8%)
5	POV	D	1103	-	34,34,51	1.36	5 (14%)	39,42,59	1.19	3 (7%)
5	POV	E	2304	-	14,14,51	1.46	3 (21%)	17,17,59	1.27	2 (11%)
5	POV	G	2304	-	14,14,51	1.45	3 (21%)	17,17,59	1.27	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	C	1116	-	-	5/10/68/68	0/4/4/4
5	POV	D	1112	-	-	13/25/25/55	-
8	NAG	F	2305	2	-	0/6/23/26	0/1/1/1
5	POV	C	1103	-	-	12/38/38/55	-
5	POV	B	1109	-	-	17/32/32/55	-
5	POV	A	1105	-	-	4/10/10/55	-
5	POV	H	2303	-	-	3/6/6/55	-
8	NAG	F	2306	2	-	2/6/23/26	0/1/1/1
5	POV	E	2302	-	-	1/5/5/55	-
5	POV	A	1107	-	-	13/25/25/55	-
5	POV	C	1105	-	-	24/43/43/55	-
6	CLR	C	1115	-	-	8/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	A	1118	-	-	31/48/48/55	-
5	POV	G	2303	-	-	3/6/6/55	-
5	POV	E	2301	-	-	19/55/55/55	-
6	CLR	B	1116	-	-	5/10/68/68	0/4/4/4
8	NAG	H	2305	2	-	0/6/23/26	0/1/1/1
5	POV	B	1101	-	-	31/48/48/55	-
6	CLR	D	1115	-	-	8/10/68/68	0/4/4/4
6	CLR	B	1118	-	-	7/10/68/68	0/4/4/4
5	POV	D	1111	-	-	21/39/39/55	-
5	POV	C	1114	-	-	4/10/10/55	-
5	POV	D	1109	-	-	17/32/32/55	-
5	POV	F	2302	-	-	1/5/5/55	-
5	POV	F	2304	-	-	3/13/13/55	-
5	POV	B	1110	-	-	4/10/10/55	-
6	CLR	B	1115	-	-	8/10/68/68	0/4/4/4
5	POV	D	1110	-	-	4/10/10/55	-
5	POV	C	1101	-	-	31/48/48/55	-
6	CLR	B	1117	-	-	5/10/68/68	0/4/4/4
5	POV	A	1120	-	-	12/38/38/55	-
5	POV	C	1111	-	-	21/39/39/55	-
8	NAG	G	2305	2	-	0/6/23/26	0/1/1/1
5	POV	B	1105	-	-	24/43/43/55	-
8	NAG	H	2306	2	-	2/6/23/26	0/1/1/1
5	POV	H	2302	-	-	1/5/5/55	-
6	CLR	D	1117	-	-	5/10/68/68	0/4/4/4
5	POV	D	1102	-	-	9/21/21/55	-
5	POV	C	1104	-	-	15/35/35/55	-
5	POV	B	1112	-	-	13/25/25/55	-
5	POV	E	2303	-	-	3/6/6/55	-
6	CLR	A	1110	-	-	8/10/68/68	0/4/4/4
6	CLR	D	1116	-	-	5/10/68/68	0/4/4/4
5	POV	G	2302	-	-	1/5/5/55	-
5	POV	A	1119	-	-	9/21/21/55	-
5	POV	C	1113	-	-	1/5/5/55	-
5	POV	H	2304	-	-	3/13/13/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	D	1105	-	-	24/43/43/55	-
8	NAG	E	2305	2	-	0/6/23/26	0/1/1/1
6	CLR	A	1111	-	-	5/10/68/68	0/4/4/4
5	POV	B	1114	-	-	4/10/10/55	-
5	POV	D	1113	-	-	1/5/5/55	-
6	CLR	D	1118	-	-	7/10/68/68	0/4/4/4
5	POV	A	1121	-	-	15/35/35/55	-
8	NAG	G	2306	2	-	2/6/23/26	0/1/1/1
5	POV	A	1109	-	-	4/10/10/55	-
5	POV	A	1106	-	-	21/39/39/55	-
5	POV	F	2301	-	-	19/55/55/55	-
5	POV	B	1104	-	-	15/35/35/55	-
6	CLR	C	1118	-	-	7/10/68/68	0/4/4/4
5	POV	C	1110	-	-	4/10/10/55	-
5	POV	D	1114	-	-	4/10/10/55	-
5	POV	A	1104	-	-	17/32/32/55	-
5	POV	B	1111	-	-	21/39/39/55	-
5	POV	B	1103	-	-	12/38/38/55	-
8	NAG	E	2306	2	-	2/6/23/26	0/1/1/1
5	POV	H	2301	-	-	19/55/55/55	-
5	POV	A	1108	-	-	1/5/5/55	-
5	POV	B	1102	-	-	9/21/21/55	-
5	POV	G	2301	-	-	19/55/55/55	-
5	POV	B	1113	-	-	1/5/5/55	-
5	POV	A	1122	-	-	24/43/43/55	-
5	POV	D	1101	-	-	31/48/48/55	-
5	POV	F	2303	-	-	3/6/6/55	-
6	CLR	C	1117	-	-	5/10/68/68	0/4/4/4
6	CLR	A	1113	-	-	7/10/68/68	0/4/4/4
5	POV	C	1109	-	-	17/32/32/55	-
6	CLR	A	1112	-	-	5/10/68/68	0/4/4/4
5	POV	C	1112	-	-	13/25/25/55	-
5	POV	C	1102	-	-	9/21/21/55	-
5	POV	D	1104	-	-	15/35/35/55	-
5	POV	D	1103	-	-	12/38/38/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	E	2304	-	-	3/13/13/55	-
5	POV	G	2304	-	-	3/13/13/55	-

All (398) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1113	CLR	C6-C5	11.16	1.57	1.33
6	C	1118	CLR	C6-C5	11.16	1.57	1.33
6	B	1118	CLR	C6-C5	11.16	1.57	1.33
6	D	1118	CLR	C6-C5	11.16	1.57	1.33
6	A	1111	CLR	C6-C5	11.05	1.57	1.33
6	B	1116	CLR	C6-C5	11.04	1.57	1.33
6	D	1116	CLR	C6-C5	11.04	1.57	1.33
6	C	1116	CLR	C6-C5	11.02	1.57	1.33
6	C	1115	CLR	C6-C5	11.01	1.57	1.33
6	B	1115	CLR	C6-C5	10.99	1.57	1.33
6	D	1115	CLR	C6-C5	10.99	1.57	1.33
6	A	1110	CLR	C6-C5	10.95	1.57	1.33
6	C	1117	CLR	C6-C5	10.78	1.56	1.33
6	A	1112	CLR	C6-C5	10.75	1.56	1.33
6	B	1117	CLR	C6-C5	10.75	1.56	1.33
6	D	1117	CLR	C6-C5	10.75	1.56	1.33
6	B	1116	CLR	C20-C17	-10.09	1.36	1.54
6	D	1116	CLR	C20-C17	-10.09	1.36	1.54
6	A	1111	CLR	C20-C17	-10.04	1.36	1.54
6	C	1116	CLR	C20-C17	-10.03	1.36	1.54
6	C	1118	CLR	C16-C17	10.00	1.75	1.54
6	B	1118	CLR	C16-C17	10.00	1.75	1.54
6	D	1118	CLR	C16-C17	10.00	1.75	1.54
6	A	1113	CLR	C16-C17	9.99	1.75	1.54
6	B	1115	CLR	C16-C17	9.99	1.75	1.54
6	D	1115	CLR	C16-C17	9.99	1.75	1.54
6	C	1115	CLR	C16-C17	9.96	1.75	1.54
6	A	1112	CLR	C16-C17	9.95	1.75	1.54
6	B	1117	CLR	C16-C17	9.95	1.75	1.54
6	D	1117	CLR	C16-C17	9.95	1.75	1.54
6	C	1117	CLR	C16-C17	9.94	1.75	1.54
6	A	1110	CLR	C16-C17	9.92	1.75	1.54
6	B	1116	CLR	C16-C17	9.76	1.74	1.54
6	D	1116	CLR	C16-C17	9.76	1.74	1.54
6	B	1117	CLR	C20-C17	-9.76	1.37	1.54
6	D	1117	CLR	C20-C17	-9.76	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1116	CLR	C16-C17	9.74	1.74	1.54
6	A	1112	CLR	C20-C17	-9.73	1.37	1.54
6	C	1117	CLR	C20-C17	-9.73	1.37	1.54
6	A	1111	CLR	C16-C17	9.72	1.74	1.54
6	B	1115	CLR	C20-C17	-9.52	1.37	1.54
6	D	1115	CLR	C20-C17	-9.52	1.37	1.54
6	C	1115	CLR	C20-C17	-9.48	1.37	1.54
6	A	1110	CLR	C20-C17	-9.47	1.37	1.54
6	A	1113	CLR	C20-C17	-9.45	1.37	1.54
6	B	1118	CLR	C20-C17	-9.45	1.37	1.54
6	D	1118	CLR	C20-C17	-9.45	1.37	1.54
6	C	1118	CLR	C20-C17	-9.45	1.37	1.54
6	A	1111	CLR	C8-C9	7.87	1.68	1.53
6	C	1116	CLR	C8-C9	7.85	1.68	1.53
6	B	1116	CLR	C8-C9	7.84	1.68	1.53
6	D	1116	CLR	C8-C9	7.84	1.68	1.53
6	A	1110	CLR	C8-C9	7.74	1.68	1.53
6	B	1115	CLR	C8-C9	7.74	1.68	1.53
6	D	1115	CLR	C8-C9	7.74	1.68	1.53
6	C	1115	CLR	C8-C9	7.72	1.68	1.53
6	B	1118	CLR	C8-C9	7.69	1.68	1.53
6	D	1118	CLR	C8-C9	7.69	1.68	1.53
6	C	1118	CLR	C8-C9	7.63	1.68	1.53
6	A	1113	CLR	C8-C9	7.62	1.68	1.53
6	A	1112	CLR	C8-C9	7.56	1.68	1.53
6	B	1117	CLR	C8-C9	7.54	1.68	1.53
6	D	1117	CLR	C8-C9	7.54	1.68	1.53
6	C	1117	CLR	C8-C9	7.52	1.68	1.53
6	A	1113	CLR	C12-C11	6.35	1.66	1.53
6	C	1118	CLR	C12-C11	6.34	1.66	1.53
6	B	1118	CLR	C12-C11	6.34	1.66	1.53
6	D	1118	CLR	C12-C11	6.34	1.66	1.53
6	A	1110	CLR	C12-C11	6.33	1.66	1.53
6	C	1115	CLR	C12-C11	6.33	1.66	1.53
6	B	1115	CLR	C12-C11	6.28	1.66	1.53
6	D	1115	CLR	C12-C11	6.28	1.66	1.53
6	C	1116	CLR	C12-C11	6.20	1.66	1.53
6	A	1111	CLR	C12-C11	6.19	1.66	1.53
6	B	1116	CLR	C12-C11	6.19	1.66	1.53
6	D	1116	CLR	C12-C11	6.19	1.66	1.53
6	A	1112	CLR	C12-C11	5.91	1.66	1.53
6	C	1117	CLR	C12-C11	5.91	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1117	CLR	C12-C11	5.85	1.65	1.53
6	D	1117	CLR	C12-C11	5.85	1.65	1.53
6	C	1118	CLR	C13-C17	5.55	1.65	1.55
6	A	1113	CLR	C13-C17	5.55	1.65	1.55
6	B	1118	CLR	C13-C17	5.54	1.65	1.55
6	D	1118	CLR	C13-C17	5.54	1.65	1.55
6	A	1110	CLR	C7-C6	5.41	1.61	1.50
6	B	1115	CLR	C13-C17	5.41	1.65	1.55
6	D	1115	CLR	C13-C17	5.41	1.65	1.55
6	A	1111	CLR	C7-C6	5.38	1.61	1.50
6	B	1115	CLR	C7-C6	5.37	1.61	1.50
6	D	1115	CLR	C7-C6	5.37	1.61	1.50
6	B	1116	CLR	C7-C6	5.37	1.61	1.50
6	D	1116	CLR	C7-C6	5.37	1.61	1.50
6	C	1116	CLR	C7-C6	5.37	1.61	1.50
6	A	1110	CLR	C13-C17	5.37	1.65	1.55
6	C	1115	CLR	C7-C6	5.36	1.61	1.50
6	C	1115	CLR	C13-C17	5.35	1.65	1.55
6	B	1118	CLR	C7-C6	5.28	1.61	1.50
6	C	1118	CLR	C7-C6	5.28	1.61	1.50
6	D	1118	CLR	C7-C6	5.28	1.61	1.50
6	A	1112	CLR	C7-C6	5.27	1.61	1.50
6	C	1117	CLR	C7-C6	5.27	1.61	1.50
6	B	1117	CLR	C7-C6	5.27	1.61	1.50
6	D	1117	CLR	C7-C6	5.27	1.61	1.50
6	A	1113	CLR	C7-C6	5.26	1.61	1.50
6	A	1112	CLR	C13-C17	5.19	1.64	1.55
6	B	1117	CLR	C13-C17	5.19	1.64	1.55
6	C	1117	CLR	C13-C17	5.19	1.64	1.55
6	D	1117	CLR	C13-C17	5.19	1.64	1.55
6	B	1116	CLR	C13-C17	4.65	1.63	1.55
6	D	1116	CLR	C13-C17	4.65	1.63	1.55
6	A	1111	CLR	C13-C17	4.61	1.63	1.55
6	C	1116	CLR	C13-C17	4.61	1.63	1.55
6	B	1116	CLR	C15-C14	4.21	1.63	1.54
6	D	1116	CLR	C15-C14	4.21	1.63	1.54
6	C	1116	CLR	C15-C14	4.20	1.63	1.54
6	A	1111	CLR	C15-C14	4.17	1.63	1.54
5	B	1112	POV	O21-C2	-4.15	1.40	1.47
5	C	1112	POV	O21-C2	-4.15	1.40	1.47
5	D	1112	POV	O21-C2	-4.15	1.40	1.47
5	A	1107	POV	O21-C2	-4.14	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1113	CLR	C15-C14	3.84	1.62	1.54
6	B	1118	CLR	C15-C14	3.84	1.62	1.54
6	D	1118	CLR	C15-C14	3.84	1.62	1.54
6	B	1117	CLR	C15-C14	3.83	1.62	1.54
6	C	1117	CLR	C15-C14	3.83	1.62	1.54
6	D	1117	CLR	C15-C14	3.83	1.62	1.54
6	C	1118	CLR	C15-C14	3.83	1.62	1.54
6	A	1110	CLR	C15-C14	3.80	1.62	1.54
6	B	1115	CLR	C15-C14	3.80	1.62	1.54
6	D	1115	CLR	C15-C14	3.80	1.62	1.54
6	A	1112	CLR	C15-C14	3.79	1.62	1.54
6	C	1115	CLR	C15-C14	3.79	1.62	1.54
5	G	2301	POV	C29-C210	3.64	1.52	1.31
5	F	2301	POV	C29-C210	3.62	1.52	1.31
5	H	2301	POV	C29-C210	3.62	1.52	1.31
5	E	2301	POV	C29-C210	3.62	1.52	1.31
5	A	1120	POV	C29-C210	3.62	1.52	1.31
5	C	1103	POV	C29-C210	3.62	1.52	1.31
5	B	1103	POV	C29-C210	3.60	1.52	1.31
5	D	1103	POV	C29-C210	3.60	1.52	1.31
5	B	1102	POV	C29-C210	3.58	1.52	1.31
5	A	1119	POV	C29-C210	3.57	1.52	1.31
5	C	1102	POV	C29-C210	3.57	1.52	1.31
5	D	1102	POV	C29-C210	3.57	1.52	1.31
5	B	1111	POV	C29-C210	3.54	1.52	1.31
5	D	1111	POV	C29-C210	3.54	1.52	1.31
6	A	1113	CLR	C13-C14	3.53	1.61	1.55
5	A	1106	POV	C29-C210	3.53	1.52	1.31
5	C	1111	POV	C29-C210	3.53	1.52	1.31
6	B	1118	CLR	C13-C14	3.52	1.61	1.55
6	D	1118	CLR	C13-C14	3.52	1.61	1.55
6	C	1117	CLR	C13-C14	3.52	1.61	1.55
6	A	1112	CLR	C13-C14	3.51	1.61	1.55
6	B	1117	CLR	C13-C14	3.51	1.61	1.55
6	D	1117	CLR	C13-C14	3.51	1.61	1.55
6	C	1118	CLR	C13-C14	3.48	1.61	1.55
6	C	1115	CLR	C13-C14	3.47	1.61	1.55
6	A	1110	CLR	C13-C14	3.45	1.61	1.55
6	B	1115	CLR	C13-C14	3.41	1.61	1.55
6	D	1115	CLR	C13-C14	3.41	1.61	1.55
6	C	1118	CLR	C22-C20	3.32	1.62	1.54
6	B	1118	CLR	C22-C20	3.32	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1118	CLR	C22-C20	3.32	1.62	1.54
6	A	1111	CLR	C13-C14	3.31	1.61	1.55
6	C	1116	CLR	C13-C14	3.31	1.61	1.55
6	A	1113	CLR	C22-C20	3.28	1.62	1.54
6	B	1116	CLR	C13-C14	3.27	1.61	1.55
6	D	1116	CLR	C13-C14	3.27	1.61	1.55
5	B	1109	POV	C29-C210	3.14	1.53	1.29
5	D	1109	POV	C29-C210	3.14	1.53	1.29
5	A	1104	POV	C29-C210	3.13	1.53	1.29
5	C	1109	POV	C29-C210	3.13	1.53	1.29
5	C	1101	POV	C29-C210	3.11	1.52	1.29
5	D	1101	POV	C29-C210	3.11	1.52	1.29
5	A	1118	POV	C29-C210	3.10	1.52	1.29
5	B	1101	POV	C29-C210	3.09	1.52	1.29
6	A	1110	CLR	C22-C20	3.09	1.62	1.54
6	C	1115	CLR	C22-C20	3.08	1.62	1.54
6	C	1118	CLR	C21-C20	3.07	1.60	1.53
6	B	1115	CLR	C22-C20	3.05	1.62	1.54
6	D	1115	CLR	C22-C20	3.05	1.62	1.54
6	A	1112	CLR	C21-C20	3.03	1.60	1.53
6	A	1113	CLR	C21-C20	3.03	1.60	1.53
6	B	1118	CLR	C21-C20	3.03	1.60	1.53
6	D	1118	CLR	C21-C20	3.03	1.60	1.53
6	C	1115	CLR	C21-C20	3.02	1.60	1.53
6	C	1117	CLR	C22-C20	3.02	1.62	1.54
6	B	1117	CLR	C21-C20	3.01	1.60	1.53
6	D	1117	CLR	C21-C20	3.01	1.60	1.53
6	A	1110	CLR	C21-C20	3.01	1.60	1.53
6	B	1115	CLR	C21-C20	3.01	1.60	1.53
6	D	1115	CLR	C21-C20	3.01	1.60	1.53
6	A	1111	CLR	C8-C14	-3.01	1.47	1.53
6	C	1116	CLR	C8-C14	-3.01	1.47	1.53
6	C	1117	CLR	C21-C20	2.99	1.60	1.53
6	A	1112	CLR	C22-C20	2.98	1.62	1.54
6	B	1117	CLR	C22-C20	2.98	1.62	1.54
6	D	1117	CLR	C22-C20	2.98	1.62	1.54
6	B	1116	CLR	C8-C14	-2.96	1.48	1.53
6	D	1116	CLR	C8-C14	-2.96	1.48	1.53
6	C	1116	CLR	C22-C20	2.94	1.62	1.54
6	A	1111	CLR	C22-C20	2.92	1.61	1.54
6	B	1116	CLR	C22-C20	2.92	1.61	1.54
6	D	1116	CLR	C22-C20	2.92	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1117	CLR	C8-C14	-2.84	1.48	1.53
6	D	1117	CLR	C8-C14	-2.84	1.48	1.53
6	A	1112	CLR	C8-C14	-2.84	1.48	1.53
5	A	1105	POV	O31-C31	2.84	1.40	1.30
6	C	1117	CLR	C8-C14	-2.83	1.48	1.53
6	B	1118	CLR	C8-C14	-2.82	1.48	1.53
6	C	1118	CLR	C8-C14	-2.82	1.48	1.53
6	D	1118	CLR	C8-C14	-2.82	1.48	1.53
5	C	1110	POV	O31-C31	2.81	1.40	1.30
6	A	1111	CLR	C21-C20	2.81	1.59	1.53
5	B	1110	POV	O31-C31	2.80	1.40	1.30
5	D	1110	POV	O31-C31	2.80	1.40	1.30
6	B	1116	CLR	C21-C20	2.80	1.59	1.53
6	D	1116	CLR	C21-C20	2.80	1.59	1.53
6	C	1116	CLR	C21-C20	2.79	1.59	1.53
6	A	1113	CLR	C8-C14	-2.76	1.48	1.53
5	D	1105	POV	O21-C2	-2.75	1.39	1.46
5	A	1122	POV	O21-C2	-2.72	1.39	1.46
5	B	1105	POV	O21-C2	-2.72	1.39	1.46
5	C	1105	POV	O21-C2	-2.72	1.39	1.46
6	B	1115	CLR	C8-C14	-2.71	1.48	1.53
6	D	1115	CLR	C8-C14	-2.71	1.48	1.53
5	B	1101	POV	O21-C2	-2.68	1.39	1.46
6	C	1115	CLR	C8-C14	-2.68	1.48	1.53
5	A	1119	POV	P-O12	2.67	1.65	1.54
5	B	1102	POV	P-O12	2.67	1.65	1.54
5	C	1102	POV	P-O12	2.67	1.65	1.54
5	E	2304	POV	P-O12	2.67	1.65	1.54
5	G	2304	POV	P-O12	2.67	1.65	1.54
5	D	1102	POV	P-O12	2.66	1.65	1.54
5	D	1101	POV	O21-C2	-2.66	1.39	1.46
5	A	1118	POV	O21-C2	-2.66	1.39	1.46
5	C	1101	POV	O21-C2	-2.66	1.39	1.46
5	F	2304	POV	P-O12	2.66	1.65	1.54
5	H	2304	POV	P-O12	2.66	1.65	1.54
6	A	1110	CLR	C8-C14	-2.66	1.48	1.53
5	A	1104	POV	P-O12	2.64	1.65	1.54
5	C	1109	POV	P-O12	2.62	1.64	1.54
5	B	1109	POV	P-O12	2.62	1.64	1.54
5	D	1109	POV	P-O12	2.62	1.64	1.54
5	A	1120	POV	O21-C2	-2.54	1.40	1.46
5	B	1103	POV	O21-C2	-2.54	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1103	POV	O21-C2	-2.54	1.40	1.46
5	D	1103	POV	O21-C2	-2.54	1.40	1.46
6	A	1111	CLR	C18-C13	2.53	1.58	1.54
5	E	2304	POV	O21-C21	2.52	1.40	1.33
5	F	2304	POV	O21-C21	2.52	1.40	1.33
5	H	2304	POV	O21-C21	2.52	1.40	1.33
5	A	1106	POV	O21-C2	-2.52	1.40	1.46
5	B	1111	POV	O21-C2	-2.52	1.40	1.46
5	C	1111	POV	O21-C2	-2.52	1.40	1.46
5	D	1111	POV	O21-C2	-2.52	1.40	1.46
5	E	2301	POV	O31-C31	2.51	1.40	1.33
5	G	2301	POV	O31-C31	2.51	1.40	1.33
5	E	2301	POV	O21-C2	-2.51	1.40	1.46
6	C	1116	CLR	C18-C13	2.50	1.58	1.54
5	G	2304	POV	O21-C21	2.49	1.40	1.33
5	F	2301	POV	O31-C31	2.49	1.40	1.33
5	H	2301	POV	O31-C31	2.49	1.40	1.33
6	B	1116	CLR	C18-C13	2.48	1.58	1.54
6	D	1116	CLR	C18-C13	2.48	1.58	1.54
5	G	2301	POV	O21-C2	-2.48	1.40	1.46
5	F	2301	POV	O21-C2	-2.47	1.40	1.46
5	H	2301	POV	O21-C2	-2.47	1.40	1.46
5	B	1104	POV	O21-C2	-2.46	1.40	1.46
6	C	1115	CLR	C7-C8	2.45	1.57	1.53
6	B	1115	CLR	C7-C8	2.44	1.57	1.53
6	D	1115	CLR	C7-C8	2.44	1.57	1.53
5	D	1104	POV	O21-C2	-2.44	1.40	1.46
5	C	1111	POV	O31-C31	2.44	1.40	1.33
5	A	1106	POV	O31-C31	2.43	1.40	1.33
5	B	1111	POV	O31-C31	2.43	1.40	1.33
5	D	1111	POV	O31-C31	2.43	1.40	1.33
6	A	1110	CLR	C7-C8	2.42	1.57	1.53
5	B	1103	POV	O31-C31	2.42	1.40	1.33
5	A	1121	POV	O21-C2	-2.41	1.40	1.46
5	C	1104	POV	O21-C2	-2.41	1.40	1.46
5	A	1104	POV	O21-C2	-2.40	1.40	1.46
5	B	1109	POV	O21-C2	-2.40	1.40	1.46
5	C	1109	POV	O21-C2	-2.40	1.40	1.46
5	D	1109	POV	O21-C2	-2.40	1.40	1.46
5	A	1120	POV	O31-C31	2.40	1.40	1.33
5	C	1103	POV	O31-C31	2.40	1.40	1.33
5	D	1103	POV	O31-C31	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	POV	O31-C31	2.39	1.40	1.33
6	B	1116	CLR	C7-C8	2.38	1.57	1.53
6	D	1116	CLR	C7-C8	2.38	1.57	1.53
5	C	1109	POV	O31-C31	2.36	1.40	1.33
5	B	1109	POV	O31-C31	2.36	1.40	1.33
5	D	1109	POV	O31-C31	2.36	1.40	1.33
5	A	1121	POV	O31-C31	2.36	1.40	1.33
5	B	1104	POV	O31-C31	2.36	1.40	1.33
5	C	1104	POV	O31-C31	2.36	1.40	1.33
6	A	1111	CLR	C7-C8	2.36	1.57	1.53
5	D	1104	POV	O31-C31	2.35	1.40	1.33
6	C	1116	CLR	C7-C8	2.34	1.57	1.53
5	A	1122	POV	O31-C31	2.32	1.40	1.33
5	B	1105	POV	O31-C31	2.32	1.40	1.33
5	C	1105	POV	O31-C31	2.32	1.40	1.33
5	A	1104	POV	O21-C21	2.31	1.40	1.34
5	B	1109	POV	O21-C21	2.31	1.40	1.34
5	D	1109	POV	O21-C21	2.31	1.40	1.34
5	B	1101	POV	O31-C3	-2.30	1.39	1.45
5	D	1105	POV	O31-C31	2.30	1.40	1.33
5	A	1118	POV	O31-C3	-2.29	1.39	1.45
5	C	1101	POV	O31-C3	-2.29	1.39	1.45
5	C	1109	POV	O21-C21	2.29	1.40	1.34
5	A	1104	POV	O31-C3	-2.28	1.40	1.45
5	D	1101	POV	O31-C3	-2.27	1.40	1.45
5	B	1109	POV	O31-C3	-2.26	1.40	1.45
5	C	1109	POV	O31-C3	-2.26	1.40	1.45
5	D	1109	POV	O31-C3	-2.26	1.40	1.45
6	A	1112	CLR	C7-C8	2.25	1.56	1.53
5	D	1101	POV	O31-C31	2.25	1.39	1.33
5	A	1118	POV	O31-C31	2.24	1.39	1.33
5	C	1101	POV	O31-C31	2.24	1.39	1.33
5	B	1101	POV	O31-C31	2.24	1.39	1.33
5	A	1104	POV	P-O13	-2.23	1.46	1.54
5	B	1109	POV	P-O13	-2.23	1.46	1.54
5	C	1109	POV	P-O13	-2.23	1.46	1.54
5	D	1109	POV	P-O13	-2.23	1.46	1.54
5	A	1119	POV	P-O13	-2.23	1.46	1.54
5	B	1102	POV	P-O13	-2.23	1.46	1.54
5	C	1102	POV	P-O13	-2.23	1.46	1.54
5	D	1102	POV	P-O13	-2.23	1.46	1.54
5	A	1121	POV	O21-C21	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1104	POV	O21-C21	2.22	1.40	1.34
5	D	1104	POV	O21-C21	2.22	1.40	1.34
5	B	1104	POV	O21-C21	2.22	1.40	1.34
6	B	1117	CLR	C7-C8	2.20	1.56	1.53
6	D	1117	CLR	C7-C8	2.20	1.56	1.53
6	C	1117	CLR	C7-C8	2.20	1.56	1.53
5	A	1121	POV	O31-C3	-2.19	1.40	1.45
5	B	1104	POV	O31-C3	-2.19	1.40	1.45
5	C	1104	POV	O31-C3	-2.19	1.40	1.45
5	D	1105	POV	O31-C3	-2.19	1.40	1.45
5	E	2304	POV	P-O13	-2.19	1.46	1.54
5	G	2304	POV	P-O13	-2.19	1.46	1.54
5	B	1105	POV	O31-C3	-2.19	1.40	1.45
5	A	1122	POV	O31-C3	-2.18	1.40	1.45
5	C	1105	POV	O31-C3	-2.18	1.40	1.45
5	F	2304	POV	P-O13	-2.17	1.46	1.54
5	H	2304	POV	P-O13	-2.17	1.46	1.54
5	D	1102	POV	O21-C21	2.17	1.39	1.33
5	A	1119	POV	O21-C21	2.17	1.39	1.33
5	B	1102	POV	O21-C21	2.17	1.39	1.33
5	C	1102	POV	O21-C21	2.17	1.39	1.33
5	D	1104	POV	O31-C3	-2.14	1.40	1.45
6	B	1115	CLR	C4-C5	2.14	1.56	1.51
6	D	1115	CLR	C4-C5	2.14	1.56	1.51
5	F	2301	POV	O21-C21	2.14	1.40	1.34
5	H	2301	POV	O21-C21	2.14	1.40	1.34
5	G	2301	POV	O21-C21	2.13	1.40	1.34
6	C	1118	CLR	C7-C8	2.13	1.56	1.53
5	A	1120	POV	O21-C21	2.13	1.40	1.34
5	E	2301	POV	O21-C21	2.13	1.40	1.34
5	B	1103	POV	O21-C21	2.13	1.40	1.34
5	C	1103	POV	O21-C21	2.13	1.40	1.34
5	D	1103	POV	O21-C21	2.13	1.40	1.34
5	B	1111	POV	O31-C3	-2.11	1.40	1.45
5	D	1111	POV	O31-C3	-2.11	1.40	1.45
5	B	1103	POV	O31-C3	-2.11	1.40	1.45
6	A	1113	CLR	C7-C8	2.09	1.56	1.53
6	C	1115	CLR	C4-C5	2.09	1.56	1.51
5	A	1106	POV	O31-C3	-2.09	1.40	1.45
6	A	1110	CLR	C4-C5	2.09	1.56	1.51
5	D	1103	POV	O31-C3	-2.09	1.40	1.45
5	A	1120	POV	O31-C3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1103	POV	O31-C3	-2.08	1.40	1.45
5	C	1111	POV	O31-C3	-2.08	1.40	1.45
5	B	1105	POV	P-O13	-2.07	1.45	1.55
5	D	1105	POV	P-O13	-2.07	1.45	1.55
6	B	1118	CLR	C7-C8	2.06	1.56	1.53
6	D	1118	CLR	C7-C8	2.06	1.56	1.53
5	A	1122	POV	P-O13	-2.05	1.45	1.55
5	C	1105	POV	P-O13	-2.05	1.45	1.55
6	A	1113	CLR	C4-C5	2.05	1.56	1.51
6	B	1118	CLR	C4-C5	2.05	1.56	1.51
6	C	1118	CLR	C4-C5	2.05	1.56	1.51
6	D	1118	CLR	C4-C5	2.05	1.56	1.51
5	B	1101	POV	O21-C21	2.04	1.40	1.34
5	G	2301	POV	O31-C3	-2.03	1.40	1.45
6	A	1112	CLR	C4-C5	2.02	1.56	1.51
6	B	1117	CLR	C4-C5	2.02	1.56	1.51
6	D	1117	CLR	C4-C5	2.02	1.56	1.51
5	E	2301	POV	O31-C3	-2.02	1.40	1.45
5	F	2301	POV	O31-C3	-2.02	1.40	1.45
5	H	2301	POV	O31-C3	-2.02	1.40	1.45
6	C	1117	CLR	C4-C5	2.02	1.56	1.51
5	D	1105	POV	O21-C21	2.02	1.40	1.34
5	A	1118	POV	O21-C21	2.00	1.40	1.34
5	C	1101	POV	O21-C21	2.00	1.40	1.34
5	B	1111	POV	O21-C21	2.00	1.40	1.34
5	D	1111	POV	O21-C21	2.00	1.40	1.34

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1113	CLR	C4-C5-C6	-9.26	107.27	120.61
6	C	1118	CLR	C4-C5-C6	-9.26	107.27	120.61
6	B	1118	CLR	C4-C5-C6	-9.25	107.27	120.61
6	D	1118	CLR	C4-C5-C6	-9.25	107.27	120.61
6	A	1112	CLR	C4-C5-C6	-9.02	107.62	120.61
6	B	1117	CLR	C4-C5-C6	-9.02	107.62	120.61
6	D	1117	CLR	C4-C5-C6	-9.02	107.62	120.61
6	C	1117	CLR	C4-C5-C6	-8.99	107.66	120.61
6	C	1116	CLR	C4-C5-C6	-8.60	108.22	120.61
6	A	1111	CLR	C4-C5-C6	-8.59	108.23	120.61
6	B	1116	CLR	C4-C5-C6	-8.59	108.24	120.61
6	D	1116	CLR	C4-C5-C6	-8.59	108.24	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1115	CLR	C4-C5-C6	-8.33	108.60	120.61
6	D	1115	CLR	C4-C5-C6	-8.33	108.60	120.61
6	C	1115	CLR	C4-C5-C6	-8.32	108.62	120.61
6	A	1110	CLR	C4-C5-C6	-8.29	108.66	120.61
6	B	1115	CLR	C7-C6-C5	-6.49	113.09	125.06
6	D	1115	CLR	C7-C6-C5	-6.49	113.09	125.06
6	A	1110	CLR	C7-C6-C5	-6.48	113.11	125.06
6	C	1115	CLR	C7-C6-C5	-6.47	113.12	125.06
6	C	1117	CLR	C10-C5-C6	-6.42	113.08	122.90
6	A	1112	CLR	C10-C5-C6	-6.42	113.08	122.90
6	B	1117	CLR	C10-C5-C6	-6.40	113.10	122.90
6	D	1117	CLR	C10-C5-C6	-6.40	113.10	122.90
6	C	1116	CLR	C7-C6-C5	-6.33	113.38	125.06
6	B	1116	CLR	C7-C6-C5	-6.33	113.38	125.06
6	D	1116	CLR	C7-C6-C5	-6.33	113.38	125.06
6	A	1111	CLR	C7-C6-C5	-6.32	113.41	125.06
6	C	1115	CLR	C10-C5-C6	-6.13	113.53	122.90
6	A	1110	CLR	C10-C5-C6	-6.12	113.53	122.90
6	B	1115	CLR	C10-C5-C6	-6.11	113.56	122.90
6	D	1115	CLR	C10-C5-C6	-6.11	113.56	122.90
6	B	1116	CLR	C10-C5-C6	-5.99	113.73	122.90
6	D	1116	CLR	C10-C5-C6	-5.99	113.73	122.90
6	A	1111	CLR	C10-C5-C6	-5.98	113.76	122.90
6	C	1117	CLR	C7-C6-C5	-5.95	114.09	125.06
6	C	1116	CLR	C10-C5-C6	-5.95	113.80	122.90
6	A	1112	CLR	C7-C6-C5	-5.95	114.09	125.06
6	B	1117	CLR	C7-C6-C5	-5.94	114.11	125.06
6	D	1117	CLR	C7-C6-C5	-5.94	114.11	125.06
6	B	1118	CLR	C7-C6-C5	-5.25	115.38	125.06
6	D	1118	CLR	C7-C6-C5	-5.25	115.38	125.06
6	A	1113	CLR	C7-C6-C5	-5.25	115.38	125.06
6	C	1118	CLR	C7-C6-C5	-5.24	115.39	125.06
6	A	1113	CLR	C10-C5-C6	-5.06	115.16	122.90
6	C	1118	CLR	C10-C5-C6	-5.05	115.17	122.90
6	B	1118	CLR	C10-C5-C6	-5.05	115.18	122.90
6	D	1118	CLR	C10-C5-C6	-5.05	115.18	122.90
6	C	1115	CLR	C14-C8-C9	4.74	115.44	109.09
8	G	2305	NAG	C1-O5-C5	4.72	118.58	112.19
8	E	2305	NAG	C1-O5-C5	4.72	118.58	112.19
6	A	1110	CLR	C14-C8-C9	4.71	115.40	109.09
8	F	2305	NAG	C1-O5-C5	4.70	118.56	112.19
8	H	2305	NAG	C1-O5-C5	4.70	118.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1115	CLR	C14-C8-C9	4.69	115.37	109.09
6	D	1115	CLR	C14-C8-C9	4.69	115.37	109.09
6	C	1115	CLR	C12-C13-C17	4.63	123.50	116.57
6	A	1110	CLR	C12-C13-C17	4.61	123.47	116.57
6	B	1115	CLR	C12-C13-C17	4.61	123.47	116.57
6	D	1115	CLR	C12-C13-C17	4.61	123.47	116.57
6	A	1111	CLR	C14-C8-C9	4.56	115.19	109.09
6	C	1116	CLR	C14-C8-C9	4.55	115.18	109.09
6	B	1116	CLR	C14-C8-C9	4.53	115.15	109.09
6	D	1116	CLR	C14-C8-C9	4.53	115.15	109.09
6	B	1117	CLR	C12-C13-C17	4.27	122.97	116.57
6	D	1117	CLR	C12-C13-C17	4.27	122.97	116.57
6	C	1118	CLR	C18-C13-C12	-4.26	103.86	110.59
6	B	1118	CLR	C18-C13-C12	-4.26	103.87	110.59
6	D	1118	CLR	C18-C13-C12	-4.26	103.87	110.59
6	C	1117	CLR	C12-C13-C17	4.25	122.94	116.57
6	A	1113	CLR	C18-C13-C12	-4.25	103.88	110.59
6	A	1112	CLR	C12-C13-C17	4.23	122.90	116.57
5	C	1111	POV	O21-C21-C22	4.14	120.42	111.50
5	A	1106	POV	O21-C21-C22	4.13	120.41	111.50
5	B	1111	POV	O21-C21-C22	4.13	120.40	111.50
5	D	1111	POV	O21-C21-C22	4.13	120.40	111.50
5	A	1107	POV	C2-O21-C21	-4.13	112.57	117.88
5	B	1112	POV	C2-O21-C21	-4.12	112.58	117.88
5	C	1112	POV	C2-O21-C21	-4.12	112.58	117.88
5	D	1112	POV	C2-O21-C21	-4.12	112.58	117.88
5	C	1112	POV	O21-C21-C22	4.09	120.32	111.50
5	A	1107	POV	O21-C21-C22	4.09	120.31	111.50
5	B	1112	POV	O21-C21-C22	4.07	120.28	111.50
5	D	1112	POV	O21-C21-C22	4.07	120.28	111.50
5	A	1120	POV	O21-C21-C22	4.06	120.24	111.50
5	B	1103	POV	O21-C21-C22	4.06	120.24	111.50
5	C	1103	POV	O21-C21-C22	4.06	120.24	111.50
5	D	1103	POV	O21-C21-C22	4.06	120.24	111.50
5	B	1109	POV	O21-C21-C22	4.04	120.21	111.50
5	C	1109	POV	O21-C21-C22	4.04	120.21	111.50
5	D	1109	POV	O21-C21-C22	4.04	120.21	111.50
5	A	1104	POV	O21-C21-C22	4.03	120.18	111.50
5	D	1104	POV	O21-C21-C22	4.00	120.12	111.50
5	B	1104	POV	O21-C21-C22	4.00	120.11	111.50
5	A	1121	POV	O21-C21-C22	3.98	120.07	111.50
5	C	1104	POV	O21-C21-C22	3.98	120.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1116	CLR	C13-C17-C20	-3.92	113.34	119.49
6	A	1111	CLR	C13-C17-C20	-3.92	113.35	119.49
6	B	1116	CLR	C13-C17-C20	-3.92	113.35	119.49
6	D	1116	CLR	C13-C17-C20	-3.92	113.35	119.49
5	B	1101	POV	O21-C21-C22	3.91	119.93	111.50
5	D	1101	POV	O21-C21-C22	3.91	119.92	111.50
6	B	1118	CLR	C12-C13-C17	3.89	122.40	116.57
6	D	1118	CLR	C12-C13-C17	3.89	122.40	116.57
5	A	1118	POV	O21-C21-C22	3.89	119.89	111.50
5	C	1101	POV	O21-C21-C22	3.89	119.89	111.50
6	A	1113	CLR	C12-C13-C17	3.87	122.36	116.57
6	C	1118	CLR	C12-C13-C17	3.85	122.33	116.57
5	G	2301	POV	O21-C21-C22	3.82	119.74	111.50
5	E	2301	POV	O21-C21-C22	3.82	119.74	111.50
5	D	1105	POV	O21-C21-C22	3.80	119.70	111.50
5	F	2301	POV	O21-C21-C22	3.80	119.69	111.50
5	H	2301	POV	O21-C21-C22	3.80	119.69	111.50
5	A	1122	POV	O21-C21-C22	3.78	119.66	111.50
5	B	1105	POV	O21-C21-C22	3.78	119.66	111.50
5	C	1105	POV	O21-C21-C22	3.78	119.66	111.50
6	B	1118	CLR	C18-C13-C14	-3.69	104.83	111.71
6	D	1118	CLR	C18-C13-C14	-3.69	104.83	111.71
6	A	1113	CLR	C18-C13-C14	-3.68	104.85	111.71
6	C	1118	CLR	C18-C13-C14	-3.67	104.87	111.71
6	B	1117	CLR	C18-C13-C14	-3.65	104.92	111.71
6	D	1117	CLR	C18-C13-C14	-3.65	104.92	111.71
6	A	1110	CLR	C18-C13-C12	-3.64	104.83	110.59
6	B	1115	CLR	C18-C13-C12	-3.64	104.84	110.59
6	D	1115	CLR	C18-C13-C12	-3.64	104.84	110.59
6	C	1115	CLR	C18-C13-C12	-3.64	104.85	110.59
6	A	1112	CLR	C18-C13-C14	-3.63	104.95	111.71
6	C	1117	CLR	C18-C13-C14	-3.63	104.95	111.71
6	B	1117	CLR	C18-C13-C12	-3.58	104.93	110.59
6	D	1117	CLR	C18-C13-C12	-3.58	104.93	110.59
6	C	1117	CLR	C18-C13-C12	-3.58	104.94	110.59
6	A	1112	CLR	C18-C13-C12	-3.55	104.97	110.59
6	C	1117	CLR	C12-C13-C14	3.51	112.71	107.27
6	A	1112	CLR	C12-C13-C14	3.50	112.70	107.27
6	B	1117	CLR	C12-C13-C14	3.50	112.70	107.27
6	D	1117	CLR	C12-C13-C14	3.50	112.70	107.27
6	C	1118	CLR	C17-C13-C14	3.47	104.18	100.07
6	C	1116	CLR	C12-C13-C17	3.46	121.76	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1111	CLR	C12-C13-C17	3.46	121.75	116.57
6	B	1118	CLR	C17-C13-C14	3.46	104.17	100.07
6	D	1118	CLR	C17-C13-C14	3.46	104.17	100.07
6	B	1116	CLR	C12-C13-C17	3.45	121.74	116.57
6	D	1116	CLR	C12-C13-C17	3.45	121.74	116.57
6	A	1113	CLR	C17-C13-C14	3.44	104.14	100.07
6	A	1113	CLR	C4-C5-C10	-3.41	111.89	116.42
6	A	1113	CLR	C1-C2-C3	3.39	114.81	110.47
6	B	1118	CLR	C11-C9-C8	-3.38	106.89	111.75
6	D	1118	CLR	C11-C9-C8	-3.38	106.89	111.75
6	B	1118	CLR	C4-C5-C10	-3.38	111.93	116.42
6	D	1118	CLR	C4-C5-C10	-3.38	111.93	116.42
6	C	1118	CLR	C1-C2-C3	3.37	114.80	110.47
6	A	1113	CLR	C11-C9-C8	-3.37	106.89	111.75
6	C	1118	CLR	C11-C9-C8	-3.37	106.89	111.75
6	C	1118	CLR	C4-C5-C10	-3.37	111.94	116.42
6	B	1118	CLR	C1-C2-C3	3.36	114.78	110.47
6	D	1118	CLR	C1-C2-C3	3.36	114.78	110.47
6	B	1116	CLR	C12-C13-C14	3.28	112.36	107.27
6	D	1116	CLR	C12-C13-C14	3.28	112.36	107.27
6	A	1111	CLR	C12-C13-C14	3.27	112.34	107.27
6	B	1115	CLR	C7-C8-C9	-3.26	105.76	109.71
6	D	1115	CLR	C7-C8-C9	-3.26	105.76	109.71
6	C	1116	CLR	C12-C13-C14	3.24	112.29	107.27
6	A	1110	CLR	C7-C8-C9	-3.24	105.79	109.71
6	C	1115	CLR	C7-C8-C9	-3.23	105.80	109.71
6	C	1117	CLR	C21-C20-C22	-3.17	105.39	110.36
6	A	1112	CLR	C21-C20-C22	-3.16	105.42	110.36
6	B	1117	CLR	C21-C20-C22	-3.15	105.42	110.36
6	D	1117	CLR	C21-C20-C22	-3.15	105.42	110.36
5	A	1122	POV	O31-C31-C32	3.15	121.80	111.91
5	C	1105	POV	O31-C31-C32	3.15	121.80	111.91
5	B	1105	POV	O31-C31-C32	3.14	121.78	111.91
5	D	1105	POV	O31-C31-C32	3.14	121.75	111.91
6	A	1111	CLR	C21-C20-C17	-3.11	108.16	112.92
6	B	1116	CLR	C21-C20-C17	-3.11	108.16	112.92
6	D	1116	CLR	C21-C20-C17	-3.11	108.16	112.92
6	B	1116	CLR	C1-C10-C5	3.10	114.44	108.75
6	D	1116	CLR	C1-C10-C5	3.10	114.44	108.75
6	C	1116	CLR	C1-C10-C5	3.10	114.43	108.75
6	C	1116	CLR	C21-C20-C17	-3.10	108.17	112.92
6	A	1111	CLR	C1-C10-C5	3.09	114.42	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1116	CLR	C21-C20-C22	-3.08	105.54	110.36
6	D	1116	CLR	C21-C20-C22	-3.08	105.54	110.36
6	A	1111	CLR	C21-C20-C22	-3.04	105.59	110.36
6	C	1116	CLR	C21-C20-C22	-3.03	105.61	110.36
6	C	1115	CLR	C18-C13-C14	-3.00	106.12	111.71
6	A	1110	CLR	C18-C13-C14	-2.99	106.13	111.71
6	A	1111	CLR	C18-C13-C12	-2.99	105.87	110.59
6	B	1115	CLR	C18-C13-C14	-2.98	106.15	111.71
6	D	1115	CLR	C18-C13-C14	-2.98	106.15	111.71
6	C	1116	CLR	C18-C13-C12	-2.98	105.88	110.59
6	B	1116	CLR	C18-C13-C12	-2.97	105.89	110.59
6	D	1116	CLR	C18-C13-C12	-2.97	105.89	110.59
6	B	1115	CLR	C1-C10-C5	2.94	114.13	108.75
6	D	1115	CLR	C1-C10-C5	2.94	114.13	108.75
6	B	1115	CLR	C17-C13-C14	2.93	103.55	100.07
6	D	1115	CLR	C17-C13-C14	2.93	103.55	100.07
6	A	1111	CLR	C7-C8-C9	-2.92	106.17	109.71
6	C	1115	CLR	C1-C10-C5	2.92	114.10	108.75
6	C	1116	CLR	C7-C8-C9	-2.92	106.18	109.71
6	A	1110	CLR	C1-C10-C5	2.91	114.08	108.75
6	A	1110	CLR	C17-C13-C14	2.89	103.50	100.07
6	B	1116	CLR	C7-C8-C9	-2.89	106.21	109.71
6	D	1116	CLR	C7-C8-C9	-2.89	106.21	109.71
6	C	1115	CLR	C17-C13-C14	2.88	103.49	100.07
5	G	2301	POV	O31-C31-C32	2.83	120.79	111.91
5	F	2301	POV	O31-C31-C32	2.82	120.75	111.91
5	H	2301	POV	O31-C31-C32	2.82	120.75	111.91
5	E	2301	POV	O31-C31-C32	2.82	120.75	111.91
5	A	1106	POV	O31-C31-C32	2.82	120.75	111.91
5	B	1111	POV	O31-C31-C32	2.81	120.71	111.91
5	D	1111	POV	O31-C31-C32	2.81	120.71	111.91
5	C	1111	POV	O31-C31-C32	2.80	120.70	111.91
5	B	1101	POV	O31-C31-C32	2.77	120.59	111.91
5	A	1118	POV	O31-C31-C32	2.76	120.56	111.91
5	C	1101	POV	O31-C31-C32	2.76	120.56	111.91
6	C	1118	CLR	C9-C10-C5	2.76	113.97	109.65
6	B	1118	CLR	C9-C10-C5	2.75	113.97	109.65
6	D	1118	CLR	C9-C10-C5	2.75	113.97	109.65
6	A	1112	CLR	C9-C10-C5	2.75	113.96	109.65
6	A	1113	CLR	C11-C9-C10	2.75	116.70	113.08
5	D	1101	POV	O31-C31-C32	2.75	120.52	111.91
6	C	1118	CLR	C11-C9-C10	2.74	116.69	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1118	CLR	C11-C9-C10	2.73	116.68	113.08
6	D	1118	CLR	C11-C9-C10	2.73	116.68	113.08
6	C	1117	CLR	C9-C10-C5	2.72	113.92	109.65
6	B	1117	CLR	C9-C10-C5	2.71	113.89	109.65
6	D	1117	CLR	C9-C10-C5	2.71	113.89	109.65
6	A	1113	CLR	C9-C10-C5	2.71	113.89	109.65
8	F	2306	NAG	C1-O5-C5	2.70	115.85	112.19
8	H	2306	NAG	C1-O5-C5	2.70	115.85	112.19
8	G	2306	NAG	C1-O5-C5	2.69	115.84	112.19
8	E	2306	NAG	C1-O5-C5	2.68	115.82	112.19
6	B	1115	CLR	C18-C13-C17	-2.65	106.78	111.71
6	D	1115	CLR	C18-C13-C17	-2.65	106.78	111.71
6	B	1118	CLR	C12-C13-C14	2.64	111.37	107.27
6	D	1118	CLR	C12-C13-C14	2.64	111.37	107.27
6	C	1118	CLR	C12-C13-C14	2.64	111.37	107.27
5	D	1103	POV	O31-C31-C32	2.64	120.19	111.91
5	D	1102	POV	O21-C21-C22	2.64	120.19	111.91
5	A	1119	POV	O21-C21-C22	2.64	120.19	111.91
5	B	1102	POV	O21-C21-C22	2.64	120.19	111.91
5	C	1102	POV	O21-C21-C22	2.64	120.19	111.91
5	A	1120	POV	O31-C31-C32	2.63	120.17	111.91
5	C	1103	POV	O31-C31-C32	2.63	120.17	111.91
6	A	1113	CLR	C12-C13-C14	2.62	111.34	107.27
6	C	1115	CLR	C18-C13-C17	-2.62	106.82	111.71
5	B	1103	POV	O31-C31-C32	2.62	120.13	111.91
6	A	1110	CLR	C18-C13-C17	-2.61	106.85	111.71
5	B	1104	POV	O31-C31-C32	2.56	119.93	111.91
5	A	1121	POV	O31-C31-C32	2.55	119.92	111.91
5	C	1104	POV	O31-C31-C32	2.55	119.92	111.91
5	E	2304	POV	O21-C21-C22	2.55	119.91	111.91
5	G	2304	POV	O21-C21-C22	2.55	119.90	111.91
5	D	1104	POV	O31-C31-C32	2.54	119.88	111.91
5	F	2304	POV	O21-C21-C22	2.54	119.86	111.91
5	H	2304	POV	O21-C21-C22	2.54	119.86	111.91
5	F	2304	POV	O13-P-O14	-2.53	100.78	110.68
5	H	2304	POV	O13-P-O14	-2.53	100.78	110.68
8	E	2305	NAG	O5-C1-C2	2.51	115.25	111.29
5	E	2304	POV	O13-P-O14	-2.51	100.85	110.68
5	G	2304	POV	O13-P-O14	-2.50	100.89	110.68
5	A	1104	POV	O31-C31-C32	2.49	119.72	111.91
8	F	2305	NAG	O5-C1-C2	2.49	115.22	111.29
8	G	2305	NAG	O5-C1-C2	2.49	115.22	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	2305	NAG	O5-C1-C2	2.49	115.22	111.29
5	C	1109	POV	O31-C31-C32	2.48	119.69	111.91
5	D	1102	POV	O13-P-O14	-2.48	100.98	110.68
6	B	1117	CLR	C4-C5-C10	-2.48	113.13	116.42
6	D	1117	CLR	C4-C5-C10	-2.48	113.13	116.42
5	B	1109	POV	O31-C31-C32	2.47	119.67	111.91
5	D	1109	POV	O31-C31-C32	2.47	119.67	111.91
5	A	1119	POV	O13-P-O14	-2.47	101.01	110.68
5	B	1102	POV	O13-P-O14	-2.47	101.01	110.68
5	C	1102	POV	O13-P-O14	-2.47	101.01	110.68
6	B	1116	CLR	C16-C17-C20	2.46	115.96	112.15
6	D	1116	CLR	C16-C17-C20	2.46	115.96	112.15
5	A	1104	POV	O13-P-O14	-2.46	101.04	110.68
6	C	1116	CLR	C16-C17-C20	2.45	115.95	112.15
6	A	1112	CLR	C4-C5-C10	-2.45	113.16	116.42
5	B	1109	POV	O13-P-O14	-2.45	101.09	110.68
5	D	1109	POV	O13-P-O14	-2.45	101.09	110.68
6	A	1111	CLR	C16-C17-C20	2.45	115.94	112.15
5	C	1109	POV	O13-P-O14	-2.44	101.13	110.68
6	C	1117	CLR	C4-C5-C10	-2.44	113.18	116.42
6	A	1111	CLR	C18-C13-C14	-2.43	107.19	111.71
6	B	1116	CLR	C18-C13-C14	-2.42	107.21	111.71
6	D	1116	CLR	C18-C13-C14	-2.42	107.21	111.71
6	A	1110	CLR	C21-C20-C22	-2.41	106.58	110.36
6	C	1116	CLR	C18-C13-C14	-2.41	107.21	111.71
6	C	1115	CLR	C21-C20-C22	-2.41	106.58	110.36
6	B	1115	CLR	C21-C20-C22	-2.40	106.60	110.36
6	D	1115	CLR	C21-C20-C22	-2.40	106.60	110.36
6	A	1112	CLR	C13-C17-C20	-2.39	115.74	119.49
6	C	1117	CLR	C13-C17-C20	-2.39	115.74	119.49
6	B	1117	CLR	C13-C17-C20	-2.38	115.76	119.49
6	D	1117	CLR	C13-C17-C20	-2.38	115.76	119.49
6	A	1110	CLR	C12-C13-C14	2.36	110.94	107.27
6	B	1115	CLR	C12-C13-C14	2.36	110.94	107.27
6	D	1115	CLR	C12-C13-C14	2.36	110.94	107.27
6	C	1115	CLR	C12-C13-C14	2.36	110.93	107.27
5	A	1122	POV	O13-P-O14	-2.35	100.61	112.24
5	C	1105	POV	O13-P-O14	-2.35	100.61	112.24
5	D	1105	POV	O13-P-O14	-2.35	100.64	112.24
5	B	1105	POV	O13-P-O14	-2.35	100.65	112.24
6	B	1117	CLR	C1-C10-C9	-2.34	105.46	108.73
6	D	1117	CLR	C1-C10-C9	-2.34	105.46	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2301	POV	O13-P-O14	-2.33	100.70	112.24
5	G	2301	POV	O13-P-O14	-2.33	100.72	112.24
5	F	2301	POV	O13-P-O14	-2.33	100.73	112.24
5	H	2301	POV	O13-P-O14	-2.33	100.73	112.24
5	A	1104	POV	C28-C29-C210	-2.33	112.58	131.07
5	B	1109	POV	C28-C29-C210	-2.32	112.60	131.07
5	D	1109	POV	C28-C29-C210	-2.32	112.60	131.07
6	A	1112	CLR	C1-C10-C9	-2.32	105.48	108.73
5	C	1109	POV	C28-C29-C210	-2.32	112.61	131.07
6	C	1117	CLR	C1-C10-C9	-2.31	105.49	108.73
6	B	1116	CLR	C15-C14-C13	2.31	106.63	103.84
6	D	1116	CLR	C15-C14-C13	2.31	106.63	103.84
6	A	1111	CLR	C15-C14-C13	2.29	106.60	103.84
6	C	1116	CLR	C15-C14-C13	2.24	106.55	103.84
6	A	1113	CLR	C13-C17-C20	-2.22	116.01	119.49
6	C	1118	CLR	C13-C17-C20	-2.22	116.01	119.49
5	A	1118	POV	C28-C29-C210	-2.21	113.46	131.07
5	C	1101	POV	C28-C29-C210	-2.21	113.47	131.07
5	B	1101	POV	C28-C29-C210	-2.21	113.50	131.07
5	D	1101	POV	C28-C29-C210	-2.21	113.51	131.07
6	B	1117	CLR	C1-C10-C5	2.21	112.79	108.75
6	D	1117	CLR	C1-C10-C5	2.21	112.79	108.75
6	B	1115	CLR	C9-C10-C5	2.21	113.11	109.65
6	D	1115	CLR	C9-C10-C5	2.21	113.11	109.65
6	B	1118	CLR	C13-C17-C20	-2.20	116.04	119.49
6	D	1118	CLR	C13-C17-C20	-2.20	116.04	119.49
5	D	1101	POV	O13-P-O14	-2.20	101.35	112.24
5	A	1106	POV	O13-P-O14	-2.20	101.36	112.24
5	C	1111	POV	O13-P-O14	-2.20	101.38	112.24
6	A	1110	CLR	C9-C10-C5	2.20	113.10	109.65
6	A	1112	CLR	C14-C8-C9	2.20	112.03	109.09
5	A	1120	POV	O13-P-O14	-2.20	101.39	112.24
5	B	1103	POV	O13-P-O14	-2.20	101.39	112.24
5	C	1103	POV	O13-P-O14	-2.20	101.39	112.24
5	D	1103	POV	O13-P-O14	-2.19	101.39	112.24
5	A	1118	POV	O13-P-O14	-2.19	101.40	112.24
5	C	1101	POV	O13-P-O14	-2.19	101.40	112.24
6	C	1115	CLR	C9-C10-C5	2.19	113.09	109.65
5	B	1101	POV	O13-P-O14	-2.19	101.40	112.24
6	B	1116	CLR	C9-C10-C5	2.19	113.09	109.65
6	D	1116	CLR	C9-C10-C5	2.19	113.09	109.65
5	D	1104	POV	O13-P-O14	-2.19	101.41	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1111	POV	O13-P-O14	-2.19	101.41	112.24
5	D	1111	POV	O13-P-O14	-2.19	101.41	112.24
6	A	1112	CLR	C1-C10-C5	2.18	112.75	108.75
5	A	1121	POV	O13-P-O14	-2.18	101.45	112.24
5	B	1104	POV	O13-P-O14	-2.18	101.45	112.24
5	C	1104	POV	O13-P-O14	-2.18	101.45	112.24
6	B	1117	CLR	C14-C8-C9	2.18	112.01	109.09
6	D	1117	CLR	C14-C8-C9	2.18	112.01	109.09
6	B	1117	CLR	C18-C13-C17	-2.18	107.65	111.71
6	C	1117	CLR	C18-C13-C17	-2.18	107.65	111.71
6	D	1117	CLR	C18-C13-C17	-2.18	107.65	111.71
6	A	1112	CLR	C18-C13-C17	-2.17	107.66	111.71
6	A	1111	CLR	C9-C10-C5	2.17	113.05	109.65
6	A	1112	CLR	C1-C2-C3	2.17	113.25	110.47
6	C	1117	CLR	C1-C2-C3	2.17	113.25	110.47
6	C	1117	CLR	C1-C10-C5	2.16	112.72	108.75
6	A	1112	CLR	C11-C9-C8	-2.16	108.64	111.75
5	B	1112	POV	O13-P-O14	-2.16	101.58	112.24
5	D	1112	POV	O13-P-O14	-2.16	101.58	112.24
5	C	1112	POV	O13-P-O14	-2.16	101.58	112.24
6	C	1116	CLR	C9-C10-C5	2.16	113.03	109.65
5	A	1107	POV	O13-P-O14	-2.15	101.59	112.24
6	B	1117	CLR	C11-C9-C8	-2.15	108.66	111.75
6	D	1117	CLR	C11-C9-C8	-2.15	108.66	111.75
6	C	1117	CLR	C14-C8-C9	2.15	111.96	109.09
6	B	1116	CLR	C1-C10-C9	-2.14	105.74	108.73
6	D	1116	CLR	C1-C10-C9	-2.14	105.74	108.73
6	B	1117	CLR	C1-C2-C3	2.14	113.21	110.47
6	D	1117	CLR	C1-C2-C3	2.14	113.21	110.47
6	C	1117	CLR	C11-C9-C8	-2.13	108.68	111.75
6	C	1116	CLR	C1-C10-C9	-2.13	105.76	108.73
6	C	1117	CLR	C8-C7-C6	2.12	115.78	112.73
6	B	1117	CLR	C8-C7-C6	2.12	115.77	112.73
6	D	1117	CLR	C8-C7-C6	2.12	115.77	112.73
6	A	1111	CLR	C1-C10-C9	-2.12	105.77	108.73
6	A	1112	CLR	C8-C7-C6	2.12	115.77	112.73
6	A	1110	CLR	C13-C17-C20	-2.10	116.20	119.49
6	C	1115	CLR	C13-C17-C20	-2.09	116.22	119.49
6	C	1115	CLR	C19-C10-C5	-2.07	105.00	108.34
6	B	1115	CLR	C13-C17-C20	-2.06	116.26	119.49
6	D	1115	CLR	C13-C17-C20	-2.06	116.26	119.49
6	A	1110	CLR	C19-C10-C5	-2.06	105.02	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	B	1115	CLR	C19-C10-C5	-2.05	105.02	108.34
6	D	1115	CLR	C19-C10-C5	-2.05	105.02	108.34
5	C	1110	POV	C33-C32-C31	-2.01	109.41	114.47
5	A	1105	POV	C33-C32-C31	-2.01	109.42	114.47

There are no chirality outliers.

All (816) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1104	POV	O21-C2-C3-O31
5	A	1104	POV	C211-C210-C29-C28
5	A	1106	POV	C211-C210-C29-C28
5	A	1106	POV	O12-C11-C12-N
5	A	1107	POV	C1-O11-P-O14
5	A	1107	POV	O12-C11-C12-N
5	A	1118	POV	C11-O12-P-O11
5	A	1118	POV	C11-O12-P-O14
5	A	1118	POV	O21-C2-C3-O31
5	A	1119	POV	O11-C1-C2-O21
5	A	1120	POV	C211-C210-C29-C28
5	A	1121	POV	C1-O11-P-O14
5	A	1121	POV	O21-C2-C3-O31
5	A	1121	POV	O12-C11-C12-N
5	A	1122	POV	C1-O11-P-O12
5	A	1122	POV	C1-O11-P-O13
5	A	1122	POV	C11-O12-P-O13
5	A	1122	POV	O32-C31-O31-C3
5	E	2301	POV	C1-O11-P-O12
5	E	2301	POV	O12-C11-C12-N
5	E	2304	POV	C1-O11-P-O14
5	B	1101	POV	C11-O12-P-O11
5	B	1101	POV	C11-O12-P-O14
5	B	1101	POV	O21-C2-C3-O31
5	B	1102	POV	O11-C1-C2-O21
5	B	1103	POV	C211-C210-C29-C28
5	B	1104	POV	C1-O11-P-O14
5	B	1104	POV	O21-C2-C3-O31
5	B	1104	POV	O12-C11-C12-N
5	B	1105	POV	C1-O11-P-O12
5	B	1105	POV	C1-O11-P-O13
5	B	1105	POV	C11-O12-P-O13
5	B	1105	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
5	B	1109	POV	O21-C2-C3-O31
5	B	1109	POV	C211-C210-C29-C28
5	B	1111	POV	C211-C210-C29-C28
5	B	1111	POV	O12-C11-C12-N
5	B	1112	POV	C1-O11-P-O14
5	B	1112	POV	O12-C11-C12-N
5	F	2301	POV	C1-O11-P-O12
5	F	2301	POV	O12-C11-C12-N
5	F	2304	POV	C1-O11-P-O14
5	C	1101	POV	C11-O12-P-O11
5	C	1101	POV	C11-O12-P-O14
5	C	1101	POV	O21-C2-C3-O31
5	C	1102	POV	O11-C1-C2-O21
5	C	1103	POV	C211-C210-C29-C28
5	C	1104	POV	C1-O11-P-O14
5	C	1104	POV	O21-C2-C3-O31
5	C	1104	POV	O12-C11-C12-N
5	C	1105	POV	C1-O11-P-O12
5	C	1105	POV	C1-O11-P-O13
5	C	1105	POV	C11-O12-P-O13
5	C	1105	POV	O32-C31-O31-C3
5	C	1109	POV	O21-C2-C3-O31
5	C	1109	POV	C211-C210-C29-C28
5	C	1111	POV	C211-C210-C29-C28
5	C	1111	POV	O12-C11-C12-N
5	C	1112	POV	C1-O11-P-O14
5	C	1112	POV	O12-C11-C12-N
5	G	2301	POV	C1-O11-P-O12
5	G	2301	POV	O12-C11-C12-N
5	G	2304	POV	C1-O11-P-O14
5	D	1101	POV	C11-O12-P-O11
5	D	1101	POV	C11-O12-P-O14
5	D	1101	POV	O21-C2-C3-O31
5	D	1102	POV	O11-C1-C2-O21
5	D	1103	POV	C211-C210-C29-C28
5	D	1104	POV	C1-O11-P-O14
5	D	1104	POV	O21-C2-C3-O31
5	D	1104	POV	O12-C11-C12-N
5	D	1105	POV	C1-O11-P-O12
5	D	1105	POV	C1-O11-P-O13
5	D	1105	POV	C11-O12-P-O13
5	D	1105	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
5	D	1109	POV	O21-C2-C3-O31
5	D	1109	POV	C211-C210-C29-C28
5	D	1111	POV	C211-C210-C29-C28
5	D	1111	POV	O12-C11-C12-N
5	D	1112	POV	C1-O11-P-O14
5	D	1112	POV	O12-C11-C12-N
5	H	2301	POV	C1-O11-P-O12
5	H	2301	POV	O12-C11-C12-N
5	H	2304	POV	C1-O11-P-O14
6	A	1111	CLR	C13-C17-C20-C21
6	B	1116	CLR	C13-C17-C20-C21
6	C	1116	CLR	C13-C17-C20-C21
6	D	1116	CLR	C13-C17-C20-C21
5	A	1106	POV	O32-C31-O31-C3
5	E	2301	POV	O32-C31-O31-C3
5	B	1111	POV	O32-C31-O31-C3
5	F	2301	POV	O32-C31-O31-C3
5	C	1111	POV	O32-C31-O31-C3
5	G	2301	POV	O32-C31-O31-C3
5	D	1111	POV	O32-C31-O31-C3
5	H	2301	POV	O32-C31-O31-C3
5	A	1106	POV	C32-C31-O31-C3
5	A	1122	POV	C32-C31-O31-C3
5	E	2301	POV	C32-C31-O31-C3
5	B	1105	POV	C32-C31-O31-C3
5	B	1111	POV	C32-C31-O31-C3
5	F	2301	POV	C32-C31-O31-C3
5	C	1105	POV	C32-C31-O31-C3
5	C	1111	POV	C32-C31-O31-C3
5	G	2301	POV	C32-C31-O31-C3
5	D	1105	POV	C32-C31-O31-C3
5	D	1111	POV	C32-C31-O31-C3
5	H	2301	POV	C32-C31-O31-C3
5	A	1120	POV	O32-C31-O31-C3
5	B	1103	POV	O32-C31-O31-C3
5	C	1103	POV	O32-C31-O31-C3
5	D	1103	POV	O32-C31-O31-C3
6	A	1111	CLR	C16-C17-C20-C21
6	B	1116	CLR	C16-C17-C20-C21
6	C	1116	CLR	C16-C17-C20-C21
6	D	1116	CLR	C16-C17-C20-C21
6	A	1111	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
6	B	1116	CLR	C13-C17-C20-C22
6	C	1116	CLR	C13-C17-C20-C22
6	D	1116	CLR	C13-C17-C20-C22
5	A	1120	POV	C32-C31-O31-C3
5	B	1103	POV	C32-C31-O31-C3
5	C	1103	POV	C32-C31-O31-C3
5	D	1103	POV	C32-C31-O31-C3
5	A	1119	POV	C211-C210-C29-C28
5	B	1102	POV	C211-C210-C29-C28
5	C	1102	POV	C211-C210-C29-C28
5	D	1102	POV	C211-C210-C29-C28
8	E	2306	NAG	O5-C5-C6-O6
8	F	2306	NAG	O5-C5-C6-O6
8	G	2306	NAG	O5-C5-C6-O6
8	H	2306	NAG	O5-C5-C6-O6
5	A	1106	POV	C22-C21-O21-C2
5	B	1111	POV	C22-C21-O21-C2
5	C	1111	POV	C22-C21-O21-C2
5	D	1111	POV	C22-C21-O21-C2
6	A	1111	CLR	C16-C17-C20-C22
6	B	1116	CLR	C16-C17-C20-C22
6	C	1116	CLR	C16-C17-C20-C22
6	D	1116	CLR	C16-C17-C20-C22
6	A	1110	CLR	C17-C20-C22-C23
6	A	1113	CLR	C17-C20-C22-C23
6	B	1115	CLR	C17-C20-C22-C23
6	B	1118	CLR	C17-C20-C22-C23
6	C	1115	CLR	C17-C20-C22-C23
6	C	1118	CLR	C17-C20-C22-C23
6	D	1115	CLR	C17-C20-C22-C23
6	D	1118	CLR	C17-C20-C22-C23
8	E	2306	NAG	C4-C5-C6-O6
8	F	2306	NAG	C4-C5-C6-O6
8	G	2306	NAG	C4-C5-C6-O6
8	H	2306	NAG	C4-C5-C6-O6
6	A	1110	CLR	C21-C20-C22-C23
6	B	1115	CLR	C21-C20-C22-C23
6	C	1115	CLR	C21-C20-C22-C23
6	D	1115	CLR	C21-C20-C22-C23
5	A	1119	POV	C22-C21-O21-C2
5	B	1102	POV	C22-C21-O21-C2
5	C	1102	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
5	D	1102	POV	C22-C21-O21-C2
6	A	1113	CLR	C21-C20-C22-C23
6	B	1118	CLR	C21-C20-C22-C23
6	C	1118	CLR	C21-C20-C22-C23
6	D	1118	CLR	C21-C20-C22-C23
5	A	1121	POV	C31-C32-C33-C34
5	B	1104	POV	C31-C32-C33-C34
5	C	1104	POV	C31-C32-C33-C34
5	D	1104	POV	C31-C32-C33-C34
5	A	1120	POV	C31-C32-C33-C34
5	B	1103	POV	C31-C32-C33-C34
5	C	1103	POV	C31-C32-C33-C34
5	D	1103	POV	C31-C32-C33-C34
5	A	1119	POV	O22-C21-O21-C2
5	B	1102	POV	O22-C21-O21-C2
5	C	1102	POV	O22-C21-O21-C2
5	D	1102	POV	O22-C21-O21-C2
5	A	1122	POV	C31-C32-C33-C34
5	E	2301	POV	C31-C32-C33-C34
5	E	2304	POV	C21-C22-C23-C24
5	B	1105	POV	C31-C32-C33-C34
5	F	2301	POV	C31-C32-C33-C34
5	F	2304	POV	C21-C22-C23-C24
5	C	1105	POV	C31-C32-C33-C34
5	G	2301	POV	C31-C32-C33-C34
5	G	2304	POV	C21-C22-C23-C24
5	D	1105	POV	C31-C32-C33-C34
5	H	2301	POV	C31-C32-C33-C34
5	H	2304	POV	C21-C22-C23-C24
6	A	1112	CLR	C20-C22-C23-C24
6	B	1117	CLR	C20-C22-C23-C24
6	C	1117	CLR	C20-C22-C23-C24
6	D	1117	CLR	C20-C22-C23-C24
5	A	1106	POV	O22-C21-O21-C2
5	B	1111	POV	O22-C21-O21-C2
5	C	1111	POV	O22-C21-O21-C2
5	D	1111	POV	O22-C21-O21-C2
6	A	1110	CLR	C22-C23-C24-C25
6	B	1115	CLR	C22-C23-C24-C25
6	C	1115	CLR	C22-C23-C24-C25
6	D	1115	CLR	C22-C23-C24-C25
5	A	1107	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
5	B	1112	POV	C2-C1-O11-P
5	C	1112	POV	C2-C1-O11-P
5	D	1112	POV	C2-C1-O11-P
5	A	1106	POV	C1-O11-P-O12
5	A	1106	POV	C11-O12-P-O11
5	A	1107	POV	C1-O11-P-O12
5	A	1121	POV	C1-O11-P-O12
5	A	1122	POV	C11-O12-P-O11
5	B	1104	POV	C1-O11-P-O12
5	B	1105	POV	C11-O12-P-O11
5	B	1111	POV	C1-O11-P-O12
5	B	1111	POV	C11-O12-P-O11
5	B	1112	POV	C1-O11-P-O12
5	C	1104	POV	C1-O11-P-O12
5	C	1105	POV	C11-O12-P-O11
5	C	1111	POV	C1-O11-P-O12
5	C	1111	POV	C11-O12-P-O11
5	C	1112	POV	C1-O11-P-O12
5	D	1104	POV	C1-O11-P-O12
5	D	1105	POV	C11-O12-P-O11
5	D	1111	POV	C1-O11-P-O12
5	D	1111	POV	C11-O12-P-O11
5	D	1112	POV	C1-O11-P-O12
5	A	1118	POV	C31-C32-C33-C34
5	B	1101	POV	C31-C32-C33-C34
5	C	1101	POV	C31-C32-C33-C34
5	D	1101	POV	C31-C32-C33-C34
5	A	1107	POV	C22-C21-O21-C2
5	B	1112	POV	C22-C21-O21-C2
5	C	1112	POV	C22-C21-O21-C2
5	D	1112	POV	C22-C21-O21-C2
5	A	1106	POV	C22-C23-C24-C25
5	A	1109	POV	C37-C38-C39-C310
5	A	1118	POV	C23-C24-C25-C26
5	A	1120	POV	C24-C25-C26-C27
5	B	1101	POV	C23-C24-C25-C26
5	B	1103	POV	C24-C25-C26-C27
5	B	1111	POV	C22-C23-C24-C25
5	B	1114	POV	C37-C38-C39-C310
5	C	1101	POV	C23-C24-C25-C26
5	C	1103	POV	C24-C25-C26-C27
5	C	1111	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
5	C	1114	POV	C37-C38-C39-C310
5	D	1101	POV	C23-C24-C25-C26
5	D	1103	POV	C24-C25-C26-C27
5	D	1111	POV	C22-C23-C24-C25
5	D	1114	POV	C37-C38-C39-C310
5	A	1109	POV	C35-C36-C37-C38
5	B	1114	POV	C35-C36-C37-C38
5	C	1114	POV	C35-C36-C37-C38
5	D	1114	POV	C35-C36-C37-C38
5	A	1107	POV	O22-C21-O21-C2
5	B	1112	POV	O22-C21-O21-C2
5	C	1112	POV	O22-C21-O21-C2
5	D	1112	POV	O22-C21-O21-C2
5	E	2301	POV	C24-C25-C26-C27
5	F	2301	POV	C24-C25-C26-C27
5	G	2301	POV	C24-C25-C26-C27
5	H	2301	POV	C24-C25-C26-C27
5	A	1106	POV	C2-C1-O11-P
5	B	1111	POV	C2-C1-O11-P
5	D	1111	POV	C2-C1-O11-P
5	A	1106	POV	C21-C22-C23-C24
5	B	1111	POV	C21-C22-C23-C24
5	C	1111	POV	C21-C22-C23-C24
5	D	1111	POV	C21-C22-C23-C24
5	A	1119	POV	C24-C25-C26-C27
5	B	1102	POV	C24-C25-C26-C27
5	C	1102	POV	C24-C25-C26-C27
5	D	1102	POV	C24-C25-C26-C27
5	A	1106	POV	C23-C24-C25-C26
5	A	1107	POV	C24-C25-C26-C27
5	B	1112	POV	C24-C25-C26-C27
5	C	1111	POV	C23-C24-C25-C26
5	C	1112	POV	C24-C25-C26-C27
5	D	1112	POV	C24-C25-C26-C27
5	B	1111	POV	C23-C24-C25-C26
5	D	1111	POV	C23-C24-C25-C26
5	E	2301	POV	C211-C212-C213-C214
5	F	2301	POV	C211-C212-C213-C214
5	G	2301	POV	C211-C212-C213-C214
5	H	2301	POV	C211-C212-C213-C214
5	A	1105	POV	C34-C35-C36-C37
5	B	1110	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	C	1110	POV	C34-C35-C36-C37
5	D	1110	POV	C34-C35-C36-C37
5	A	1118	POV	C311-C310-C39-C38
5	B	1101	POV	C311-C310-C39-C38
5	C	1101	POV	C311-C310-C39-C38
5	D	1101	POV	C311-C310-C39-C38
5	A	1104	POV	C24-C25-C26-C27
5	B	1109	POV	C24-C25-C26-C27
5	C	1109	POV	C24-C25-C26-C27
5	D	1109	POV	C24-C25-C26-C27
5	A	1120	POV	C22-C21-O21-C2
5	B	1103	POV	C22-C21-O21-C2
5	C	1103	POV	C22-C21-O21-C2
5	D	1103	POV	C22-C21-O21-C2
5	A	1118	POV	C311-C312-C313-C314
5	B	1101	POV	C311-C312-C313-C314
5	C	1101	POV	C311-C312-C313-C314
5	D	1101	POV	C311-C312-C313-C314
5	E	2301	POV	C26-C27-C28-C29
5	F	2301	POV	C26-C27-C28-C29
5	G	2301	POV	C26-C27-C28-C29
5	H	2301	POV	C26-C27-C28-C29
5	A	1118	POV	C32-C31-O31-C3
5	B	1101	POV	C32-C31-O31-C3
5	C	1101	POV	C32-C31-O31-C3
5	D	1101	POV	C32-C31-O31-C3
5	A	1118	POV	C33-C34-C35-C36
5	C	1101	POV	C33-C34-C35-C36
5	D	1101	POV	C33-C34-C35-C36
5	B	1101	POV	C33-C34-C35-C36
5	A	1120	POV	O22-C21-O21-C2
5	B	1103	POV	O22-C21-O21-C2
5	C	1103	POV	O22-C21-O21-C2
5	D	1103	POV	O22-C21-O21-C2
5	C	1111	POV	C2-C1-O11-P
5	A	1122	POV	C37-C38-C39-C310
5	B	1105	POV	C37-C38-C39-C310
5	C	1105	POV	C37-C38-C39-C310
5	D	1105	POV	C37-C38-C39-C310
5	A	1118	POV	C24-C25-C26-C27
5	B	1101	POV	C24-C25-C26-C27
5	C	1101	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
5	D	1101	POV	C24-C25-C26-C27
5	A	1118	POV	C22-C21-O21-C2
5	B	1101	POV	C22-C21-O21-C2
5	C	1101	POV	C22-C21-O21-C2
5	D	1101	POV	C22-C21-O21-C2
5	A	1118	POV	C211-C210-C29-C28
5	B	1101	POV	C211-C210-C29-C28
5	C	1101	POV	C211-C210-C29-C28
5	D	1101	POV	C211-C210-C29-C28
6	A	1112	CLR	C13-C17-C20-C21
6	B	1117	CLR	C13-C17-C20-C21
6	C	1117	CLR	C13-C17-C20-C21
6	D	1117	CLR	C13-C17-C20-C21
5	E	2301	POV	C34-C35-C36-C37
5	F	2301	POV	C34-C35-C36-C37
5	H	2301	POV	C34-C35-C36-C37
5	A	1104	POV	C26-C27-C28-C29
5	B	1109	POV	C26-C27-C28-C29
5	C	1109	POV	C26-C27-C28-C29
5	D	1109	POV	C26-C27-C28-C29
5	G	2301	POV	C34-C35-C36-C37
5	A	1118	POV	C25-C26-C27-C28
5	A	1118	POV	C37-C38-C39-C310
5	B	1101	POV	C25-C26-C27-C28
5	B	1101	POV	C37-C38-C39-C310
5	C	1101	POV	C25-C26-C27-C28
5	C	1101	POV	C37-C38-C39-C310
5	D	1101	POV	C25-C26-C27-C28
5	D	1101	POV	C37-C38-C39-C310
5	A	1121	POV	C21-C22-C23-C24
5	B	1104	POV	C21-C22-C23-C24
5	C	1104	POV	C21-C22-C23-C24
5	D	1104	POV	C21-C22-C23-C24
5	A	1105	POV	C37-C38-C39-C310
5	C	1110	POV	C37-C38-C39-C310
5	A	1122	POV	C22-C21-O21-C2
5	B	1105	POV	C22-C21-O21-C2
5	C	1105	POV	C22-C21-O21-C2
5	D	1105	POV	C22-C21-O21-C2
5	A	1122	POV	O11-C1-C2-O21
5	B	1105	POV	O11-C1-C2-O21
5	C	1105	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
5	D	1105	POV	O11-C1-C2-O21
5	B	1110	POV	C37-C38-C39-C310
5	D	1110	POV	C37-C38-C39-C310
5	A	1118	POV	O32-C31-O31-C3
5	C	1101	POV	O32-C31-O31-C3
5	E	2301	POV	C27-C28-C29-C210
5	F	2301	POV	C27-C28-C29-C210
5	G	2301	POV	C27-C28-C29-C210
5	H	2301	POV	C27-C28-C29-C210
5	A	1107	POV	C23-C24-C25-C26
5	B	1112	POV	C23-C24-C25-C26
5	C	1112	POV	C23-C24-C25-C26
5	D	1112	POV	C23-C24-C25-C26
5	A	1118	POV	O22-C21-O21-C2
5	A	1122	POV	O22-C21-O21-C2
5	B	1101	POV	O22-C21-O21-C2
5	B	1105	POV	O22-C21-O21-C2
5	C	1101	POV	O22-C21-O21-C2
5	C	1105	POV	O22-C21-O21-C2
5	D	1101	POV	O22-C21-O21-C2
5	D	1105	POV	O22-C21-O21-C2
5	A	1109	POV	C32-C33-C34-C35
5	B	1114	POV	C32-C33-C34-C35
5	C	1114	POV	C32-C33-C34-C35
5	D	1114	POV	C32-C33-C34-C35
5	B	1101	POV	O32-C31-O31-C3
5	D	1101	POV	O32-C31-O31-C3
5	A	1104	POV	C33-C34-C35-C36
5	C	1109	POV	C33-C34-C35-C36
5	B	1109	POV	C33-C34-C35-C36
5	D	1109	POV	C33-C34-C35-C36
5	A	1106	POV	O11-C1-C2-C3
5	E	2301	POV	O11-C1-C2-C3
5	B	1111	POV	O11-C1-C2-C3
5	F	2301	POV	O11-C1-C2-C3
5	C	1111	POV	O11-C1-C2-C3
5	G	2301	POV	O11-C1-C2-C3
5	D	1111	POV	O11-C1-C2-C3
5	H	2301	POV	O11-C1-C2-C3
5	E	2304	POV	C22-C23-C24-C25
5	F	2304	POV	C22-C23-C24-C25
5	H	2304	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
5	G	2304	POV	C22-C23-C24-C25
6	A	1110	CLR	C13-C17-C20-C21
6	B	1115	CLR	C13-C17-C20-C21
6	C	1115	CLR	C13-C17-C20-C21
6	D	1115	CLR	C13-C17-C20-C21
5	A	1109	POV	C33-C34-C35-C36
5	A	1121	POV	C1-C2-C3-O31
5	B	1104	POV	C1-C2-C3-O31
5	B	1114	POV	C33-C34-C35-C36
5	C	1104	POV	C1-C2-C3-O31
5	D	1104	POV	C1-C2-C3-O31
5	D	1114	POV	C33-C34-C35-C36
5	C	1114	POV	C33-C34-C35-C36
5	A	1119	POV	C211-C212-C213-C214
5	B	1102	POV	C211-C212-C213-C214
5	C	1102	POV	C211-C212-C213-C214
5	D	1102	POV	C211-C212-C213-C214
5	E	2301	POV	C215-C216-C217-C218
5	A	1122	POV	C33-C34-C35-C36
5	F	2301	POV	C215-C216-C217-C218
5	C	1105	POV	C33-C34-C35-C36
5	G	2301	POV	C215-C216-C217-C218
5	H	2301	POV	C215-C216-C217-C218
5	B	1105	POV	C33-C34-C35-C36
5	D	1105	POV	C33-C34-C35-C36
5	A	1106	POV	C31-C32-C33-C34
5	B	1111	POV	C31-C32-C33-C34
5	C	1111	POV	C31-C32-C33-C34
5	D	1111	POV	C31-C32-C33-C34
5	A	1104	POV	C32-C31-O31-C3
5	B	1109	POV	C32-C31-O31-C3
5	C	1109	POV	C32-C31-O31-C3
5	D	1109	POV	C32-C31-O31-C3
6	A	1113	CLR	C13-C17-C20-C21
6	B	1118	CLR	C13-C17-C20-C21
6	C	1118	CLR	C13-C17-C20-C21
6	D	1118	CLR	C13-C17-C20-C21
5	B	1105	POV	C39-C310-C311-C312
5	D	1105	POV	C39-C310-C311-C312
5	A	1122	POV	C39-C310-C311-C312
5	C	1105	POV	C39-C310-C311-C312
5	B	1104	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	D	1104	POV	C33-C34-C35-C36
5	A	1121	POV	C33-C34-C35-C36
5	C	1104	POV	C33-C34-C35-C36
6	A	1112	CLR	C16-C17-C20-C21
6	A	1113	CLR	C16-C17-C20-C21
6	B	1117	CLR	C16-C17-C20-C21
6	B	1118	CLR	C16-C17-C20-C21
6	C	1117	CLR	C16-C17-C20-C21
6	C	1118	CLR	C16-C17-C20-C21
6	D	1117	CLR	C16-C17-C20-C21
6	D	1118	CLR	C16-C17-C20-C21
6	A	1110	CLR	C16-C17-C20-C21
6	B	1115	CLR	C16-C17-C20-C21
6	C	1115	CLR	C16-C17-C20-C21
6	D	1115	CLR	C16-C17-C20-C21
5	A	1122	POV	C24-C25-C26-C27
5	B	1105	POV	C24-C25-C26-C27
5	C	1105	POV	C24-C25-C26-C27
5	D	1105	POV	C24-C25-C26-C27
6	A	1113	CLR	C13-C17-C20-C22
6	B	1118	CLR	C13-C17-C20-C22
6	C	1118	CLR	C13-C17-C20-C22
6	D	1118	CLR	C13-C17-C20-C22
5	B	1109	POV	O32-C31-O31-C3
5	D	1109	POV	O32-C31-O31-C3
5	A	1121	POV	O11-C1-C2-C3
5	A	1122	POV	O11-C1-C2-C3
5	B	1104	POV	O11-C1-C2-C3
5	B	1105	POV	O11-C1-C2-C3
5	C	1104	POV	O11-C1-C2-C3
5	C	1105	POV	O11-C1-C2-C3
5	D	1104	POV	O11-C1-C2-C3
5	D	1105	POV	O11-C1-C2-C3
5	A	1104	POV	O32-C31-O31-C3
5	C	1109	POV	O32-C31-O31-C3
5	A	1104	POV	C21-C22-C23-C24
5	B	1109	POV	C21-C22-C23-C24
5	C	1109	POV	C21-C22-C23-C24
5	D	1109	POV	C21-C22-C23-C24
5	A	1118	POV	C34-C35-C36-C37
5	B	1101	POV	C34-C35-C36-C37
5	C	1101	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	D	1101	POV	C34-C35-C36-C37
5	A	1105	POV	C311-C310-C39-C38
5	C	1110	POV	C311-C310-C39-C38
5	B	1110	POV	C311-C310-C39-C38
5	D	1110	POV	C311-C310-C39-C38
5	A	1104	POV	C1-C2-C3-O31
5	A	1118	POV	C1-C2-C3-O31
5	B	1101	POV	C1-C2-C3-O31
5	B	1109	POV	C1-C2-C3-O31
5	C	1101	POV	C1-C2-C3-O31
5	C	1109	POV	C1-C2-C3-O31
5	D	1101	POV	C1-C2-C3-O31
5	D	1109	POV	C1-C2-C3-O31
5	A	1122	POV	C22-C23-C24-C25
5	B	1105	POV	C22-C23-C24-C25
5	C	1105	POV	C22-C23-C24-C25
5	A	1120	POV	C22-C23-C24-C25
5	B	1103	POV	C22-C23-C24-C25
5	C	1103	POV	C22-C23-C24-C25
5	D	1103	POV	C22-C23-C24-C25
5	D	1105	POV	C22-C23-C24-C25
5	A	1106	POV	O11-C1-C2-O21
5	E	2301	POV	O11-C1-C2-O21
5	B	1111	POV	O11-C1-C2-O21
5	F	2301	POV	O11-C1-C2-O21
5	C	1111	POV	O11-C1-C2-O21
5	G	2301	POV	O11-C1-C2-O21
5	D	1111	POV	O11-C1-C2-O21
5	H	2301	POV	O11-C1-C2-O21
6	A	1110	CLR	C13-C17-C20-C22
6	B	1115	CLR	C13-C17-C20-C22
6	C	1115	CLR	C13-C17-C20-C22
6	D	1115	CLR	C13-C17-C20-C22
5	E	2301	POV	C211-C210-C29-C28
5	F	2301	POV	C211-C210-C29-C28
5	G	2301	POV	C211-C210-C29-C28
5	H	2301	POV	C211-C210-C29-C28
5	E	2301	POV	C213-C214-C215-C216
5	F	2301	POV	C213-C214-C215-C216
5	G	2301	POV	C213-C214-C215-C216
5	H	2301	POV	C213-C214-C215-C216
5	D	1101	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
5	A	1118	POV	C39-C310-C311-C312
5	E	2303	POV	C31-C32-C33-C34
5	B	1101	POV	C39-C310-C311-C312
5	F	2303	POV	C31-C32-C33-C34
5	C	1101	POV	C39-C310-C311-C312
5	G	2303	POV	C31-C32-C33-C34
5	H	2303	POV	C31-C32-C33-C34
6	A	1113	CLR	C16-C17-C20-C22
6	B	1118	CLR	C16-C17-C20-C22
6	C	1118	CLR	C16-C17-C20-C22
6	D	1118	CLR	C16-C17-C20-C22
5	A	1120	POV	O11-C1-C2-C3
5	B	1103	POV	O11-C1-C2-C3
5	C	1103	POV	O11-C1-C2-C3
5	D	1103	POV	O11-C1-C2-C3
5	A	1118	POV	C22-C23-C24-C25
5	B	1101	POV	C22-C23-C24-C25
5	C	1101	POV	C22-C23-C24-C25
5	D	1101	POV	C22-C23-C24-C25
5	E	2301	POV	C29-C210-C211-C212
5	F	2301	POV	C29-C210-C211-C212
5	G	2301	POV	C29-C210-C211-C212
5	H	2301	POV	C29-C210-C211-C212
6	A	1112	CLR	C13-C17-C20-C22
6	B	1117	CLR	C13-C17-C20-C22
6	C	1117	CLR	C13-C17-C20-C22
6	D	1117	CLR	C13-C17-C20-C22
5	A	1119	POV	C23-C24-C25-C26
5	C	1102	POV	C23-C24-C25-C26
5	B	1102	POV	C23-C24-C25-C26
5	D	1102	POV	C23-C24-C25-C26
5	A	1106	POV	C1-C2-C3-O31
5	B	1111	POV	C1-C2-C3-O31
5	C	1111	POV	C1-C2-C3-O31
5	D	1111	POV	C1-C2-C3-O31
5	A	1118	POV	O11-C1-C2-O21
5	A	1120	POV	O11-C1-C2-O21
5	A	1121	POV	O11-C1-C2-O21
5	B	1101	POV	O11-C1-C2-O21
5	B	1103	POV	O11-C1-C2-O21
5	B	1104	POV	O11-C1-C2-O21
5	C	1101	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
5	C	1103	POV	O11-C1-C2-O21
5	C	1104	POV	O11-C1-C2-O21
5	D	1101	POV	O11-C1-C2-O21
5	D	1103	POV	O11-C1-C2-O21
5	D	1104	POV	O11-C1-C2-O21
5	E	2303	POV	C33-C34-C35-C36
5	F	2303	POV	C33-C34-C35-C36
5	G	2303	POV	C33-C34-C35-C36
5	H	2303	POV	C33-C34-C35-C36
5	A	1106	POV	O21-C2-C3-O31
5	B	1111	POV	O21-C2-C3-O31
5	C	1111	POV	O21-C2-C3-O31
5	D	1111	POV	O21-C2-C3-O31
6	A	1110	CLR	C20-C22-C23-C24
6	B	1115	CLR	C20-C22-C23-C24
6	C	1115	CLR	C20-C22-C23-C24
6	D	1115	CLR	C20-C22-C23-C24
5	A	1106	POV	C24-C25-C26-C27
5	C	1111	POV	C24-C25-C26-C27
5	B	1111	POV	C24-C25-C26-C27
5	D	1111	POV	C24-C25-C26-C27
6	A	1111	CLR	C23-C24-C25-C27
5	A	1106	POV	C1-O11-P-O13
5	A	1106	POV	C11-O12-P-O13
5	A	1106	POV	C11-O12-P-O14
5	A	1107	POV	C1-O11-P-O13
5	A	1118	POV	C11-O12-P-O13
5	A	1122	POV	C1-O11-P-O14
5	A	1122	POV	C11-O12-P-O14
5	B	1101	POV	C11-O12-P-O13
5	B	1105	POV	C1-O11-P-O14
5	B	1105	POV	C11-O12-P-O14
5	B	1111	POV	C1-O11-P-O13
5	B	1111	POV	C11-O12-P-O13
5	B	1111	POV	C11-O12-P-O14
5	B	1112	POV	C1-O11-P-O13
5	C	1101	POV	C11-O12-P-O13
5	C	1105	POV	C1-O11-P-O14
5	C	1105	POV	C11-O12-P-O14
5	C	1111	POV	C1-O11-P-O13
5	C	1111	POV	C11-O12-P-O13
5	C	1111	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
5	C	1112	POV	C1-O11-P-O13
5	D	1101	POV	C11-O12-P-O13
5	D	1105	POV	C1-O11-P-O14
5	D	1105	POV	C11-O12-P-O14
5	D	1111	POV	C1-O11-P-O13
5	D	1111	POV	C11-O12-P-O13
5	D	1111	POV	C11-O12-P-O14
5	D	1112	POV	C1-O11-P-O13
6	B	1116	CLR	C23-C24-C25-C27
6	C	1116	CLR	C23-C24-C25-C27
6	D	1116	CLR	C23-C24-C25-C27
5	A	1121	POV	C32-C31-O31-C3
5	B	1104	POV	C32-C31-O31-C3
5	C	1104	POV	C32-C31-O31-C3
5	D	1104	POV	C32-C31-O31-C3
5	A	1104	POV	C25-C26-C27-C28
5	A	1105	POV	C36-C37-C38-C39
5	B	1109	POV	C25-C26-C27-C28
5	B	1110	POV	C36-C37-C38-C39
5	C	1109	POV	C25-C26-C27-C28
5	D	1109	POV	C25-C26-C27-C28
5	D	1110	POV	C36-C37-C38-C39
5	E	2301	POV	C21-C22-C23-C24
5	F	2301	POV	C21-C22-C23-C24
5	G	2301	POV	C21-C22-C23-C24
5	H	2301	POV	C21-C22-C23-C24
5	C	1110	POV	C36-C37-C38-C39
5	D	1101	POV	C35-C36-C37-C38
5	A	1118	POV	C35-C36-C37-C38
5	B	1101	POV	C35-C36-C37-C38
5	C	1101	POV	C35-C36-C37-C38
5	A	1104	POV	O11-C1-C2-O21
5	B	1109	POV	O11-C1-C2-O21
5	C	1109	POV	O11-C1-C2-O21
5	D	1109	POV	O11-C1-C2-O21
5	A	1122	POV	C11-C12-N-C13
5	B	1105	POV	C11-C12-N-C13
5	C	1105	POV	C11-C12-N-C13
5	D	1105	POV	C11-C12-N-C13
5	A	1118	POV	O12-C11-C12-N
5	A	1120	POV	O12-C11-C12-N
5	B	1101	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
5	B	1103	POV	O12-C11-C12-N
5	C	1101	POV	O12-C11-C12-N
5	C	1103	POV	O12-C11-C12-N
5	D	1101	POV	O12-C11-C12-N
5	D	1103	POV	O12-C11-C12-N
5	A	1104	POV	C22-C23-C24-C25
5	B	1109	POV	C22-C23-C24-C25
5	C	1109	POV	C22-C23-C24-C25
5	D	1109	POV	C22-C23-C24-C25
5	D	1104	POV	O32-C31-O31-C3
5	A	1121	POV	C32-C33-C34-C35
5	C	1104	POV	C32-C33-C34-C35
5	B	1104	POV	C32-C33-C34-C35
5	D	1104	POV	C32-C33-C34-C35
5	A	1122	POV	C36-C37-C38-C39
5	C	1105	POV	C36-C37-C38-C39
5	A	1121	POV	O32-C31-O31-C3
5	C	1104	POV	O32-C31-O31-C3
5	D	1105	POV	C36-C37-C38-C39
5	B	1105	POV	C36-C37-C38-C39
5	B	1104	POV	O32-C31-O31-C3
5	A	1122	POV	C11-C12-N-C14
5	A	1122	POV	C11-C12-N-C15
5	B	1105	POV	C11-C12-N-C14
5	B	1105	POV	C11-C12-N-C15
5	C	1105	POV	C11-C12-N-C14
5	C	1105	POV	C11-C12-N-C15
5	D	1105	POV	C11-C12-N-C14
5	D	1105	POV	C11-C12-N-C15
5	B	1102	POV	C22-C23-C24-C25
5	D	1102	POV	C22-C23-C24-C25
6	C	1115	CLR	C16-C17-C20-C22
5	A	1119	POV	C22-C23-C24-C25
5	C	1102	POV	C22-C23-C24-C25
5	A	1118	POV	O11-C1-C2-C3
5	B	1101	POV	O11-C1-C2-C3
5	C	1101	POV	O11-C1-C2-C3
5	D	1101	POV	O11-C1-C2-C3
6	B	1115	CLR	C16-C17-C20-C22
6	D	1115	CLR	C16-C17-C20-C22
6	A	1110	CLR	C16-C17-C20-C22
5	A	1118	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
5	A	1120	POV	C11-O12-P-O11
5	E	2301	POV	C11-O12-P-O11
5	B	1101	POV	C1-O11-P-O12
5	B	1103	POV	C11-O12-P-O11
5	F	2301	POV	C11-O12-P-O11
5	C	1101	POV	C1-O11-P-O12
5	C	1103	POV	C11-O12-P-O11
5	G	2301	POV	C11-O12-P-O11
5	D	1101	POV	C1-O11-P-O12
5	D	1103	POV	C11-O12-P-O11
5	H	2301	POV	C11-O12-P-O11
5	A	1118	POV	C32-C33-C34-C35
5	C	1101	POV	C32-C33-C34-C35
5	A	1118	POV	C27-C28-C29-C210
5	B	1101	POV	C27-C28-C29-C210
5	C	1101	POV	C27-C28-C29-C210
5	D	1101	POV	C27-C28-C29-C210
5	B	1101	POV	C32-C33-C34-C35
5	D	1101	POV	C32-C33-C34-C35
5	D	1105	POV	C311-C310-C39-C38
5	A	1122	POV	C311-C310-C39-C38
5	B	1105	POV	C311-C310-C39-C38
5	C	1105	POV	C311-C310-C39-C38
5	E	2303	POV	C34-C35-C36-C37
5	F	2303	POV	C34-C35-C36-C37
5	G	2303	POV	C34-C35-C36-C37
5	H	2303	POV	C34-C35-C36-C37
6	A	1112	CLR	C16-C17-C20-C22
6	B	1117	CLR	C16-C17-C20-C22
6	C	1117	CLR	C16-C17-C20-C22
6	D	1117	CLR	C16-C17-C20-C22
5	A	1104	POV	O31-C31-C32-C33
5	B	1109	POV	O31-C31-C32-C33
5	C	1109	POV	O31-C31-C32-C33
5	D	1109	POV	O31-C31-C32-C33
5	E	2302	POV	C24-C25-C26-C27
5	F	2302	POV	C24-C25-C26-C27
5	G	2302	POV	C24-C25-C26-C27
5	H	2302	POV	C24-C25-C26-C27
5	A	1104	POV	O11-C1-C2-C3
5	B	1109	POV	O11-C1-C2-C3
5	C	1109	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	D	1109	POV	O11-C1-C2-C3
5	G	2301	POV	C33-C34-C35-C36
5	E	2301	POV	C33-C34-C35-C36
5	F	2301	POV	C33-C34-C35-C36
5	H	2301	POV	C33-C34-C35-C36
5	A	1104	POV	C2-C1-O11-P
5	B	1109	POV	C2-C1-O11-P
5	C	1109	POV	C2-C1-O11-P
5	D	1109	POV	C2-C1-O11-P
5	A	1107	POV	C21-C22-C23-C24
5	C	1112	POV	C21-C22-C23-C24
5	B	1112	POV	C21-C22-C23-C24
5	D	1112	POV	C21-C22-C23-C24
5	B	1109	POV	O21-C21-C22-C23
5	C	1109	POV	O21-C21-C22-C23
5	D	1109	POV	O21-C21-C22-C23
5	A	1104	POV	O21-C21-C22-C23
5	A	1107	POV	O21-C21-C22-C23
5	B	1112	POV	O21-C21-C22-C23
5	D	1112	POV	O21-C21-C22-C23
5	C	1112	POV	O21-C21-C22-C23
5	A	1119	POV	C26-C27-C28-C29
5	B	1102	POV	C26-C27-C28-C29
5	C	1102	POV	C26-C27-C28-C29
5	D	1102	POV	C26-C27-C28-C29
5	A	1108	POV	C23-C24-C25-C26
5	C	1113	POV	C23-C24-C25-C26
5	B	1113	POV	C23-C24-C25-C26
5	D	1113	POV	C23-C24-C25-C26
5	A	1104	POV	O22-C21-C22-C23
5	B	1109	POV	O22-C21-C22-C23
5	B	1112	POV	O22-C21-C22-C23
5	C	1112	POV	O22-C21-C22-C23
5	D	1109	POV	O22-C21-C22-C23
5	D	1112	POV	O22-C21-C22-C23
5	A	1118	POV	C310-C311-C312-C313
5	C	1101	POV	C310-C311-C312-C313
5	A	1107	POV	O22-C21-C22-C23
5	C	1109	POV	O22-C21-C22-C23
5	B	1101	POV	C310-C311-C312-C313
5	D	1101	POV	C310-C311-C312-C313
5	A	1121	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	B	1104	POV	C34-C35-C36-C37
5	C	1104	POV	C34-C35-C36-C37
5	D	1104	POV	C34-C35-C36-C37
5	A	1118	POV	C1-O11-P-O14
5	B	1101	POV	C1-O11-P-O14
5	C	1101	POV	C1-O11-P-O14
5	D	1101	POV	C1-O11-P-O14
6	A	1113	CLR	C22-C23-C24-C25
6	B	1118	CLR	C22-C23-C24-C25
6	C	1118	CLR	C22-C23-C24-C25
6	D	1118	CLR	C22-C23-C24-C25
5	A	1107	POV	C12-C11-O12-P
5	A	1121	POV	C12-C11-O12-P
5	A	1122	POV	C12-C11-O12-P
5	B	1104	POV	C12-C11-O12-P
5	B	1105	POV	C12-C11-O12-P
5	B	1112	POV	C12-C11-O12-P
5	C	1104	POV	C12-C11-O12-P
5	C	1105	POV	C12-C11-O12-P
5	C	1112	POV	C12-C11-O12-P
5	D	1104	POV	C12-C11-O12-P
5	D	1105	POV	C12-C11-O12-P
5	D	1112	POV	C12-C11-O12-P
5	A	1118	POV	C36-C37-C38-C39
5	C	1101	POV	C36-C37-C38-C39
5	D	1101	POV	C36-C37-C38-C39
5	B	1101	POV	C36-C37-C38-C39

There are no ring outliers.

43 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1116	CLR	4	0
5	B	1109	POV	1	0
5	A	1105	POV	1	0
5	C	1105	POV	1	0
6	C	1115	CLR	8	0
5	A	1118	POV	2	0
6	B	1116	CLR	5	0
5	B	1101	POV	2	0
6	D	1115	CLR	7	0
6	B	1118	CLR	6	0

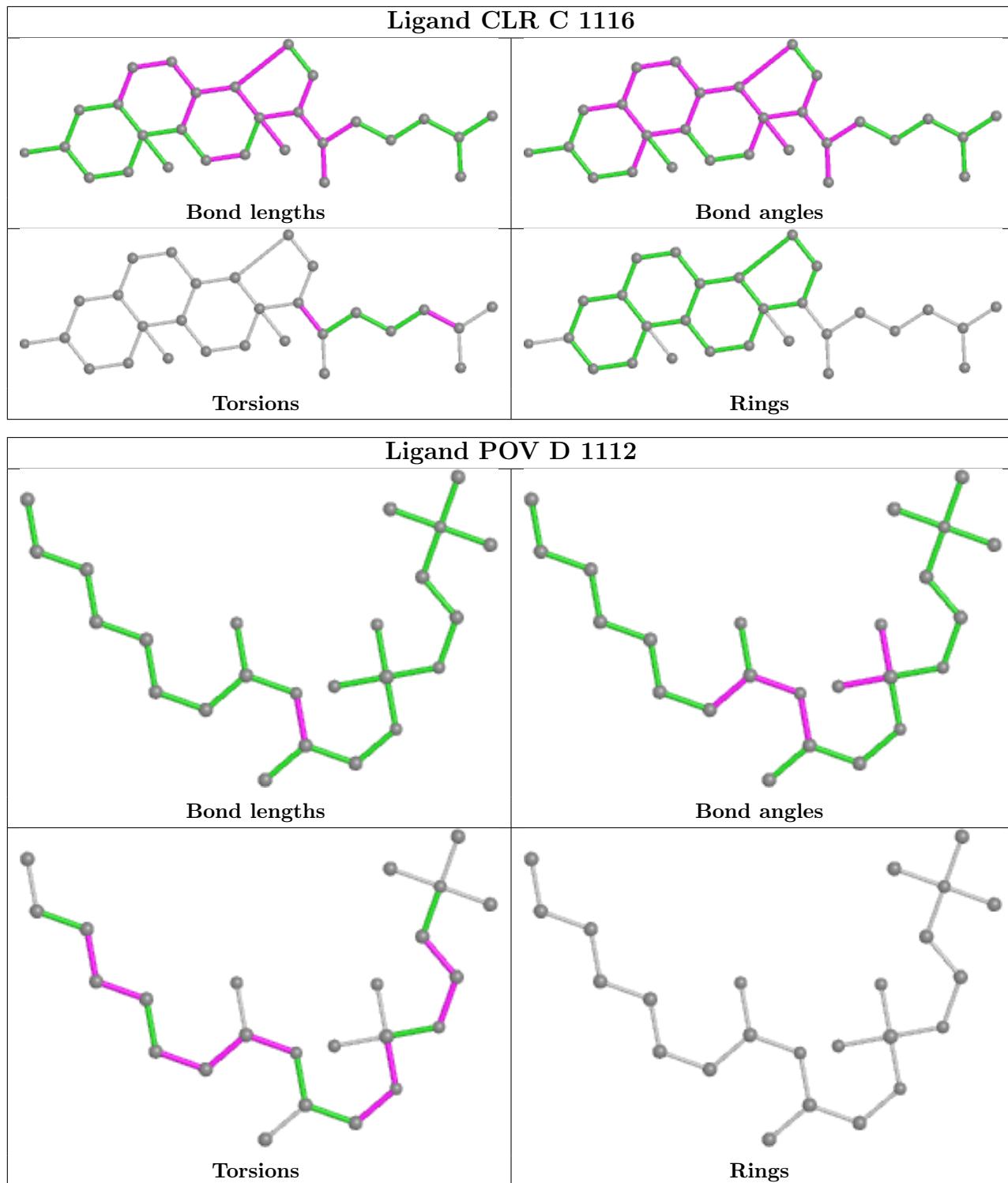
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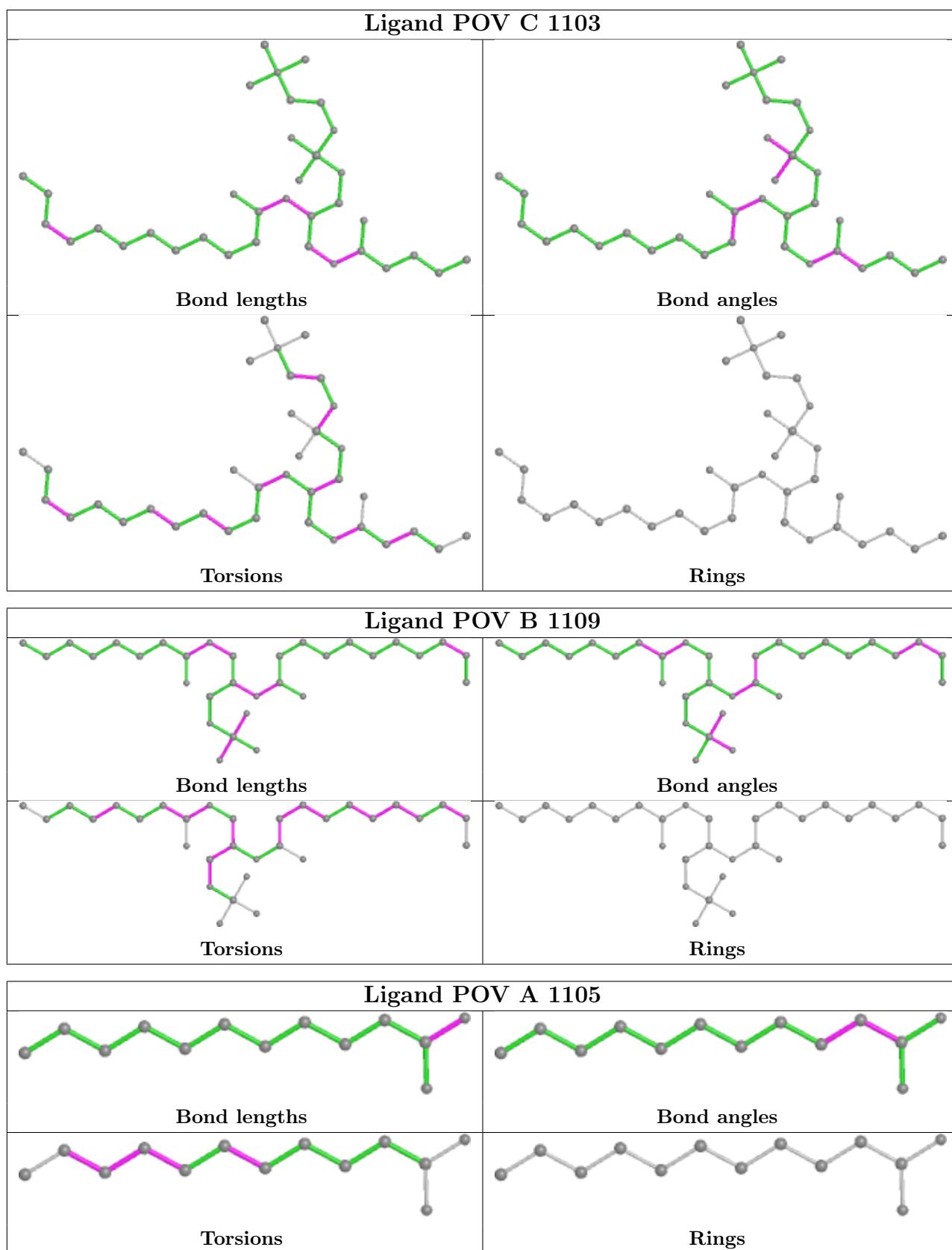
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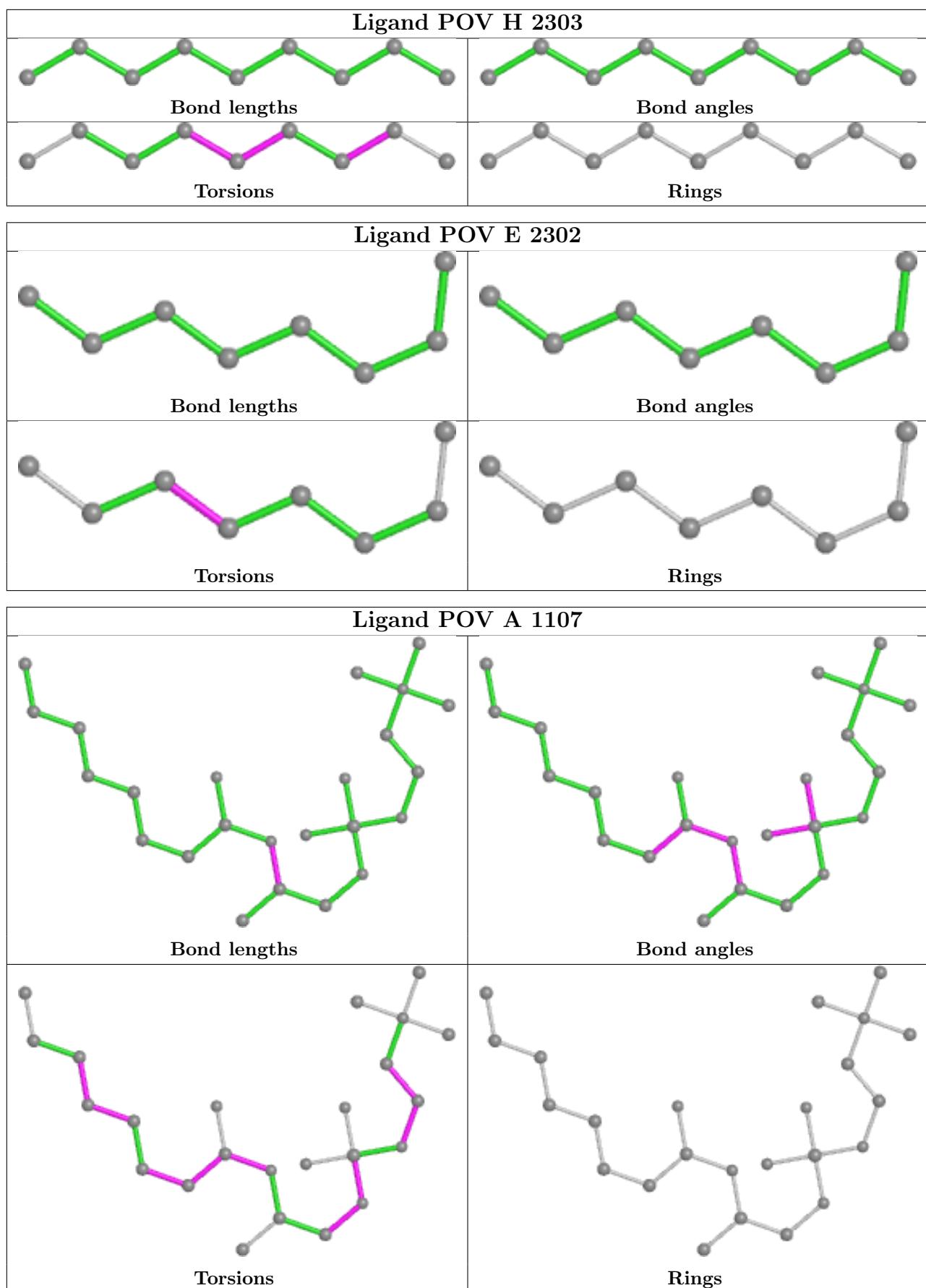
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1111	POV	1	0
5	D	1109	POV	2	0
5	B	1110	POV	1	0
6	B	1115	CLR	7	0
5	D	1110	POV	1	0
5	C	1101	POV	2	0
6	B	1117	CLR	5	0
5	A	1120	POV	1	0
5	C	1111	POV	1	0
5	B	1105	POV	1	0
6	D	1117	CLR	7	0
5	C	1104	POV	2	0
5	B	1112	POV	1	0
6	A	1110	CLR	8	0
6	D	1116	CLR	4	0
5	D	1105	POV	1	0
6	A	1111	CLR	5	0
6	D	1118	CLR	6	0
5	A	1121	POV	2	0
5	A	1106	POV	1	0
5	B	1104	POV	2	0
6	C	1118	CLR	6	0
5	C	1110	POV	1	0
5	A	1104	POV	1	0
5	B	1111	POV	2	0
5	A	1122	POV	1	0
5	D	1101	POV	2	0
6	C	1117	CLR	4	0
6	A	1113	CLR	6	0
5	C	1109	POV	2	0
6	A	1112	CLR	5	0
5	D	1104	POV	2	0
5	D	1103	POV	2	0

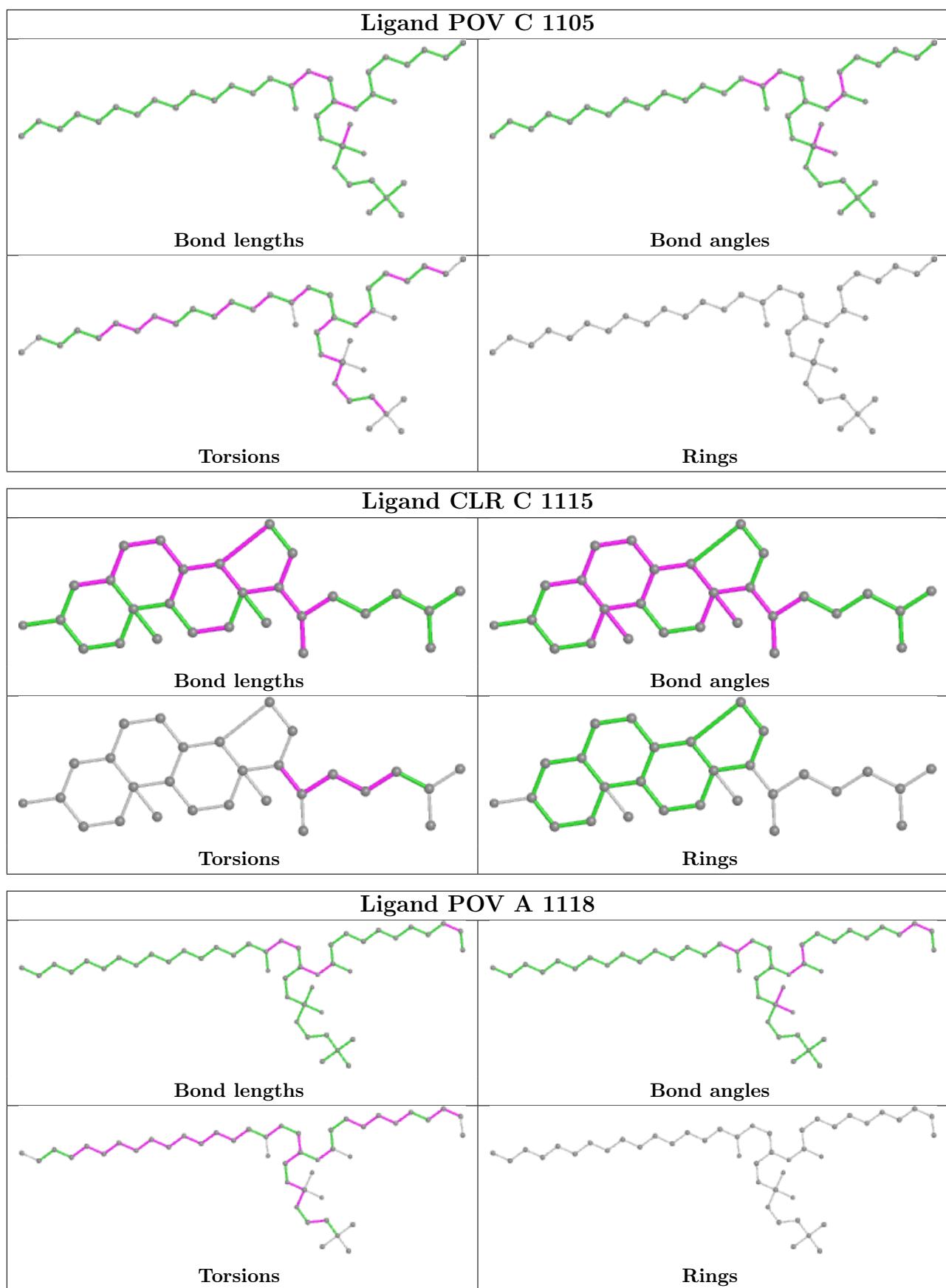
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

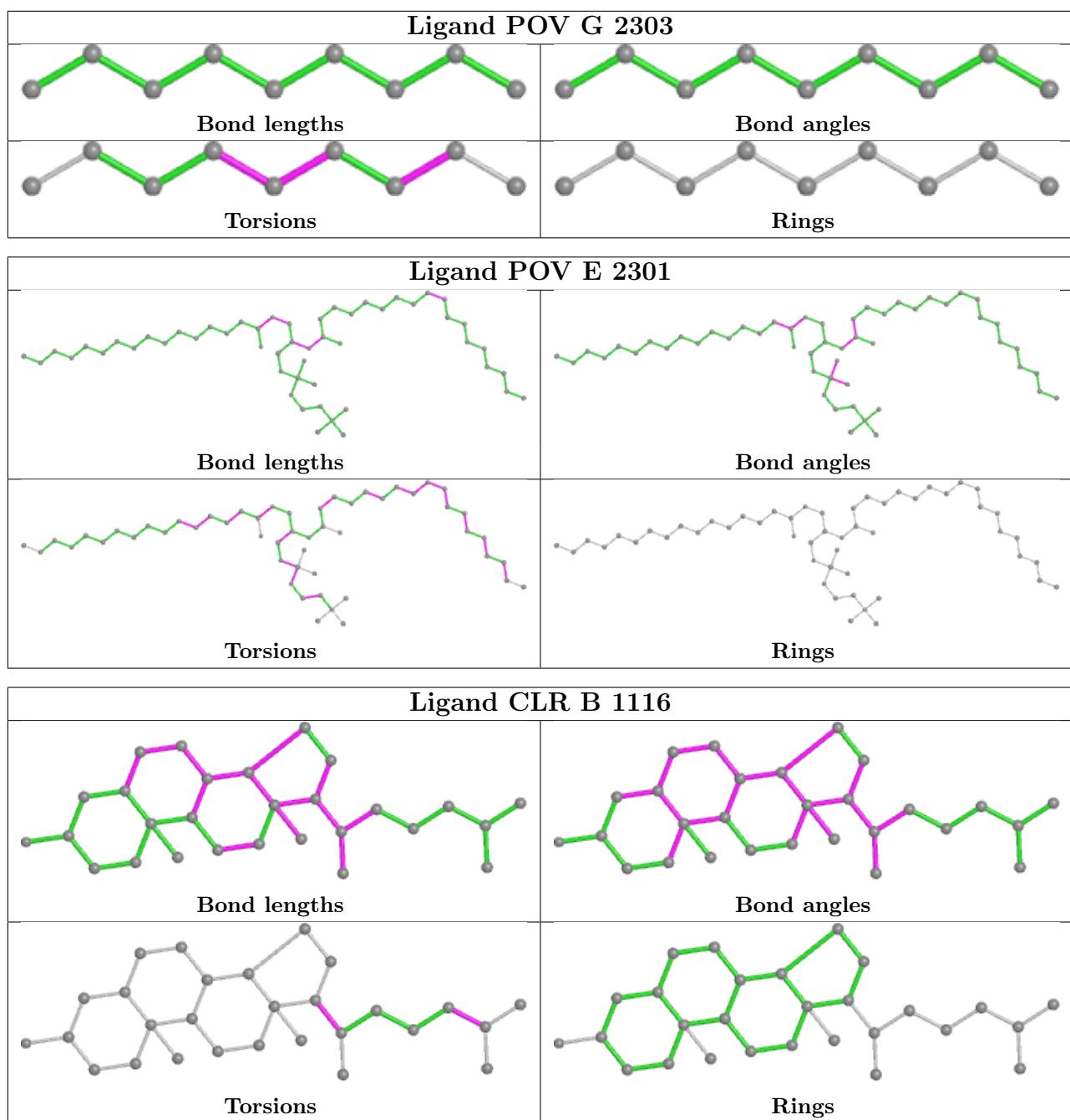
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

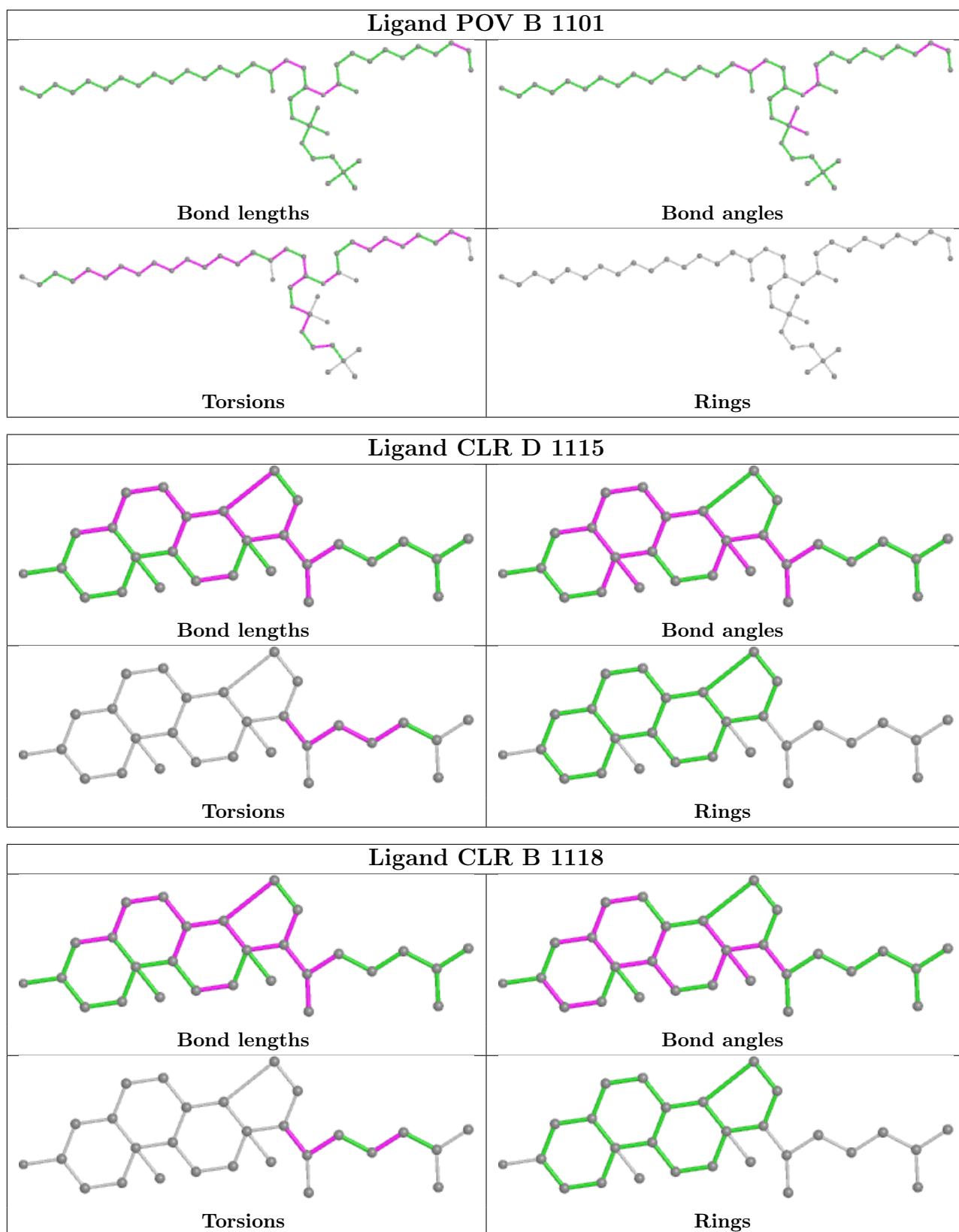


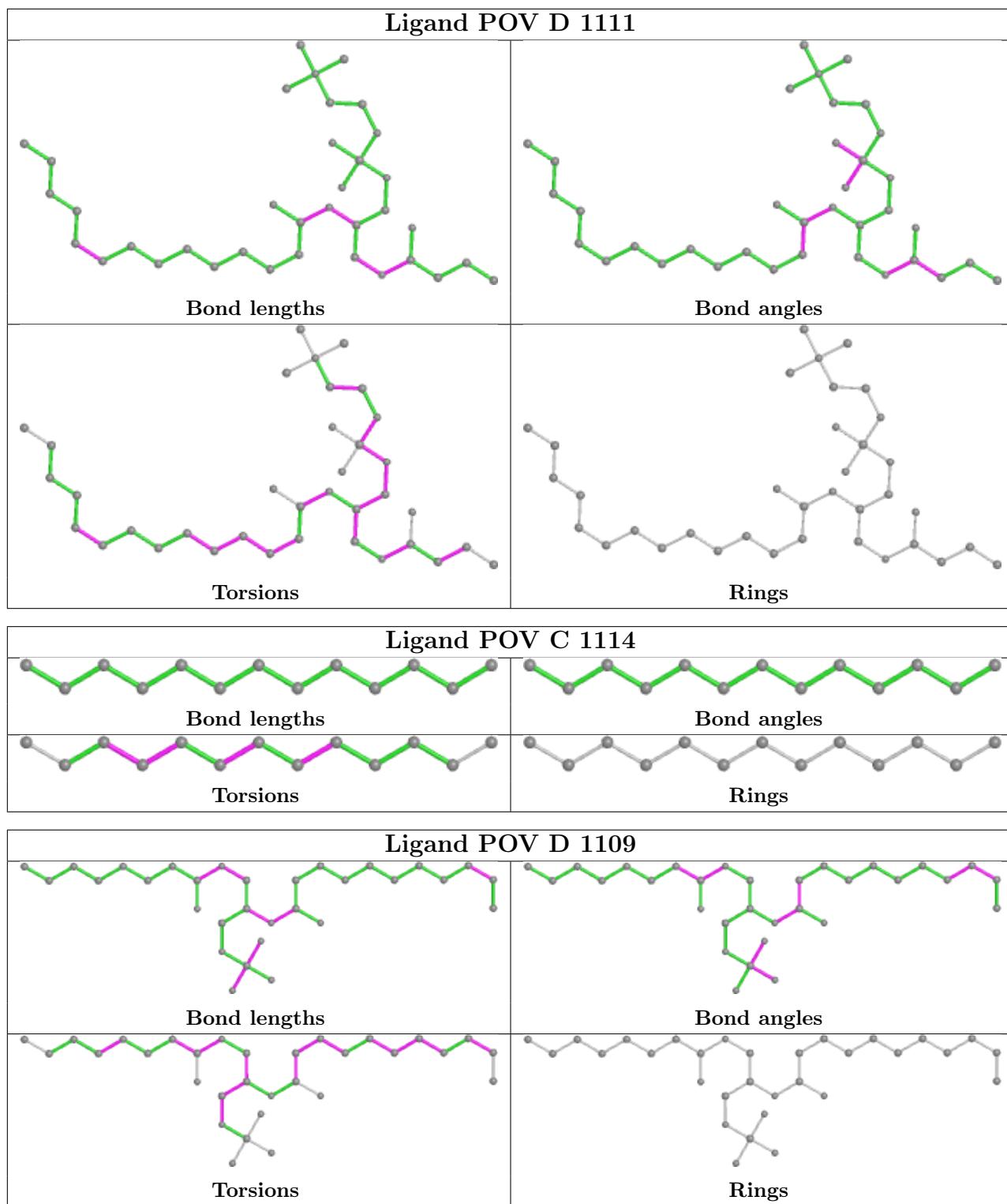


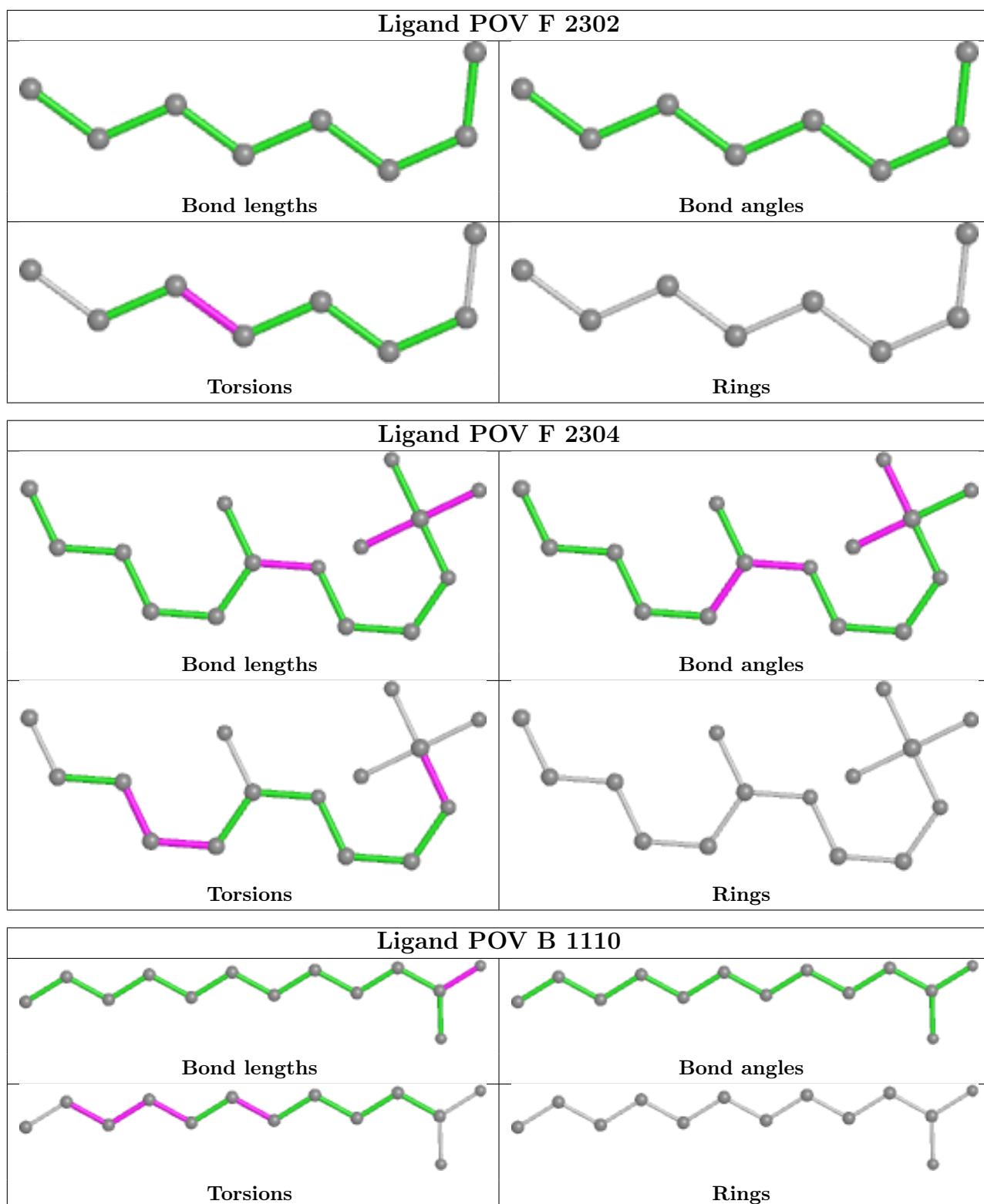


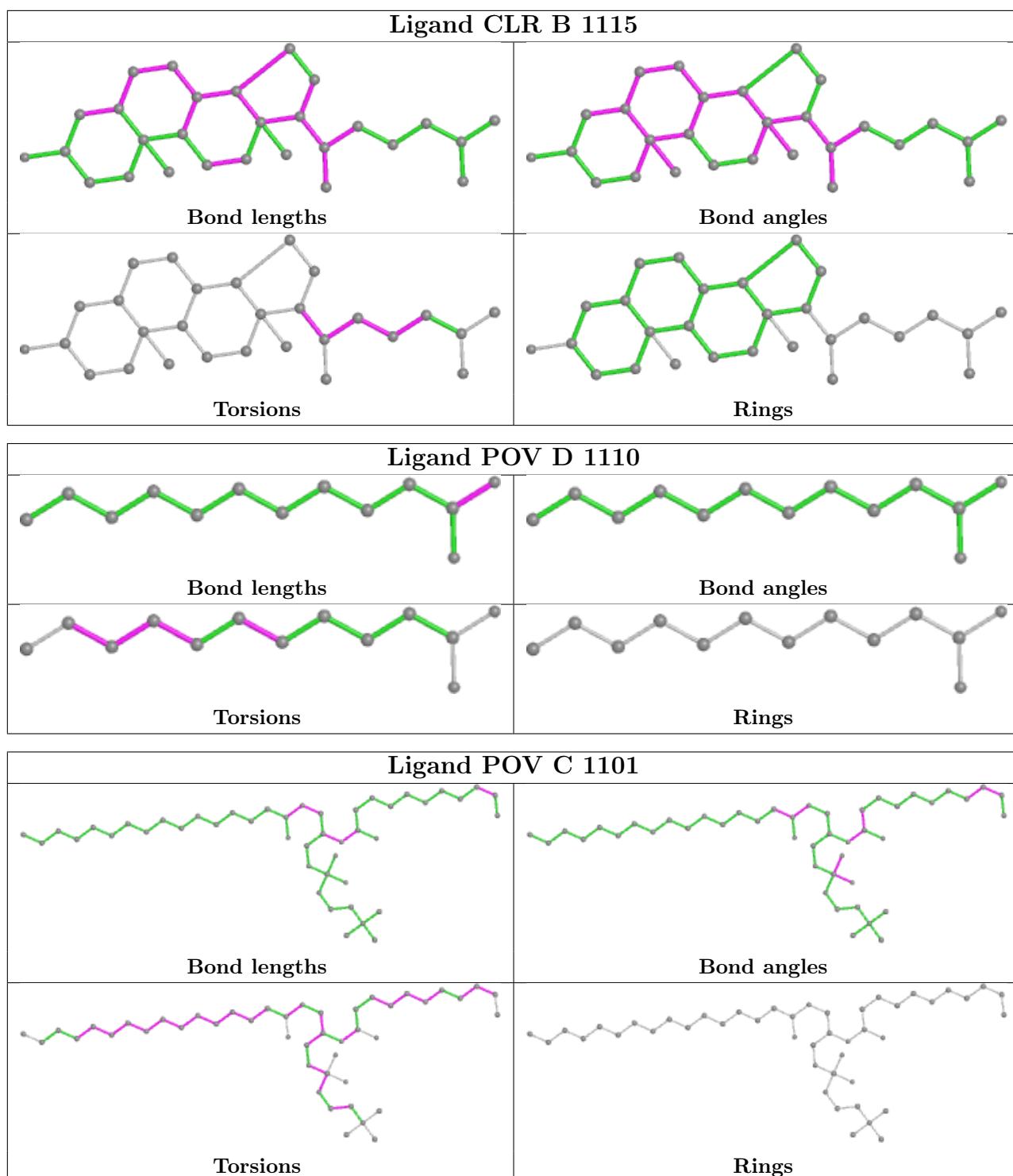


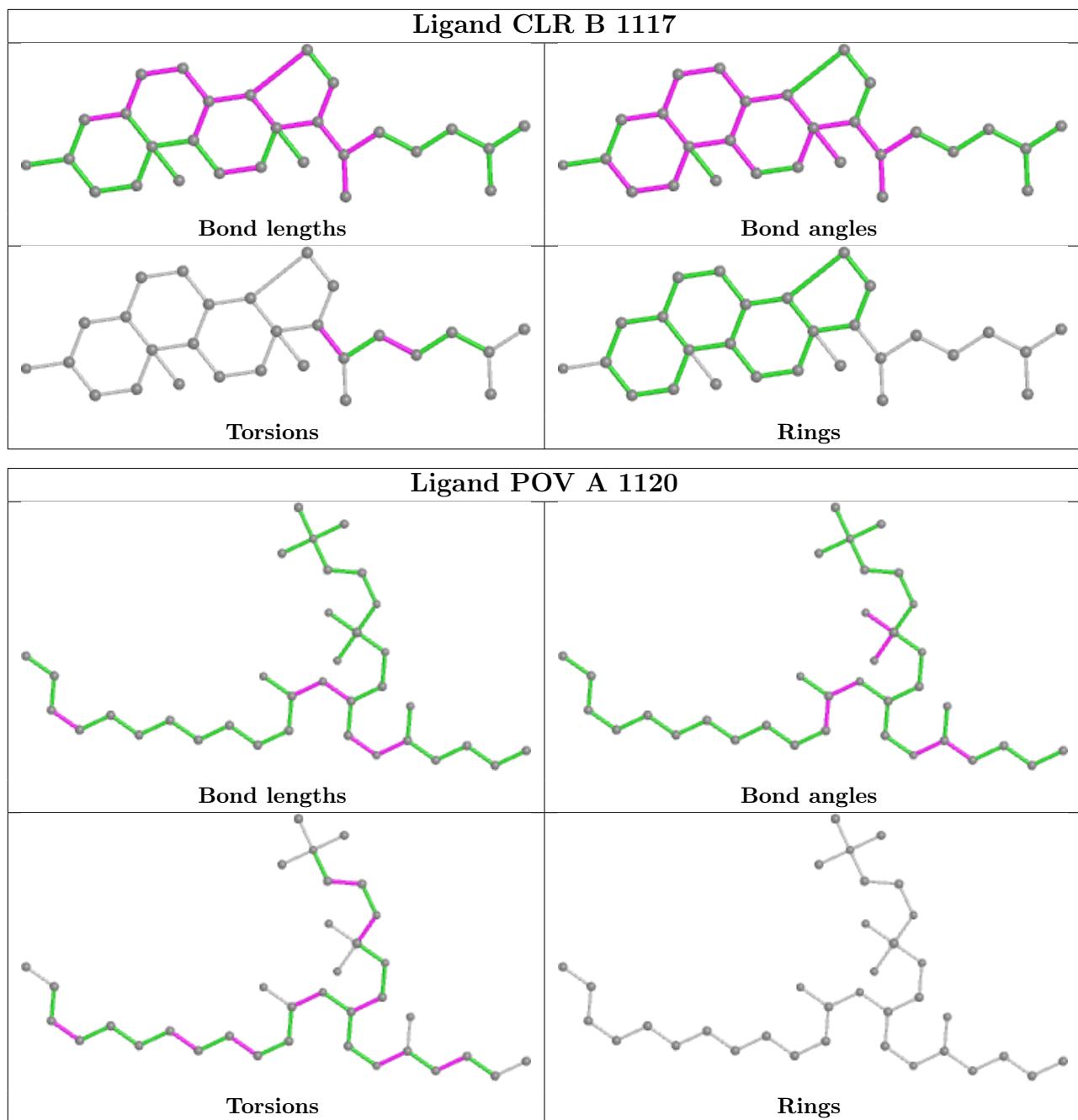


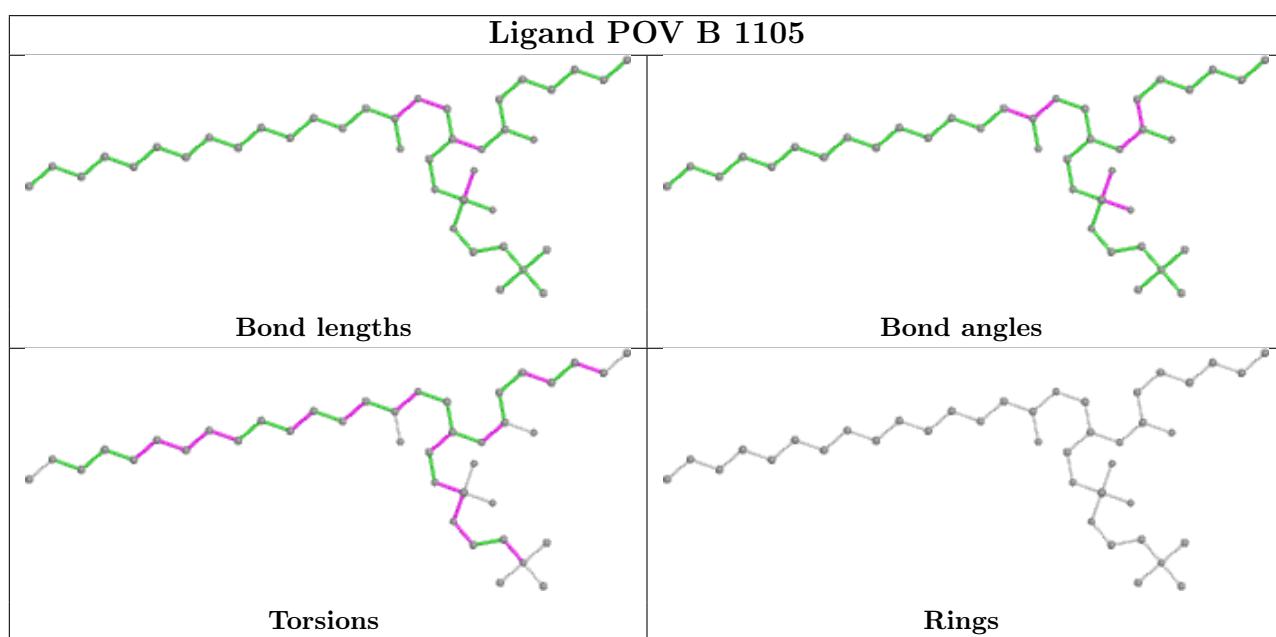
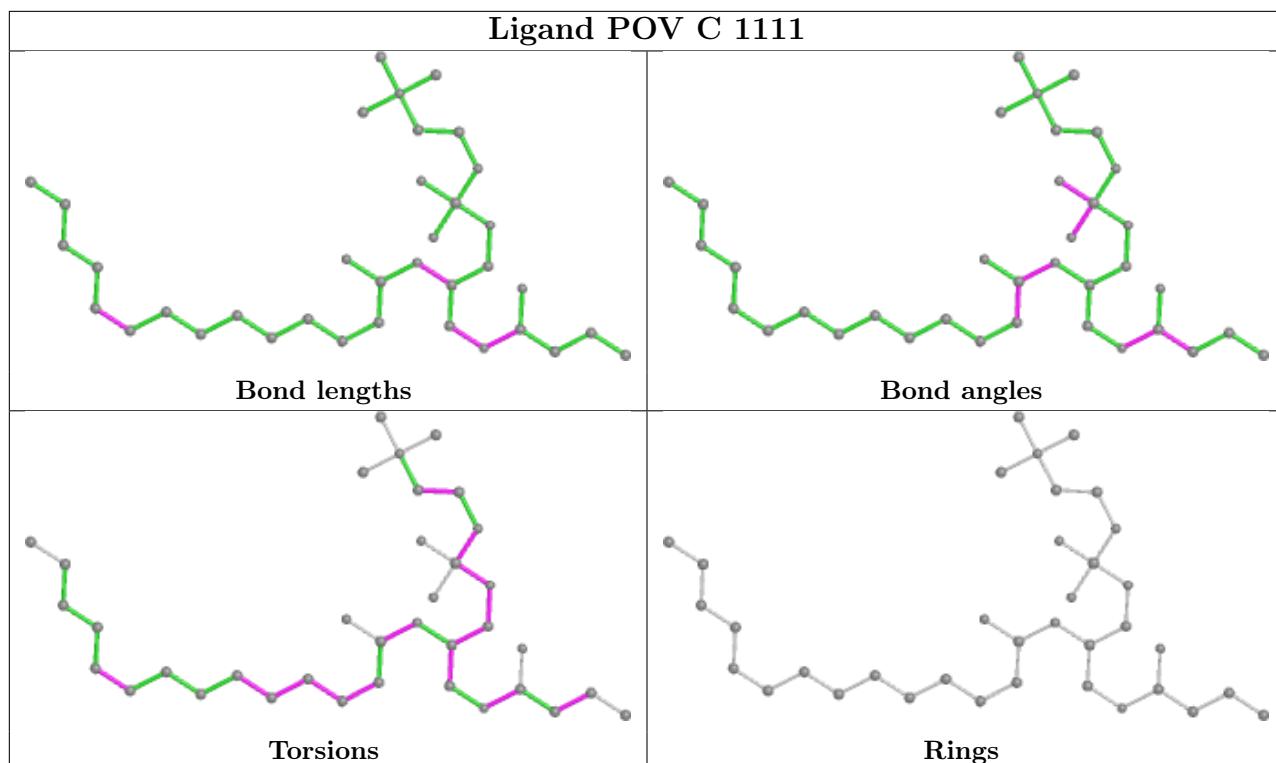


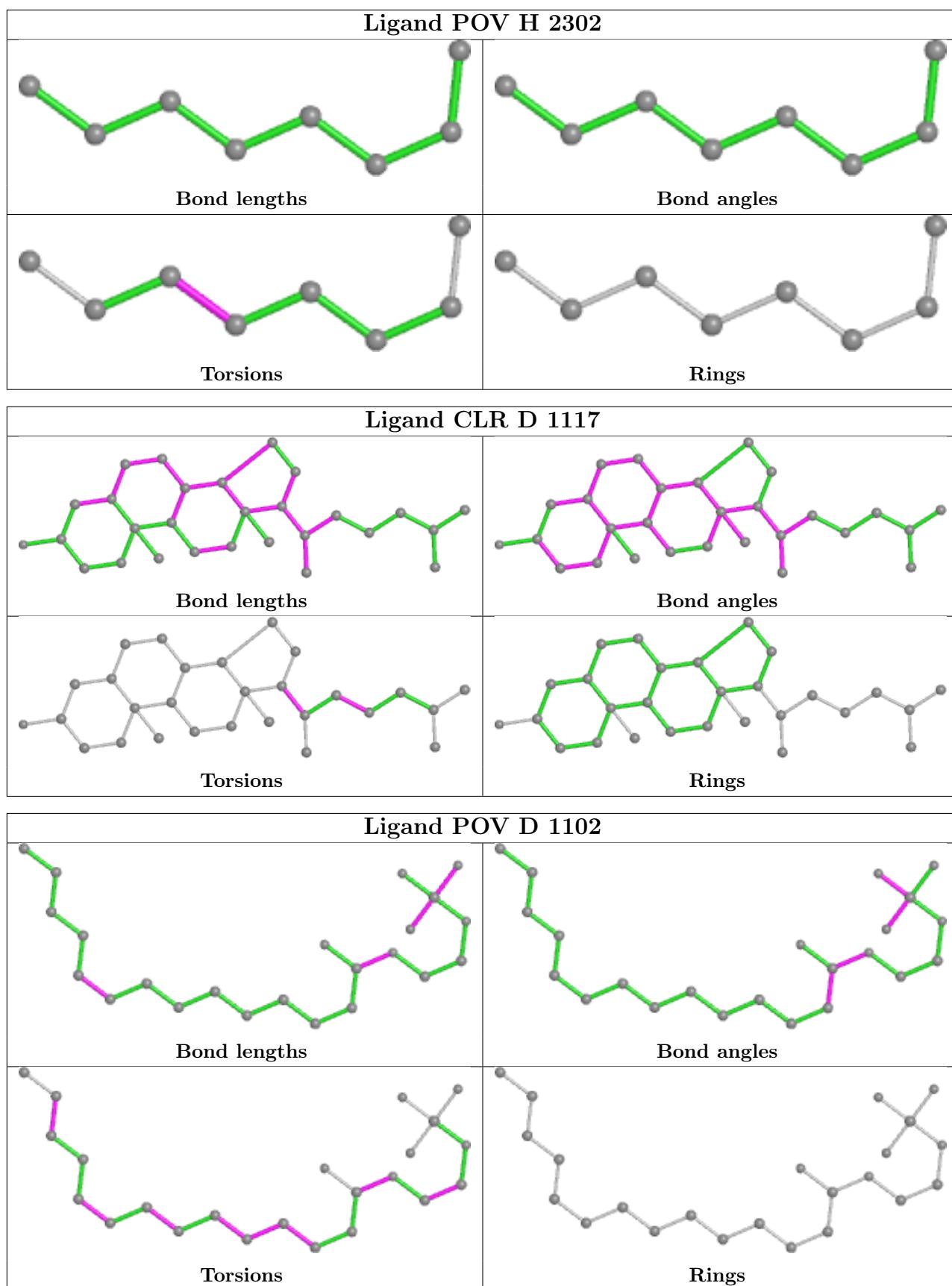


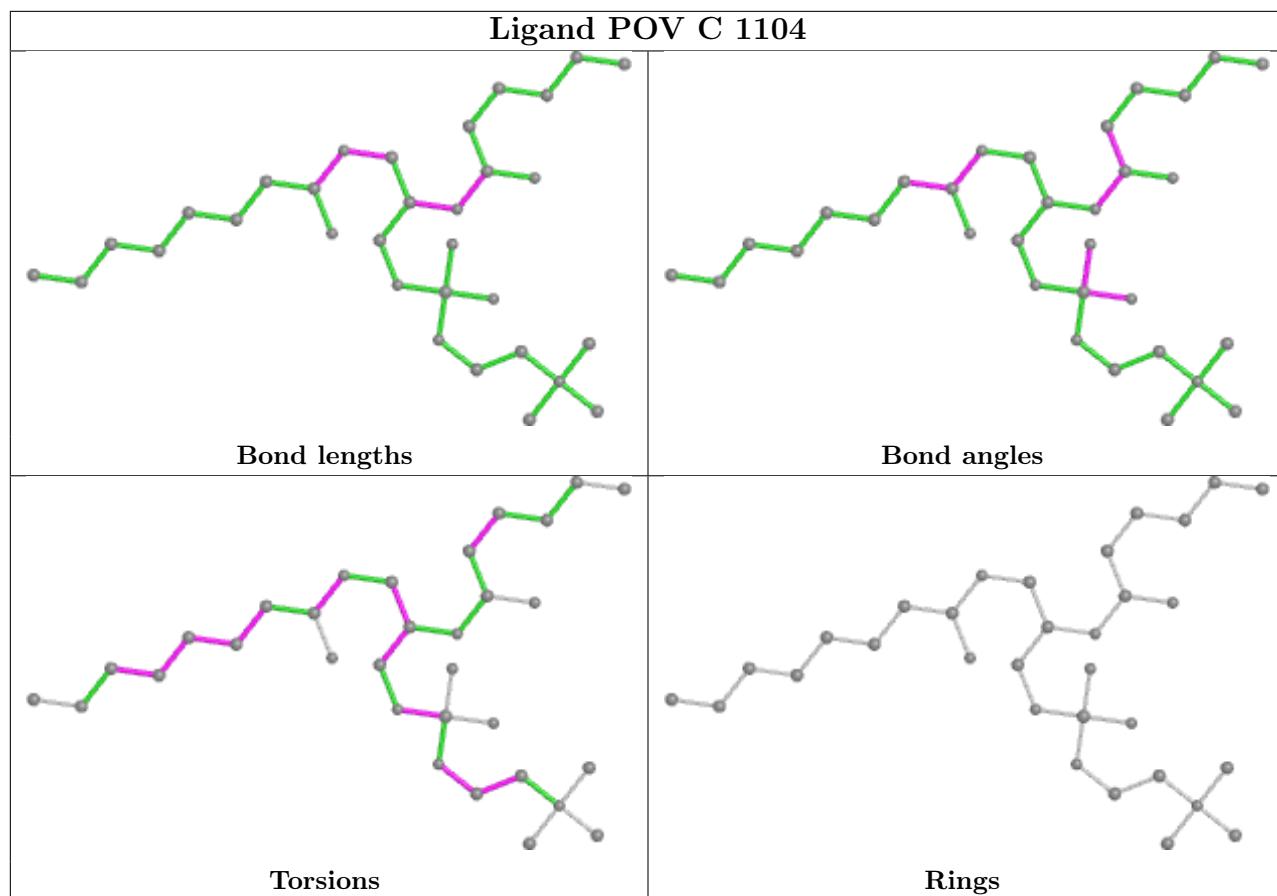


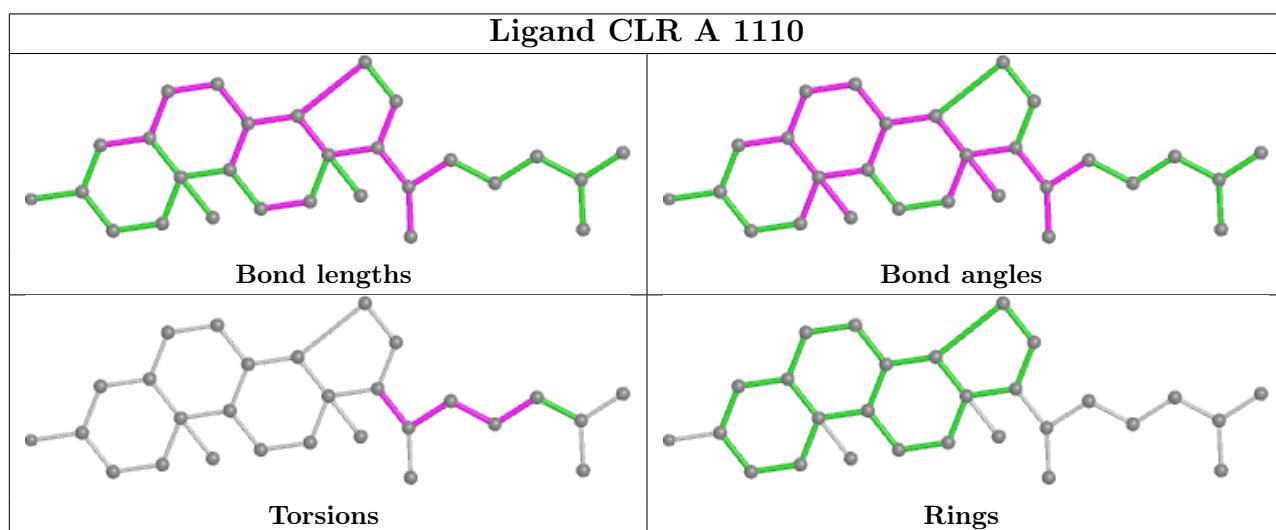
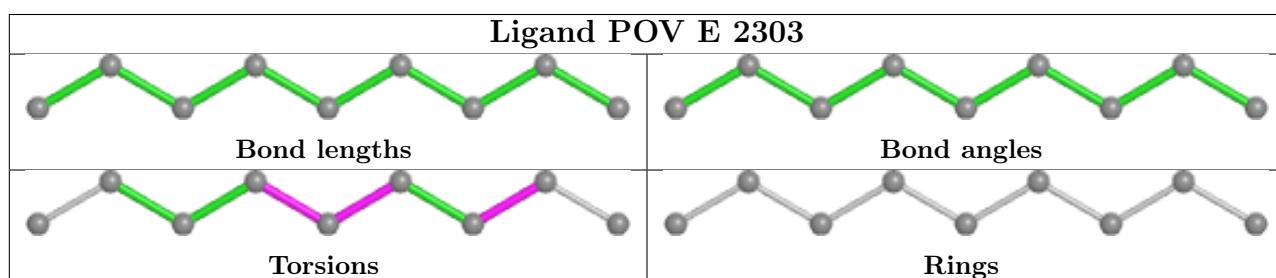
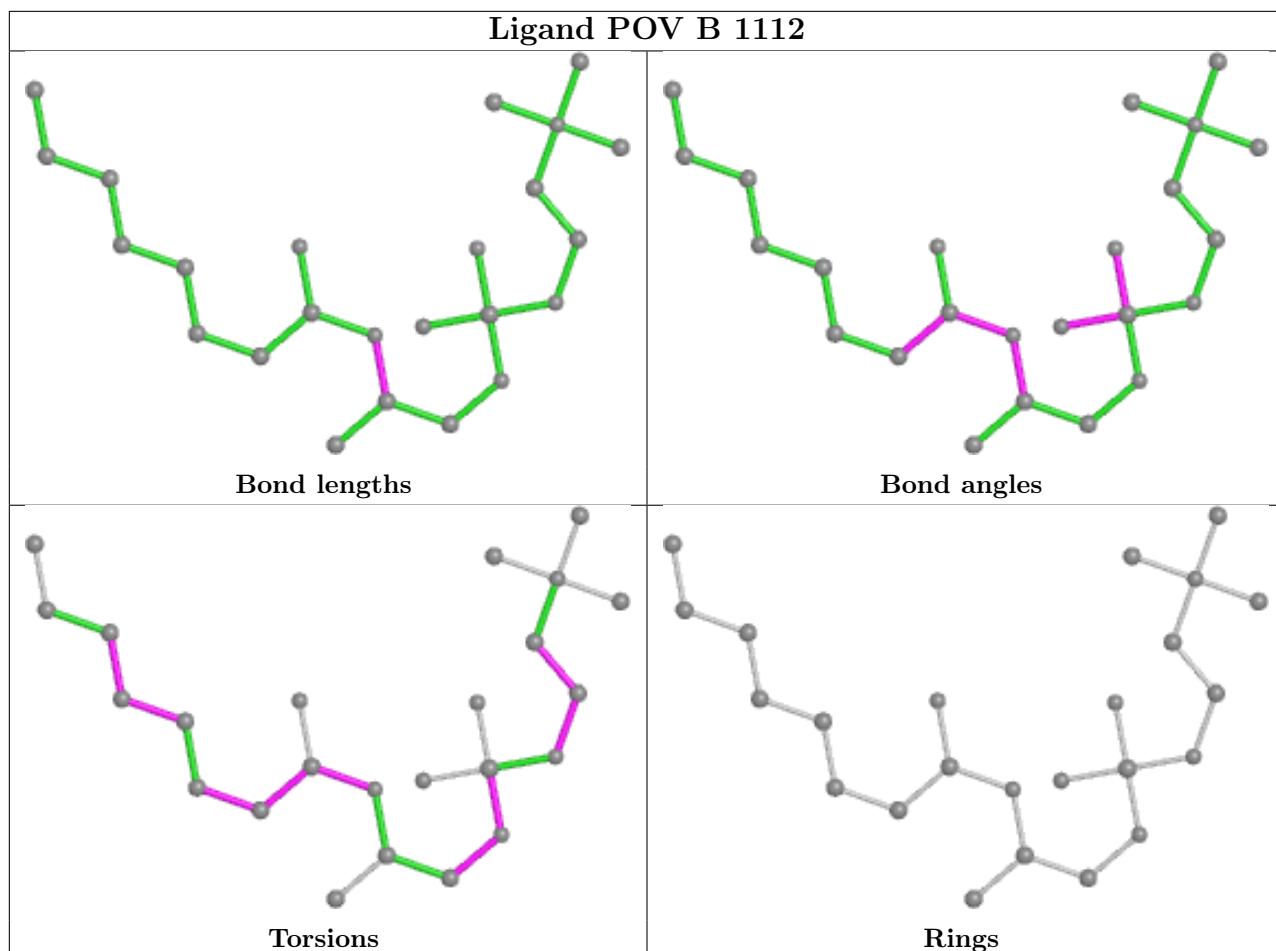


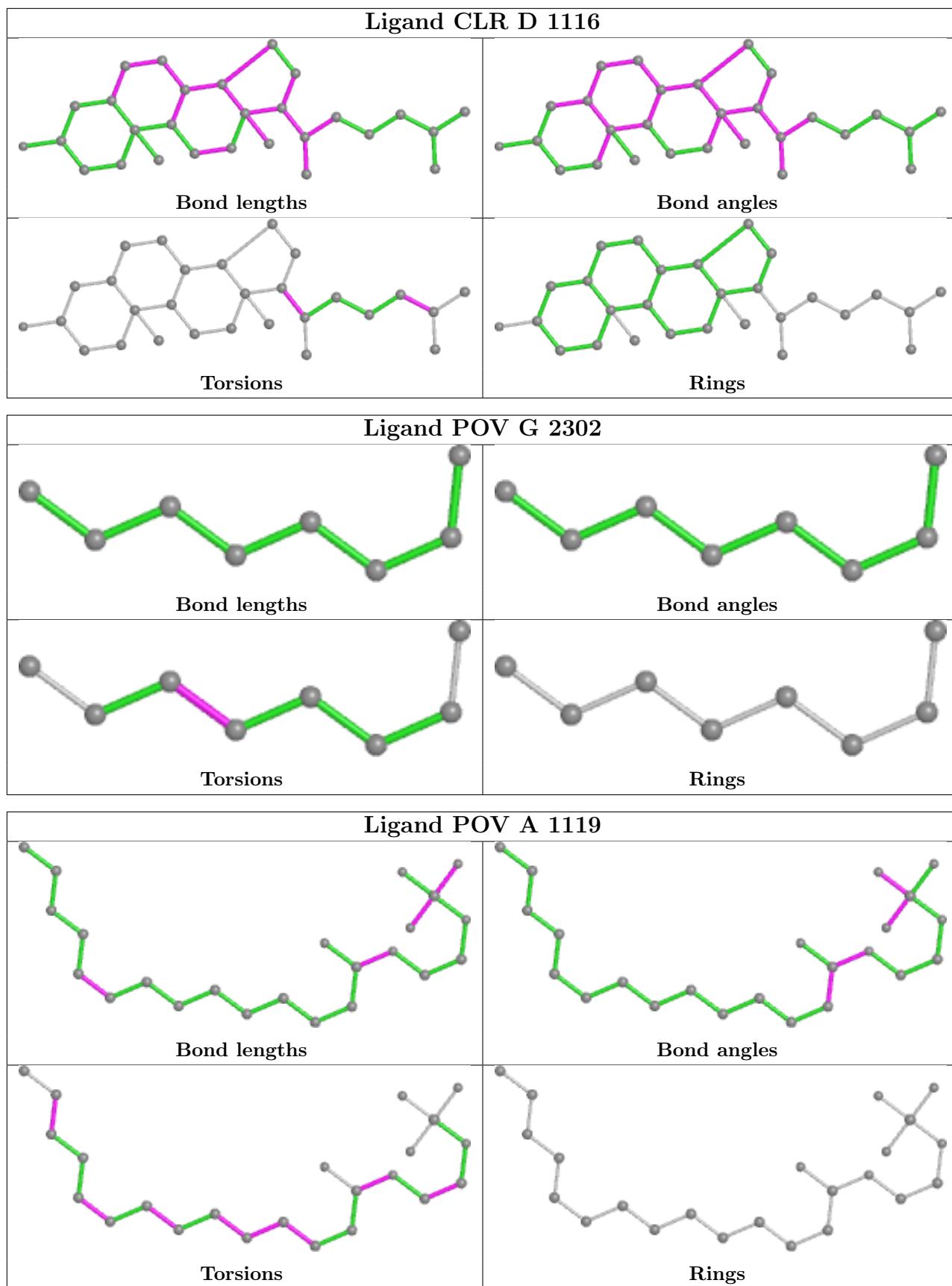


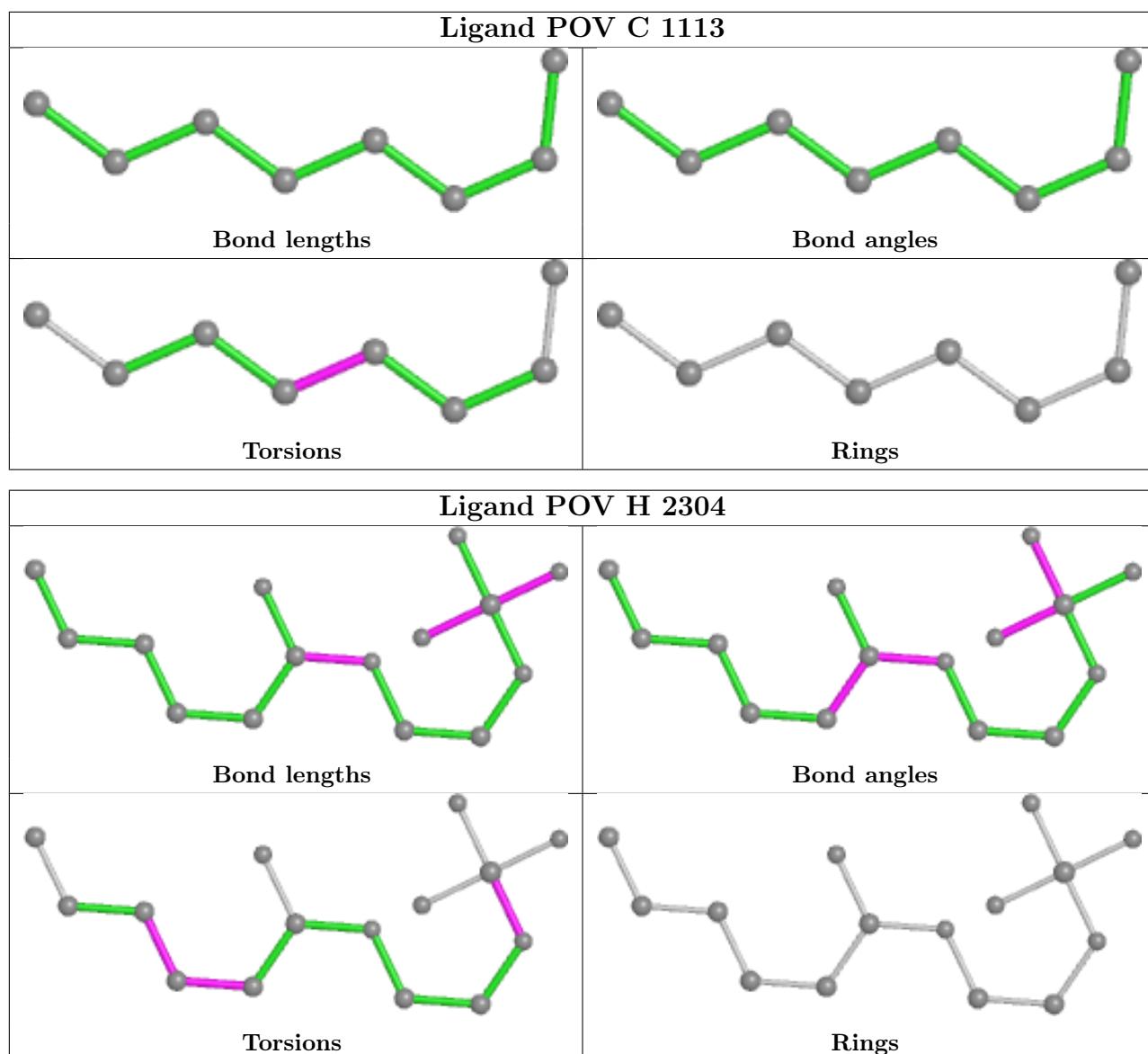


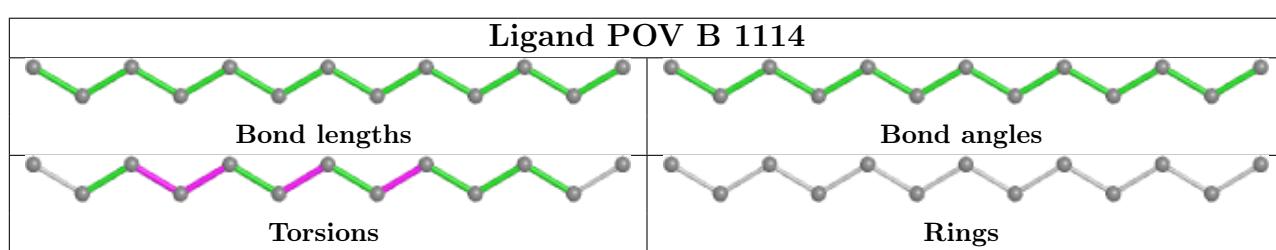
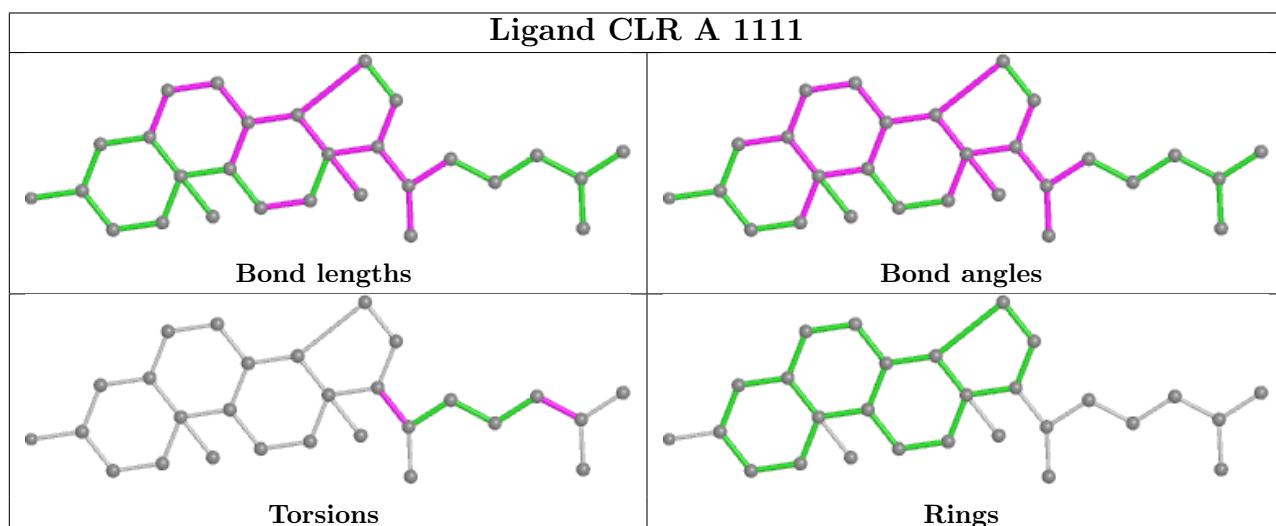
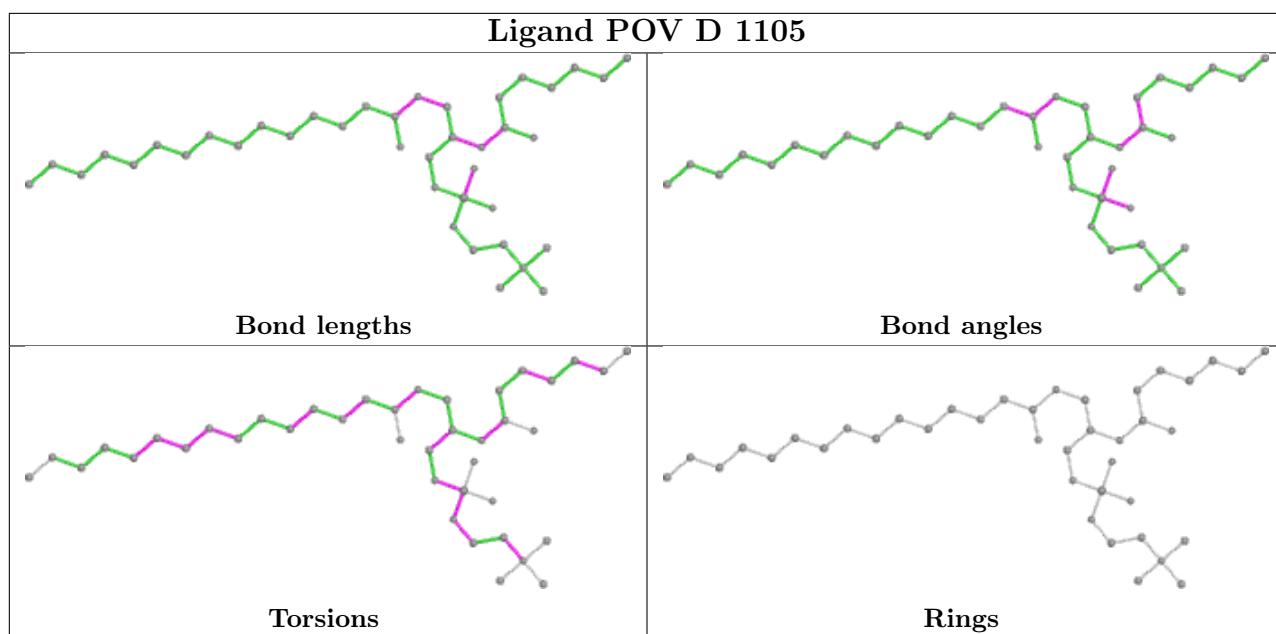


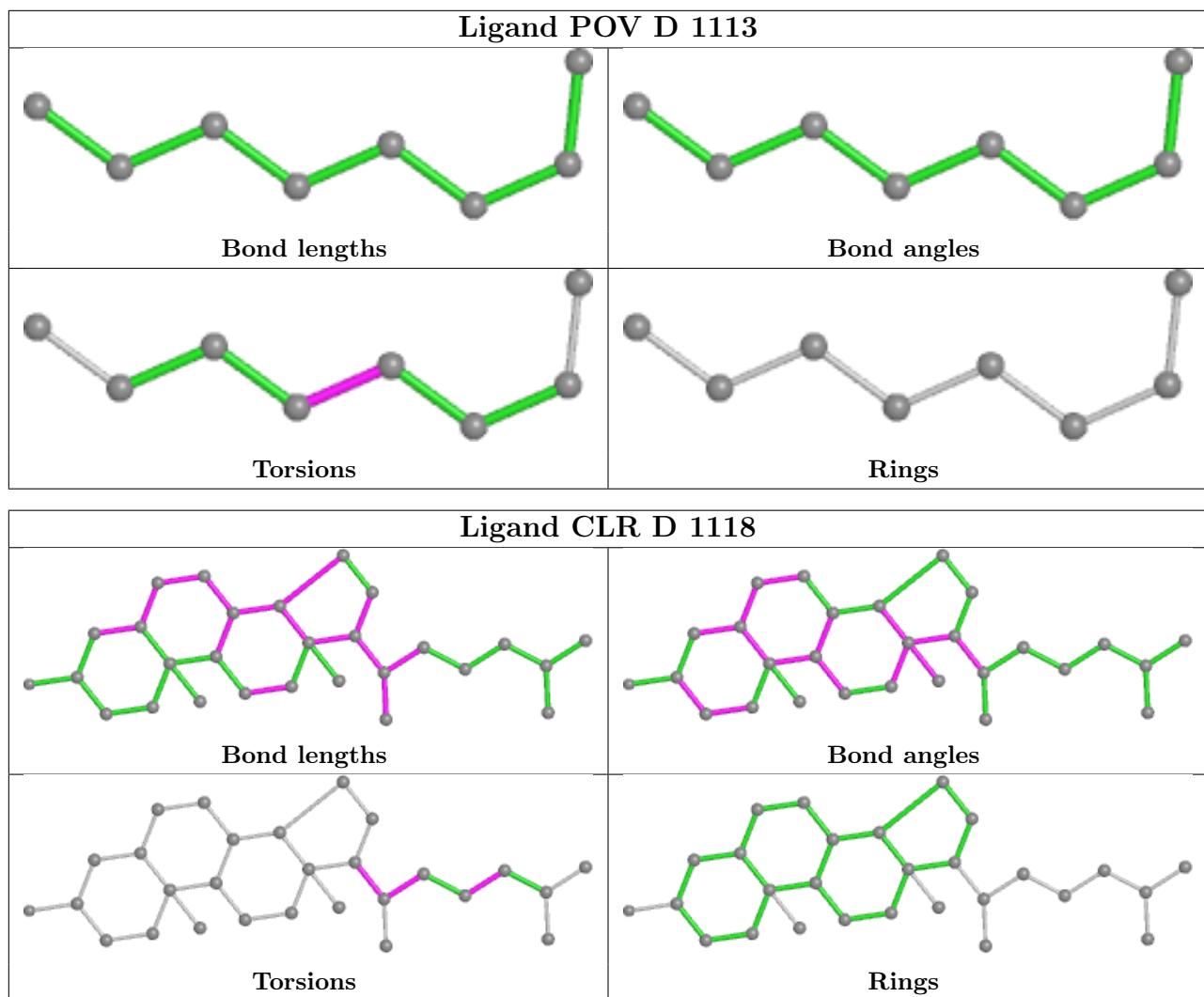


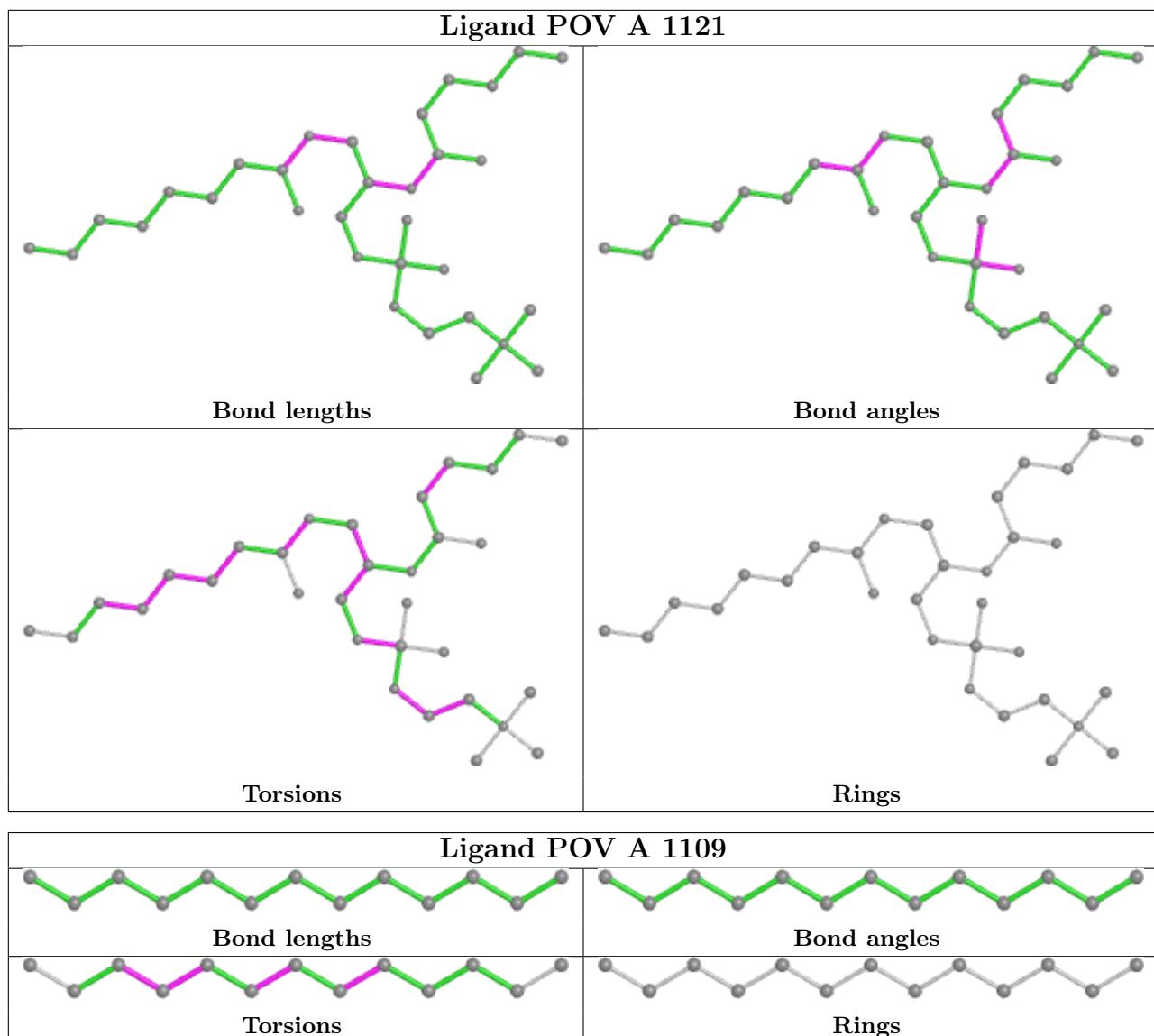


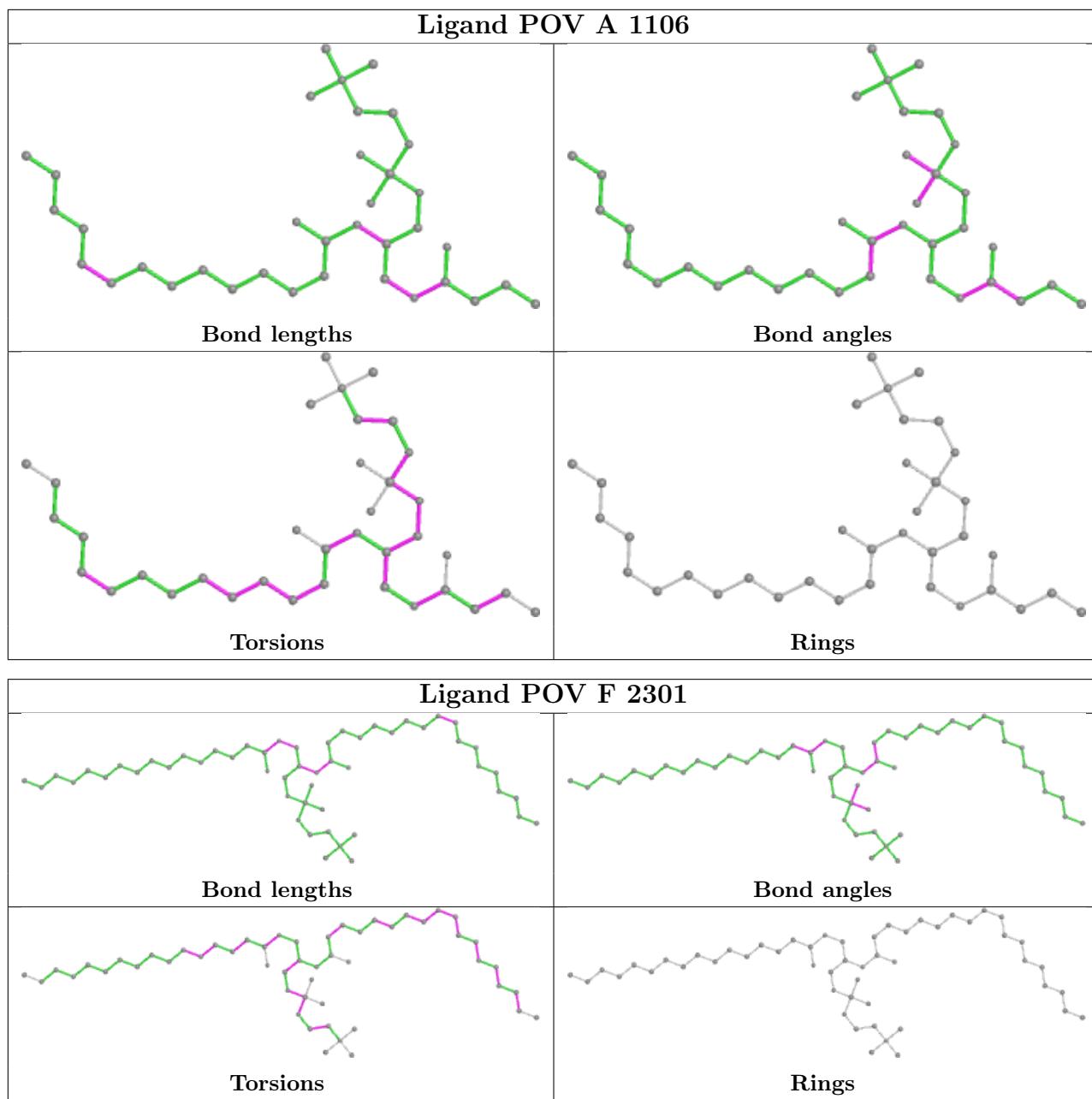


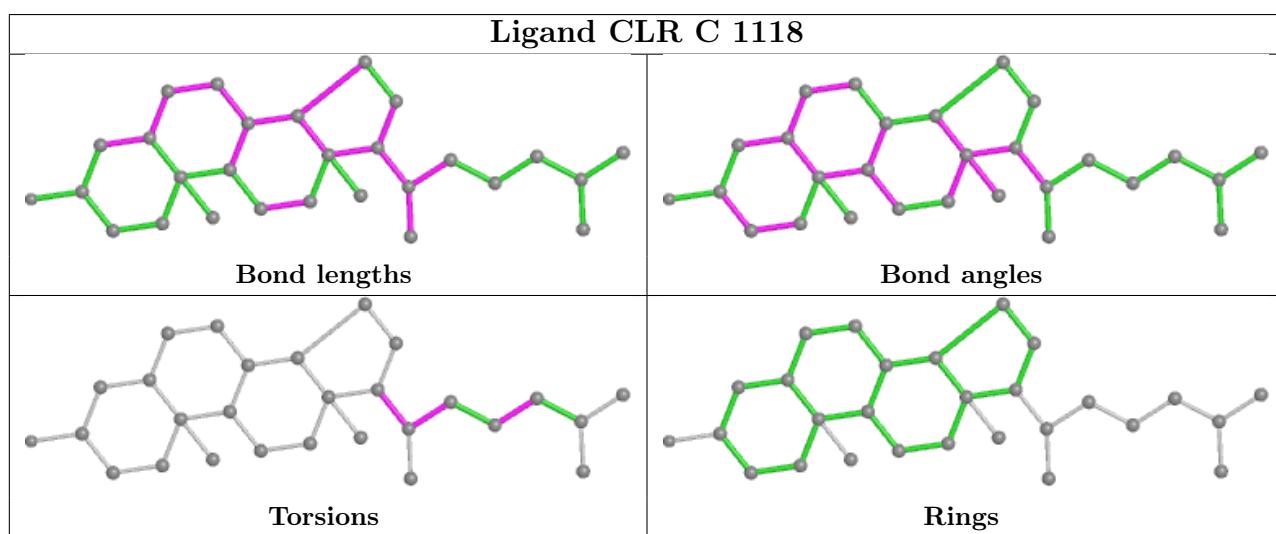
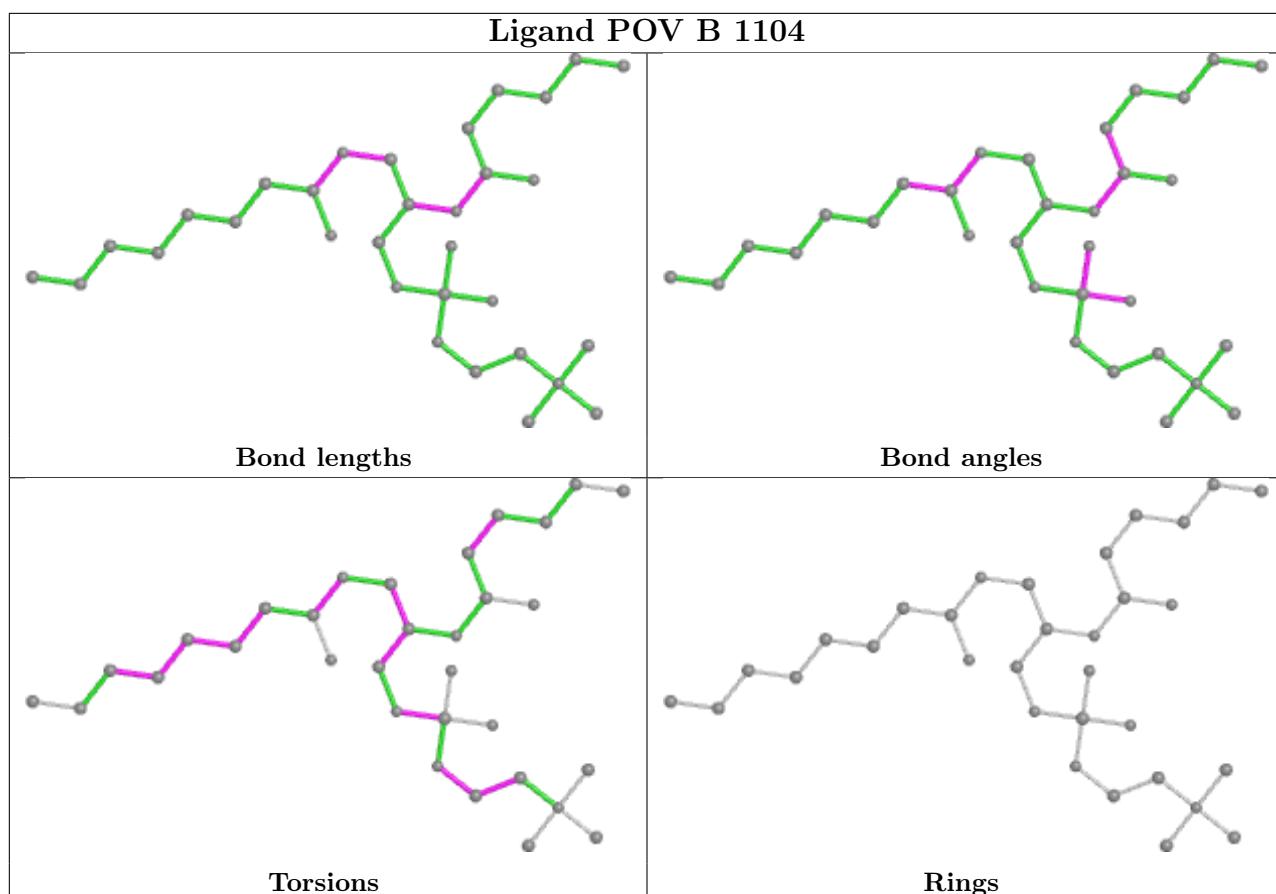


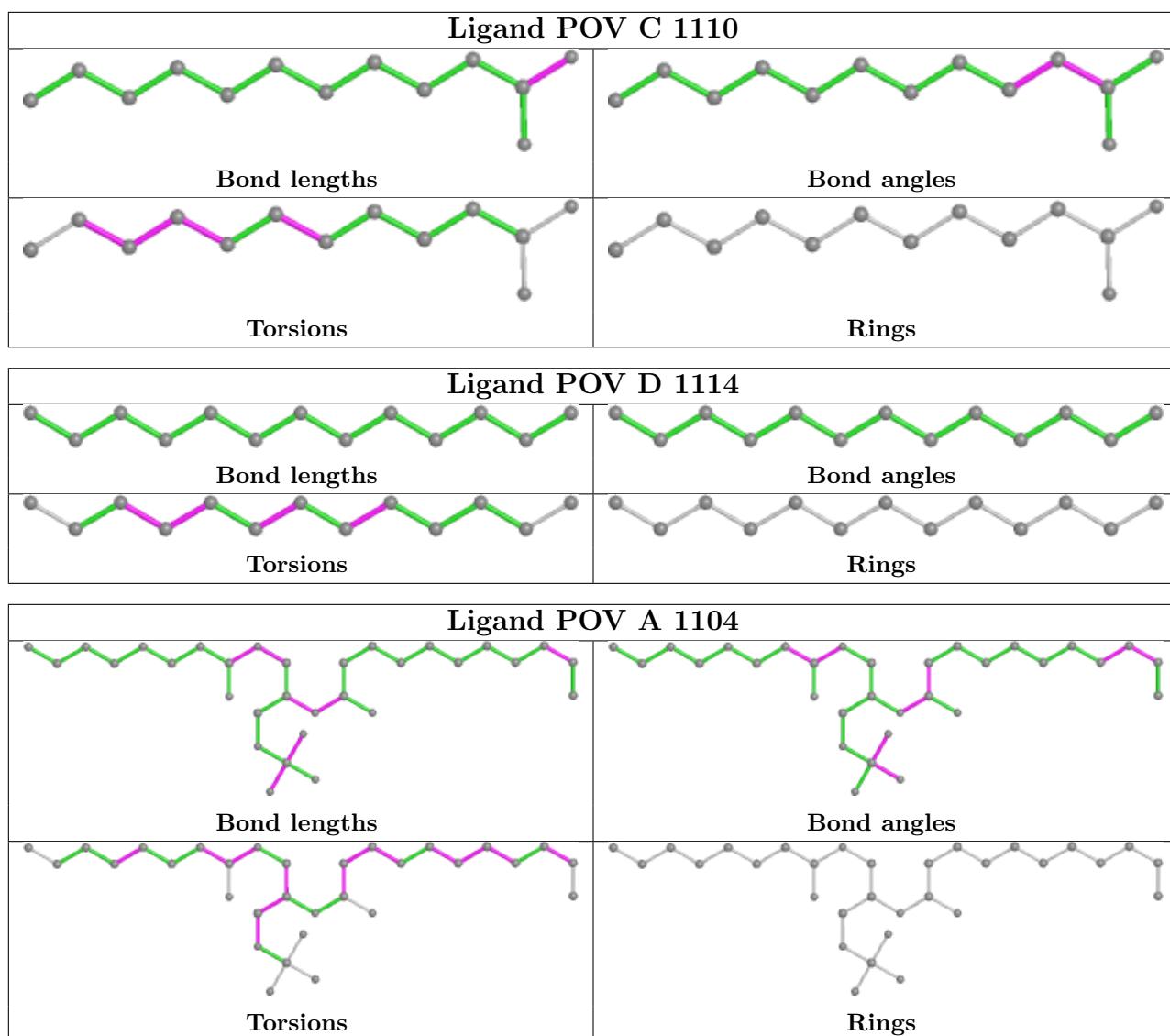


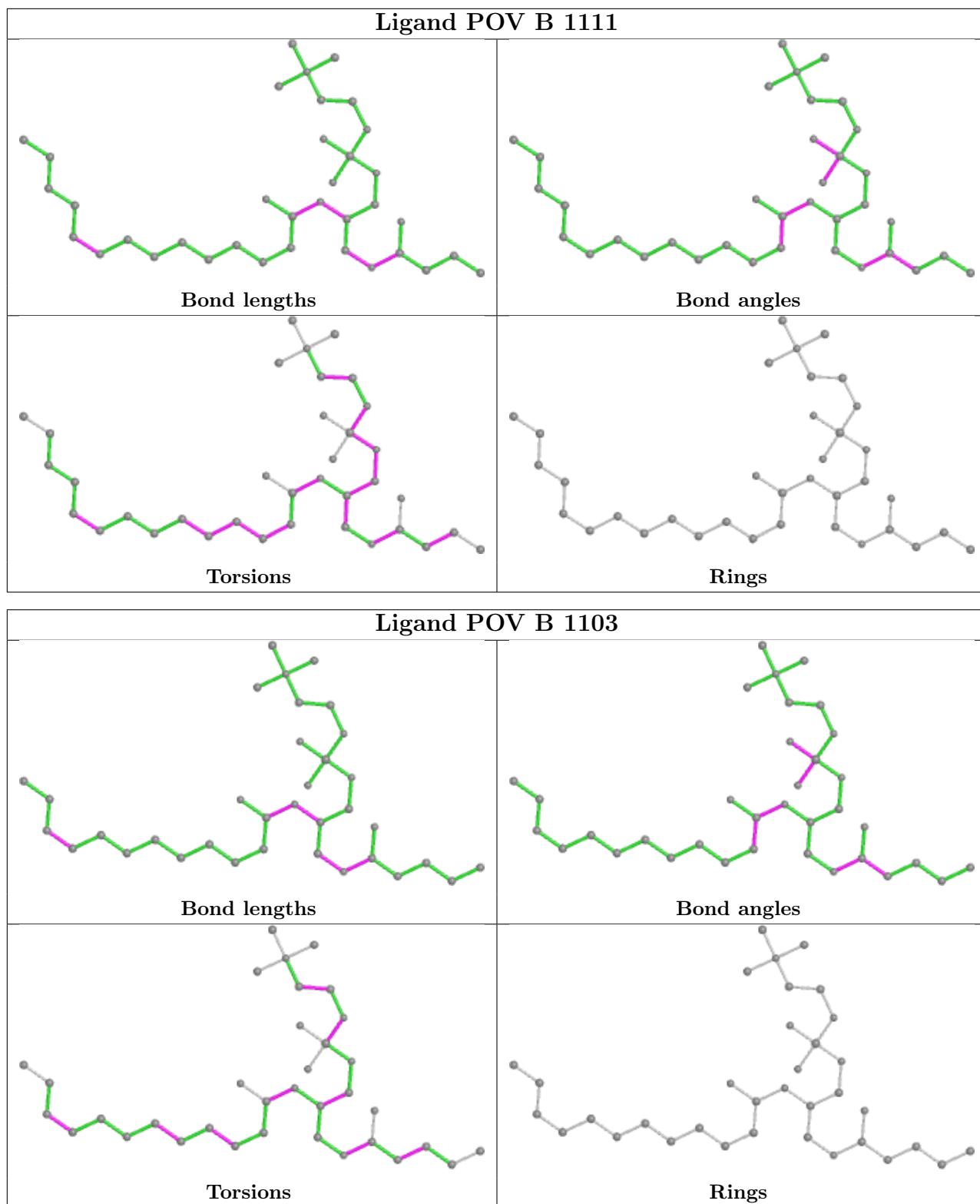


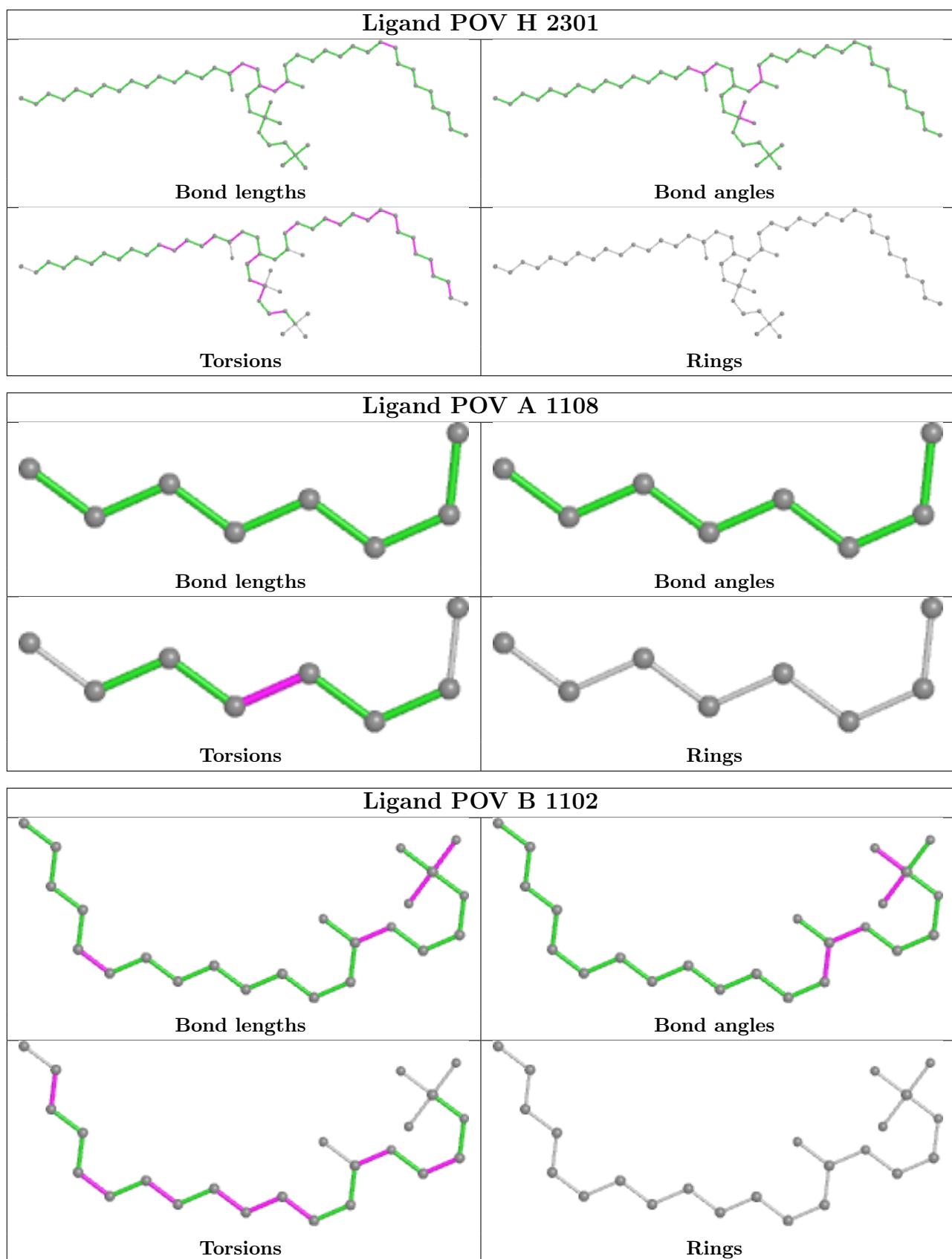


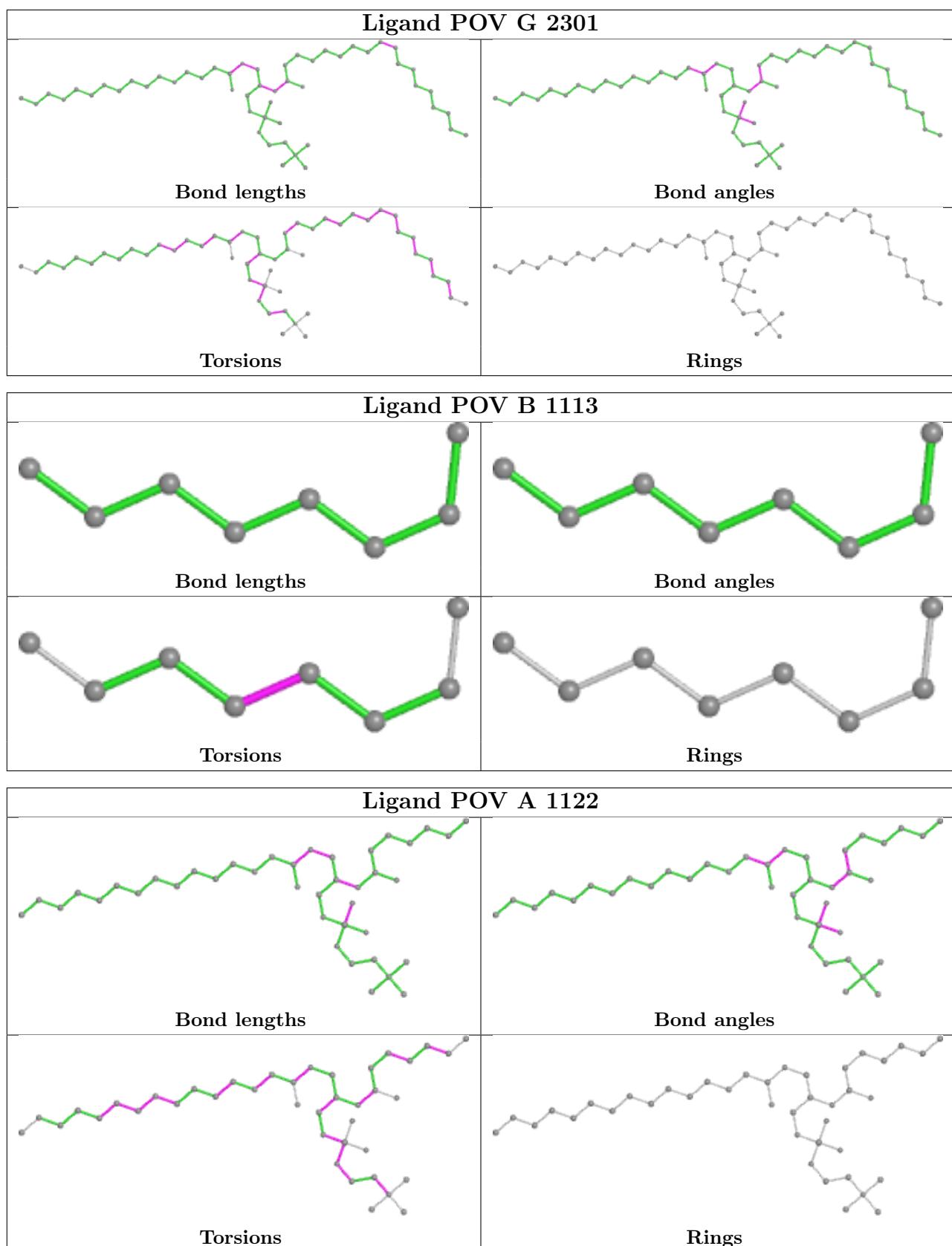


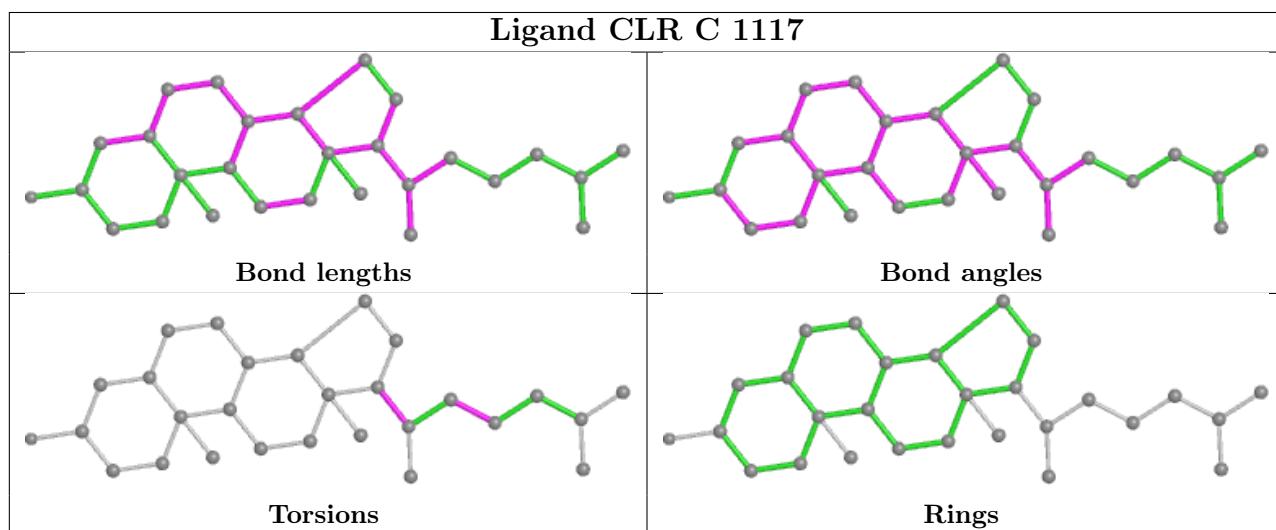
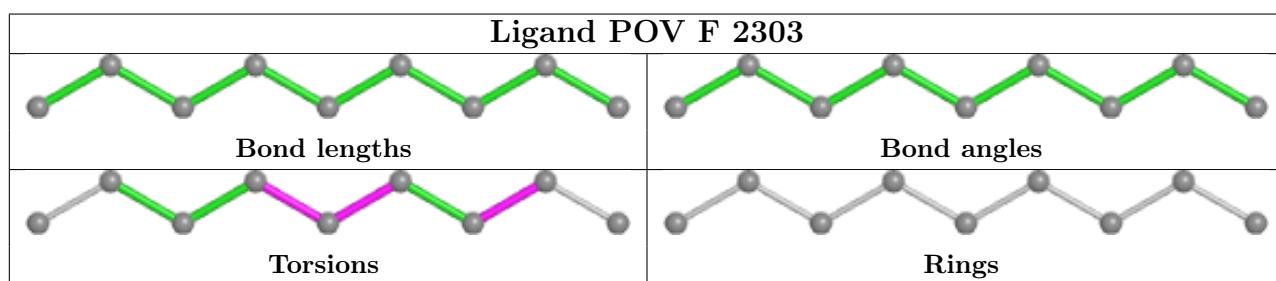
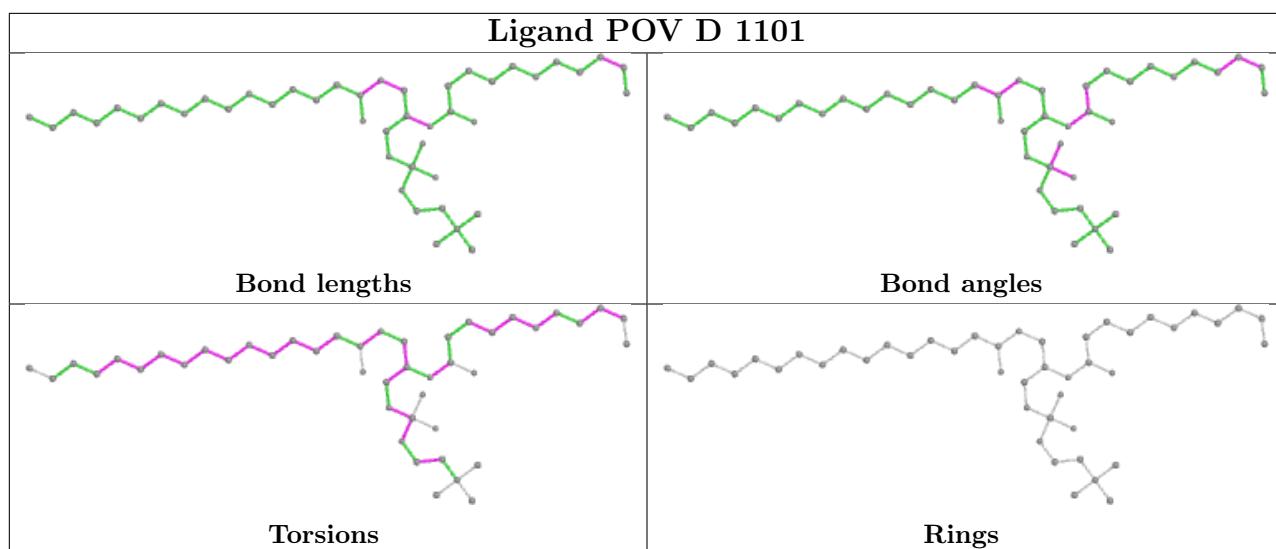


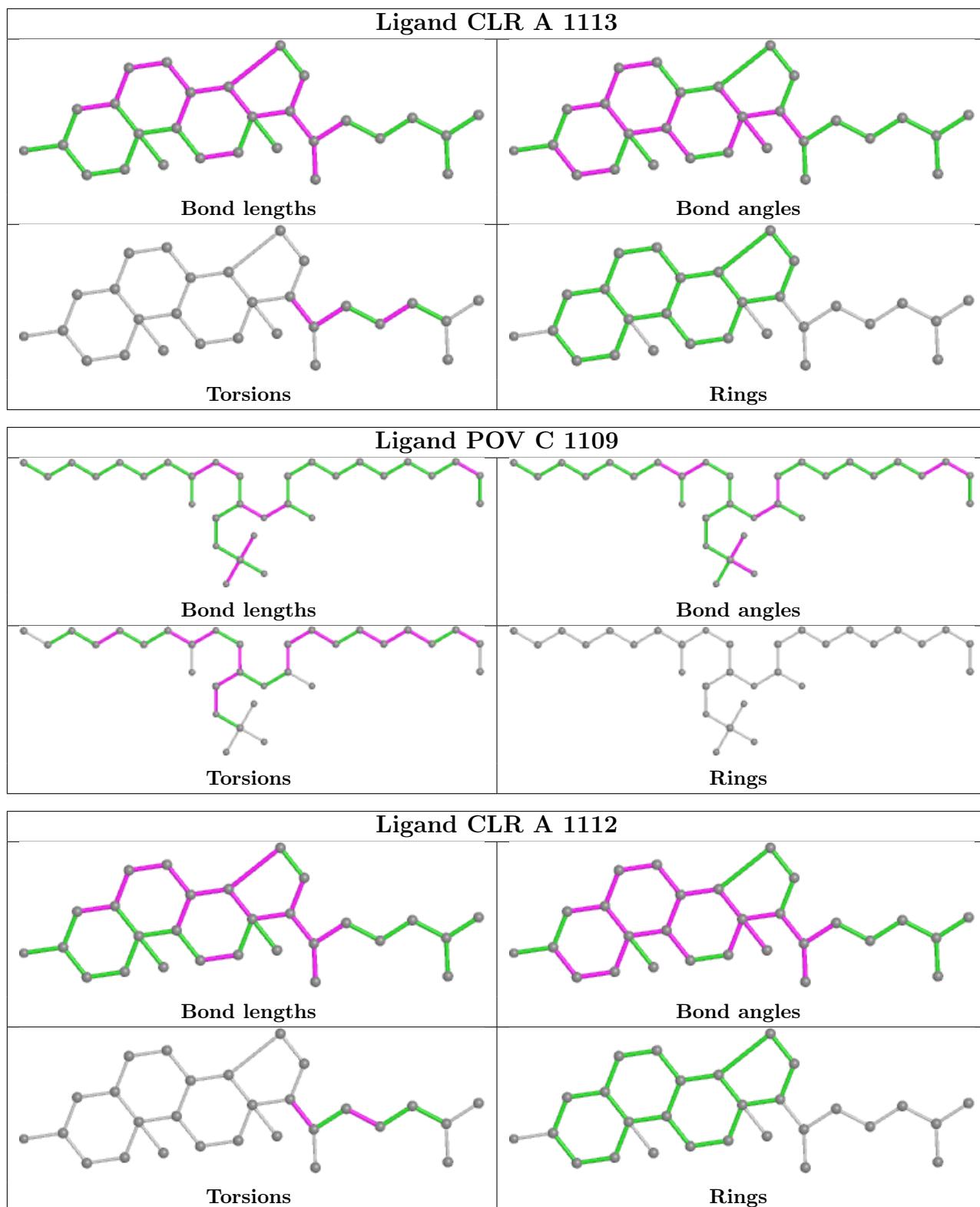


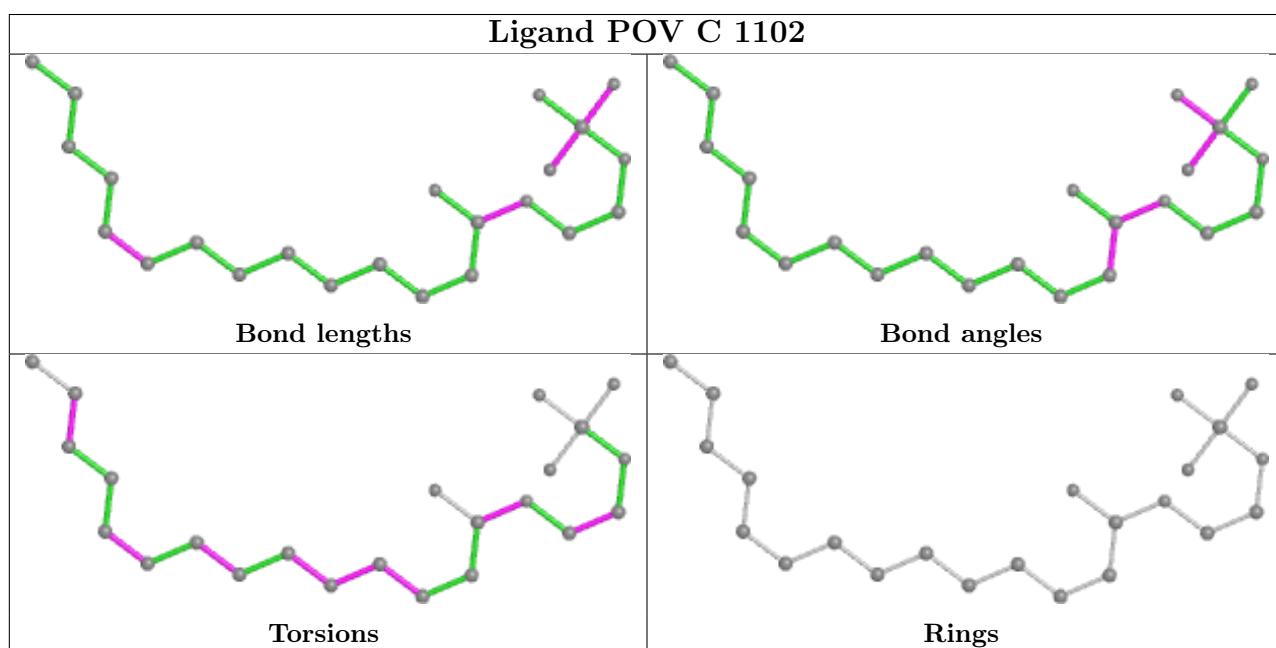
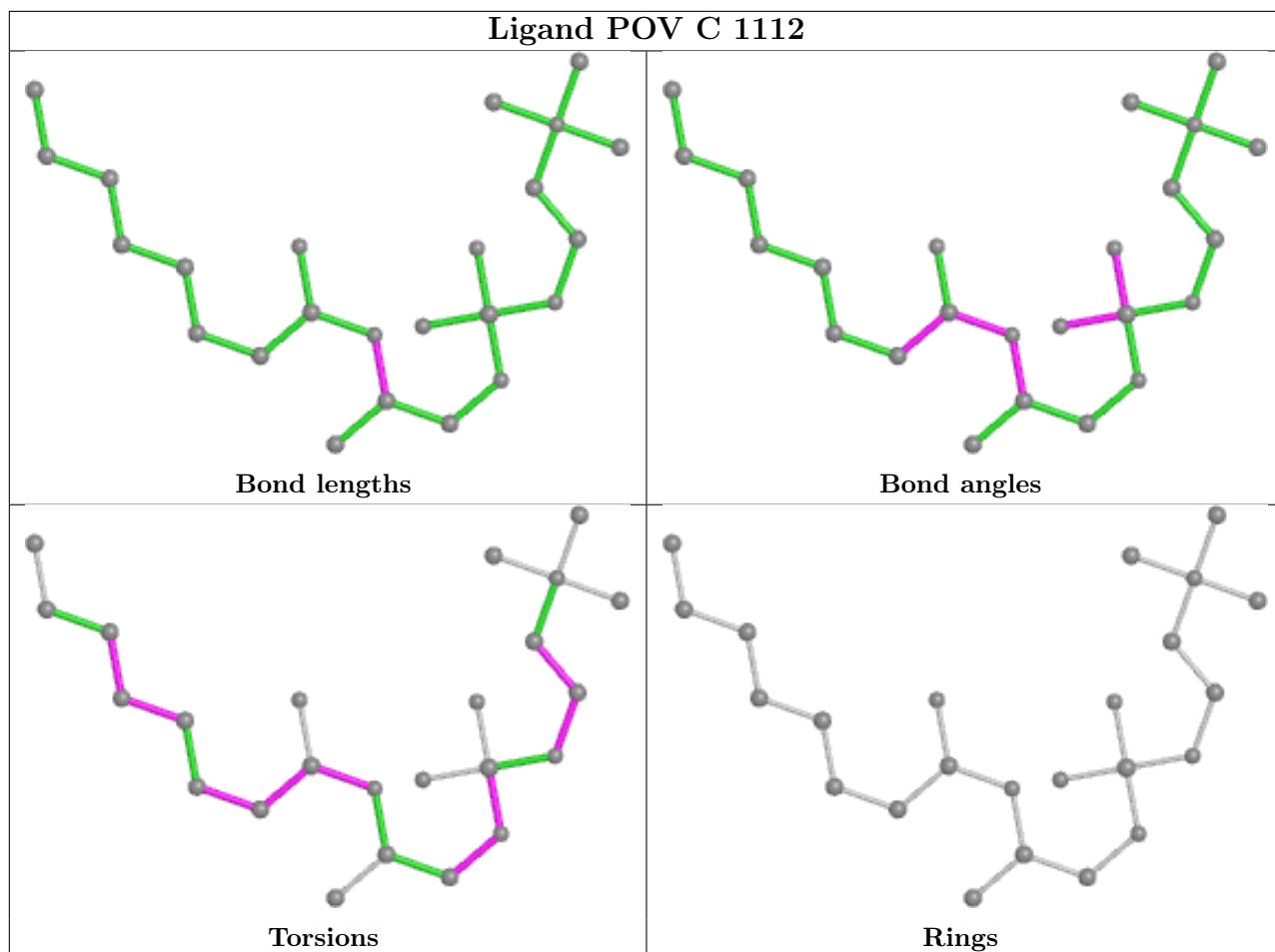


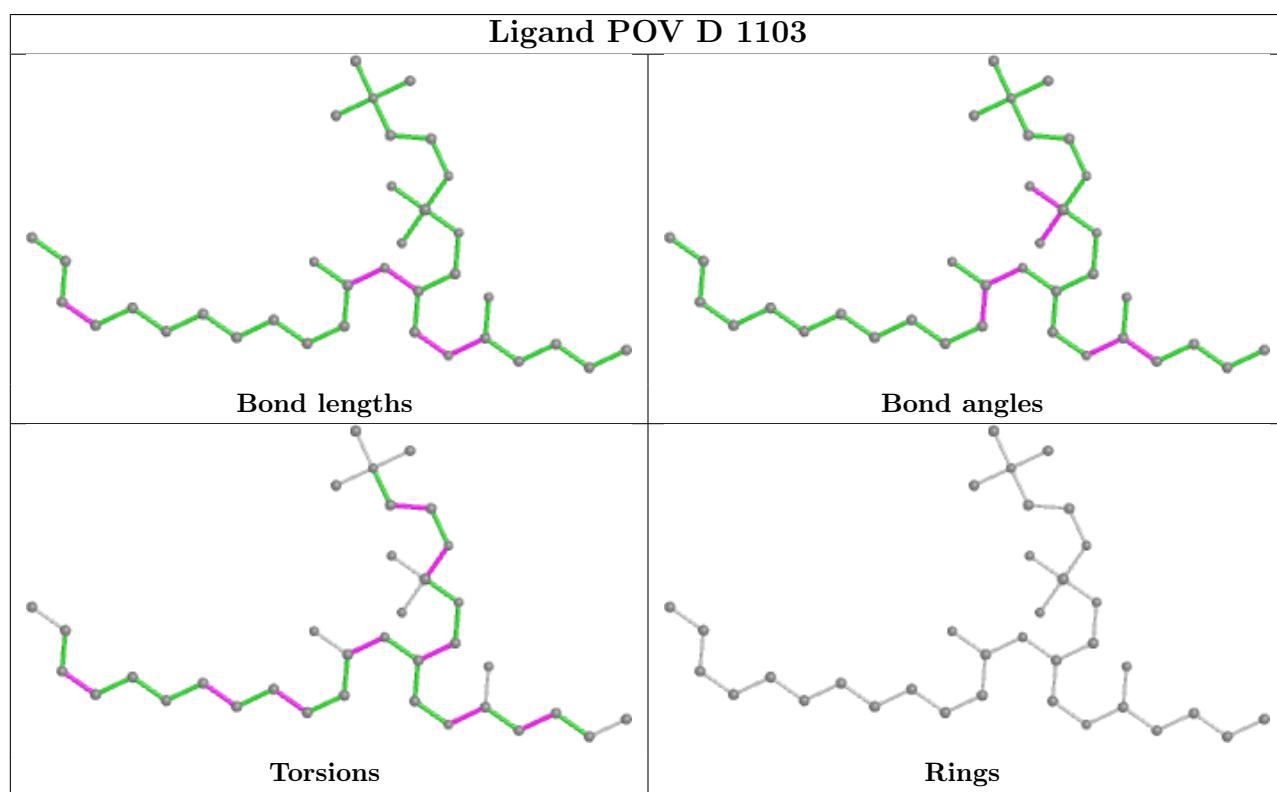
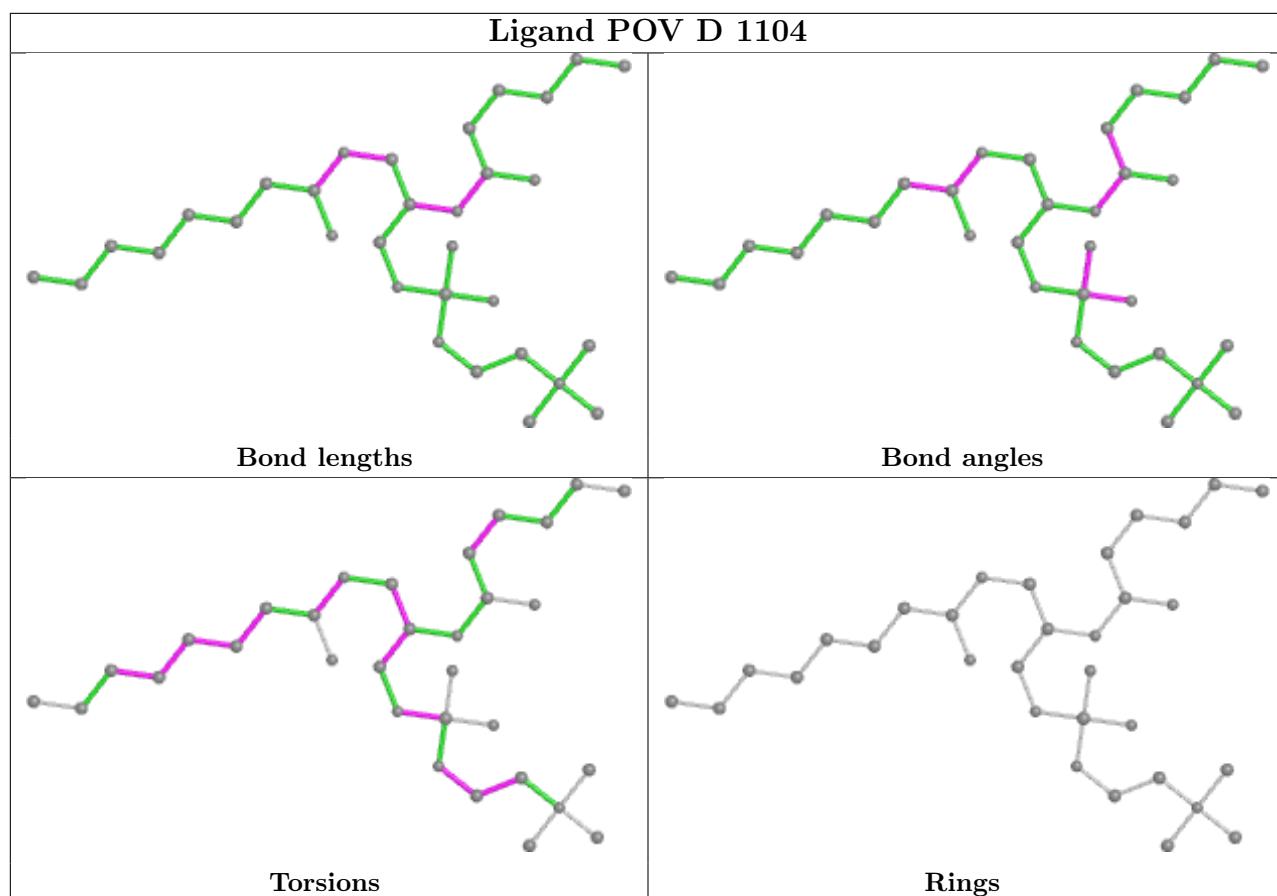


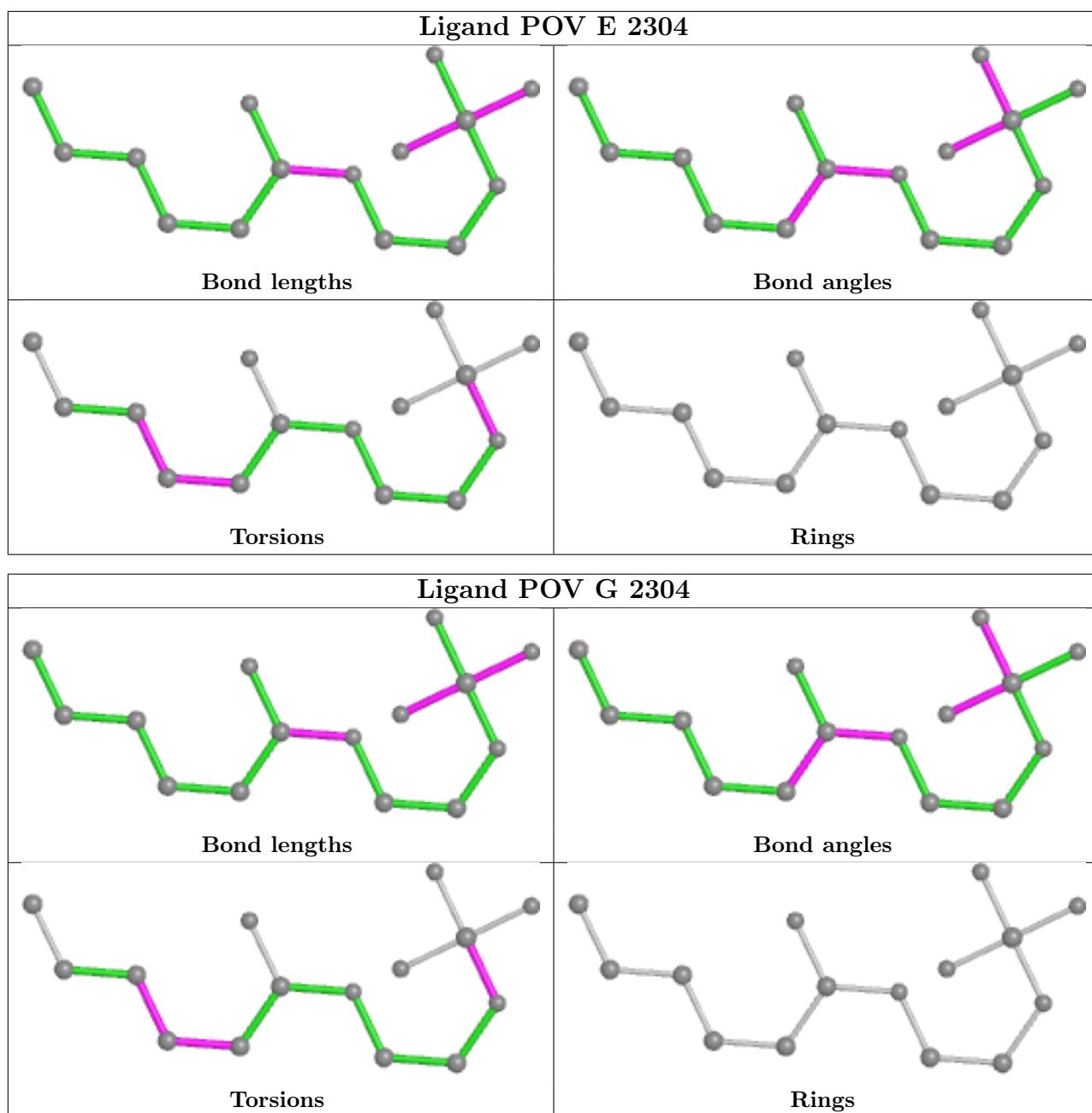












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

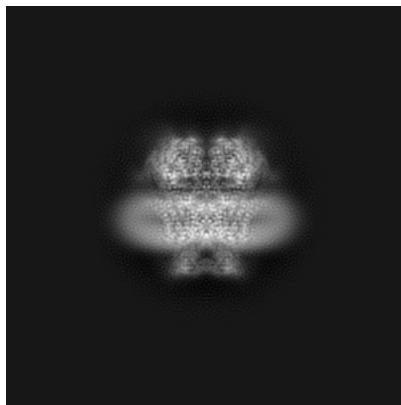
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21025. These allow visual inspection of the internal detail of the map and identification of artifacts.

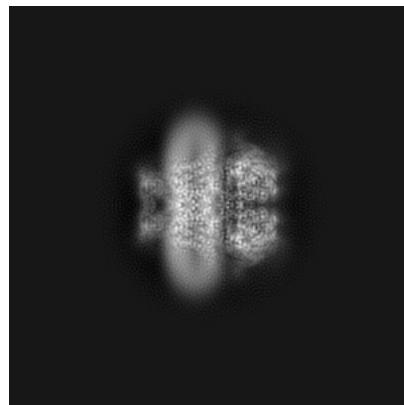
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

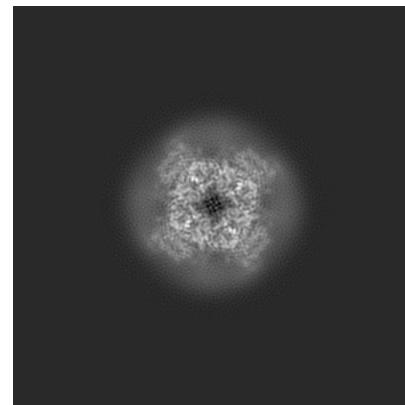
6.1.1 Primary map



X



Y

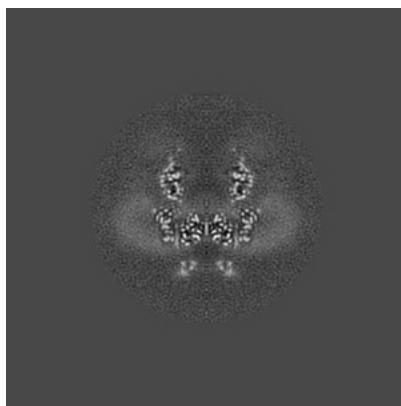


Z

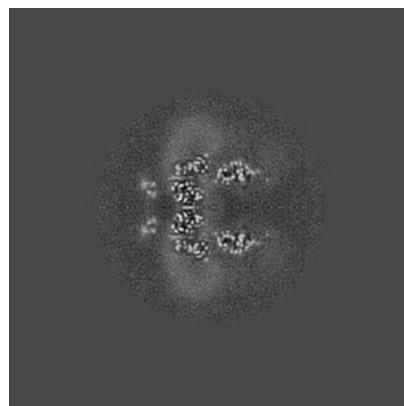
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

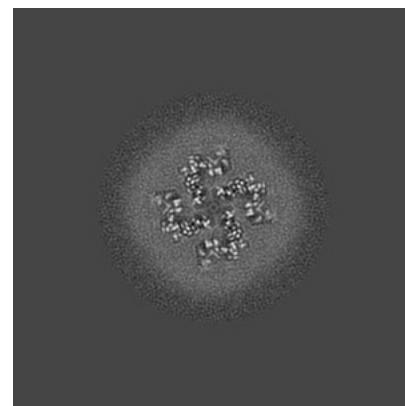
6.2.1 Primary map



X Index: 192



Y Index: 192

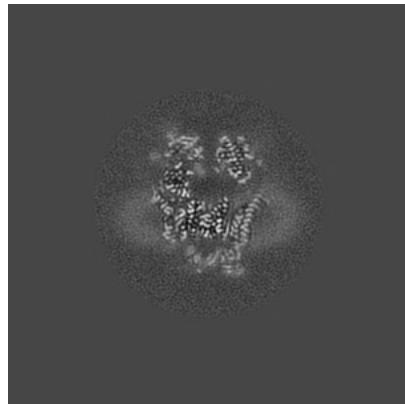


Z Index: 192

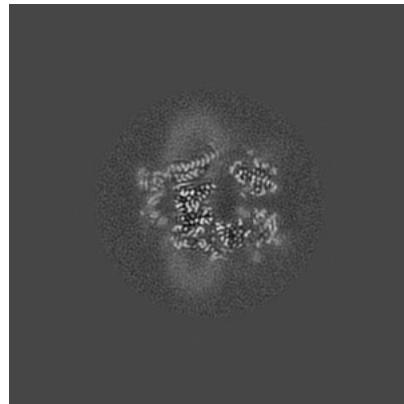
The images above show central slices of the map in three orthogonal directions.

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

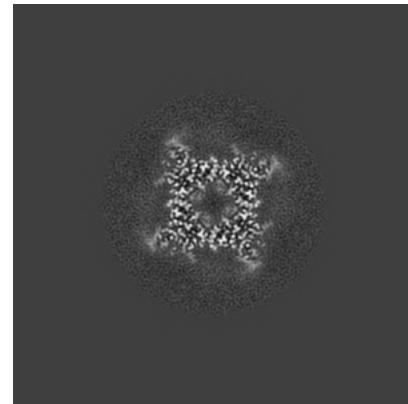
6.3.1 Primary map



X Index: 205



Y Index: 179



Z Index: 222

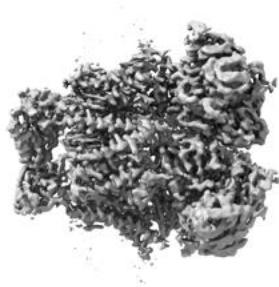
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [\(i\)](#)

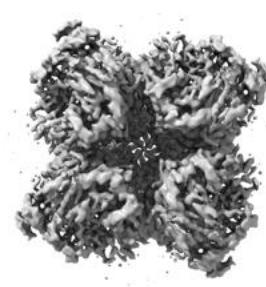
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

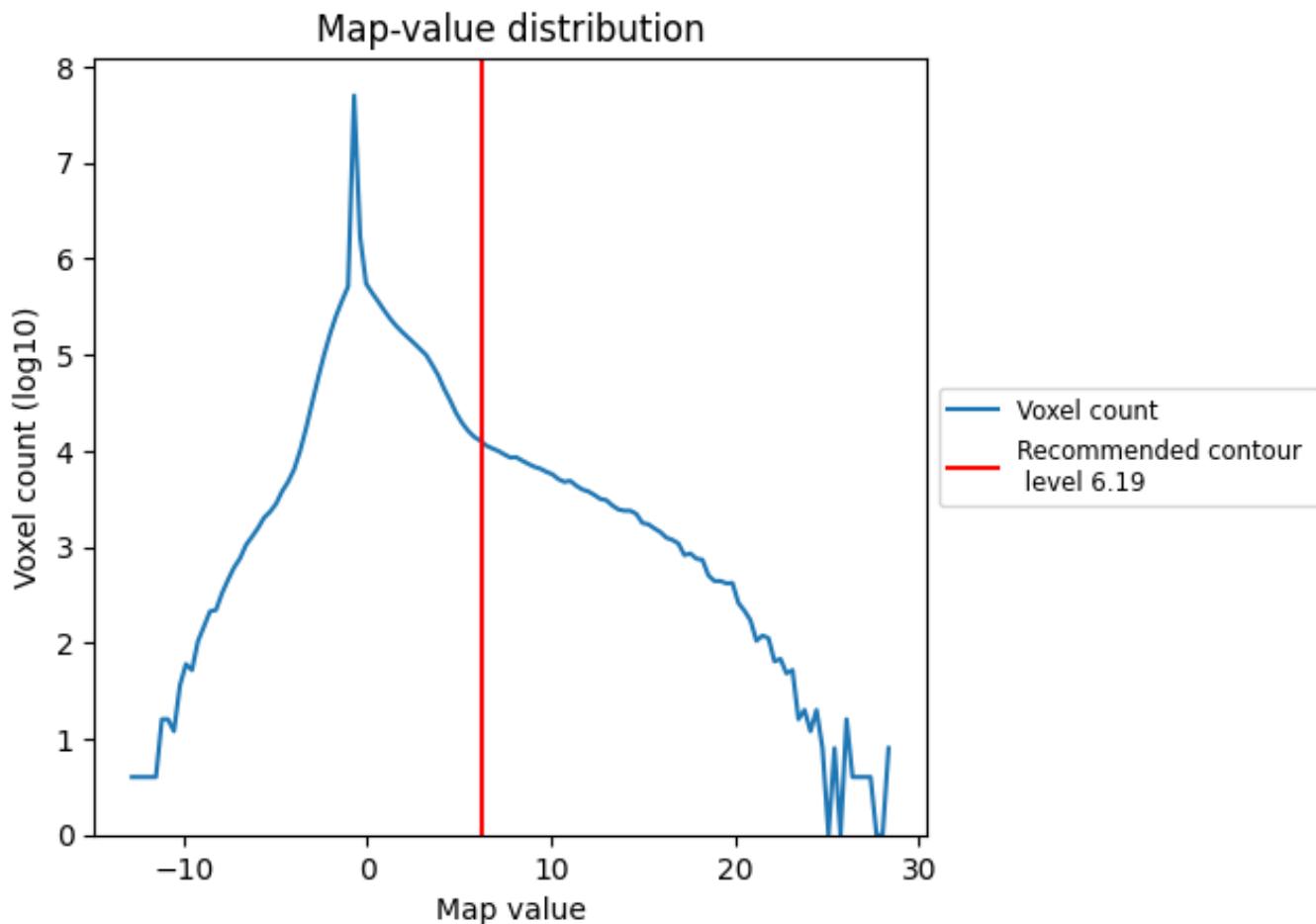
6.5 Mask visualisation

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

7 Map analysis (i)

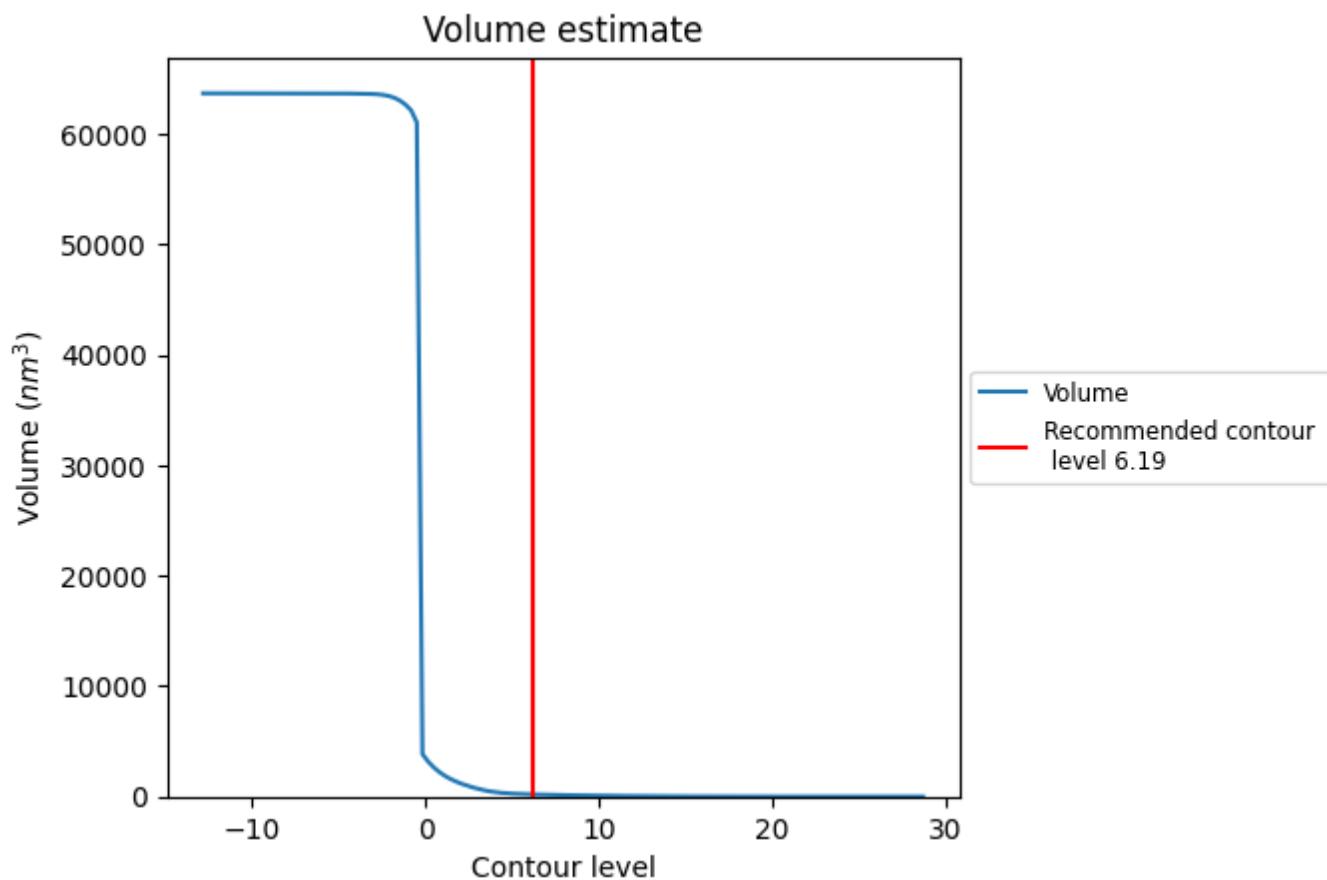
This section contains the results of statistical analysis of the map.

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.

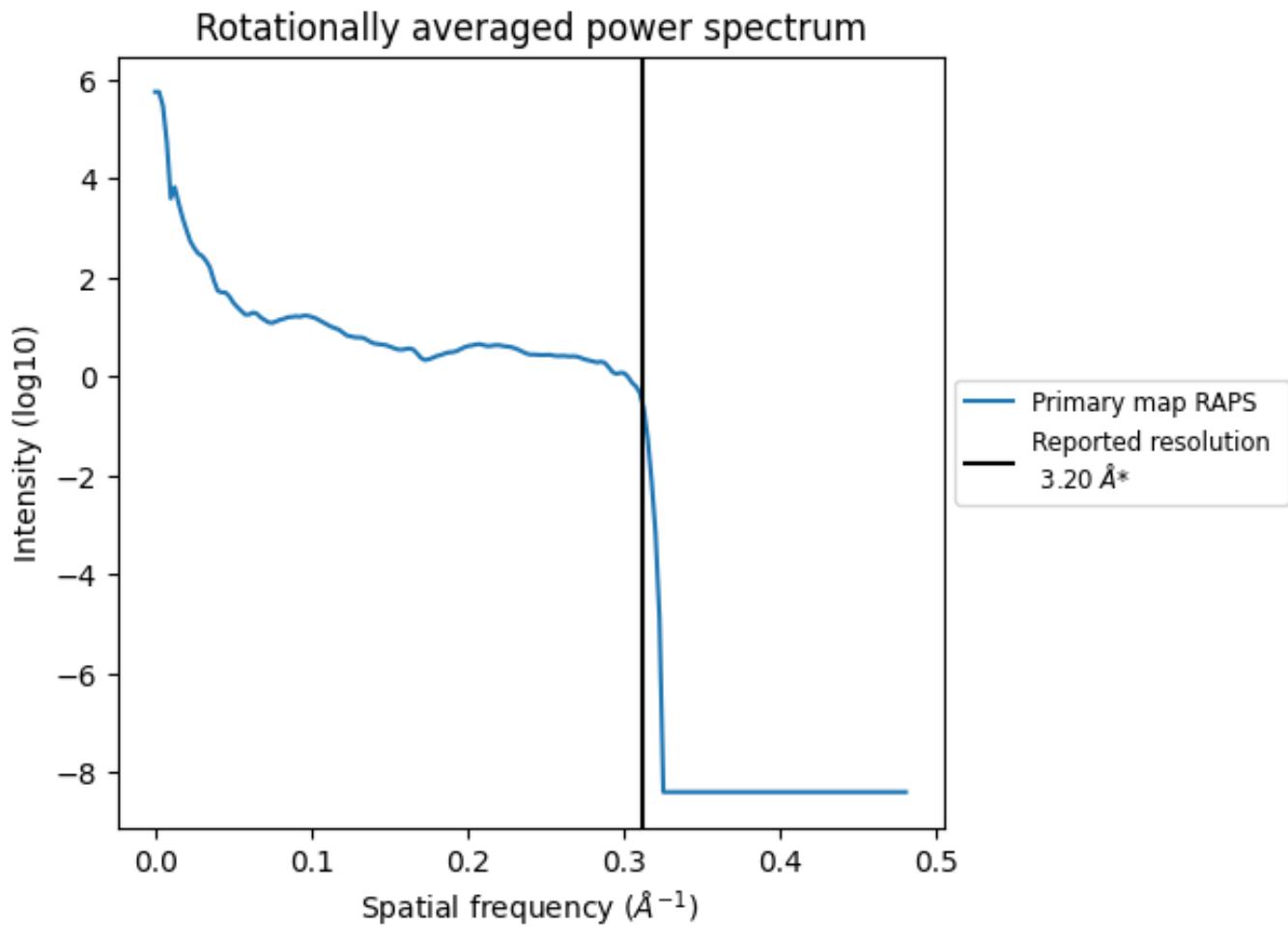
7.2 Volume estimate (i)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 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 0.312\AA^{-1}

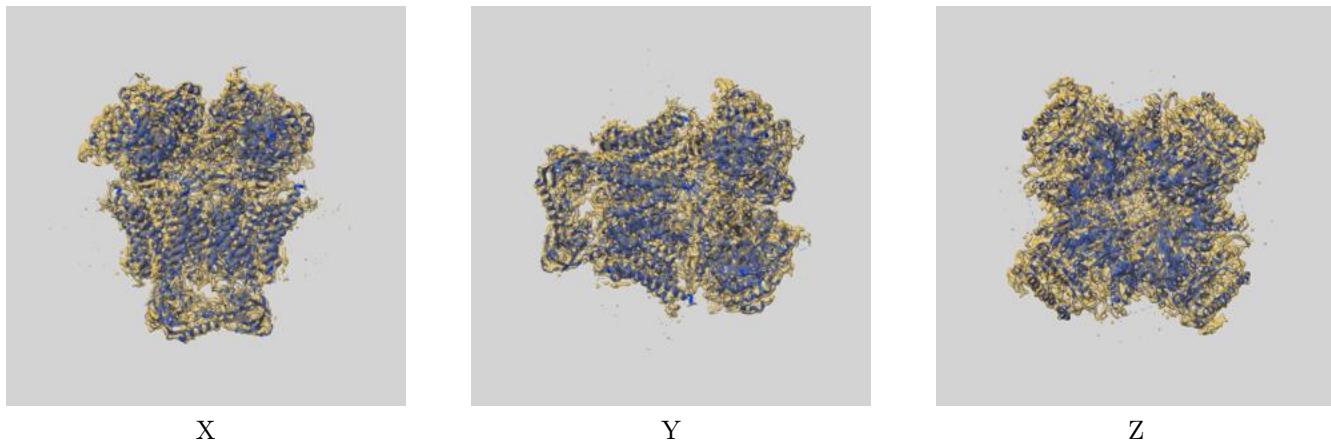
8 Fourier-Shell correlation

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

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

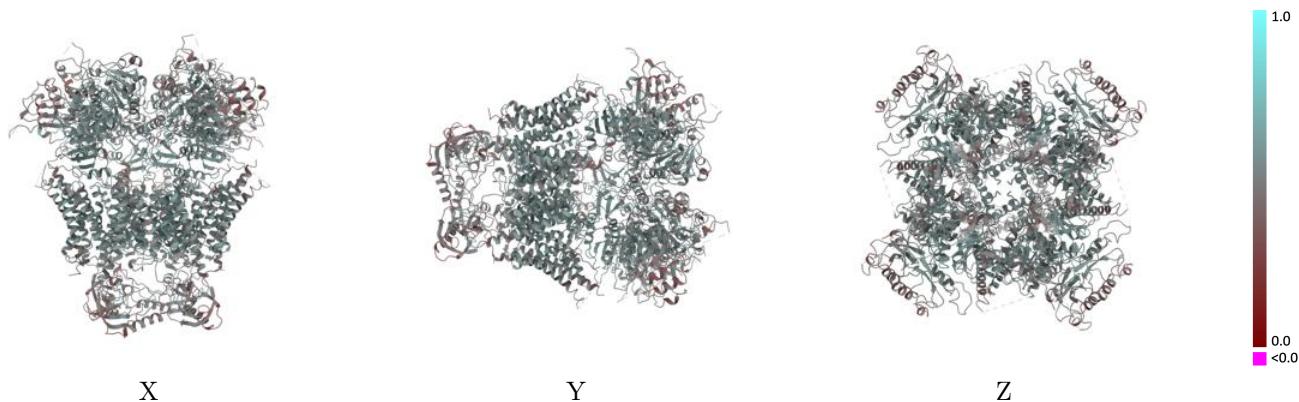
This section contains information regarding the fit between EMDB map EMD-21025 and PDB model 6V22. Per-residue inclusion information can be found in section 3 on page 12.

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



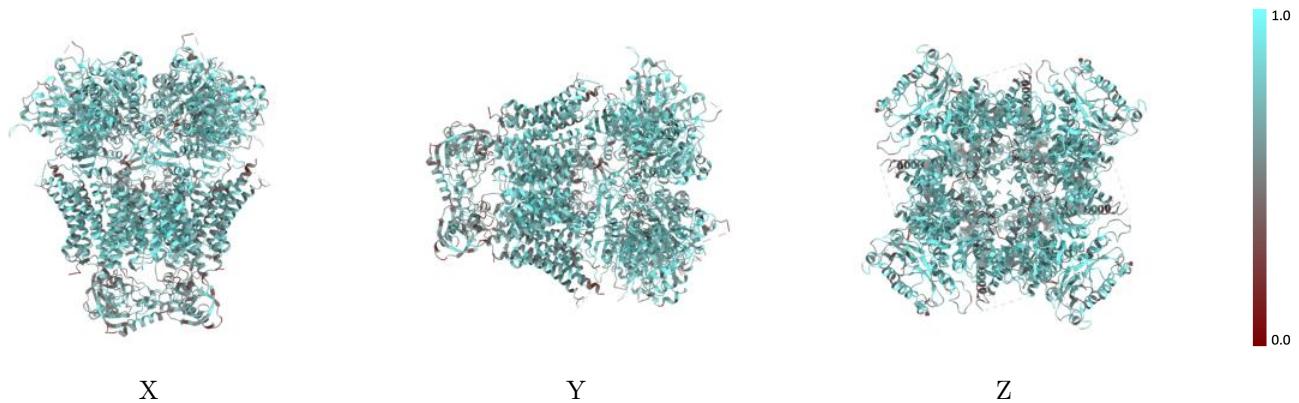
The images above show the 3D surface view of the map at the recommended contour level 6.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



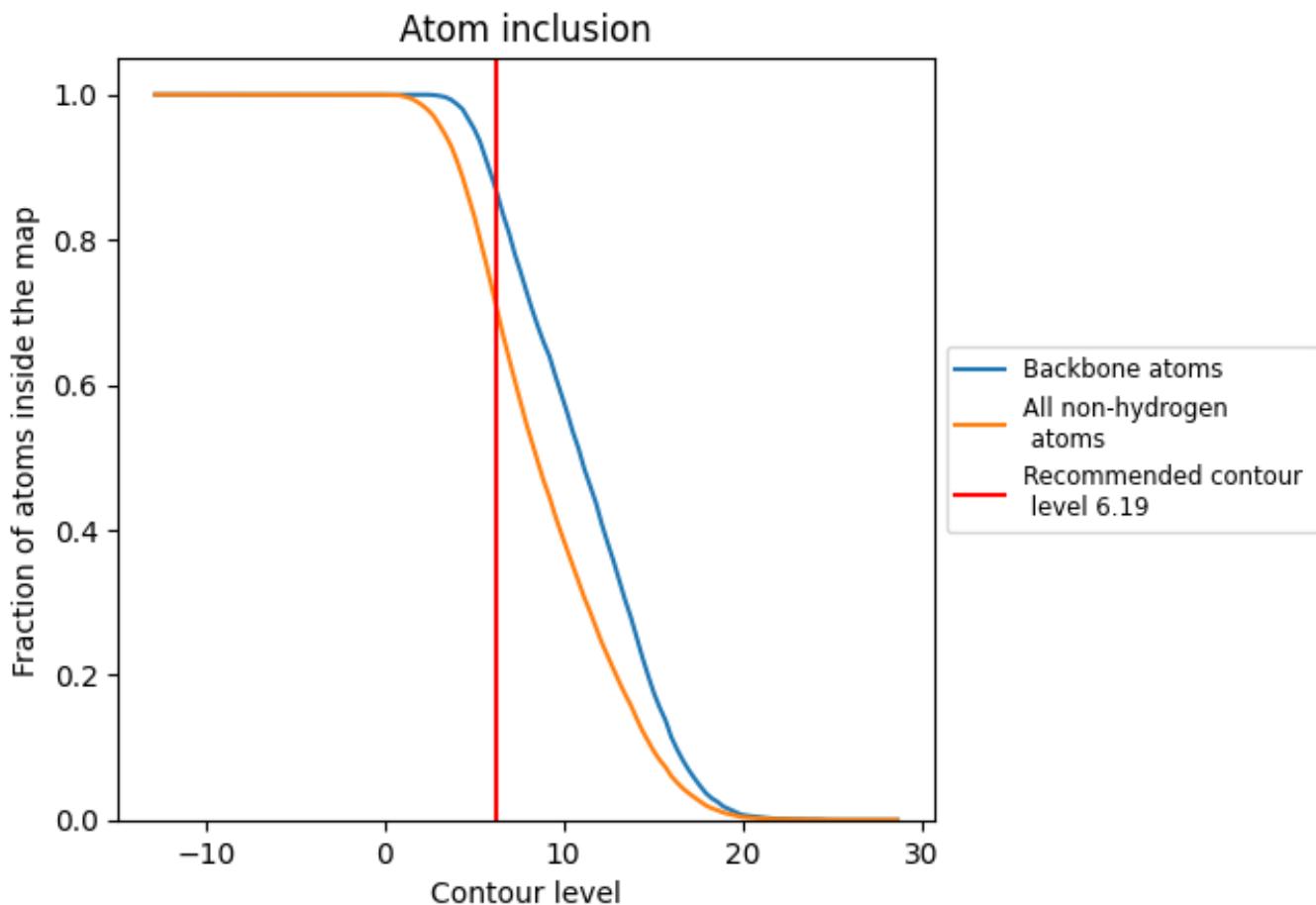
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.19).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (6.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7136	0.5080
A	0.7414	0.5180
B	0.7403	0.5180
C	0.7400	0.5190
D	0.7403	0.5170
E	0.5946	0.4650
F	0.5946	0.4650
G	0.5940	0.4670
H	0.5946	0.4680

