



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 02:40 AM JST

PDB ID : 9JDM / pdb_00009jdm
EMDB ID : EMD-61396
Title : Cryo-EM structure of human TRPV3 determined in MSP2N2 nanodisc
Authors : Lu, X.; Yao, J.
Deposited on : 2024-08-31
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

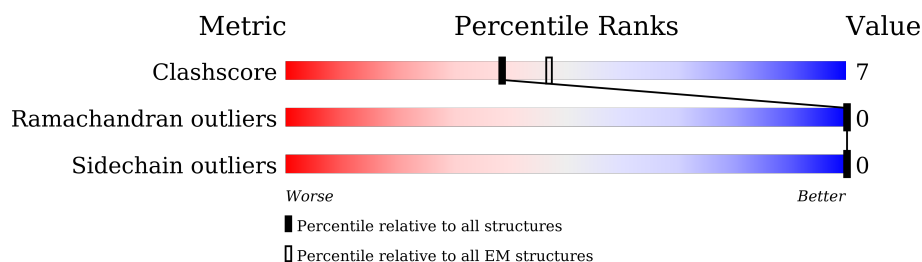
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	799	
1	B	799	
1	C	799	
1	D	799	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20992 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 Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	610	Total	C	N	O	S	0	0
			4946	3224	809	882	31		
1	D	610	Total	C	N	O	S	0	0
			4946	3224	809	882	31		
1	B	610	Total	C	N	O	S	0	0
			4946	3224	809	882	31		
1	C	610	Total	C	N	O	S	0	0
			4946	3224	809	882	31		

There are 40 discrepancies between the modelled and reference sequences:

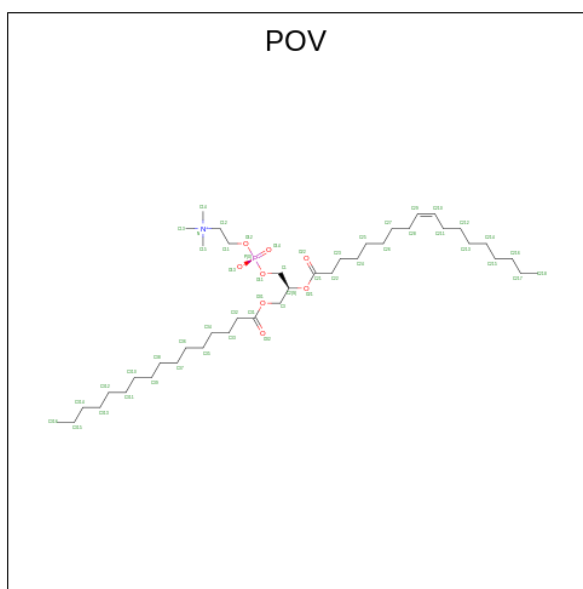
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ILE	variant	UNP Q8NET8
A	791	SER	-	expression tag	UNP Q8NET8
A	792	ASN	-	expression tag	UNP Q8NET8
A	793	SER	-	expression tag	UNP Q8NET8
A	794	LEU	-	expression tag	UNP Q8NET8
A	795	GLU	-	expression tag	UNP Q8NET8
A	796	VAL	-	expression tag	UNP Q8NET8
A	797	LEU	-	expression tag	UNP Q8NET8
A	798	PHE	-	expression tag	UNP Q8NET8
A	799	GLN	-	expression tag	UNP Q8NET8
D	25	VAL	ILE	variant	UNP Q8NET8
D	791	SER	-	expression tag	UNP Q8NET8
D	792	ASN	-	expression tag	UNP Q8NET8
D	793	SER	-	expression tag	UNP Q8NET8
D	794	LEU	-	expression tag	UNP Q8NET8
D	795	GLU	-	expression tag	UNP Q8NET8
D	796	VAL	-	expression tag	UNP Q8NET8
D	797	LEU	-	expression tag	UNP Q8NET8
D	798	PHE	-	expression tag	UNP Q8NET8
D	799	GLN	-	expression tag	UNP Q8NET8
B	25	VAL	ILE	variant	UNP Q8NET8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	791	SER	-	expression tag	UNP Q8NET8
B	792	ASN	-	expression tag	UNP Q8NET8
B	793	SER	-	expression tag	UNP Q8NET8
B	794	LEU	-	expression tag	UNP Q8NET8
B	795	GLU	-	expression tag	UNP Q8NET8
B	796	VAL	-	expression tag	UNP Q8NET8
B	797	LEU	-	expression tag	UNP Q8NET8
B	798	PHE	-	expression tag	UNP Q8NET8
B	799	GLN	-	expression tag	UNP Q8NET8
C	25	VAL	ILE	variant	UNP Q8NET8
C	791	SER	-	expression tag	UNP Q8NET8
C	792	ASN	-	expression tag	UNP Q8NET8
C	793	SER	-	expression tag	UNP Q8NET8
C	794	LEU	-	expression tag	UNP Q8NET8
C	795	GLU	-	expression tag	UNP Q8NET8
C	796	VAL	-	expression tag	UNP Q8NET8
C	797	LEU	-	expression tag	UNP Q8NET8
C	798	PHE	-	expression tag	UNP Q8NET8
C	799	GLN	-	expression tag	UNP Q8NET8

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			46	36	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
2	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	D	1	Total	C	N	O	P	0
			48	38	1	8	1	
2	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
2	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	B	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			34	24	1	8	1	

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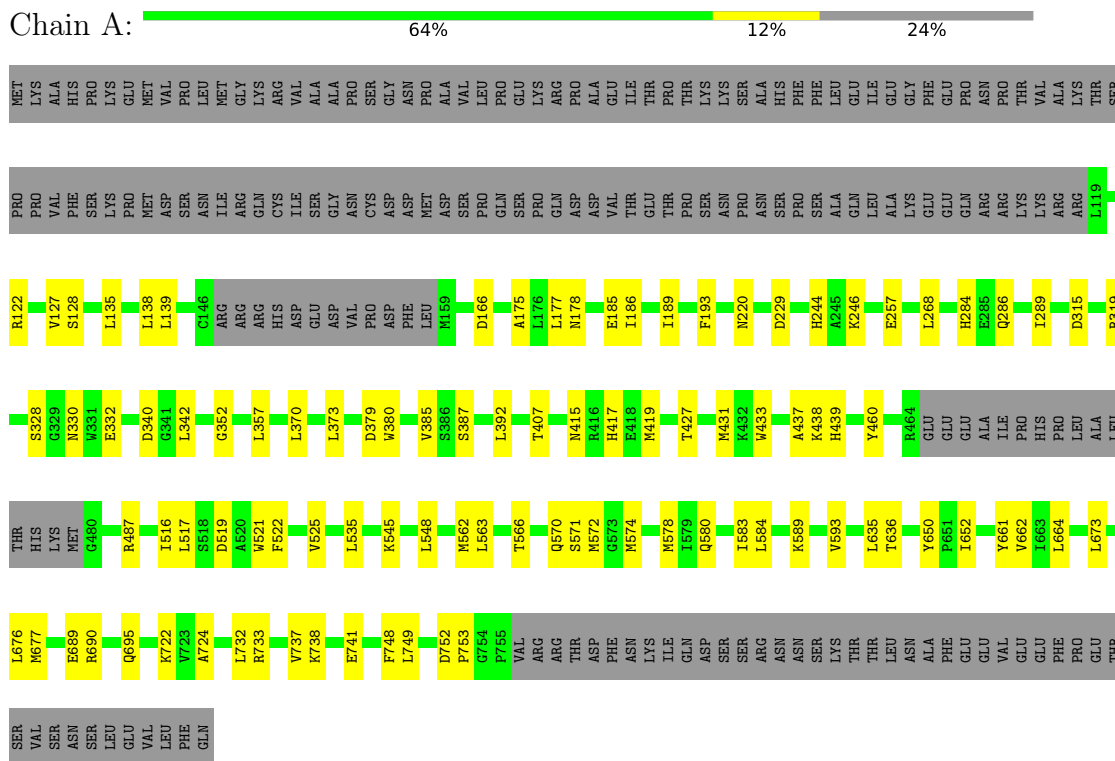
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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
2	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	C	1	Total	C	N	O	P	0
			39	29	1	8	1	

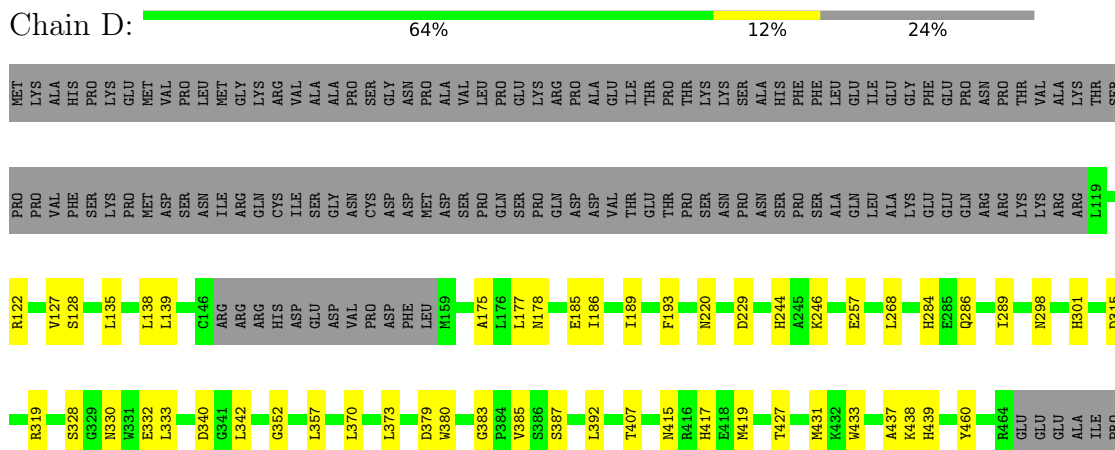
3 Residue-property plots

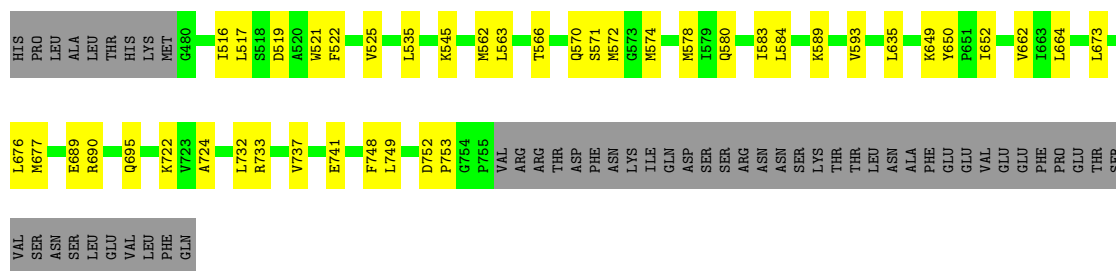
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Transient receptor potential cation channel subfamily V member 3



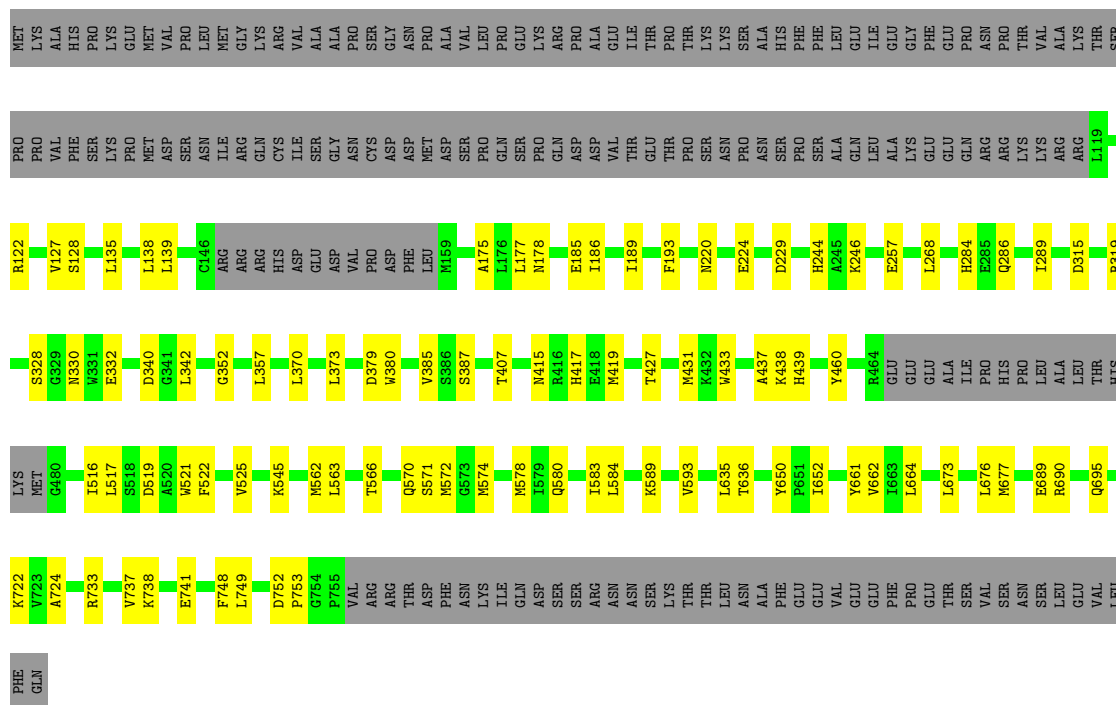
- Molecule 1: Transient receptor potential cation channel subfamily V member 3





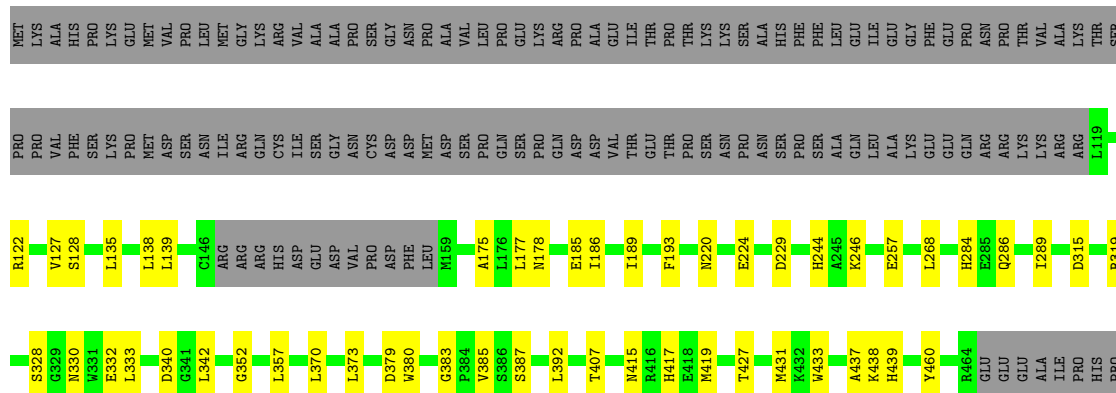
- Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain B: 65% 12% 24%



- Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain C: 64% 12% 24%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-1400	Depositor
Maximum defocus (nm)	-2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.10	0/5053	0.30	2/6836 (0.0%)
1	B	0.11	0/5053	0.30	2/6836 (0.0%)
1	C	0.11	0/5053	0.30	2/6836 (0.0%)
1	D	0.10	0/5053	0.30	2/6836 (0.0%)
All	All	0.10	0/20212	0.30	8/27344 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	752	ASP	CA-C-N	-6.80	113.68	120.21
1	C	752	ASP	C-N-CA	-6.80	113.68	120.21
1	A	752	ASP	CA-C-N	-6.78	113.70	120.21
1	A	752	ASP	C-N-CA	-6.78	113.70	120.21
1	D	752	ASP	CA-C-N	-6.78	113.70	120.21
1	D	752	ASP	C-N-CA	-6.78	113.70	120.21
1	B	752	ASP	CA-C-N	-6.78	113.70	120.21
1	B	752	ASP	C-N-CA	-6.78	113.70	120.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4946	0	5008	79	0
1	B	4946	0	5008	79	0
1	C	4946	0	5008	78	0
1	D	4946	0	5008	80	0
2	A	302	0	431	13	0
2	B	302	0	431	13	0
2	C	302	0	431	16	0
2	D	302	0	431	13	0
All	All	20992	0	21756	304	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 7.

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:PHE:HZ	1:C:178:ASN:OD1	1.66	0.77
1:B:178:ASN:OD1	1:C:748:PHE:HZ	1.68	0.76
1:B:128:SER:HB2	1:B:178:ASN:HD22	1.52	0.75
1:A:748:PHE:HZ	1:D:178:ASN:OD1	1.69	0.75
1:A:178:ASN:OD1	1:B:748:PHE:HZ	1.69	0.75
1:D:748:PHE:CZ	1:C:178:ASN:OD1	2.40	0.75
1:C:128:SER:HB2	1:C:178:ASN:HD22	1.52	0.75
1:A:128:SER:HB2	1:A:178:ASN:HD22	1.52	0.74
1:D:128:SER:HB2	1:D:178:ASN:HD22	1.52	0.74
1:B:676:LEU:HD21	1:C:578:MET:HE1	1.71	0.73
1:A:578:MET:HE1	1:D:676:LEU:HD21	1.71	0.73
1:B:178:ASN:OD1	1:C:748:PHE:CZ	2.42	0.73
1:A:676:LEU:HD21	1:B:578:MET:HE1	1.70	0.72
1:A:178:ASN:OD1	1:B:748:PHE:CZ	2.42	0.72
1:C:128:SER:CB	1:C:178:ASN:HD22	2.03	0.72
1:B:128:SER:CB	1:B:178:ASN:HD22	2.03	0.71
1:D:578:MET:HE1	1:C:676:LEU:HD21	1.72	0.71
1:A:748:PHE:CZ	1:D:178:ASN:OD1	2.42	0.71
1:A:128:SER:CB	1:A:178:ASN:HD22	2.03	0.71
1:D:128:SER:CB	1:D:178:ASN:HD22	2.03	0.71
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.75	0.69
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.75	0.68
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.75	0.68
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.75	0.67
1:D:340:ASP:OD2	1:D:342:LEU:CD1	2.46	0.64
1:A:340:ASP:OD2	1:A:342:LEU:CD1	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ASP:OD2	1:C:342:LEU:CD1	2.46	0.63
1:B:340:ASP:OD2	1:B:342:LEU:CD1	2.46	0.63
1:A:722:LYS:HG3	1:A:724:ALA:H	1.67	0.60
1:D:722:LYS:HG3	1:D:724:ALA:H	1.67	0.59
1:B:722:LYS:HG3	1:B:724:ALA:H	1.67	0.59
1:C:352:GLY:O	1:C:415:ASN:ND2	2.36	0.59
1:A:352:GLY:O	1:A:415:ASN:ND2	2.36	0.59
1:C:722:LYS:HG3	1:C:724:ALA:H	1.67	0.59
1:D:352:GLY:O	1:D:415:ASN:ND2	2.36	0.58
1:D:289:ILE:HD12	1:D:289:ILE:H	1.68	0.58
1:B:289:ILE:H	1:B:289:ILE:HD12	1.68	0.58
1:C:289:ILE:HD12	1:C:289:ILE:H	1.68	0.58
1:B:352:GLY:O	1:B:415:ASN:ND2	2.36	0.58
1:A:589:LYS:HE3	2:A:805:POV:H3	1.85	0.58
1:A:289:ILE:HD12	1:A:289:ILE:H	1.68	0.58
1:D:589:LYS:HE3	2:D:807:POV:H3	1.85	0.58
1:B:589:LYS:HE3	2:B:805:POV:H3	1.85	0.57
1:C:589:LYS:HE3	2:C:807:POV:H3	1.85	0.57
1:A:571:SER:HB2	1:D:589:LYS:HE2	1.86	0.57
1:D:519:ASP:N	1:D:519:ASP:OD1	2.37	0.57
1:C:519:ASP:OD1	1:C:519:ASP:N	2.37	0.57
1:B:519:ASP:OD1	1:B:519:ASP:N	2.37	0.56
1:A:229:ASP:OD1	1:A:229:ASP:N	2.39	0.56
1:B:574:MET:HE1	1:B:689:GLU:HG2	1.88	0.56
1:A:574:MET:HE1	1:A:689:GLU:HG2	1.88	0.56
1:C:229:ASP:OD1	1:C:229:ASP:N	2.38	0.56
1:A:589:LYS:HE2	1:B:571:SER:HB2	1.86	0.56
1:D:229:ASP:OD1	1:D:229:ASP:N	2.39	0.56
1:B:589:LYS:HE2	1:C:571:SER:HB2	1.87	0.56
1:D:128:SER:OG	1:D:178:ASN:ND2	2.39	0.56
1:D:571:SER:HB2	1:C:589:LYS:HE2	1.88	0.56
1:C:574:MET:HE1	1:C:689:GLU:HG2	1.88	0.56
1:D:574:MET:HE1	1:D:689:GLU:HG2	1.88	0.56
1:C:128:SER:OG	1:C:178:ASN:ND2	2.39	0.56
1:A:128:SER:OG	1:A:178:ASN:ND2	2.39	0.55
1:D:438:LYS:HG2	2:D:804:POV:H3A	1.89	0.55
1:B:128:SER:OG	1:B:178:ASN:ND2	2.39	0.55
1:C:438:LYS:HG2	2:C:804:POV:H3A	1.89	0.55
1:C:122:ARG:HB3	1:C:138:LEU:HD21	1.89	0.55
1:B:522:PHE:HA	1:B:525:VAL:HG22	1.89	0.54
1:A:438:LYS:HG2	2:A:802:POV:H3A	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASP:N	1:A:519:ASP:OD1	2.37	0.54
1:B:438:LYS:HG2	2:B:802:POV:H3A	1.89	0.54
1:C:328:SER:OG	1:C:330:ASN:OD1	2.25	0.54
1:C:583:ILE:HD13	2:C:806:POV:H24	1.90	0.54
1:D:583:ILE:HD13	2:D:806:POV:H24	1.90	0.54
1:C:244:HIS:O	1:C:246:LYS:NZ	2.41	0.54
1:A:522:PHE:HA	1:A:525:VAL:HG22	1.89	0.54
1:D:522:PHE:HA	1:D:525:VAL:HG22	1.89	0.54
1:B:244:HIS:O	1:B:246:LYS:NZ	2.41	0.54
1:B:328:SER:OG	1:B:330:ASN:OD1	2.25	0.54
1:B:229:ASP:OD1	1:B:229:ASP:N	2.39	0.53
1:D:122:ARG:HB3	1:D:138:LEU:HD21	1.89	0.53
1:B:122:ARG:HB3	1:B:138:LEU:HD21	1.89	0.53
1:A:122:ARG:HB3	1:A:138:LEU:HD21	1.89	0.53
1:A:244:HIS:O	1:A:246:LYS:NZ	2.41	0.53
1:B:127:VAL:HB	1:B:175:ALA:HB2	1.90	0.53
1:A:127:VAL:HB	1:A:175:ALA:HB2	1.90	0.53
1:B:583:ILE:HD13	2:B:804:POV:H24	1.90	0.53
1:D:244:HIS:O	1:D:246:LYS:NZ	2.41	0.53
1:A:417:HIS:HB2	1:A:690:ARG:HE	1.74	0.53
1:C:127:VAL:HB	1:C:175:ALA:HB2	1.90	0.53
1:D:127:VAL:HB	1:D:175:ALA:HB2	1.90	0.53
1:A:583:ILE:HD13	2:A:804:POV:H24	1.90	0.52
1:A:328:SER:OG	1:A:330:ASN:OD1	2.25	0.52
1:C:522:PHE:HA	1:C:525:VAL:HG22	1.89	0.52
1:B:417:HIS:HB2	1:B:690:ARG:HE	1.74	0.52
1:D:417:HIS:HB2	1:D:690:ARG:HE	1.74	0.52
1:A:128:SER:CB	1:A:178:ASN:ND2	2.72	0.52
1:A:517:LEU:HB3	1:A:521:TRP:HB2	1.92	0.52
1:D:517:LEU:HB3	1:D:521:TRP:HB2	1.92	0.52
1:A:284:HIS:ND1	1:A:286:GLN:OE1	2.44	0.51
1:B:517:LEU:HB3	1:B:521:TRP:HB2	1.92	0.51
1:B:128:SER:CB	1:B:178:ASN:ND2	2.72	0.51
1:C:517:LEU:HB3	1:C:521:TRP:HB2	1.92	0.51
1:D:128:SER:CB	1:D:178:ASN:ND2	2.72	0.51
1:B:284:HIS:ND1	1:B:286:GLN:OE1	2.43	0.51
1:C:220:ASN:OD1	1:C:268:LEU:HD22	2.11	0.51
1:C:407:THR:HG23	1:C:419:MET:HE2	1.92	0.51
1:B:407:THR:HG23	1:B:419:MET:HE2	1.92	0.51
1:B:330:ASN:ND2	1:B:332:GLU:OE1	2.40	0.51
1:C:128:SER:CB	1:C:178:ASN:ND2	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:ND1	1:D:286:GLN:OE1	2.43	0.51
1:C:417:HIS:HB2	1:C:690:ARG:HE	1.74	0.51
2:A:801:POV:O14	1:B:460:TYR:OH	2.28	0.51
1:D:635:LEU:HD21	1:D:662:VAL:HG22	1.93	0.51
1:C:330:ASN:ND2	1:C:332:GLU:OE1	2.40	0.50
1:B:635:LEU:HD21	1:B:662:VAL:HG22	1.93	0.50
1:C:284:HIS:ND1	1:C:286:GLN:OE1	2.44	0.50
1:B:516:ILE:HB	1:B:584:LEU:HD13	1.93	0.50
1:D:516:ILE:HB	1:D:584:LEU:HD13	1.93	0.50
1:B:220:ASN:OD1	1:B:268:LEU:HD22	2.11	0.50
2:B:801:POV:O14	1:C:460:TYR:OH	2.29	0.50
1:C:370:LEU:HD12	1:C:373:LEU:HD22	1.93	0.50
1:A:330:ASN:ND2	1:A:332:GLU:OE1	2.40	0.50
1:D:220:ASN:OD1	1:D:268:LEU:HD22	2.11	0.50
1:D:407:THR:HG23	1:D:419:MET:HE2	1.92	0.50
1:A:635:LEU:HD21	1:A:662:VAL:HG22	1.93	0.50
1:D:370:LEU:HD12	1:D:373:LEU:HD22	1.93	0.50
1:A:220:ASN:OD1	1:A:268:LEU:HD22	2.11	0.49
1:A:407:THR:HG23	1:A:419:MET:HE2	1.92	0.49
1:C:695:GLN:NE2	2:C:806:POV:O13	2.45	0.49
1:A:516:ILE:HB	1:A:584:LEU:HD13	1.93	0.49
1:A:695:GLN:NE2	2:A:804:POV:O13	2.45	0.49
2:D:807:POV:H28	2:D:807:POV:H37	1.94	0.49
2:B:805:POV:H28	2:B:805:POV:H37	1.94	0.49
1:B:370:LEU:HD12	1:B:373:LEU:HD22	1.93	0.49
1:C:635:LEU:HD21	1:C:662:VAL:HG22	1.93	0.49
1:B:695:GLN:NE2	2:B:804:POV:O13	2.45	0.49
1:C:516:ILE:HB	1:C:584:LEU:HD13	1.93	0.49
1:A:460:TYR:OH	2:D:803:POV:O14	2.30	0.49
1:D:695:GLN:NE2	2:D:806:POV:O13	2.45	0.49
2:A:805:POV:H37	2:A:805:POV:H28	1.94	0.49
2:C:807:POV:H37	2:C:807:POV:H28	1.94	0.49
1:A:166:ASP:OD1	1:A:166:ASP:N	2.39	0.48
1:A:370:LEU:HD12	1:A:373:LEU:HD22	1.93	0.48
1:D:460:TYR:OH	2:C:803:POV:O14	2.31	0.48
1:D:315:ASP:OD1	1:D:319:ARG:NH1	2.47	0.48
1:D:328:SER:OG	1:D:330:ASN:OD1	2.25	0.48
1:D:387:SER:OG	1:D:733:ARG:NH1	2.44	0.48
1:C:315:ASP:OD1	1:C:319:ARG:NH1	2.47	0.48
1:A:315:ASP:OD1	1:A:319:ARG:NH1	2.47	0.48
2:A:805:POV:H15A	2:A:805:POV:H1A	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASP:OD2	1:A:342:LEU:HD12	2.14	0.48
2:B:805:POV:H1A	2:B:805:POV:H15A	1.96	0.48
1:C:387:SER:OG	1:C:733:ARG:NH1	2.44	0.47
1:B:340:ASP:OD2	1:B:342:LEU:HD12	2.14	0.47
1:D:673:LEU:O	1:D:677:MET:HG3	2.15	0.47
1:C:673:LEU:O	1:C:677:MET:HG3	2.15	0.47
1:D:652:ILE:HB	2:D:801:POV:H1A	1.97	0.47
2:D:807:POV:H15A	2:D:807:POV:H1A	1.96	0.47
1:B:315:ASP:OD1	1:B:319:ARG:NH1	2.47	0.47
1:A:652:ILE:HB	2:A:806:POV:H1A	1.97	0.47
1:D:330:ASN:ND2	1:D:332:GLU:OE1	2.40	0.47
1:D:357:LEU:HD22	1:D:419:MET:HE3	1.96	0.47
1:C:340:ASP:OD2	1:C:342:LEU:HD12	2.14	0.47
2:C:807:POV:H15A	2:C:807:POV:H1A	1.96	0.47
1:A:387:SER:OG	1:A:733:ARG:NH1	2.44	0.47
1:D:128:SER:HB2	1:D:178:ASN:ND2	2.26	0.47
1:B:357:LEU:HD22	1:B:419:MET:HE3	1.96	0.47
1:C:676:LEU:HD23	1:C:676:LEU:HA	1.79	0.47
1:A:357:LEU:HD22	1:A:419:MET:HE3	1.96	0.47
1:A:673:LEU:O	1:A:677:MET:HG3	2.15	0.46
1:D:340:ASP:OD2	1:D:342:LEU:HD12	2.14	0.46
1:C:566:THR:HB	1:C:572:MET:HB3	1.97	0.46
1:A:570:GLN:O	1:A:574:MET:HG2	2.16	0.46
1:B:570:GLN:O	1:B:574:MET:HG2	2.16	0.46
1:C:357:LEU:HD22	1:C:419:MET:HE3	1.96	0.46
1:B:673:LEU:O	1:B:677:MET:HG3	2.15	0.46
1:C:570:GLN:O	1:C:574:MET:HG2	2.16	0.46
1:B:652:ILE:HB	2:B:806:POV:H1A	1.98	0.46
1:C:738:LYS:HA	1:C:738:LYS:HD3	1.76	0.46
1:A:664:LEU:HD21	2:B:804:POV:H37	1.97	0.46
1:D:566:THR:HB	1:D:572:MET:HB3	1.97	0.46
1:B:664:LEU:HD21	2:C:806:POV:H37	1.98	0.46
1:A:128:SER:HB2	1:A:178:ASN:ND2	2.26	0.46
2:A:804:POV:H37	1:D:664:LEU:HD21	1.97	0.46
1:D:570:GLN:O	1:D:574:MET:HG2	2.16	0.45
1:A:593:VAL:HG13	1:B:563:LEU:HD21	1.99	0.45
1:B:562:MET:HE3	1:B:562:MET:HB3	1.86	0.45
1:C:652:ILE:HB	2:C:801:POV:H1A	1.98	0.45
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.86	0.45
1:A:566:THR:HB	1:A:572:MET:HB3	1.97	0.45
1:B:566:THR:HB	1:B:572:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:SER:HB2	1:B:178:ASN:ND2	2.26	0.45
1:A:563:LEU:O	1:A:566:THR:OG1	2.30	0.45
1:A:563:LEU:HD21	1:D:593:VAL:HG13	2.00	0.44
1:A:379:ASP:HA	1:A:749:LEU:HB3	2.00	0.44
2:D:806:POV:H37	1:C:664:LEU:HD21	1.99	0.44
1:B:387:SER:OG	1:B:733:ARG:NH1	2.45	0.44
1:B:738:LYS:HD3	1:B:738:LYS:HA	1.76	0.44
1:A:562:MET:HE3	1:A:562:MET:HB3	1.86	0.44
1:B:379:ASP:HA	1:B:749:LEU:HB3	2.00	0.44
1:B:593:VAL:HG13	1:C:563:LEU:HD21	1.99	0.44
1:A:562:MET:HE2	2:A:802:POV:H21B	2.00	0.44
1:C:379:ASP:HA	1:C:749:LEU:HB3	2.00	0.44
1:D:379:ASP:HA	1:D:749:LEU:HB3	2.00	0.44
1:B:562:MET:HE2	2:B:802:POV:H21B	2.00	0.44
1:B:741:GLU:OE2	1:B:741:GLU:N	2.51	0.44
1:A:741:GLU:N	1:A:741:GLU:OE2	2.51	0.43
1:C:741:GLU:N	1:C:741:GLU:OE2	2.51	0.43
1:D:741:GLU:OE2	1:D:741:GLU:N	2.51	0.43
1:C:562:MET:HE2	2:C:804:POV:H21B	2.00	0.43
1:B:439:HIS:HB3	2:B:802:POV:H37A	2.00	0.43
1:D:562:MET:HE2	2:D:804:POV:H21B	2.00	0.43
1:A:439:HIS:HB3	2:A:802:POV:H37A	2.00	0.43
1:A:636:THR:HG1	1:A:661:TYR:HH	1.66	0.43
1:D:562:MET:HE3	1:D:562:MET:HB3	1.86	0.43
1:A:650:TYR:OH	1:B:545:LYS:O	2.36	0.43
1:D:439:HIS:HB3	2:D:804:POV:H37A	2.00	0.43
1:D:649:LYS:H	1:D:649:LYS:HG2	1.55	0.43
2:B:807:POV:H316	1:C:583:ILE:HD11	2.01	0.43
1:C:257:GLU:OE1	1:C:257:GLU:N	2.52	0.43
1:C:562:MET:HE3	1:C:562:MET:HB3	1.86	0.43
1:C:643:ASN:O	1:C:646:GLN:NE2	2.48	0.43
1:A:257:GLU:OE1	1:A:257:GLU:N	2.52	0.43
1:B:636:THR:HG1	1:B:661:TYR:HH	1.66	0.43
1:C:333:LEU:HD23	1:C:333:LEU:HA	1.91	0.43
1:A:545:LYS:O	1:D:650:TYR:OH	2.37	0.42
1:D:676:LEU:HA	1:D:676:LEU:HD23	1.79	0.42
1:B:257:GLU:N	1:B:257:GLU:OE1	2.52	0.42
1:B:427:THR:O	1:B:431:MET:HG3	2.19	0.42
1:B:563:LEU:O	1:B:566:THR:OG1	2.30	0.42
1:D:385:VAL:HG22	1:D:737:VAL:HG22	2.01	0.42
1:B:139:LEU:HD21	1:B:193:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:806:POV:H14B	2:C:806:POV:H11	1.88	0.42
1:A:427:THR:O	1:A:431:MET:HG3	2.20	0.42
1:A:574:MET:HG2	1:A:574:MET:H	1.66	0.42
1:D:517:LEU:HD13	1:D:521:TRP:CE3	2.55	0.42
1:C:139:LEU:HD21	1:C:193:PHE:HB2	2.01	0.42
1:C:427:THR:O	1:C:431:MET:HG3	2.20	0.42
1:D:563:LEU:HD21	1:C:593:VAL:HG13	2.01	0.42
1:A:385:VAL:HG22	1:A:737:VAL:HG22	2.01	0.42
1:A:583:ILE:HD11	2:D:802:POV:H316	2.01	0.42
2:D:806:POV:H14B	2:D:806:POV:H11	1.88	0.42
1:C:439:HIS:HB3	2:C:804:POV:H37A	2.00	0.42
1:C:658:LEU:HD12	1:C:658:LEU:HA	1.90	0.42
1:D:257:GLU:N	1:D:257:GLU:OE1	2.52	0.42
1:D:583:ILE:HD11	2:C:802:POV:H316	2.01	0.42
1:A:517:LEU:HD13	1:A:521:TRP:CE3	2.55	0.42
1:D:535:LEU:HD23	1:D:535:LEU:HA	1.86	0.42
1:B:517:LEU:HD13	1:B:521:TRP:CE3	2.55	0.42
2:A:807:POV:H316	1:B:583:ILE:HD11	2.01	0.41
1:D:563:LEU:O	1:D:566:THR:OG1	2.30	0.41
1:C:517:LEU:HD13	1:C:521:TRP:CE3	2.55	0.41
2:C:801:POV:H37A	2:C:801:POV:H34	1.95	0.41
2:C:803:POV:H24	2:C:803:POV:H27A	1.78	0.41
1:A:177:LEU:H	1:A:177:LEU:HD12	1.85	0.41
1:D:433:TRP:CE2	1:D:438:LYS:HG3	2.55	0.41
1:B:177:LEU:HD12	1:B:177:LEU:H	1.85	0.41
1:B:650:TYR:OH	1:C:545:LYS:O	2.38	0.41
1:A:738:LYS:HD3	1:A:738:LYS:HA	1.76	0.41
1:C:433:TRP:CE2	1:C:438:LYS:HG3	2.55	0.41
2:C:804:POV:H13B	2:C:804:POV:H11	1.93	0.41
1:A:139:LEU:HD21	1:A:193:PHE:HB2	2.01	0.41
1:D:139:LEU:HD21	1:D:193:PHE:HB2	2.01	0.41
1:D:427:THR:O	1:D:431:MET:HG3	2.20	0.41
1:A:487:ARG:H	1:A:487:ARG:HG2	1.75	0.41
1:C:380:TRP:CE3	1:C:753:PRO:HB3	2.56	0.41
1:A:433:TRP:CE2	1:A:438:LYS:HG3	2.55	0.41
1:D:135:LEU:HD22	1:D:186:ILE:HB	2.03	0.41
1:B:385:VAL:HG22	1:B:737:VAL:HG22	2.01	0.41
1:C:286:GLN:OE1	1:C:286:GLN:N	2.54	0.41
1:C:563:LEU:O	1:C:566:THR:OG1	2.30	0.41
1:A:185:GLU:O	1:A:189:ILE:HG13	2.21	0.41
1:B:380:TRP:CE3	1:B:753:PRO:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:TRP:CE2	1:B:438:LYS:HG3	2.55	0.41
1:B:676:LEU:HA	1:B:676:LEU:HD23	1.79	0.41
1:A:135:LEU:HD22	1:A:186:ILE:HB	2.03	0.41
1:D:580:GLN:HE22	1:D:584:LEU:HD11	1.86	0.41
1:C:392:LEU:HD11	1:C:732:LEU:HB2	2.03	0.41
1:A:548:LEU:HD23	1:D:649:LYS:HE3	2.03	0.40
2:A:804:POV:H11	2:A:804:POV:H14B	1.88	0.40
1:D:570:GLN:NE2	1:D:689:GLU:OE1	2.54	0.40
1:B:286:GLN:OE1	1:B:286:GLN:N	2.54	0.40
1:B:574:MET:HG2	1:B:574:MET:H	1.66	0.40
2:B:806:POV:H37A	2:B:806:POV:H34	1.95	0.40
1:C:385:VAL:HG22	1:C:737:VAL:HG22	2.01	0.40
1:A:392:LEU:HD11	1:A:732:LEU:HB2	2.03	0.40
1:D:298:ASN:H	1:D:301:HIS:HB2	1.87	0.40
1:B:135:LEU:HD22	1:B:186:ILE:HB	2.03	0.40
1:B:224:GLU:OE1	1:C:383:GLY:N	2.54	0.40
1:C:135:LEU:HD22	1:C:186:ILE:HB	2.03	0.40
1:C:185:GLU:O	1:C:189:ILE:HG13	2.21	0.40
1:A:580:GLN:HE22	1:A:584:LEU:HD11	1.87	0.40
1:D:383:GLY:N	1:C:224:GLU:OE1	2.54	0.40
1:B:636:THR:OG1	1:B:661:TYR:OH	2.38	0.40
1:A:380:TRP:CE3	1:A:753:PRO:HB3	2.56	0.40
1:D:177:LEU:H	1:D:177:LEU:HD12	1.85	0.40
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.91	0.40
1:B:570:GLN:NE2	1:B:689:GLU:OE1	2.54	0.40
1:D:185:GLU:O	1:D:189:ILE:HG13	2.21	0.40
1:D:380:TRP:CE3	1:D:753:PRO:HB3	2.56	0.40
1:D:392:LEU:HD11	1:D:732:LEU:HB2	2.03	0.40
1:D:545:LYS:O	1:C:650:TYR:OH	2.39	0.40
1:B:185:GLU:O	1:B:189:ILE:HG13	2.21	0.40
1:B:580:GLN:HE22	1:B:584:LEU:HD11	1.87	0.40
1:C:177:LEU:HD12	1:C:177:LEU:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/799 (76%)	561 (93%)	43 (7%)	0	100	100
1	B	604/799 (76%)	561 (93%)	43 (7%)	0	100	100
1	C	604/799 (76%)	561 (93%)	43 (7%)	0	100	100
1	D	604/799 (76%)	561 (93%)	43 (7%)	0	100	100
All	All	2416/3196 (76%)	2244 (93%)	172 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	538/712 (76%)	538 (100%)	0	100	100
1	B	538/712 (76%)	538 (100%)	0	100	100
1	C	538/712 (76%)	538 (100%)	0	100	100
1	D	538/712 (76%)	538 (100%)	0	100	100
All	All	2152/2848 (76%)	2152 (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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	182	ASN
1	A	244	HIS
1	A	394	ASN
1	A	735	ASN
1	A	745	HIS

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Mol	Chain	Res	Type
1	D	178	ASN
1	D	182	ASN
1	D	244	HIS
1	D	314	ASN
1	D	735	ASN
1	D	745	HIS
1	B	178	ASN
1	B	182	ASN
1	B	244	HIS
1	B	394	ASN
1	B	735	ASN
1	C	178	ASN
1	C	182	ASN
1	C	244	HIS
1	C	394	ASN
1	C	735	ASN
1	C	745	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	D	803	-	45,45,51	0.53	0	50,53,59	0.47	0
2	POV	B	805	-	38,38,51	0.57	0	44,46,59	0.53	0
2	POV	C	802	-	51,51,51	0.50	0	57,59,59	0.46	0
2	POV	C	803	-	45,45,51	0.53	0	50,53,59	0.47	0
2	POV	C	807	-	38,38,51	0.58	0	44,46,59	0.53	0
2	POV	B	802	-	43,43,51	0.54	0	49,51,59	0.48	0
2	POV	B	807	-	51,51,51	0.50	0	57,59,59	0.46	0
2	POV	C	806	-	38,38,51	0.56	0	44,46,59	0.52	0
2	POV	C	804	-	43,43,51	0.53	0	49,51,59	0.48	0
2	POV	B	803	-	47,47,51	0.51	0	53,55,59	0.48	0
2	POV	B	806	-	33,33,51	0.58	0	39,41,59	0.68	1 (2%)
2	POV	B	804	-	38,38,51	0.56	0	44,46,59	0.53	0
2	POV	D	805	-	47,47,51	0.51	0	53,55,59	0.48	0
2	POV	A	805	-	38,38,51	0.58	0	44,46,59	0.53	0
2	POV	C	801	-	33,33,51	0.59	0	39,41,59	0.68	1 (2%)
2	POV	D	806	-	38,38,51	0.56	0	44,46,59	0.53	0
2	POV	A	807	-	51,51,51	0.50	0	57,59,59	0.46	0
2	POV	A	803	-	47,47,51	0.51	0	53,55,59	0.48	0
2	POV	D	807	-	38,38,51	0.58	0	44,46,59	0.53	0
2	POV	A	802	-	43,43,51	0.54	0	49,51,59	0.48	0
2	POV	D	802	-	51,51,51	0.50	0	57,59,59	0.46	0
2	POV	D	804	-	43,43,51	0.54	0	49,51,59	0.48	0
2	POV	A	804	-	38,38,51	0.56	0	44,46,59	0.53	0
2	POV	A	806	-	33,33,51	0.58	0	39,41,59	0.68	1 (2%)
2	POV	B	801	-	45,45,51	0.53	0	50,53,59	0.47	0
2	POV	D	801	-	33,33,51	0.58	0	39,41,59	0.68	1 (2%)
2	POV	C	805	-	47,47,51	0.51	0	53,55,59	0.48	0
2	POV	A	801	-	45,45,51	0.53	0	50,53,59	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	803	-	-	12/49/49/55	-
2	POV	B	805	-	-	12/42/42/55	-
2	POV	C	802	-	-	17/55/55/55	-
2	POV	C	803	-	-	12/49/49/55	-
2	POV	C	807	-	-	12/42/42/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	802	-	-	14/47/47/55	-
2	POV	B	807	-	-	17/55/55/55	-
2	POV	C	806	-	-	16/42/42/55	-
2	POV	C	804	-	-	14/47/47/55	-
2	POV	B	803	-	-	13/51/51/55	-
2	POV	B	806	-	-	15/37/37/55	-
2	POV	B	804	-	-	16/42/42/55	-
2	POV	D	805	-	-	13/51/51/55	-
2	POV	A	805	-	-	12/42/42/55	-
2	POV	C	801	-	-	15/37/37/55	-
2	POV	D	806	-	-	16/42/42/55	-
2	POV	A	807	-	-	17/55/55/55	-
2	POV	A	803	-	-	13/51/51/55	-
2	POV	D	807	-	-	12/42/42/55	-
2	POV	A	802	-	-	14/47/47/55	-
2	POV	D	802	-	-	17/55/55/55	-
2	POV	D	804	-	-	14/47/47/55	-
2	POV	A	804	-	-	16/42/42/55	-
2	POV	A	806	-	-	15/37/37/55	-
2	POV	B	801	-	-	12/49/49/55	-
2	POV	D	801	-	-	15/37/37/55	-
2	POV	C	805	-	-	13/51/51/55	-
2	POV	A	801	-	-	12/49/49/55	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	POV	C2-O21-C21	2.51	123.97	117.79
2	A	806	POV	C2-O21-C21	2.50	123.94	117.79
2	D	801	POV	C2-O21-C21	2.50	123.94	117.79
2	B	806	POV	C2-O21-C21	2.50	123.94	117.79

There are no chirality outliers.

All (396) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	POV	C11-O12-P-O13
2	A	802	POV	C1-O11-P-O13
2	A	802	POV	C1-O11-P-O14
2	A	802	POV	C11-O12-P-O13
2	A	803	POV	C11-O12-P-O11
2	A	803	POV	C11-O12-P-O13
2	A	803	POV	O22-C21-O21-C2
2	A	804	POV	C1-O11-P-O14
2	A	804	POV	C22-C21-O21-C2
2	A	806	POV	C1-O11-P-O12
2	A	806	POV	C1-O11-P-O13
2	A	806	POV	C1-O11-P-O14
2	A	806	POV	O12-C11-C12-N
2	A	807	POV	C11-O12-P-O11
2	A	807	POV	C11-O12-P-O13
2	A	807	POV	C11-O12-P-O14
2	D	801	POV	C1-O11-P-O12
2	D	801	POV	C1-O11-P-O13
2	D	801	POV	C1-O11-P-O14
2	D	801	POV	O12-C11-C12-N
2	D	802	POV	C11-O12-P-O11
2	D	802	POV	C11-O12-P-O13
2	D	802	POV	C11-O12-P-O14
2	D	803	POV	C11-O12-P-O13
2	D	804	POV	C1-O11-P-O13
2	D	804	POV	C1-O11-P-O14
2	D	804	POV	C11-O12-P-O13
2	D	805	POV	C11-O12-P-O11
2	D	805	POV	C11-O12-P-O13
2	D	805	POV	O22-C21-O21-C2
2	D	806	POV	C1-O11-P-O14
2	D	806	POV	C22-C21-O21-C2
2	B	801	POV	C11-O12-P-O13
2	B	802	POV	C1-O11-P-O13
2	B	802	POV	C1-O11-P-O14
2	B	802	POV	C11-O12-P-O13
2	B	803	POV	C11-O12-P-O11
2	B	803	POV	C11-O12-P-O13
2	B	803	POV	O22-C21-O21-C2
2	B	804	POV	C1-O11-P-O14
2	B	804	POV	C22-C21-O21-C2
2	B	806	POV	C1-O11-P-O12
2	B	806	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	B	806	POV	C1-O11-P-O14
2	B	806	POV	O12-C11-C12-N
2	B	807	POV	C11-O12-P-O11
2	B	807	POV	C11-O12-P-O13
2	B	807	POV	C11-O12-P-O14
2	C	801	POV	C1-O11-P-O12
2	C	801	POV	C1-O11-P-O13
2	C	801	POV	C1-O11-P-O14
2	C	801	POV	O12-C11-C12-N
2	C	802	POV	C11-O12-P-O11
2	C	802	POV	C11-O12-P-O13
2	C	802	POV	C11-O12-P-O14
2	C	803	POV	C11-O12-P-O13
2	C	804	POV	C1-O11-P-O13
2	C	804	POV	C1-O11-P-O14
2	C	804	POV	C11-O12-P-O13
2	C	805	POV	C11-O12-P-O11
2	C	805	POV	C11-O12-P-O13
2	C	805	POV	O22-C21-O21-C2
2	C	806	POV	C1-O11-P-O14
2	C	806	POV	C22-C21-O21-C2
2	A	803	POV	C22-C21-O21-C2
2	D	805	POV	C22-C21-O21-C2
2	B	803	POV	C22-C21-O21-C2
2	C	805	POV	C22-C21-O21-C2
2	A	804	POV	O22-C21-O21-C2
2	D	806	POV	O22-C21-O21-C2
2	B	804	POV	O22-C21-O21-C2
2	C	806	POV	O22-C21-O21-C2
2	A	807	POV	C2-C1-O11-P
2	D	802	POV	C2-C1-O11-P
2	B	807	POV	C2-C1-O11-P
2	C	802	POV	C2-C1-O11-P
2	A	806	POV	C32-C31-O31-C3
2	D	801	POV	C32-C31-O31-C3
2	B	806	POV	C32-C31-O31-C3
2	C	801	POV	C32-C31-O31-C3
2	A	801	POV	O21-C2-C3-O31
2	D	803	POV	O21-C2-C3-O31
2	B	801	POV	O21-C2-C3-O31
2	C	803	POV	O21-C2-C3-O31
2	A	806	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	D	801	POV	O32-C31-O31-C3
2	B	806	POV	O32-C31-O31-C3
2	C	801	POV	O32-C31-O31-C3
2	A	802	POV	C32-C31-O31-C3
2	D	804	POV	C32-C31-O31-C3
2	B	802	POV	C32-C31-O31-C3
2	C	804	POV	C32-C31-O31-C3
2	A	802	POV	O32-C31-O31-C3
2	D	804	POV	O32-C31-O31-C3
2	B	802	POV	O32-C31-O31-C3
2	C	804	POV	O32-C31-O31-C3
2	A	801	POV	C11-O12-P-O11
2	A	802	POV	C1-O11-P-O12
2	A	802	POV	C11-O12-P-O11
2	A	805	POV	C11-O12-P-O11
2	A	806	POV	C11-O12-P-O11
2	A	807	POV	C1-O11-P-O12
2	D	801	POV	C11-O12-P-O11
2	D	802	POV	C1-O11-P-O12
2	D	803	POV	C11-O12-P-O11
2	D	804	POV	C1-O11-P-O12
2	D	804	POV	C11-O12-P-O11
2	D	807	POV	C11-O12-P-O11
2	B	801	POV	C11-O12-P-O11
2	B	802	POV	C1-O11-P-O12
2	B	802	POV	C11-O12-P-O11
2	B	805	POV	C11-O12-P-O11
2	B	806	POV	C11-O12-P-O11
2	B	807	POV	C1-O11-P-O12
2	C	801	POV	C11-O12-P-O11
2	C	802	POV	C1-O11-P-O12
2	C	803	POV	C11-O12-P-O11
2	C	804	POV	C1-O11-P-O12
2	C	804	POV	C11-O12-P-O11
2	C	807	POV	C11-O12-P-O11
2	A	803	POV	C21-C22-C23-C24
2	D	805	POV	C21-C22-C23-C24
2	B	803	POV	C21-C22-C23-C24
2	C	805	POV	C21-C22-C23-C24
2	A	802	POV	C210-C211-C212-C213
2	D	804	POV	C210-C211-C212-C213
2	B	802	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
2	C	804	POV	C210-C211-C212-C213
2	D	805	POV	C34-C35-C36-C37
2	C	805	POV	C34-C35-C36-C37
2	A	803	POV	C34-C35-C36-C37
2	B	803	POV	C34-C35-C36-C37
2	A	804	POV	C311-C312-C313-C314
2	B	804	POV	C311-C312-C313-C314
2	C	806	POV	C311-C312-C313-C314
2	D	806	POV	C311-C312-C313-C314
2	A	804	POV	C36-C37-C38-C39
2	D	806	POV	C36-C37-C38-C39
2	B	804	POV	C36-C37-C38-C39
2	C	806	POV	C36-C37-C38-C39
2	D	802	POV	C312-C313-C314-C315
2	C	802	POV	C312-C313-C314-C315
2	A	807	POV	C312-C313-C314-C315
2	B	807	POV	C312-C313-C314-C315
2	A	805	POV	C33-C34-C35-C36
2	D	807	POV	C33-C34-C35-C36
2	B	805	POV	C33-C34-C35-C36
2	C	807	POV	C33-C34-C35-C36
2	A	804	POV	C32-C31-O31-C3
2	D	806	POV	C32-C31-O31-C3
2	B	804	POV	C32-C31-O31-C3
2	C	806	POV	C32-C31-O31-C3
2	A	805	POV	C22-C21-O21-C2
2	D	807	POV	C22-C21-O21-C2
2	B	805	POV	C22-C21-O21-C2
2	C	807	POV	C22-C21-O21-C2
2	A	802	POV	C22-C23-C24-C25
2	C	804	POV	C22-C23-C24-C25
2	A	805	POV	O22-C21-O21-C2
2	D	807	POV	O22-C21-O21-C2
2	B	805	POV	O22-C21-O21-C2
2	C	807	POV	O22-C21-O21-C2
2	D	804	POV	C22-C23-C24-C25
2	B	802	POV	C22-C23-C24-C25
2	A	804	POV	O32-C31-O31-C3
2	D	806	POV	O32-C31-O31-C3
2	B	804	POV	O32-C31-O31-C3
2	C	806	POV	O32-C31-O31-C3
2	A	801	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	D	803	POV	C1-C2-C3-O31
2	B	801	POV	C1-C2-C3-O31
2	C	803	POV	C1-C2-C3-O31
2	A	803	POV	C32-C31-O31-C3
2	D	805	POV	C32-C31-O31-C3
2	B	803	POV	C32-C31-O31-C3
2	C	805	POV	C32-C31-O31-C3
2	A	806	POV	O11-C1-C2-O21
2	D	801	POV	O11-C1-C2-O21
2	B	806	POV	O11-C1-C2-O21
2	C	801	POV	O11-C1-C2-O21
2	A	803	POV	O32-C31-O31-C3
2	D	805	POV	O32-C31-O31-C3
2	B	803	POV	O32-C31-O31-C3
2	C	805	POV	O32-C31-O31-C3
2	A	807	POV	O11-C1-C2-C3
2	D	802	POV	O11-C1-C2-C3
2	B	807	POV	O11-C1-C2-C3
2	C	802	POV	O11-C1-C2-C3
2	A	805	POV	O11-C1-C2-O21
2	A	807	POV	O11-C1-C2-O21
2	D	802	POV	O11-C1-C2-O21
2	D	807	POV	O11-C1-C2-O21
2	B	805	POV	O11-C1-C2-O21
2	B	807	POV	O11-C1-C2-O21
2	C	802	POV	O11-C1-C2-O21
2	C	807	POV	O11-C1-C2-O21
2	D	807	POV	C23-C24-C25-C26
2	A	805	POV	C23-C24-C25-C26
2	A	807	POV	C215-C216-C217-C218
2	D	802	POV	C215-C216-C217-C218
2	B	805	POV	C23-C24-C25-C26
2	B	807	POV	C215-C216-C217-C218
2	C	802	POV	C215-C216-C217-C218
2	C	807	POV	C23-C24-C25-C26
2	A	802	POV	O21-C2-C3-O31
2	A	803	POV	O21-C2-C3-O31
2	D	804	POV	O21-C2-C3-O31
2	D	805	POV	O21-C2-C3-O31
2	B	802	POV	O21-C2-C3-O31
2	B	803	POV	O21-C2-C3-O31
2	C	804	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	C	805	POV	O21-C2-C3-O31
2	B	801	POV	C311-C312-C313-C314
2	C	803	POV	C311-C312-C313-C314
2	A	801	POV	C311-C312-C313-C314
2	D	803	POV	C311-C312-C313-C314
2	A	806	POV	O22-C21-O21-C2
2	D	801	POV	O22-C21-O21-C2
2	B	806	POV	O22-C21-O21-C2
2	C	801	POV	O22-C21-O21-C2
2	B	803	POV	C25-C26-C27-C28
2	A	806	POV	C22-C21-O21-C2
2	D	801	POV	C22-C21-O21-C2
2	B	806	POV	C22-C21-O21-C2
2	C	801	POV	C22-C21-O21-C2
2	A	803	POV	C25-C26-C27-C28
2	C	805	POV	C25-C26-C27-C28
2	D	805	POV	C25-C26-C27-C28
2	A	805	POV	O11-C1-C2-C3
2	A	806	POV	O11-C1-C2-C3
2	D	801	POV	O11-C1-C2-C3
2	D	807	POV	O11-C1-C2-C3
2	B	805	POV	O11-C1-C2-C3
2	B	806	POV	O11-C1-C2-C3
2	C	801	POV	O11-C1-C2-C3
2	C	807	POV	O11-C1-C2-C3
2	A	805	POV	C24-C25-C26-C27
2	D	807	POV	C24-C25-C26-C27
2	B	805	POV	C24-C25-C26-C27
2	C	807	POV	C24-C25-C26-C27
2	A	803	POV	C1-C2-C3-O31
2	D	805	POV	C1-C2-C3-O31
2	B	803	POV	C1-C2-C3-O31
2	C	805	POV	C1-C2-C3-O31
2	A	804	POV	C11-O12-P-O11
2	D	806	POV	C11-O12-P-O11
2	B	804	POV	C11-O12-P-O11
2	C	806	POV	C11-O12-P-O11
2	B	807	POV	C32-C33-C34-C35
2	A	807	POV	C32-C33-C34-C35
2	D	802	POV	C32-C33-C34-C35
2	C	802	POV	C32-C33-C34-C35
2	A	804	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
2	A	805	POV	C1-O11-P-O13
2	A	805	POV	C11-O12-P-O14
2	A	806	POV	C11-O12-P-O14
2	A	807	POV	C1-O11-P-O14
2	D	801	POV	C11-O12-P-O14
2	D	802	POV	C1-O11-P-O14
2	D	806	POV	C11-O12-P-O13
2	D	807	POV	C1-O11-P-O13
2	D	807	POV	C11-O12-P-O14
2	B	804	POV	C11-O12-P-O13
2	B	805	POV	C1-O11-P-O13
2	B	805	POV	C11-O12-P-O14
2	B	806	POV	C11-O12-P-O14
2	B	807	POV	C1-O11-P-O14
2	C	801	POV	C11-O12-P-O14
2	C	802	POV	C1-O11-P-O14
2	C	806	POV	C11-O12-P-O13
2	C	807	POV	C1-O11-P-O13
2	C	807	POV	C11-O12-P-O14
2	A	801	POV	O11-C1-C2-C3
2	A	803	POV	O11-C1-C2-C3
2	A	804	POV	O11-C1-C2-C3
2	D	803	POV	O11-C1-C2-C3
2	D	805	POV	O11-C1-C2-C3
2	D	806	POV	O11-C1-C2-C3
2	B	801	POV	O11-C1-C2-C3
2	B	803	POV	O11-C1-C2-C3
2	B	804	POV	O11-C1-C2-C3
2	C	803	POV	O11-C1-C2-C3
2	C	805	POV	O11-C1-C2-C3
2	C	806	POV	O11-C1-C2-C3
2	A	801	POV	O11-C1-C2-O21
2	A	802	POV	O11-C1-C2-O21
2	A	803	POV	O11-C1-C2-O21
2	A	804	POV	O11-C1-C2-O21
2	D	803	POV	O11-C1-C2-O21
2	D	804	POV	O11-C1-C2-O21
2	D	805	POV	O11-C1-C2-O21
2	D	806	POV	O11-C1-C2-O21
2	B	801	POV	O11-C1-C2-O21
2	B	802	POV	O11-C1-C2-O21
2	B	803	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
2	B	804	POV	O11-C1-C2-O21
2	C	803	POV	O11-C1-C2-O21
2	C	804	POV	O11-C1-C2-O21
2	C	805	POV	O11-C1-C2-O21
2	C	806	POV	O11-C1-C2-O21
2	A	804	POV	C34-C35-C36-C37
2	C	806	POV	C34-C35-C36-C37
2	D	806	POV	C34-C35-C36-C37
2	B	804	POV	C34-C35-C36-C37
2	B	807	POV	C24-C25-C26-C27
2	C	802	POV	C24-C25-C26-C27
2	A	802	POV	C1-C2-C3-O31
2	A	804	POV	O12-C11-C12-N
2	A	807	POV	O12-C11-C12-N
2	A	807	POV	C24-C25-C26-C27
2	D	802	POV	O12-C11-C12-N
2	D	802	POV	C24-C25-C26-C27
2	D	804	POV	C1-C2-C3-O31
2	D	806	POV	O12-C11-C12-N
2	B	802	POV	C1-C2-C3-O31
2	B	804	POV	O12-C11-C12-N
2	B	807	POV	O12-C11-C12-N
2	C	802	POV	O12-C11-C12-N
2	C	804	POV	C1-C2-C3-O31
2	C	806	POV	O12-C11-C12-N
2	D	803	POV	C36-C37-C38-C39
2	A	801	POV	C36-C37-C38-C39
2	B	801	POV	C36-C37-C38-C39
2	C	803	POV	C36-C37-C38-C39
2	A	806	POV	C3-C2-O21-C21
2	D	801	POV	C3-C2-O21-C21
2	B	806	POV	C3-C2-O21-C21
2	C	801	POV	C3-C2-O21-C21
2	C	802	POV	C33-C34-C35-C36
2	D	802	POV	C33-C34-C35-C36
2	B	807	POV	C33-C34-C35-C36
2	A	807	POV	C33-C34-C35-C36
2	D	803	POV	C21-C22-C23-C24
2	A	801	POV	C21-C22-C23-C24
2	B	801	POV	C21-C22-C23-C24
2	C	803	POV	C21-C22-C23-C24
2	A	807	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	D	802	POV	C1-C2-C3-O31
2	B	807	POV	C1-C2-C3-O31
2	C	802	POV	C1-C2-C3-O31
2	D	803	POV	C24-C25-C26-C27
2	A	801	POV	C24-C25-C26-C27
2	C	803	POV	C24-C25-C26-C27
2	B	801	POV	C24-C25-C26-C27
2	A	807	POV	C21-C22-C23-C24
2	D	802	POV	C21-C22-C23-C24
2	B	807	POV	C21-C22-C23-C24
2	C	802	POV	C21-C22-C23-C24
2	A	804	POV	C310-C311-C312-C313
2	D	806	POV	C310-C311-C312-C313
2	C	806	POV	C310-C311-C312-C313
2	B	804	POV	C310-C311-C312-C313
2	D	802	POV	C25-C26-C27-C28
2	B	807	POV	C25-C26-C27-C28
2	C	802	POV	C25-C26-C27-C28
2	A	807	POV	C25-C26-C27-C28
2	A	802	POV	O11-C1-C2-C3
2	D	804	POV	O11-C1-C2-C3
2	B	802	POV	O11-C1-C2-C3
2	C	804	POV	O11-C1-C2-C3
2	B	806	POV	C33-C34-C35-C36
2	C	803	POV	C22-C23-C24-C25
2	A	806	POV	C33-C34-C35-C36
2	A	801	POV	C22-C23-C24-C25
2	D	801	POV	C33-C34-C35-C36
2	D	803	POV	C22-C23-C24-C25
2	B	801	POV	C22-C23-C24-C25
2	C	801	POV	C33-C34-C35-C36
2	A	804	POV	C32-C33-C34-C35
2	D	806	POV	C32-C33-C34-C35
2	B	804	POV	C32-C33-C34-C35
2	C	806	POV	C32-C33-C34-C35
2	C	803	POV	C34-C35-C36-C37
2	A	801	POV	C34-C35-C36-C37
2	D	803	POV	C34-C35-C36-C37
2	B	801	POV	C34-C35-C36-C37
2	C	807	POV	C311-C310-C39-C38
2	A	805	POV	C311-C310-C39-C38
2	D	807	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
2	B	805	POV	C311-C310-C39-C38
2	B	802	POV	C25-C26-C27-C28
2	A	802	POV	C25-C26-C27-C28
2	A	804	POV	C35-C36-C37-C38
2	D	804	POV	C25-C26-C27-C28
2	D	806	POV	C35-C36-C37-C38
2	B	804	POV	C35-C36-C37-C38
2	C	804	POV	C25-C26-C27-C28
2	C	806	POV	C35-C36-C37-C38
2	A	806	POV	C25-C26-C27-C28
2	B	806	POV	C25-C26-C27-C28
2	D	801	POV	C25-C26-C27-C28
2	C	801	POV	C25-C26-C27-C28
2	D	807	POV	C35-C36-C37-C38
2	C	807	POV	C35-C36-C37-C38
2	A	805	POV	C35-C36-C37-C38
2	B	805	POV	C35-C36-C37-C38

There are no ring outliers.

24 monomers are involved in 55 short contacts:

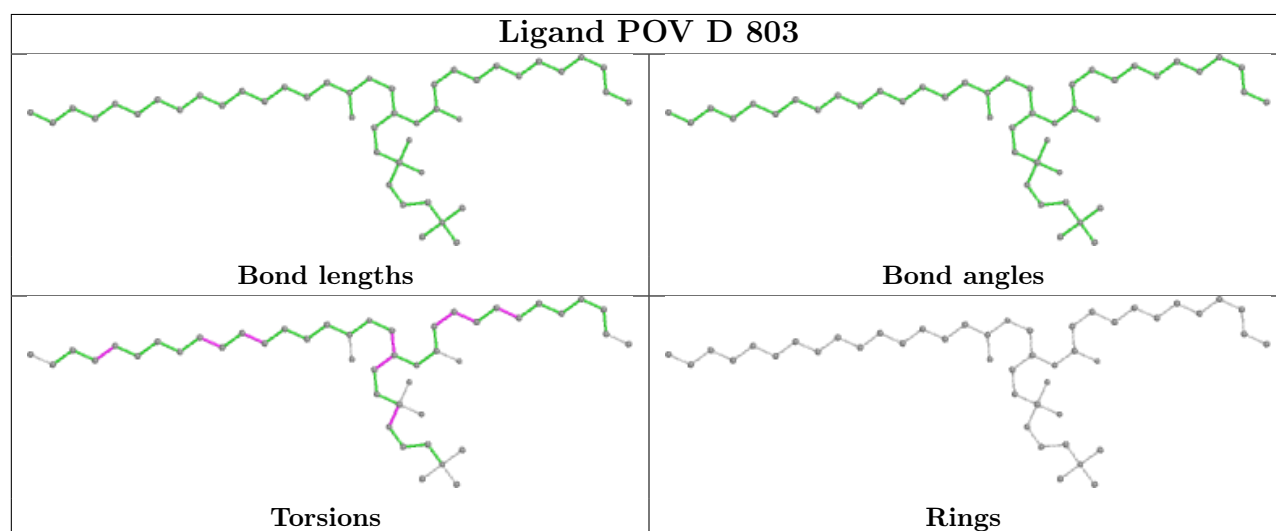
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	803	POV	1	0
2	B	805	POV	3	0
2	C	802	POV	1	0
2	C	803	POV	2	0
2	C	807	POV	3	0
2	B	802	POV	3	0
2	B	807	POV	1	0
2	C	806	POV	4	0
2	C	804	POV	4	0
2	B	806	POV	2	0
2	B	804	POV	3	0
2	A	805	POV	3	0
2	C	801	POV	2	0
2	D	806	POV	4	0
2	A	807	POV	1	0
2	D	807	POV	3	0
2	A	802	POV	3	0
2	D	802	POV	1	0
2	D	804	POV	3	0
2	A	804	POV	4	0

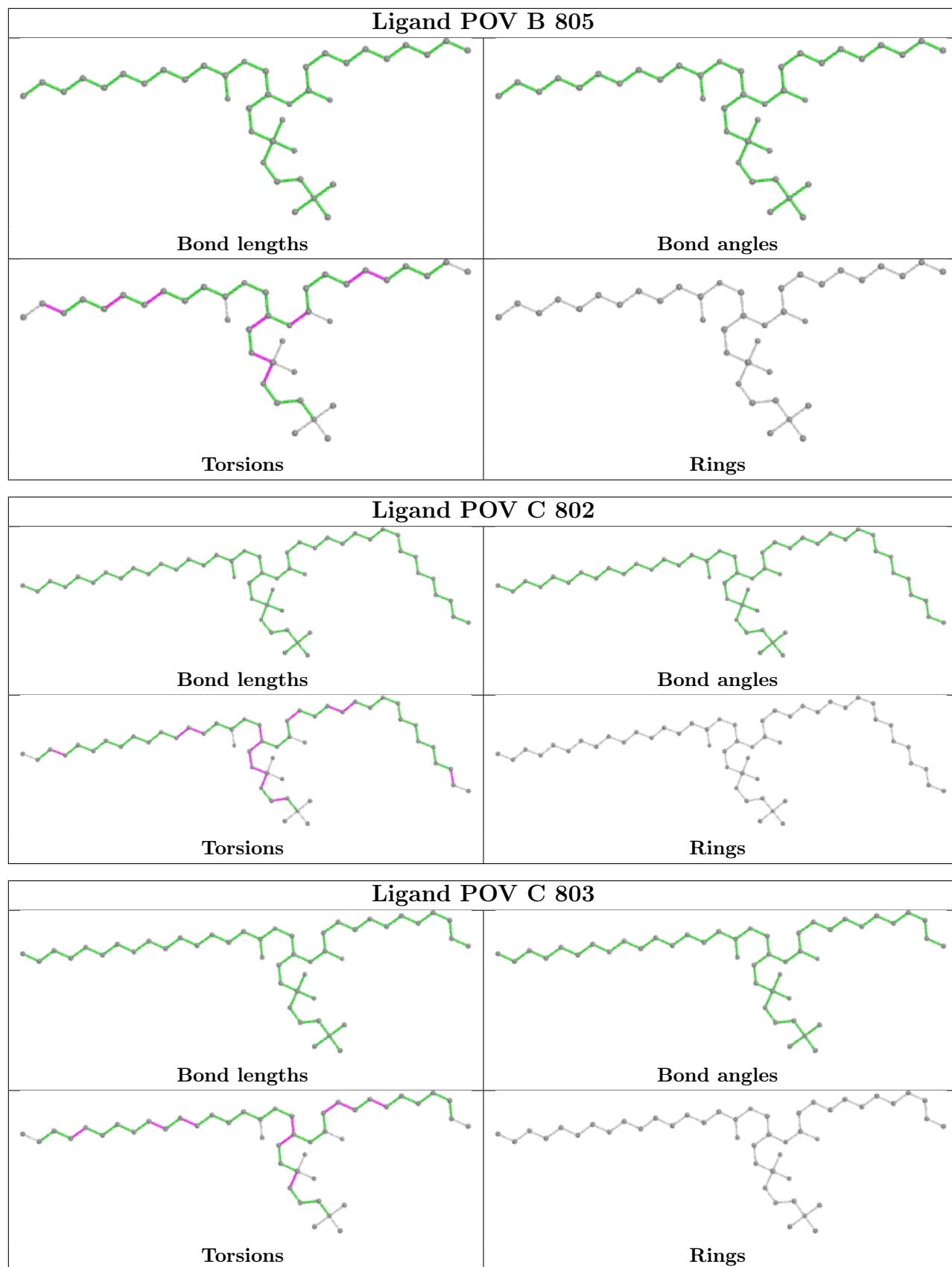
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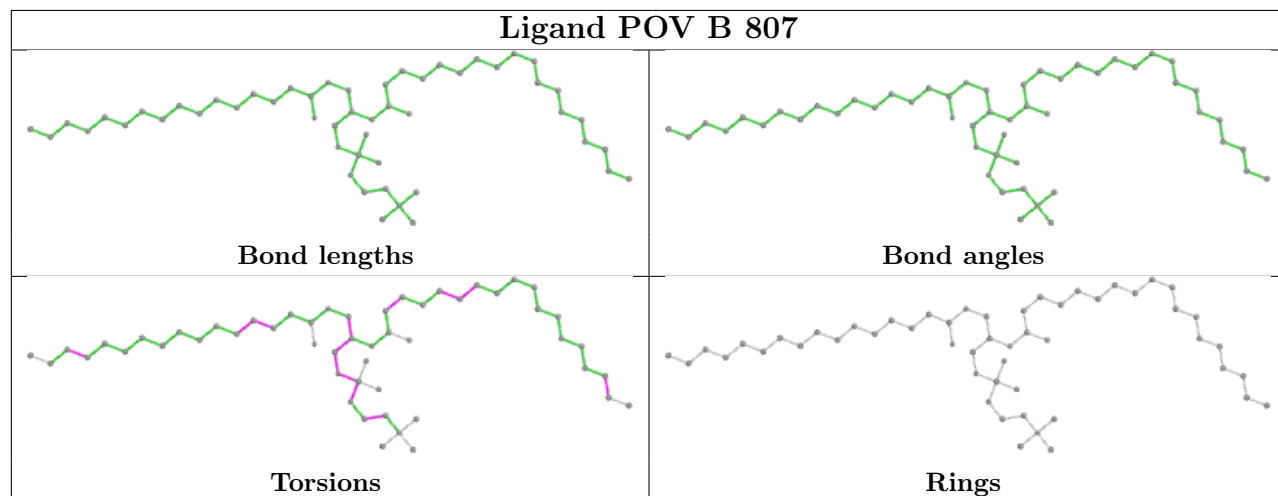
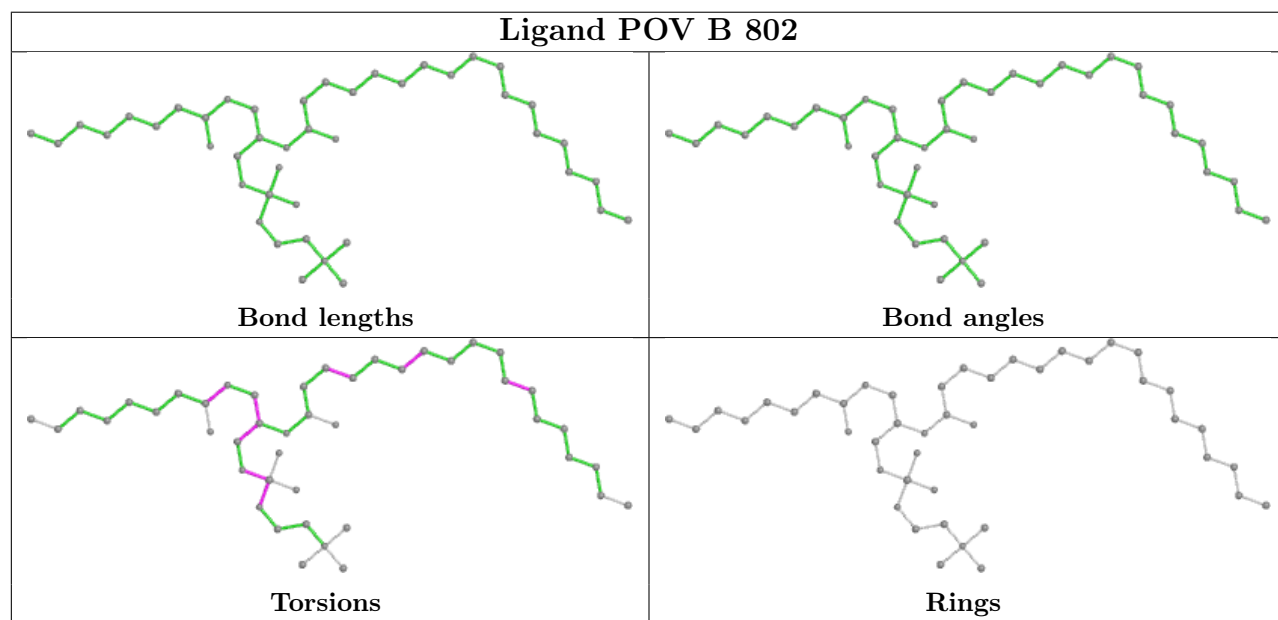
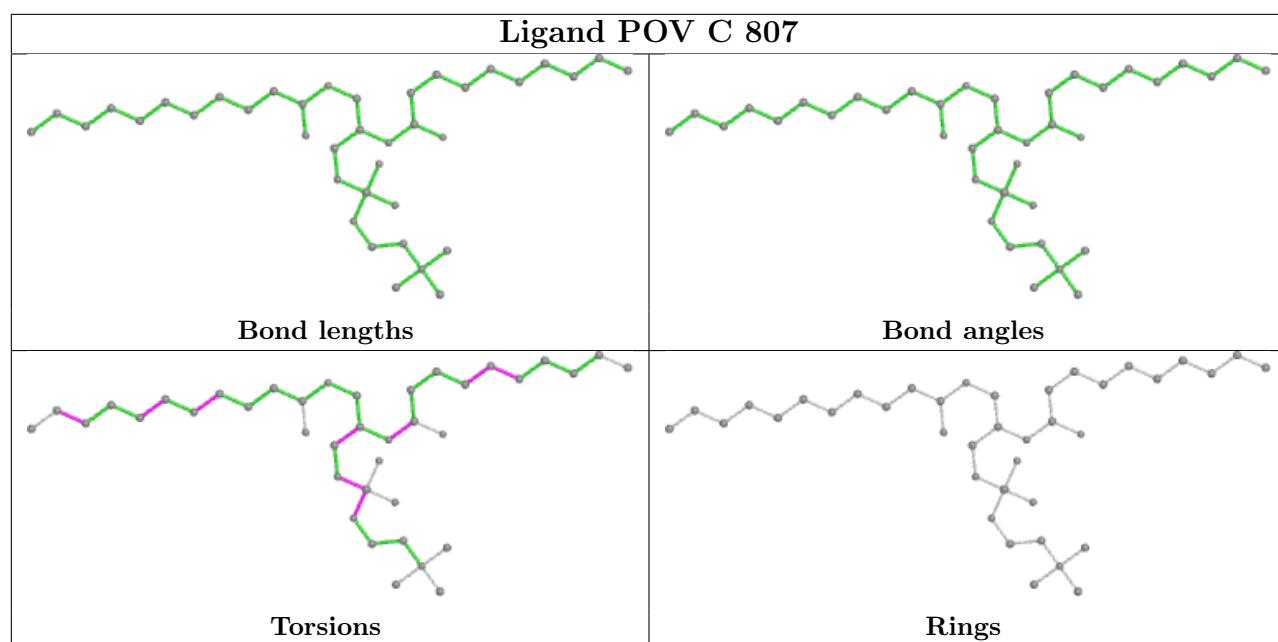
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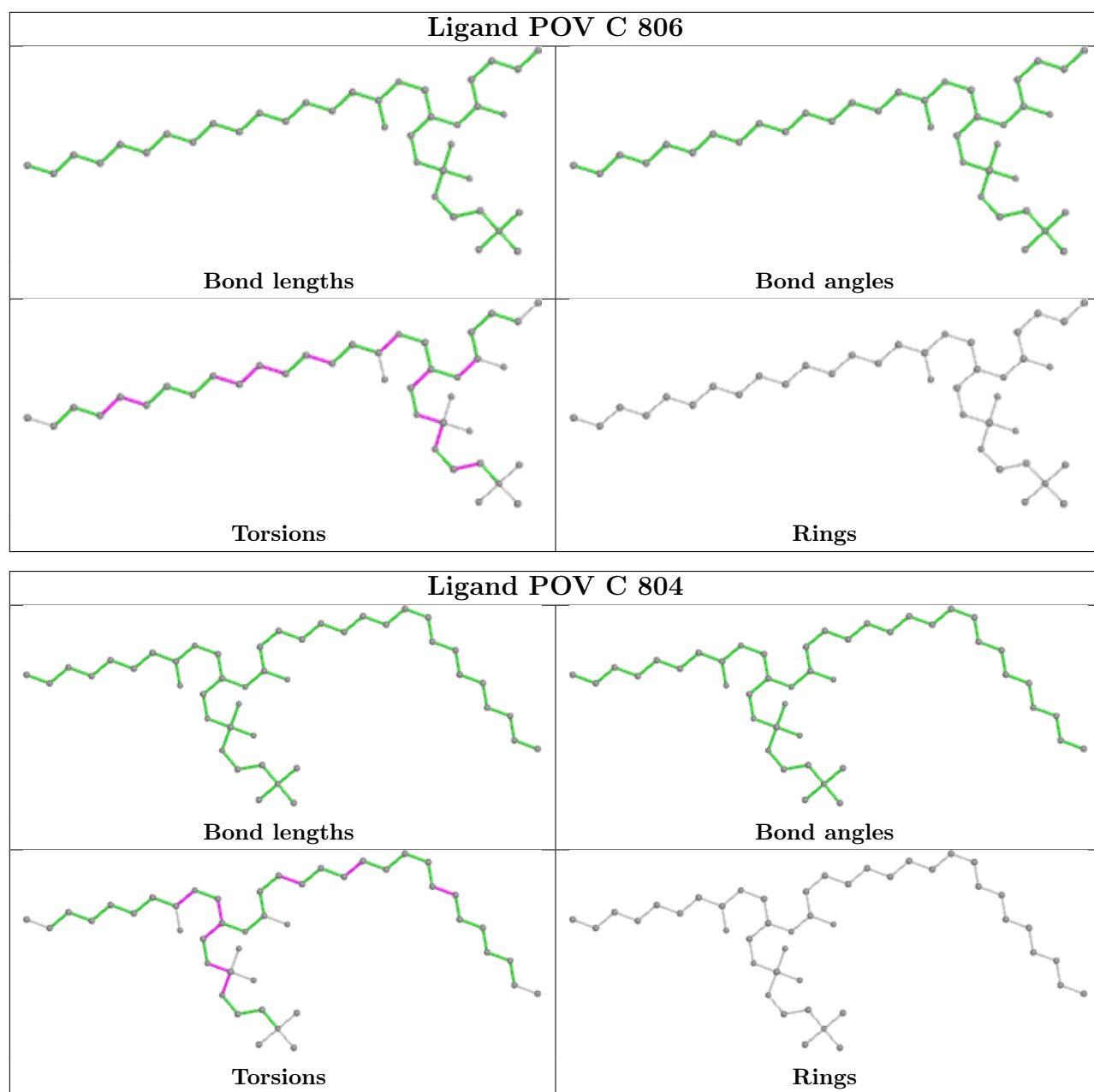
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	806	POV	1	0
2	B	801	POV	1	0
2	D	801	POV	1	0
2	A	801	POV	1	0

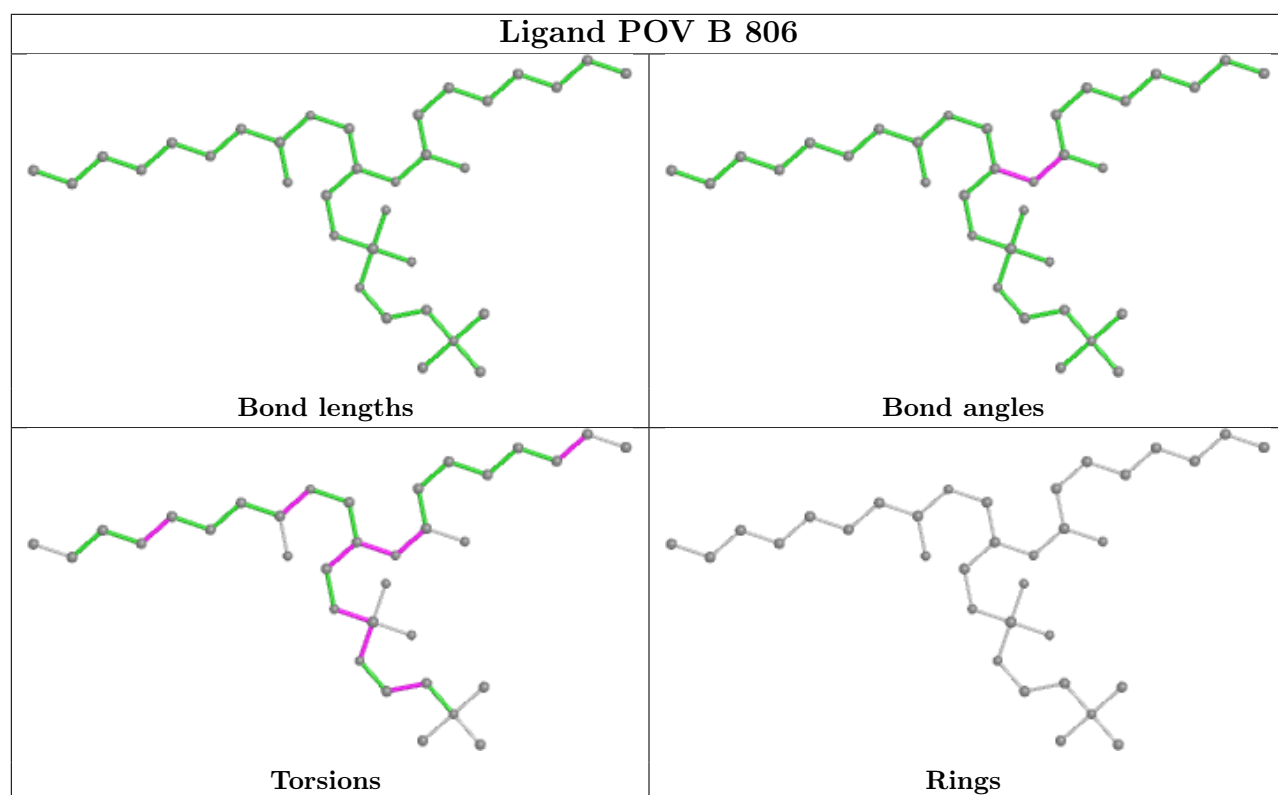
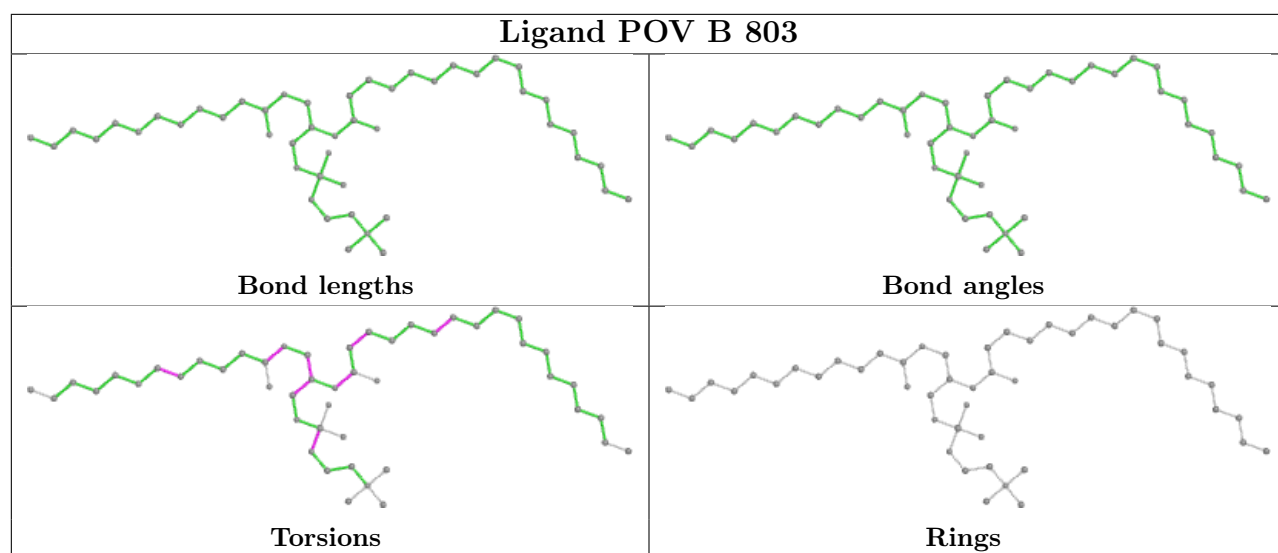
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

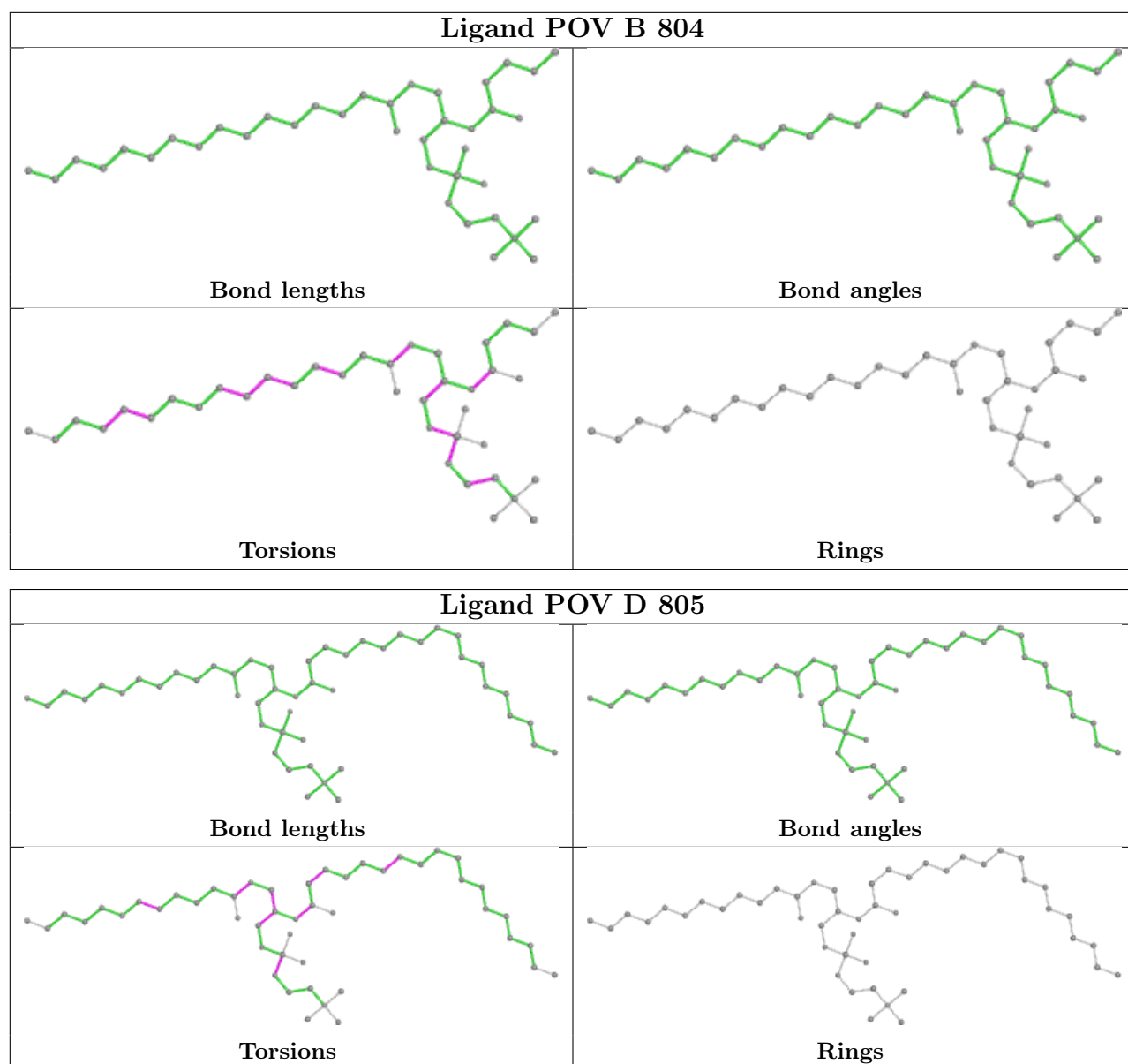


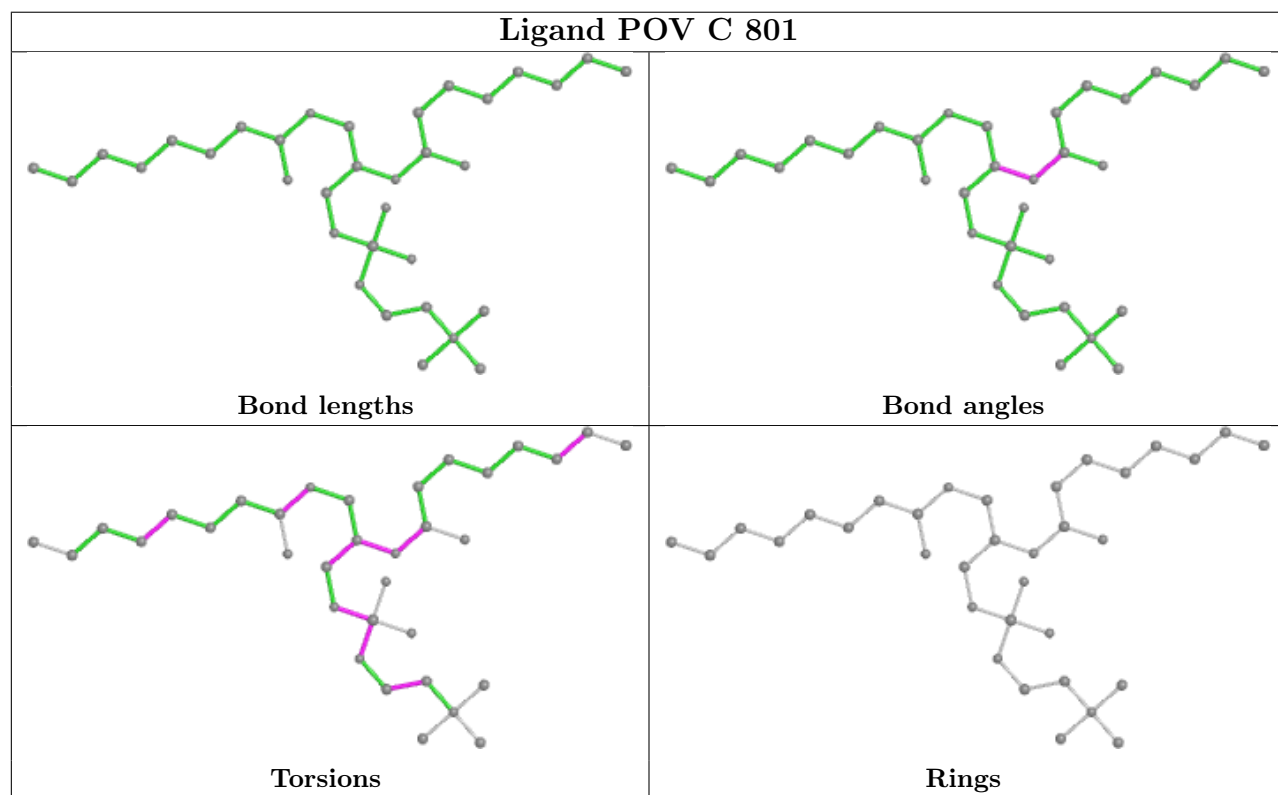
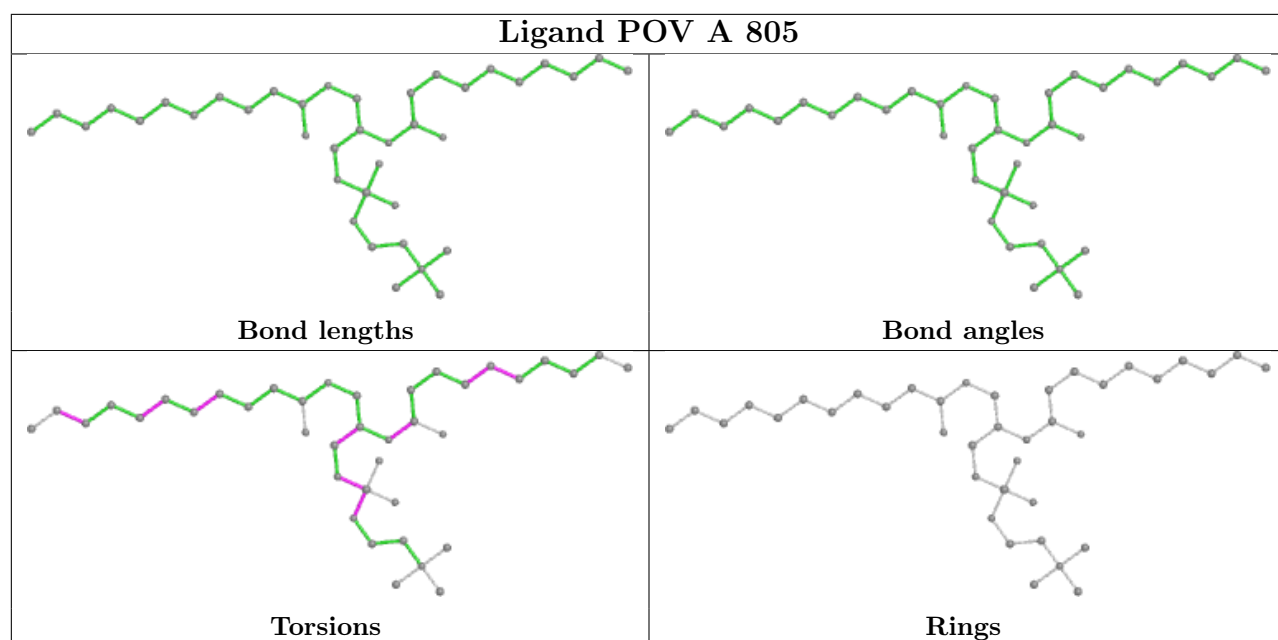


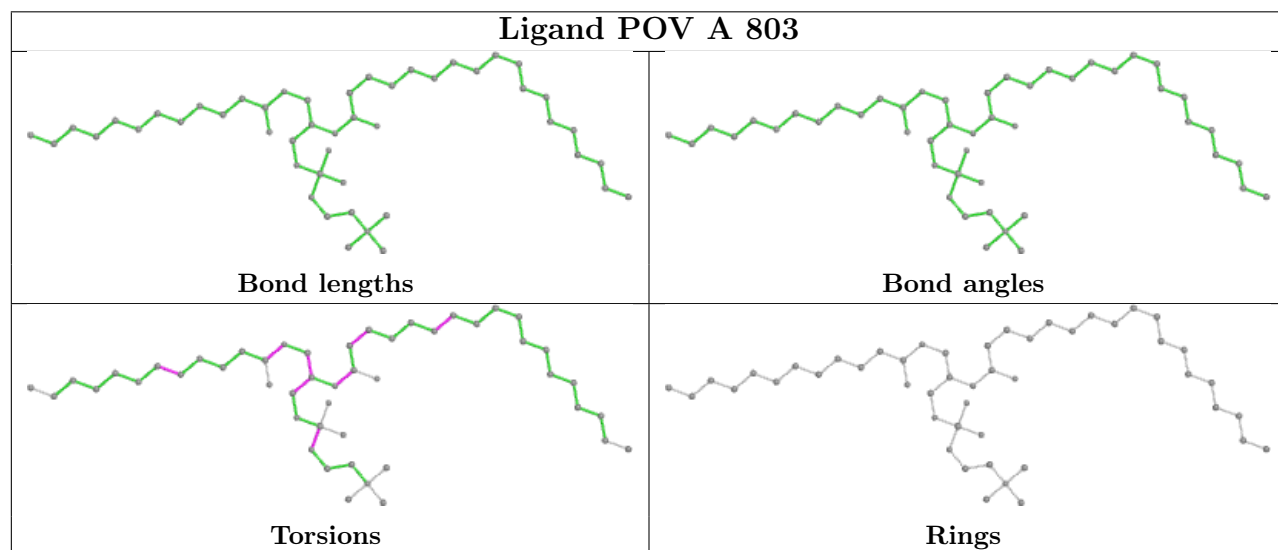
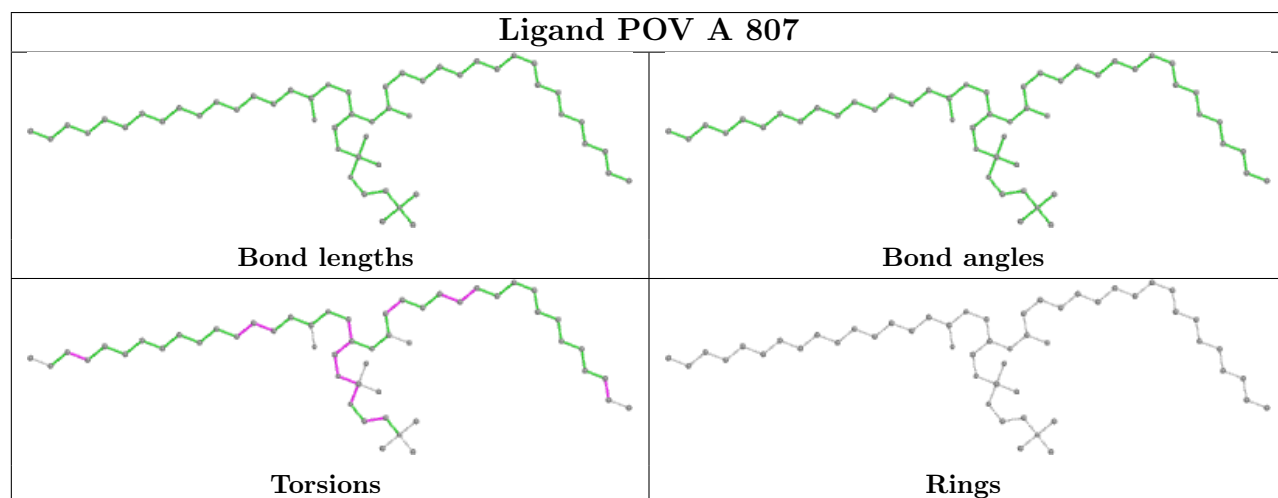
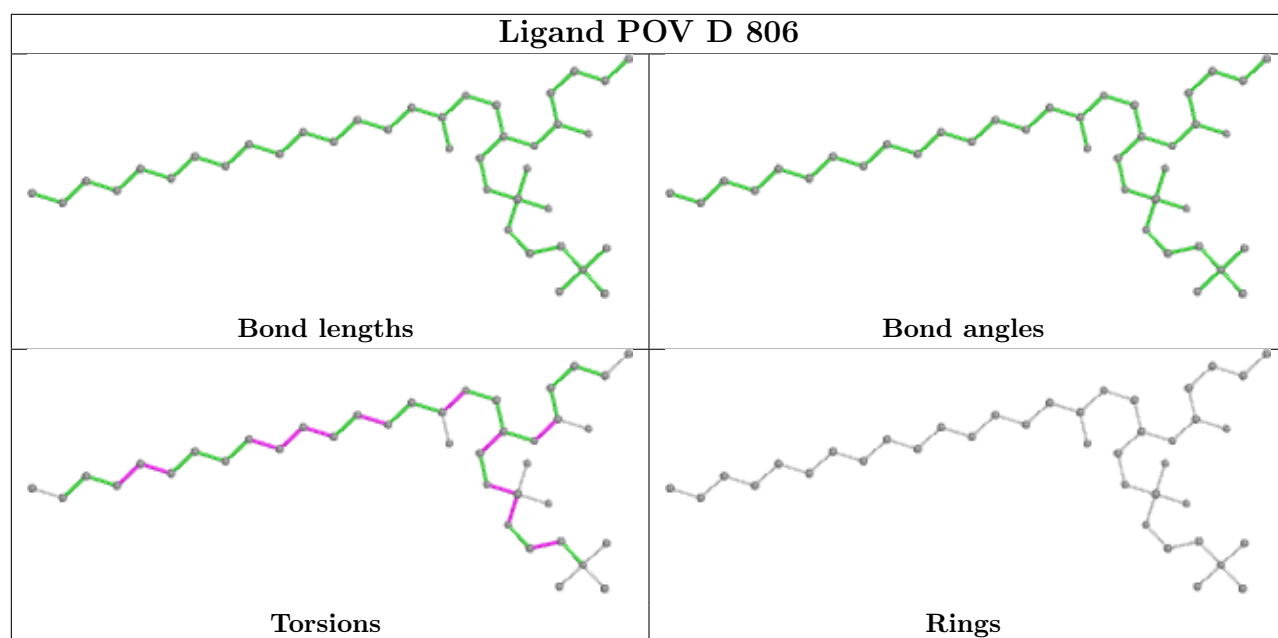


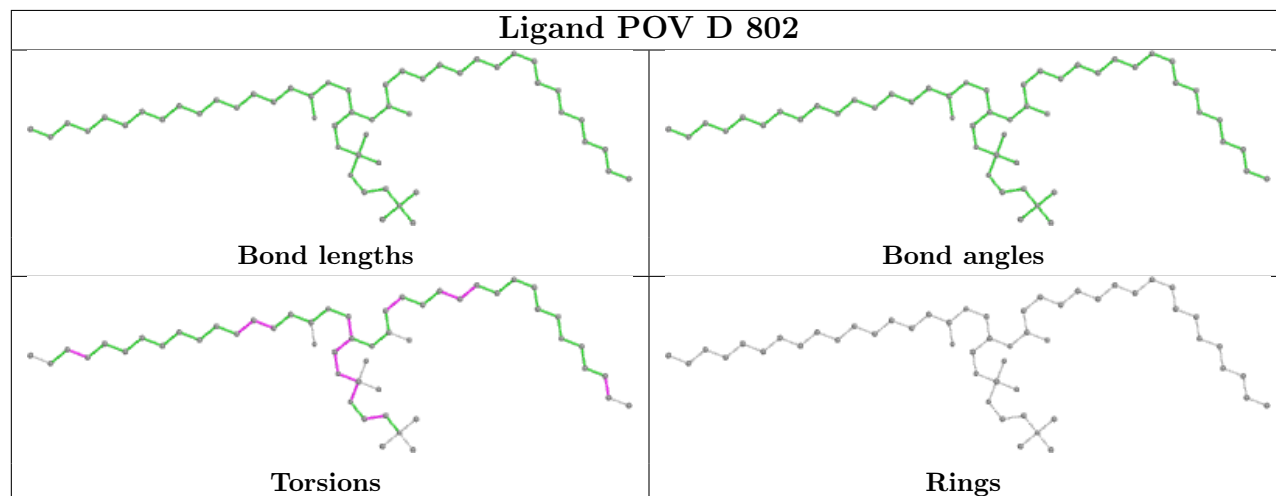
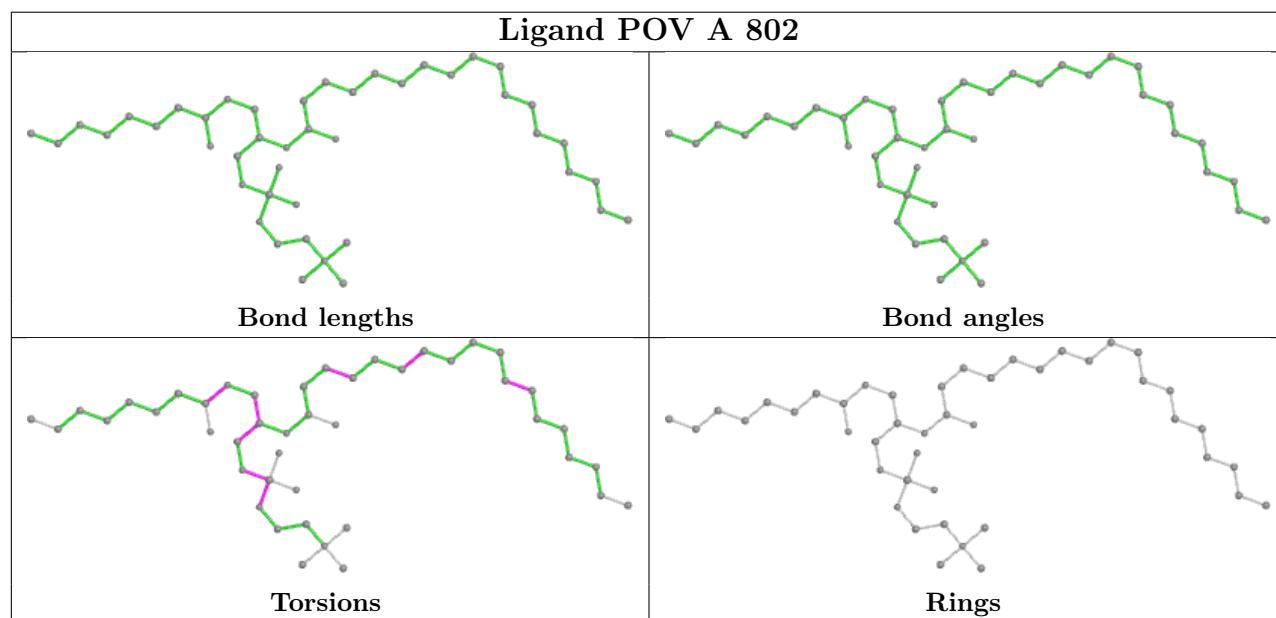
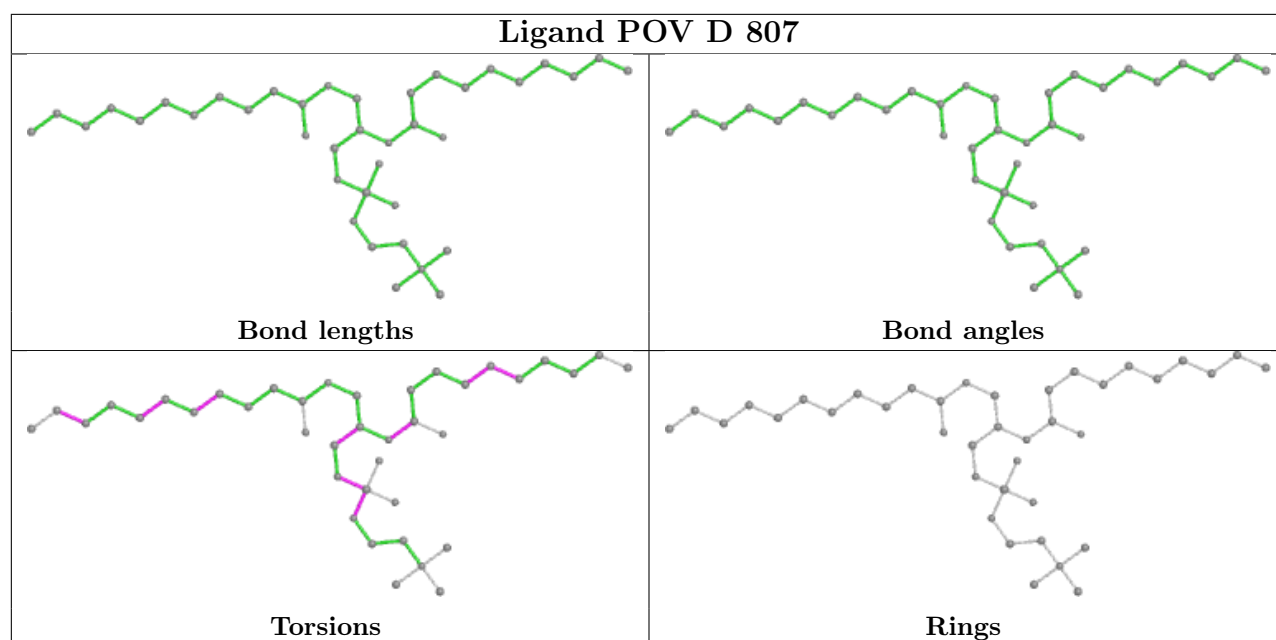


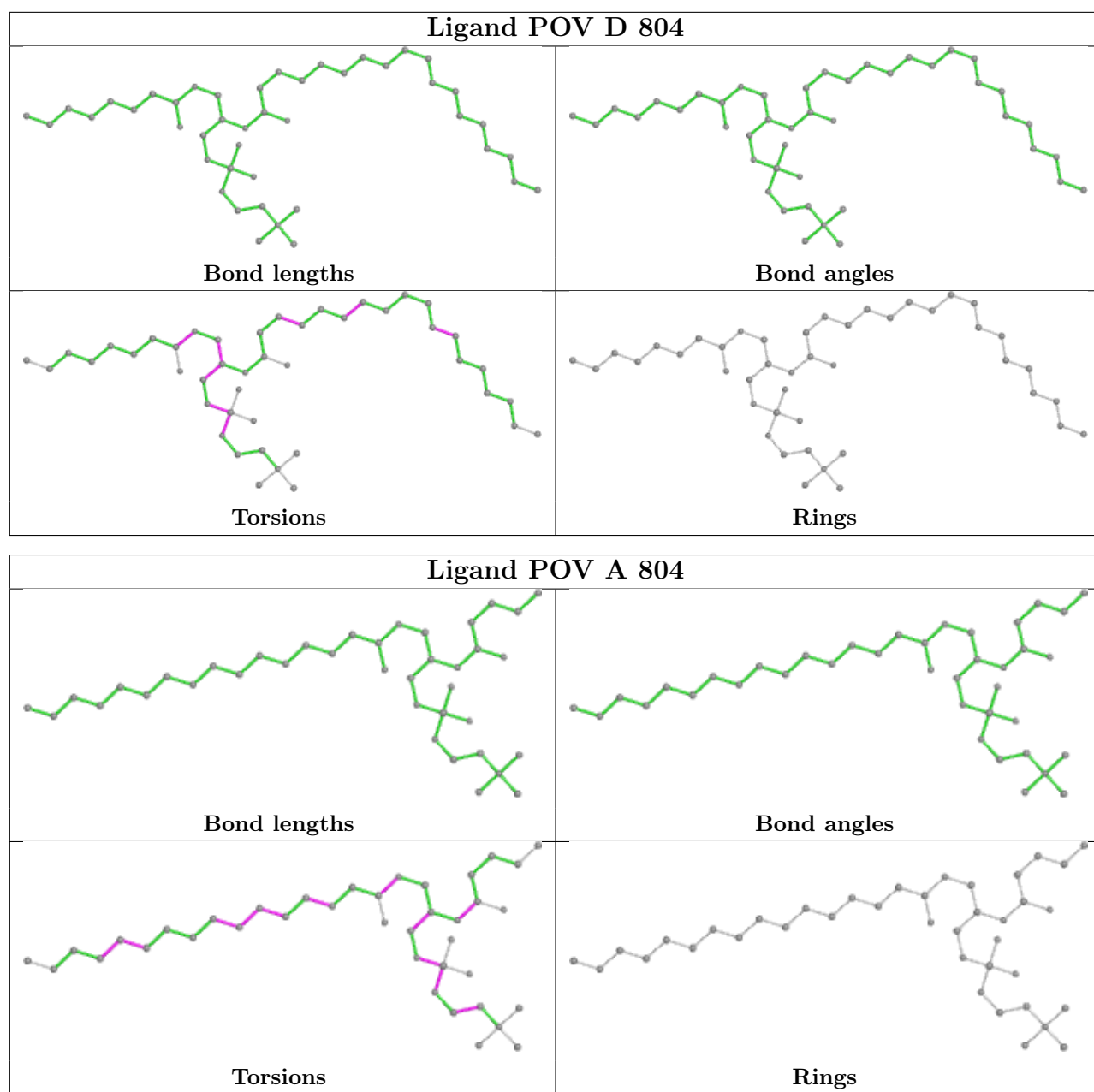


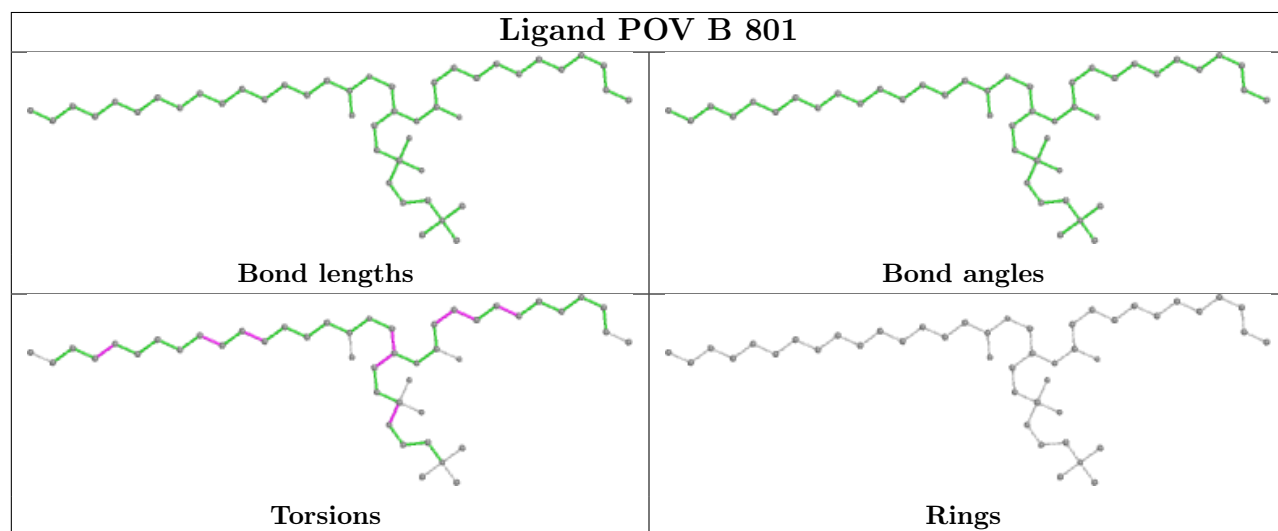
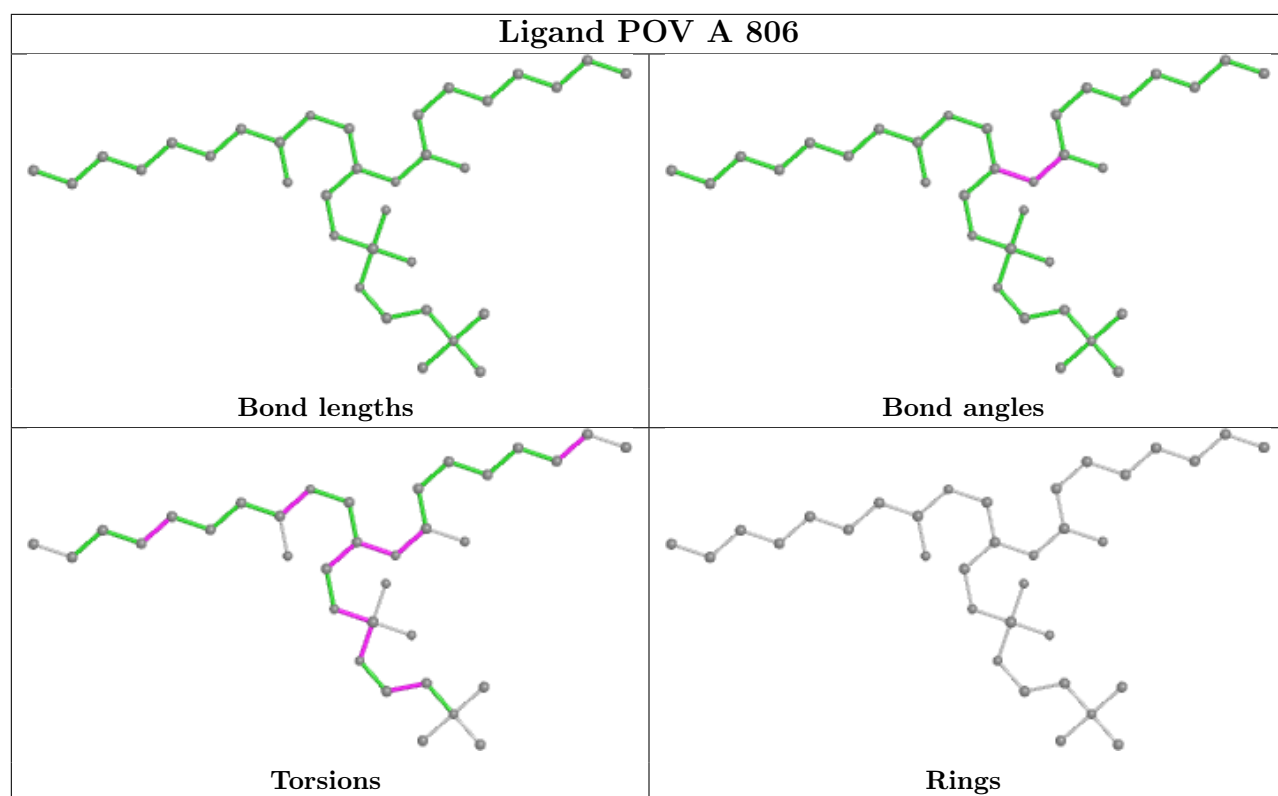


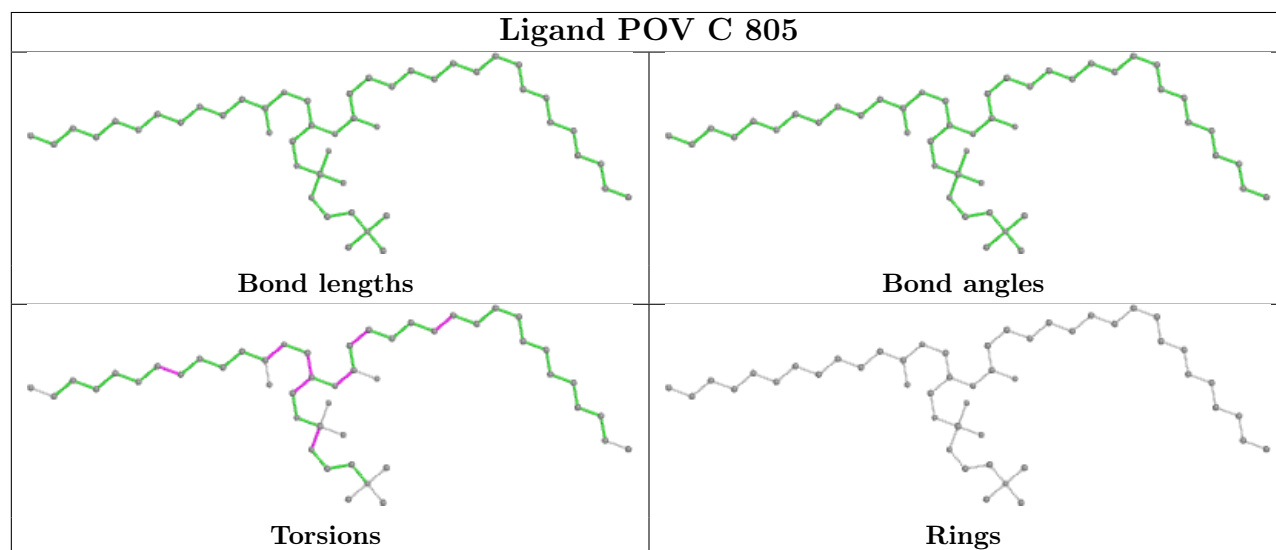
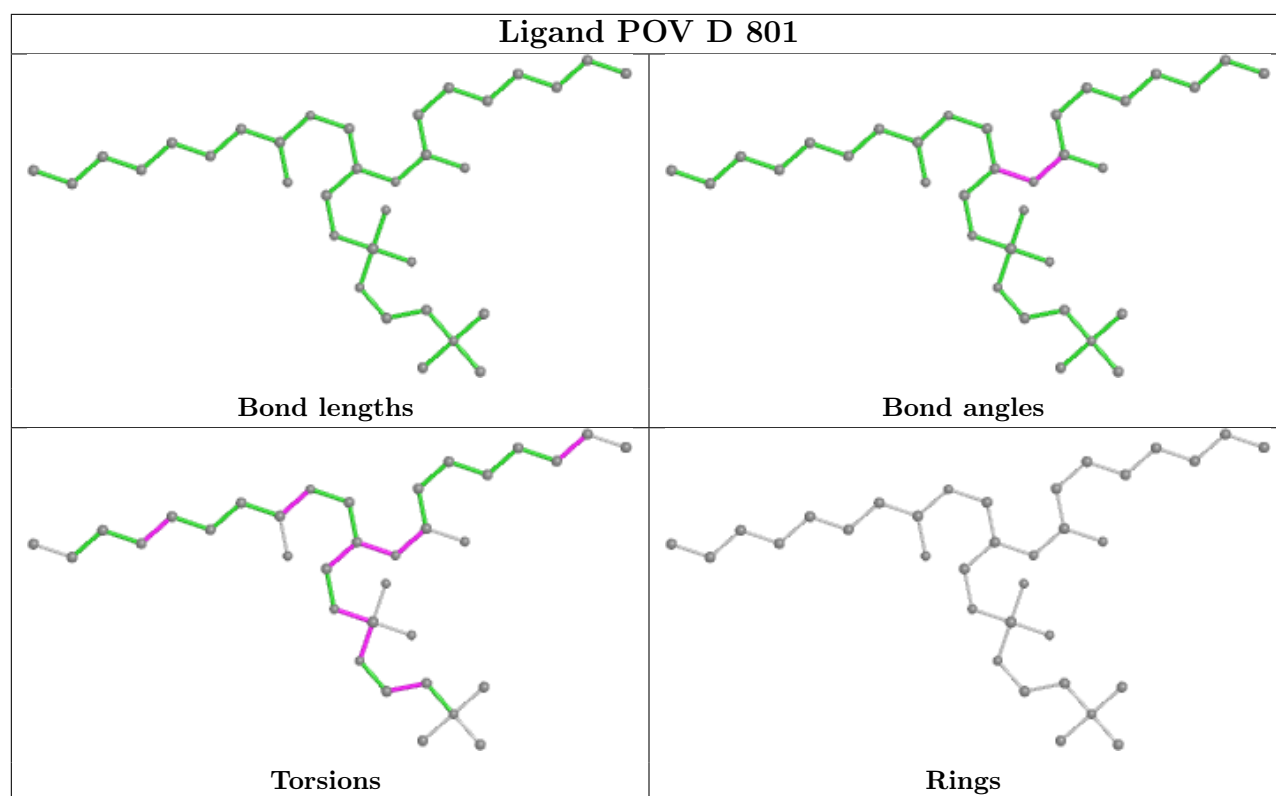


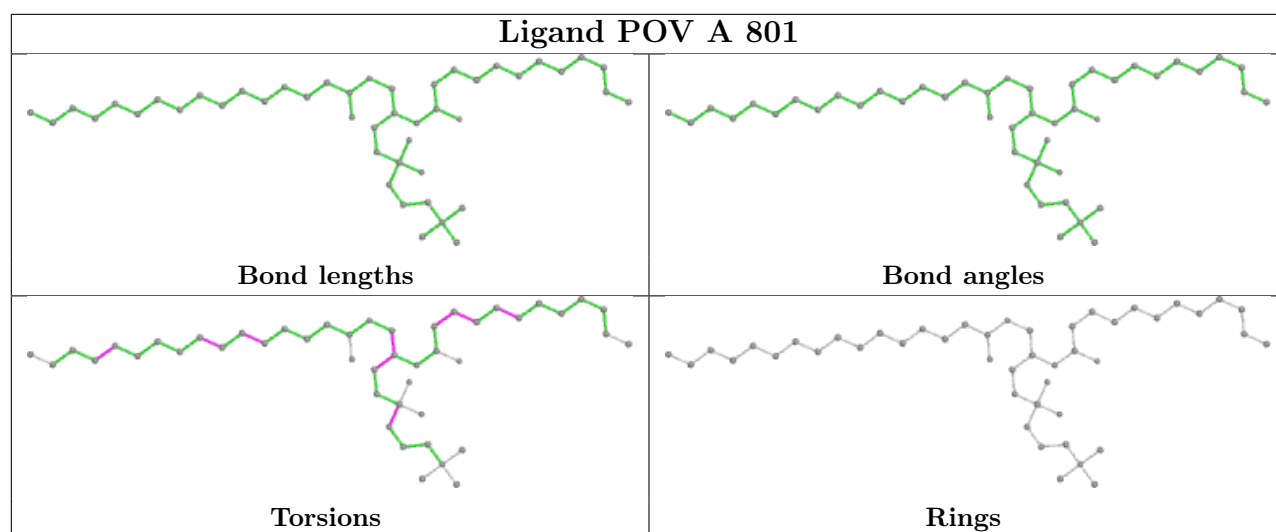












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.