



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:07 AM UTC

PDB ID : 6LGP / pdb_00006lgp
EMDB ID : EMD-0882
Title : cryo-EM structure of TRPV3 in lipid nanodisc
Authors : Shimada, H.; Kusakizako, T.; Nishizawa, T.; Nureki, O.
Deposited on : 2019-12-05
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

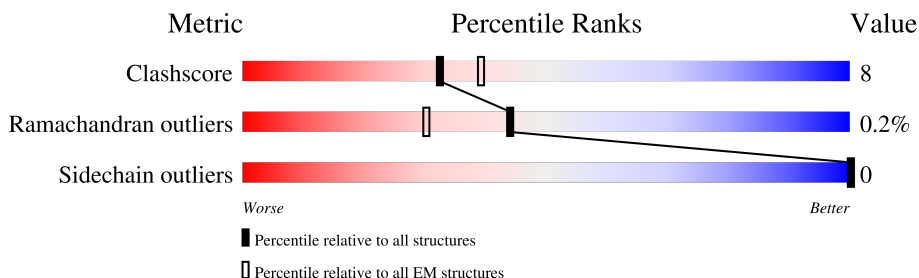
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	639	
1	B	639	
1	C	639	
1	D	639	

2 Entry composition [i](#)

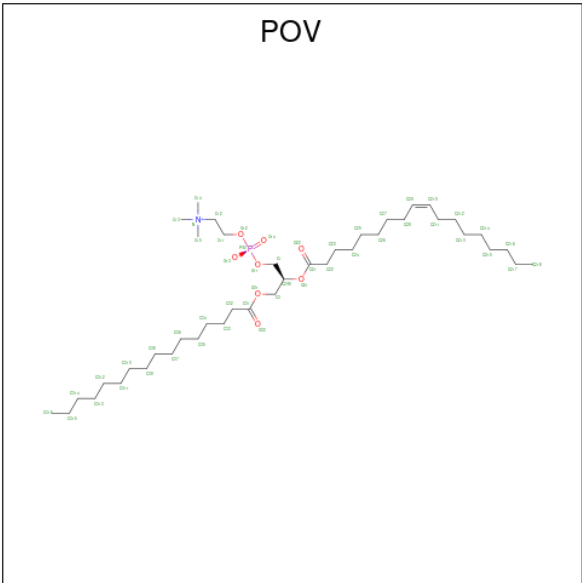
There are 3 unique types of molecules in this entry. The entry contains 21212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	622	Total	C	N	O	S	0	0
			5061	3292	833	906	30		
1	B	622	Total	C	N	O	S	0	0
			5061	3292	833	906	30		
1	C	622	Total	C	N	O	S	0	0
			5061	3292	833	906	30		
1	D	622	Total	C	N	O	S	0	0
			5061	3292	833	906	30		

- 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).



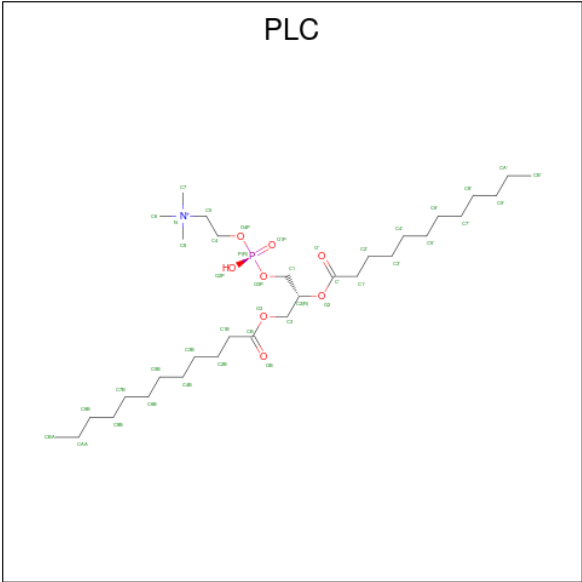
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			46	36	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C				0
			13	13				
2	A	1	Total	C				0
			13	13				
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	B	1	Total	C				0
			13	13				
2	B	1	Total	C				0
			13	13				
2	B	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				0
			13	13				
2	C	1	Total	C				0
			13	13				
2	C	1	Total	C	N	O	P	0
			52	42	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				0
			13	13				
2	D	1	Total	C				0
			13	13				

- Molecule 3 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$) (labeled as "Ligand of Interest" by depositor).

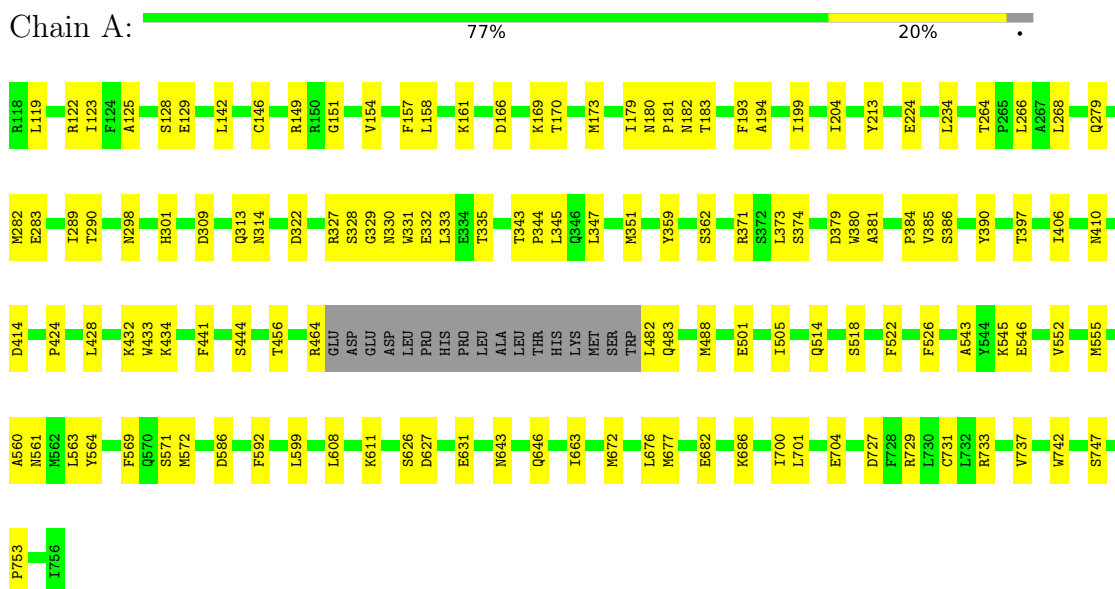


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	A	1	Total	C	O	P		0
			36	27	8	1		
3	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	B	1	Total	C	O	P		0
			36	27	8	1		
3	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	C	1	Total	C	O	P		0
			36	27	8	1		
3	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	D	1	Total	C	O	P		0
			36	27	8	1		

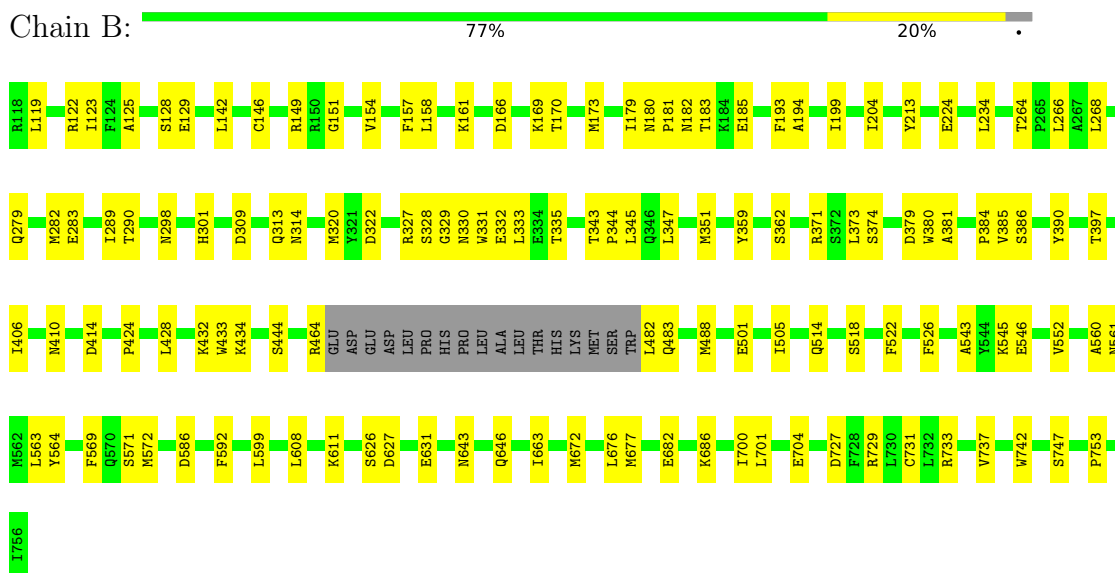
3 Residue-property plots [i](#)

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

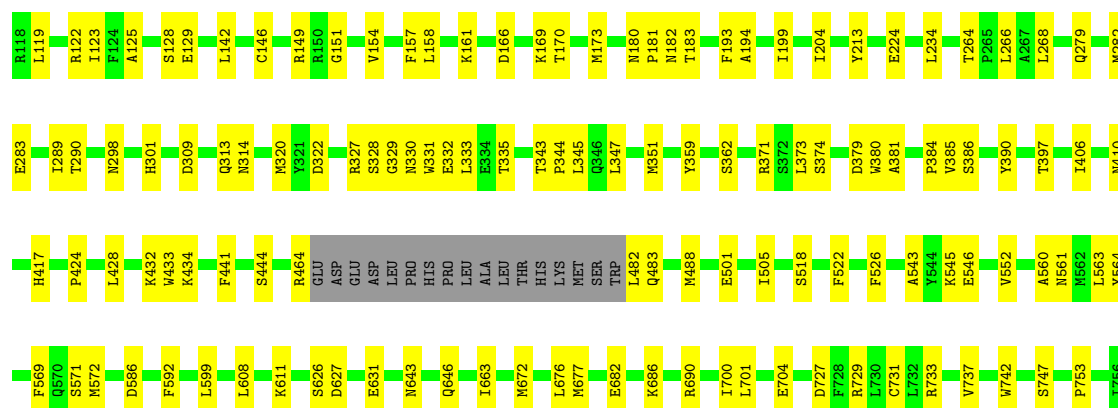


- Molecule 1: Transient receptor potential cation channel subfamily V member 3



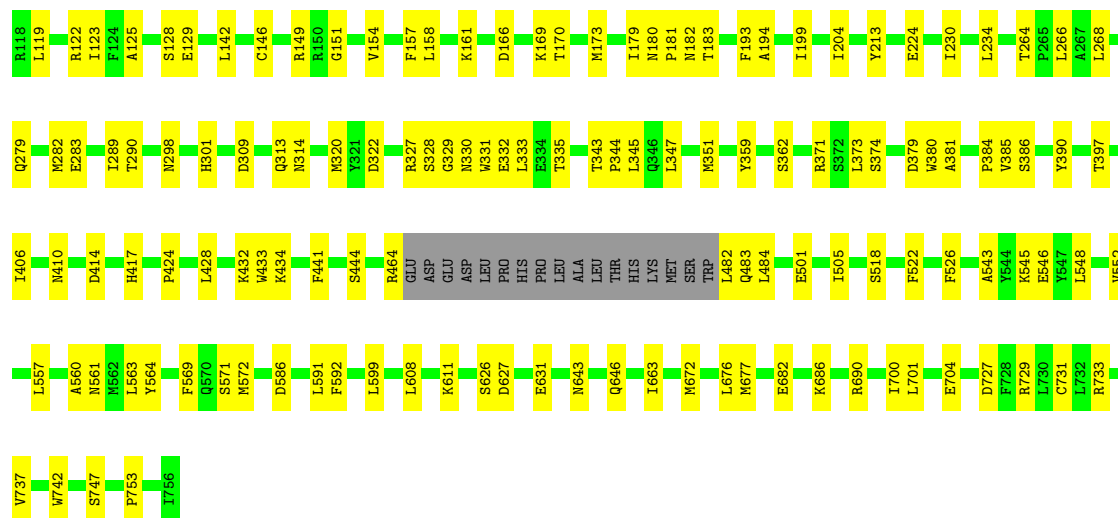
- Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain C:  77% 20% .



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

Chain D:  76% 21% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	106947	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, 50, 50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	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: POV, PLC

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	0.33	0/5168	0.47	0/6992
1	B	0.33	0/5168	0.47	0/6992
1	C	0.33	0/5168	0.47	0/6992
1	D	0.33	0/5168	0.47	0/6992
All	All	0.33	0/20672	0.47	0/27968

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	5061	0	5138	90	0
1	B	5061	0	5138	92	0
1	C	5061	0	5138	89	0
1	D	5061	0	5138	96	0
2	A	124	0	193	5	0
2	B	124	0	193	6	0
2	C	124	0	193	5	0
2	D	124	0	193	6	0
3	A	118	0	172	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	118	0	172	8	0
3	C	118	0	172	8	0
3	D	118	0	172	7	0
All	All	21212	0	22012	366	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 8.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HH22	1:A:154:VAL:HG22	1.47	0.80
1:B:149:ARG:HH22	1:B:154:VAL:HG22	1.47	0.80
1:C:149:ARG:HH22	1:C:154:VAL:HG22	1.47	0.80
1:D:149:ARG:HH22	1:D:154:VAL:HG22	1.47	0.80
1:C:569:PHE:HE2	3:C:804:PLC:H8'2	1.51	0.76
1:D:379:ASP:OD2	1:D:733:ARG:NH1	2.19	0.75
1:B:379:ASP:OD2	1:B:733:ARG:NH1	2.19	0.75
1:B:569:PHE:HE2	3:B:804:PLC:H8'2	1.51	0.75
1:A:379:ASP:OD2	1:A:733:ARG:NH1	2.19	0.75
1:D:569:PHE:HE2	3:D:805:PLC:H8'2	1.51	0.75
1:A:569:PHE:HE2	3:A:1003:PLC:H8'2	1.51	0.74
1:C:379:ASP:OD2	1:C:733:ARG:NH1	2.19	0.74
1:A:213:TYR:OH	1:B:753:PRO:O	2.06	0.73
1:B:213:TYR:OH	1:C:753:PRO:O	2.06	0.73
1:A:753:PRO:O	1:D:213:TYR:OH	2.06	0.72
1:C:213:TYR:OH	1:D:753:PRO:O	2.06	0.70
1:A:682:GLU:O	1:A:686:LYS:NZ	2.25	0.69
1:B:682:GLU:O	1:B:686:LYS:NZ	2.25	0.69
1:D:682:GLU:O	1:D:686:LYS:NZ	2.25	0.68
1:C:682:GLU:O	1:C:686:LYS:NZ	2.25	0.68
1:D:224:GLU:HB3	1:D:268:LEU:HD21	1.78	0.66
1:A:224:GLU:HB3	1:A:268:LEU:HD21	1.78	0.66
1:D:289:ILE:HG23	1:D:290:THR:HG23	1.79	0.65
1:B:146:CYS:HA	1:B:149:ARG:HH21	1.62	0.65
1:D:727:ASP:OD2	1:D:729:ARG:NH1	2.30	0.65
1:A:289:ILE:HG23	1:A:290:THR:HG23	1.79	0.65
1:A:727:ASP:OD2	1:A:729:ARG:NH1	2.30	0.65
1:B:224:GLU:HB3	1:B:268:LEU:HD21	1.78	0.64
1:C:146:CYS:HA	1:C:149:ARG:HH21	1.62	0.64
2:C:807:POV:H21A	3:D:804:PLC:H8A1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:HB3	1:C:268:LEU:HD21	1.78	0.64
1:B:727:ASP:OD2	1:B:729:ARG:NH1	2.30	0.64
2:B:807:POV:H21A	3:C:803:PLC:H8A1	1.79	0.64
1:C:727:ASP:OD2	1:C:729:ARG:NH1	2.30	0.64
1:A:146:CYS:HA	1:A:149:ARG:HH21	1.62	0.63
1:B:289:ILE:HG23	1:B:290:THR:HG23	1.79	0.63
1:B:626:SER:HB3	3:B:803:PLC:H1A2	1.80	0.63
1:C:289:ILE:HG23	1:C:290:THR:HG23	1.79	0.63
1:A:626:SER:HB3	3:A:1002:PLC:H1A2	1.80	0.63
2:A:1006:POV:H21A	3:B:803:PLC:H8A1	1.79	0.63
1:D:146:CYS:HA	1:D:149:ARG:HH21	1.62	0.63
3:A:1002:PLC:H8A1	2:D:801:POV:H21A	1.79	0.63
1:D:626:SER:HB3	3:D:804:PLC:H1A2	1.80	0.63
1:C:626:SER:HB3	3:C:803:PLC:H1A2	1.80	0.62
1:C:643:ASN:O	1:C:646:GLN:NE2	2.35	0.59
1:B:643:ASN:O	1:B:646:GLN:NE2	2.35	0.59
1:A:643:ASN:O	1:A:646:GLN:NE2	2.35	0.58
1:B:180:ASN:O	1:B:182:ASN:N	2.37	0.57
1:C:180:ASN:O	1:C:182:ASN:N	2.37	0.57
1:A:180:ASN:O	1:A:182:ASN:N	2.37	0.57
1:D:180:ASN:O	1:D:182:ASN:N	2.37	0.57
1:A:663:ILE:HG12	2:A:1006:POV:H21E	1.87	0.57
1:B:663:ILE:HG12	2:B:807:POV:H21E	1.87	0.56
1:C:663:ILE:HG12	2:C:807:POV:H21E	1.87	0.56
1:D:643:ASN:O	1:D:646:GLN:NE2	2.35	0.56
1:D:663:ILE:HG12	2:D:801:POV:H21E	1.87	0.56
1:A:592:PHE:HB2	2:A:1005:POV:H311	1.88	0.55
1:A:433:TRP:HB2	1:A:700:ILE:HD11	1.88	0.55
1:D:592:PHE:HB2	2:D:807:POV:H311	1.88	0.55
1:B:433:TRP:HB2	1:B:700:ILE:HD11	1.88	0.55
1:C:282:MET:HE2	1:C:327:ARG:HB3	1.89	0.55
1:C:672:MET:HE2	1:C:676:LEU:HD11	1.89	0.55
1:D:282:MET:HE2	1:D:327:ARG:HB3	1.89	0.55
1:B:397:THR:HG21	1:B:701:LEU:HD11	1.89	0.55
1:D:672:MET:HE2	1:D:676:LEU:HD11	1.89	0.55
1:C:397:THR:HG21	1:C:701:LEU:HD11	1.89	0.54
1:D:432:LYS:NZ	1:D:704:GLU:OE2	2.41	0.54
1:B:672:MET:HE2	1:B:676:LEU:HD11	1.89	0.54
1:C:518:SER:O	2:C:802:POV:H14	2.07	0.54
1:C:128:SER:C	1:C:180:ASN:HD21	2.15	0.54
1:A:518:SER:O	2:A:1001:POV:H14	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:PHE:HB2	2:C:806:POV:H311	1.88	0.54
1:D:433:TRP:HB2	1:D:700:ILE:HD11	1.88	0.54
1:A:282:MET:HE2	1:A:327:ARG:HB3	1.89	0.54
1:B:592:PHE:HB2	2:B:806:POV:H311	1.88	0.54
1:C:433:TRP:HB2	1:C:700:ILE:HD11	1.88	0.54
1:B:128:SER:C	1:B:180:ASN:HD21	2.15	0.54
1:B:282:MET:HE2	1:B:327:ARG:HB3	1.89	0.54
1:B:522:PHE:CE1	1:B:564:TYR:HB2	2.43	0.54
1:D:128:SER:C	1:D:180:ASN:HD21	2.15	0.54
1:D:397:THR:HG21	1:D:701:LEU:HD11	1.89	0.54
1:A:599:LEU:HB3	3:A:1002:PLC:H9'2	1.90	0.54
1:A:672:MET:HE2	1:A:676:LEU:HD11	1.89	0.54
1:C:522:PHE:CE1	1:C:564:TYR:HB2	2.43	0.54
1:D:518:SER:O	2:D:803:POV:H14	2.07	0.54
1:A:290:THR:HG22	1:A:333:LEU:HD13	1.91	0.53
1:A:432:LYS:NZ	1:A:704:GLU:OE2	2.41	0.53
1:A:522:PHE:CE1	1:A:564:TYR:HB2	2.43	0.53
1:B:518:SER:O	2:B:802:POV:H14	2.07	0.53
1:D:522:PHE:CE1	1:D:564:TYR:HB2	2.43	0.53
1:A:397:THR:HG21	1:A:701:LEU:HD11	1.89	0.53
1:C:599:LEU:HB3	3:C:803:PLC:H9'2	1.90	0.53
1:D:290:THR:HG22	1:D:333:LEU:HD13	1.91	0.53
1:B:290:THR:HG22	1:B:333:LEU:HD13	1.91	0.53
1:C:290:THR:HG22	1:C:333:LEU:HD13	1.91	0.53
1:C:432:LYS:NZ	1:C:704:GLU:OE2	2.41	0.53
1:B:328:SER:OG	1:B:329:GLY:N	2.42	0.53
1:C:125:ALA:O	1:C:129:GLU:HG2	2.08	0.53
1:B:599:LEU:HB3	3:B:803:PLC:H9'2	1.90	0.53
1:B:125:ALA:O	1:B:129:GLU:HG2	2.08	0.53
1:A:128:SER:C	1:A:180:ASN:HD21	2.15	0.52
1:A:328:SER:OG	1:A:329:GLY:N	2.42	0.52
1:B:432:LYS:NZ	1:B:704:GLU:OE2	2.41	0.52
1:C:169:LYS:HA	1:C:173:MET:HE3	1.92	0.52
1:C:309:ASP:OD1	1:C:309:ASP:N	2.40	0.52
1:D:125:ALA:O	1:D:129:GLU:HG2	2.08	0.52
1:A:125:ALA:O	1:A:129:GLU:HG2	2.08	0.52
1:D:169:LYS:HA	1:D:173:MET:HE3	1.92	0.52
1:C:142:LEU:HD21	1:C:158:LEU:HG	1.92	0.52
1:C:149:ARG:HH11	1:C:151:GLY:HA3	1.75	0.52
1:D:149:ARG:HH11	1:D:151:GLY:HA3	1.75	0.52
1:D:599:LEU:HB3	3:D:804:PLC:H9'2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:HD21	1:B:158:LEU:HG	1.92	0.52
1:B:169:LYS:HA	1:B:173:MET:HE3	1.92	0.52
1:A:169:LYS:HA	1:A:173:MET:HE3	1.92	0.51
1:D:142:LEU:HD21	1:D:158:LEU:HG	1.92	0.51
1:C:371:ARG:NH1	1:C:747:SER:O	2.44	0.51
1:B:149:ARG:HH11	1:B:151:GLY:HA3	1.75	0.51
1:A:149:ARG:HH11	1:A:151:GLY:HA3	1.75	0.51
1:A:301:HIS:NE2	1:A:344:PRO:HD3	2.25	0.51
1:C:301:HIS:NE2	1:C:344:PRO:HD3	2.25	0.51
1:C:561:ASN:O	1:C:564:TYR:HB3	2.11	0.51
1:B:371:ARG:NH1	1:B:747:SER:O	2.44	0.51
1:A:142:LEU:HD21	1:A:158:LEU:HG	1.92	0.51
1:A:371:ARG:NH1	1:A:747:SER:O	2.44	0.51
1:A:444:SER:HB2	2:A:1004:POV:H34	1.93	0.51
1:A:561:ASN:O	1:A:564:TYR:HB3	2.11	0.51
1:B:561:ASN:O	1:B:564:TYR:HB3	2.11	0.51
1:D:444:SER:HB2	2:D:806:POV:H34	1.93	0.51
1:B:301:HIS:NE2	1:B:344:PRO:HD3	2.25	0.51
1:D:301:HIS:NE2	1:D:344:PRO:HD3	2.25	0.51
1:D:371:ARG:NH1	1:D:747:SER:O	2.44	0.51
1:C:381:ALA:HA	1:C:386:SER:HA	1.93	0.50
1:D:381:ALA:HA	1:D:386:SER:HA	1.93	0.50
1:D:561:ASN:O	1:D:564:TYR:HB3	2.11	0.50
1:B:128:SER:O	1:B:180:ASN:ND2	2.40	0.50
1:C:374:SER:O	1:C:729:ARG:NH2	2.45	0.50
1:D:322:ASP:HB3	1:D:359:TYR:OH	2.12	0.50
1:B:322:ASP:HB3	1:B:359:TYR:OH	2.12	0.50
1:B:374:SER:O	1:B:729:ARG:NH2	2.45	0.50
1:A:546:GLU:O	1:A:546:GLU:HG2	2.12	0.50
1:B:546:GLU:O	1:B:546:GLU:HG2	2.12	0.50
1:D:546:GLU:O	1:D:546:GLU:HG2	2.12	0.50
1:A:322:ASP:HB3	1:A:359:TYR:OH	2.12	0.50
1:C:322:ASP:HB3	1:C:359:TYR:OH	2.12	0.50
1:B:381:ALA:HA	1:B:386:SER:HA	1.93	0.50
1:C:444:SER:HB2	2:C:805:POV:H34	1.93	0.50
1:D:128:SER:O	1:D:180:ASN:ND2	2.40	0.50
1:A:381:ALA:HA	1:A:386:SER:HA	1.93	0.49
1:C:328:SER:OG	1:C:329:GLY:N	2.42	0.49
1:C:522:PHE:CD1	1:C:564:TYR:HB2	2.47	0.49
1:C:546:GLU:HG2	1:C:546:GLU:O	2.12	0.49
1:D:522:PHE:CD1	1:D:564:TYR:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:SER:O	1:A:729:ARG:NH2	2.45	0.49
1:B:444:SER:HB2	2:B:805:POV:H34	1.93	0.49
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.43	0.49
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.43	0.49
1:D:374:SER:O	1:D:729:ARG:NH2	2.45	0.49
1:B:571:SER:OG	1:B:572:MET:N	2.46	0.49
1:A:128:SER:O	1:A:180:ASN:ND2	2.40	0.49
1:A:571:SER:OG	1:A:572:MET:N	2.46	0.49
1:B:522:PHE:CD1	1:B:564:TYR:HB2	2.47	0.49
1:B:119:LEU:O	1:B:123:ILE:HG12	2.13	0.48
1:A:522:PHE:CD1	1:A:564:TYR:HB2	2.47	0.48
1:C:119:LEU:O	1:C:123:ILE:HG12	2.13	0.48
1:A:298:ASN:OD1	1:A:301:HIS:ND1	2.43	0.48
1:A:119:LEU:O	1:A:123:ILE:HG12	2.13	0.48
1:C:180:ASN:O	1:C:183:THR:N	2.47	0.48
1:D:119:LEU:O	1:D:123:ILE:HG12	2.13	0.48
1:C:166:ASP:OD2	1:C:166:ASP:N	2.47	0.48
1:B:298:ASN:OD1	1:B:301:HIS:ND1	2.43	0.48
1:C:406:ILE:O	1:C:410:ASN:HB2	2.14	0.48
1:A:464:ARG:HG3	1:D:611:LYS:HZ1	1.77	0.48
1:B:180:ASN:O	1:B:183:THR:N	2.47	0.47
1:B:406:ILE:O	1:B:410:ASN:HB2	2.14	0.47
1:A:180:ASN:O	1:A:183:THR:N	2.47	0.47
1:B:569:PHE:CE2	3:B:804:PLC:H8'2	2.41	0.47
1:D:180:ASN:O	1:D:183:THR:N	2.47	0.47
1:A:385:VAL:HG12	1:A:737:VAL:HG22	1.96	0.47
1:B:166:ASP:OD2	1:B:166:ASP:N	2.47	0.47
1:D:571:SER:OG	1:D:572:MET:N	2.46	0.47
1:C:385:VAL:HG12	1:C:737:VAL:HG22	1.96	0.47
3:C:803:PLC:HTA2	3:C:803:PLC:H6A2	1.97	0.47
3:D:804:PLC:HTA2	3:D:804:PLC:H6A2	1.97	0.47
1:D:414:ASP:OD1	1:D:414:ASP:N	2.48	0.47
1:A:406:ILE:O	1:A:410:ASN:HB2	2.14	0.47
1:A:414:ASP:OD1	1:A:414:ASP:N	2.48	0.47
3:A:1007:PLC:H32	3:A:1007:PLC:H1A1	1.61	0.47
1:C:571:SER:OG	1:C:572:MET:N	2.46	0.47
1:C:611:LYS:NZ	1:D:464:ARG:HG3	2.30	0.47
1:D:406:ILE:O	1:D:410:ASN:HB2	2.14	0.47
1:D:204:ILE:HD11	1:D:234:LEU:HD23	1.97	0.47
1:A:569:PHE:CE2	3:A:1003:PLC:H8'2	2.41	0.46
1:B:414:ASP:OD1	1:B:414:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD12	1:B:122:ARG:HD2	1.97	0.46
1:C:119:LEU:HD12	1:C:122:ARG:HD2	1.97	0.46
1:A:204:ILE:HD11	1:A:234:LEU:HD23	1.97	0.46
1:D:385:VAL:HG12	1:D:737:VAL:HG22	1.96	0.46
1:A:611:LYS:NZ	1:B:464:ARG:HG3	2.30	0.46
1:B:385:VAL:HG12	1:B:737:VAL:HG22	1.96	0.46
3:B:803:PLC:H6A2	3:B:803:PLC:HTA2	1.97	0.46
1:D:166:ASP:N	1:D:166:ASP:OD2	2.47	0.46
1:A:309:ASP:OD1	1:A:309:ASP:N	2.40	0.46
1:D:119:LEU:HD12	1:D:122:ARG:HD2	1.97	0.46
1:A:464:ARG:HG3	1:D:611:LYS:NZ	2.30	0.46
1:B:611:LYS:NZ	1:C:464:ARG:HG3	2.30	0.46
1:C:543:ALA:HB1	1:C:545:LYS:HE3	1.98	0.46
3:D:802:PLC:H32	3:D:802:PLC:H1A1	1.61	0.46
1:B:384:PRO:HG3	1:B:742:TRP:CH2	2.51	0.46
1:C:384:PRO:HG3	1:C:742:TRP:CH2	2.51	0.46
1:D:347:LEU:O	1:D:351:MET:HG2	2.16	0.46
1:B:204:ILE:HD11	1:B:234:LEU:HD23	1.97	0.45
1:C:279:GLN:O	1:C:283:GLU:HG2	2.16	0.45
1:D:328:SER:OG	1:D:329:GLY:N	2.42	0.45
1:A:384:PRO:HG3	1:A:742:TRP:CH2	2.51	0.45
1:B:362:SER:HB3	1:B:390:TYR:HE2	1.82	0.45
1:B:543:ALA:HB1	1:B:545:LYS:HE3	1.98	0.45
1:C:128:SER:O	1:C:180:ASN:ND2	2.40	0.45
1:C:204:ILE:HD11	1:C:234:LEU:HD23	1.97	0.45
1:D:362:SER:HB3	1:D:390:TYR:HE2	1.82	0.45
1:D:543:ALA:HB1	1:D:545:LYS:HE3	1.98	0.45
1:A:362:SER:HB3	1:A:390:TYR:HE2	1.82	0.45
1:D:384:PRO:HG3	1:D:742:TRP:CH2	2.51	0.45
1:A:179:ILE:HD12	1:A:179:ILE:HA	1.84	0.45
1:A:301:HIS:CE1	1:A:344:PRO:HD3	2.52	0.45
1:A:347:LEU:O	1:A:351:MET:HG2	2.16	0.45
1:A:488:MET:HE3	1:A:488:MET:HB2	1.90	0.45
1:C:301:HIS:CE1	1:C:344:PRO:HD3	2.52	0.45
1:A:543:ALA:HB1	1:A:545:LYS:HE3	1.98	0.45
1:B:279:GLN:O	1:B:283:GLU:HG2	2.16	0.45
1:D:301:HIS:CE1	1:D:344:PRO:HD3	2.52	0.45
1:A:119:LEU:HD12	1:A:122:ARG:HD2	1.97	0.45
1:A:157:PHE:O	1:A:161:LYS:HG2	2.17	0.45
1:A:434:LYS:HE2	1:A:434:LYS:HB3	1.76	0.45
1:A:611:LYS:HZ1	1:B:464:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1002:PLC:HTA2	3:A:1002:PLC:H6A2	1.97	0.45
1:B:347:LEU:O	1:B:351:MET:HG2	2.16	0.45
1:C:347:LEU:O	1:C:351:MET:HG2	2.16	0.45
1:D:309:ASP:OD1	1:D:309:ASP:N	2.40	0.45
1:B:301:HIS:CE1	1:B:344:PRO:HD3	2.52	0.45
1:A:279:GLN:O	1:A:283:GLU:HG2	2.16	0.45
1:D:157:PHE:O	1:D:161:LYS:HG2	2.17	0.45
1:D:170:THR:H	1:D:173:MET:HE3	1.82	0.45
1:D:279:GLN:O	1:D:283:GLU:HG2	2.16	0.45
1:B:157:PHE:O	1:B:161:LYS:HG2	2.17	0.44
1:C:569:PHE:CE2	3:C:804:PLC:H8'2	2.41	0.44
1:A:194:ALA:HB1	1:A:199:ILE:O	2.18	0.44
1:B:170:THR:H	1:B:173:MET:HE3	1.82	0.44
1:B:194:ALA:HB1	1:B:199:ILE:O	2.18	0.44
1:B:488:MET:HE3	1:B:488:MET:HB2	1.90	0.44
1:C:434:LYS:HE2	1:C:434:LYS:HB3	1.76	0.44
1:D:373:LEU:HD23	1:D:373:LEU:H	1.83	0.44
1:B:627:ASP:O	1:B:631:GLU:HG2	2.18	0.44
1:A:501:GLU:O	1:A:505:ILE:HG13	2.18	0.44
1:B:501:GLU:O	1:B:505:ILE:HG13	2.18	0.44
1:C:157:PHE:O	1:C:161:LYS:HG2	2.17	0.44
1:C:501:GLU:O	1:C:505:ILE:HG13	2.18	0.44
1:C:170:THR:H	1:C:173:MET:HE3	1.82	0.44
1:B:373:LEU:H	1:B:373:LEU:HD23	1.83	0.43
1:C:362:SER:HB3	1:C:390:TYR:HE2	1.82	0.43
1:D:501:GLU:O	1:D:505:ILE:HG13	2.18	0.43
1:C:194:ALA:HB1	1:C:199:ILE:O	2.18	0.43
1:C:627:ASP:O	1:C:631:GLU:HG2	2.18	0.43
1:D:390:TYR:O	1:D:731:CYS:HB3	2.19	0.43
1:D:557:LEU:HD12	1:D:557:LEU:HA	1.81	0.43
1:A:170:THR:H	1:A:173:MET:HE3	1.82	0.43
1:A:373:LEU:HD23	1:A:373:LEU:H	1.83	0.43
1:A:424:PRO:O	1:A:428:LEU:HB2	2.18	0.43
1:A:433:TRP:O	1:A:433:TRP:CD1	2.71	0.43
1:A:627:ASP:O	1:A:631:GLU:HG2	2.18	0.43
1:D:194:ALA:HB1	1:D:199:ILE:O	2.18	0.43
1:D:320:MET:HE2	1:D:320:MET:HB2	1.92	0.43
1:D:433:TRP:O	1:D:433:TRP:CD1	2.71	0.43
1:A:166:ASP:OD2	1:A:166:ASP:N	2.47	0.43
1:B:424:PRO:O	1:B:428:LEU:HB2	2.18	0.43
1:B:434:LYS:HE2	1:B:434:LYS:HB3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:LEU:HD13	1:C:552:VAL:HG21	2.01	0.43
1:C:424:PRO:O	1:C:428:LEU:HB2	2.18	0.43
1:D:424:PRO:O	1:D:428:LEU:HB2	2.18	0.43
1:A:560:ALA:O	1:A:563:LEU:HB2	2.18	0.43
1:A:586:ASP:OD2	1:A:677:MET:HA	2.19	0.43
1:B:158:LEU:HD21	1:B:193:PHE:HE2	1.84	0.43
1:B:390:TYR:O	1:B:731:CYS:HB3	2.19	0.43
1:A:390:TYR:O	1:A:731:CYS:HB3	2.19	0.43
1:B:433:TRP:O	1:B:433:TRP:CD1	2.71	0.43
1:A:482:LEU:HD23	1:A:483:GLN:HG2	2.01	0.43
1:D:560:ALA:O	1:D:563:LEU:HB2	2.18	0.43
1:A:264:THR:HG22	1:A:266:LEU:H	1.84	0.43
1:C:560:ALA:O	1:C:563:LEU:HB2	2.18	0.43
1:D:313:GLN:HG3	1:D:314:ASN:O	2.19	0.43
1:B:563:LEU:HD23	1:B:563:LEU:HA	1.80	0.43
1:C:373:LEU:HD23	1:C:373:LEU:H	1.83	0.43
1:B:264:THR:HG22	1:B:266:LEU:H	1.84	0.42
1:C:482:LEU:HD23	1:C:483:GLN:HG2	2.01	0.42
1:C:586:ASP:OD2	1:C:677:MET:HA	2.19	0.42
1:A:608:LEU:HD13	1:B:552:VAL:HG21	2.01	0.42
1:B:313:GLN:HG3	1:B:314:ASN:O	2.19	0.42
1:B:560:ALA:O	1:B:563:LEU:HB2	2.18	0.42
1:C:397:THR:OG1	1:C:704:GLU:OE1	2.30	0.42
1:C:611:LYS:HZ1	1:D:464:ARG:HG3	1.84	0.42
1:D:627:ASP:O	1:D:631:GLU:HG2	2.18	0.42
1:C:433:TRP:CD1	1:C:433:TRP:O	2.71	0.42
1:A:330:ASN:HB3	1:A:332:GLU:H	1.85	0.42
1:C:264:THR:HG22	1:C:266:LEU:H	1.84	0.42
1:C:390:TYR:O	1:C:731:CYS:HB3	2.19	0.42
1:D:264:THR:HG22	1:D:266:LEU:H	1.84	0.42
1:A:158:LEU:HD21	1:A:193:PHE:HE2	1.84	0.42
1:C:158:LEU:HD21	1:C:193:PHE:HE2	1.84	0.42
1:C:608:LEU:HD13	1:D:552:VAL:HG21	2.01	0.42
1:B:330:ASN:HB3	1:B:332:GLU:H	1.85	0.42
1:D:158:LEU:HD21	1:D:193:PHE:HE2	1.84	0.42
1:D:563:LEU:HD23	1:D:563:LEU:HA	1.80	0.42
1:D:586:ASP:OD2	1:D:677:MET:HA	2.19	0.42
1:A:313:GLN:HG3	1:A:314:ASN:O	2.19	0.42
1:A:343:THR:HG22	1:A:345:LEU:H	1.85	0.42
1:A:552:VAL:HG21	1:D:608:LEU:HD13	2.01	0.42
1:C:313:GLN:HG3	1:C:314:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ILE:HA	1:D:179:ILE:HD12	1.84	0.42
1:D:343:THR:HG22	1:D:345:LEU:H	1.85	0.42
1:B:586:ASP:OD2	1:B:677:MET:HA	2.19	0.42
3:B:801:PLC:H32	3:B:801:PLC:H1A1	1.61	0.42
1:D:482:LEU:HD23	1:D:483:GLN:HG2	2.01	0.42
1:C:331:TRP:O	1:C:335:THR:HG23	2.20	0.42
1:D:434:LYS:HE2	1:D:434:LYS:HB3	1.76	0.41
1:D:484:LEU:HD12	1:D:484:LEU:HA	1.92	0.41
1:C:320:MET:HE2	1:C:320:MET:HB2	1.92	0.41
1:A:331:TRP:O	1:A:335:THR:HG23	2.20	0.41
1:B:179:ILE:HD12	1:B:179:ILE:HA	1.84	0.41
1:C:563:LEU:HD23	1:C:563:LEU:HA	1.80	0.41
1:D:397:THR:OG1	1:D:704:GLU:OE1	2.30	0.41
1:B:343:THR:HG22	1:B:345:LEU:H	1.85	0.41
1:C:330:ASN:HB3	1:C:332:GLU:H	1.85	0.41
1:C:488:MET:HE3	1:C:488:MET:HB2	1.90	0.41
1:D:548:LEU:HD23	1:D:548:LEU:HA	1.92	0.41
1:B:526:PHE:CE1	1:B:561:ASN:HB3	2.56	0.41
1:C:343:THR:HG22	1:C:345:LEU:H	1.85	0.41
1:D:330:ASN:HB3	1:D:332:GLU:H	1.85	0.41
1:A:456:THR:OG1	1:A:555:MET:SD	2.71	0.41
1:B:185:GLU:OE2	1:B:185:GLU:N	2.53	0.41
1:B:309:ASP:OD1	1:B:309:ASP:N	2.40	0.41
1:B:320:MET:HE2	1:B:320:MET:HB2	1.92	0.41
1:B:331:TRP:O	1:B:335:THR:HG23	2.20	0.41
1:B:482:LEU:HD23	1:B:483:GLN:HG2	2.01	0.41
1:D:230:ILE:H	1:D:230:ILE:HG13	1.68	0.41
1:D:331:TRP:O	1:D:335:THR:HG23	2.20	0.41
1:A:441:PHE:HD2	3:A:1003:PLC:H5'1	1.86	0.41
1:B:482:LEU:HD23	1:B:483:GLN:N	2.37	0.41
1:B:514:GLN:O	1:B:518:SER:OG	2.18	0.41
1:D:501:GLU:OE2	2:D:806:POV:H313	2.21	0.41
1:A:514:GLN:O	1:A:518:SER:OG	2.18	0.40
1:A:526:PHE:CE1	1:A:561:ASN:HB3	2.56	0.40
1:B:501:GLU:OE2	2:B:805:POV:H313	2.21	0.40
3:C:801:PLC:H32	3:C:801:PLC:H1A1	1.61	0.40
1:D:417:HIS:HB2	1:D:690:ARG:HB3	2.03	0.40
1:D:441:PHE:HD2	3:D:805:PLC:H5'1	1.86	0.40
1:A:380:TRP:CB	1:A:753:PRO:HA	2.51	0.40
1:C:441:PHE:HD2	3:C:804:PLC:H5'1	1.86	0.40
1:C:526:PHE:CE1	1:C:561:ASN:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:TRP:CB	1:D:753:PRO:HA	2.51	0.40
3:A:1002:PLC:H31	3:A:1002:PLC:H1A1	1.80	0.40
1:C:380:TRP:CB	1:C:753:PRO:HA	2.51	0.40
1:C:417:HIS:HB2	1:C:690:ARG:HB3	2.03	0.40
1:B:380:TRP:CB	1:B:753:PRO:HA	2.51	0.40
3:B:803:PLC:H31	3:B:803:PLC:H1A1	1.80	0.40
1:D:526:PHE:CE1	1:D:561:ASN:HB3	2.56	0.40
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.92	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	618/639 (97%)	545 (88%)	72 (12%)	1 (0%)	43	71
1	B	618/639 (97%)	545 (88%)	72 (12%)	1 (0%)	43	71
1	C	618/639 (97%)	545 (88%)	72 (12%)	1 (0%)	43	71
1	D	618/639 (97%)	545 (88%)	72 (12%)	1 (0%)	43	71
All	All	2472/2556 (97%)	2180 (88%)	288 (12%)	4 (0%)	44	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	PRO
1	B	181	PRO
1	C	181	PRO
1	D	181	PRO

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	554/570 (97%)	554 (100%)	0	100	100
1	B	554/570 (97%)	554 (100%)	0	100	100
1	C	554/570 (97%)	554 (100%)	0	100	100
1	D	554/570 (97%)	554 (100%)	0	100	100
All	All	2216/2280 (97%)	2216 (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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	216	GLN
1	A	244	HIS
1	A	297	ASN
1	A	346	GLN
1	A	671	ASN
1	A	683	ASN
1	B	197	ASN
1	B	216	GLN
1	B	244	HIS
1	B	297	ASN
1	B	346	GLN
1	B	671	ASN
1	B	683	ASN
1	C	197	ASN
1	C	216	GLN
1	C	244	HIS
1	C	297	ASN
1	C	346	GLN
1	C	671	ASN
1	C	683	ASN
1	D	197	ASN

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Mol	Chain	Res	Type
1	D	216	GLN
1	D	244	HIS
1	D	297	ASN
1	D	346	GLN
1	D	671	ASN
1	D	683	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	PLC	B	801	-	39,39,41	0.31	0	45,47,49	0.36	0
2	POV	B	806	-	12,12,51	0.11	0	11,11,59	0.10	0
3	PLC	D	805	-	35,35,41	0.41	0	38,40,49	0.62	1 (2%)
3	PLC	B	804	-	35,35,41	0.41	0	38,40,49	0.62	1 (2%)
2	POV	B	802	-	45,45,51	0.32	0	51,53,59	0.36	0
2	POV	C	806	-	12,12,51	0.11	0	11,11,59	0.10	0
3	PLC	A	1003	-	35,35,41	0.41	0	38,40,49	0.62	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	A	1005	-	12,12,51	0.11	0	11,11,59	0.10	0
3	PLC	C	804	-	35,35,41	0.41	0	38,40,49	0.62	1 (2%)
2	POV	D	807	-	12,12,51	0.11	0	11,11,59	0.10	0
2	POV	D	801	-	51,51,51	0.30	0	57,59,59	0.38	0
2	POV	A	1004	-	12,12,51	0.13	0	11,11,59	0.09	0
3	PLC	C	801	-	39,39,41	0.31	0	45,47,49	0.36	0
3	PLC	D	802	-	39,39,41	0.31	0	45,47,49	0.36	0
3	PLC	C	803	-	41,41,41	0.32	0	47,49,49	0.51	0
3	PLC	A	1007	-	39,39,41	0.31	0	45,47,49	0.36	0
2	POV	D	806	-	12,12,51	0.13	0	11,11,59	0.09	0
2	POV	A	1006	-	51,51,51	0.30	0	57,59,59	0.38	0
2	POV	C	807	-	51,51,51	0.30	0	57,59,59	0.38	0
2	POV	D	803	-	45,45,51	0.32	0	51,53,59	0.36	0
3	PLC	D	804	-	41,41,41	0.32	0	47,49,49	0.51	0
2	POV	C	805	-	12,12,51	0.13	0	11,11,59	0.09	0
2	POV	C	802	-	45,45,51	0.32	0	51,53,59	0.36	0
2	POV	B	805	-	12,12,51	0.13	0	11,11,59	0.09	0
2	POV	B	807	-	51,51,51	0.30	0	57,59,59	0.38	0
2	POV	A	1001	-	45,45,51	0.32	0	51,53,59	0.36	0
3	PLC	A	1002	-	41,41,41	0.32	0	47,49,49	0.51	0
3	PLC	B	803	-	41,41,41	0.32	0	47,49,49	0.51	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
3	PLC	B	801	-	-	8/43/43/45	-
2	POV	B	806	-	-	0/10/10/55	-
3	PLC	D	805	-	-	3/37/37/45	-
3	PLC	B	804	-	-	3/37/37/45	-
2	POV	B	802	-	-	5/49/49/55	-
2	POV	C	806	-	-	0/10/10/55	-
3	PLC	A	1003	-	-	3/37/37/45	-
2	POV	A	1005	-	-	0/10/10/55	-
3	PLC	C	804	-	-	3/37/37/45	-
2	POV	D	807	-	-	0/10/10/55	-
2	POV	D	801	-	-	8/55/55/55	-
2	POV	A	1004	-	-	1/10/10/55	-
3	PLC	C	801	-	-	8/43/43/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLC	D	802	-	-	8/43/43/45	-
3	PLC	C	803	-	-	9/45/45/45	-
3	PLC	A	1007	-	-	8/43/43/45	-
2	POV	D	806	-	-	1/10/10/55	-
2	POV	A	1006	-	-	8/55/55/55	-
2	POV	C	807	-	-	8/55/55/55	-
2	POV	D	803	-	-	5/49/49/55	-
3	PLC	D	804	-	-	9/45/45/45	-
2	POV	C	805	-	-	1/10/10/55	-
2	POV	C	802	-	-	5/49/49/55	-
2	POV	B	805	-	-	1/10/10/55	-
2	POV	B	807	-	-	8/55/55/55	-
2	POV	A	1001	-	-	5/49/49/55	-
3	PLC	A	1002	-	-	9/45/45/45	-
3	PLC	B	803	-	-	9/45/45/45	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	PLC	O2P-P-O1P	2.33	119.93	110.83
3	B	804	PLC	O2P-P-O1P	2.33	119.93	110.83
3	C	804	PLC	O2P-P-O1P	2.33	119.93	110.83
3	D	805	PLC	O2P-P-O1P	2.33	119.93	110.83

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	POV	C1-O11-P-O14
2	B	802	POV	C1-O11-P-O14
2	C	802	POV	C1-O11-P-O14
2	D	803	POV	C1-O11-P-O14
3	A	1002	PLC	C1B-CB-O3-C3
3	A	1002	PLC	OB-CB-O3-C3
3	A	1002	PLC	C1-O3P-P-O2P
3	A	1002	PLC	C1-O3P-P-O4P
3	A	1003	PLC	C1'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	1003	PLC	O'-C'-O2-C2
3	A	1007	PLC	C1B-CB-O3-C3
3	A	1007	PLC	OB-CB-O3-C3
3	B	801	PLC	C1B-CB-O3-C3
3	B	801	PLC	OB-CB-O3-C3
3	B	803	PLC	C1B-CB-O3-C3
3	B	803	PLC	OB-CB-O3-C3
3	B	803	PLC	C1-O3P-P-O2P
3	B	803	PLC	C1-O3P-P-O4P
3	B	804	PLC	C1'-C'-O2-C2
3	B	804	PLC	O'-C'-O2-C2
3	C	801	PLC	C1B-CB-O3-C3
3	C	801	PLC	OB-CB-O3-C3
3	C	803	PLC	C1B-CB-O3-C3
3	C	803	PLC	OB-CB-O3-C3
3	C	803	PLC	C1-O3P-P-O2P
3	C	803	PLC	C1-O3P-P-O4P
3	C	804	PLC	C1'-C'-O2-C2
3	C	804	PLC	O'-C'-O2-C2
3	D	802	PLC	C1B-CB-O3-C3
3	D	802	PLC	OB-CB-O3-C3
3	D	804	PLC	C1B-CB-O3-C3
3	D	804	PLC	OB-CB-O3-C3
3	D	804	PLC	C1-O3P-P-O2P
3	D	804	PLC	C1-O3P-P-O4P
3	D	805	PLC	C1'-C'-O2-C2
3	D	805	PLC	O'-C'-O2-C2
3	A	1007	PLC	C3B-C4B-C5B-C6B
3	B	801	PLC	C3B-C4B-C5B-C6B
3	C	801	PLC	C3B-C4B-C5B-C6B
3	D	802	PLC	C3B-C4B-C5B-C6B
2	A	1006	POV	C36-C37-C38-C39
2	B	807	POV	C36-C37-C38-C39
2	C	807	POV	C36-C37-C38-C39
2	D	801	POV	C36-C37-C38-C39
3	A	1002	PLC	O3P-C1-C2-O2
3	B	803	PLC	O3P-C1-C2-O2
3	C	803	PLC	O3P-C1-C2-O2
3	D	804	PLC	O3P-C1-C2-O2
3	A	1002	PLC	O4P-C4-C5-N
3	B	803	PLC	O4P-C4-C5-N
3	C	803	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
3	D	804	PLC	O4P-C4-C5-N
2	A	1006	POV	C23-C24-C25-C26
2	B	807	POV	C23-C24-C25-C26
2	C	807	POV	C23-C24-C25-C26
2	D	801	POV	C23-C24-C25-C26
2	A	1001	POV	O11-C1-C2-C3
2	B	802	POV	O11-C1-C2-C3
2	C	802	POV	O11-C1-C2-C3
2	D	803	POV	O11-C1-C2-C3
3	A	1007	PLC	C4B-C5B-C6B-C7B
3	B	801	PLC	C4B-C5B-C6B-C7B
3	C	801	PLC	C4B-C5B-C6B-C7B
3	D	802	PLC	C4B-C5B-C6B-C7B
2	A	1006	POV	C29-C210-C211-C212
2	B	807	POV	C29-C210-C211-C212
2	C	807	POV	C29-C210-C211-C212
2	D	801	POV	C29-C210-C211-C212
2	A	1001	POV	C11-O12-P-O14
2	A	1006	POV	C1-O11-P-O14
2	A	1006	POV	C11-O12-P-O14
2	B	802	POV	C11-O12-P-O14
2	B	807	POV	C1-O11-P-O14
2	B	807	POV	C11-O12-P-O14
2	C	802	POV	C11-O12-P-O14
2	C	807	POV	C1-O11-P-O14
2	C	807	POV	C11-O12-P-O14
2	D	801	POV	C1-O11-P-O14
2	D	801	POV	C11-O12-P-O14
2	D	803	POV	C11-O12-P-O14
3	A	1002	PLC	C1-C2-O2-C'
3	B	803	PLC	C1-C2-O2-C'
3	C	803	PLC	C1-C2-O2-C'
3	D	804	PLC	C1-C2-O2-C'
3	A	1002	PLC	O3P-C1-C2-C3
3	B	803	PLC	O3P-C1-C2-C3
3	C	803	PLC	O3P-C1-C2-C3
3	D	804	PLC	O3P-C1-C2-C3
2	A	1006	POV	C26-C27-C28-C29
2	B	807	POV	C26-C27-C28-C29
2	C	807	POV	C26-C27-C28-C29
2	D	801	POV	C26-C27-C28-C29
3	A	1007	PLC	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
3	B	801	PLC	C1B-C2B-C3B-C4B
3	C	801	PLC	C1B-C2B-C3B-C4B
3	D	802	PLC	C1B-C2B-C3B-C4B
2	A	1001	POV	O11-C1-C2-O21
2	B	802	POV	O11-C1-C2-O21
2	C	802	POV	O11-C1-C2-O21
2	D	803	POV	O11-C1-C2-O21
3	A	1002	PLC	C6B-C7B-C8B-C9B
3	B	803	PLC	C6B-C7B-C8B-C9B
3	C	803	PLC	C6B-C7B-C8B-C9B
3	D	804	PLC	C6B-C7B-C8B-C9B
2	A	1004	POV	C37-C38-C39-C310
2	B	805	POV	C37-C38-C39-C310
2	C	805	POV	C37-C38-C39-C310
2	D	806	POV	C37-C38-C39-C310
3	A	1007	PLC	C1-C2-O2-C'
3	B	801	PLC	C1-C2-O2-C'
3	C	801	PLC	C1-C2-O2-C'
3	D	802	PLC	C1-C2-O2-C'
3	A	1003	PLC	O2-C2-C3-O3
3	B	804	PLC	O2-C2-C3-O3
3	C	804	PLC	O2-C2-C3-O3
3	D	805	PLC	O2-C2-C3-O3
2	A	1001	POV	C33-C34-C35-C36
2	A	1006	POV	C34-C35-C36-C37
2	B	802	POV	C33-C34-C35-C36
2	B	807	POV	C34-C35-C36-C37
2	C	802	POV	C33-C34-C35-C36
2	C	807	POV	C34-C35-C36-C37
2	D	801	POV	C34-C35-C36-C37
2	D	803	POV	C33-C34-C35-C36
3	A	1007	PLC	C4-C5-N-C7
3	B	801	PLC	C4-C5-N-C7
3	C	801	PLC	C4-C5-N-C7
3	D	802	PLC	C4-C5-N-C7
3	A	1007	PLC	C2B-C1B-CB-O3
3	B	801	PLC	C2B-C1B-CB-O3
3	C	801	PLC	C2B-C1B-CB-O3
3	D	802	PLC	C2B-C1B-CB-O3
2	A	1006	POV	C32-C33-C34-C35
2	B	807	POV	C32-C33-C34-C35
2	C	807	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	D	801	POV	C32-C33-C34-C35

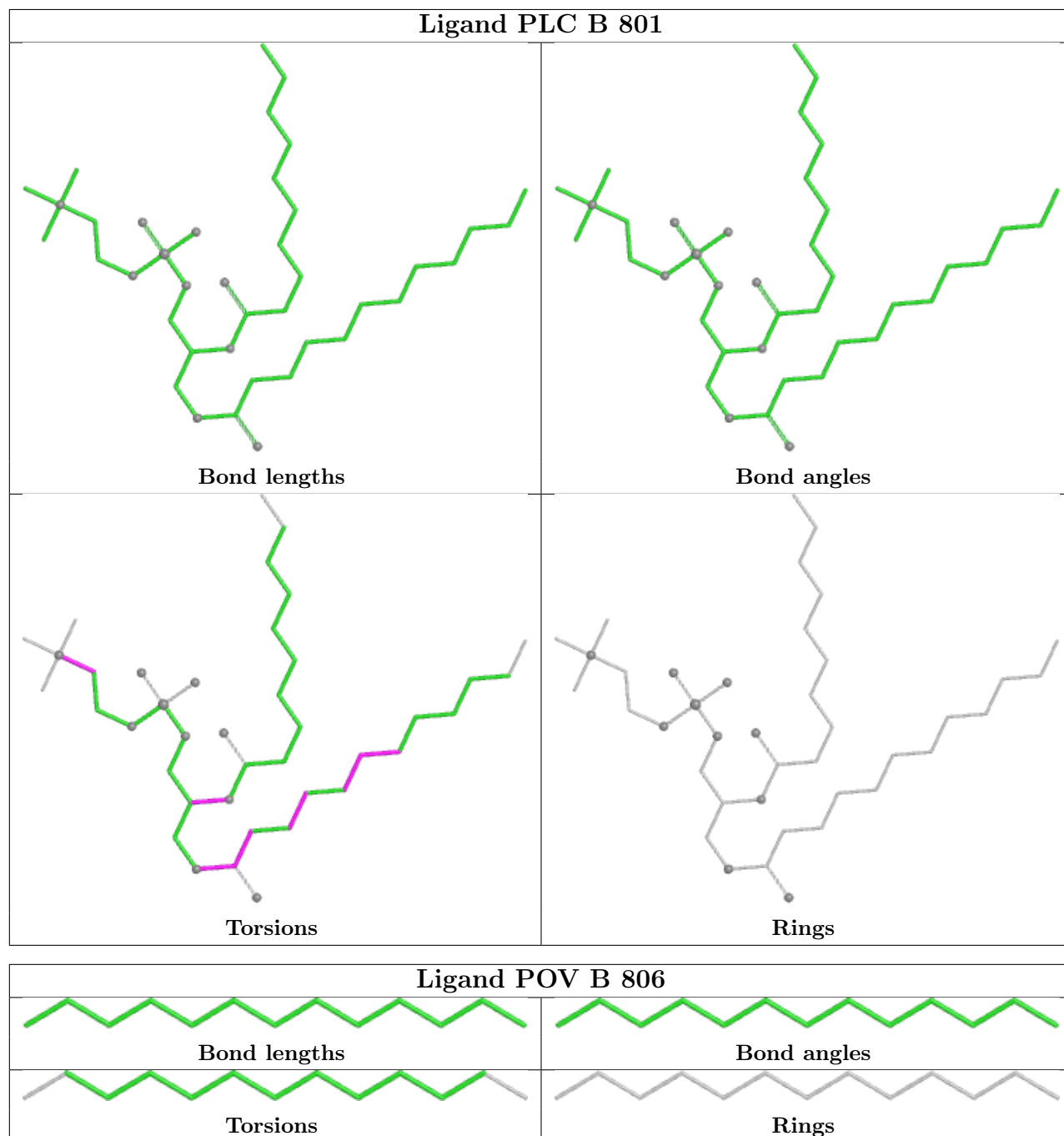
There are no ring outliers.

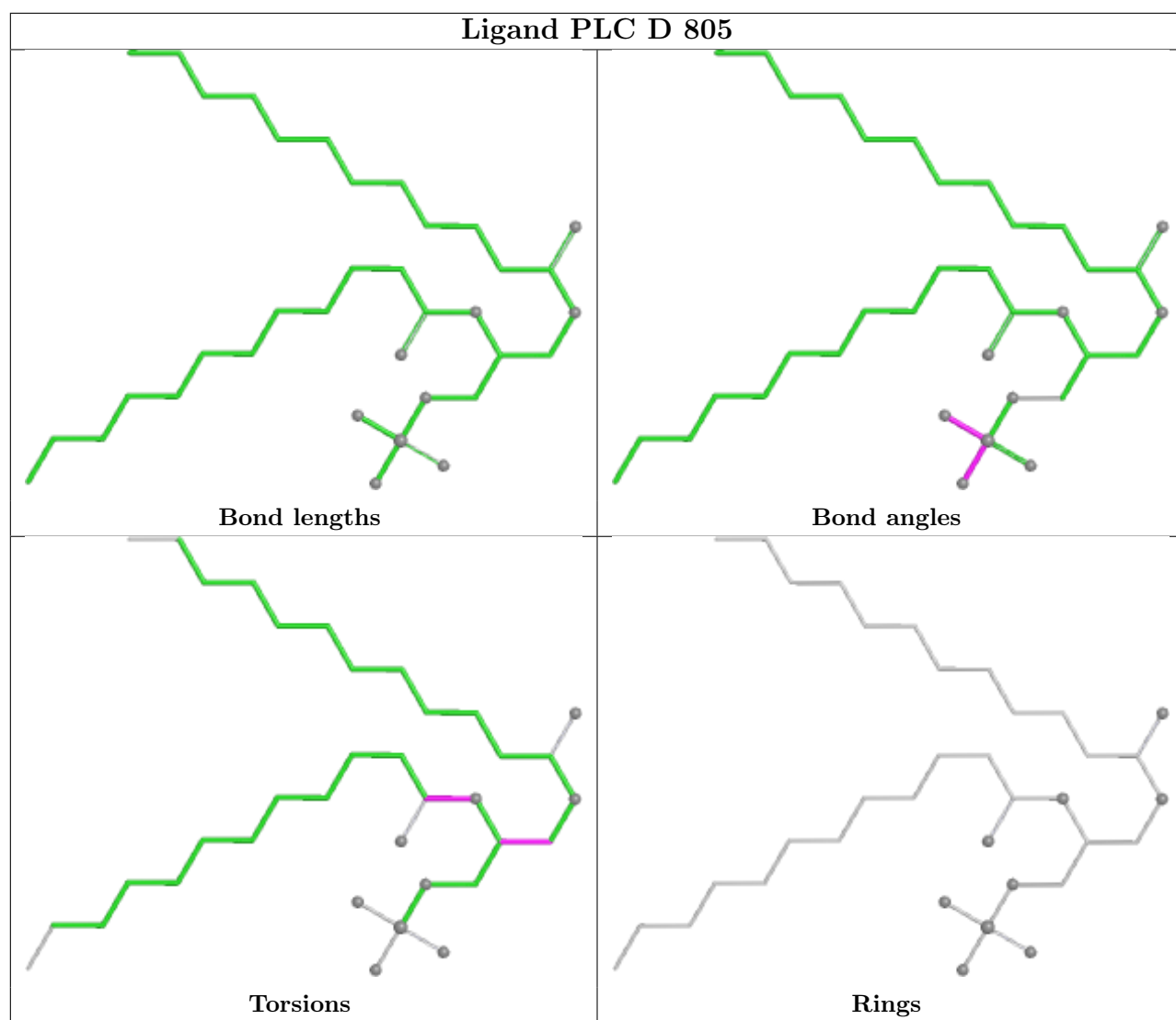
28 monomers are involved in 50 short contacts:

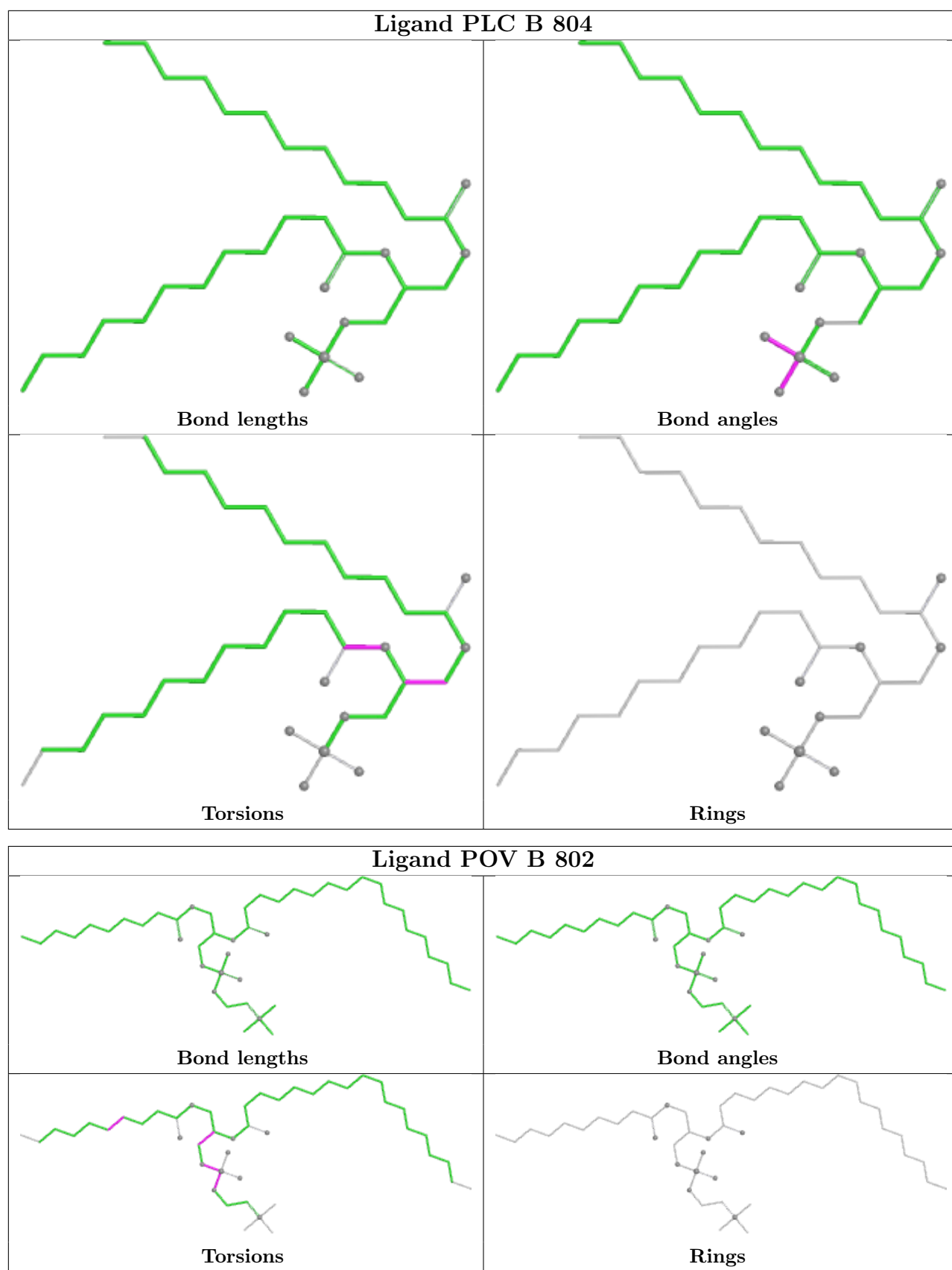
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	PLC	1	0
2	B	806	POV	1	0
3	D	805	PLC	2	0
3	B	804	PLC	2	0
2	B	802	POV	1	0
2	C	806	POV	1	0
3	A	1003	PLC	3	0
2	A	1005	POV	1	0
3	C	804	PLC	3	0
2	D	807	POV	1	0
2	D	801	POV	2	0
2	A	1004	POV	1	0
3	C	801	PLC	1	0
3	D	802	PLC	1	0
3	C	803	PLC	4	0
3	A	1007	PLC	1	0
2	D	806	POV	2	0
2	A	1006	POV	2	0
2	C	807	POV	2	0
2	D	803	POV	1	0
3	D	804	PLC	4	0
2	C	805	POV	1	0
2	C	802	POV	1	0
2	B	805	POV	2	0
2	B	807	POV	2	0
2	A	1001	POV	1	0
3	A	1002	PLC	5	0
3	B	803	PLC	5	0

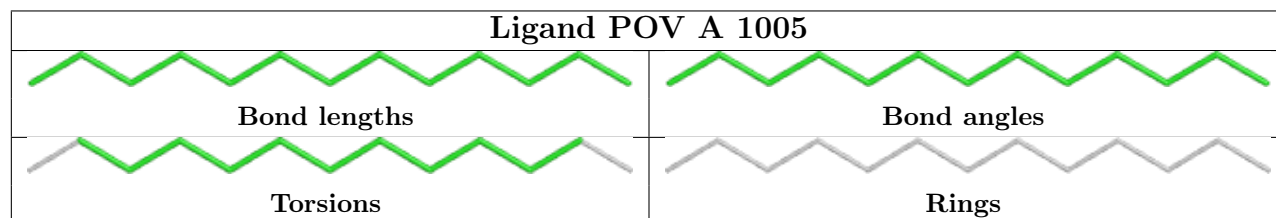
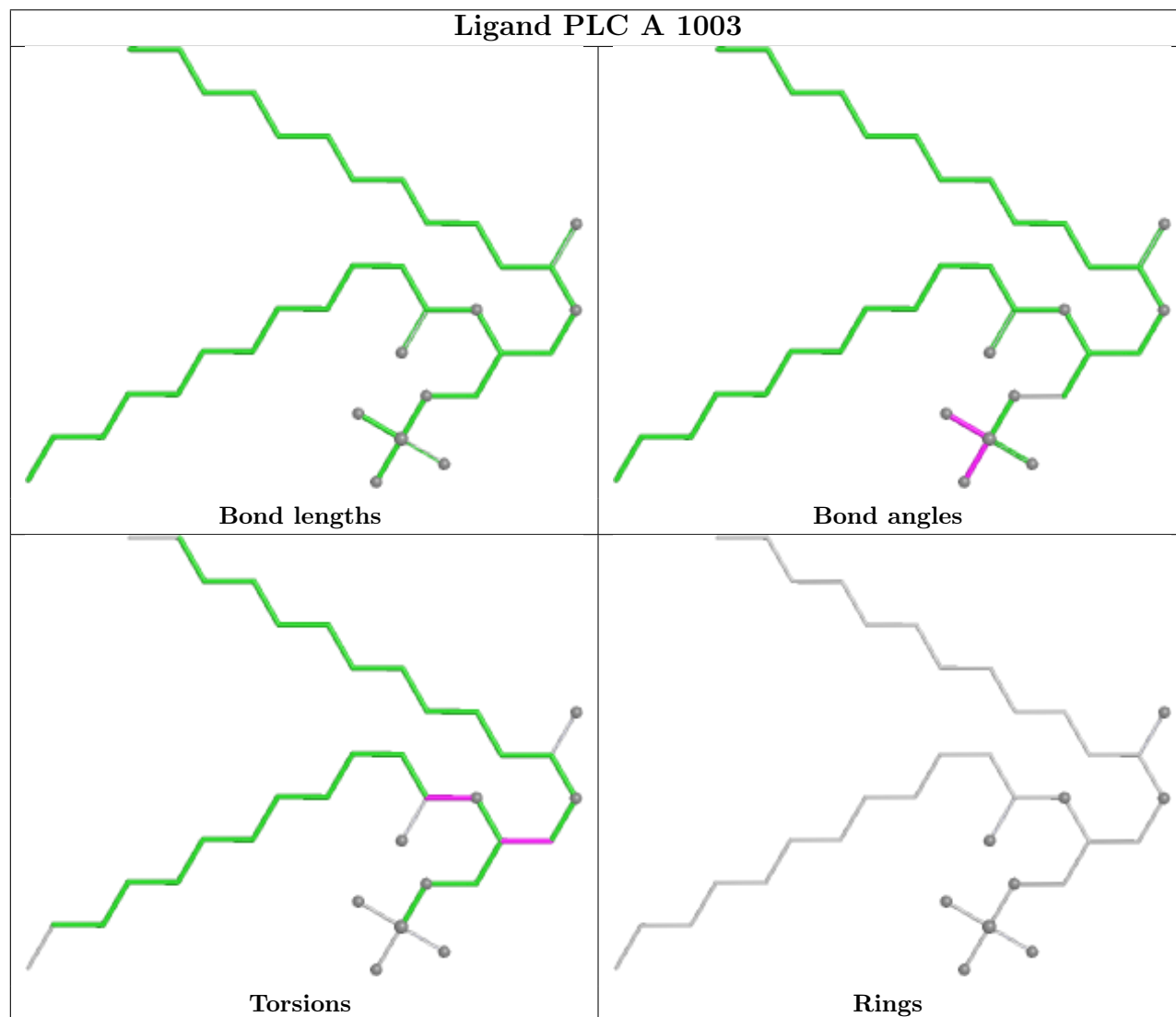
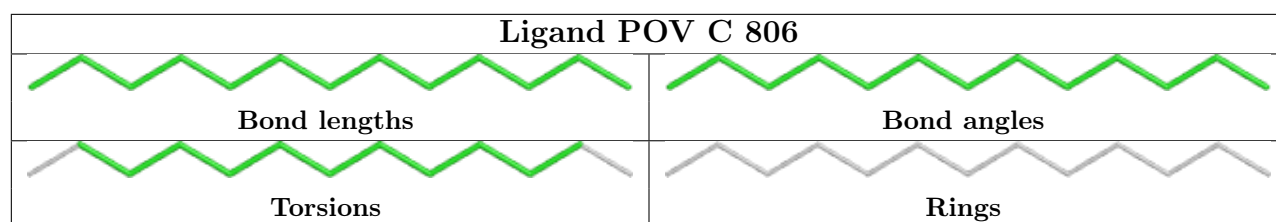
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

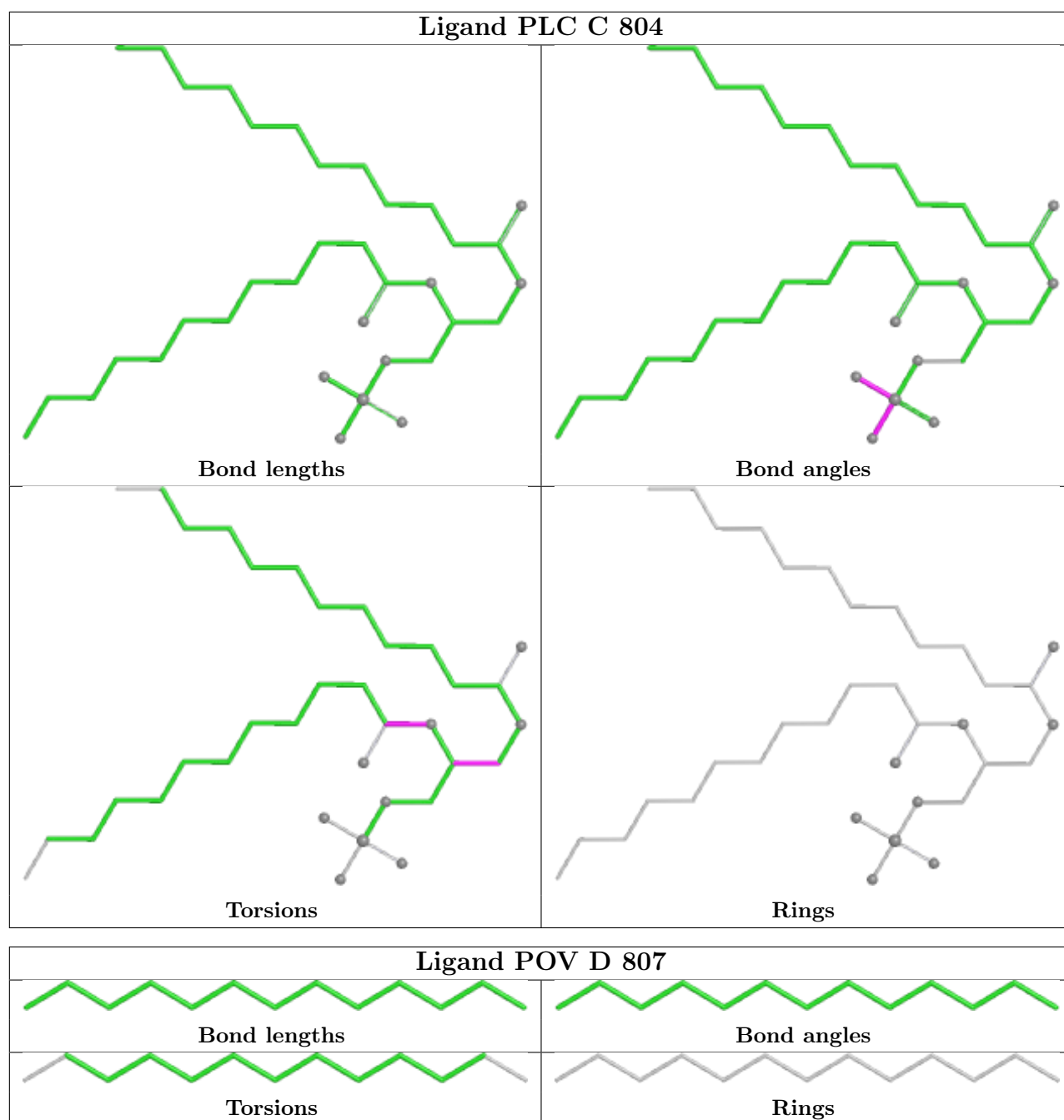
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

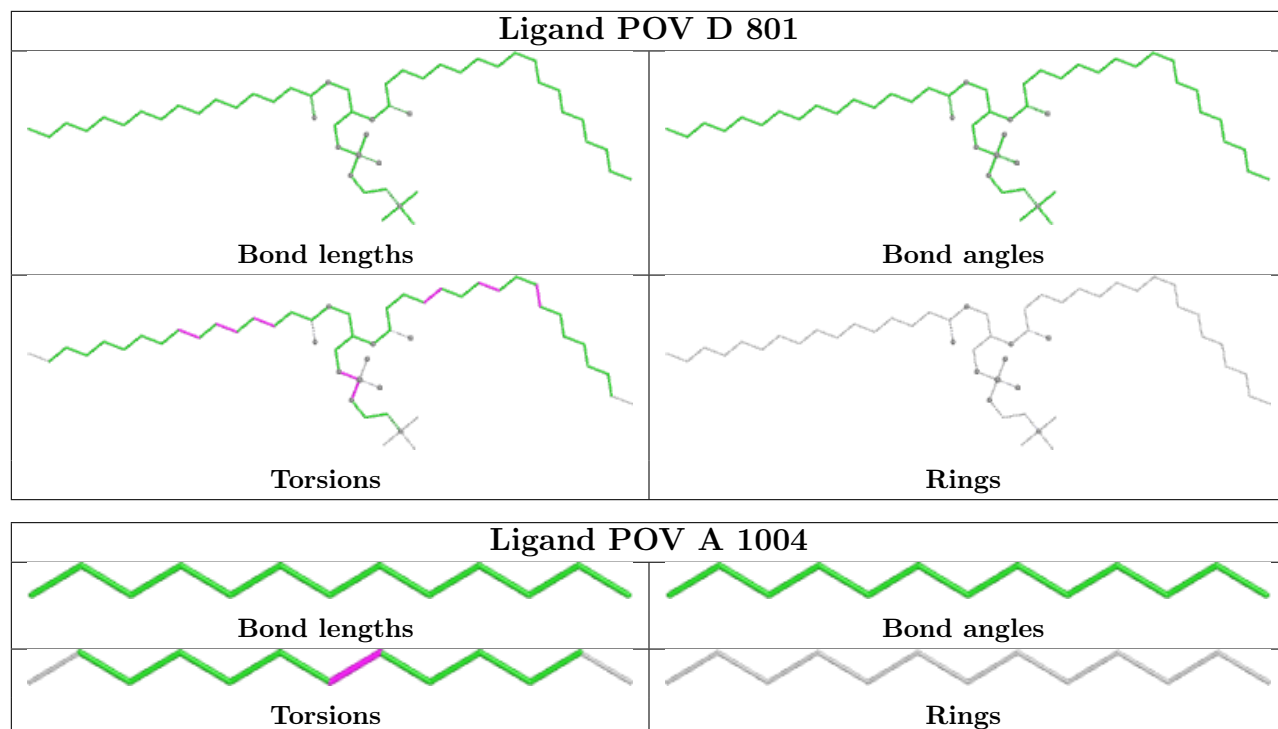


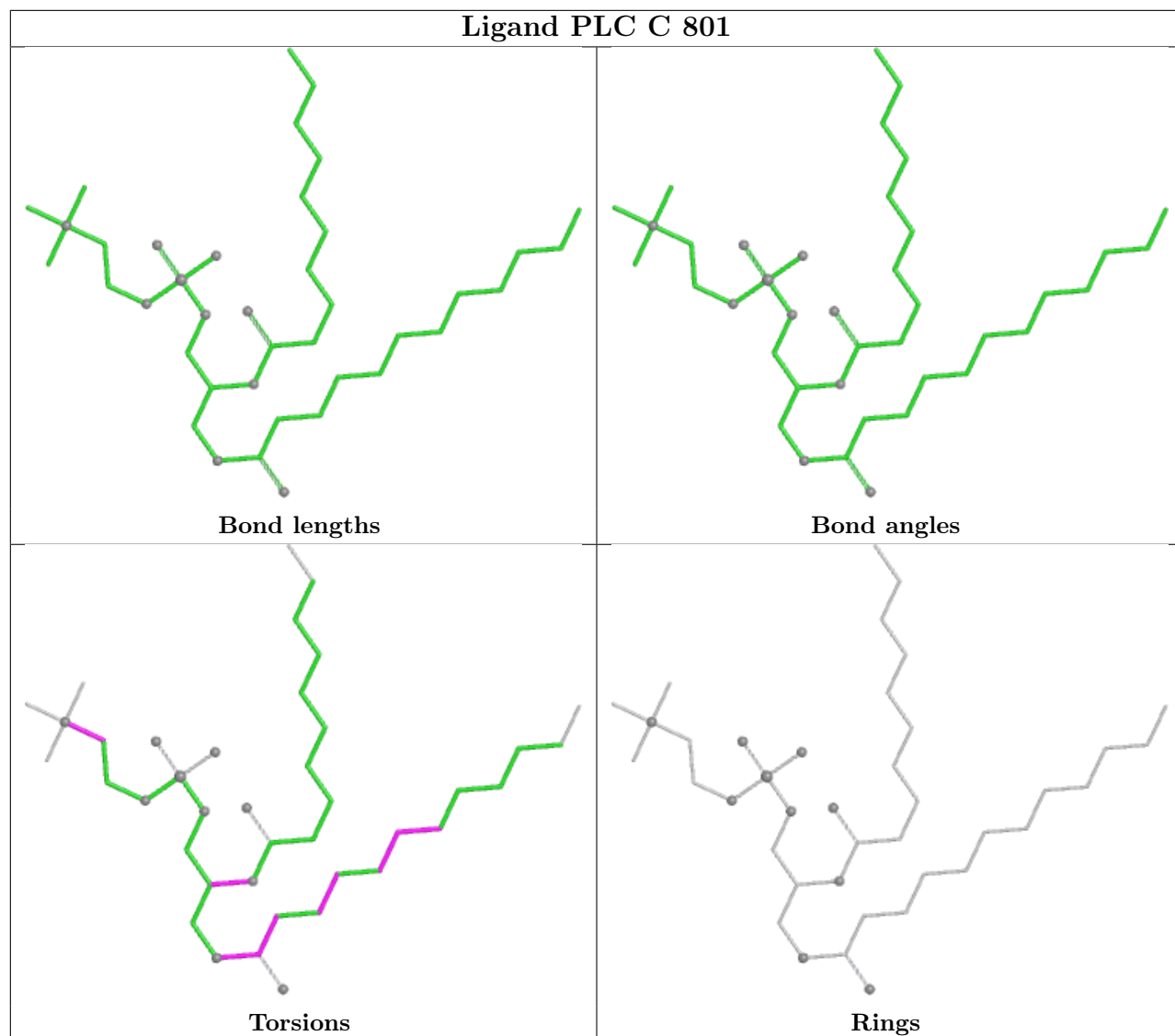


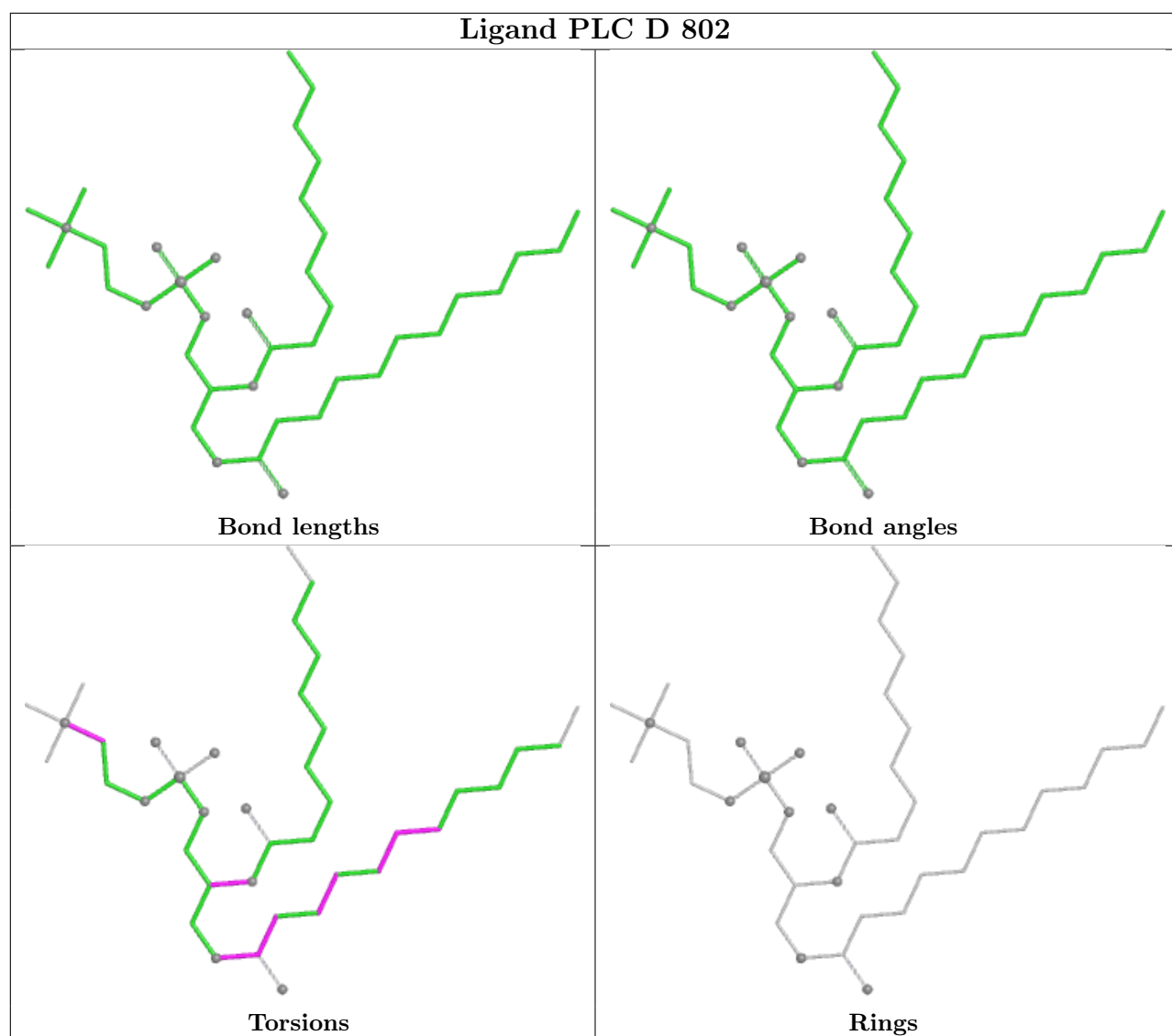


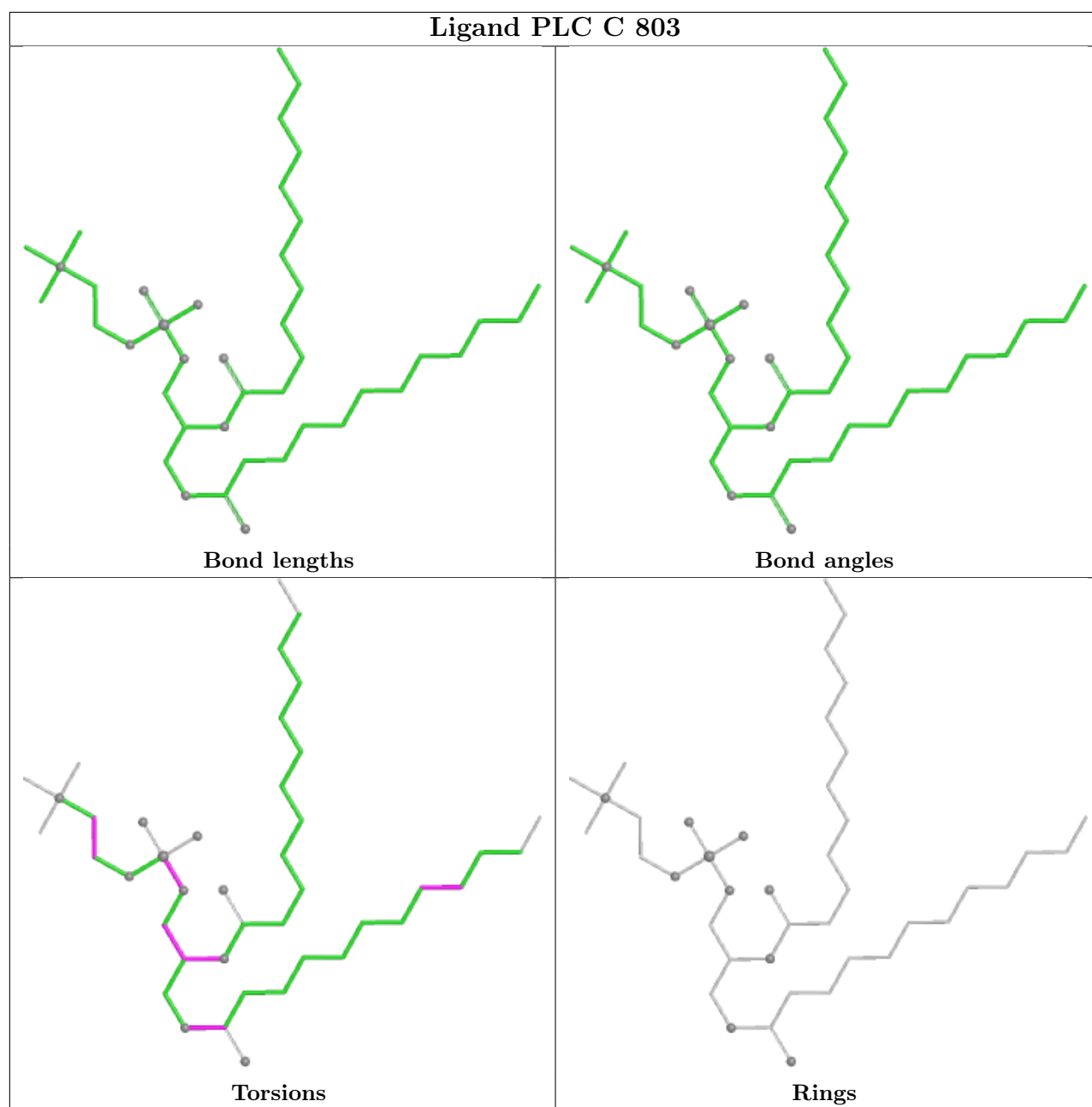


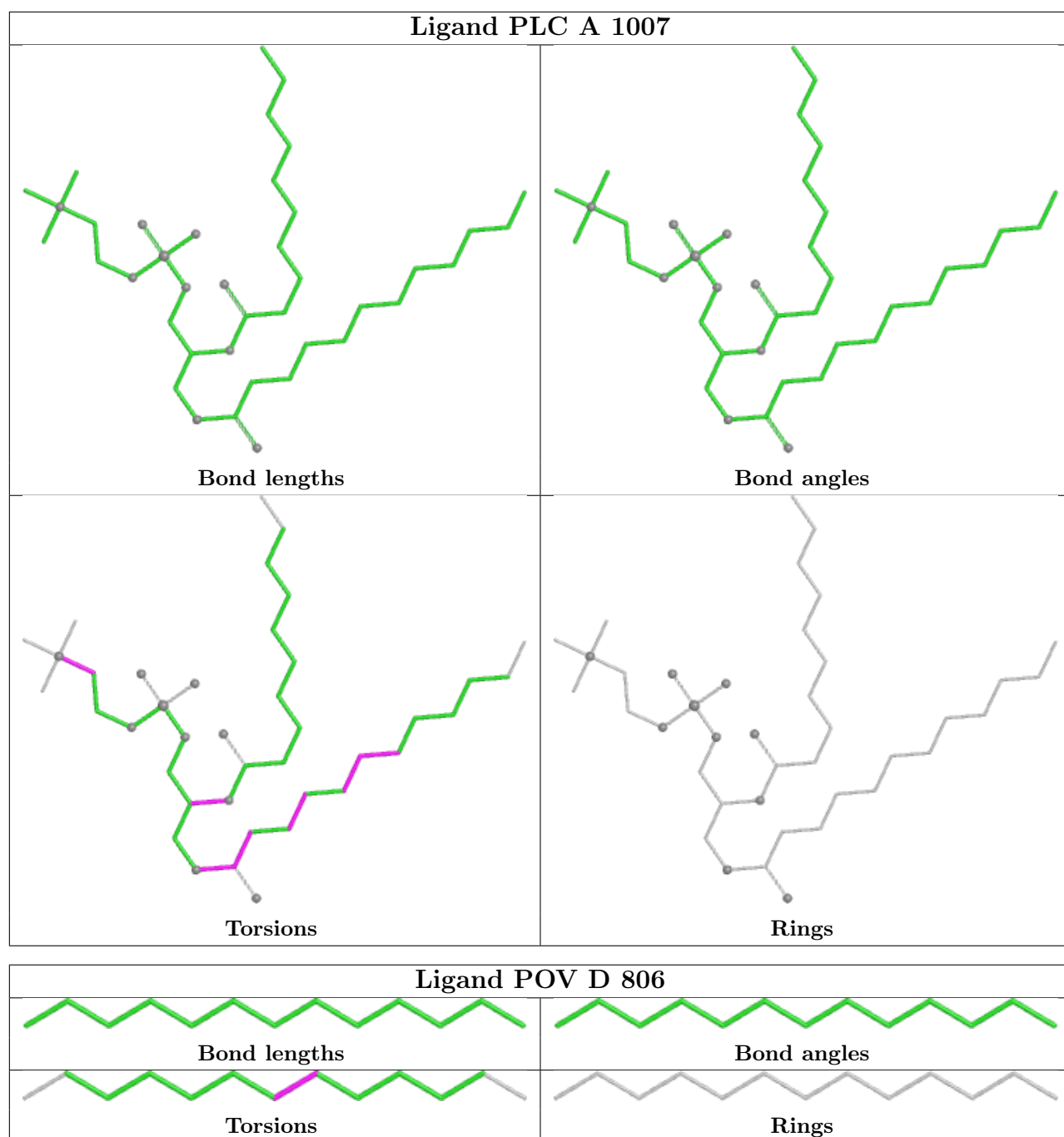


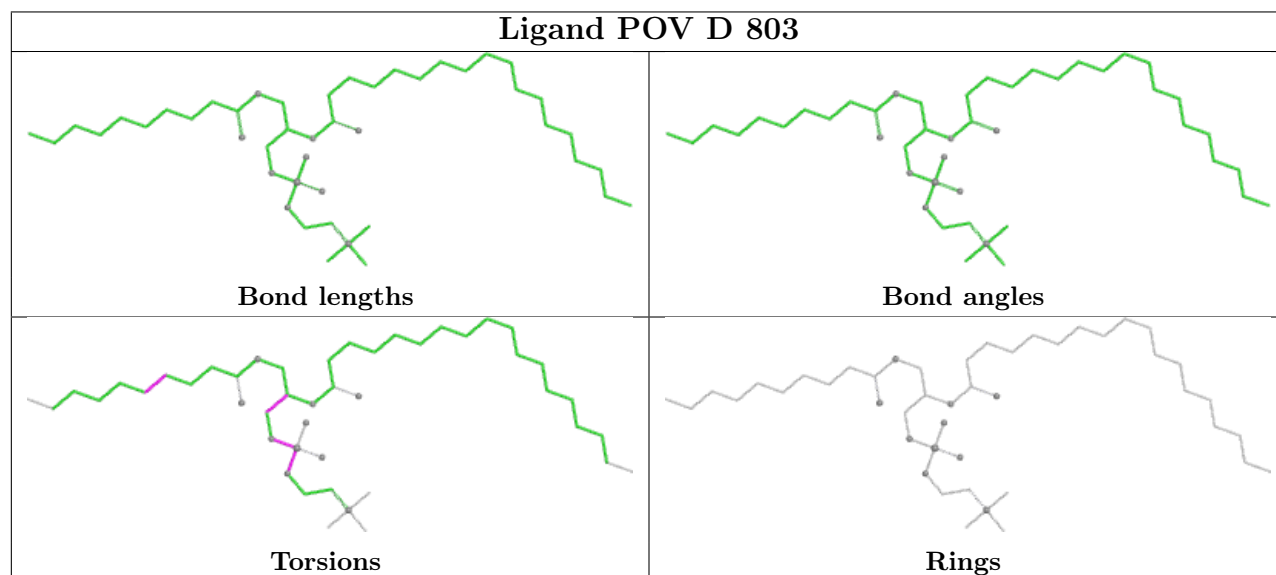
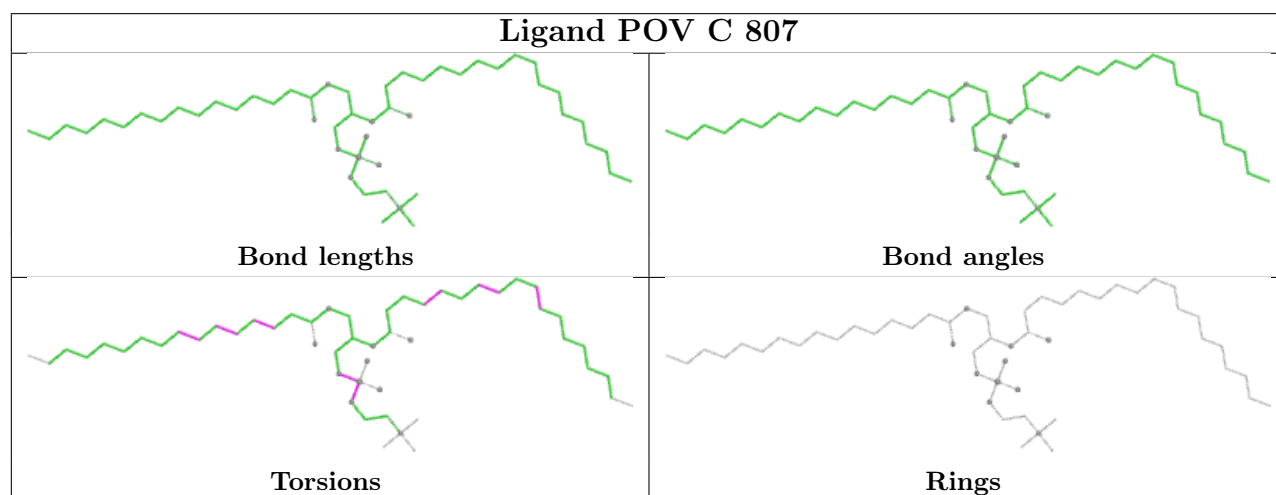
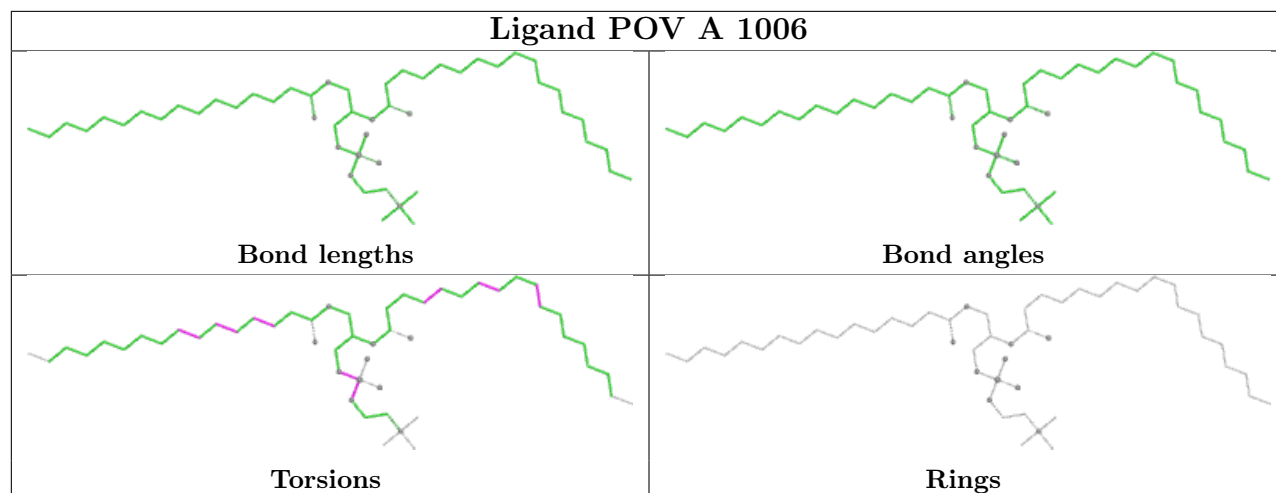


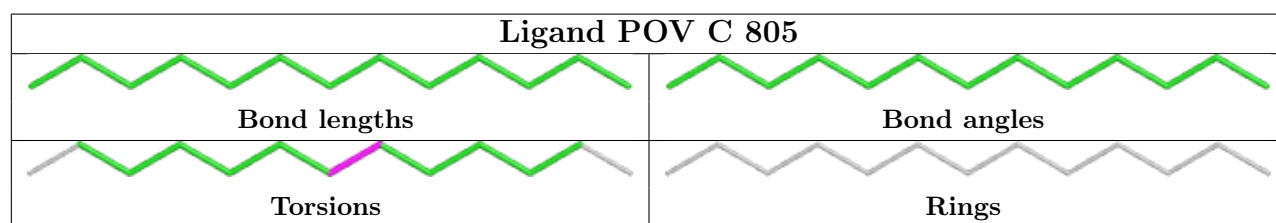
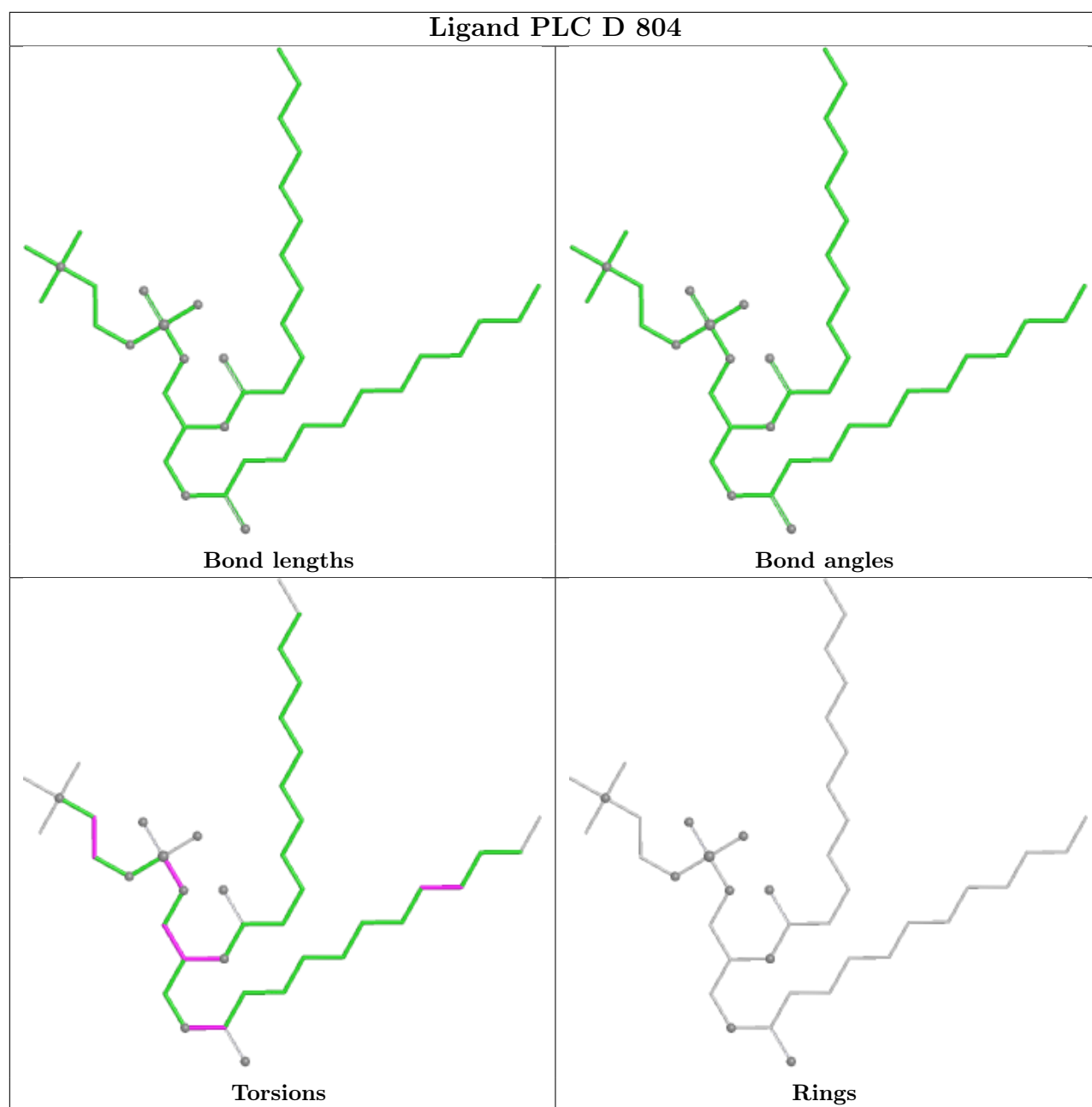


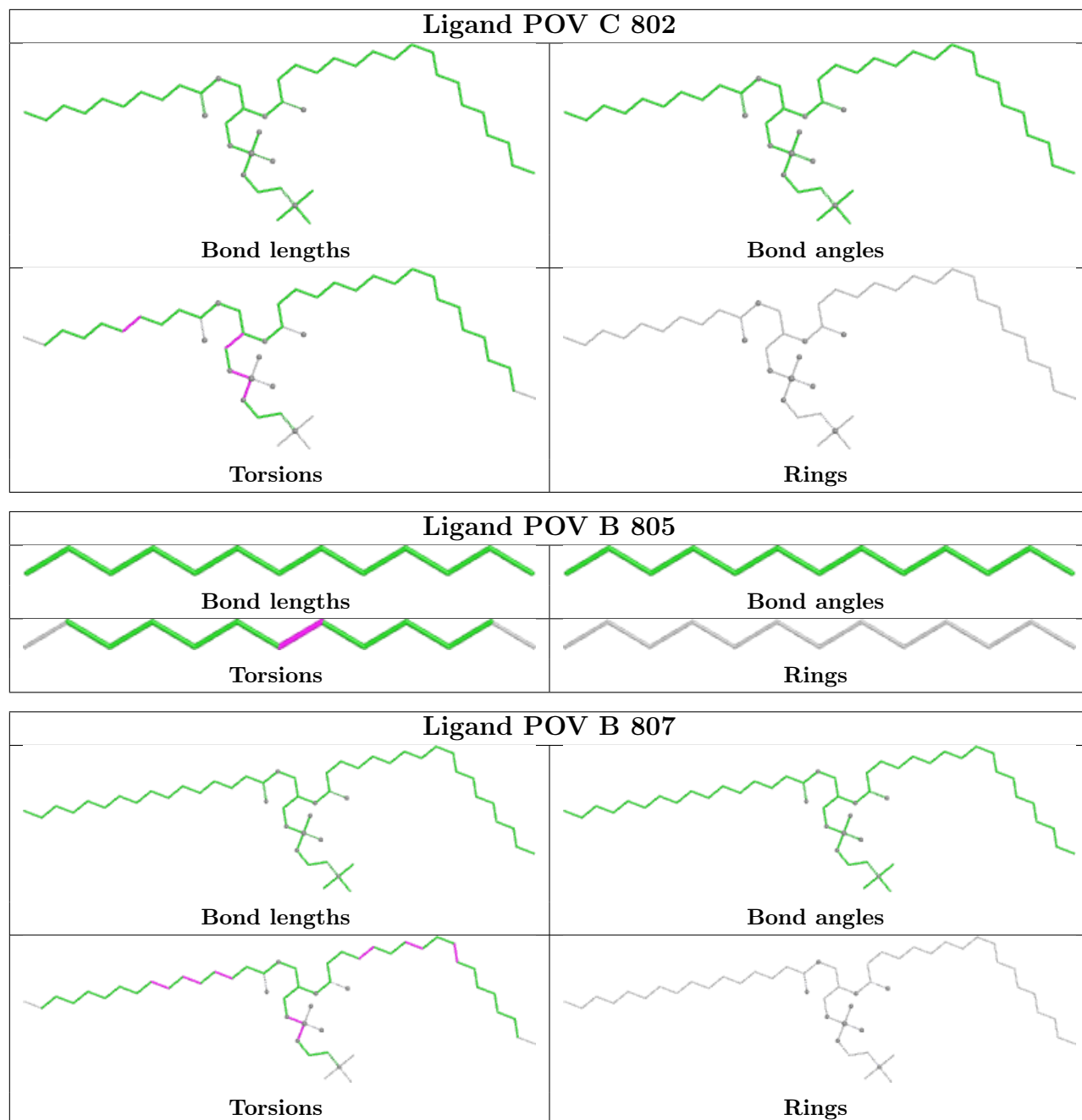


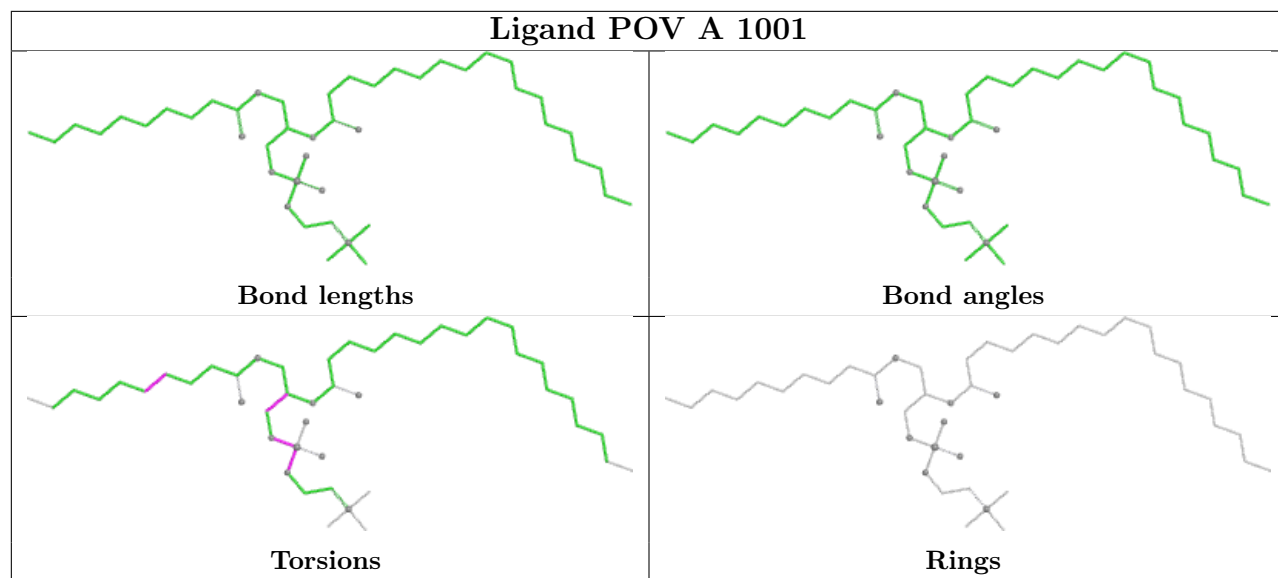


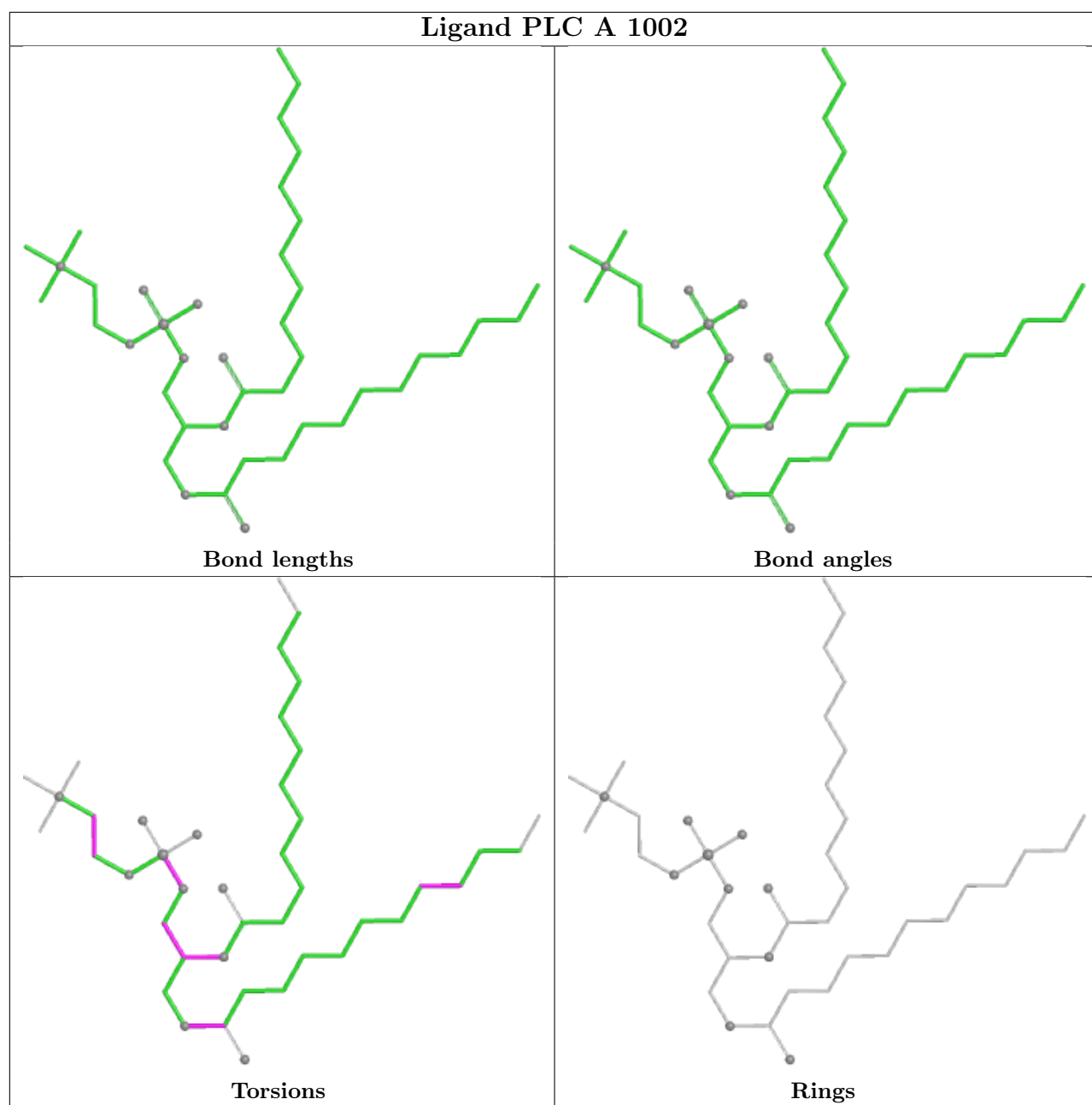


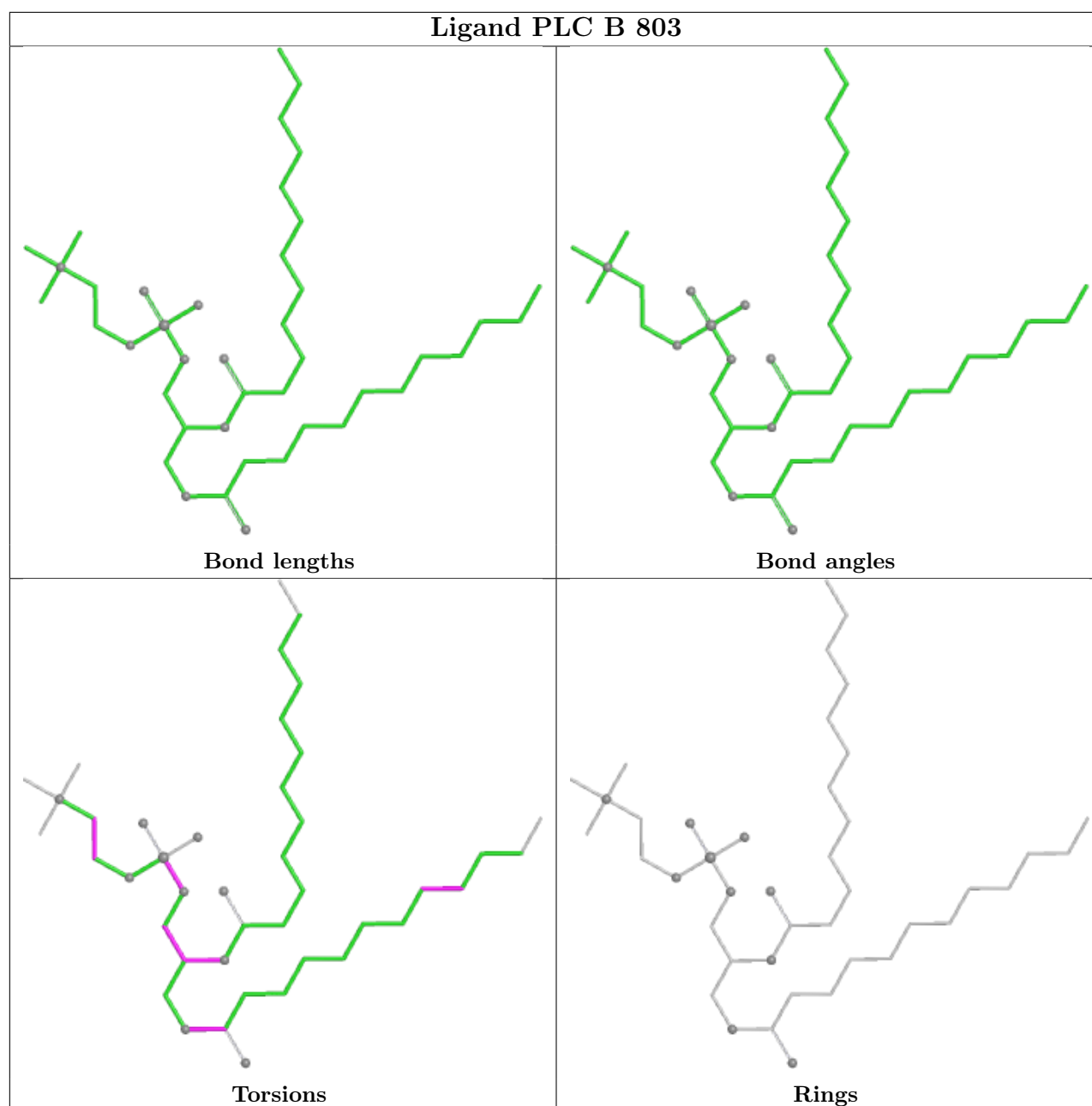












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0882. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.