



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2021 – 04:21 am BST

PDB ID : 6ZHW
Title : Ultrafast Structural Response to Charge Redistribution Within a Photosynthetic Reaction Centre - 1 ps structure
Authors : Baath, P.; Dods, R.; Branden, G.; Neutze, R.
Deposited on : 2020-06-23
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

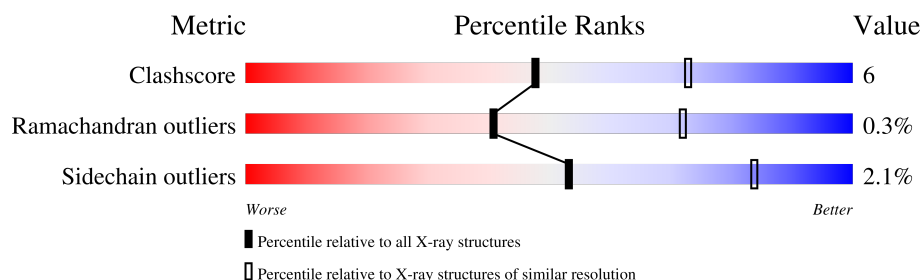
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	336	89% 9% ..
2	H	258	83% 14% .
3	L	273	86% 14%
4	M	323	89% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	M	407	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 11472 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	0
			2018	1292	344	380	2			

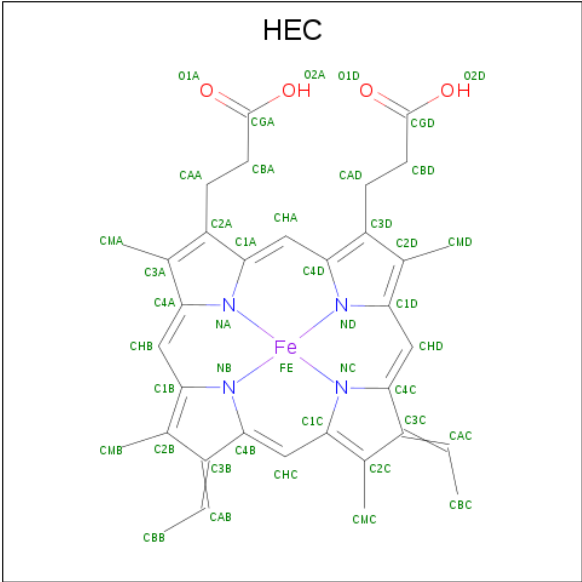
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	41	0
			2508	1678	409	413	8			

- Molecule 4 is a protein called Reaction center protein M chain.

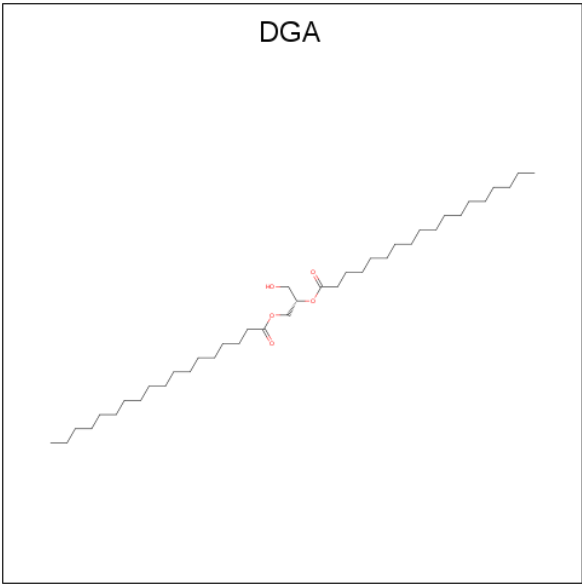
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	51	0
			2977	1983	491	490	13			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



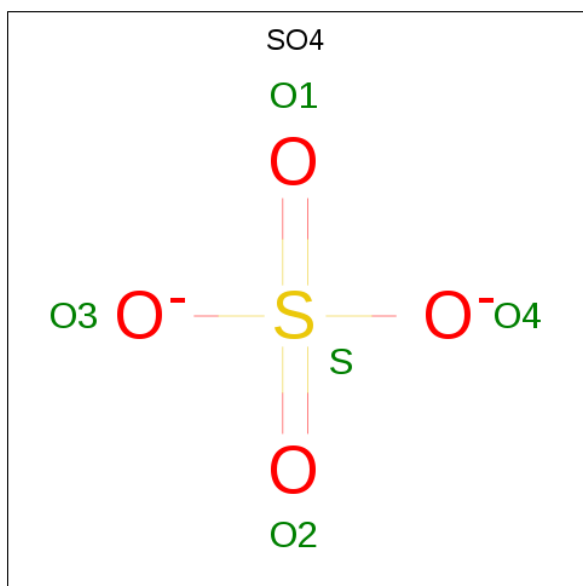
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



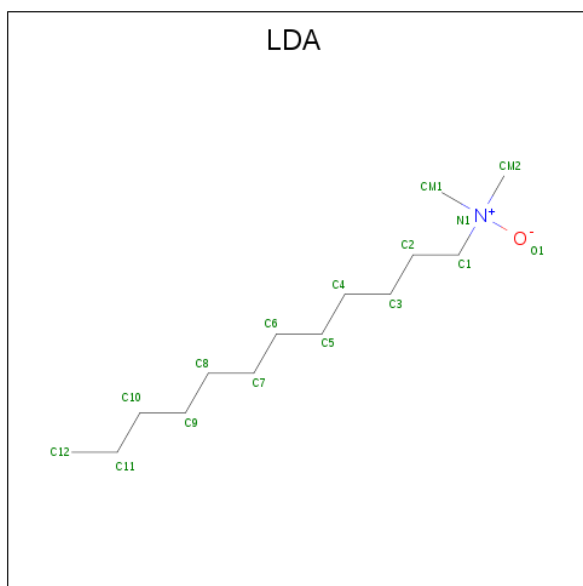
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

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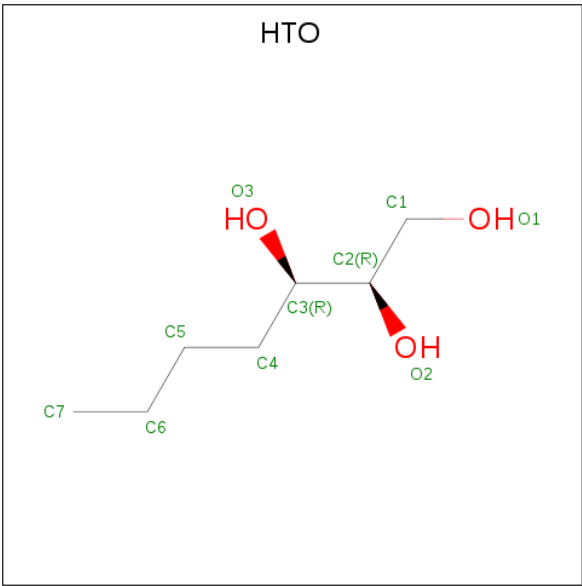
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



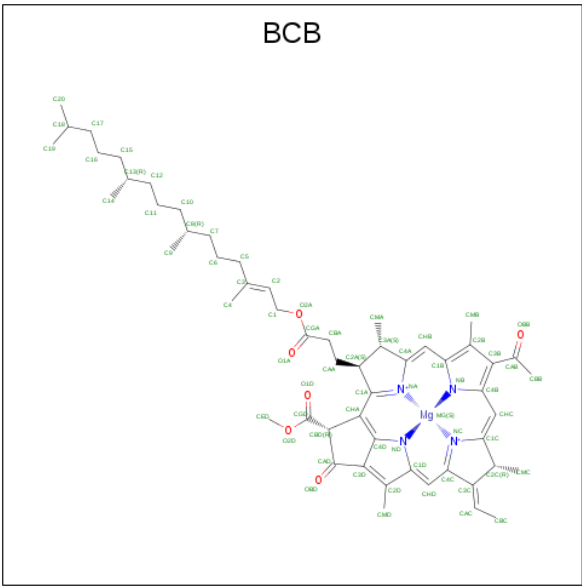
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



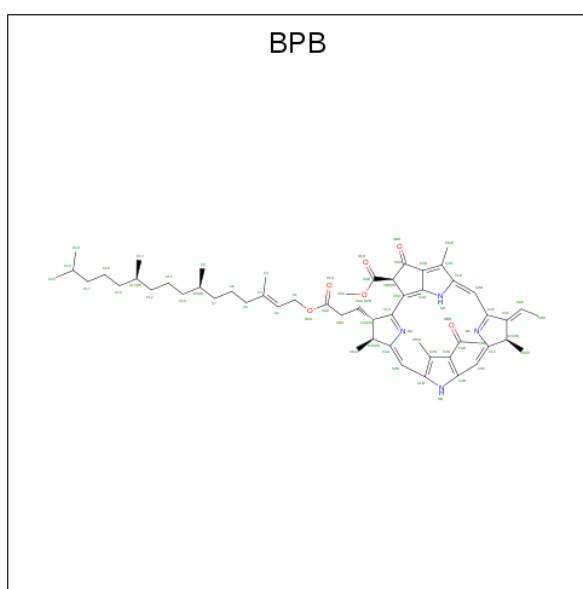
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆) (labeled as "Ligand of Interest" by depositor).

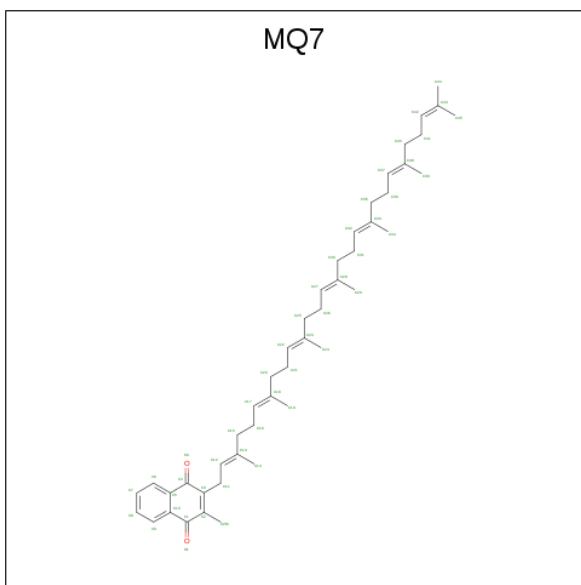


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	1
			130	110	8	12		
11	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

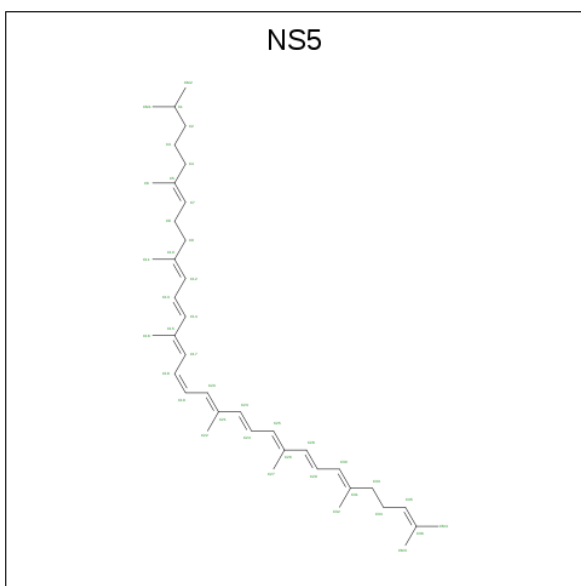
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	1
			2	2		

- Molecule 13 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	1
			96	92	4		

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	C	0	0
			40	40		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	56	Total 56	O 56	0	0
15	H	26	Total 26	O 26	0	0
15	L	25	Total 25	O 25	0	0
15	M	39	Total 39	O 39	0	0

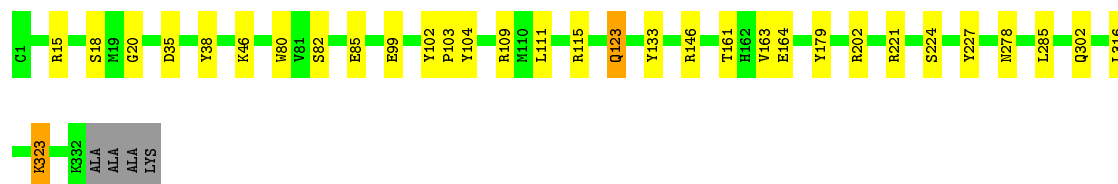
3 Residue-property plots [i](#)

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.


Note EDS was not executed.

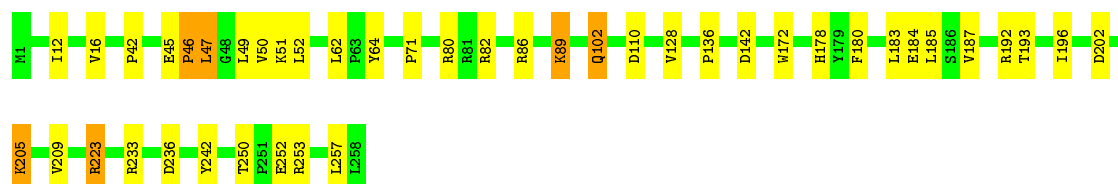
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 




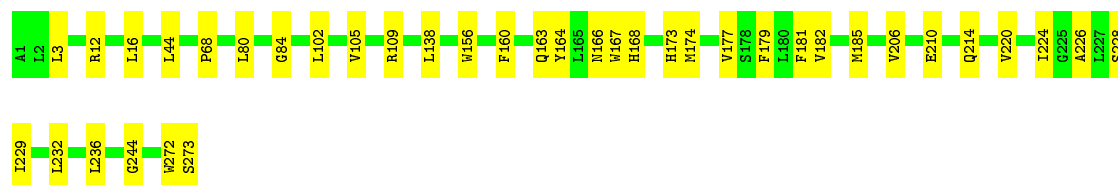
- Molecule 2: Reaction center protein H chain

Chain H: 



- Molecule 3: Reaction center protein L chain

Chain L: 



- Molecule 4: Reaction center protein M chain

Chain M: 





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	226.50Å 226.50Å 113.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.55 – 2.80	Depositor
% Data completeness (in resolution range)	98.7 (35.55-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0158, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

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: LDA, NS5, SO4, BCB, DGA, MQ7, BPB, FME, HEC, HTO, FE

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	C	0.42	0/2669	0.57	0/3637
2	H	0.43	0/2055	0.60	0/2807
3	L	0.43	0/2612	0.56	0/3568
4	M	0.45	0/3101	0.55	0/4242
All	All	0.43	0/10437	0.57	0/14254

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	C	2602	0	2578	25	0
2	H	2018	0	2020	37	0
3	L	2508	0	2390	42	0
4	M	2977	0	2832	24	0
5	C	172	0	120	4	0
6	C	37	0	58	0	0
7	C	15	0	0	0	0
7	H	25	0	0	0	0
7	M	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	48	0	93	5	0
8	L	32	0	62	2	0
8	M	32	0	62	0	0
9	H	20	0	32	0	0
9	L	10	0	16	0	0
10	L	330	0	360	18	0
10	M	132	0	144	6	0
11	L	195	0	222	14	0
12	M	2	0	0	0	0
13	M	96	0	128	1	0
14	M	40	0	60	2	0
15	C	56	0	0	0	0
15	H	26	0	0	1	0
15	L	25	0	0	0	0
15	M	39	0	0	0	0
All	All	11472	0	11177	137	0

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

All (137) 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)
2:H:205:LYS:HD3	2:H:205:LYS:H	1.46	0.80
1:C:161:THR:HG21	3:L:273:SER:O	1.83	0.79
4:M:160:CYS:O	4:M:164:THR:HG23	1.82	0.78
2:H:184:GLU:OE2	2:H:193:THR:HG21	1.82	0.77
11:L:305:BPB:HHC	11:L:305:BPB:HBBB	1.67	0.77
1:C:161:THR:HB	1:C:164:GLU:HG3	1.68	0.75
2:H:42:PRO:HD3	8:H:708:LDA:H121	1.68	0.75
4:M:38:LEU:HD23	4:M:46:ILE:HD11	1.73	0.71
1:C:161:THR:HG22	1:C:163:VAL:H	1.56	0.69
1:C:20:GLY:O	3:L:163[B]:GLN:NE2	2.28	0.67
1:C:161:THR:HG22	1:C:163:VAL:N	2.12	0.65
2:H:89:LYS:H	2:H:89:LYS:HE2	1.61	0.64
2:H:250:THR:OG1	2:H:253:ARG:HG3	1.97	0.64
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.63	0.63
1:C:111:LEU:O	1:C:115:ARG:HG3	1.99	0.62
4:M:251[B]:ARG:NH1	4:M:257[B]:ASN:OD1	2.31	0.62
2:H:45:GLU:HG3	2:H:46:PRO:HD2	1.81	0.60
2:H:80:ARG:CZ	2:H:82:ARG:HD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:ILE:HD12	2:H:242:TYR:CZ	2.37	0.60
3:L:3:LEU:HD11	4:M:251[B]:ARG:HD2	1.83	0.59
3:L:181:PHE:HB3	11:L:305:BPB:HBBA	1.83	0.58
3:L:244[A]:GLY:O	10:L:301[A]:BCB:HED3	2.04	0.58
2:H:128:VAL:HG22	3:L:210:GLU:CD	2.24	0.57
2:H:205:LYS:H	2:H:205:LYS:CD	2.15	0.57
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	1.86	0.57
3:L:182:VAL:HG13	3:L:236[B]:LEU:HD22	1.86	0.57
4:M:120:MET:HG3	10:M:403[B]:BCB:H202	1.87	0.56
4:M:190:ARG:O	4:M:190:ARG:HD2	2.05	0.56
3:L:181:PHE:CD2	11:L:305:BPB:HBB	2.41	0.56
3:L:185:MET:CE	10:L:304:BCB:H41	2.36	0.55
2:H:196:ILE:HD12	2:H:242:TYR:CE1	2.42	0.55
4:M:253[B]:THR:HG22	4:M:254:ILE:HG23	1.89	0.55
1:C:123:GLN:NE2	1:C:123:GLN:H	2.05	0.54
3:L:224:ILE:HG12	3:L:228:SER:HB2	1.90	0.54
10:L:304:BCB:HBB3	10:M:403[A]:BCB:H62	1.89	0.54
2:H:89:LYS:HE3	2:H:110:ASP:HB3	1.90	0.54
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.44	0.53
2:H:183:LEU:HB2	2:H:196:ILE:CG2	2.39	0.53
2:H:142:ASP:OD1	2:H:142:ASP:N	2.35	0.53
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.44	0.52
3:L:16:LEU:HD11	3:L:105:VAL:CG2	2.39	0.52
1:C:323:LYS:H	1:C:323:LYS:CD	2.22	0.52
4:M:102:MET:HE1	4:M:164:THR:HG22	1.91	0.52
2:H:180:PHE:CE2	4:M:12:ALA:HB2	2.46	0.51
8:H:707:LDA:H123	10:L:302[B]:BCB:HED3	1.93	0.51
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	1.93	0.51
2:H:12:ILE:O	2:H:16:VAL:HG23	2.11	0.51
1:C:227:TYR:HH	4:M:183:TRP:HD1	1.59	0.51
2:H:62:LEU:O	8:H:708:LDA:HM21	2.11	0.50
10:L:302[B]:BCB:HMB1	10:L:302[B]:BCB:HBB2	1.93	0.50
3:L:3:LEU:HD11	4:M:251[A]:ARG:HD2	1.93	0.50
10:M:403[B]:BCB:HBD	10:M:403[B]:BCB:HAA1	1.92	0.50
10:L:304:BCB:HHC	10:L:304:BCB:HBB2	1.94	0.50
4:M:265[B]:ARG:NH1	7:M:407:SO4:O1	2.43	0.50
3:L:181:PHE:HB3	11:L:305:BPB:CBB	2.42	0.50
1:C:123:GLN:H	1:C:123:GLN:HE21	1.60	0.49
2:H:257:LEU:HD11	3:L:109:ARG:CZ	2.43	0.49
5:C:403:HEC:HMB1	5:C:403:HEC:HBB3	1.95	0.49
3:L:232:LEU:HG	3:L:236[B]:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:224:ILE:HG12	3:L:228:SER:CB	2.43	0.48
2:H:64:TYR:CE1	8:H:708:LDA:H11	2.48	0.48
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.48	0.48
2:H:45:GLU:O	2:H:47:LEU:N	2.47	0.48
2:H:128:VAL:CG2	3:L:210:GLU:CD	2.82	0.48
5:C:402:HEC:HHA	5:C:402:HEC:O1D	2.14	0.47
2:H:187:VAL:CG2	2:H:192:ARG:HG3	2.44	0.47
4:M:29:VAL:HG21	4:M:51:LEU:HD12	1.96	0.47
11:L:303[B]:BPB:HBBB	11:L:303[B]:BPB:HMB	1.97	0.47
3:L:232:LEU:HG	3:L:236[B]:LEU:HD11	1.96	0.47
11:L:303[A]:BPB:HMB	11:L:303[A]:BPB:HBBB	1.96	0.47
2:H:49:LEU:O	2:H:51:LYS:N	2.48	0.47
8:H:701:LDA:HM21	8:L:306:LDA:HM22	1.97	0.47
10:L:302[B]:BCB:HMD3	4:M:195[B]:TYR:HE1	1.80	0.46
3:L:167[A]:TRP:HE1	3:L:173[A]:HIS:CD2	2.34	0.46
1:C:224:SER:HA	1:C:227:TYR:HD2	1.81	0.45
2:H:45:GLU:HG3	2:H:46:PRO:CD	2.45	0.45
4:M:265[A]:ARG:NH2	7:M:407:SO4:O1	2.42	0.45
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.17	0.45
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.98	0.45
1:C:161:THR:HG21	3:L:273:SER:C	2.36	0.45
11:L:303[B]:BPB:H7A	11:L:303[B]:BPB:H11A	1.88	0.45
3:L:138:LEU:HD23	3:L:138:LEU:HA	1.78	0.44
3:L:185:MET:HE2	10:L:304:BCB:H41	1.98	0.44
8:L:306:LDA:HM21	8:L:306:LDA:H22	1.60	0.44
2:H:80:ARG:NH2	2:H:82:ARG:HD2	2.33	0.44
4:M:258[B]:ALA:HB1	4:M:262[B]:SER:OG	2.17	0.44
11:L:305:BPB:H14	11:L:305:BPB:H16A	1.61	0.44
3:L:174[B]:MET:HA	10:L:304:BCB:OBD	2.17	0.44
1:C:146:ARG:HD3	1:C:179:TYR:CE1	2.53	0.44
3:L:44:LEU:HD12	3:L:44:LEU:HA	1.70	0.44
1:C:18:SER:HB2	3:L:156[A]:TRP:CD1	2.53	0.43
2:H:89:LYS:HE3	2:H:110:ASP:CB	2.48	0.43
1:C:15:ARG:HD2	3:L:68:PRO:O	2.17	0.43
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.00	0.43
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.01	0.43
1:C:323:LYS:H	1:C:323:LYS:HD3	1.84	0.43
10:L:304:BCB:H43	10:L:304:BCB:H11	1.85	0.43
4:M:157:CYS:HA	4:M:161:ILE:HB	1.99	0.43
3:L:226:ALA:O	3:L:229:ILE:HG22	2.18	0.43
2:H:102:GLN:NE2	3:L:12:ARG:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:403[B]:BCB:H111	10:M:403[B]:BCB:H91	1.74	0.43
4:M:250[A]:TRP:CD1	13:M:402[A]:MQ7:C3	3.01	0.43
10:M:403[B]:BCB:H112	10:M:403[B]:BCB:H142	1.77	0.43
3:L:220:VAL:HG11	11:L:305:BPB:HEDA	2.00	0.42
2:H:128:VAL:HG22	3:L:210:GLU:HB2	2.01	0.42
10:L:301[A]:BCB:H62	10:L:301[A]:BCB:H41	1.93	0.42
11:L:303[B]:BPB:OBB	11:L:303[B]:BPB:HHC	2.19	0.42
14:M:404:NS5:H18	14:M:404:NS5:H161	1.86	0.42
10:L:301[A]:BCB:H151	11:L:303[A]:BPB:H5A	2.00	0.42
2:H:71:PRO:HD3	3:L:206:VAL:HG22	2.01	0.42
3:L:102:LEU:O	3:L:105:VAL:HG22	2.19	0.42
4:M:159:GLY:HA3	14:M:404:NS5:H272	2.00	0.42
1:C:109:ARG:HG2	1:C:285:LEU:HD21	2.02	0.42
1:C:202:ARG:O	1:C:221:ARG:NH2	2.47	0.42
4:M:236:ILE:HG12	4:M:260[A]:ILE:HG23	2.00	0.42
2:H:136:PRO:HA	2:H:172:TRP:HA	2.01	0.42
2:H:257:LEU:HD13	3:L:16:LEU:HD23	2.02	0.41
11:L:303[A]:BPB:OBB	11:L:303[A]:BPB:HHC	2.20	0.41
2:H:223:ARG:NH1	15:H:801:HOH:O	2.34	0.41
10:L:301[B]:BCB:H52	11:L:303[B]:BPB:CAB	2.51	0.41
2:H:257:LEU:HD12	2:H:257:LEU:H	1.86	0.41
3:L:166[B]:ASN:OD1	3:L:168[B]:HIS:HB2	2.21	0.41
10:L:302[B]:BCB:OBD	4:M:201[B]:GLY:HA2	2.20	0.41
3:L:168[A]:HIS:CE1	10:L:301[A]:BCB:HMC2	2.56	0.41
11:L:303[B]:BPB:H6	11:L:303[B]:BPB:H2	1.73	0.41
2:H:47:LEU:CD1	2:H:49:LEU:HB3	2.51	0.41
3:L:174[B]:MET:HE3	10:L:304:BCB:O1D	2.20	0.41
3:L:177[B]:VAL:HG11	10:L:304:BCB:C3D	2.51	0.41
3:L:80:LEU:HA	3:L:84:GLY:HA3	2.02	0.40
3:L:164[B]:TYR:CD1	3:L:164[B]:TYR:N	2.88	0.40
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.56	0.40
3:L:168[B]:HIS:CE1	10:L:301[B]:BCB:HMC2	2.56	0.40
4:M:282:ILE:HD11	10:M:403[B]:BCB:OBD	2.22	0.40
4:M:200[B]:HIS:CE1	4:M:204[B]:ILE:HD11	2.56	0.40
2:H:183:LEU:HB2	2:H:196:ILE:HG22	2.02	0.40
2:H:250:THR:HB	2:H:252:GLU:OE2	2.22	0.40
3:L:179:PHE:HA	3:L:182:VAL:HG12	2.04	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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	330/336 (98%)	320 (97%)	10 (3%)	0	100	100
2	H	256/258 (99%)	248 (97%)	5 (2%)	3 (1%)	13	39
3	L	312/273 (114%)	296 (95%)	16 (5%)	0	100	100
4	M	372/323 (115%)	356 (96%)	15 (4%)	1 (0%)	41	72
All	All	1270/1190 (107%)	1220 (96%)	46 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE
2	H	46	PRO
2	H	47	LEU
2	H	50	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	281/282 (100%)	277 (99%)	4 (1%)	67	90
2	H	212/212 (100%)	202 (95%)	10 (5%)	26	59
3	L	253/218 (116%)	250 (99%)	3 (1%)	71	92
4	M	288/249 (116%)	282 (98%)	6 (2%)	53	84
All	All	1034/961 (108%)	1011 (98%)	23 (2%)	53	83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	46	LYS
1	C	123	GLN
1	C	323	LYS
2	H	52	LEU
2	H	86	ARG
2	H	89	LYS
2	H	102	GLN
2	H	178	HIS
2	H	185	LEU
2	H	205	LYS
2	H	223	ARG
2	H	233	ARG
2	H	236	ASP
3	L	160[A]	PHE
3	L	160[B]	PHE
3	L	272	TRP
4	M	27	ASP
4	M	194[A]	PHE
4	M	194[B]	PHE
4	M	214[A]	PHE
4	M	214[B]	PHE
4	M	290	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
1	C	123	GLN
1	C	302	GLN
1	C	310	GLN
2	H	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	H	1	2	8,9,10	0.98	0	7,9,11	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	1/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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	$\# Z > 2$
8	LDA	H	701	-	12,15,15	0.36	0	14,17,17	0.76	0
7	SO4	M	406	-	4,4,4	0.16	0	6,6,6	0.17	0
10	BCB	L	301[A]	-	60,74,74	2.81	19 (31%)	48,115,115	2.30	16 (33%)
14	NS5	M	404	-	39,39,39	1.39	2 (5%)	44,46,46	2.04	14 (31%)
6	DGA	C	405	1	36,36,43	1.18	3 (8%)	38,38,45	1.17	3 (7%)
7	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.39	0
7	SO4	M	409	-	4,4,4	0.15	0	6,6,6	0.18	0
10	BCB	L	302[B]	-	60,74,74	2.77	20 (33%)	48,115,115	2.19	16 (33%)
8	LDA	L	307	-	12,15,15	0.39	0	14,17,17	0.64	0
7	SO4	M	407	-	4,4,4	0.14	0	6,6,6	0.25	0
9	HTO	H	709	-	9,9,9	0.85	0	10,10,10	0.59	0
10	BCB	L	302[A]	-	60,74,74	2.75	19 (31%)	48,115,115	2.34	17 (35%)
7	SO4	C	408	-	4,4,4	0.16	0	6,6,6	0.11	0
5	HEC	C	403	1	26,50,50	1.53	4 (15%)	18,82,82	1.93	8 (44%)
7	SO4	H	705	-	4,4,4	0.27	0	6,6,6	0.36	0
11	BPB	L	303[B]	-	64,70,70	2.09	15 (23%)	64,101,101	2.06	16 (25%)
7	SO4	H	703	-	4,4,4	0.22	0	6,6,6	0.12	0
7	SO4	H	702	-	4,4,4	0.23	0	6,6,6	0.33	0
5	HEC	C	404	1	26,50,50	1.58	3 (11%)	18,82,82	1.95	7 (38%)
13	MQ7	M	402[B]	-	49,49,49	1.51	2 (4%)	60,63,63	1.42	12 (20%)
7	SO4	H	706	-	4,4,4	0.18	0	6,6,6	0.09	0
7	SO4	M	408	-	4,4,4	0.30	0	6,6,6	0.27	0
9	HTO	H	710	-	9,9,9	0.85	0	10,10,10	1.04	1 (10%)
8	LDA	M	412	-	12,15,15	0.42	0	14,17,17	0.55	0
5	HEC	C	401	1	26,50,50	1.64	4 (15%)	18,82,82	2.71	6 (33%)
11	BPB	L	303[A]	-	64,70,70	2.11	16 (25%)	64,101,101	1.97	17 (26%)
9	HTO	L	308	-	9,9,9	0.72	0	10,10,10	1.20	1 (10%)
5	HEC	C	402	1	26,50,50	1.51	3 (11%)	18,82,82	2.22	8 (44%)
10	BCB	L	304	-	60,74,74	2.70	20 (33%)	48,115,115	2.30	14 (29%)
13	MQ7	M	402[A]	-	49,49,49	1.53	2 (4%)	60,63,63	1.57	14 (23%)
7	SO4	H	704	-	4,4,4	0.12	0	6,6,6	0.16	0
11	BPB	L	305	-	64,70,70	2.18	16 (25%)	64,101,101	1.89	14 (21%)
10	BCB	M	403[B]	-	60,74,74	2.73	21 (35%)	48,115,115	2.40	19 (39%)
7	SO4	C	407	-	4,4,4	0.16	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	LDA	H	707	-	12,15,15	0.36	0	14,17,17	0.82	0
7	SO4	M	405	-	4,4,4	0.11	0	6,6,6	0.26	0
8	LDA	H	708	-	12,15,15	0.27	0	14,17,17	0.84	0
7	SO4	M	410	-	4,4,4	0.28	0	6,6,6	0.33	0
8	LDA	M	413	-	12,15,15	0.48	0	14,17,17	0.52	0
10	BCB	L	301[B]	-	60,74,74	2.79	22 (36%)	48,115,115	2.25	14 (29%)
8	LDA	L	306	-	12,15,15	0.39	0	14,17,17	0.70	0
10	BCB	M	403[A]	-	60,74,74	2.81	21 (35%)	48,115,115	2.32	16 (33%)
7	SO4	M	411	-	4,4,4	0.25	0	6,6,6	0.21	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
8	LDA	H	701	-	-	3/13/13/13	-
10	BCB	L	301[A]	-	-	12/41/177/177	-
14	NS5	M	404	-	-	10/43/43/43	-
6	DGA	C	405	1	-	15/37/37/45	-
10	BCB	L	302[B]	-	-	8/41/177/177	-
8	LDA	L	307	-	-	10/13/13/13	-
9	HTO	H	709	-	-	4/10/10/10	-
10	BCB	L	302[A]	-	-	10/41/177/177	-
5	HEC	C	403	1	-	0/6/54/54	-
11	BPB	L	303[B]	-	-	13/47/105/105	0/5/6/6
5	HEC	C	404	1	-	0/6/54/54	-
13	MQ7	M	402[B]	-	-	1/41/61/61	0/2/2/2
9	HTO	H	710	-	-	0/10/10/10	-
8	LDA	M	412	-	-	4/13/13/13	-
5	HEC	C	401	1	-	0/6/54/54	-
11	BPB	L	303[A]	-	-	6/47/105/105	0/5/6/6
9	HTO	L	308	-	-	4/10/10/10	-
5	HEC	C	402	1	-	1/6/54/54	-
10	BCB	L	304	-	-	15/41/177/177	-
13	MQ7	M	402[A]	-	-	0/41/61/61	0/2/2/2
11	BPB	L	305	-	-	8/47/105/105	0/5/6/6
10	BCB	M	403[B]	-	-	17/41/177/177	-
8	LDA	H	707	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LDA	H	708	-	-	7/13/13/13	-
8	LDA	M	413	-	-	4/13/13/13	-
10	BCB	L	301[B]	-	-	16/41/177/177	-
8	LDA	L	306	-	-	5/13/13/13	-
10	BCB	M	403[A]	-	-	14/41/177/177	-

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402[A]	MQ7	C3-C2	8.62	1.51	1.35
10	M	403[A]	BCB	CHB-C4A	-8.46	1.33	1.52
10	L	301[B]	BCB	CHB-C4A	-8.44	1.33	1.52
10	L	301[A]	BCB	CHB-C4A	-8.39	1.33	1.52
10	L	302[B]	BCB	CHB-C4A	-8.29	1.33	1.52
10	L	304	BCB	CHB-C4A	-8.14	1.34	1.52
13	M	402[B]	MQ7	C3-C2	8.08	1.50	1.35
10	M	403[B]	BCB	CHB-C4A	-8.05	1.34	1.52
10	L	302[A]	BCB	CHB-C4A	-7.96	1.34	1.52
10	M	403[A]	BCB	C1D-ND	-7.91	1.33	1.50
10	L	301[B]	BCB	C1D-ND	-7.85	1.33	1.50
10	L	301[A]	BCB	C1D-ND	-7.84	1.33	1.50
10	L	302[B]	BCB	C1D-ND	-7.73	1.34	1.50
10	L	302[A]	BCB	C1D-ND	-7.68	1.34	1.50
10	M	403[B]	BCB	C1D-ND	-7.63	1.34	1.50
10	L	304	BCB	C1D-ND	-7.51	1.34	1.50
14	M	404	NS5	C35-C36	7.35	1.53	1.32
10	M	403[A]	BCB	C4B-NB	-6.95	1.35	1.50
10	L	301[A]	BCB	C4B-NB	-6.94	1.35	1.50
11	L	305	BPB	CAC-C3C	6.93	1.52	1.33
10	M	403[A]	BCB	C1B-NB	-6.91	1.35	1.50
10	L	301[A]	BCB	C1B-NB	-6.85	1.35	1.50
10	M	403[B]	BCB	C4B-NB	-6.83	1.35	1.50
10	L	301[B]	BCB	C1B-NB	-6.82	1.35	1.50
10	M	403[B]	BCB	C1B-NB	-6.68	1.36	1.50
10	L	301[B]	BCB	C4B-NB	-6.63	1.36	1.50
11	L	303[A]	BPB	CAC-C3C	6.58	1.51	1.33
10	L	302[A]	BCB	C1B-NB	-6.58	1.36	1.50
10	L	302[B]	BCB	C1B-NB	-6.57	1.36	1.50
11	L	303[B]	BPB	CAC-C3C	6.55	1.51	1.33
10	L	302[A]	BCB	C4B-NB	-6.54	1.36	1.50
10	L	304	BCB	C1B-NB	-6.35	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	304	BCB	C4B-NB	-6.32	1.36	1.50
10	L	302[B]	BCB	C4B-NB	-6.13	1.37	1.50
10	L	301[A]	BCB	C4D-ND	-5.60	1.38	1.50
10	L	302[A]	BCB	C4D-ND	-5.58	1.38	1.50
11	L	305	BPB	C3B-C4B	5.52	1.48	1.41
10	L	302[B]	BCB	C4D-ND	-5.49	1.38	1.50
11	L	303[A]	BPB	C3B-C4B	5.49	1.48	1.41
10	L	301[B]	BCB	C4D-ND	-5.45	1.38	1.50
10	M	403[A]	BCB	O2D-CGD	5.44	1.46	1.33
5	C	401	HEC	C3B-C2B	-5.42	1.35	1.40
13	M	402[B]	MQ7	C10-C5	5.38	1.49	1.40
10	L	304	BCB	C4D-ND	-5.37	1.38	1.50
11	L	303[B]	BPB	O2D-CGD	5.24	1.46	1.33
10	M	403[B]	BCB	C4D-ND	-5.22	1.39	1.50
10	M	403[A]	BCB	C4D-ND	-5.21	1.39	1.50
11	L	303[A]	BPB	O2D-CGD	5.21	1.45	1.33
10	L	302[B]	BCB	O2D-CGD	5.20	1.45	1.33
11	L	303[A]	BPB	C3B-C2B	5.15	1.48	1.39
11	L	303[B]	BPB	C3B-C2B	5.12	1.48	1.39
11	L	305	BPB	O2A-CGA	5.10	1.48	1.33
10	M	403[B]	BCB	O2D-CGD	5.08	1.45	1.33
5	C	404	HEC	C3B-C2B	-5.07	1.35	1.40
11	L	305	BPB	CHD-C1D	5.00	1.48	1.38
10	L	304	BCB	O2D-CGD	5.00	1.45	1.33
10	L	304	BCB	CHD-C1D	-4.99	1.45	1.53
10	M	403[A]	BCB	CHD-C1D	-4.96	1.45	1.53
11	L	303[B]	BPB	CHD-C1D	4.95	1.48	1.38
11	L	305	BPB	O2D-CGD	4.90	1.45	1.33
10	L	301[A]	BCB	O2D-CGD	4.89	1.45	1.33
10	L	302[B]	BCB	CHD-C1D	-4.87	1.46	1.53
10	L	301[B]	BCB	O2D-CGD	4.87	1.45	1.33
10	L	302[A]	BCB	O2D-CGD	4.86	1.45	1.33
10	L	302[A]	BCB	CHD-C1D	-4.86	1.46	1.53
10	L	301[A]	BCB	CHD-C1D	-4.84	1.46	1.53
11	L	303[A]	BPB	CHD-C1D	4.84	1.48	1.38
11	L	303[B]	BPB	C1A-NA	-4.81	1.27	1.36
11	L	305	BPB	C1A-NA	-4.78	1.27	1.36
11	L	303[B]	BPB	C3B-C4B	4.74	1.47	1.41
11	L	303[A]	BPB	C1A-NA	-4.71	1.27	1.36
10	L	302[A]	BCB	CHD-C4C	-4.69	1.45	1.53
10	M	403[A]	BCB	CHD-C4C	-4.68	1.45	1.53
11	L	305	BPB	C4C-NC	-4.67	1.26	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	305	BPB	C3B-C2B	4.64	1.47	1.39
10	L	302[B]	BCB	OBD-CAD	4.62	1.29	1.21
10	L	301[B]	BCB	OBD-CAD	4.53	1.28	1.21
10	L	301[B]	BCB	CHD-C1D	-4.52	1.46	1.53
13	M	402[A]	MQ7	C10-C5	4.50	1.48	1.40
10	L	301[A]	BCB	OBD-CAD	4.48	1.28	1.21
5	C	402	HEC	C3B-C2B	-4.45	1.36	1.40
10	L	301[A]	BCB	CHD-C4C	-4.44	1.45	1.53
5	C	403	HEC	C3B-C2B	-4.43	1.36	1.40
10	M	403[B]	BCB	CHD-C1D	-4.39	1.46	1.53
10	L	302[B]	BCB	CHD-C4C	-4.36	1.45	1.53
10	M	403[B]	BCB	OBD-CAD	4.30	1.28	1.21
10	L	302[A]	BCB	OBD-CAD	4.29	1.28	1.21
10	L	302[B]	BCB	O2A-CGA	4.27	1.45	1.33
10	L	301[B]	BCB	O2A-CGA	4.26	1.45	1.33
10	M	403[A]	BCB	OBD-CAD	4.22	1.28	1.21
10	L	301[A]	BCB	O2A-CGA	4.18	1.45	1.33
10	L	302[A]	BCB	O2A-CGA	4.16	1.45	1.33
10	L	301[B]	BCB	CHB-C1B	-4.13	1.47	1.53
11	L	303[B]	BPB	O2A-CGA	4.12	1.45	1.33
10	M	403[A]	BCB	O2A-CGA	4.09	1.45	1.33
10	L	301[A]	BCB	CHB-C1B	-4.08	1.47	1.53
10	M	403[B]	BCB	O2A-CGA	4.07	1.45	1.33
10	L	301[B]	BCB	CHD-C4C	-4.06	1.46	1.53
10	L	304	BCB	CHD-C4C	-4.06	1.46	1.53
11	L	303[A]	BPB	C4C-NC	-4.04	1.27	1.36
10	M	403[A]	BCB	CHB-C1B	-3.99	1.47	1.53
10	L	304	BCB	O2A-CGA	3.98	1.45	1.33
11	L	303[A]	BPB	O2A-CGA	3.96	1.44	1.33
10	L	304	BCB	OBD-CAD	3.94	1.28	1.21
10	L	302[B]	BCB	CHB-C1B	-3.89	1.47	1.53
10	M	403[B]	BCB	CHD-C4C	-3.89	1.46	1.53
10	M	403[B]	BCB	CBD-CAD	-3.86	1.47	1.53
10	L	302[B]	BCB	C1A-CHA	-3.81	1.48	1.54
11	L	303[B]	BPB	C4C-NC	-3.76	1.28	1.36
10	L	301[A]	BCB	CBD-CAD	-3.72	1.47	1.53
10	L	302[A]	BCB	CHC-C4B	-3.72	1.47	1.53
10	M	403[B]	BCB	CHB-C1B	-3.70	1.47	1.53
10	L	302[A]	BCB	C1A-CHA	-3.69	1.48	1.54
10	L	304	BCB	CHB-C1B	-3.61	1.48	1.53
10	L	302[B]	BCB	C2D-C1D	-3.61	1.46	1.53
5	C	401	HEC	C3C-C2C	-3.59	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	305	BPB	OBD-CAD	3.59	1.28	1.22
10	M	403[B]	BCB	CHC-C4B	-3.55	1.48	1.53
5	C	404	HEC	C3C-C2C	-3.51	1.37	1.40
10	L	304	BCB	C1A-CHA	-3.48	1.48	1.54
11	L	303[B]	BPB	OBD-CAD	3.48	1.28	1.22
10	L	301[B]	BCB	C4A-C3A	-3.48	1.49	1.53
10	M	403[A]	BCB	CBD-CAD	-3.46	1.47	1.53
10	L	302[A]	BCB	C2D-C1D	-3.43	1.47	1.53
10	L	301[A]	BCB	CHC-C4B	-3.41	1.48	1.53
11	L	303[A]	BPB	OBD-CAD	3.37	1.28	1.22
6	C	405	DGA	OG2-CB1	3.35	1.43	1.34
10	L	301[B]	BCB	CBD-CAD	-3.34	1.48	1.53
10	L	301[A]	BCB	C2D-C1D	-3.33	1.47	1.53
10	M	403[A]	BCB	CHC-C4B	-3.33	1.48	1.53
10	L	304	BCB	C2D-C1D	-3.32	1.47	1.53
10	L	302[A]	BCB	CHB-C1B	-3.32	1.48	1.53
5	C	402	HEC	C3C-C2C	-3.31	1.37	1.40
11	L	303[A]	BPB	C3D-C2D	3.28	1.48	1.39
10	M	403[A]	BCB	C2D-C1D	-3.15	1.47	1.53
11	L	303[B]	BPB	C3D-C2D	3.13	1.47	1.39
10	M	403[B]	BCB	C1A-CHA	-3.05	1.49	1.54
11	L	305	BPB	C3D-C2D	3.04	1.47	1.39
6	C	405	DGA	OG1-CA1	3.00	1.42	1.33
10	L	301[B]	BCB	C1A-CHA	-2.94	1.49	1.54
10	L	301[B]	BCB	CHC-C4B	-2.94	1.49	1.53
5	C	403	HEC	C3C-C2C	-2.87	1.37	1.40
11	L	303[B]	BPB	C1C-NC	-2.86	1.33	1.38
10	L	304	BCB	C3B-C2B	-2.85	1.47	1.55
10	L	301[B]	BCB	C2D-C1D	-2.84	1.48	1.53
10	L	302[B]	BCB	CHC-C4B	-2.84	1.49	1.53
11	L	303[B]	BPB	CHD-C4C	2.83	1.47	1.40
10	L	301[B]	BCB	C2B-C1B	-2.83	1.48	1.53
11	L	305	BPB	C1C-NC	-2.82	1.33	1.38
10	M	403[B]	BCB	C4A-C3A	-2.81	1.50	1.53
6	C	405	DGA	OG2-CG2	-2.77	1.42	1.47
10	L	304	BCB	CHC-C4B	-2.77	1.49	1.53
11	L	303[A]	BPB	CHD-C4C	2.76	1.46	1.40
10	M	403[B]	BCB	C2D-C1D	-2.76	1.48	1.53
11	L	303[A]	BPB	C1C-NC	-2.74	1.33	1.38
10	M	403[A]	BCB	C2B-C1B	-2.74	1.48	1.53
10	L	304	BCB	C3B-CAB	-2.71	1.49	1.52
10	L	301[A]	BCB	C4A-C3A	-2.68	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302[B]	BCB	C3B-C2B	-2.66	1.48	1.55
10	L	301[A]	BCB	C2B-C1B	-2.64	1.48	1.53
10	L	302[A]	BCB	C3B-C2B	-2.64	1.48	1.55
10	L	302[B]	BCB	C3D-C2D	-2.64	1.48	1.55
10	M	403[A]	BCB	C3B-C2B	-2.61	1.48	1.55
10	L	302[A]	BCB	C3D-C2D	-2.59	1.48	1.55
10	M	403[B]	BCB	CHA-CBD	-2.59	1.45	1.53
10	L	301[A]	BCB	C3B-C2B	-2.57	1.48	1.55
5	C	403	HEC	C3C-C4C	2.55	1.47	1.43
10	L	302[A]	BCB	CBD-CAD	-2.52	1.49	1.53
10	L	301[B]	BCB	C3D-C2D	-2.50	1.48	1.55
10	L	301[B]	BCB	C3B-C2B	-2.46	1.48	1.55
10	M	403[A]	BCB	C1A-CHA	-2.44	1.50	1.54
11	L	305	BPB	CHD-C4C	2.42	1.46	1.40
10	M	403[B]	BCB	C3B-C2B	-2.41	1.49	1.55
10	L	304	BCB	CHC-C1C	-2.41	1.47	1.52
10	M	403[A]	BCB	C3D-C2D	-2.39	1.49	1.55
10	L	302[B]	BCB	CBD-CAD	-2.39	1.49	1.53
10	M	403[B]	BCB	C3D-C2D	-2.36	1.49	1.55
10	L	301[A]	BCB	C1A-CHA	-2.34	1.50	1.54
10	L	302[B]	BCB	C4A-C3A	-2.33	1.50	1.53
10	L	301[A]	BCB	C3D-C2D	-2.33	1.49	1.55
5	C	403	HEC	C1A-C2A	2.31	1.47	1.42
10	L	304	BCB	C3D-C2D	-2.31	1.49	1.55
11	L	305	BPB	C1B-CHB	2.25	1.49	1.41
11	L	303[B]	BPB	C4D-ND	2.24	1.41	1.36
10	L	302[B]	BCB	C3B-CAB	-2.24	1.49	1.52
10	L	304	BCB	C2B-C1B	-2.20	1.49	1.53
11	L	305	BPB	C4D-ND	2.17	1.41	1.36
10	M	403[A]	BCB	CHA-CBD	-2.16	1.46	1.53
11	L	303[A]	BPB	C4D-ND	2.13	1.41	1.36
5	C	401	HEC	C3C-C4C	2.13	1.46	1.43
10	L	302[A]	BCB	CHC-C1C	-2.13	1.47	1.52
11	L	303[A]	BPB	C4B-CHC	2.11	1.49	1.41
5	C	402	HEC	C4D-ND	2.11	1.40	1.36
5	C	404	HEC	C3C-C4C	2.10	1.46	1.43
10	L	304	BCB	CBD-CAD	-2.10	1.49	1.53
10	M	403[B]	BCB	C2B-C1B	-2.10	1.49	1.53
11	L	305	BPB	C4B-CHC	2.09	1.49	1.41
10	M	403[A]	BCB	CHC-C1C	-2.09	1.47	1.52
11	L	303[B]	BPB	C4B-CHC	2.09	1.49	1.41
11	L	305	BPB	C4C-C3C	2.09	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403[B]	BCB	CHC-C1C	-2.08	1.47	1.52
10	M	403[A]	BCB	C4A-C3A	-2.07	1.51	1.53
10	L	302[A]	BCB	C3B-CAB	-2.06	1.49	1.52
10	L	301[B]	BCB	CHA-CBD	-2.05	1.47	1.53
10	L	302[B]	BCB	C2A-C3A	-2.05	1.51	1.54
10	L	301[B]	BCB	C2A-C3A	-2.03	1.51	1.54
10	L	301[B]	BCB	CBD-CGD	-2.03	1.48	1.52
11	L	303[A]	BPB	C4C-C3C	2.03	1.50	1.45
14	M	404	NS5	C23-C21	2.02	1.50	1.45
11	L	303[A]	BPB	C1B-CHB	2.02	1.48	1.41
5	C	401	HEC	C1A-C2A	2.01	1.47	1.42
11	L	303[B]	BPB	C1B-CHB	2.00	1.48	1.41

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301[B]	BCB	CMB-C2B-C3B	8.15	134.52	114.29
10	M	403[A]	BCB	CMB-C2B-C3B	7.81	133.68	114.29
10	L	301[A]	BCB	CMB-C2B-C3B	7.73	133.50	114.29
10	M	403[B]	BCB	CMB-C2B-C3B	7.52	132.96	114.29
10	L	302[A]	BCB	CMB-C2B-C3B	7.30	132.42	114.29
5	C	401	HEC	CBA-CAA-C2A	-7.27	99.08	112.48
10	L	302[B]	BCB	CMB-C2B-C3B	7.10	131.92	114.29
11	L	303[B]	BPB	CBC-CAC-C3C	-6.35	108.15	126.72
11	L	305	BPB	CMD-C2D-C1D	6.24	134.67	125.06
10	L	304	BCB	CMB-C2B-C3B	6.22	129.72	114.29
11	L	303[B]	BPB	CMD-C2D-C1D	6.10	134.45	125.06
11	L	303[A]	BPB	CBC-CAC-C3C	-6.08	108.94	126.72
10	M	403[B]	BCB	CHA-CBD-CGD	-5.94	101.59	115.02
11	L	303[B]	BPB	O2D-CGD-CBD	5.80	121.57	111.27
11	L	303[A]	BPB	CMD-C2D-C1D	5.75	133.92	125.06
10	L	302[A]	BCB	C3B-C4B-NB	5.73	114.21	103.75
10	L	304	BCB	C1-C2-C3	-5.56	116.43	126.04
10	M	403[B]	BCB	C3B-C4B-NB	5.48	113.75	103.75
11	L	303[A]	BPB	O2D-CGD-CBD	5.39	120.85	111.27
10	L	304	BCB	OBD-CAD-C3D	-5.32	117.37	126.73
11	L	305	BPB	O2D-CGD-CBD	5.28	120.65	111.27
11	L	305	BPB	CBC-CAC-C3C	-5.26	111.32	126.72
10	M	403[A]	BCB	C3B-C4B-NB	5.21	113.25	103.75
10	L	301[B]	BCB	C3B-C4B-NB	5.11	113.08	103.75
10	M	403[A]	BCB	CHA-CBD-CGD	-5.08	103.53	115.02
10	L	301[A]	BCB	C3B-C4B-NB	5.08	113.02	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	HEC	CBA-CAA-C2A	-5.06	103.16	112.48
10	L	302[B]	BCB	C3B-C4B-NB	5.05	112.96	103.75
5	C	401	HEC	CBD-CAD-C3D	-4.97	103.31	112.49
11	L	303[B]	BPB	OBD-CAD-C3D	-4.97	116.57	128.52
14	M	404	NS5	C19-C20-C21	-4.93	120.27	127.31
10	M	403[B]	BCB	O2D-CGD-O1D	-4.68	114.69	123.84
10	L	302[B]	BCB	O2D-CGD-CBD	4.67	122.07	111.11
10	L	304	BCB	C3B-C4B-NB	4.60	112.14	103.75
10	M	403[B]	BCB	O2D-CGD-CBD	4.56	121.81	111.11
10	L	302[A]	BCB	O2D-CGD-CBD	4.51	121.71	111.11
14	M	404	NS5	CM4-C36-C35	-4.36	110.05	122.65
10	L	302[A]	BCB	OBD-CAD-C3D	-4.30	119.17	126.73
10	M	403[A]	BCB	O2D-CGD-CBD	4.28	121.17	111.11
10	L	301[A]	BCB	CHA-CBD-CGD	-4.28	105.33	115.02
6	C	405	DGA	OG2-CB1-CB2	4.25	120.66	111.50
10	L	301[B]	BCB	O2D-CGD-CBD	4.21	120.99	111.11
10	M	403[A]	BCB	O2D-CGD-O1D	-4.14	115.74	123.84
5	C	404	HEC	CAD-CBD-CGD	-4.11	105.77	112.67
14	M	404	NS5	C11-C10-C9	3.99	121.99	115.27
10	L	301[A]	BCB	O2D-CGD-CBD	3.98	120.47	111.11
10	L	304	BCB	O2D-CGD-CBD	3.93	120.34	111.11
14	M	404	NS5	C34-C35-C36	-3.89	114.47	127.75
10	L	301[B]	BCB	C1D-CHD-C4C	3.86	120.59	112.37
11	L	303[A]	BPB	CMB-C2B-C3B	3.82	131.82	124.68
11	L	305	BPB	CMD-C2D-C3D	-3.80	118.86	127.61
10	L	304	BCB	CBA-CAA-C2A	-3.77	110.60	115.72
10	L	302[A]	BCB	CBA-CAA-C2A	-3.75	110.61	115.72
5	C	401	HEC	CMC-C2C-C1C	-3.75	122.70	128.46
11	L	303[B]	BPB	CMD-C2D-C3D	-3.75	118.99	127.61
10	L	302[B]	BCB	OBD-CAD-C3D	-3.75	120.14	126.73
10	L	304	BCB	C1D-CHD-C4C	3.70	120.26	112.37
5	C	402	HEC	CAD-CBD-CGD	-3.69	106.48	112.67
11	L	303[B]	BPB	CMB-C2B-C3B	3.68	131.57	124.68
10	L	301[A]	BCB	CBB-CAB-C3B	3.67	120.55	116.80
14	M	404	NS5	CM3-C36-C35	-3.66	112.06	122.65
14	M	404	NS5	C18-C17-C15	-3.66	122.08	127.31
10	L	301[A]	BCB	OBD-CAD-C3D	-3.54	120.50	126.73
10	L	302[A]	BCB	C6-C5-C3	-3.54	104.18	113.45
11	L	305	BPB	O2A-CGA-CBA	3.52	122.94	111.91
10	L	302[B]	BCB	C1D-CHD-C4C	3.51	119.86	112.37
5	C	403	HEC	CMC-C2C-C1C	-3.46	123.15	128.46
13	M	402[A]	MQ7	C19-C18-C20	3.46	121.09	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302[B]	BCB	O1D-CGD-CBD	-3.46	117.69	124.54
10	L	304	BCB	O2A-CGA-CBA	3.44	122.70	111.91
10	L	301[A]	BCB	O2D-CGD-O1D	-3.44	117.12	123.84
10	M	403[A]	BCB	CBB-CAB-C3B	3.42	120.29	116.80
13	M	402[A]	MQ7	C39-C38-C40	3.41	121.01	115.27
10	L	302[A]	BCB	C1D-CHD-C4C	3.40	119.62	112.37
10	L	301[B]	BCB	C4-C3-C5	3.38	120.96	115.27
10	L	301[A]	BCB	C1D-CHD-C4C	3.37	119.55	112.37
14	M	404	NS5	C32-C31-C33	3.35	120.90	115.27
10	L	302[A]	BCB	O1D-CGD-CBD	-3.34	117.92	124.54
11	L	303[A]	BPB	CMD-C2D-C3D	-3.34	119.94	127.61
5	C	401	HEC	CMC-C2C-C3C	3.33	129.74	125.82
10	L	301[B]	BCB	CHA-CBD-CGD	-3.33	107.49	115.02
10	L	302[A]	BCB	C1-C2-C3	-3.32	120.29	126.04
11	L	303[B]	BPB	C4D-ND-C1D	-3.29	100.84	106.76
10	L	301[B]	BCB	CBB-CAB-C3B	3.27	120.14	116.80
11	L	303[A]	BPB	C3C-C4C-NC	3.23	114.75	109.58
10	M	403[B]	BCB	C1D-CHD-C4C	3.23	119.25	112.37
11	L	303[B]	BPB	C3C-C4C-NC	3.23	114.74	109.58
10	L	301[A]	BCB	O2A-CGA-CBA	3.22	122.00	111.91
10	L	304	BCB	C4-C3-C5	3.19	120.63	115.27
11	L	305	BPB	C1-O2A-CGA	3.16	124.73	116.44
10	L	301[A]	BCB	C4-C3-C5	3.13	120.54	115.27
10	M	403[A]	BCB	CMD-C2D-C3D	3.11	122.02	114.29
10	M	403[A]	BCB	OBD-CAD-C3D	-3.11	121.26	126.73
11	L	303[A]	BPB	C4D-ND-C1D	-3.10	101.19	106.76
10	L	304	BCB	CMD-C2D-C3D	3.08	121.94	114.29
10	L	304	BCB	C4-C3-C2	-3.07	115.81	123.68
5	C	403	HEC	CMC-C2C-C3C	3.04	129.40	125.82
9	L	308	HTO	C5-C4-C3	-3.04	109.18	114.18
5	C	402	HEC	CMD-C2D-C1D	-3.00	123.85	128.46
11	L	305	BPB	C3C-C4C-NC	3.00	114.38	109.58
10	L	302[B]	BCB	CBB-CAB-C3B	3.00	119.86	116.80
13	M	402[B]	MQ7	C39-C38-C40	2.98	120.29	115.27
13	M	402[A]	MQ7	C29-C28-C30	2.98	120.29	115.27
10	L	302[B]	BCB	C6-C5-C3	-2.95	105.72	113.45
11	L	303[A]	BPB	CAD-C3D-C2D	2.95	155.02	140.80
5	C	402	HEC	CMC-C2C-C1C	-2.95	123.94	128.46
11	L	305	BPB	CAD-C3D-C2D	2.94	154.99	140.80
11	L	303[B]	BPB	O2D-CGD-O1D	-2.93	118.10	123.84
13	M	402[A]	MQ7	C21-C22-C23	-2.93	120.61	127.66
5	C	404	HEC	CMA-C3A-C2A	2.92	130.44	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	404	NS5	C18-C19-C20	2.91	129.44	123.47
13	M	402[B]	MQ7	C19-C18-C20	2.91	120.16	115.27
10	L	301[A]	BCB	O2A-CGA-O1A	-2.88	116.33	123.59
10	L	301[A]	BCB	CMD-C2D-C3D	2.87	121.42	114.29
10	M	403[B]	BCB	CBB-CAB-C3B	2.85	119.71	116.80
11	L	303[A]	BPB	O2A-CGA-CBA	2.83	120.79	111.91
10	L	301[B]	BCB	C4A-C3A-C2A	-2.83	99.53	103.86
6	C	405	DGA	OG1-CA1-CA2	2.79	120.65	111.91
5	C	404	HEC	CMC-C2C-C1C	-2.78	124.20	128.46
10	M	403[B]	BCB	OBD-CAD-C3D	-2.77	121.86	126.73
11	L	305	BPB	C4D-ND-C1D	-2.76	101.79	106.76
11	L	305	BPB	OBD-CAD-C3D	-2.76	121.89	128.52
13	M	402[B]	MQ7	C16-C17-C18	-2.75	121.03	127.66
10	M	403[A]	BCB	C1D-CHD-C4C	2.74	118.20	112.37
10	L	301[B]	BCB	OBD-CAD-C3D	-2.73	121.93	126.73
5	C	403	HEC	CBA-CAA-C2A	-2.72	107.47	112.48
10	L	304	BCB	O2A-CGA-O1A	-2.71	116.75	123.59
11	L	303[B]	BPB	CHD-C4C-C3C	-2.71	120.79	125.11
11	L	303[B]	BPB	CAD-C3D-C2D	2.71	153.85	140.80
10	L	302[A]	BCB	C4-C3-C5	2.71	119.82	115.27
10	L	301[B]	BCB	O2A-CGA-CBA	2.67	120.29	111.91
5	C	402	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
5	C	404	HEC	CBA-CAA-C2A	-2.67	107.57	112.48
13	M	402[A]	MQ7	C16-C17-C18	-2.65	121.27	127.66
10	L	302[A]	BCB	CBB-CAB-C3B	2.65	119.50	116.80
5	C	403	HEC	CMD-C2D-C1D	-2.65	124.39	128.46
13	M	402[B]	MQ7	C34-C33-C35	2.65	119.73	115.27
10	L	301[B]	BCB	CHC-C4B-C3B	2.64	124.64	118.17
10	L	302[A]	BCB	O2A-CGA-CBA	2.64	120.18	111.91
11	L	303[B]	BPB	C4-C3-C5	2.62	119.68	115.27
10	M	403[A]	BCB	CHC-C4B-C3B	2.61	124.57	118.17
11	L	303[A]	BPB	OBD-CAD-C3D	-2.60	122.27	128.52
11	L	303[A]	BPB	CMA-C3A-C4A	-2.59	104.84	112.09
14	M	404	NS5	C12-C13-C14	-2.58	115.16	123.22
5	C	403	HEC	C1D-C2D-C3D	2.58	108.79	107.00
11	L	303[A]	BPB	O2D-CGD-O1D	-2.57	118.82	123.84
10	M	403[A]	BCB	C4A-C3A-C2A	-2.56	99.94	103.86
10	L	301[B]	BCB	O2D-CGD-O1D	-2.56	118.84	123.84
10	L	304	BCB	O2D-CGD-O1D	-2.55	118.85	123.84
6	C	405	DGA	OG2-CG2-CG1	2.54	112.02	106.13
13	M	402[B]	MQ7	C21-C22-C23	-2.53	121.57	127.66
10	M	403[B]	BCB	C1-O2A-CGA	2.52	123.07	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	402[A]	MQ7	C45-C43-C44	2.50	120.12	114.60
13	M	402[B]	MQ7	C29-C28-C30	2.48	119.44	115.27
11	L	305	BPB	C4B-CHC-C1C	2.48	131.76	128.57
10	L	302[B]	BCB	O2A-CGA-CBA	2.47	119.67	111.91
10	L	302[B]	BCB	CBA-CAA-C2A	-2.47	112.36	115.72
10	L	302[B]	BCB	C4-C3-C5	2.46	119.42	115.27
11	L	303[A]	BPB	C4B-CHC-C1C	2.46	131.74	128.57
10	M	403[B]	BCB	CHC-C4B-C3B	2.45	124.19	118.17
10	L	302[A]	BCB	CMD-C2D-C3D	2.45	120.38	114.29
13	M	402[A]	MQ7	C26-C27-C28	-2.44	121.79	127.66
10	L	301[A]	BCB	C1-C2-C3	-2.44	121.83	126.04
10	L	301[A]	BCB	CHC-C4B-C3B	2.43	124.13	118.17
13	M	402[B]	MQ7	C26-C27-C28	-2.43	121.81	127.66
5	C	404	HEC	CMB-C2B-C1B	-2.43	124.73	128.46
11	L	305	BPB	O1D-CGD-CBD	-2.42	119.52	124.48
11	L	303[A]	BPB	O2A-CGA-O1A	-2.41	117.51	123.59
10	L	302[B]	BCB	CHC-C4B-C3B	2.41	124.07	118.17
10	L	302[A]	BCB	CED-O2D-CGD	2.40	121.36	115.94
10	L	302[A]	BCB	O2A-CGA-O1A	-2.39	117.55	123.59
10	L	302[B]	BCB	CMD-C2D-C3D	2.35	120.14	114.29
10	M	403[B]	BCB	C4-C3-C5	2.34	119.21	115.27
10	M	403[B]	BCB	CMD-C2D-C3D	2.32	120.06	114.29
10	M	403[B]	BCB	C1-C2-C3	-2.32	122.03	126.04
10	L	304	BCB	CHC-C4B-C3B	2.31	123.84	118.17
13	M	402[B]	MQ7	C12-C11-C3	-2.31	105.82	112.05
13	M	402[A]	MQ7	C34-C33-C35	2.30	119.14	115.27
13	M	402[B]	MQ7	C24-C23-C25	2.30	119.14	115.27
10	M	403[B]	BCB	C6-C5-C3	-2.30	107.44	113.45
10	M	403[B]	BCB	O2A-CGA-CBA	2.28	119.05	111.91
5	C	402	HEC	CMB-C2B-C3B	2.28	128.50	125.82
10	L	302[B]	BCB	C1-C2-C3	-2.27	122.12	126.04
10	M	403[B]	BCB	O2A-CGA-O1A	-2.26	117.88	123.59
10	M	403[A]	BCB	C4-C3-C5	2.26	119.08	115.27
5	C	402	HEC	CMC-C2C-C3C	2.26	128.48	125.82
5	C	401	HEC	CAD-CBD-CGD	2.25	116.45	112.67
10	L	302[A]	BCB	C4A-C3A-C2A	-2.24	100.44	103.86
11	L	305	BPB	CED-O2D-CGD	2.23	120.98	115.94
10	M	403[B]	BCB	C4D-C3D-CAD	-2.23	99.66	104.73
10	L	302[B]	BCB	OBB-CAB-C3B	-2.21	119.18	121.52
10	M	403[B]	BCB	CBA-CAA-C2A	-2.21	112.71	115.72
10	M	403[A]	BCB	O2A-CGA-O1A	-2.21	118.02	123.59
10	L	301[B]	BCB	O1D-CGD-CBD	-2.21	120.17	124.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	402[A]	MQ7	C12-C11-C3	-2.21	106.10	112.05
10	L	301[B]	BCB	O2A-CGA-O1A	-2.20	118.04	123.59
13	M	402[A]	MQ7	C14-C13-C15	2.20	118.97	115.27
10	M	403[A]	BCB	C4D-C3D-CAD	-2.20	99.73	104.73
5	C	403	HEC	CMB-C2B-C1B	-2.19	125.10	128.46
11	L	303[B]	BPB	C4B-CHC-C1C	2.19	131.39	128.57
10	M	403[A]	BCB	C7-C6-C5	-2.18	107.43	113.36
13	M	402[A]	MQ7	C5-C4-C3	2.18	122.42	118.42
11	L	303[A]	BPB	C2D-C1D-ND	2.17	113.07	109.79
5	C	404	HEC	CMD-C2D-C1D	-2.17	125.13	128.46
14	M	404	NS5	C8-C7-C5	-2.16	122.45	127.66
10	M	403[B]	BCB	OBD-CAD-CBD	-2.16	122.31	127.49
11	L	303[B]	BPB	O2A-CGA-CBA	2.15	118.64	111.91
9	H	710	HTO	C5-C4-C3	-2.14	110.66	114.18
11	L	303[A]	BPB	CHD-C4C-C3C	-2.13	121.70	125.11
13	M	402[A]	MQ7	O4-C4-C5	-2.13	118.12	121.56
13	M	402[A]	MQ7	C24-C23-C25	2.13	118.85	115.27
14	M	404	NS5	C16-C15-C14	2.13	121.43	118.08
10	M	403[A]	BCB	OBD-CAD-CBD	-2.12	122.40	127.49
10	L	302[A]	BCB	CHC-C4B-C3B	2.10	123.32	118.17
10	L	301[A]	BCB	OBB-CAB-C3B	-2.10	119.31	121.52
5	C	401	HEC	C4B-C3B-C2B	2.09	108.61	106.35
13	M	402[A]	MQ7	C41-C42-C43	-2.09	120.60	127.75
5	C	403	HEC	CMB-C2B-C3B	2.09	128.28	125.82
10	L	301[A]	BCB	C4A-C3A-C2A	-2.09	100.67	103.86
5	C	402	HEC	CMA-C3A-C2A	2.08	128.86	124.94
11	L	303[B]	BPB	O1D-CGD-CBD	-2.06	120.26	124.48
10	L	302[B]	BCB	C4A-C3A-C2A	-2.06	100.71	103.86
13	M	402[B]	MQ7	C2M-C2-C1	2.06	119.69	116.27
5	C	404	HEC	CBD-CAD-C3D	2.05	116.27	112.49
14	M	404	NS5	C14-C15-C17	-2.05	115.79	118.94
13	M	402[B]	MQ7	C2M-C2-C3	-2.05	121.05	124.40
11	L	305	BPB	O2D-CGD-O1D	-2.05	119.83	123.84
14	M	404	NS5	C30-C29-C28	-2.04	116.84	123.22
5	C	403	HEC	CAA-CBA-CGA	-2.04	109.25	112.67
11	L	303[A]	BPB	O1D-CGD-CBD	-2.03	120.33	124.48
14	M	404	NS5	C22-C21-C20	-2.02	120.09	122.92
13	M	402[B]	MQ7	C45-C43-C44	2.02	119.06	114.60
11	L	303[B]	BPB	C2D-C1D-ND	2.01	112.83	109.79

There are no chirality outliers.

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
8	H	707	LDA	C2-C1-N1-O1
8	H	707	LDA	C2-C1-N1-CM1
8	H	707	LDA	C2-C1-N1-CM2
8	H	707	LDA	N1-C1-C2-C3
8	L	307	LDA	C2-C1-N1-O1
8	L	307	LDA	C2-C1-N1-CM1
8	M	413	LDA	C2-C1-N1-CM1
8	M	413	LDA	C2-C1-N1-CM2
9	H	709	HTO	C1-C2-C3-O3
9	H	709	HTO	O2-C2-C3-O3
9	H	709	HTO	O2-C2-C3-C4
9	L	308	HTO	O2-C2-C3-C4
10	L	301[A]	BCB	C2B-C3B-CAB-OBB
10	L	301[A]	BCB	C2B-C3B-CAB-CBB
10	L	301[A]	BCB	C2-C3-C5-C6
10	L	301[A]	BCB	C4-C3-C5-C6
10	L	301[B]	BCB	C2B-C3B-CAB-OBB
10	L	301[B]	BCB	C2B-C3B-CAB-CBB
10	L	302[A]	BCB	C2B-C3B-CAB-OBB
10	L	302[A]	BCB	C2B-C3B-CAB-CBB
10	M	403[A]	BCB	C2A-CAA-CBA-CGA
10	M	403[A]	BCB	C2B-C3B-CAB-OBB
10	M	403[A]	BCB	C2B-C3B-CAB-CBB
10	M	403[A]	BCB	C2C-C3C-CAC-CBC
10	M	403[A]	BCB	CAD-CBD-CGD-O1D
10	M	403[A]	BCB	CAD-CBD-CGD-O2D
10	M	403[B]	BCB	C2B-C3B-CAB-OBB
10	M	403[B]	BCB	C2B-C3B-CAB-CBB
10	M	403[B]	BCB	C2C-C3C-CAC-CBC
10	M	403[B]	BCB	CAD-CBD-CGD-O1D
10	M	403[B]	BCB	CAD-CBD-CGD-O2D
11	L	303[A]	BPB	O2A-C1-C2-C3
11	L	303[A]	BPB	C2C-C3C-CAC-CBC
11	L	303[B]	BPB	C2C-C3C-CAC-CBC
11	L	305	BPB	C2C-C3C-CAC-CBC
14	M	404	NS5	C34-C35-C36-CM3
10	L	304	BCB	CBD-CGD-O2D-CED
11	L	303[B]	BPB	CBD-CGD-O2D-CED
10	M	403[B]	BCB	C2A-CAA-CBA-CGA
11	L	305	BPB	CBA-CGA-O2A-C1
10	L	302[B]	BCB	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	M	404	NS5	C13-C14-C15-C16
11	L	303[B]	BPB	O1D-CGD-O2D-CED
10	L	304	BCB	O1D-CGD-O2D-CED
11	L	305	BPB	O1A-CGA-O2A-C1
10	L	301[A]	BCB	C13-C15-C16-C17
10	M	403[B]	BCB	C8-C10-C11-C12
10	M	403[A]	BCB	C8-C10-C11-C12
10	M	403[B]	BCB	C12-C13-C15-C16
10	L	302[B]	BCB	C8-C10-C11-C12
10	L	304	BCB	C3-C5-C6-C7
10	L	301[B]	BCB	C15-C16-C17-C18
10	M	403[B]	BCB	C16-C17-C18-C19
8	H	708	LDA	C3-C4-C5-C6
10	L	301[B]	BCB	C16-C17-C18-C20
10	M	403[B]	BCB	CBA-CGA-O2A-C1
8	L	306	LDA	C2-C3-C4-C5
8	M	412	LDA	C5-C6-C7-C8
6	C	405	DGA	CA2-CA1-OG1-CG1
6	C	405	DGA	CBB-CAB-CB9-CB8
10	M	403[B]	BCB	C14-C13-C15-C16
10	L	301[B]	BCB	C16-C17-C18-C19
8	H	708	LDA	C5-C6-C7-C8
10	L	302[B]	BCB	C13-C15-C16-C17
8	L	307	LDA	C7-C8-C9-C10
10	M	403[B]	BCB	O1A-CGA-O2A-C1
6	C	405	DGA	CCB-CDB-CEB-CFB
11	L	303[B]	BPB	C4-C3-C5-C6
11	L	303[A]	BPB	C2-C3-C5-C6
11	L	303[B]	BPB	C2-C3-C5-C6
6	C	405	DGA	OA1-CA1-OG1-CG1
8	M	413	LDA	C6-C7-C8-C9
8	L	307	LDA	C3-C4-C5-C6
8	L	306	LDA	C5-C6-C7-C8
10	L	302[A]	BCB	C12-C13-C15-C16
11	L	303[B]	BPB	C13-C15-C16-C17
14	M	404	NS5	C34-C35-C36-CM4
11	L	305	BPB	C13-C15-C16-C17
8	L	307	LDA	C6-C7-C8-C9
11	L	303[A]	BPB	C4-C3-C5-C6
8	L	306	LDA	C3-C4-C5-C6
8	H	701	LDA	C6-C7-C8-C9
11	L	303[A]	BPB	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	L	307	LDA	C4-C5-C6-C7
10	M	403[A]	BCB	C13-C15-C16-C17
8	L	306	LDA	C1-C2-C3-C4
8	H	708	LDA	C9-C10-C11-C12
14	M	404	NS5	C7-C8-C9-C10
9	H	709	HTO	C4-C5-C6-C7
8	H	701	LDA	C4-C5-C6-C7
10	M	403[B]	BCB	C2-C1-O2A-CGA
9	L	308	HTO	O2-C2-C3-O3
10	L	301[A]	BCB	CAD-CBD-CGD-O2D
10	L	301[B]	BCB	C12-C13-C15-C16
10	M	403[A]	BCB	C12-C13-C15-C16
10	M	403[A]	BCB	C14-C13-C15-C16
6	C	405	DGA	CB9-CAB-CBB-CCB
8	H	708	LDA	N1-C1-C2-C3
10	L	302[A]	BCB	C13-C15-C16-C17
8	L	307	LDA	C9-C10-C11-C12
9	L	308	HTO	C1-C2-C3-O3
8	H	707	LDA	C1-C2-C3-C4
14	M	404	NS5	C3-C4-C5-C6
10	L	302[B]	BCB	C2B-C3B-CAB-OB
10	L	302[B]	BCB	C2B-C3B-CAB-CBB
8	L	307	LDA	C1-C2-C3-C4
9	L	308	HTO	C4-C5-C6-C7
8	H	707	LDA	C6-C7-C8-C9
10	L	301[B]	BCB	C14-C13-C15-C16
10	L	302[A]	BCB	C14-C13-C15-C16
10	M	403[B]	BCB	C16-C17-C18-C20
11	L	303[B]	BPB	C15-C16-C17-C18
10	L	304	BCB	C5-C6-C7-C8
11	L	303[B]	BPB	C8-C10-C11-C12
8	H	708	LDA	C6-C7-C8-C9
10	L	301[B]	BCB	C2C-C3C-CAC-CBC
10	L	302[A]	BCB	C2C-C3C-CAC-CBC
10	L	302[B]	BCB	C2C-C3C-CAC-CBC
10	L	304	BCB	C2C-C3C-CAC-CBC
11	L	303[A]	BPB	CAD-CBD-CGD-O2D
11	L	305	BPB	CAD-CBD-CGD-O2D
6	C	405	DGA	CA3-CA4-CA5-CA6
8	L	307	LDA	C2-C1-N1-CM2
11	L	305	BPB	CHA-CBD-CGD-O1D
6	C	405	DGA	CA9-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
8	L	306	LDA	C4-C5-C6-C7
6	C	405	DGA	CB6-CB7-CB8-CB9
8	M	413	LDA	C2-C1-N1-O1
10	L	301[B]	BCB	C6-C7-C8-C10
8	H	708	LDA	C7-C8-C9-C10
8	L	307	LDA	C11-C10-C9-C8
10	L	301[A]	BCB	C16-C17-C18-C20
14	M	404	NS5	C13-C14-C15-C17
6	C	405	DGA	CB2-CB3-CB4-CB5
11	L	305	BPB	C4-C3-C5-C6
10	L	301[A]	BCB	CAD-CBD-CGD-O1D
10	L	301[B]	BCB	C6-C7-C8-C9
14	M	404	NS5	C10-C12-C13-C14
14	M	404	NS5	C23-C24-C25-C26
6	C	405	DGA	CAB-CBB-CCB-CDB
10	L	301[A]	BCB	C16-C17-C18-C19
10	M	403[B]	BCB	C11-C10-C8-C9
11	L	303[B]	BPB	C6-C7-C8-C9
10	L	304	BCB	C8-C10-C11-C12
10	M	403[A]	BCB	O2A-C1-C2-C3
11	L	303[B]	BPB	O2A-C1-C2-C3
8	H	708	LDA	C2-C3-C4-C5
10	L	301[A]	BCB	C1A-C2A-CAA-CBA
10	M	403[A]	BCB	C1A-C2A-CAA-CBA
8	H	701	LDA	C9-C10-C11-C12
10	L	304	BCB	C11-C10-C8-C7
11	L	303[B]	BPB	C12-C13-C15-C16
10	L	302[A]	BCB	CHA-CBD-CGD-O1D
10	L	304	BCB	CHA-CBD-CGD-O1D
13	M	402[B]	MQ7	C39-C38-C40-C41
5	C	402	HEC	C3D-CAD-CBD-CGD
10	L	304	BCB	C10-C11-C12-C13
10	L	301[B]	BCB	C4-C3-C5-C6
10	L	304	BCB	C4-C3-C5-C6
10	L	304	BCB	C11-C10-C8-C9
11	L	303[B]	BPB	C14-C13-C15-C16
11	L	303[B]	BPB	CAD-CBD-CGD-O2D
10	M	403[A]	BCB	C15-C16-C17-C18
10	L	302[A]	BCB	C3A-C2A-CAA-CBA
10	L	304	BCB	C3A-C2A-CAA-CBA
8	M	412	LDA	C3-C4-C5-C6
10	L	301[B]	BCB	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	L	301[A]	BCB	CHA-CBD-CGD-O1D
10	L	302[B]	BCB	CHA-CBD-CGD-O1D
10	L	304	BCB	CHA-CBD-CGD-O2D
10	L	301[B]	BCB	CAD-CBD-CGD-O2D
8	M	412	LDA	C6-C7-C8-C9
10	L	301[B]	BCB	CBA-CGA-O2A-C1
14	M	404	NS5	C3-C4-C5-C7
10	L	301[B]	BCB	C11-C10-C8-C9
10	L	304	BCB	C4B-C3B-CAB-OB
10	M	403[A]	BCB	C16-C17-C18-C20
6	C	405	DGA	CBB-CCB-CDB-CEB
10	L	301[A]	BCB	C15-C16-C17-C18
6	C	405	DGA	OB1-CB1-OG2-CG2
10	L	304	BCB	C2-C3-C5-C6
11	L	305	BPB	C2-C3-C5-C6
10	L	302[A]	BCB	C8-C10-C11-C12
8	M	412	LDA	C4-C5-C6-C7
6	C	405	DGA	CB1-CB2-CB3-CB4
10	M	403[B]	BCB	CAA-CBA-CGA-O2A
10	L	301[B]	BCB	C2-C3-C5-C6
10	L	302[A]	BCB	CHA-CBD-CGD-O2D
10	L	302[B]	BCB	CHA-CBD-CGD-O2D
10	M	403[B]	BCB	CAA-CBA-CGA-O1A
14	M	404	NS5	C31-C33-C34-C35

There are no ring outliers.

20 monomers are involved in 49 short contacts:

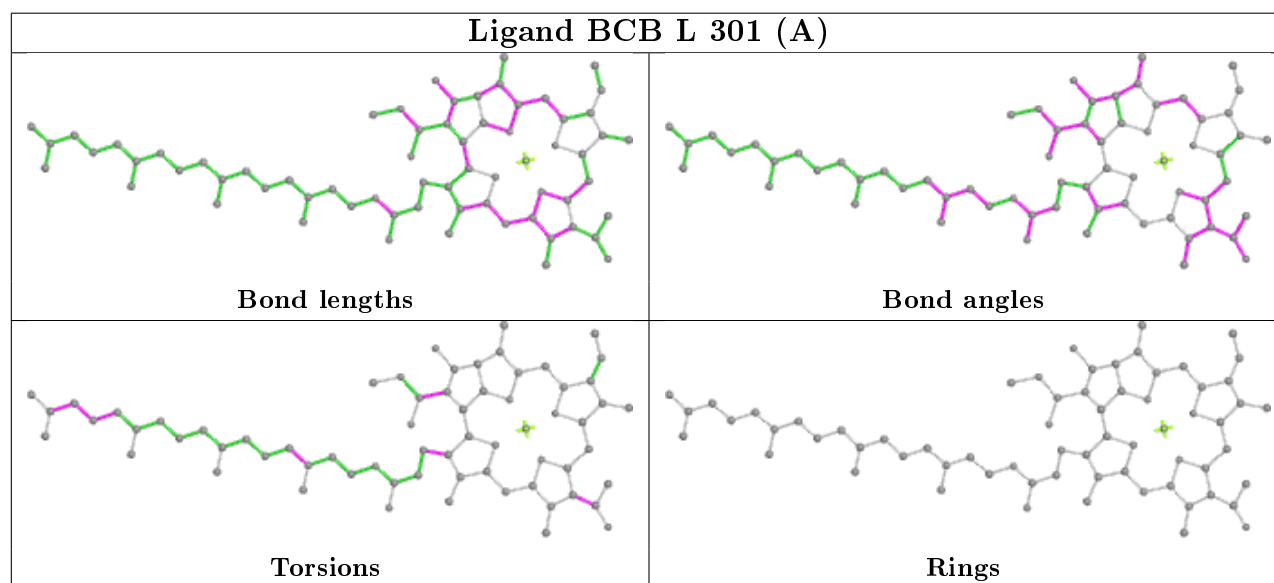
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	701	LDA	1	0
10	L	301[A]	BCB	4	0
14	M	404	NS5	2	0
10	L	302[B]	BCB	4	0
7	M	407	SO4	2	0
5	C	403	HEC	2	0
11	L	303[B]	BPB	5	0
5	C	404	HEC	1	0
5	C	401	HEC	1	0
11	L	303[A]	BPB	3	0
5	C	402	HEC	1	0
10	L	304	BCB	8	0
13	M	402[A]	MQ7	1	0

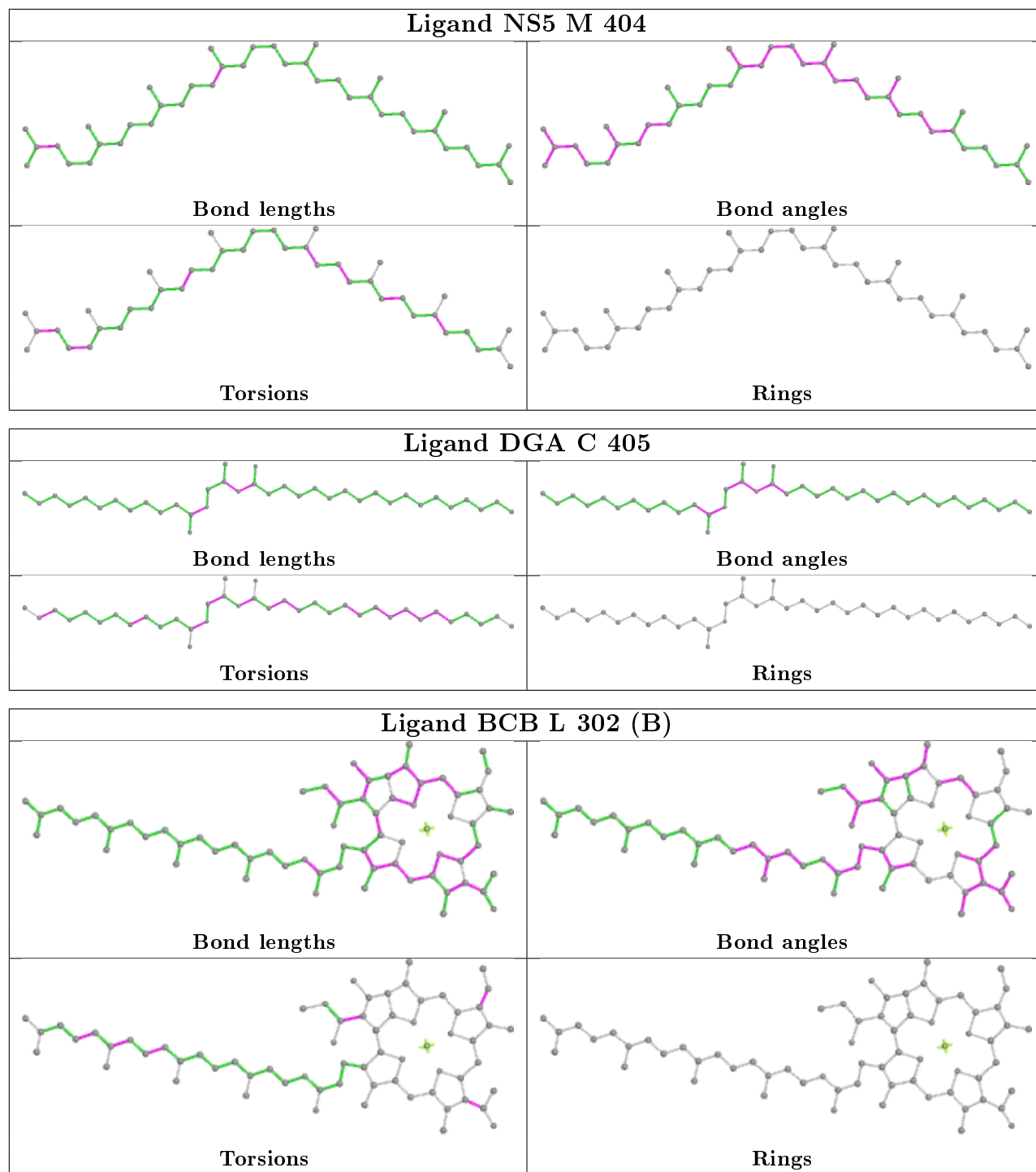
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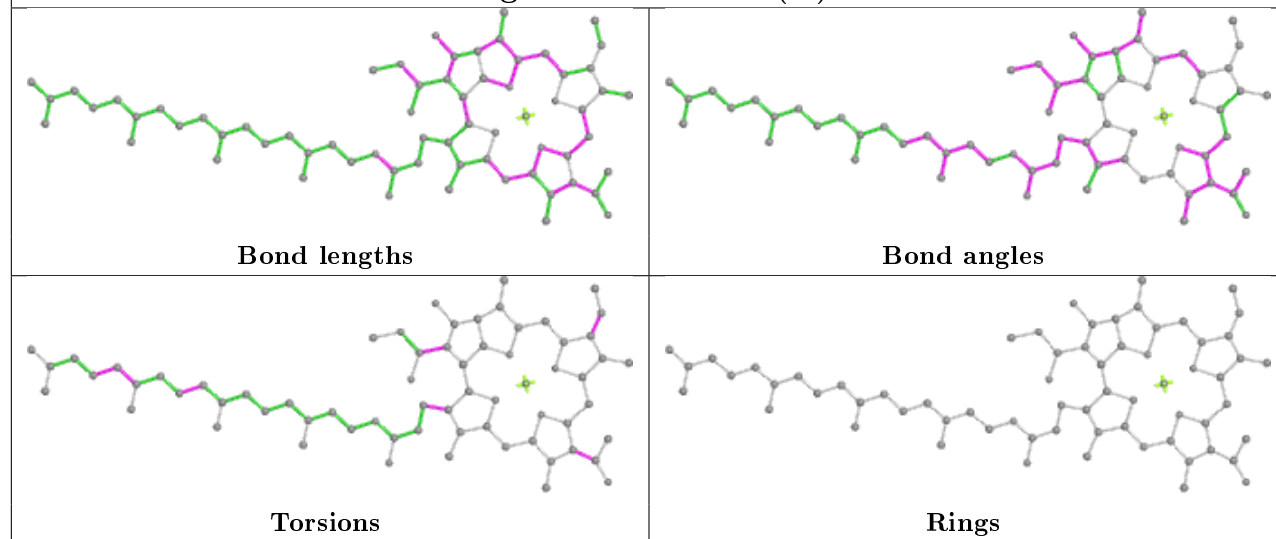
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	305	BPB	6	0
10	M	403[B]	BCB	5	0
8	H	707	LDA	1	0
8	H	708	LDA	3	0
10	L	301[B]	BCB	2	0
8	L	306	LDA	2	0
10	M	403[A]	BCB	1	0

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.

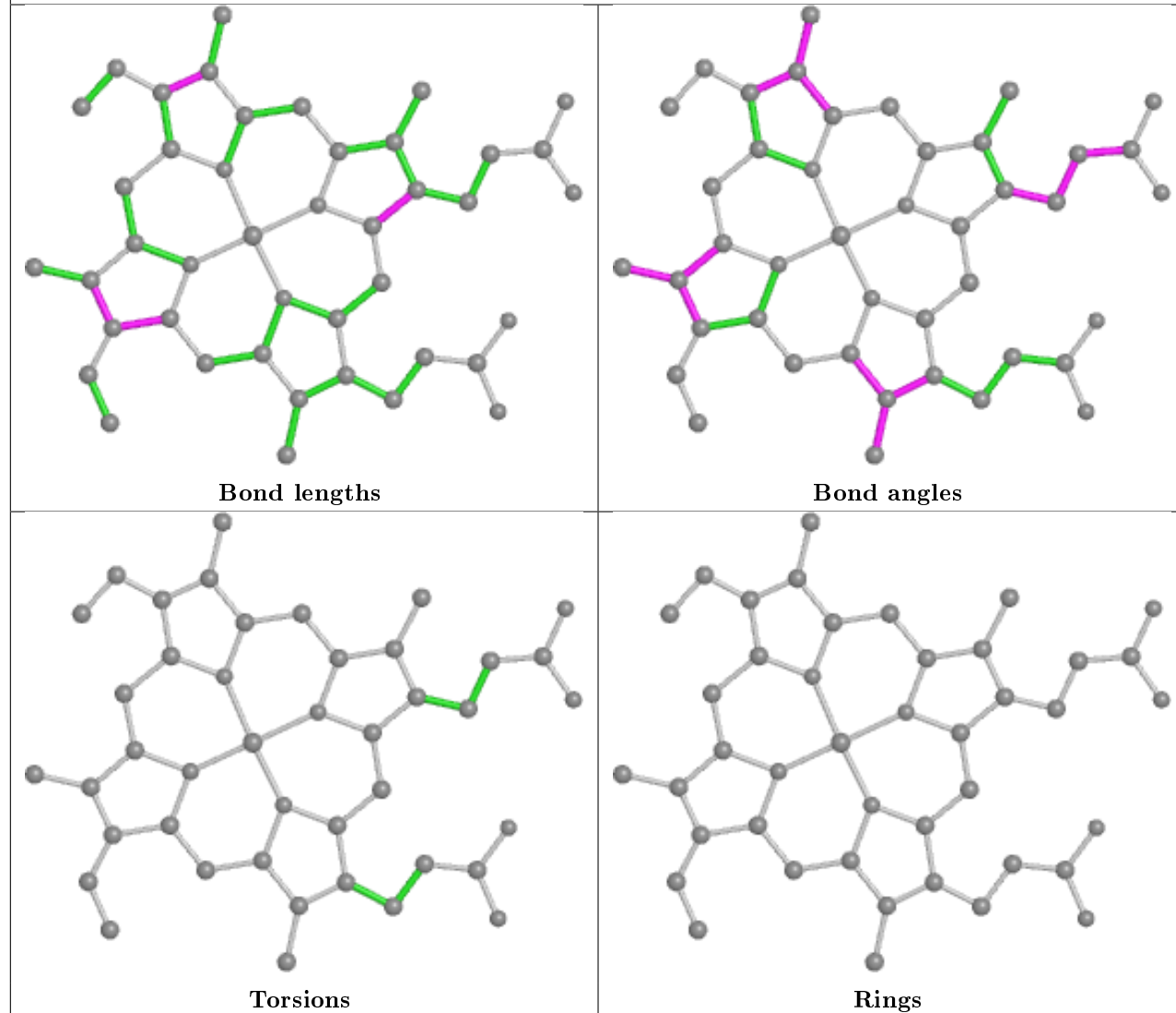




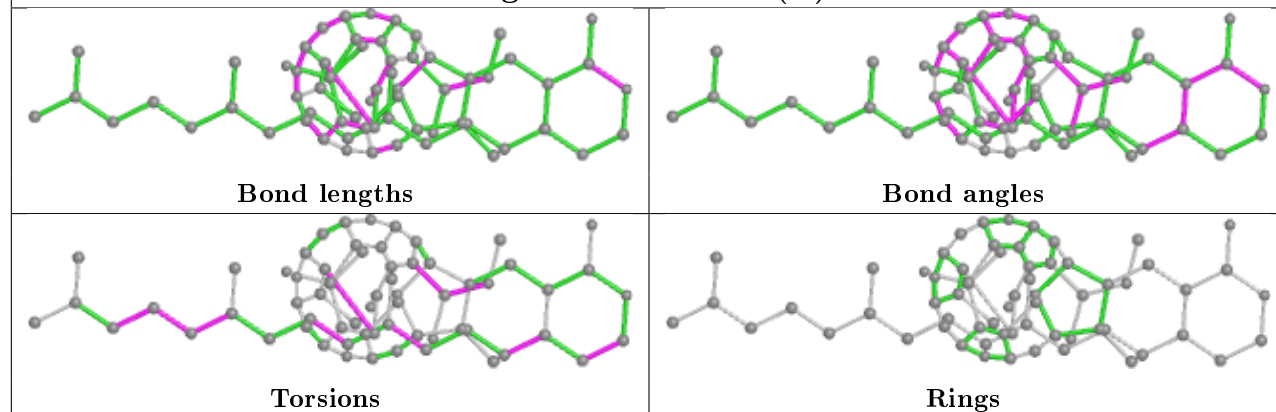
Ligand BCB L 302 (A)



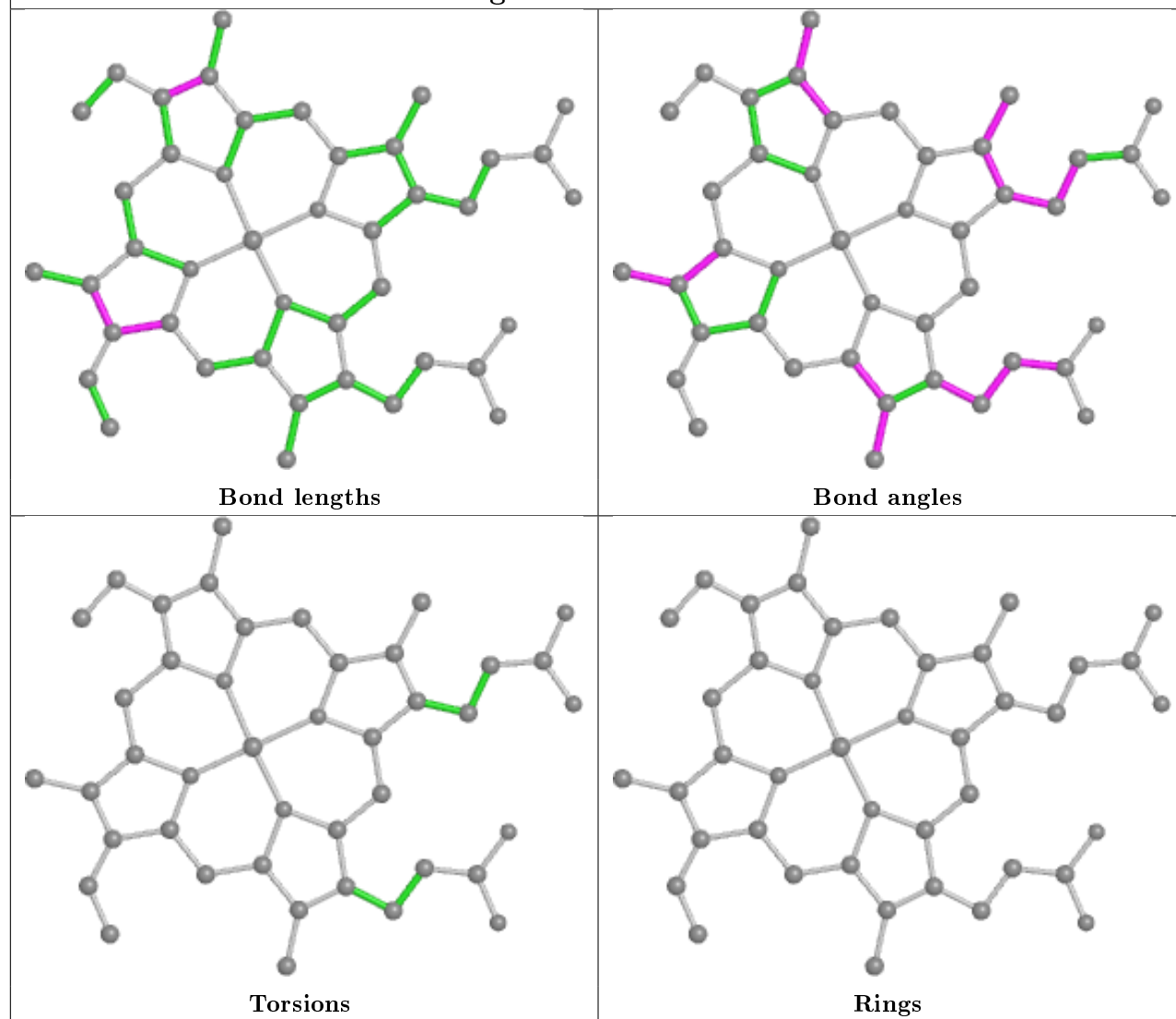
Ligand HEC C 403

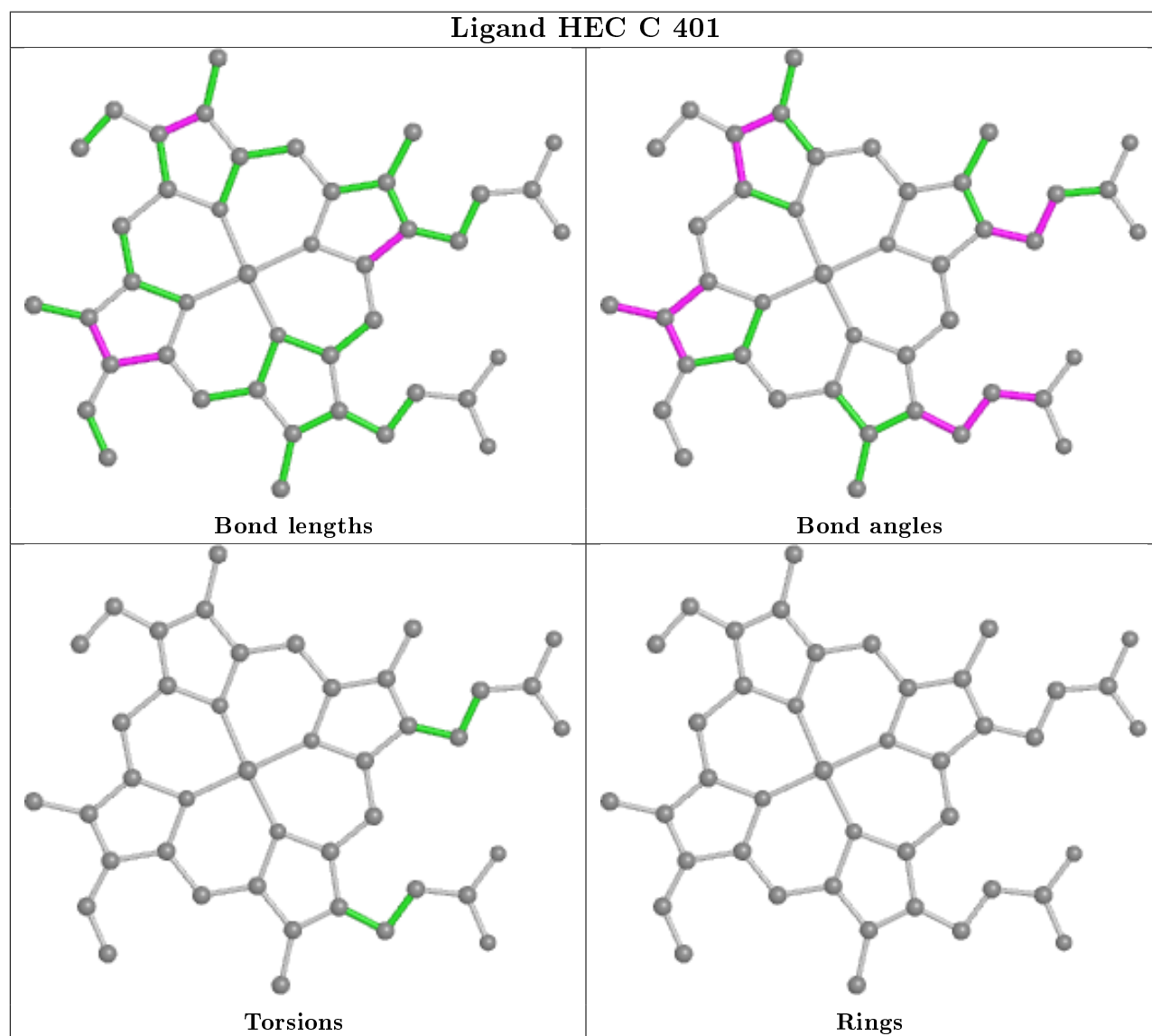
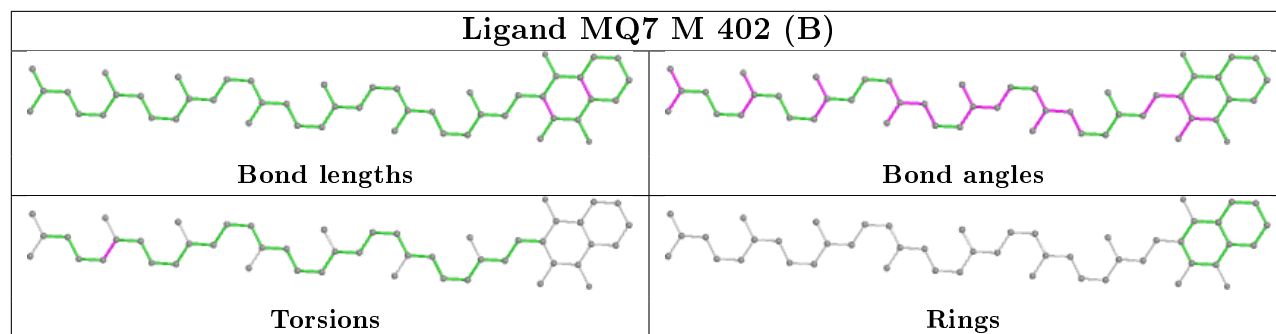


Ligand BPB L 303 (B)

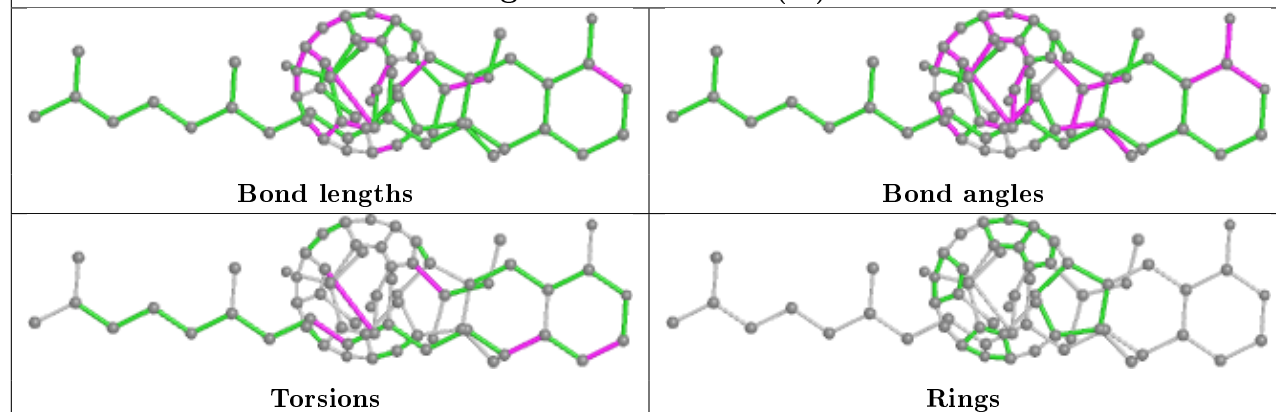


Ligand HEC C 404

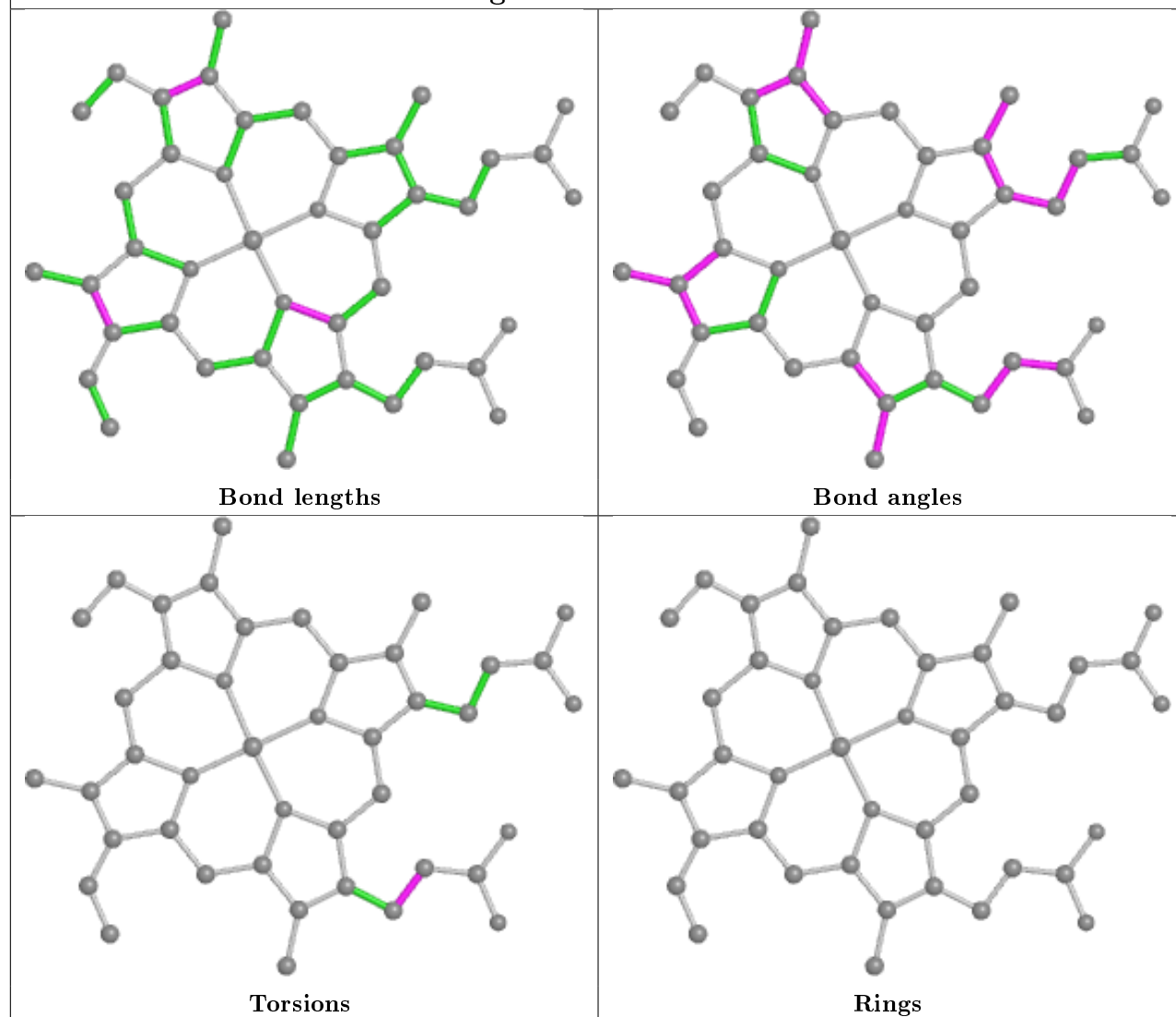


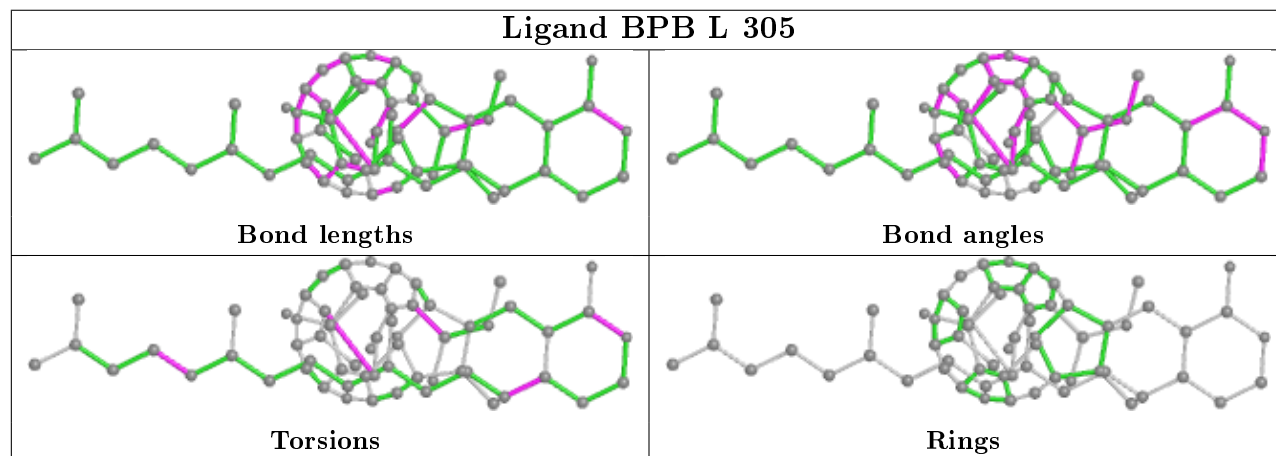
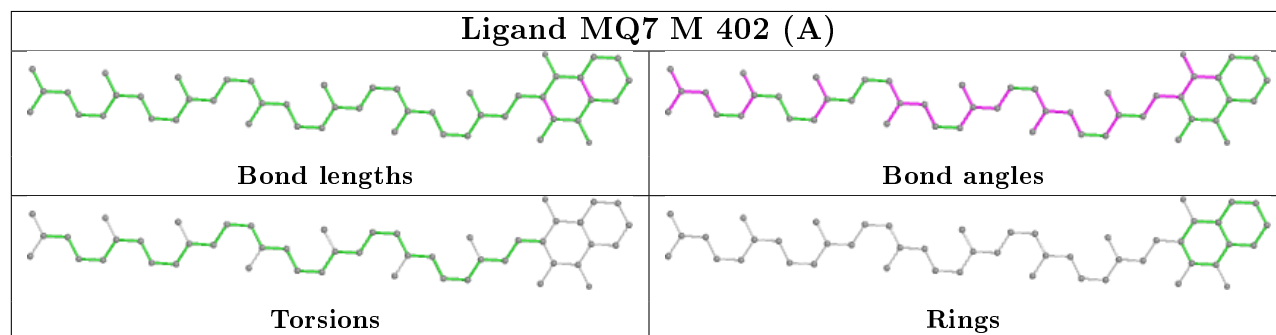
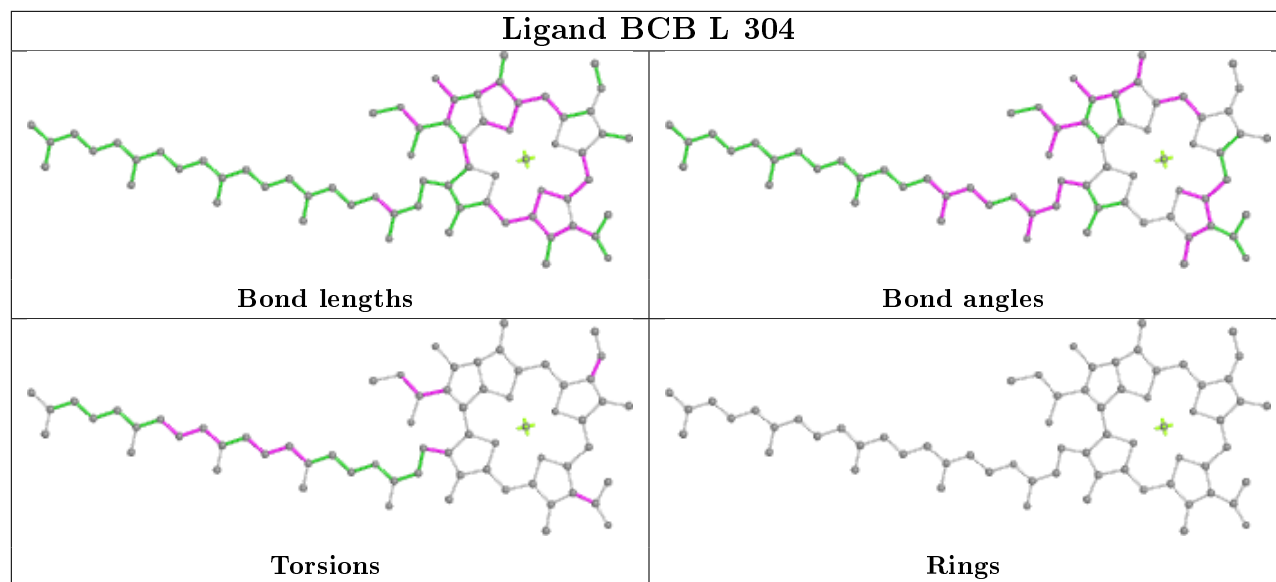


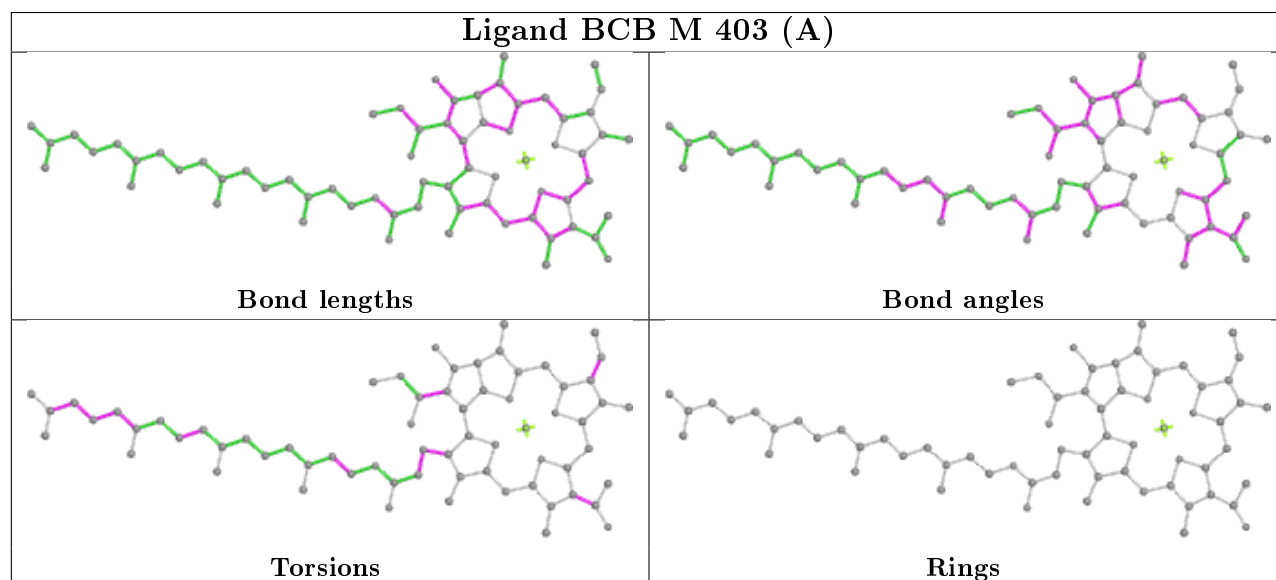
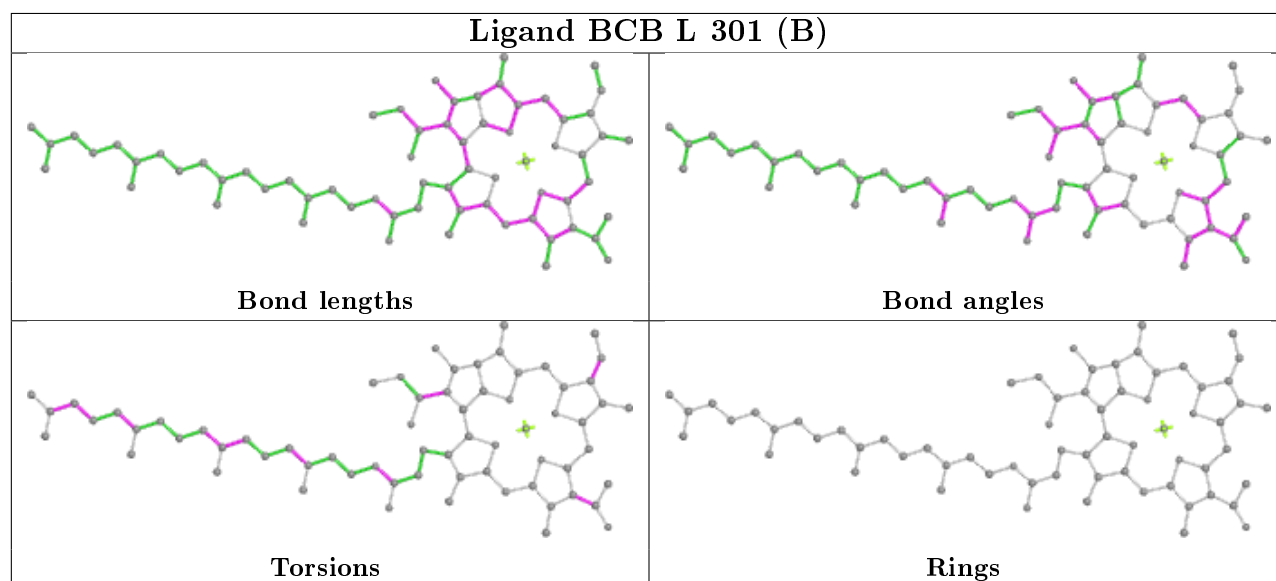
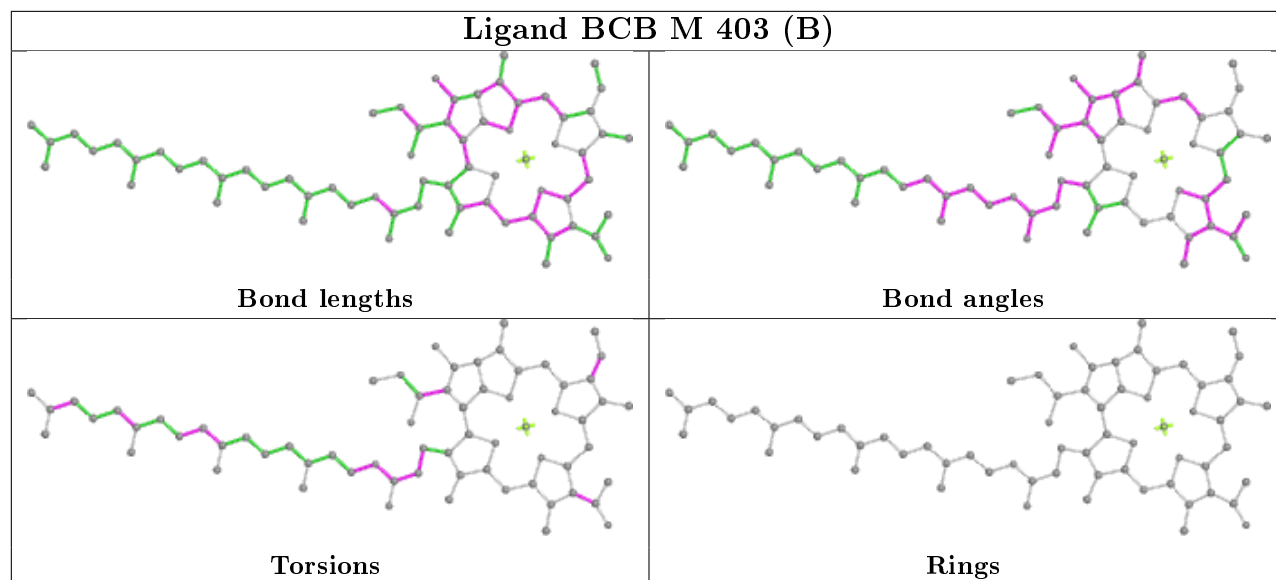
Ligand BPB L 303 (A)



Ligand HEC C 402







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.