



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:26 PM UTC

PDB ID : 8I48 / pdb_00008i48
EMDB ID : EMD-35164
Title : Cryo-EM structure of nanodisc (PE:PS:PC) reconstituted GLIC at pH 4 in closed state
Authors : Bharambe, N.; Li, Z.; Basak, S.
Deposited on : 2023-01-18
Resolution : 2.74 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

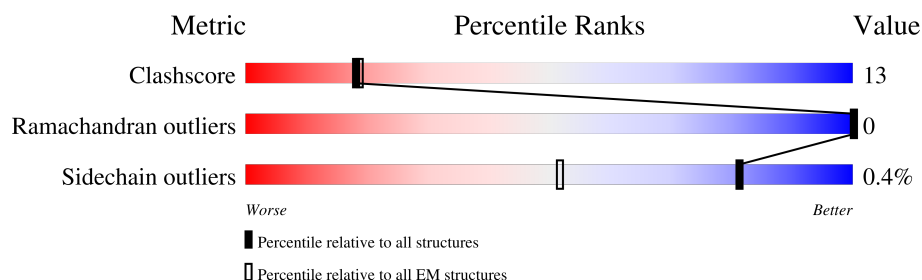
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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	312	74%	26%
1	B	312	75%	25%
1	C	312	75%	25%
1	D	312	74%	26%
1	E	312	74%	26%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14270 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.

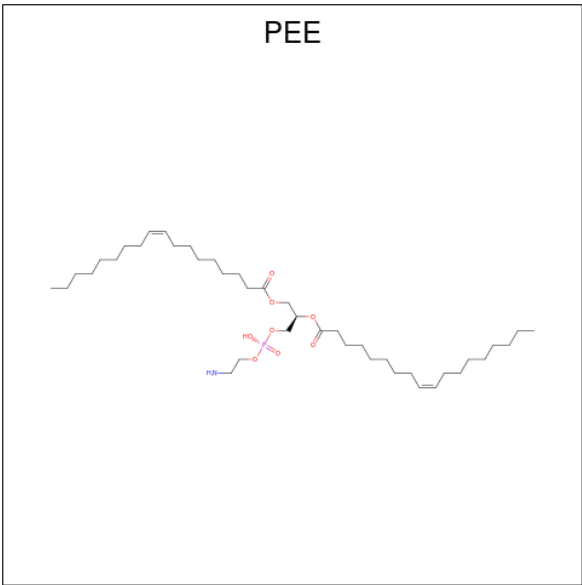
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	312	Total	C	N	O	S	1	0
			2540	1672	409	455	4		
1	C	312	Total	C	N	O	S	1	0
			2540	1672	409	455	4		
1	D	312	Total	C	N	O	S	1	0
			2540	1672	409	455	4		
1	B	312	Total	C	N	O	S	1	0
			2540	1672	409	455	4		
1	E	312	Total	C	N	O	S	1	0
			2540	1672	409	455	4		

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Cl	0
			1	1	
2	C	1	Total	Cl	0
			1	1	
2	D	1	Total	Cl	0
			1	1	
2	B	1	Total	Cl	0
			1	1	
2	E	1	Total	Cl	0
			1	1	

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	O	P		0
			32	23	8	1		
3	A	1	Total	C	O	P		0
			26	17	8	1		
3	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	A	1	Total	C	O	P		0
			26	17	8	1		
3	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
3	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	C	1	Total	C	O	P		0
			32	23	8	1		
3	C	1	Total	C	O	P		0
			26	17	8	1		
3	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	C	1	Total	C	O	P		0
			26	17	8	1		
3	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	C	1	Total	C	N	O	P	0
			34	24	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	C	1	Total	C	N	O	P	0
			42	32	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
			32	23	8	1		
3	D	1	Total	C	O	P		0
			26	17	8	1		
3	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	D	1	Total	C	O	P		0
			26	17	8	1		
3	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	D	1	Total	C	N	O	P	0
			34	24	1	8	1	
3	D	1	Total	C	N	O	P	0
			38	28	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
			32	23	8	1		
3	B	1	Total	C	O	P		0
			26	17	8	1		
3	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	B	1	Total	C	O	P		0
			26	17	8	1		
3	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	B	1	Total	C	N	O	P	0
			34	24	1	8	1	
3	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	E	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	E	1	Total	C	O	P		0
			32	23	8	1		
3	E	1	Total	C	O	P		0
			26	17	8	1		

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Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	E	1	Total	C	O	P		0
			26	17	8	1		
3	E	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	E	1	Total	C	N	O	P	0
			34	24	1	8	1	
3	E	1	Total	C	N	O	P	0
			38	28	1	8	1	

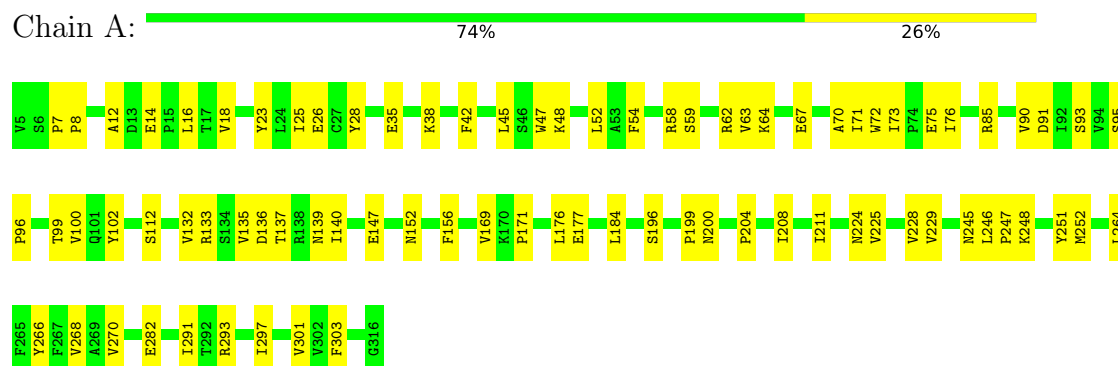
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	32	Total	O	0
			32	32	
4	C	32	Total	O	0
			32	32	
4	D	32	Total	O	0
			32	32	
4	B	32	Total	O	0
			32	32	
4	E	32	Total	O	0
			32	32	

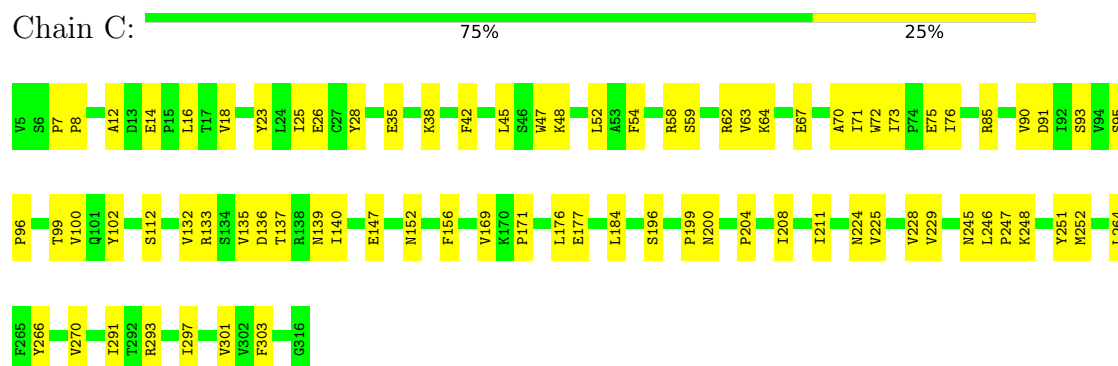
3 Residue-property plots

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.

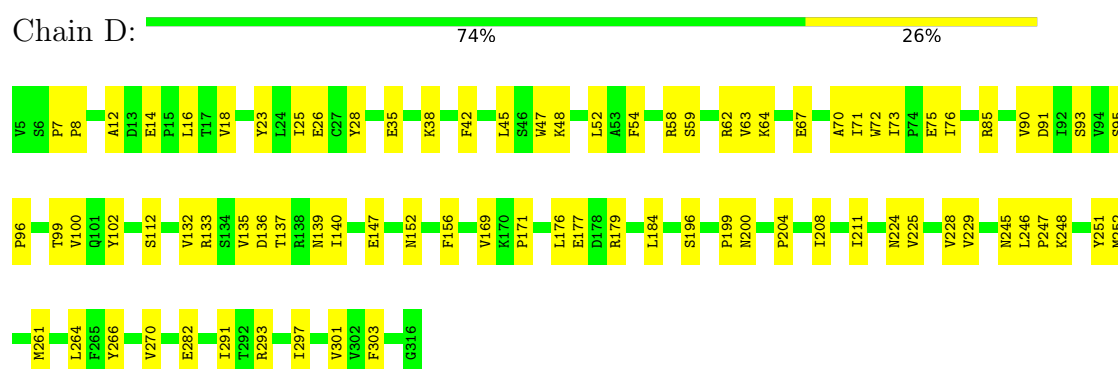
- Molecule 1: Proton-gated ion channel



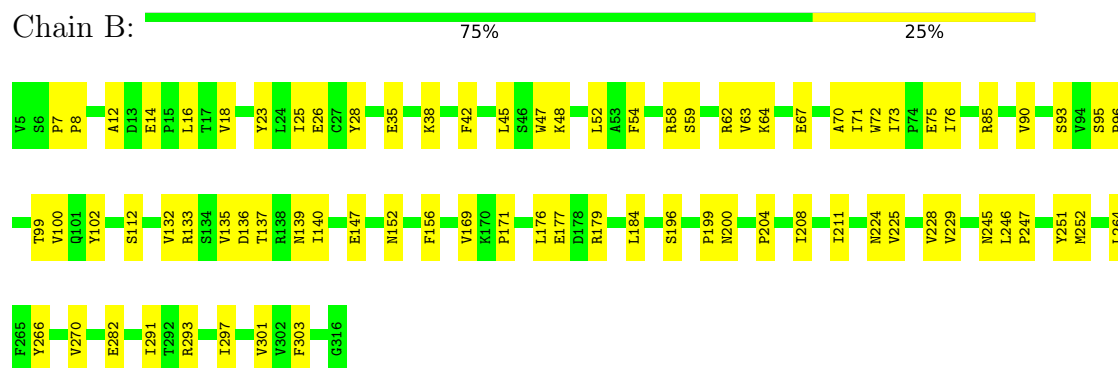
- Molecule 1: Proton-gated ion channel



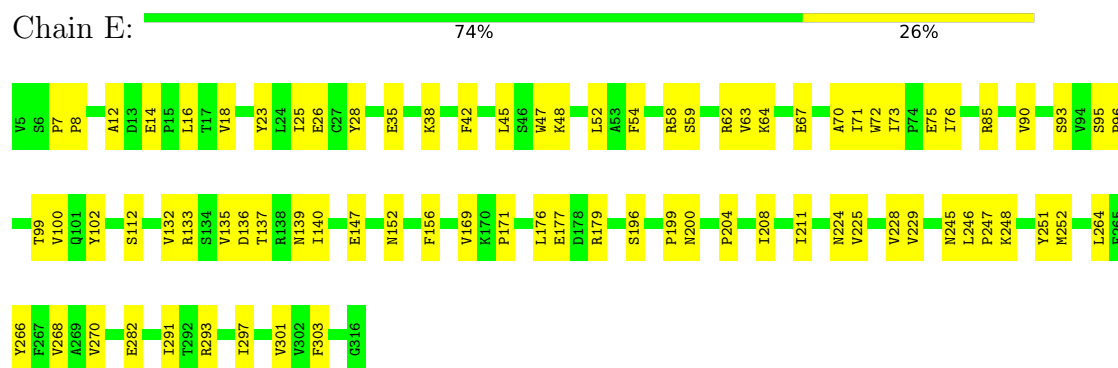
- Molecule 1: Proton-gated ion channel



● Molecule 1: Proton-gated ion channel



● Molecule 1: Proton-gated ion channel



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	254591	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 ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: CL, PEE

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	0.22	0/2608	0.50	0/3564
1	B	0.22	0/2608	0.50	0/3564
1	C	0.22	0/2608	0.50	0/3564
1	D	0.22	0/2608	0.50	0/3564
1	E	0.22	0/2608	0.50	0/3564
All	All	0.22	0/13040	0.50	0/17820

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	2540	0	2560	76	0
1	B	2540	0	2560	77	0
1	C	2540	0	2560	75	0
1	D	2540	0	2560	77	0
1	E	2540	0	2560	77	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
2	C	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	1	0
2	E	1	0	0	1	0
3	A	281	0	351	9	0
3	B	281	0	351	9	0
3	C	281	0	351	10	0
3	D	281	0	351	13	0
3	E	281	0	351	11	0
4	A	32	0	0	0	0
4	B	32	0	0	0	0
4	C	32	0	0	0	0
4	D	32	0	0	0	0
4	E	32	0	0	0	0
All	All	14270	0	14555	378	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 13.

All (378) 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:B:252:MET:HA	3:B:409:PEE:H11	1.55	0.89
1:C:252:MET:HA	3:C:408:PEE:H11	1.55	0.88
1:A:252:MET:HA	3:A:408:PEE:H11	1.55	0.88
1:E:252:MET:HA	3:E:409:PEE:H11	1.55	0.87
1:D:252:MET:HA	3:D:409:PEE:H11	1.55	0.86
1:A:67:GLU:HB3	1:A:70:ALA:HB3	1.59	0.84
1:B:67:GLU:HB3	1:B:70:ALA:HB3	1.59	0.84
1:C:16:LEU:HD11	1:C:47:TRP:HB2	1.60	0.83
1:D:67:GLU:HB3	1:D:70:ALA:HB3	1.59	0.82
1:A:16:LEU:HD11	1:A:47:TRP:HB2	1.60	0.82
1:C:67:GLU:HB3	1:C:70:ALA:HB3	1.59	0.82
1:E:16:LEU:HD11	1:E:47:TRP:HB2	1.60	0.81
1:D:16:LEU:HD11	1:D:47:TRP:HB2	1.60	0.81
1:B:16:LEU:HD11	1:B:47:TRP:HB2	1.60	0.81
1:E:67:GLU:HB3	1:E:70:ALA:HB3	1.59	0.81
1:D:71:ILE:HD13	1:D:73:ILE:HG13	1.64	0.80
1:C:71:ILE:HD13	1:C:73:ILE:HG13	1.64	0.79
1:E:71:ILE:HD13	1:E:73:ILE:HG13	1.64	0.79
1:B:71:ILE:HD13	1:B:73:ILE:HG13	1.64	0.78
1:A:71:ILE:HD13	1:A:73:ILE:HG13	1.64	0.77
1:D:54:PHE:HB3	1:D:96:PRO:HA	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:PHE:HB3	1:E:96:PRO:HA	1.73	0.71
1:A:54:PHE:HB3	1:A:96:PRO:HA	1.73	0.71
1:C:54:PHE:HB3	1:C:96:PRO:HA	1.73	0.70
1:B:54:PHE:HB3	1:B:96:PRO:HA	1.73	0.70
1:A:199:PRO:HG3	3:B:409:PEE:H10	1.74	0.69
1:B:95:SER:OG	1:B:99:THR:N	2.27	0.68
1:A:95:SER:OG	1:A:99:THR:N	2.27	0.68
1:D:199:PRO:HG3	3:E:409:PEE:H10	1.76	0.68
3:A:408:PEE:H10	1:E:199:PRO:HG3	1.75	0.68
1:C:95:SER:OG	1:C:99:THR:N	2.27	0.68
1:E:95:SER:OG	1:E:99:THR:N	2.27	0.67
3:C:408:PEE:H10	1:B:199:PRO:HG3	1.76	0.67
1:A:25:ILE:HD11	1:A:42:PHE:CE1	2.30	0.67
1:C:25:ILE:HD11	1:C:42:PHE:CE1	2.30	0.67
1:D:25:ILE:HD11	1:D:42:PHE:CE1	2.30	0.67
1:B:25:ILE:HD11	1:B:42:PHE:CE1	2.30	0.67
1:D:95:SER:OG	1:D:99:THR:N	2.27	0.66
1:E:25:ILE:HD11	1:E:42:PHE:CE1	2.30	0.66
1:C:199:PRO:HG3	3:D:409:PEE:H10	1.78	0.65
1:B:75:GLU:N	1:B:75:GLU:OE1	2.30	0.65
1:C:75:GLU:OE1	1:C:75:GLU:N	2.30	0.64
1:A:75:GLU:OE1	1:A:75:GLU:N	2.30	0.64
1:D:75:GLU:N	1:D:75:GLU:OE1	2.30	0.63
1:A:252:MET:SD	1:A:252:MET:N	2.68	0.63
1:A:176:LEU:HG	1:A:177:GLU:HG2	1.81	0.63
1:E:75:GLU:N	1:E:75:GLU:OE1	2.30	0.63
1:C:176:LEU:HG	1:C:177:GLU:HG2	1.81	0.63
1:D:176:LEU:HG	1:D:177:GLU:HG2	1.81	0.63
1:C:270:VAL:HG11	1:B:211:ILE:HG23	1.80	0.62
1:D:252:MET:SD	1:D:252:MET:N	2.68	0.62
1:C:252:MET:SD	1:C:252:MET:N	2.68	0.62
1:B:176:LEU:HG	1:B:177:GLU:HG2	1.81	0.62
1:A:133:ARG:NH2	1:E:90:VAL:O	2.32	0.62
1:E:176:LEU:HG	1:E:177:GLU:HG2	1.81	0.61
1:B:252:MET:SD	1:B:252:MET:N	2.68	0.60
1:D:90:VAL:O	1:E:133:ARG:NH2	2.34	0.60
1:C:133:ARG:NH2	1:B:90:VAL:O	2.35	0.59
1:E:252:MET:SD	1:E:252:MET:N	2.68	0.59
1:C:25:ILE:HG22	1:C:26:GLU:OE1	2.03	0.58
1:D:25:ILE:HG22	1:D:26:GLU:OE1	2.03	0.58
1:A:90:VAL:O	1:B:133:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PRO:HG2	1:B:16:LEU:HD22	1.85	0.58
1:B:25:ILE:HG22	1:B:26:GLU:OE1	2.03	0.58
1:E:8:PRO:HG2	1:E:16:LEU:HD22	1.85	0.58
1:E:25:ILE:HG22	1:E:26:GLU:OE1	2.03	0.58
1:A:25:ILE:HG22	1:A:26:GLU:OE1	2.03	0.58
1:C:72:TRP:CH2	1:C:140:ILE:HD11	2.39	0.58
1:B:72:TRP:CH2	1:B:140:ILE:HD11	2.39	0.58
1:A:8:PRO:HG2	1:A:16:LEU:HD22	1.85	0.58
1:C:8:PRO:HG2	1:C:16:LEU:HD22	1.85	0.57
1:A:25:ILE:HG22	1:A:26:GLU:CD	2.29	0.57
1:D:8:PRO:HG2	1:D:16:LEU:HD22	1.85	0.57
1:D:25:ILE:HG22	1:D:26:GLU:CD	2.29	0.57
1:D:72:TRP:CH2	1:D:140:ILE:HD11	2.39	0.57
1:B:25:ILE:HG22	1:B:26:GLU:CD	2.29	0.57
1:C:211:ILE:HG23	1:D:270:VAL:HG11	1.85	0.57
1:D:211:ILE:HG23	1:E:270:VAL:HG11	1.87	0.57
1:E:25:ILE:HG22	1:E:26:GLU:CD	2.29	0.57
1:E:72:TRP:CH2	1:E:140:ILE:HD11	2.39	0.57
1:A:72:TRP:CH2	1:A:140:ILE:HD11	2.39	0.56
1:E:35:GLU:HG3	1:E:112:SER:O	2.05	0.56
1:A:211:ILE:HG23	1:B:270:VAL:HG11	1.86	0.56
1:C:25:ILE:HG22	1:C:26:GLU:CD	2.29	0.56
1:B:35:GLU:HG3	1:B:112:SER:O	2.05	0.56
1:A:35:GLU:HG3	1:A:112:SER:O	2.05	0.56
1:D:35:GLU:HG3	1:D:112:SER:O	2.05	0.56
1:A:270:VAL:HG11	1:E:211:ILE:HG23	1.86	0.55
1:C:35:GLU:HG3	1:C:112:SER:O	2.05	0.55
1:B:282:GLU:OE2	3:B:401:PEE:N	2.40	0.55
1:D:136:ASP:OD1	1:D:137:THR:N	2.39	0.54
1:A:7:PRO:HB3	1:A:135:VAL:HG21	1.89	0.54
1:C:45:LEU:HD13	1:C:102:TYR:CD2	2.43	0.54
1:B:7:PRO:HB3	1:B:135:VAL:HG21	1.89	0.54
1:C:136:ASP:OD1	1:C:137:THR:N	2.40	0.54
1:A:54:PHE:HD1	1:A:58:ARG:NH2	2.06	0.54
1:E:54:PHE:HD1	1:E:58:ARG:NH2	2.06	0.54
1:C:35:GLU:OE2	1:B:156:PHE:CE1	2.61	0.54
1:E:136:ASP:OD1	1:E:137:THR:N	2.40	0.53
1:E:45:LEU:HD13	1:E:102:TYR:CD2	2.43	0.53
1:D:54:PHE:HD1	1:D:58:ARG:NH2	2.06	0.53
1:B:45:LEU:HD13	1:B:102:TYR:CD2	2.43	0.53
1:C:7:PRO:HB3	1:C:135:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:PRO:HB3	1:E:135:VAL:HG21	1.89	0.53
1:D:45:LEU:HD13	1:D:102:TYR:CD2	2.43	0.53
1:A:45:LEU:HD13	1:A:102:TYR:CD2	2.43	0.53
1:B:54:PHE:HD1	1:B:58:ARG:NH2	2.06	0.53
1:D:7:PRO:HB3	1:D:135:VAL:HG21	1.89	0.53
3:E:409:PEE:O1P	3:E:409:PEE:N	2.42	0.53
1:C:54:PHE:HD1	1:C:58:ARG:NH2	2.06	0.52
3:C:408:PEE:O1P	3:C:408:PEE:N	2.42	0.52
1:E:282:GLU:OE2	3:E:401:PEE:N	2.43	0.52
1:A:71:ILE:HD12	1:A:71:ILE:O	2.10	0.52
1:E:59:SER:HB2	1:E:63:VAL:HG23	1.92	0.52
3:A:408:PEE:O1P	3:A:408:PEE:N	2.42	0.52
1:B:136:ASP:OD1	1:B:137:THR:N	2.39	0.52
1:C:71:ILE:HD12	1:C:71:ILE:O	2.10	0.51
1:A:35:GLU:OE2	1:E:156:PHE:CE1	2.63	0.51
1:C:291:ILE:HD11	3:C:406:PEE:H14	1.93	0.51
1:D:282:GLU:OE2	3:D:401:PEE:N	2.43	0.51
3:B:409:PEE:O1P	3:B:409:PEE:N	2.42	0.51
1:A:282:GLU:OE2	3:A:409:PEE:N	2.43	0.51
1:B:291:ILE:HD11	3:B:407:PEE:H14	1.93	0.51
1:E:71:ILE:HD12	1:E:71:ILE:O	2.10	0.51
1:D:291:ILE:HD11	3:D:407:PEE:H14	1.93	0.51
1:A:156:PHE:CE1	1:B:35:GLU:OE2	2.63	0.51
1:C:59:SER:HB2	1:C:63:VAL:HG23	1.92	0.51
1:D:71:ILE:O	1:D:71:ILE:HD12	2.10	0.51
1:B:71:ILE:O	1:B:71:ILE:HD12	2.10	0.51
1:B:64:LYS:HB2	1:B:93:SER:HB2	1.93	0.51
1:E:291:ILE:HD11	3:E:407:PEE:H14	1.93	0.51
1:C:64:LYS:HB2	1:C:93:SER:HB2	1.93	0.50
1:A:59:SER:HB2	1:A:63:VAL:HG23	1.92	0.50
1:D:59:SER:HB2	1:D:63:VAL:HG23	1.92	0.50
1:D:156:PHE:CE1	1:E:35:GLU:OE2	2.64	0.50
3:C:408:PEE:H6	1:B:200:ASN:HD21	1.57	0.50
1:B:45:LEU:HB2	1:B:102:TYR:HB3	1.94	0.50
1:A:291:ILE:HD11	3:A:406:PEE:H14	1.93	0.50
1:B:59:SER:HB2	1:B:63:VAL:HG23	1.92	0.50
1:E:297:ILE:O	1:E:301:VAL:HG23	2.12	0.50
1:C:246:LEU:HD23	1:C:247:PRO:HD2	1.94	0.50
1:D:64:LYS:HB2	1:D:93:SER:HB2	1.93	0.50
1:B:266:TYR:O	1:B:270:VAL:HG23	2.12	0.50
1:D:45:LEU:HB2	1:D:102:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HD11	1:B:42:PHE:HE1	1.77	0.50
1:B:297:ILE:O	1:B:301:VAL:HG23	2.12	0.50
1:C:297:ILE:O	1:C:301:VAL:HG23	2.12	0.49
1:E:64:LYS:HB2	1:E:93:SER:HB2	1.93	0.49
1:A:45:LEU:HB2	1:A:102:TYR:HB3	1.94	0.49
1:A:132:VAL:HG21	1:A:140:ILE:HG21	1.94	0.49
1:D:266:TYR:O	1:D:270:VAL:HG23	2.12	0.49
1:E:266:TYR:O	1:E:270:VAL:HG23	2.12	0.49
1:A:64:LYS:HB2	1:A:93:SER:HB2	1.93	0.49
1:A:266:TYR:O	1:A:270:VAL:HG23	2.12	0.49
1:E:132:VAL:HG21	1:E:140:ILE:HG21	1.94	0.49
1:E:246:LEU:HD23	1:E:247:PRO:HD2	1.94	0.49
1:C:266:TYR:O	1:C:270:VAL:HG23	2.12	0.49
1:E:45:LEU:HB2	1:E:102:TYR:HB3	1.94	0.49
1:E:52:LEU:CD2	1:E:71:ILE:HG22	2.43	0.49
1:A:246:LEU:HD23	1:A:247:PRO:HD2	1.94	0.49
1:A:297:ILE:O	1:A:301:VAL:HG23	2.12	0.49
1:D:246:LEU:HD23	1:D:247:PRO:HD2	1.94	0.49
1:D:297:ILE:O	1:D:301:VAL:HG23	2.12	0.49
1:B:28:TYR:CE2	1:B:38:LYS:HD3	2.48	0.49
1:A:52:LEU:CD2	1:A:71:ILE:HG22	2.43	0.49
1:D:52:LEU:CD2	1:D:71:ILE:HG22	2.43	0.49
1:B:246:LEU:HD23	1:B:247:PRO:HD2	1.94	0.48
1:A:54:PHE:CE2	1:A:62:ARG:HA	2.48	0.48
1:B:225:VAL:O	1:B:229:VAL:HG23	2.14	0.48
1:A:28:TYR:CE2	1:A:38:LYS:HD3	2.48	0.48
1:C:52:LEU:CD2	1:C:71:ILE:HG22	2.43	0.48
1:C:200:ASN:HD21	3:D:409:PEE:H5	1.61	0.48
1:D:54:PHE:CE2	1:D:62:ARG:HA	2.48	0.48
1:A:136:ASP:OD1	1:A:137:THR:N	2.40	0.48
1:C:45:LEU:HB2	1:C:102:TYR:HB3	1.94	0.48
1:C:54:PHE:CE2	1:C:62:ARG:HA	2.48	0.48
1:B:132:VAL:HG21	1:B:140:ILE:HG21	1.94	0.48
1:E:48:LYS:HA	1:E:99:THR:HA	1.95	0.48
1:C:132:VAL:HG21	1:C:140:ILE:HG21	1.94	0.48
1:D:132:VAL:HG21	1:D:140:ILE:HG21	1.94	0.48
1:B:52:LEU:CD2	1:B:71:ILE:HG22	2.43	0.48
1:B:54:PHE:CE2	1:B:62:ARG:HA	2.49	0.48
1:C:225:VAL:O	1:C:229:VAL:HG23	2.13	0.48
1:E:225:VAL:O	1:E:229:VAL:HG23	2.13	0.48
1:A:225:VAL:O	1:A:229:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TYR:CE2	1:C:38:LYS:HD3	2.48	0.48
1:C:48:LYS:HA	1:C:99:THR:HA	1.95	0.48
1:D:48:LYS:HA	1:D:99:THR:HA	1.95	0.48
1:D:200:ASN:HD21	3:E:409:PEE:H6	1.60	0.48
1:B:48:LYS:HA	1:B:99:THR:HA	1.95	0.48
1:A:72:TRP:HH2	1:A:140:ILE:HD11	1.79	0.48
1:C:16:LEU:N	1:C:139:ASN:O	2.44	0.48
1:D:62:ARG:HB3	1:D:96:PRO:HD3	1.96	0.48
1:D:72:TRP:HH2	1:D:140:ILE:HD11	1.79	0.48
1:D:225:VAL:O	1:D:229:VAL:HG23	2.13	0.48
1:C:62:ARG:HB3	1:C:96:PRO:HD3	1.96	0.48
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.77	0.48
1:E:54:PHE:CE2	1:E:62:ARG:HA	2.49	0.48
1:E:28:TYR:CE2	1:E:38:LYS:HD3	2.48	0.47
1:A:48:LYS:HA	1:A:99:THR:HA	1.95	0.47
1:C:45:LEU:HD13	1:C:102:TYR:HD2	1.79	0.47
3:D:409:PEE:O1P	3:D:409:PEE:N	2.42	0.47
1:C:251:TYR:HB2	1:C:252:MET:SD	2.55	0.47
1:D:45:LEU:HD13	1:D:102:TYR:HD2	1.79	0.47
1:B:62:ARG:HB3	1:B:96:PRO:HD3	1.96	0.47
1:E:25:ILE:HD11	1:E:42:PHE:HE1	1.76	0.47
1:D:28:TYR:CE2	1:D:38:LYS:HD3	2.48	0.47
1:B:45:LEU:HD13	1:B:102:TYR:HD2	1.79	0.47
1:B:95:SER:HG	1:B:99:THR:H	1.56	0.47
1:E:95:SER:HG	1:E:99:THR:H	1.57	0.47
1:D:251:TYR:HB2	1:D:252:MET:SD	2.55	0.47
1:C:200:ASN:ND2	3:D:409:PEE:H5	2.13	0.47
1:B:251:TYR:HB2	1:B:252:MET:SD	2.55	0.47
1:E:251:TYR:HB2	1:E:252:MET:SD	2.55	0.47
1:E:62:ARG:HB3	1:E:96:PRO:HD3	1.96	0.47
1:D:16:LEU:N	1:D:139:ASN:O	2.44	0.46
1:E:196:SER:O	1:E:200:ASN:HB2	2.15	0.46
1:A:196:SER:O	1:A:200:ASN:HB2	2.15	0.46
1:E:16:LEU:N	1:E:139:ASN:O	2.44	0.46
1:D:23:TYR:HE1	1:D:152:ASN:OD1	1.98	0.46
1:C:25:ILE:HD11	1:C:42:PHE:HE1	1.76	0.46
1:D:25:ILE:HD11	1:D:42:PHE:HE1	1.76	0.46
1:A:62:ARG:HB3	1:A:96:PRO:HD3	1.96	0.46
1:A:248:LYS:HA	1:A:248:LYS:HD3	1.75	0.46
1:A:251:TYR:HB2	1:A:252:MET:SD	2.55	0.46
1:D:248:LYS:HA	1:D:248:LYS:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:SER:O	1:B:200:ASN:HB2	2.15	0.46
1:A:23:TYR:HE1	1:A:152:ASN:OD1	1.98	0.46
1:A:25:ILE:HD11	1:A:42:PHE:HE1	1.77	0.46
1:C:196:SER:O	1:C:200:ASN:HB2	2.15	0.46
1:E:72:TRP:HH2	1:E:140:ILE:HD11	1.79	0.46
1:E:45:LEU:HD13	1:E:102:TYR:HD2	1.79	0.46
1:C:23:TYR:CE1	1:C:152:ASN:OD1	2.69	0.46
1:D:23:TYR:CE1	1:D:152:ASN:OD1	2.69	0.46
1:D:196:SER:O	1:D:200:ASN:HB2	2.15	0.46
1:E:23:TYR:HE1	1:E:152:ASN:OD1	1.98	0.45
1:C:72:TRP:HH2	1:C:140:ILE:HD11	1.79	0.45
1:A:45:LEU:HD13	1:A:102:TYR:HD2	1.79	0.45
1:B:16:LEU:N	1:B:139:ASN:O	2.44	0.45
1:D:264:LEU:HD11	3:D:409:PEE:H31	1.99	0.45
1:B:18:VAL:HG11	1:B:45:LEU:HD23	1.99	0.45
1:E:264:LEU:HD11	3:E:409:PEE:H31	1.99	0.45
1:A:23:TYR:CE1	1:A:152:ASN:OD1	2.69	0.45
1:A:199:PRO:CG	3:B:409:PEE:H10	2.46	0.45
3:A:403:PEE:H13	3:A:406:PEE:H17	1.99	0.45
1:B:23:TYR:HE1	1:B:152:ASN:OD1	1.98	0.45
1:B:252:MET:N	1:B:252:MET:HE3	2.32	0.45
1:E:23:TYR:CE1	1:E:152:ASN:OD1	2.69	0.45
1:C:23:TYR:HE1	1:C:152:ASN:OD1	1.99	0.45
1:E:18:VAL:HG11	1:E:45:LEU:HD23	1.99	0.45
1:A:135:VAL:HG22	1:A:136:ASP:H	1.82	0.45
3:B:404:PEE:H13	3:B:407:PEE:H17	1.99	0.45
1:D:18:VAL:HG11	1:D:45:LEU:HD23	1.99	0.45
1:D:224:ASN:O	1:D:228:VAL:HG23	2.17	0.45
1:B:135:VAL:HG22	1:B:136:ASP:H	1.82	0.45
3:E:404:PEE:H13	3:E:407:PEE:H17	1.99	0.45
1:C:76:ILE:O	1:C:85:ARG:NH1	2.50	0.44
1:D:252:MET:N	1:D:252:MET:HE3	2.32	0.44
1:B:23:TYR:CE1	1:B:152:ASN:OD1	2.69	0.44
1:B:224:ASN:O	1:B:228:VAL:HG23	2.17	0.44
3:D:404:PEE:H13	3:D:407:PEE:H17	1.99	0.44
1:E:224:ASN:O	1:E:228:VAL:HG23	2.17	0.44
1:E:252:MET:N	1:E:252:MET:HE3	2.32	0.44
1:A:224:ASN:O	1:A:228:VAL:HG23	2.17	0.44
1:A:252:MET:N	1:A:252:MET:HE3	2.32	0.44
1:C:252:MET:N	1:C:252:MET:HE3	2.32	0.44
1:B:264:LEU:HD11	3:B:409:PEE:H31	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:HG11	1:A:45:LEU:HD23	1.99	0.44
1:C:91:ASP:HB3	1:D:179:ARG:NH1	2.33	0.44
1:C:224:ASN:O	1:C:228:VAL:HG23	2.17	0.44
1:B:35:GLU:CG	1:B:35:GLU:O	2.65	0.44
1:E:76:ILE:O	1:E:85:ARG:NH1	2.50	0.44
3:C:403:PEE:H13	3:C:406:PEE:H17	1.99	0.44
1:D:76:ILE:O	1:D:85:ARG:NH1	2.51	0.44
1:A:16:LEU:N	1:A:139:ASN:O	2.44	0.44
1:C:28:TYR:HE2	1:C:38:LYS:HD3	1.83	0.44
1:D:47:TRP:HZ3	1:D:102:TYR:HB2	1.83	0.44
1:B:76:ILE:O	1:B:85:ARG:NH1	2.50	0.44
1:E:204:PRO:O	1:E:208:ILE:HG13	2.18	0.44
1:A:35:GLU:O	1:A:35:GLU:CG	2.65	0.44
1:C:264:LEU:HD11	3:C:408:PEE:H31	1.99	0.44
1:D:35:GLU:O	1:D:35:GLU:CG	2.65	0.44
1:D:47:TRP:O	1:D:100:VAL:N	2.51	0.44
1:D:204:PRO:O	1:D:208:ILE:HG13	2.18	0.44
1:D:28:TYR:HE2	1:D:38:LYS:HD3	1.83	0.44
1:B:72:TRP:HH2	1:B:140:ILE:HD11	1.79	0.44
1:A:204:PRO:O	1:A:208:ILE:HG13	2.18	0.44
1:C:135:VAL:HG22	1:C:136:ASP:H	1.82	0.44
1:C:248:LYS:HA	1:C:248:LYS:HD3	1.74	0.44
1:B:47:TRP:HZ3	1:B:102:TYR:HB2	1.83	0.44
1:E:35:GLU:CG	1:E:35:GLU:O	2.65	0.44
1:E:135:VAL:HG22	1:E:136:ASP:H	1.82	0.44
1:C:18:VAL:HG11	1:C:45:LEU:HD23	1.99	0.43
1:E:47:TRP:HZ3	1:E:102:TYR:HB2	1.83	0.43
1:A:47:TRP:HZ3	1:A:102:TYR:HB2	1.83	0.43
1:C:35:GLU:CG	1:C:35:GLU:O	2.65	0.43
1:C:204:PRO:O	1:C:208:ILE:HG13	2.18	0.43
1:E:28:TYR:HE2	1:E:38:LYS:HD3	1.83	0.43
1:A:12:ALA:HB1	1:A:14:GLU:OE1	2.19	0.43
1:C:169:VAL:O	1:C:171:PRO:HD3	2.18	0.43
1:C:199:PRO:CG	3:D:409:PEE:H10	2.46	0.43
1:D:135:VAL:HG22	1:D:136:ASP:H	1.82	0.43
1:E:248:LYS:HA	1:E:248:LYS:HD3	1.75	0.43
1:C:12:ALA:HB1	1:C:14:GLU:OE1	2.19	0.43
1:A:264:LEU:HD11	3:A:408:PEE:H31	1.99	0.43
1:B:204:PRO:O	1:B:208:ILE:HG13	2.18	0.43
1:E:12:ALA:HB1	1:E:14:GLU:OE1	2.19	0.43
1:E:169:VAL:O	1:E:171:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:O	1:A:171:PRO:HD3	2.18	0.43
1:C:47:TRP:HZ3	1:C:102:TYR:HB2	1.83	0.43
1:C:47:TRP:O	1:C:100:VAL:N	2.51	0.43
1:D:169:VAL:O	1:D:171:PRO:HD3	2.18	0.43
1:C:90:VAL:O	1:D:133:ARG:NH2	2.52	0.43
1:D:12:ALA:HB1	1:D:14:GLU:OE1	2.19	0.43
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.77	0.43
1:A:28:TYR:HE2	1:A:38:LYS:HD3	1.83	0.42
1:C:8:PRO:HD3	1:C:72:TRP:CE3	2.54	0.42
1:B:12:ALA:HB1	1:B:14:GLU:OE1	2.18	0.42
1:E:8:PRO:HD3	1:E:72:TRP:CE3	2.54	0.42
1:A:8:PRO:HD3	1:A:72:TRP:CE3	2.54	0.42
1:A:76:ILE:O	1:A:85:ARG:NH1	2.51	0.42
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.77	0.42
3:D:407:PEE:H56	3:D:407:PEE:H63	1.88	0.42
1:B:28:TYR:HE2	1:B:38:LYS:HD3	1.83	0.42
1:B:85:ARG:HD3	2:B:402:CL:CL	2.57	0.42
1:E:85:ARG:HD3	2:E:402:CL:CL	2.57	0.42
1:B:169:VAL:O	1:B:171:PRO:HD3	2.18	0.42
1:B:47:TRP:O	1:B:100:VAL:N	2.51	0.42
1:D:85:ARG:HD3	2:D:402:CL:CL	2.57	0.42
1:D:199:PRO:CG	3:E:409:PEE:H10	2.46	0.42
1:B:54:PHE:HD2	1:B:96:PRO:HB3	1.84	0.42
1:E:54:PHE:HD2	1:E:96:PRO:HB3	1.84	0.42
1:D:54:PHE:HD2	1:D:96:PRO:HB3	1.84	0.42
1:A:85:ARG:HD3	2:A:401:CL:CL	2.57	0.42
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.77	0.42
1:D:8:PRO:HD3	1:D:72:TRP:CE3	2.54	0.42
3:A:408:PEE:H10	1:E:199:PRO:CG	2.47	0.42
1:B:8:PRO:HD3	1:B:72:TRP:CE3	2.54	0.42
1:C:85:ARG:HD3	2:C:401:CL:CL	2.57	0.42
1:D:91:ASP:HB3	1:E:179:ARG:NH1	2.35	0.42
3:E:407:PEE:H56	3:E:407:PEE:H63	1.88	0.42
1:C:147:GLU:CD	1:C:147:GLU:H	2.29	0.41
1:E:47:TRP:O	1:E:100:VAL:N	2.51	0.41
1:E:54:PHE:CE1	1:E:63:VAL:HB	2.55	0.41
1:C:54:PHE:CE1	1:C:63:VAL:HB	2.55	0.41
1:A:54:PHE:CE1	1:A:63:VAL:HB	2.55	0.41
1:A:54:PHE:HD2	1:A:96:PRO:HB3	1.84	0.41
1:C:245:ASN:OD1	1:C:245:ASN:C	2.63	0.41
1:A:47:TRP:O	1:A:100:VAL:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CD1	1:A:156:PHE:O	2.74	0.41
1:C:54:PHE:HD2	1:C:96:PRO:HB3	1.84	0.41
1:A:245:ASN:OD1	1:A:245:ASN:C	2.63	0.41
1:B:54:PHE:CE1	1:B:63:VAL:HB	2.55	0.41
1:B:147:GLU:CD	1:B:147:GLU:H	2.29	0.41
1:E:156:PHE:O	1:E:156:PHE:CD1	2.74	0.41
1:A:303:PHE:HD2	3:A:407:PEE:H63	1.86	0.41
1:C:303:PHE:HD2	3:C:407:PEE:H63	1.86	0.41
1:D:303:PHE:HD2	3:D:408:PEE:H63	1.86	0.41
1:D:54:PHE:CE1	1:D:63:VAL:HB	2.55	0.41
1:B:156:PHE:O	1:B:156:PHE:CD1	2.74	0.41
1:B:245:ASN:OD1	1:B:245:ASN:C	2.63	0.41
1:E:303:PHE:HD2	3:E:408:PEE:H63	1.86	0.41
3:C:406:PEE:H56	3:C:406:PEE:H63	1.88	0.41
3:C:408:PEE:H10	1:B:199:PRO:CG	2.46	0.41
1:D:147:GLU:H	1:D:147:GLU:CD	2.29	0.41
1:B:303:PHE:HD2	3:B:408:PEE:H63	1.86	0.41
1:A:91:ASP:HB3	1:B:179:ARG:NH1	2.36	0.41
1:D:156:PHE:O	1:D:156:PHE:CD1	2.74	0.41
1:D:245:ASN:OD1	1:D:245:ASN:C	2.63	0.40
1:E:54:PHE:CE1	1:E:58:ARG:HB3	2.57	0.40
1:A:147:GLU:H	1:A:147:GLU:CD	2.29	0.40
1:C:156:PHE:CD1	1:C:156:PHE:O	2.74	0.40
1:A:264:LEU:O	1:A:268:VAL:HG23	2.22	0.40
1:D:261:MET:HG3	3:D:409:PEE:H51	2.03	0.40
1:B:54:PHE:CE1	1:B:58:ARG:HB3	2.57	0.40
1:E:245:ASN:OD1	1:E:245:ASN:C	2.63	0.40
1:E:264:LEU:O	1:E:268:VAL:HG23	2.22	0.40
1:E:147:GLU:H	1:E:147:GLU:CD	2.29	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	311/312 (100%)	296 (95%)	15 (5%)	0	100	100
1	B	311/312 (100%)	297 (96%)	14 (4%)	0	100	100
1	C	311/312 (100%)	297 (96%)	14 (4%)	0	100	100
1	D	311/312 (100%)	297 (96%)	14 (4%)	0	100	100
1	E	311/312 (100%)	297 (96%)	14 (4%)	0	100	100
All	All	1555/1560 (100%)	1484 (95%)	71 (5%)	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	281/280 (100%)	279 (99%)	2 (1%)	76	85
1	B	281/280 (100%)	279 (99%)	2 (1%)	76	85
1	C	281/280 (100%)	279 (99%)	2 (1%)	76	85
1	D	281/280 (100%)	279 (99%)	2 (1%)	76	85
1	E	281/280 (100%)	279 (99%)	2 (1%)	76	85
All	All	1405/1400 (100%)	1395 (99%)	10 (1%)	81	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293[A]	ARG
1	A	293[B]	ARG
1	C	293[A]	ARG
1	C	293[B]	ARG
1	D	293[A]	ARG
1	D	293[B]	ARG
1	B	293[A]	ARG
1	B	293[B]	ARG
1	E	293[A]	ARG
1	E	293[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	200	ASN
1	C	200	ASN
1	D	200	ASN
1	B	200	ASN
1	E	200	ASN

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](#)

Of 45 ligands modelled in this entry, 5 are monoatomic - leaving 40 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	$\# Z > 2$
3	PEE	D	407	-	40,40,50	0.99	2 (5%)	43,45,55	0.68	0
3	PEE	B	403	-	31,31,50	0.99	2 (6%)	34,36,55	1.22	2 (5%)
3	PEE	B	408	-	33,33,50	0.82	1 (3%)	36,38,55	0.73	1 (2%)
3	PEE	C	403	-	25,25,50	0.81	1 (4%)	28,30,55	1.24	2 (7%)
3	PEE	D	408	-	33,33,50	0.83	1 (3%)	36,38,55	0.73	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEE	E	405	-	41,41,50	0.99	2 (4%)	44,46,55	0.67	0
3	PEE	D	404	-	25,25,50	0.82	1 (4%)	28,30,55	1.24	2 (7%)
3	PEE	A	406	-	40,40,50	0.99	2 (5%)	43,45,55	0.68	0
3	PEE	B	401	-	41,41,50	0.98	2 (4%)	44,46,55	0.76	0
3	PEE	A	408	-	37,37,50	0.83	1 (2%)	40,42,55	0.62	0
3	PEE	E	406	-	25,25,50	1.11	2 (8%)	28,30,55	1.30	2 (7%)
3	PEE	A	409	-	41,41,50	0.98	2 (4%)	44,46,55	0.76	0
3	PEE	E	407	-	40,40,50	0.99	2 (5%)	43,45,55	0.68	0
3	PEE	C	405	-	25,25,50	1.10	2 (8%)	28,30,55	1.30	2 (7%)
3	PEE	C	402	-	31,31,50	0.99	2 (6%)	34,36,55	1.22	2 (5%)
3	PEE	C	407	-	33,33,50	0.83	1 (3%)	36,38,55	0.73	1 (2%)
3	PEE	C	404	-	41,41,50	0.98	2 (4%)	44,46,55	0.67	0
3	PEE	A	403	-	25,25,50	0.82	1 (4%)	28,30,55	1.24	2 (7%)
3	PEE	D	405	-	41,41,50	0.98	2 (4%)	44,46,55	0.67	0
3	PEE	C	406	-	40,40,50	0.99	2 (5%)	43,45,55	0.68	0
3	PEE	B	406	-	25,25,50	1.11	2 (8%)	28,30,55	1.30	3 (10%)
3	PEE	E	409	-	37,37,50	0.83	1 (2%)	40,42,55	0.62	0
3	PEE	B	409	-	37,37,50	0.83	1 (2%)	40,42,55	0.62	0
3	PEE	E	403	-	31,31,50	1.00	2 (6%)	34,36,55	1.22	2 (5%)
3	PEE	C	408	-	37,37,50	0.83	1 (2%)	40,42,55	0.62	0
3	PEE	B	407	-	40,40,50	0.99	2 (5%)	43,45,55	0.68	0
3	PEE	D	403	-	31,31,50	1.00	2 (6%)	34,36,55	1.22	2 (5%)
3	PEE	E	401	-	41,41,50	0.98	2 (4%)	44,46,55	0.76	0
3	PEE	E	404	-	25,25,50	0.82	1 (4%)	28,30,55	1.24	2 (7%)
3	PEE	E	408	-	33,33,50	0.82	1 (3%)	36,38,55	0.73	1 (2%)
3	PEE	D	406	-	25,25,50	1.11	2 (8%)	28,30,55	1.30	3 (10%)
3	PEE	B	405	-	41,41,50	0.99	2 (4%)	44,46,55	0.67	0
3	PEE	A	402	-	31,31,50	0.99	2 (6%)	34,36,55	1.22	2 (5%)
3	PEE	D	401	-	41,41,50	0.98	2 (4%)	44,46,55	0.76	0
3	PEE	D	409	-	37,37,50	0.83	1 (2%)	40,42,55	0.62	0
3	PEE	A	407	-	33,33,50	0.82	1 (3%)	36,38,55	0.73	1 (2%)
3	PEE	C	409	-	41,41,50	0.98	2 (4%)	44,46,55	0.76	0
3	PEE	A	405	-	25,25,50	1.11	2 (8%)	28,30,55	1.30	3 (10%)
3	PEE	B	404	-	25,25,50	0.82	1 (4%)	28,30,55	1.24	2 (7%)
3	PEE	A	404	-	41,41,50	0.98	2 (4%)	44,46,55	0.67	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	PEE	D	407	-	-	12/44/44/54	-
3	PEE	B	403	-	-	10/33/33/54	-
3	PEE	B	408	-	-	12/37/37/54	-
3	PEE	C	403	-	-	3/27/27/54	-
3	PEE	D	408	-	-	12/37/37/54	-
3	PEE	E	405	-	-	16/45/45/54	-
3	PEE	D	404	-	-	3/27/27/54	-
3	PEE	A	406	-	-	12/44/44/54	-
3	PEE	B	401	-	-	23/45/45/54	-
3	PEE	A	408	-	-	6/41/41/54	-
3	PEE	E	406	-	-	6/27/27/54	-
3	PEE	A	409	-	-	23/45/45/54	-
3	PEE	E	407	-	-	12/44/44/54	-
3	PEE	C	405	-	-	6/27/27/54	-
3	PEE	C	402	-	-	10/33/33/54	-
3	PEE	C	407	-	-	12/37/37/54	-
3	PEE	C	404	-	-	16/45/45/54	-
3	PEE	A	403	-	-	3/27/27/54	-
3	PEE	D	405	-	-	16/45/45/54	-
3	PEE	C	406	-	-	12/44/44/54	-
3	PEE	B	406	-	-	6/27/27/54	-
3	PEE	E	409	-	-	6/41/41/54	-
3	PEE	B	409	-	-	6/41/41/54	-
3	PEE	E	403	-	-	10/33/33/54	-
3	PEE	C	408	-	-	6/41/41/54	-
3	PEE	B	407	-	-	12/44/44/54	-
3	PEE	D	403	-	-	10/33/33/54	-
3	PEE	E	401	-	-	23/45/45/54	-
3	PEE	E	404	-	-	3/27/27/54	-
3	PEE	E	408	-	-	12/37/37/54	-
3	PEE	D	406	-	-	6/27/27/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	B	405	-	-	16/45/45/54	-
3	PEE	A	402	-	-	10/33/33/54	-
3	PEE	D	401	-	-	23/45/45/54	-
3	PEE	D	409	-	-	6/41/41/54	-
3	PEE	A	407	-	-	12/37/37/54	-
3	PEE	C	409	-	-	23/45/45/54	-
3	PEE	A	405	-	-	6/27/27/54	-
3	PEE	B	404	-	-	3/27/27/54	-
3	PEE	A	404	-	-	16/45/45/54	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	409	PEE	C39-C38	3.71	1.52	1.31
3	D	403	PEE	C39-C38	3.71	1.52	1.31
3	E	403	PEE	C39-C38	3.71	1.52	1.31
3	C	409	PEE	C39-C38	3.71	1.52	1.31
3	E	401	PEE	C39-C38	3.71	1.52	1.31
3	E	409	PEE	C18-C19	3.71	1.52	1.31
3	E	407	PEE	C39-C38	3.71	1.52	1.31
3	B	409	PEE	C18-C19	3.71	1.52	1.31
3	C	402	PEE	C39-C38	3.71	1.52	1.31
3	C	406	PEE	C39-C38	3.71	1.52	1.31
3	B	403	PEE	C39-C38	3.71	1.52	1.31
3	A	406	PEE	C39-C38	3.71	1.52	1.31
3	B	405	PEE	C39-C38	3.70	1.52	1.31
3	C	404	PEE	C39-C38	3.70	1.52	1.31
3	B	405	PEE	C18-C19	3.70	1.52	1.31
3	A	404	PEE	C39-C38	3.70	1.52	1.31
3	A	408	PEE	C18-C19	3.70	1.52	1.31
3	D	409	PEE	C18-C19	3.70	1.52	1.31
3	E	405	PEE	C18-C19	3.70	1.52	1.31
3	B	401	PEE	C39-C38	3.70	1.52	1.31
3	D	405	PEE	C39-C38	3.70	1.52	1.31
3	D	401	PEE	C39-C38	3.70	1.52	1.31
3	A	402	PEE	C39-C38	3.70	1.52	1.31
3	D	407	PEE	C39-C38	3.70	1.52	1.31
3	E	405	PEE	C39-C38	3.70	1.52	1.31
3	B	407	PEE	C39-C38	3.69	1.52	1.31
3	C	408	PEE	C18-C19	3.69	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	405	PEE	C18-C19	3.69	1.52	1.31
3	C	409	PEE	C18-C19	3.69	1.52	1.31
3	B	401	PEE	C18-C19	3.69	1.52	1.31
3	A	409	PEE	C18-C19	3.69	1.52	1.31
3	D	401	PEE	C18-C19	3.69	1.52	1.31
3	A	404	PEE	C18-C19	3.68	1.52	1.31
3	C	404	PEE	C18-C19	3.68	1.52	1.31
3	E	401	PEE	C18-C19	3.67	1.52	1.31
3	C	405	PEE	C19-C18	3.67	1.52	1.29
3	E	406	PEE	C19-C18	3.67	1.52	1.29
3	D	407	PEE	C19-C18	3.67	1.52	1.29
3	B	407	PEE	C19-C18	3.67	1.52	1.29
3	D	406	PEE	C19-C18	3.66	1.52	1.29
3	B	406	PEE	C19-C18	3.66	1.52	1.29
3	A	405	PEE	C19-C18	3.66	1.52	1.29
3	A	406	PEE	C19-C18	3.65	1.52	1.29
3	C	406	PEE	C19-C18	3.65	1.52	1.29
3	E	407	PEE	C19-C18	3.65	1.52	1.29
3	A	407	PEE	C38-C39	3.18	1.52	1.29
3	B	408	PEE	C38-C39	3.18	1.52	1.29
3	E	408	PEE	C38-C39	3.18	1.52	1.29
3	C	407	PEE	C38-C39	3.17	1.52	1.29
3	D	408	PEE	C38-C39	3.16	1.52	1.29
3	B	404	PEE	P-O4P	2.96	1.65	1.54
3	D	406	PEE	P-O4P	2.96	1.65	1.54
3	A	403	PEE	P-O4P	2.96	1.65	1.54
3	D	404	PEE	P-O4P	2.95	1.65	1.54
3	A	402	PEE	P-O4P	2.95	1.65	1.54
3	D	403	PEE	P-O4P	2.95	1.65	1.54
3	E	403	PEE	P-O4P	2.95	1.65	1.54
3	B	406	PEE	P-O4P	2.95	1.65	1.54
3	B	403	PEE	P-O4P	2.94	1.65	1.54
3	E	404	PEE	P-O4P	2.94	1.65	1.54
3	C	402	PEE	P-O4P	2.94	1.65	1.54
3	C	403	PEE	P-O4P	2.93	1.65	1.54
3	A	405	PEE	P-O4P	2.93	1.65	1.54
3	E	406	PEE	P-O4P	2.92	1.65	1.54
3	C	405	PEE	P-O4P	2.91	1.65	1.54

All (38) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	403	PEE	O4P-P-O3P	-5.30	92.84	106.67
3	D	406	PEE	O4P-P-O3P	-5.30	92.85	106.67
3	C	405	PEE	O4P-P-O3P	-5.30	92.86	106.67
3	A	405	PEE	O4P-P-O3P	-5.29	92.87	106.67
3	D	403	PEE	O4P-P-O3P	-5.29	92.87	106.67
3	B	406	PEE	O4P-P-O3P	-5.29	92.87	106.67
3	E	406	PEE	O4P-P-O3P	-5.29	92.88	106.67
3	A	402	PEE	O4P-P-O3P	-5.29	92.88	106.67
3	B	404	PEE	O4P-P-O3P	-5.28	92.89	106.67
3	B	403	PEE	O4P-P-O3P	-5.28	92.89	106.67
3	A	403	PEE	O4P-P-O3P	-5.28	92.90	106.67
3	C	402	PEE	O4P-P-O3P	-5.28	92.90	106.67
3	C	403	PEE	O4P-P-O3P	-5.28	92.91	106.67
3	D	404	PEE	O4P-P-O3P	-5.27	92.92	106.67
3	E	404	PEE	O4P-P-O3P	-5.27	92.92	106.67
3	B	404	PEE	O2P-P-O1P	2.23	119.54	110.83
3	A	403	PEE	O2P-P-O1P	2.23	119.53	110.83
3	D	404	PEE	O2P-P-O1P	2.23	119.53	110.83
3	C	403	PEE	O2P-P-O1P	2.23	119.50	110.83
3	E	403	PEE	O2P-P-O1P	2.22	119.49	110.83
3	E	404	PEE	O2P-P-O1P	2.22	119.49	110.83
3	A	407	PEE	C37-C38-C39	-2.22	113.67	130.48
3	C	407	PEE	C37-C38-C39	-2.22	113.67	130.48
3	B	408	PEE	C37-C38-C39	-2.22	113.68	130.48
3	C	402	PEE	O2P-P-O1P	2.22	119.47	110.83
3	D	408	PEE	C37-C38-C39	-2.22	113.69	130.48
3	E	408	PEE	C37-C38-C39	-2.22	113.69	130.48
3	B	403	PEE	O2P-P-O1P	2.22	119.47	110.83
3	D	406	PEE	O2P-P-O1P	2.21	119.46	110.83
3	D	403	PEE	O2P-P-O1P	2.21	119.46	110.83
3	B	406	PEE	O2P-P-O1P	2.21	119.46	110.83
3	A	402	PEE	O2P-P-O1P	2.21	119.45	110.83
3	E	406	PEE	O2P-P-O1P	2.21	119.44	110.83
3	C	405	PEE	O2P-P-O1P	2.21	119.43	110.83
3	A	405	PEE	O2P-P-O1P	2.20	119.43	110.83
3	D	406	PEE	O3P-P-O1P	2.02	111.89	106.44
3	A	405	PEE	O3P-P-O1P	2.01	111.87	106.44
3	B	406	PEE	O3P-P-O1P	2.00	111.86	106.44

There are no chirality outliers.

All (440) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	PEE	O2-C2-C3-O3
3	A	404	PEE	O2-C2-C3-O3
3	A	404	PEE	C1-O3P-P-O2P
3	A	404	PEE	C1-O3P-P-O4P
3	A	404	PEE	C4-O4P-P-O3P
3	A	404	PEE	C4-O4P-P-O2P
3	A	404	PEE	C4-O4P-P-O1P
3	A	406	PEE	C4-O4P-P-O3P
3	A	406	PEE	C4-O4P-P-O2P
3	A	407	PEE	C1-O3P-P-O2P
3	A	407	PEE	C1-O3P-P-O1P
3	A	407	PEE	C4-O4P-P-O3P
3	A	407	PEE	C37-C38-C39-C40
3	A	408	PEE	C4-O4P-P-O3P
3	A	408	PEE	C4-O4P-P-O2P
3	A	408	PEE	C4-O4P-P-O1P
3	A	408	PEE	C5-C4-O4P-P
3	A	409	PEE	C1-O3P-P-O2P
3	A	409	PEE	C1-O3P-P-O1P
3	A	409	PEE	C1-O3P-P-O4P
3	A	409	PEE	C4-O4P-P-O1P
3	C	403	PEE	O2-C2-C3-O3
3	C	404	PEE	O2-C2-C3-O3
3	C	404	PEE	C1-O3P-P-O2P
3	C	404	PEE	C1-O3P-P-O4P
3	C	404	PEE	C4-O4P-P-O3P
3	C	404	PEE	C4-O4P-P-O2P
3	C	404	PEE	C4-O4P-P-O1P
3	C	406	PEE	C4-O4P-P-O3P
3	C	406	PEE	C4-O4P-P-O2P
3	C	407	PEE	C1-O3P-P-O2P
3	C	407	PEE	C1-O3P-P-O1P
3	C	407	PEE	C4-O4P-P-O3P
3	C	407	PEE	C37-C38-C39-C40
3	C	408	PEE	C4-O4P-P-O3P
3	C	408	PEE	C4-O4P-P-O2P
3	C	408	PEE	C4-O4P-P-O1P
3	C	408	PEE	C5-C4-O4P-P
3	C	409	PEE	C1-O3P-P-O2P
3	C	409	PEE	C1-O3P-P-O1P
3	C	409	PEE	C1-O3P-P-O4P
3	C	409	PEE	C4-O4P-P-O1P
3	D	401	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	D	401	PEE	C1-O3P-P-O1P
3	D	401	PEE	C1-O3P-P-O4P
3	D	401	PEE	C4-O4P-P-O1P
3	D	404	PEE	O2-C2-C3-O3
3	D	405	PEE	O2-C2-C3-O3
3	D	405	PEE	C1-O3P-P-O2P
3	D	405	PEE	C1-O3P-P-O4P
3	D	405	PEE	C4-O4P-P-O3P
3	D	405	PEE	C4-O4P-P-O2P
3	D	405	PEE	C4-O4P-P-O1P
3	D	407	PEE	C4-O4P-P-O3P
3	D	407	PEE	C4-O4P-P-O2P
3	D	408	PEE	C1-O3P-P-O2P
3	D	408	PEE	C1-O3P-P-O1P
3	D	408	PEE	C4-O4P-P-O3P
3	D	408	PEE	C37-C38-C39-C40
3	D	409	PEE	C4-O4P-P-O3P
3	D	409	PEE	C4-O4P-P-O2P
3	D	409	PEE	C4-O4P-P-O1P
3	D	409	PEE	C5-C4-O4P-P
3	B	401	PEE	C1-O3P-P-O2P
3	B	401	PEE	C1-O3P-P-O1P
3	B	401	PEE	C1-O3P-P-O4P
3	B	401	PEE	C4-O4P-P-O1P
3	B	404	PEE	O2-C2-C3-O3
3	B	405	PEE	O2-C2-C3-O3
3	B	405	PEE	C1-O3P-P-O2P
3	B	405	PEE	C1-O3P-P-O4P
3	B	405	PEE	C4-O4P-P-O3P
3	B	405	PEE	C4-O4P-P-O2P
3	B	405	PEE	C4-O4P-P-O1P
3	B	407	PEE	C4-O4P-P-O3P
3	B	407	PEE	C4-O4P-P-O2P
3	B	408	PEE	C1-O3P-P-O2P
3	B	408	PEE	C1-O3P-P-O1P
3	B	408	PEE	C4-O4P-P-O3P
3	B	408	PEE	C37-C38-C39-C40
3	B	409	PEE	C4-O4P-P-O3P
3	B	409	PEE	C4-O4P-P-O2P
3	B	409	PEE	C4-O4P-P-O1P
3	B	409	PEE	C5-C4-O4P-P
3	E	401	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	E	401	PEE	C1-O3P-P-O1P
3	E	401	PEE	C1-O3P-P-O4P
3	E	401	PEE	C4-O4P-P-O1P
3	E	404	PEE	O2-C2-C3-O3
3	E	405	PEE	O2-C2-C3-O3
3	E	405	PEE	C1-O3P-P-O2P
3	E	405	PEE	C1-O3P-P-O4P
3	E	405	PEE	C4-O4P-P-O3P
3	E	405	PEE	C4-O4P-P-O2P
3	E	405	PEE	C4-O4P-P-O1P
3	E	407	PEE	C4-O4P-P-O3P
3	E	407	PEE	C4-O4P-P-O2P
3	E	408	PEE	C1-O3P-P-O2P
3	E	408	PEE	C1-O3P-P-O1P
3	E	408	PEE	C4-O4P-P-O3P
3	E	408	PEE	C37-C38-C39-C40
3	E	409	PEE	C4-O4P-P-O3P
3	E	409	PEE	C4-O4P-P-O2P
3	E	409	PEE	C4-O4P-P-O1P
3	E	409	PEE	C5-C4-O4P-P
3	A	409	PEE	C31-C30-O3-C3
3	C	409	PEE	C31-C30-O3-C3
3	D	401	PEE	C31-C30-O3-C3
3	B	401	PEE	C31-C30-O3-C3
3	E	401	PEE	C31-C30-O3-C3
3	A	405	PEE	C11-C10-O2-C2
3	C	405	PEE	C11-C10-O2-C2
3	B	406	PEE	C11-C10-O2-C2
3	A	409	PEE	O5-C30-O3-C3
3	C	409	PEE	O5-C30-O3-C3
3	D	401	PEE	O5-C30-O3-C3
3	B	401	PEE	O5-C30-O3-C3
3	E	401	PEE	O5-C30-O3-C3
3	A	406	PEE	C37-C38-C39-C40
3	C	406	PEE	C37-C38-C39-C40
3	D	407	PEE	C37-C38-C39-C40
3	B	407	PEE	C37-C38-C39-C40
3	E	407	PEE	C37-C38-C39-C40
3	D	406	PEE	C11-C10-O2-C2
3	E	406	PEE	C11-C10-O2-C2
3	A	406	PEE	C30-C31-C32-C33
3	C	406	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	D	407	PEE	C30-C31-C32-C33
3	B	407	PEE	C30-C31-C32-C33
3	E	407	PEE	C30-C31-C32-C33
3	A	405	PEE	O4-C10-O2-C2
3	C	405	PEE	O4-C10-O2-C2
3	D	406	PEE	O4-C10-O2-C2
3	B	406	PEE	O4-C10-O2-C2
3	E	406	PEE	O4-C10-O2-C2
3	A	402	PEE	C37-C38-C39-C40
3	A	409	PEE	C37-C38-C39-C40
3	C	402	PEE	C37-C38-C39-C40
3	C	409	PEE	C37-C38-C39-C40
3	D	401	PEE	C37-C38-C39-C40
3	D	403	PEE	C37-C38-C39-C40
3	B	401	PEE	C37-C38-C39-C40
3	B	403	PEE	C37-C38-C39-C40
3	E	401	PEE	C37-C38-C39-C40
3	E	403	PEE	C37-C38-C39-C40
3	A	402	PEE	C11-C10-O2-C2
3	A	406	PEE	C11-C10-O2-C2
3	A	407	PEE	C11-C10-O2-C2
3	C	402	PEE	C11-C10-O2-C2
3	C	406	PEE	C11-C10-O2-C2
3	C	407	PEE	C11-C10-O2-C2
3	D	403	PEE	C11-C10-O2-C2
3	D	407	PEE	C11-C10-O2-C2
3	D	408	PEE	C11-C10-O2-C2
3	B	403	PEE	C11-C10-O2-C2
3	B	407	PEE	C11-C10-O2-C2
3	B	408	PEE	C11-C10-O2-C2
3	E	403	PEE	C11-C10-O2-C2
3	E	407	PEE	C11-C10-O2-C2
3	E	408	PEE	C11-C10-O2-C2
3	A	406	PEE	O4-C10-O2-C2
3	A	407	PEE	O4-C10-O2-C2
3	C	406	PEE	O4-C10-O2-C2
3	C	407	PEE	O4-C10-O2-C2
3	D	407	PEE	O4-C10-O2-C2
3	D	408	PEE	O4-C10-O2-C2
3	B	407	PEE	O4-C10-O2-C2
3	B	408	PEE	O4-C10-O2-C2
3	E	407	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
3	E	408	PEE	O4-C10-O2-C2
3	A	408	PEE	C17-C18-C19-C20
3	C	408	PEE	C17-C18-C19-C20
3	D	409	PEE	C17-C18-C19-C20
3	B	409	PEE	C17-C18-C19-C20
3	E	409	PEE	C17-C18-C19-C20
3	A	402	PEE	O4-C10-O2-C2
3	C	402	PEE	O4-C10-O2-C2
3	D	403	PEE	O4-C10-O2-C2
3	B	403	PEE	O4-C10-O2-C2
3	E	403	PEE	O4-C10-O2-C2
3	A	409	PEE	C11-C10-O2-C2
3	C	409	PEE	C11-C10-O2-C2
3	D	401	PEE	C11-C10-O2-C2
3	B	401	PEE	C11-C10-O2-C2
3	E	401	PEE	C11-C10-O2-C2
3	A	405	PEE	C10-C11-C12-C13
3	C	405	PEE	C10-C11-C12-C13
3	D	406	PEE	C10-C11-C12-C13
3	B	406	PEE	C10-C11-C12-C13
3	E	406	PEE	C10-C11-C12-C13
3	A	409	PEE	C10-C11-C12-C13
3	C	409	PEE	C10-C11-C12-C13
3	D	401	PEE	C10-C11-C12-C13
3	B	401	PEE	C10-C11-C12-C13
3	E	401	PEE	C10-C11-C12-C13
3	A	409	PEE	O4-C10-O2-C2
3	C	409	PEE	O4-C10-O2-C2
3	D	401	PEE	O4-C10-O2-C2
3	B	401	PEE	O4-C10-O2-C2
3	E	401	PEE	O4-C10-O2-C2
3	A	409	PEE	C11-C12-C13-C14
3	C	409	PEE	C11-C12-C13-C14
3	D	401	PEE	C12-C13-C14-C15
3	D	401	PEE	C11-C12-C13-C14
3	B	401	PEE	C12-C13-C14-C15
3	E	401	PEE	C12-C13-C14-C15
3	A	409	PEE	C12-C13-C14-C15
3	C	409	PEE	C12-C13-C14-C15
3	B	401	PEE	C11-C12-C13-C14
3	E	401	PEE	C11-C12-C13-C14
3	A	409	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	C	409	PEE	O3P-C1-C2-C3
3	D	401	PEE	O3P-C1-C2-C3
3	B	401	PEE	O3P-C1-C2-C3
3	E	401	PEE	O3P-C1-C2-C3
3	A	403	PEE	C10-C11-C12-C13
3	C	403	PEE	C10-C11-C12-C13
3	D	404	PEE	C10-C11-C12-C13
3	B	404	PEE	C10-C11-C12-C13
3	E	404	PEE	C10-C11-C12-C13
3	A	404	PEE	C1-C2-C3-O3
3	A	409	PEE	C1-C2-C3-O3
3	C	404	PEE	C1-C2-C3-O3
3	C	409	PEE	C1-C2-C3-O3
3	D	401	PEE	C1-C2-C3-O3
3	D	405	PEE	C1-C2-C3-O3
3	B	401	PEE	C1-C2-C3-O3
3	B	405	PEE	C1-C2-C3-O3
3	E	401	PEE	C1-C2-C3-O3
3	E	405	PEE	C1-C2-C3-O3
3	A	402	PEE	C32-C33-C34-C35
3	B	403	PEE	C32-C33-C34-C35
3	C	402	PEE	C32-C33-C34-C35
3	D	403	PEE	C32-C33-C34-C35
3	E	403	PEE	C32-C33-C34-C35
3	A	405	PEE	O2-C2-C3-O3
3	C	405	PEE	O2-C2-C3-O3
3	D	406	PEE	O2-C2-C3-O3
3	B	406	PEE	O2-C2-C3-O3
3	E	406	PEE	O2-C2-C3-O3
3	A	409	PEE	C40-C41-C42-C43
3	D	401	PEE	C40-C41-C42-C43
3	B	401	PEE	C40-C41-C42-C43
3	E	401	PEE	C40-C41-C42-C43
3	C	409	PEE	C40-C41-C42-C43
3	A	405	PEE	C1-C2-C3-O3
3	C	405	PEE	C1-C2-C3-O3
3	D	406	PEE	C1-C2-C3-O3
3	B	406	PEE	C1-C2-C3-O3
3	E	406	PEE	C1-C2-C3-O3
3	A	402	PEE	O3P-C1-C2-O2
3	C	402	PEE	O3P-C1-C2-O2
3	D	403	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	408	PEE	O3P-C1-C2-O2
3	B	403	PEE	O3P-C1-C2-O2
3	B	408	PEE	O3P-C1-C2-O2
3	E	403	PEE	O3P-C1-C2-O2
3	E	408	PEE	O3P-C1-C2-O2
3	A	406	PEE	C3-C2-O2-C10
3	C	406	PEE	C3-C2-O2-C10
3	D	407	PEE	C3-C2-O2-C10
3	B	407	PEE	C3-C2-O2-C10
3	E	407	PEE	C3-C2-O2-C10
3	A	405	PEE	C16-C17-C18-C19
3	C	405	PEE	C16-C17-C18-C19
3	D	406	PEE	C16-C17-C18-C19
3	B	406	PEE	C16-C17-C18-C19
3	E	406	PEE	C16-C17-C18-C19
3	A	407	PEE	O3P-C1-C2-O2
3	C	407	PEE	O3P-C1-C2-O2
3	A	403	PEE	C1-C2-C3-O3
3	C	403	PEE	C1-C2-C3-O3
3	D	404	PEE	C1-C2-C3-O3
3	B	404	PEE	C1-C2-C3-O3
3	E	404	PEE	C1-C2-C3-O3
3	A	409	PEE	O2-C2-C3-O3
3	C	409	PEE	O2-C2-C3-O3
3	D	401	PEE	O2-C2-C3-O3
3	B	401	PEE	O2-C2-C3-O3
3	E	401	PEE	O2-C2-C3-O3
3	A	404	PEE	C31-C32-C33-C34
3	C	404	PEE	C31-C32-C33-C34
3	D	405	PEE	C31-C32-C33-C34
3	E	405	PEE	C31-C32-C33-C34
3	B	405	PEE	C31-C32-C33-C34
3	A	402	PEE	O3P-C1-C2-C3
3	C	402	PEE	O3P-C1-C2-C3
3	D	403	PEE	O3P-C1-C2-C3
3	B	403	PEE	O3P-C1-C2-C3
3	E	403	PEE	O3P-C1-C2-C3
3	A	402	PEE	C2-C1-O3P-P
3	D	403	PEE	C2-C1-O3P-P
3	E	403	PEE	C2-C1-O3P-P
3	A	409	PEE	O3P-C1-C2-O2
3	C	409	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	401	PEE	O3P-C1-C2-O2
3	B	401	PEE	O3P-C1-C2-O2
3	E	401	PEE	O3P-C1-C2-O2
3	A	407	PEE	C13-C14-C15-C16
3	D	408	PEE	C13-C14-C15-C16
3	B	408	PEE	C13-C14-C15-C16
3	E	408	PEE	C13-C14-C15-C16
3	C	407	PEE	C13-C14-C15-C16
3	A	404	PEE	C1-O3P-P-O1P
3	A	407	PEE	C1-O3P-P-O4P
3	A	407	PEE	C4-O4P-P-O1P
3	A	409	PEE	C4-O4P-P-O3P
3	A	409	PEE	C4-O4P-P-O2P
3	C	404	PEE	C1-O3P-P-O1P
3	C	407	PEE	C1-O3P-P-O4P
3	C	407	PEE	C4-O4P-P-O1P
3	C	409	PEE	C4-O4P-P-O3P
3	C	409	PEE	C4-O4P-P-O2P
3	D	401	PEE	C4-O4P-P-O3P
3	D	401	PEE	C4-O4P-P-O2P
3	D	405	PEE	C1-O3P-P-O1P
3	D	408	PEE	C1-O3P-P-O4P
3	D	408	PEE	C4-O4P-P-O1P
3	B	401	PEE	C4-O4P-P-O3P
3	B	401	PEE	C4-O4P-P-O2P
3	B	405	PEE	C1-O3P-P-O1P
3	B	408	PEE	C1-O3P-P-O4P
3	B	408	PEE	C4-O4P-P-O1P
3	E	401	PEE	C4-O4P-P-O3P
3	E	401	PEE	C4-O4P-P-O2P
3	E	405	PEE	C1-O3P-P-O1P
3	E	408	PEE	C1-O3P-P-O4P
3	E	408	PEE	C4-O4P-P-O1P
3	C	402	PEE	C2-C1-O3P-P
3	B	403	PEE	C2-C1-O3P-P
3	A	402	PEE	C3-C2-O2-C10
3	A	409	PEE	C3-C2-O2-C10
3	C	402	PEE	C3-C2-O2-C10
3	C	409	PEE	C3-C2-O2-C10
3	D	401	PEE	C3-C2-O2-C10
3	D	403	PEE	C3-C2-O2-C10
3	B	401	PEE	C3-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
3	B	403	PEE	C3-C2-O2-C10
3	E	401	PEE	C3-C2-O2-C10
3	E	403	PEE	C3-C2-O2-C10
3	D	403	PEE	C11-C12-C13-C14
3	E	403	PEE	C11-C12-C13-C14
3	A	404	PEE	C18-C19-C20-C21
3	C	404	PEE	C18-C19-C20-C21
3	D	405	PEE	C18-C19-C20-C21
3	B	405	PEE	C18-C19-C20-C21
3	E	405	PEE	C18-C19-C20-C21
3	C	402	PEE	C11-C12-C13-C14
3	B	403	PEE	C11-C12-C13-C14
3	A	402	PEE	C11-C12-C13-C14
3	A	406	PEE	C2-C1-O3P-P
3	C	406	PEE	C2-C1-O3P-P
3	D	407	PEE	C2-C1-O3P-P
3	B	407	PEE	C2-C1-O3P-P
3	E	407	PEE	C2-C1-O3P-P
3	A	404	PEE	C38-C39-C40-C41
3	C	404	PEE	C38-C39-C40-C41
3	D	405	PEE	C38-C39-C40-C41
3	B	405	PEE	C38-C39-C40-C41
3	E	405	PEE	C38-C39-C40-C41
3	A	406	PEE	C16-C17-C18-C19
3	B	407	PEE	C16-C17-C18-C19
3	A	404	PEE	C17-C18-C19-C20
3	C	404	PEE	C17-C18-C19-C20
3	D	405	PEE	C17-C18-C19-C20
3	B	405	PEE	C17-C18-C19-C20
3	E	405	PEE	C17-C18-C19-C20
3	A	404	PEE	C34-C35-C36-C37
3	C	404	PEE	C34-C35-C36-C37
3	D	405	PEE	C34-C35-C36-C37
3	B	405	PEE	C34-C35-C36-C37
3	E	405	PEE	C34-C35-C36-C37
3	C	406	PEE	C16-C17-C18-C19
3	D	407	PEE	C16-C17-C18-C19
3	E	407	PEE	C16-C17-C18-C19
3	A	407	PEE	O3P-C1-C2-C3
3	D	408	PEE	O3P-C1-C2-C3
3	B	408	PEE	O3P-C1-C2-C3
3	E	408	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	402	PEE	C38-C39-C40-C41
3	C	402	PEE	C38-C39-C40-C41
3	D	403	PEE	C38-C39-C40-C41
3	B	403	PEE	C38-C39-C40-C41
3	E	403	PEE	C38-C39-C40-C41
3	A	406	PEE	C42-C43-C44-C45
3	D	407	PEE	C42-C43-C44-C45
3	C	406	PEE	C42-C43-C44-C45
3	B	407	PEE	C42-C43-C44-C45
3	E	407	PEE	C42-C43-C44-C45
3	A	409	PEE	C18-C19-C20-C21
3	C	409	PEE	C18-C19-C20-C21
3	D	401	PEE	C18-C19-C20-C21
3	B	401	PEE	C18-C19-C20-C21
3	E	401	PEE	C18-C19-C20-C21
3	C	407	PEE	O3P-C1-C2-C3
3	C	404	PEE	C16-C17-C18-C19
3	D	405	PEE	C16-C17-C18-C19
3	E	405	PEE	C16-C17-C18-C19
3	A	404	PEE	C16-C17-C18-C19
3	B	405	PEE	C16-C17-C18-C19
3	A	406	PEE	C38-C39-C40-C41
3	A	407	PEE	C36-C37-C38-C39
3	C	407	PEE	C36-C37-C38-C39
3	D	408	PEE	C36-C37-C38-C39
3	E	407	PEE	C38-C39-C40-C41
3	E	408	PEE	C36-C37-C38-C39
3	C	406	PEE	C38-C39-C40-C41
3	D	407	PEE	C38-C39-C40-C41
3	B	407	PEE	C38-C39-C40-C41
3	B	408	PEE	C36-C37-C38-C39
3	A	404	PEE	C36-C37-C38-C39
3	C	404	PEE	C36-C37-C38-C39
3	D	405	PEE	C36-C37-C38-C39
3	B	405	PEE	C36-C37-C38-C39
3	E	405	PEE	C36-C37-C38-C39
3	A	406	PEE	C36-C37-C38-C39
3	C	406	PEE	C36-C37-C38-C39
3	D	407	PEE	C36-C37-C38-C39
3	B	407	PEE	C36-C37-C38-C39
3	E	407	PEE	C36-C37-C38-C39
3	A	408	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	C	408	PEE	C31-C32-C33-C34
3	D	409	PEE	C31-C32-C33-C34
3	B	409	PEE	C31-C32-C33-C34
3	E	409	PEE	C31-C32-C33-C34
3	A	409	PEE	C16-C17-C18-C19
3	D	401	PEE	C16-C17-C18-C19
3	B	401	PEE	C16-C17-C18-C19
3	E	401	PEE	C16-C17-C18-C19
3	C	409	PEE	C16-C17-C18-C19
3	A	404	PEE	C14-C15-C16-C17
3	C	404	PEE	C14-C15-C16-C17
3	D	405	PEE	C14-C15-C16-C17
3	E	405	PEE	C14-C15-C16-C17
3	B	405	PEE	C14-C15-C16-C17
3	A	409	PEE	C38-C39-C40-C41
3	C	409	PEE	C38-C39-C40-C41
3	D	401	PEE	C38-C39-C40-C41
3	B	401	PEE	C38-C39-C40-C41
3	E	401	PEE	C38-C39-C40-C41

There are no ring outliers.

24 monomers are involved in 52 short contacts:

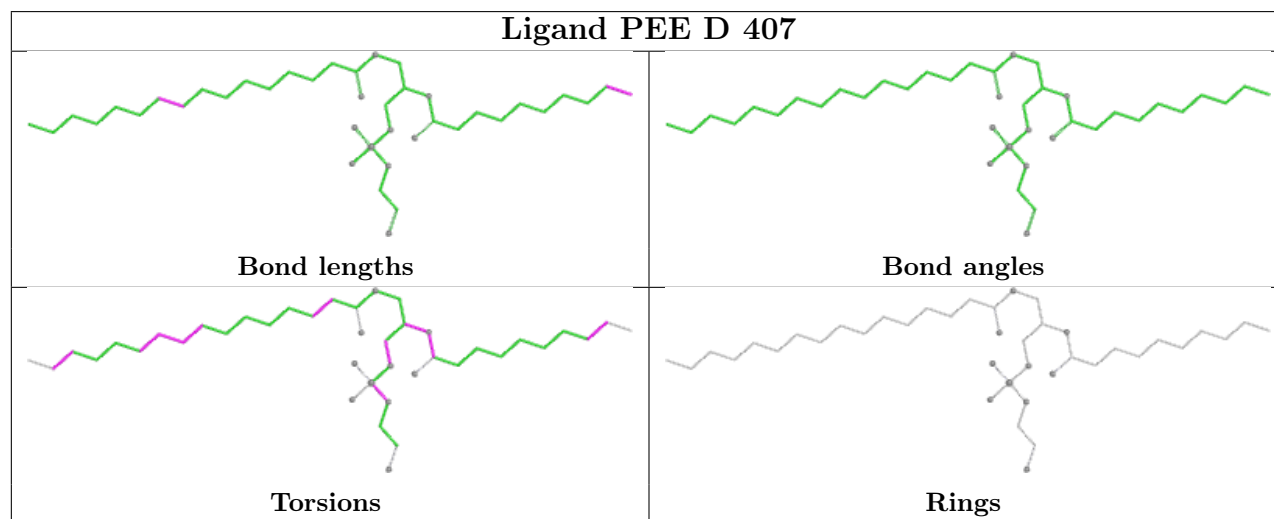
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	407	PEE	3	0
3	B	408	PEE	1	0
3	C	403	PEE	1	0
3	D	408	PEE	1	0
3	D	404	PEE	1	0
3	A	406	PEE	2	0
3	B	401	PEE	1	0
3	A	408	PEE	5	0
3	A	409	PEE	1	0
3	E	407	PEE	3	0
3	C	407	PEE	1	0
3	A	403	PEE	1	0
3	C	406	PEE	3	0
3	E	409	PEE	6	0
3	B	409	PEE	5	0
3	C	408	PEE	6	0
3	B	407	PEE	2	0
3	E	401	PEE	1	0

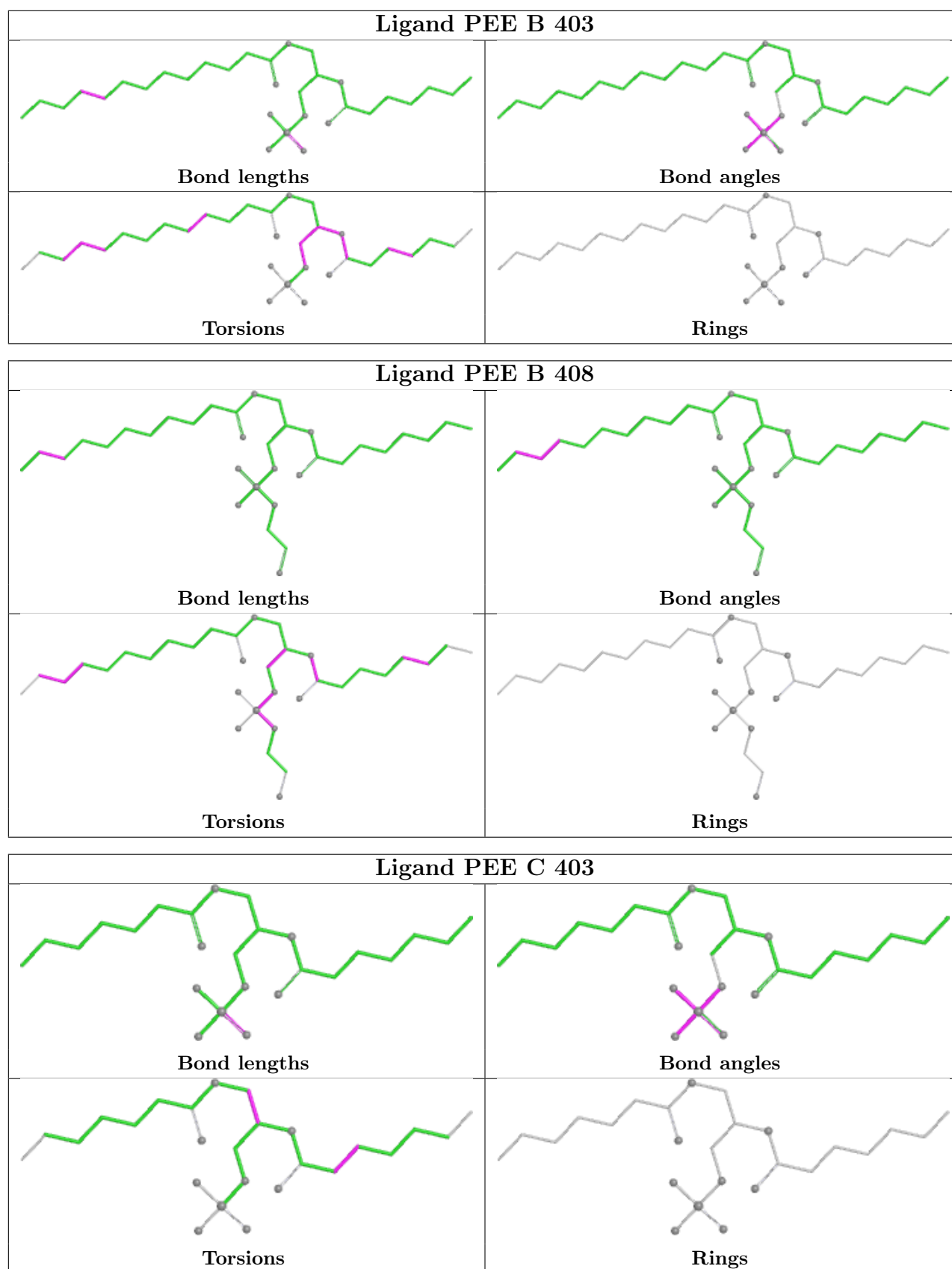
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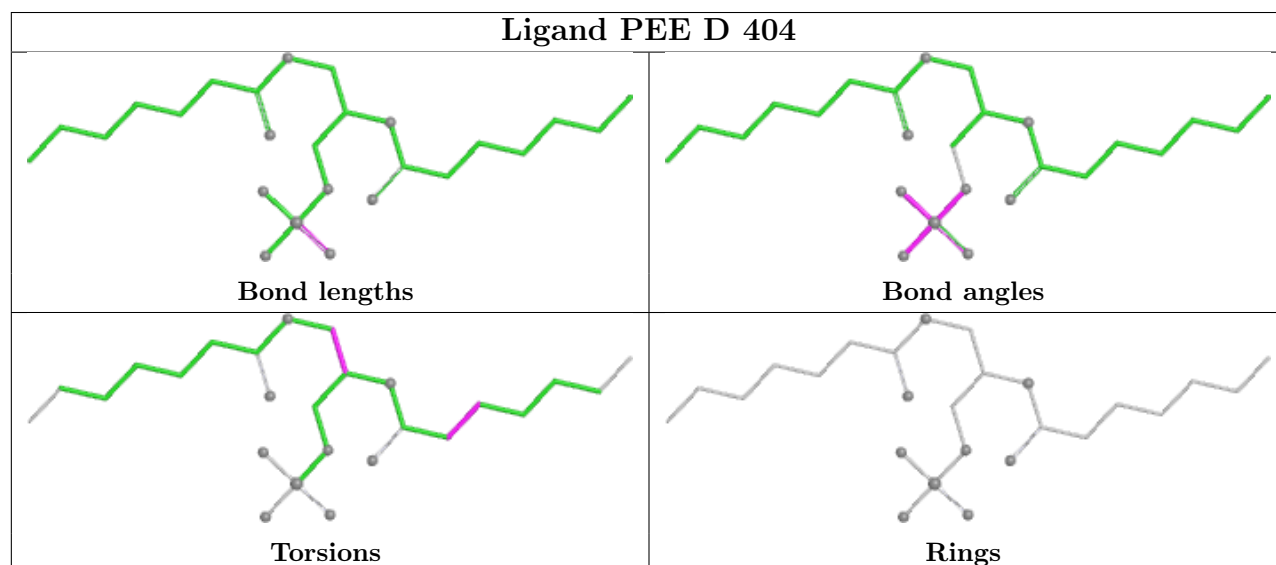
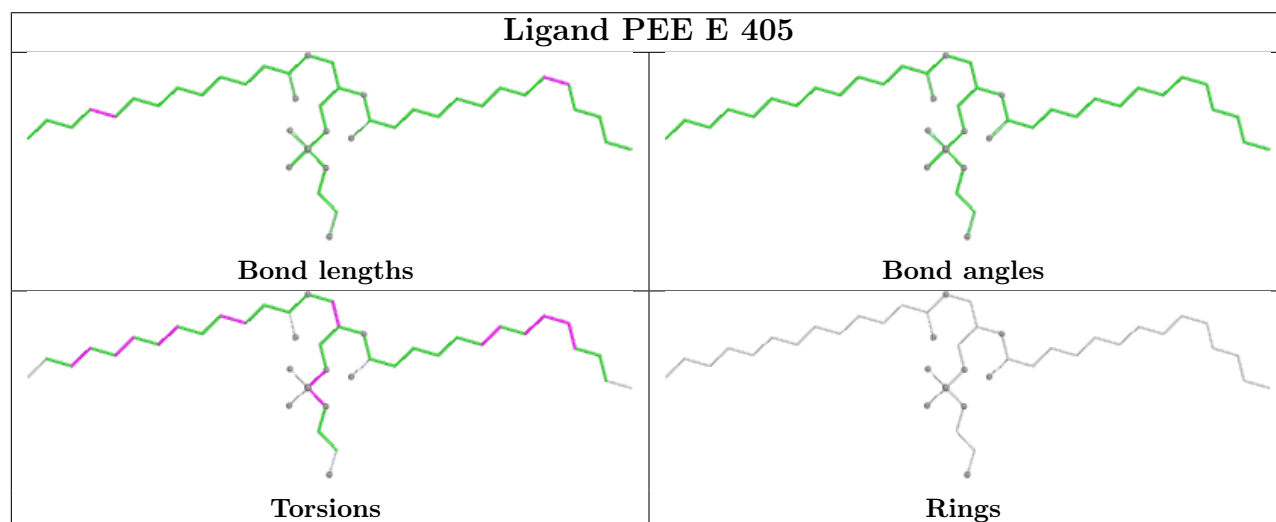
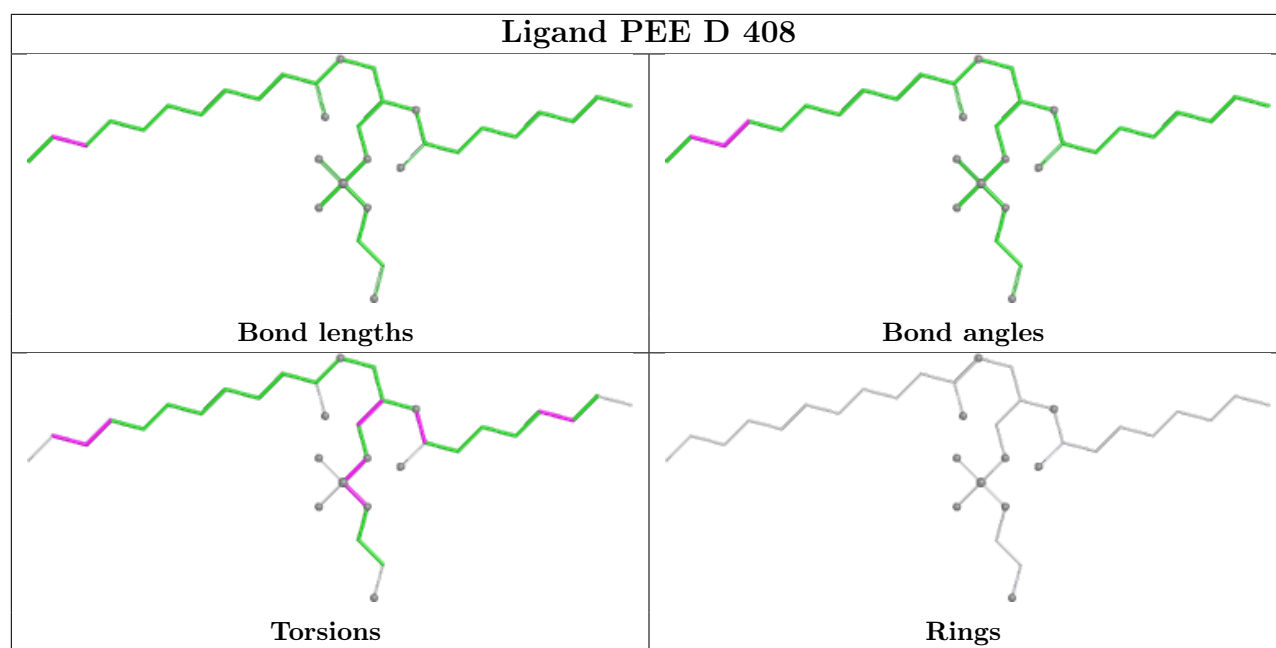
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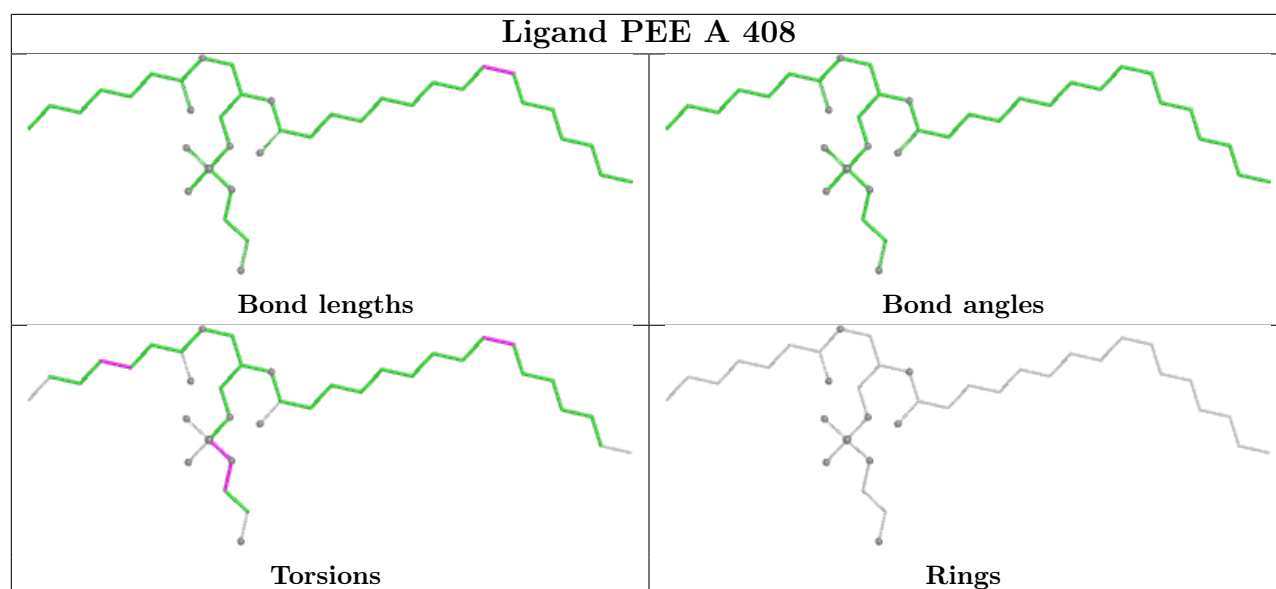
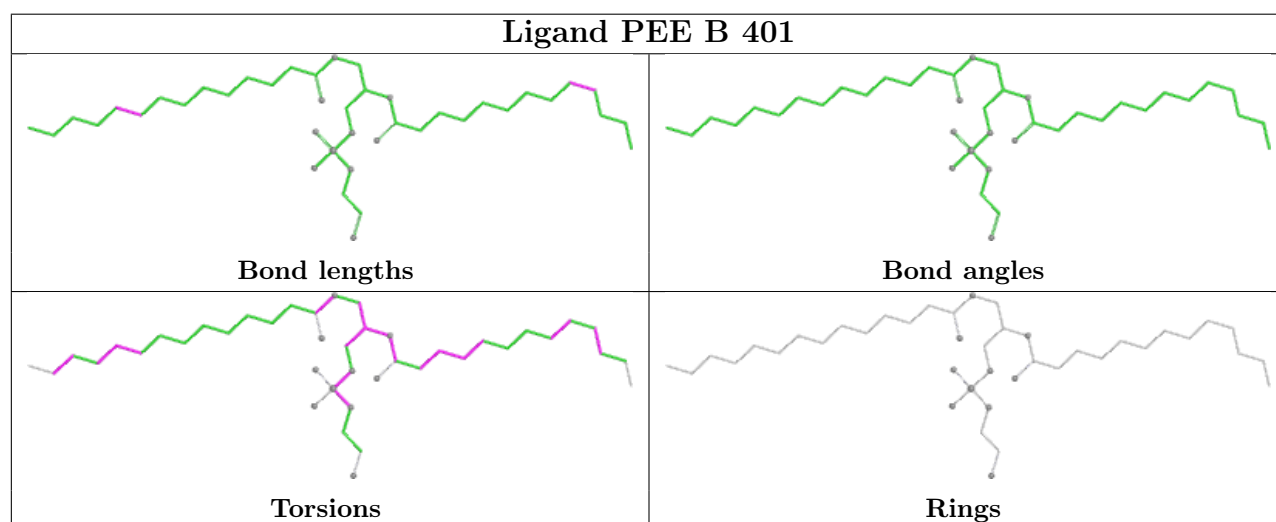
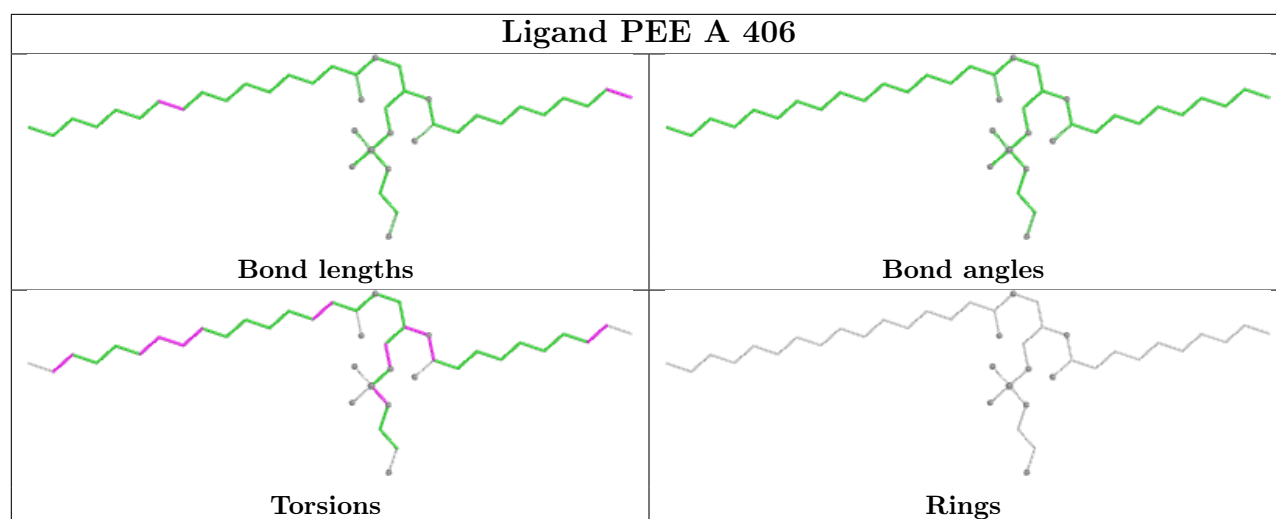
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	404	PEE	1	0
3	E	408	PEE	1	0
3	D	401	PEE	1	0
3	D	409	PEE	8	0
3	A	407	PEE	1	0
3	B	404	PEE	1	0

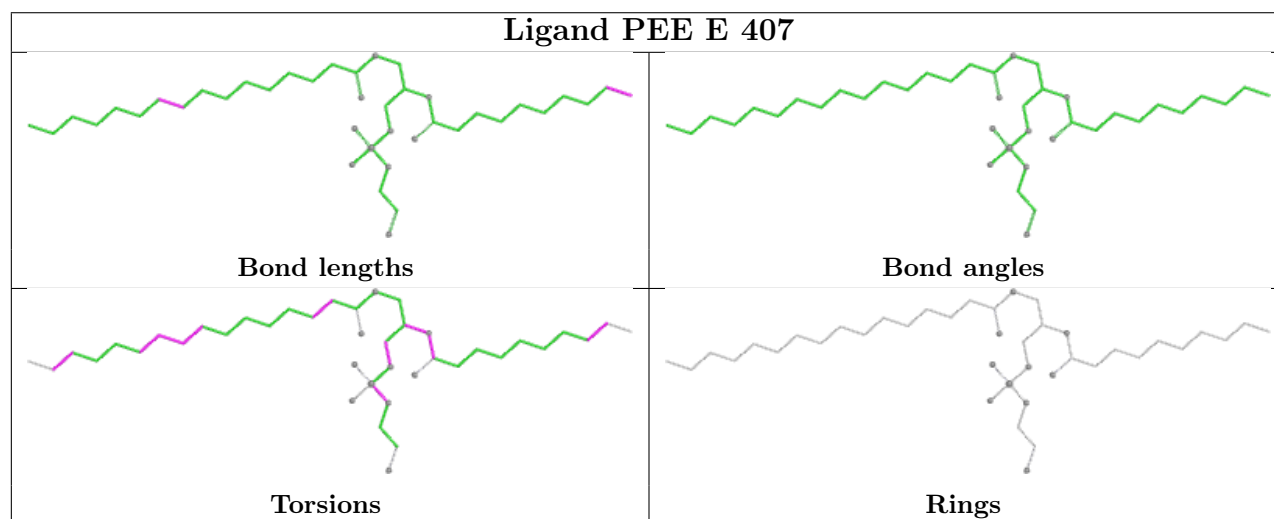
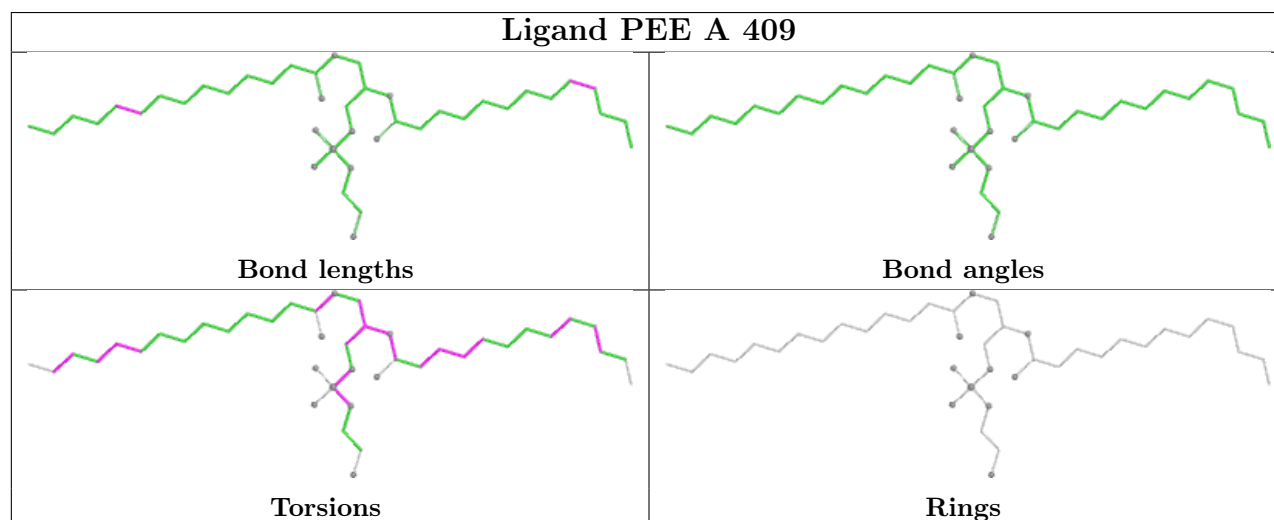
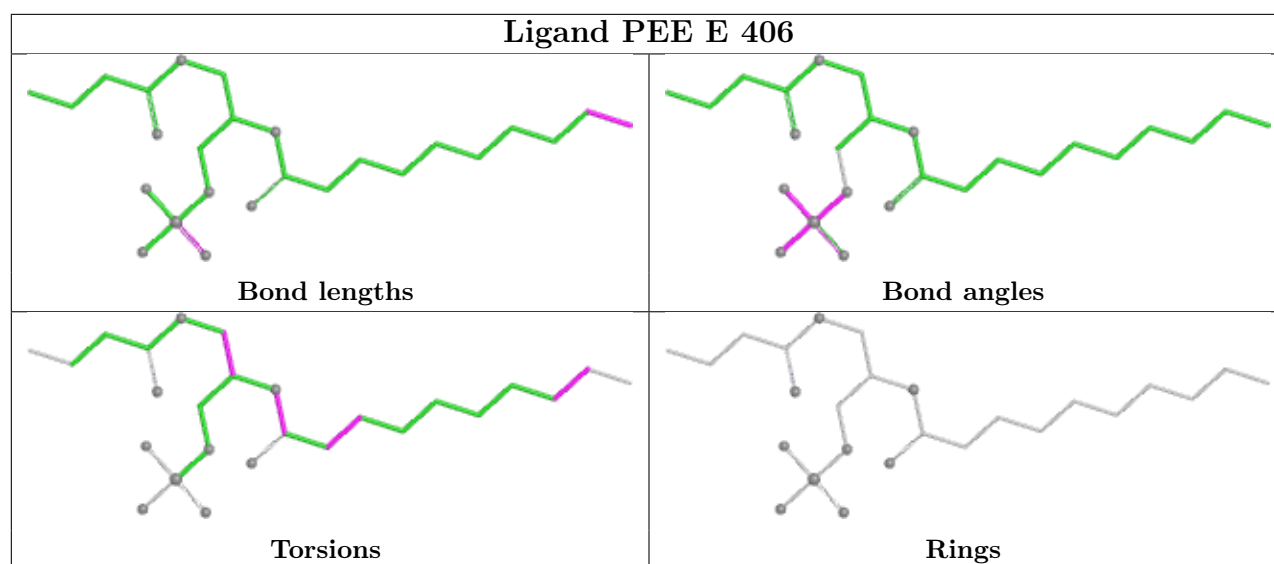
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

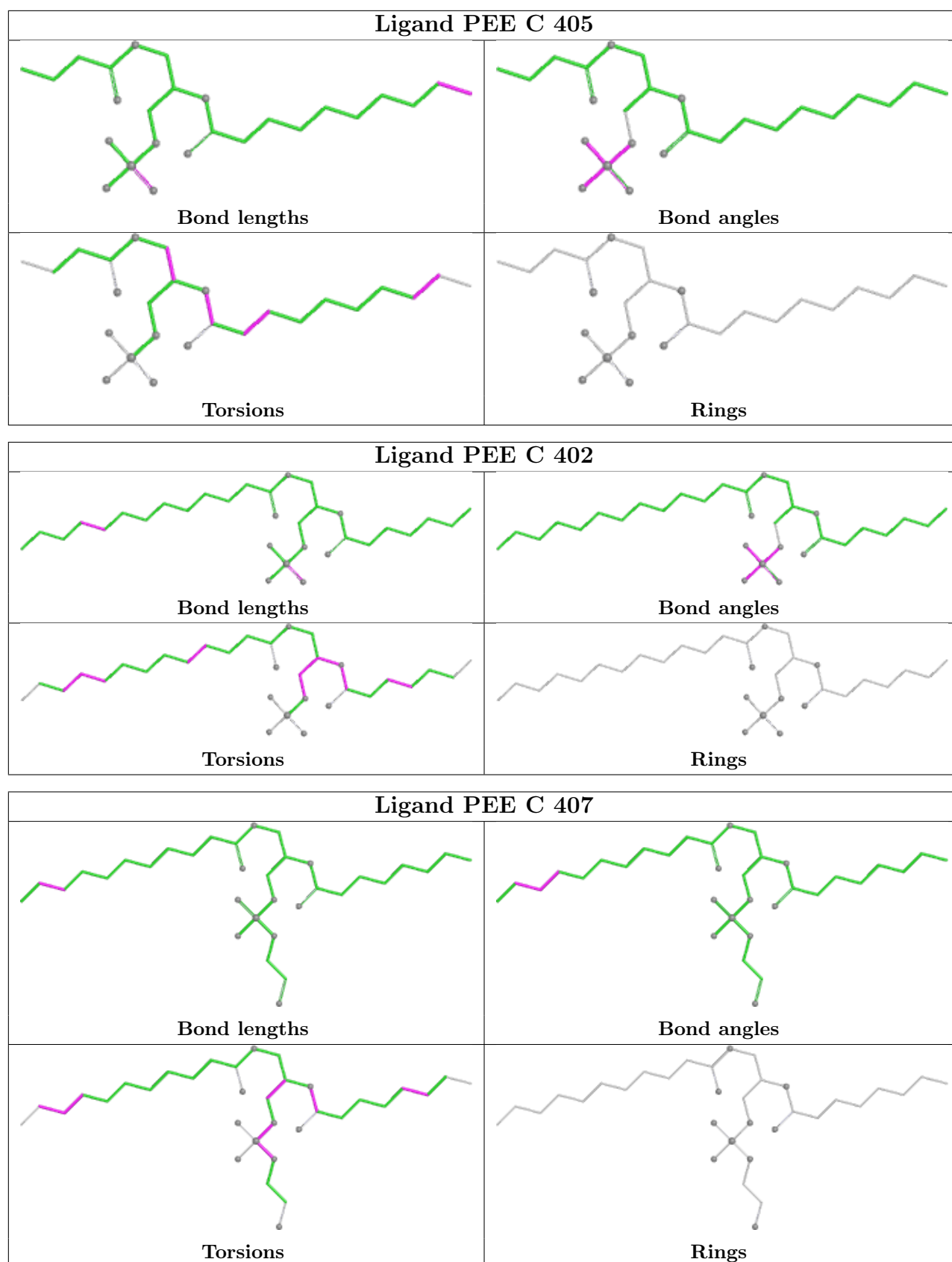


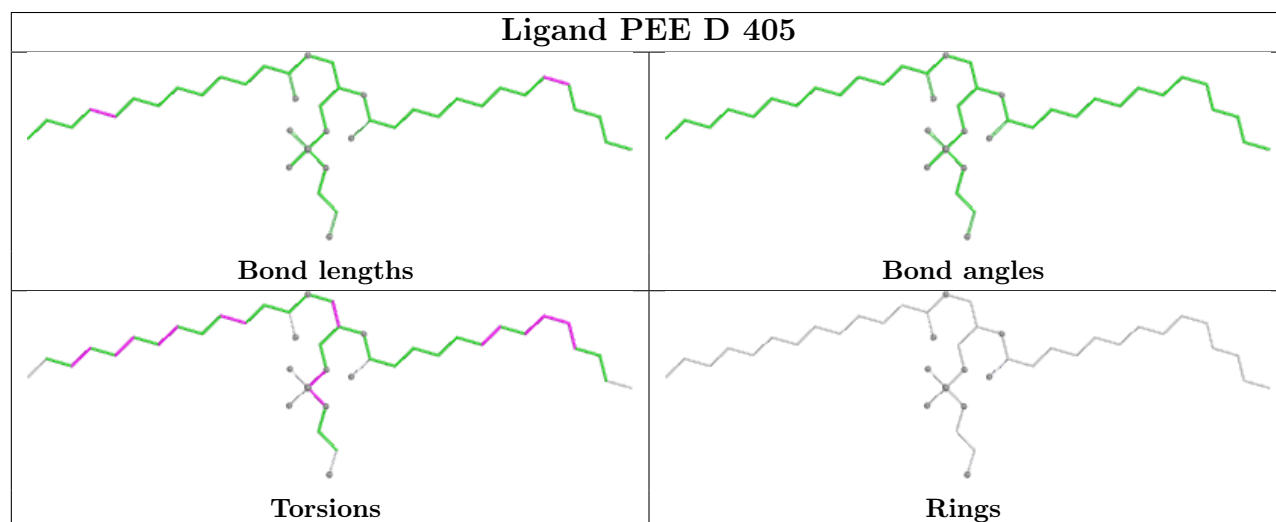
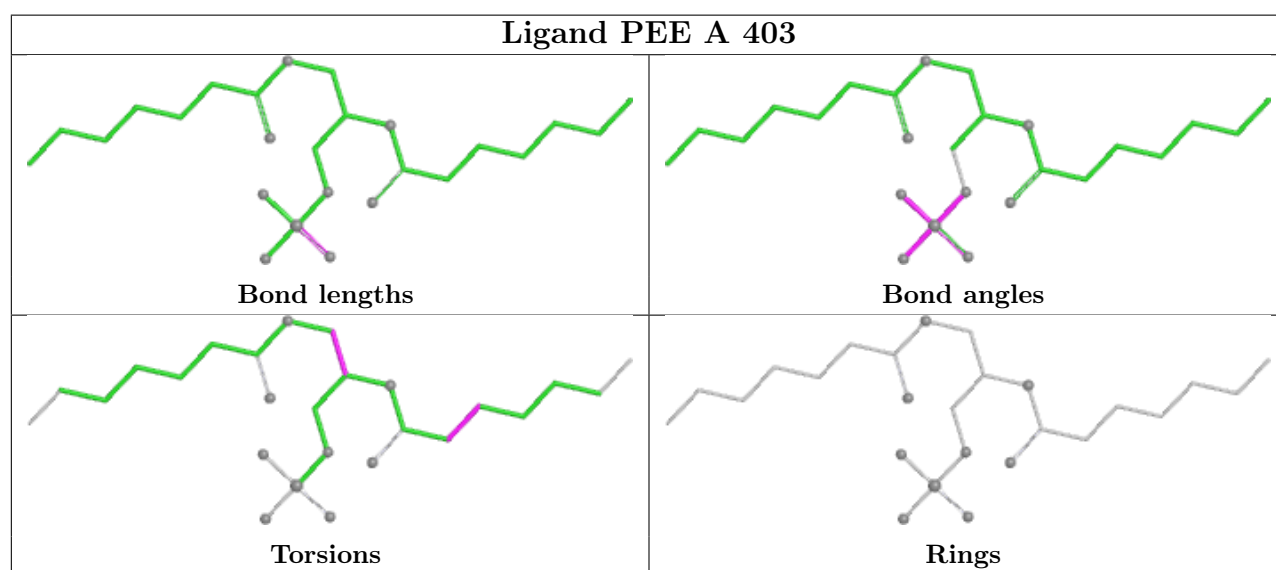
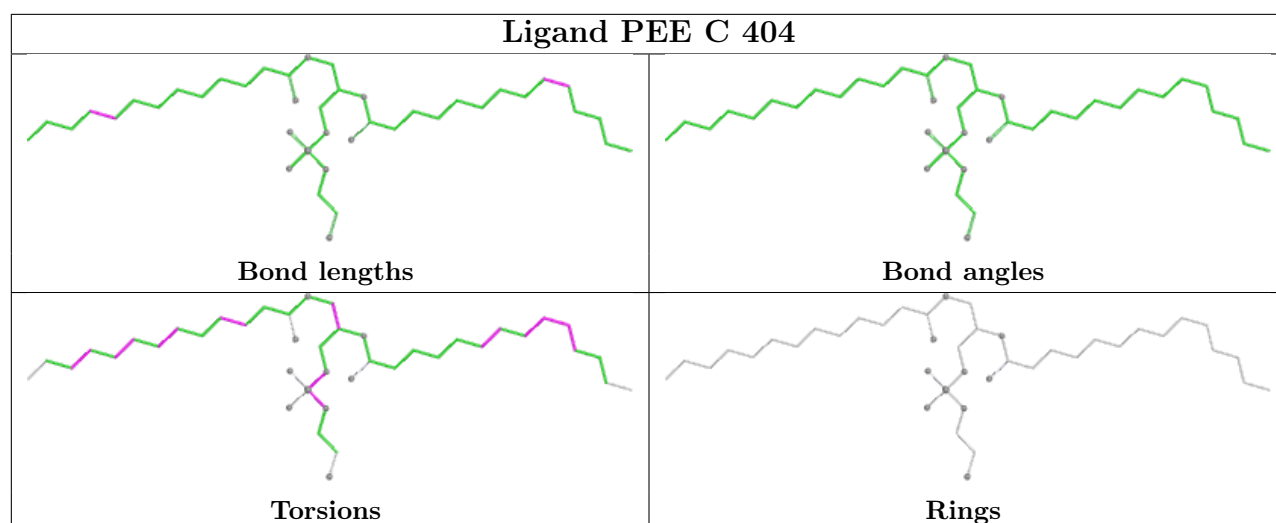


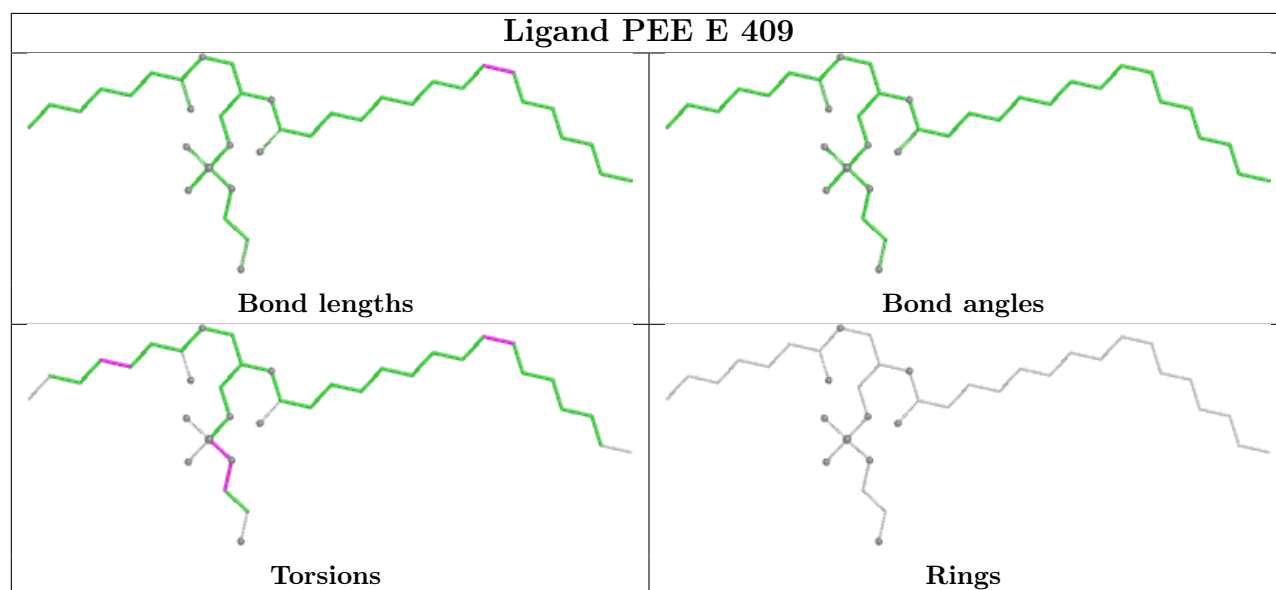
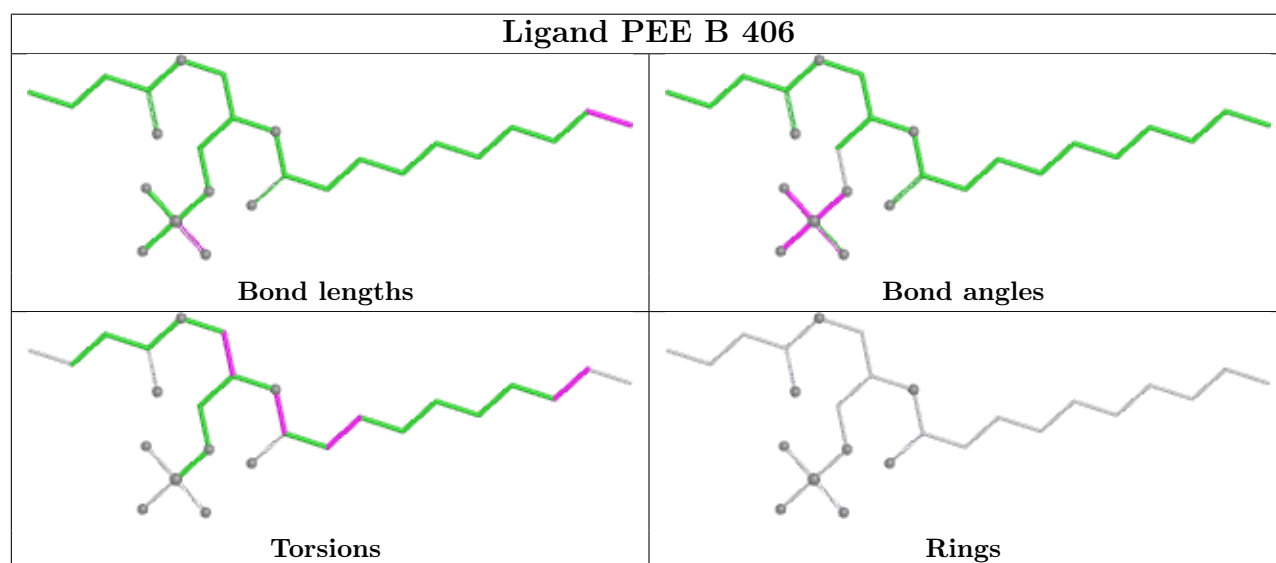
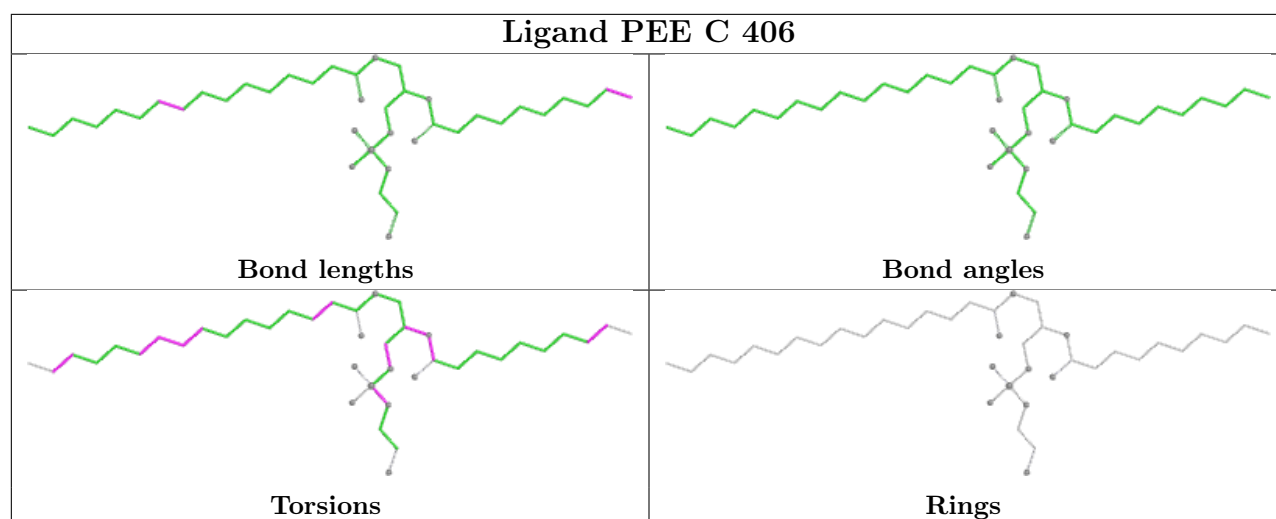


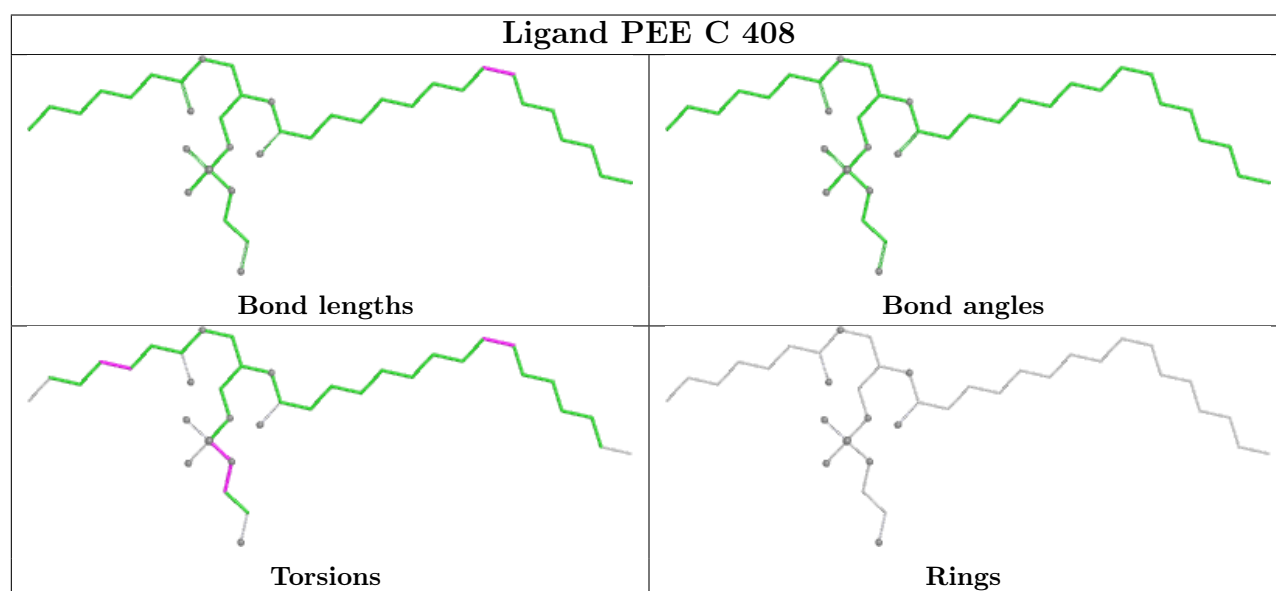
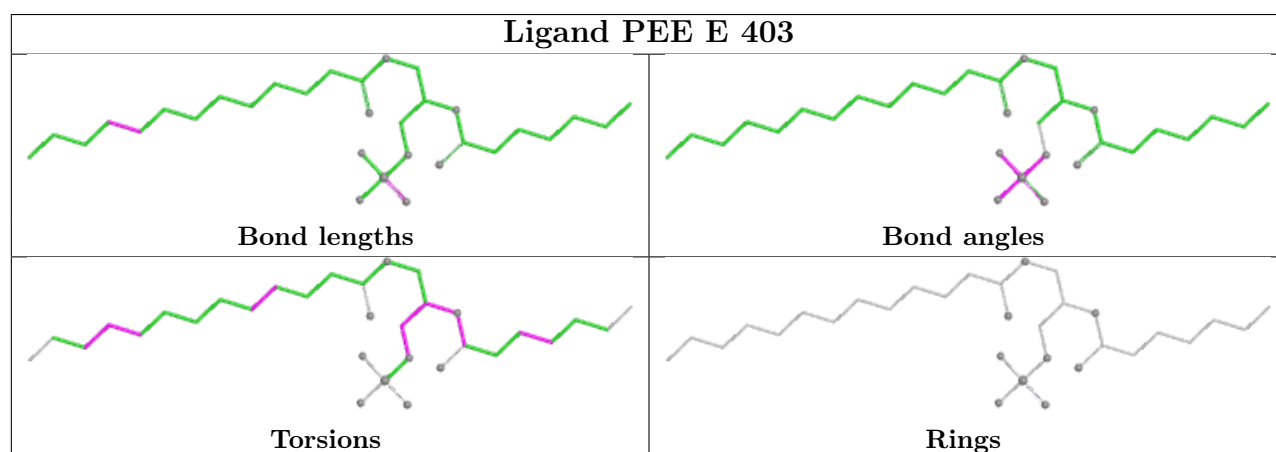
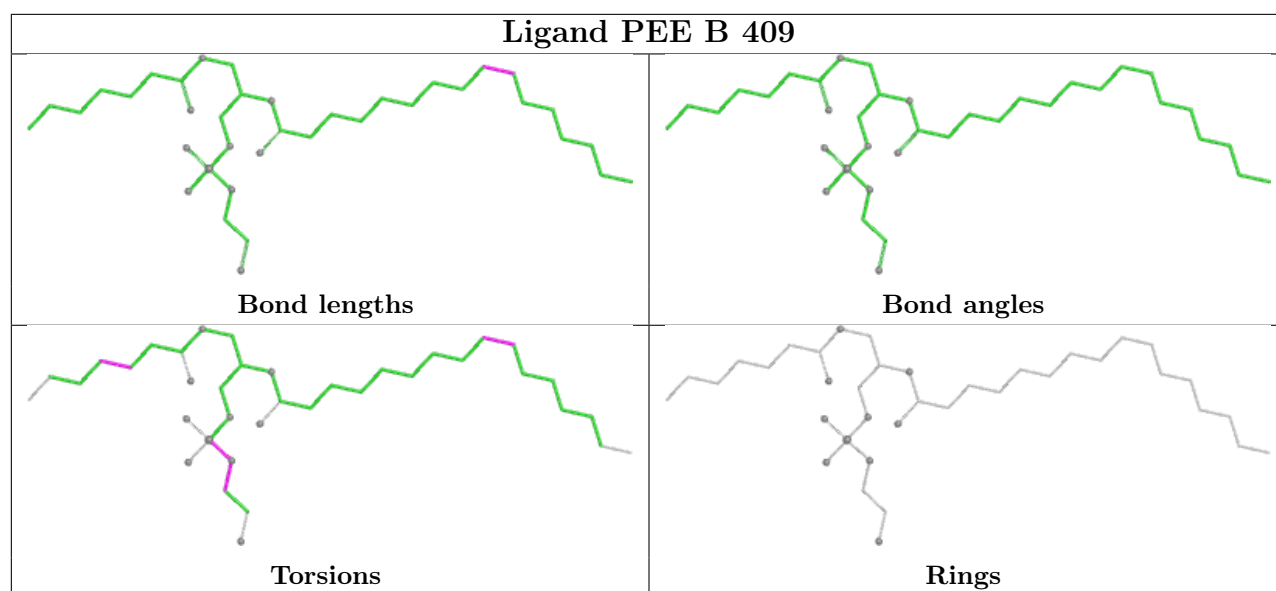


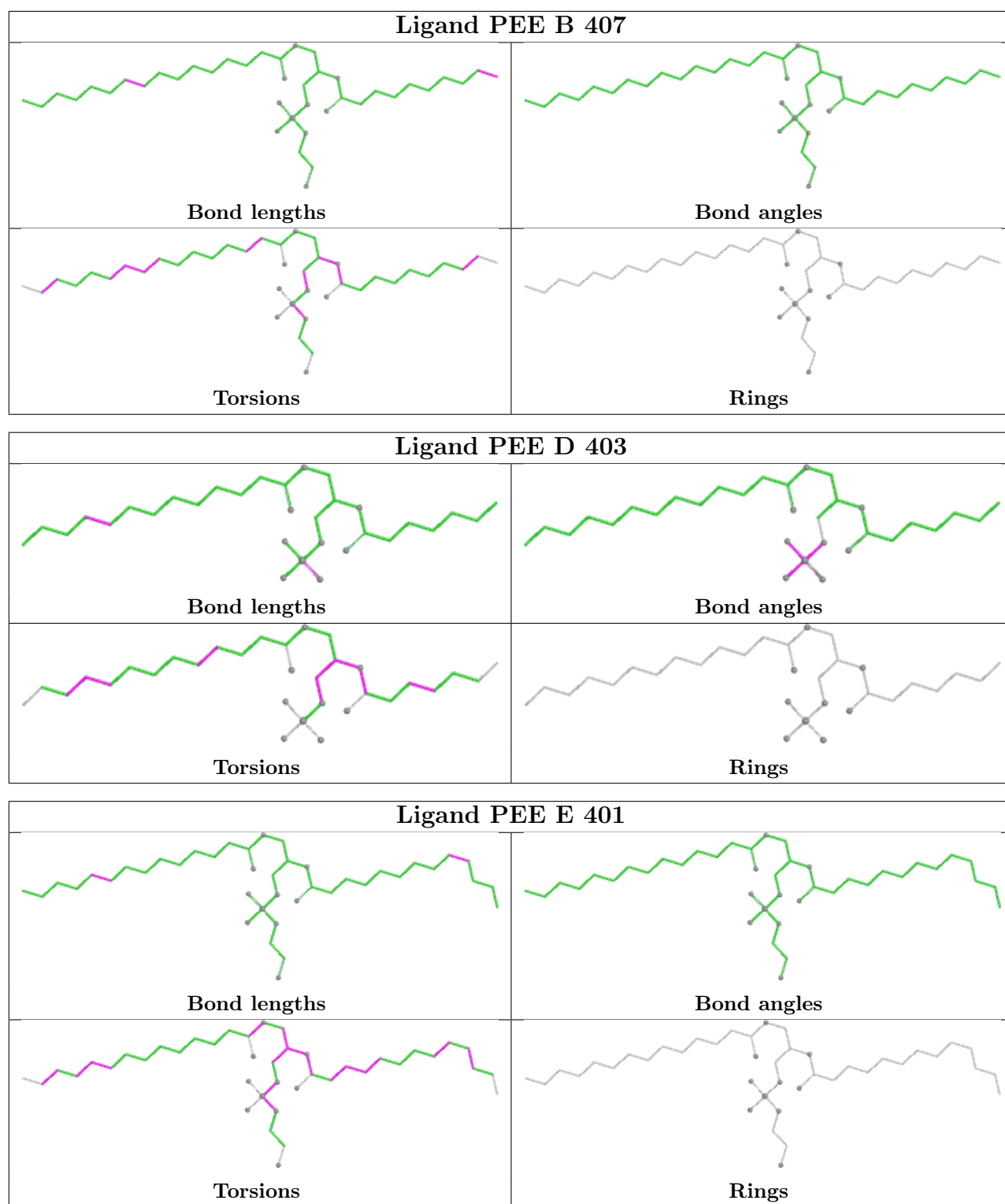


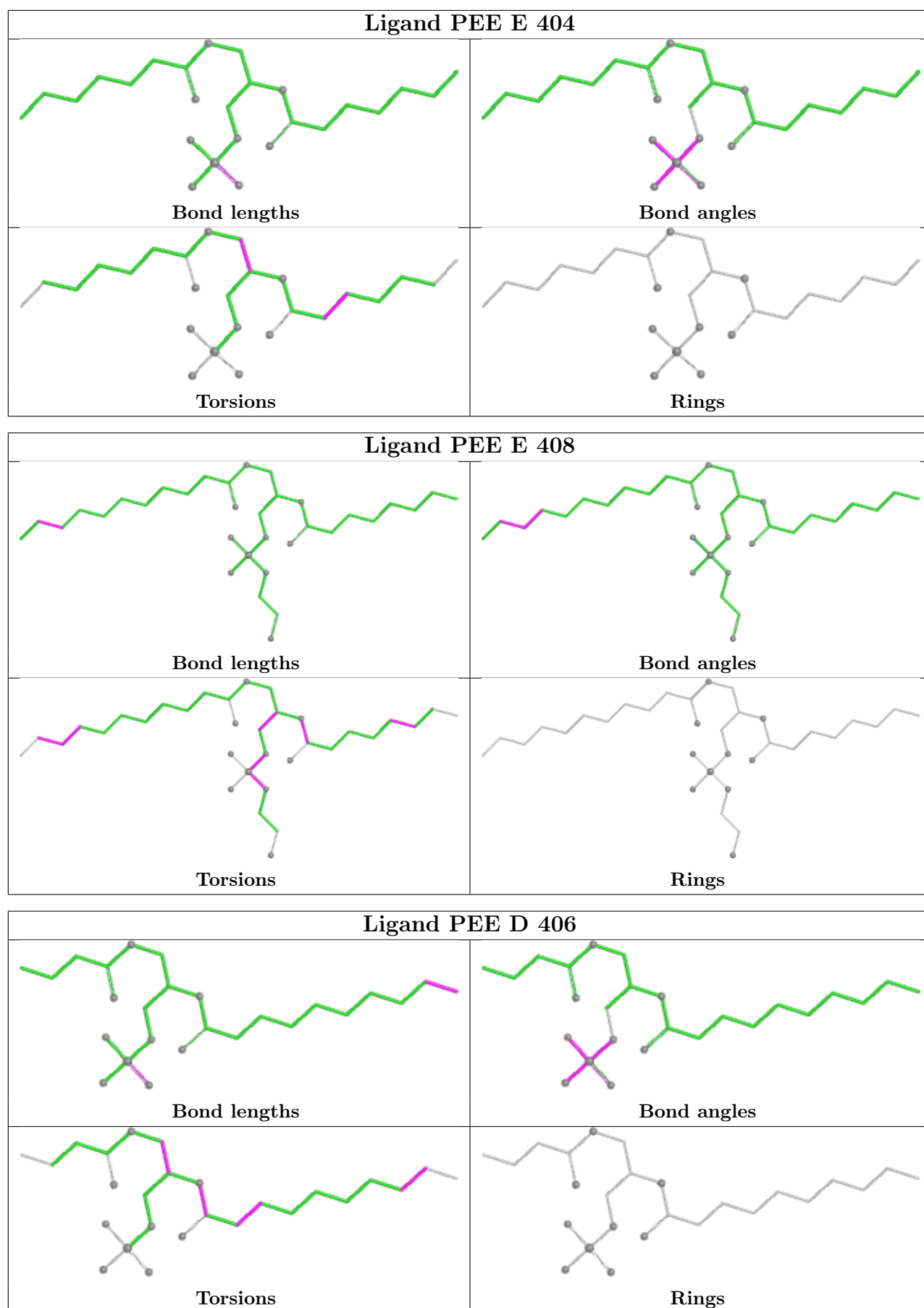


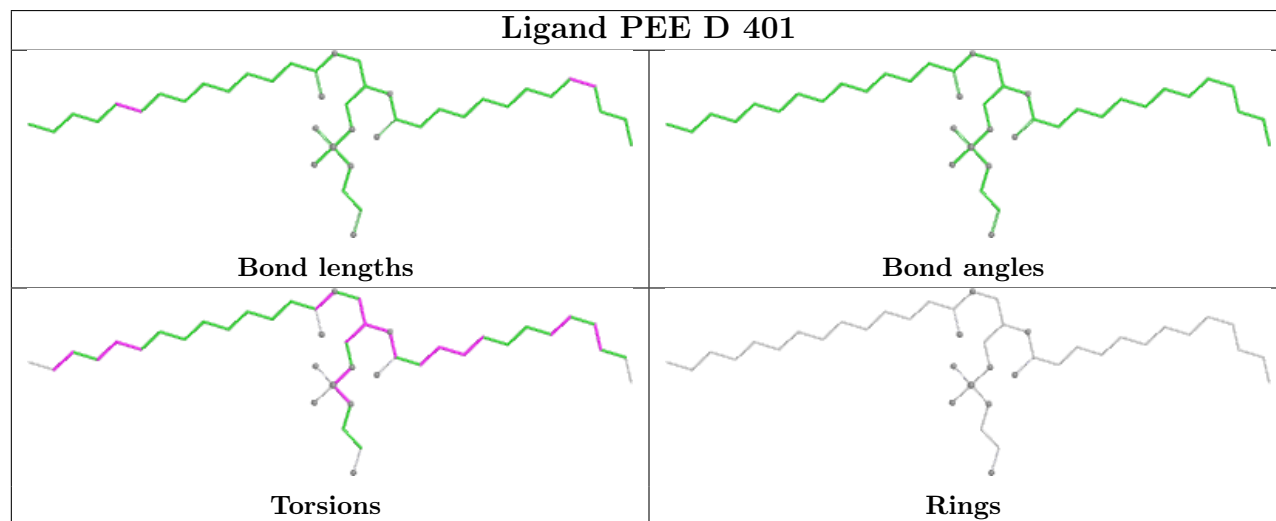
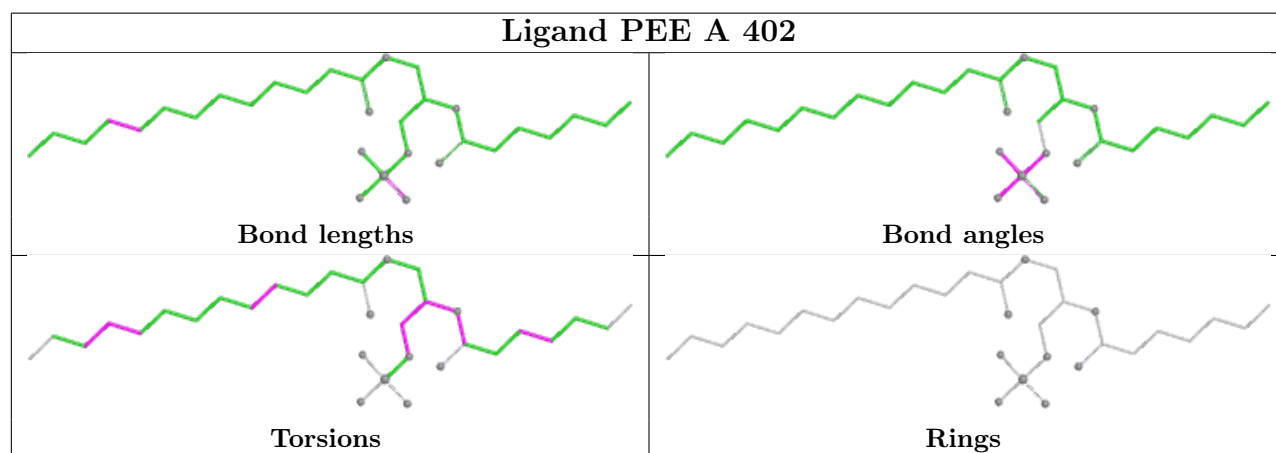
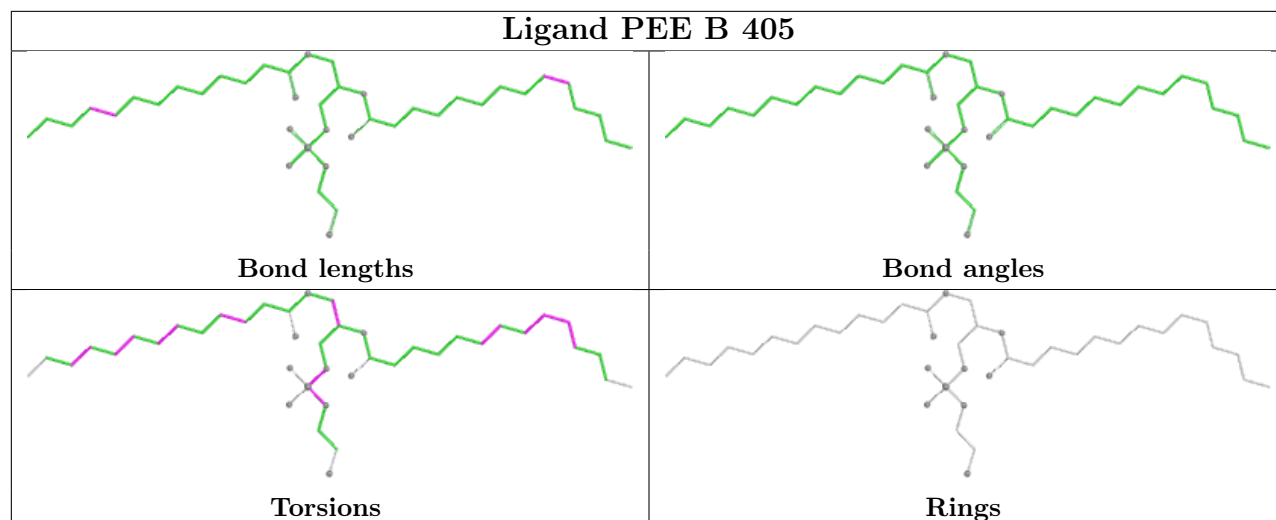


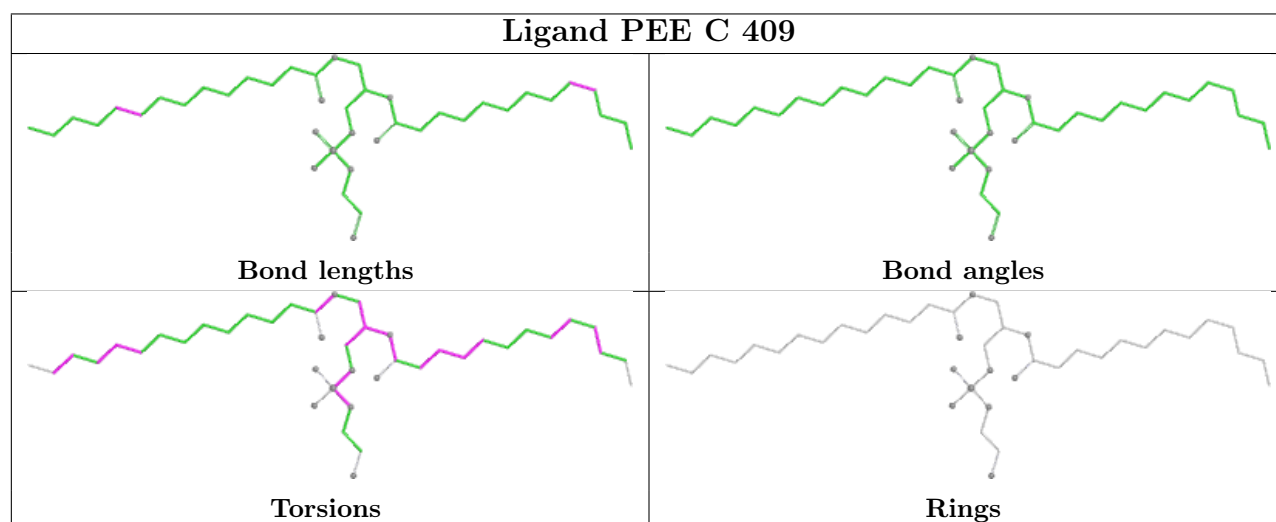
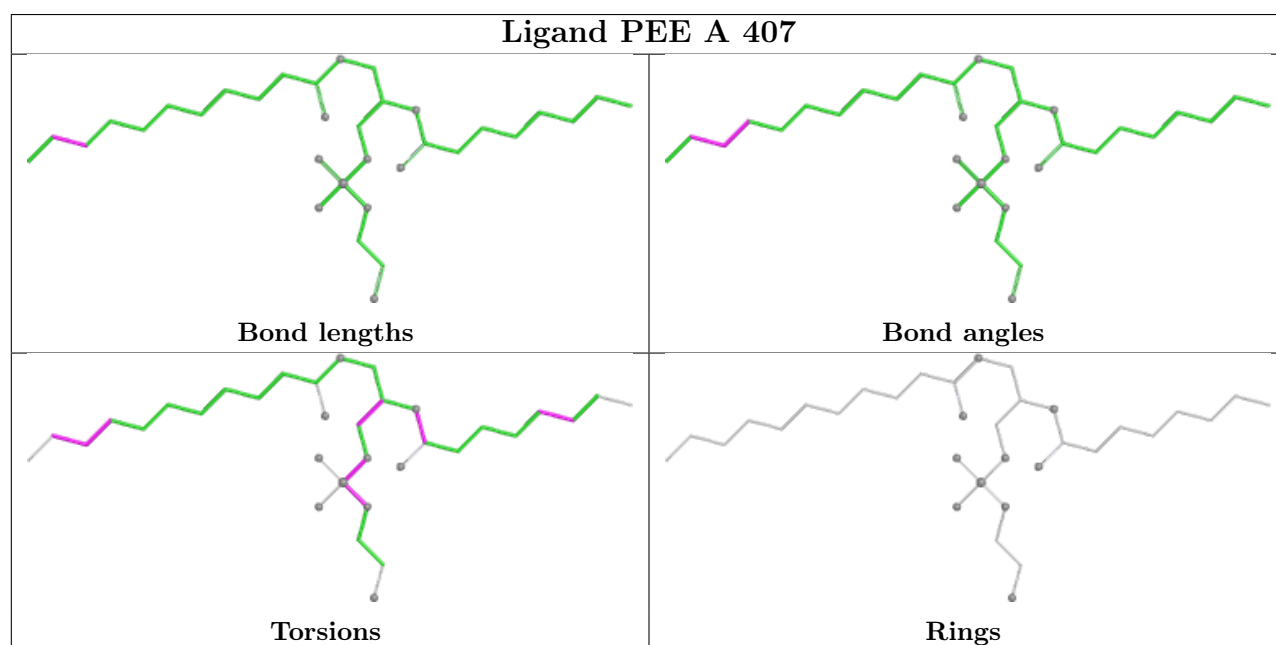
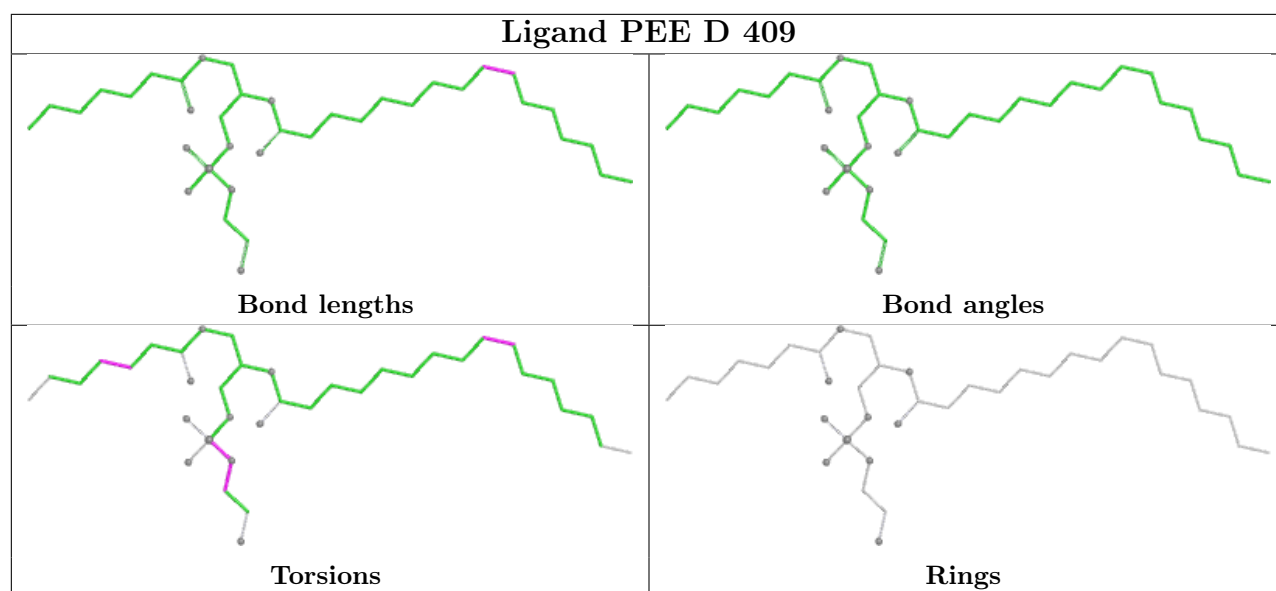


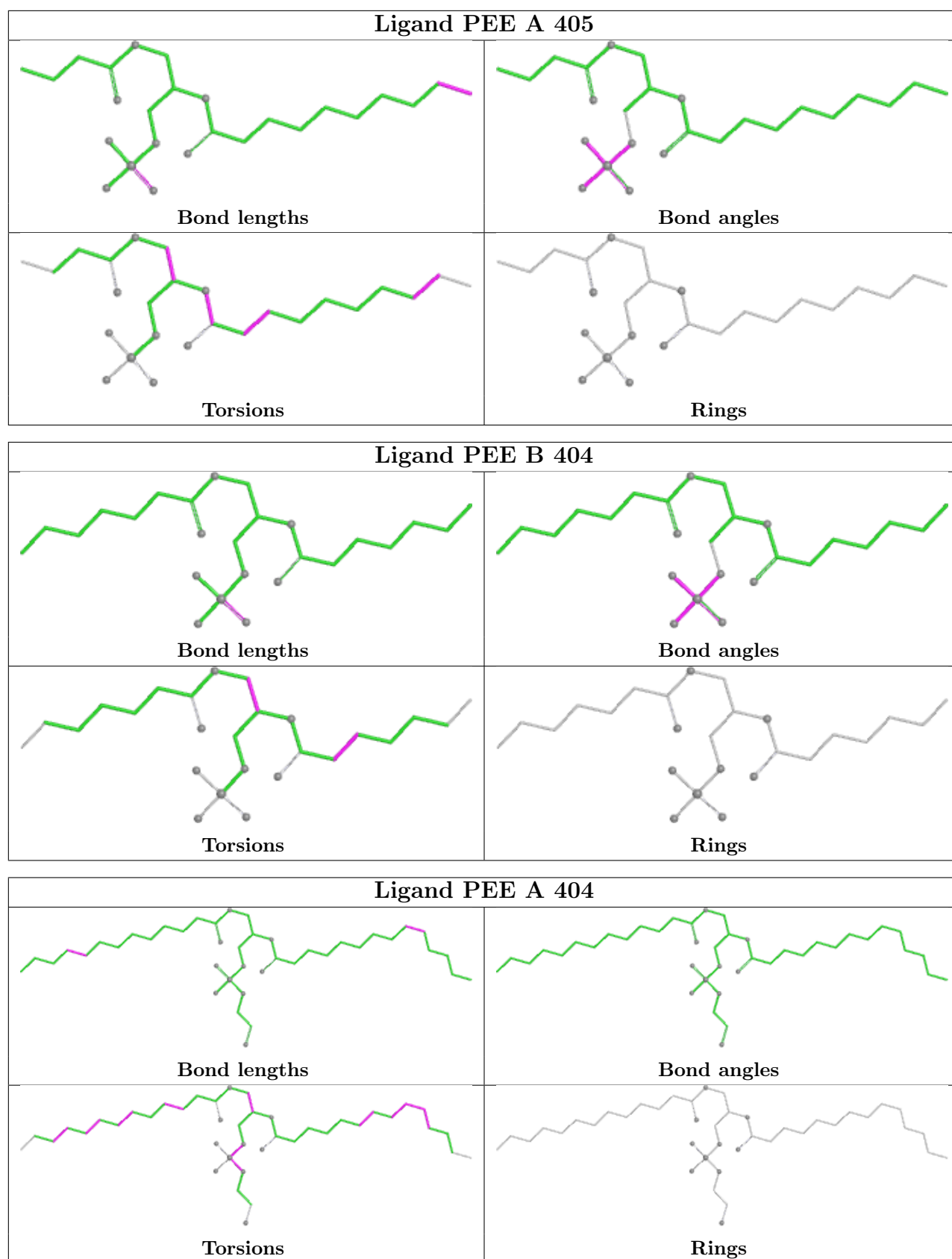












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35164. 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.