



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:59 pm BST

PDB ID : 1DXR  
Title : Photosynthetic reaction center from Rhodopseudomonas viridis - His L168 Phe mutant (terbutryn complex)  
Authors : Lancaster, C.R.D.; Bibikova, M.; Sabatino, P.; Oesterhelt, D.; Michel, H.  
Deposited on : 2000-01-15  
Resolution : 2.00 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](mailto: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.

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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) : 2.11

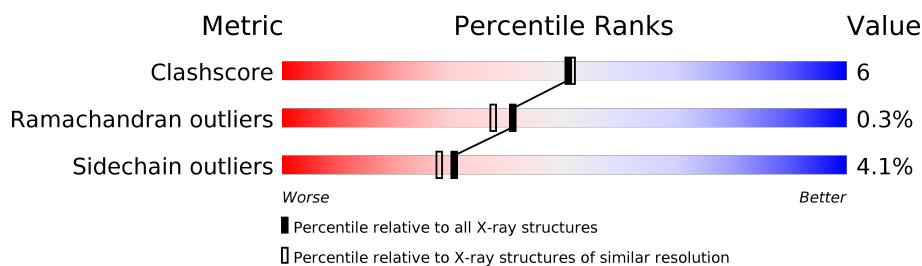
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
2	H	258	
3	L	273	
4	M	323	

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
9	BPB	M	402	X	-	-	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10777 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	39	4	0
			2636	1658	474	486	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	118	0	0
			2018	1292	344	380	2			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	13	0	0
			2172	1462	348	355	7			

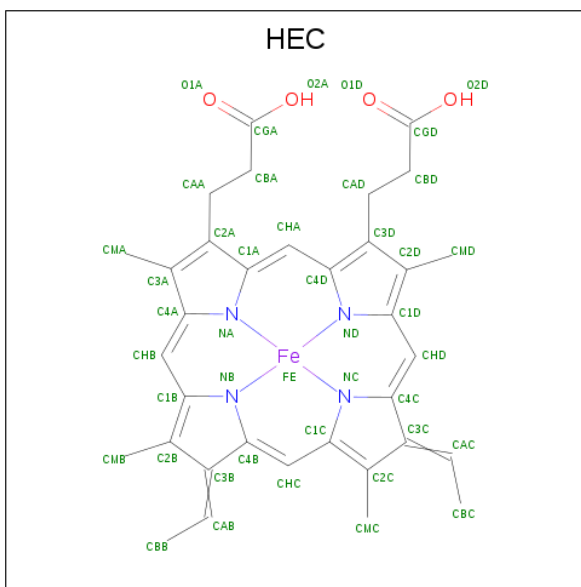
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	168	PHE	HIS	engineered mutation	UNP P06009

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

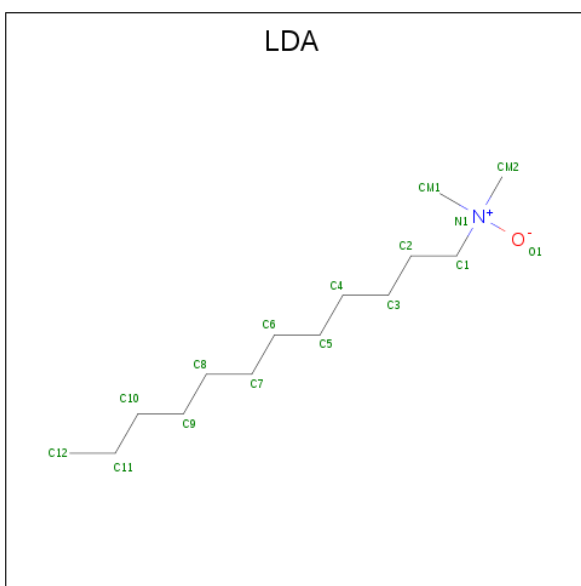
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	15	2	0
			2569	1710	421	425	13			

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



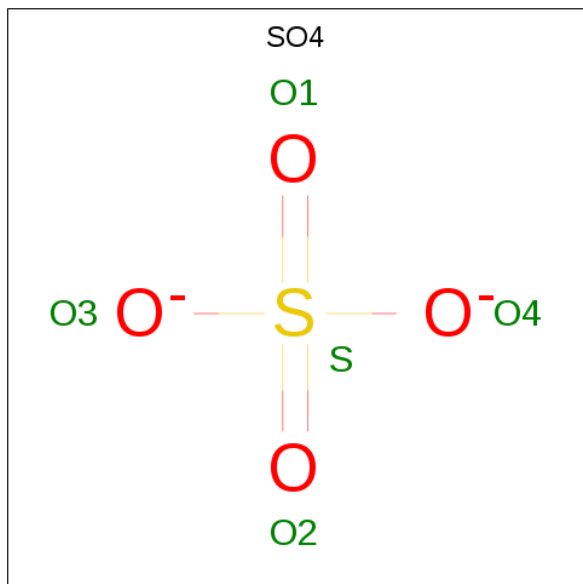
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $\text{C}_{14}\text{H}_{31}\text{NO}$ ).



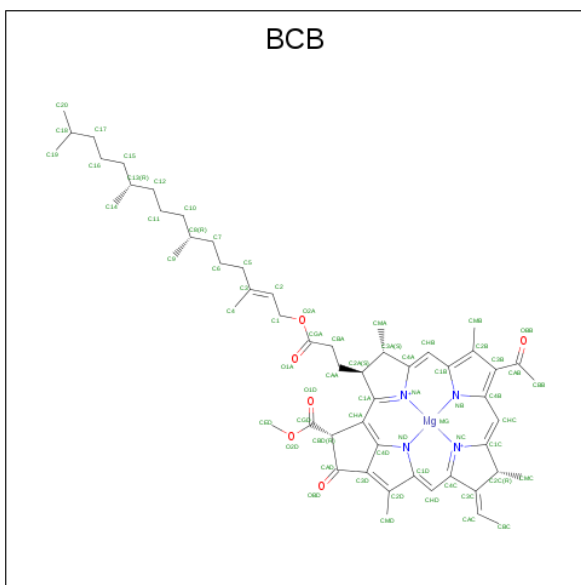
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	3	0
			16	14	1	1		
6	M	1	Total	C	N	O	4	0
			16	14	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



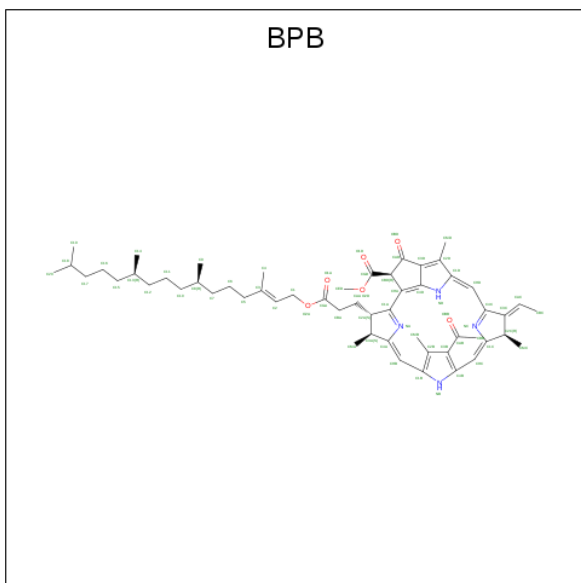
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_6$ ).

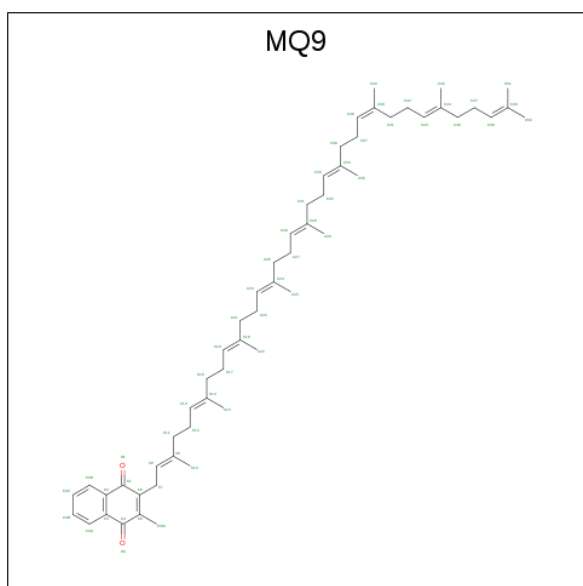


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			65	55	4	6		
9	M	1	Total	C	N	O	7	0
			65	55	4	6		

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

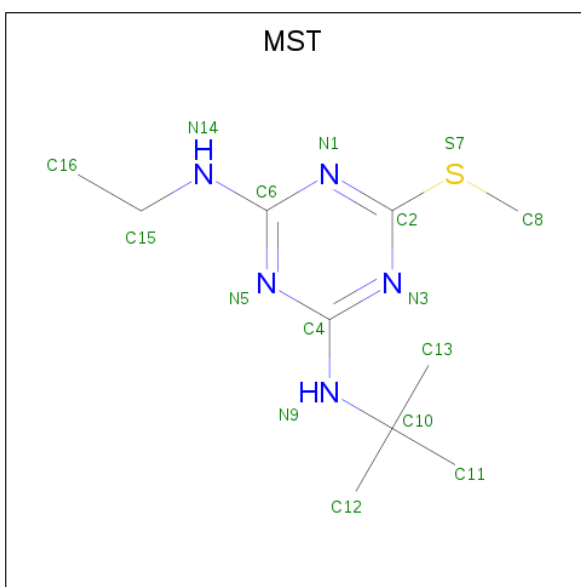
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	1	Total	Fe	0	0
			1	1		

- Molecule 11 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C<sub>56</sub>H<sub>80</sub>O<sub>2</sub>).



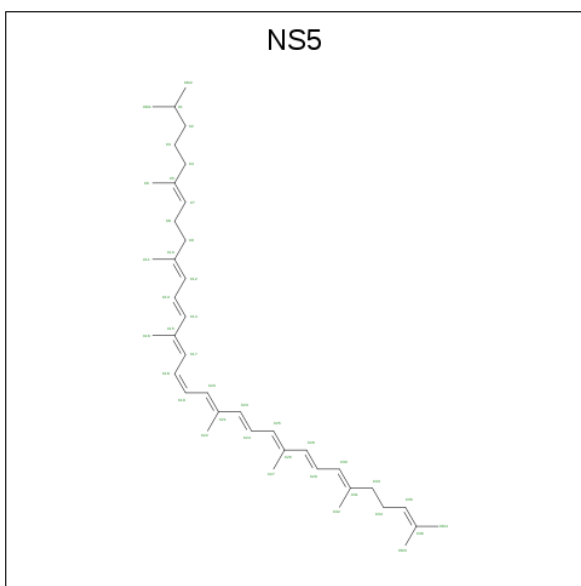
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			58	56	2		

- Molecule 12 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (three-letter code: MST) (formula: C<sub>10</sub>H<sub>19</sub>N<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

- Molecule 14 is water.

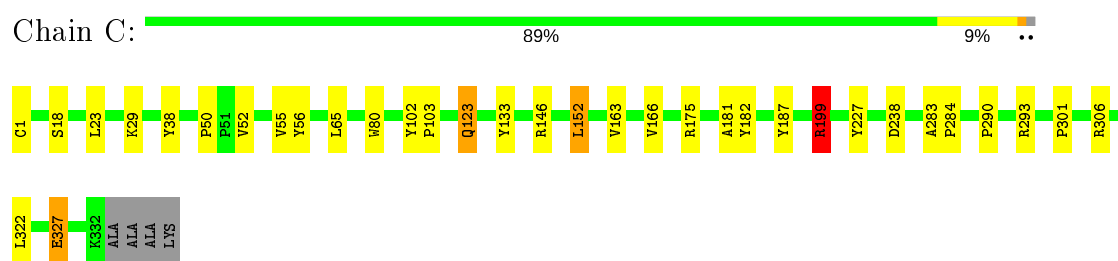
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	222	Total 222	O 222	0	0
14	H	146	Total 146	O 146	0	0
14	H	1	Total 1	O 1	0	0
14	H	2	Total 2	O 2	0	0
14	H	1	Total 1	O 1	0	0
14	L	88	Total 88	O 88	0	0
14	L	1	Total 1	O 1	0	0
14	M	120	Total 120	O 120	0	0
14	M	1	Total 1	O 1	0	0
14	M	1	Total 1	O 1	0	0
14	M	1	Total 1	O 1	0	0
14	M	1	Total 1	O 1	0	0

### 3 Residue-property plots [i](#)

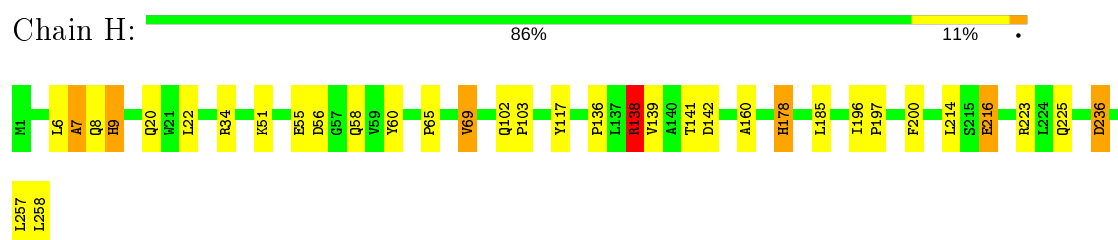
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

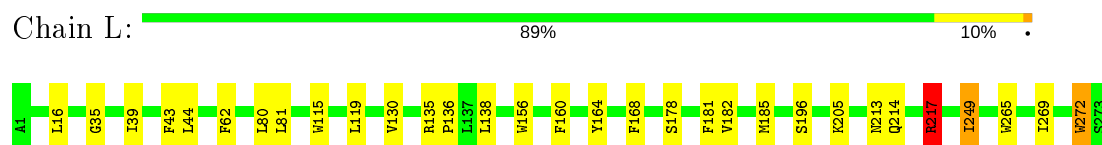
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



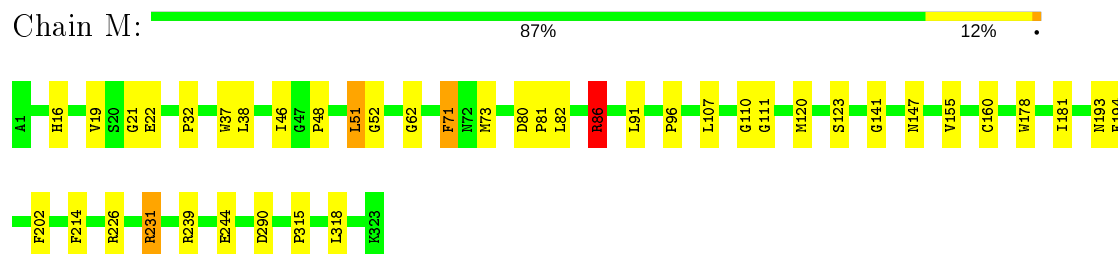
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT



#### • Molecule 4: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT



## 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, $\alpha$ , $\beta$ , $\gamma$	223.50 Å   223.50 Å   113.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.5 (10.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.194 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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, BPB, MST, BCB, FE2, SO4, HEC, MQ9, FME, NS5

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	0.49	0/2703	0.60	2/3683 (0.1%)
2	H	0.52	0/2055	0.65	1/2807 (0.0%)
3	L	0.54	0/2260	0.56	0/3085
4	M	0.52	0/2673	0.58	1/3655 (0.0%)
All	All	0.52	0/9691	0.60	4/13230 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
2	H	0	4
3	L	0	2
4	M	0	2
All	All	0	12

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199[A]	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	199[B]	ARG	NE-CZ-NH2	-6.46	117.07	120.30
4	M	231	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	H	138	ARG	NE-CZ-NH2	-5.52	117.54	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	187	TYR	Sidechain
1	C	199[A]	ARG	Sidechain
1	C	227	TYR	Sidechain
1	C	327	GLU	Mainchain
2	H	138	ARG	Sidechain
2	H	34	ARG	Sidechain
2	H	8	GLN	Peptide
2	H	9	HIS	Peptide
3	L	164	TYR	Sidechain
3	L	217	ARG	Sidechain
4	M	231	ARG	Sidechain
4	M	86	ARG	Sidechain

## 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	2636	0	2599	19	0
2	H	2018	0	2020	21	0
3	L	2172	0	2100	34	0
4	M	2569	0	2464	27	0
5	C	172	0	120	4	0
6	H	32	0	62	3	0
6	L	16	0	31	4	0
6	M	48	0	93	2	0
7	H	5	0	0	0	0
7	M	15	0	0	1	0
8	L	132	0	144	8	0
8	M	132	0	144	14	0
9	L	65	0	74	3	0
9	M	65	0	74	7	0
10	L	1	0	0	0	0
11	L	58	0	80	1	0
12	L	16	0	19	0	0
13	M	40	0	60	2	0
14	C	222	0	0	0	0
14	H	150	0	0	0	0
14	L	89	0	0	2	0
14	M	124	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10777	0	10084	113	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 (113) 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)
9:M:402:BPB:HBBB	9:M:402:BPB:HHC	1.46	0.94
8:M:400:BCB:HBB2	8:M:400:BCB:HHC	1.50	0.91
3:L:62:PHE:HD2	6:L:1274:LDA:HM11	1.48	0.77
3:L:185:MET:SD	8:M:400:BCB:H41	2.29	0.73
2:H:65:PRO:HG3	6:H:1260:LDA:H72	1.70	0.72
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.71	0.71
3:L:43:PHE:HA	11:L:501:MQ9:H512	1.72	0.70
9:M:402:BPB:HBBB	9:M:402:BPB:CHC	2.22	0.70
3:L:181:PHE:CD2	9:M:402:BPB:HBB	2.29	0.68
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.76	0.68
3:L:214:GLN:NE2	4:M:19:VAL:H	1.94	0.66
8:M:400:BCB:CBB	8:M:400:BCB:HHC	2.25	0.65
3:L:178:SER:O	3:L:182:VAL:HG23	1.97	0.65
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.78	0.65
3:L:181:PHE:HB3	9:M:402:BPB:HBBA	1.79	0.64
3:L:272:TRP:CG	4:M:86:ARG:HG3	2.33	0.64
1:C:50:PRO:HG2	1:C:55:VAL:HG22	1.81	0.63
1:C:123[A]:GLN:H	1:C:123[A]:GLN:NE2	1.97	0.62
1:C:301:PRO:HG2	5:C:402:HEC:HBD1	1.82	0.61
1:C:50:PRO:HG2	1:C:55:VAL:CG2	2.29	0.61
3:L:62:PHE:HD2	6:L:1274:LDA:CM1	2.14	0.60
3:L:62:PHE:CD2	6:L:1274:LDA:HM11	2.32	0.60
4:M:71:PHE:HB3	6:M:1326:LDA:H52	1.82	0.60
4:M:315:PRO:HA	4:M:318:LEU:HG	1.83	0.60
3:L:214:GLN:HE21	4:M:19:VAL:H	1.48	0.58
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.38	0.58
4:M:32:PRO:HG3	4:M:48:PRO:HD3	1.83	0.58
3:L:181:PHE:HB3	9:M:402:BPB:CBB	2.33	0.58
2:H:65:PRO:HG3	6:H:1260:LDA:C7	2.34	0.58
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.40	0.57
2:H:6:LEU:O	2:H:7:ALA:HB2	2.05	0.57
2:H:65:PRO:CG	6:H:1260:LDA:H72	2.35	0.57
2:H:160:ALA:HB3	2:H:214:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.88	0.56
3:L:269:ILE:HB	3:L:272:TRP:NE1	2.22	0.55
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.89	0.55
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.43	0.54
8:L:400:BCB:HBB2	8:L:400:BCB:HMB1	1.89	0.54
3:L:185:MET:SD	8:M:400:BCB:C4	2.97	0.53
2:H:55:GLU:HB2	2:H:58:GLN:HG3	1.89	0.53
3:L:62:PHE:CE2	6:L:1274:LDA:HM21	2.44	0.53
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.91	0.52
4:M:160[A]:CYS:SG	13:M:600:NS5:H322	2.51	0.51
3:L:182:VAL:HG22	8:M:400:BCB:H12	1.93	0.50
5:C:402:HEC:HMB1	5:C:402:HEC:HBB3	1.93	0.50
3:L:138:LEU:HD12	3:L:249:ILE:HD12	1.93	0.50
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.47	0.49
8:L:401:BCB:HMB1	8:L:401:BCB:CBB	2.41	0.49
4:M:62:GLY:HA3	9:M:402:BPB:H5	1.95	0.49
1:C:52:VAL:HA	1:C:55:VAL:HB	1.95	0.48
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.49	0.48
1:C:123[A]:GLN:HE21	1:C:123[A]:GLN:H	1.62	0.47
8:L:401:BCB:OBB	8:L:401:BCB:HHC	2.13	0.47
3:L:272:TRP:CD2	4:M:86:ARG:HG3	2.50	0.47
8:L:400:BCB:CBB	8:L:400:BCB:HMB1	2.44	0.46
3:L:35:GLY:O	3:L:39:ILE:HG12	2.15	0.46
8:L:401:BCB:HMB1	8:L:401:BCB:HBB2	1.98	0.46
8:L:400:BCB:H11	8:L:401:BCB:H2C	1.98	0.46
9:L:402:BPB:HHC	9:L:402:BPB:OBB	2.15	0.46
4:M:21:GLY:HA3	14:M:2021:HOH:O	2.15	0.45
8:M:400:BCB:H152	8:M:400:BCB:H111	1.84	0.45
4:M:51:LEU:HA	4:M:51:LEU:HD12	1.80	0.45
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.45
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.51	0.45
1:C:181:ALA:O	1:C:182:TYR:HB2	2.17	0.45
9:M:402:BPB:CBB	9:M:402:BPB:CHC	2.92	0.45
2:H:178:HIS:HD2	14:M:2016:HOH:O	1.98	0.44
8:M:400:BCB:HBB3	8:M:401:BCB:H41	1.98	0.44
4:M:155:VAL:HG21	8:M:401:BCB:H8	1.99	0.44
8:L:400:BCB:HHC	8:L:400:BCB:OBB	2.17	0.44
4:M:239:ARG:HD3	4:M:244:GLU:HG2	2.00	0.44
9:L:402:BPB:HMB	9:L:402:BPB:HBBB	2.00	0.44
1:C:301:PRO:CG	5:C:402:HEC:HBD1	2.46	0.44
2:H:69:VAL:HG22	3:L:205:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:80:ASP:HA	4:M:81:PRO:HD3	1.85	0.43
4:M:160[A]:CYS:SG	13:M:600:NS5:C31	3.06	0.43
4:M:120:MET:O	4:M:123:SER:HB3	2.17	0.43
3:L:272:TRP:HB3	4:M:82:LEU:HD21	1.99	0.43
2:H:69:VAL:CG2	3:L:205:LYS:HG2	2.49	0.43
3:L:214:GLN:NE2	14:L:2074:HOH:O	2.52	0.43
8:M:401:BCB:HAA2	8:M:401:BCB:HBD	2.01	0.43
4:M:178:TRP:CE3	4:M:178:TRP:HA	2.53	0.43
4:M:96:PRO:HD3	4:M:110:GLY:HA3	2.01	0.43
3:L:81:LEU:HA	3:L:81:LEU:HD23	1.83	0.42
8:M:401:BCB:HMB1	8:M:401:BCB:HBB3	2.01	0.42
2:H:102:GLN:HA	2:H:103:PRO:HD3	1.90	0.42
1:C:1:CYS:HB2	3:L:265:TRP:HB3	2.02	0.42
2:H:138:ARG:HG3	2:H:139:VAL:HG23	2.00	0.42
2:H:216:GLU:HG3	2:H:216:GLU:H	1.58	0.42
3:L:80:LEU:HD12	3:L:80:LEU:HA	1.90	0.41
8:M:401:BCB:HHC	8:M:401:BCB:OBB	2.20	0.41
2:H:136:PRO:HG2	2:H:138:ARG:HG2	2.02	0.41
3:L:168:PHE:CZ	8:L:400:BCB:HMC2	2.55	0.41
2:H:20:GLN:HG2	4:M:202:PHE:CZ	2.55	0.41
8:M:401:BCB:HMB1	8:M:401:BCB:CBB	2.50	0.41
2:H:6:LEU:O	2:H:7:ALA:CB	2.69	0.41
3:L:130:VAL:HG13	3:L:249:ILE:HG12	2.03	0.41
4:M:38:LEU:HD22	4:M:46:ILE:HD11	2.01	0.41
4:M:51:LEU:HB3	4:M:52:GLY:H	1.64	0.41
1:C:163:VAL:HG23	14:L:2087:HOH:O	2.20	0.41
1:C:238:ASP:OD2	1:C:306:ARG:NH2	2.54	0.41
3:L:182:VAL:HG22	8:M:400:BCB:C1	2.50	0.41
8:M:401:BCB:H141	8:M:401:BCB:H162	1.72	0.41
3:L:213:ASN:O	3:L:217:ARG:HB2	2.21	0.41
2:H:142:ASP:N	2:H:142:ASP:OD1	2.52	0.41
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	2.03	0.41
6:M:1324:LDA:HM11	7:M:1329:SO4:O4	2.20	0.40
3:L:196:SER:HB2	4:M:141:GLY:O	2.21	0.40
9:L:402:BPB:NC	9:L:402:BPB:ND	2.69	0.40
2:H:196:ILE:HA	2:H:197:PRO:HD3	1.98	0.40
1:C:283:ALA:N	1:C:284:PRO:CD	2.84	0.40
3:L:115:TRP:N	3:L:115:TRP:CD1	2.86	0.40
3:L:135:ARG:HB3	3:L:136:PRO:HD3	2.03	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	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	H	256/258 (99%)	245 (96%)	9 (4%)	2 (1%)	19	13
3	L	271/273 (99%)	265 (98%)	6 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	8 (2%)	1 (0%)	41	37
All	All	1184/1190 (100%)	1151 (97%)	30 (2%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	7	ALA
2	H	9	HIS
4	M	193	ASN

### 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	284/282 (101%)	273 (96%)	11 (4%)	32	30
2	H	212/212 (100%)	200 (94%)	12 (6%)	20	16
3	L	218/218 (100%)	211 (97%)	7 (3%)	39	38
4	M	251/249 (101%)	240 (96%)	11 (4%)	28	25
All	All	965/961 (100%)	924 (96%)	41 (4%)	30	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	29	LYS
1	C	38	TYR
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	146	ARG
1	C	152	LEU
1	C	166	VAL
1	C	199[A]	ARG
1	C	199[B]	ARG
1	C	322	LEU
2	H	22	LEU
2	H	51	LYS
2	H	69	VAL
2	H	141	THR
2	H	178	HIS
2	H	185	LEU
2	H	216	GLU
2	H	223	ARG
2	H	225	GLN
2	H	236	ASP
2	H	257	LEU
2	H	258	LEU
3	L	16	LEU
3	L	44	LEU
3	L	119	LEU
3	L	160	PHE
3	L	217	ARG
3	L	249	ILE
3	L	272	TRP
4	M	16	HIS
4	M	22	GLU
4	M	37	TRP
4	M	51	LEU
4	M	71	PHE
4	M	86	ARG
4	M	147	ASN
4	M	181	ILE
4	M	194	PHE
4	M	214	PHE
4	M	290	ASP

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

Mol	Chain	Res	Type
1	C	302	GLN
2	H	102	GLN
3	L	183	ASN
3	L	214	GLN
4	M	147	ASN

### 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	0.59	0	7,9,11	2.30	2 (28%)

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	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	O1-CN-N	-4.26	114.05	125.27
2	H	1	FME	CA-N-CN	-3.35	117.68	122.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA
2	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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$
9	BPB	L	402	-	64,70,70	1.10	7 (10%)	64,101,101	1.87	9 (14%)
6	LDA	M	1326	-	12,15,15	2.29	1 (8%)	14,17,17	0.56	0
7	SO4	M	1329	-	4,4,4	1.38	0	6,6,6	0.80	0
5	HEC	C	404	1	26,50,50	1.73	3 (11%)	18,82,82	1.41	3 (16%)
8	BCB	M	400	4	60,74,74	3.57	22 (36%)	48,115,115	2.67	19 (39%)
8	BCB	M	401	8,4	60,74,74	3.65	25 (41%)	48,115,115	2.64	17 (35%)
13	NS5	M	600	-	39,39,39	0.87	2 (5%)	44,46,46	1.13	4 (9%)
7	SO4	H	1261	-	4,4,4	0.55	0	6,6,6	0.38	0
5	HEC	C	402	1	26,50,50	1.63	3 (11%)	18,82,82	1.21	2 (11%)
12	MST	L	502	-	16,16,16	1.22	1 (6%)	22,22,22	1.41	2 (9%)
9	BPB	M	402	-	64,70,70	1.07	6 (9%)	64,101,101	1.79	12 (18%)
8	BCB	L	401	3	60,74,74	3.71	22 (36%)	48,115,115	2.41	14 (29%)
5	HEC	C	401	1	26,50,50	1.58	2 (7%)	18,82,82	1.38	3 (16%)
6	LDA	L	1274	-	12,15,15	2.24	1 (8%)	14,17,17	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LDA	H	1259	-	12,15,15	2.20	1 (8%)	14,17,17	0.59	0
5	HEC	C	403	1	26,50,50	1.62	3 (11%)	18,82,82	1.99	6 (33%)
6	LDA	M	1325	-	12,15,15	2.31	1 (8%)	14,17,17	0.57	0
6	LDA	H	1260	-	12,15,15	2.35	1 (8%)	14,17,17	0.49	0
11	MQ9	L	501	-	59,59,59	1.66	21 (35%)	72,75,75	1.40	12 (16%)
7	SO4	M	1327	-	4,4,4	1.15	0	6,6,6	0.42	0
7	SO4	M	1328	-	4,4,4	1.03	0	6,6,6	0.53	0
6	LDA	M	1324	-	12,15,15	1.84	1 (8%)	14,17,17	0.58	0
8	BCB	L	400	8,3	60,74,74	3.65	23 (38%)	48,115,115	2.42	18 (37%)

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	BCB	M	401	8,4	-	8/41/177/177	-
5	HEC	C	403	1	-	0/6/54/54	-
6	LDA	M	1324	-	-	3/13/13/13	-
9	BPB	L	402	-	-	3/47/105/105	0/5/6/6
6	LDA	M	1326	-	-	2/13/13/13	-
5	HEC	C	402	1	-	0/6/54/54	-
12	MST	L	502	-	-	0/10/10/10	0/1/1/1
8	BCB	M	400	4	-	7/41/177/177	-
6	LDA	M	1325	-	-	3/13/13/13	-
9	BPB	M	402	-	1/1/18/23	2/47/105/105	0/5/6/6
8	BCB	L	401	3	-	6/41/177/177	-
5	HEC	C	404	1	-	0/6/54/54	-
13	NS5	M	600	-	-	11/43/43/43	-
5	HEC	C	401	1	-	0/6/54/54	-
6	LDA	L	1274	-	-	3/13/13/13	-
6	LDA	H	1259	-	-	5/13/13/13	-
11	MQ9	L	501	-	-	4/53/73/73	0/2/2/2
6	LDA	H	1260	-	-	4/13/13/13	-
8	BCB	L	400	8,3	-	9/41/177/177	-

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	401	BCB	C1A-CHA	-9.87	1.38	1.54
8	L	400	BCB	CHD-C1D	-9.13	1.39	1.53
8	L	401	BCB	CHB-C1B	-9.09	1.39	1.53
8	M	400	BCB	CHC-C4B	-8.88	1.39	1.53
8	L	400	BCB	CHB-C1B	-8.75	1.39	1.53
8	M	401	BCB	CHB-C1B	-8.54	1.40	1.53
8	M	401	BCB	C1A-CHA	-8.39	1.40	1.54
8	M	400	BCB	CHD-C1D	-8.37	1.40	1.53
8	M	401	BCB	CHD-C1D	-8.35	1.40	1.53
8	M	400	BCB	CHB-C1B	-8.26	1.40	1.53
8	L	401	BCB	CHD-C4C	-8.26	1.39	1.53
8	L	401	BCB	CHD-C1D	-8.22	1.40	1.53
6	H	1260	LDA	O1-N1	-8.11	1.23	1.42
8	M	401	BCB	CHC-C4B	-8.08	1.40	1.53
8	L	400	BCB	CHC-C4B	-8.04	1.40	1.53
6	M	1326	LDA	O1-N1	-7.93	1.23	1.42
8	M	400	BCB	C1A-CHA	-7.90	1.41	1.54
8	L	400	BCB	CHD-C4C	-7.89	1.40	1.53
8	M	400	BCB	CHD-C4C	-7.84	1.40	1.53
6	M	1325	LDA	O1-N1	-7.78	1.24	1.42
8	L	401	BCB	CHC-C4B	-7.68	1.41	1.53
6	L	1274	LDA	O1-N1	-7.62	1.24	1.42
6	H	1259	LDA	O1-N1	-7.55	1.24	1.42
8	L	400	BCB	C3D-C2D	-7.41	1.35	1.55
8	M	401	BCB	C3B-C2B	-7.37	1.36	1.55
8	M	401	BCB	CHD-C4C	-7.33	1.41	1.53
8	L	401	BCB	C3B-C2B	-7.22	1.36	1.55
8	L	401	BCB	C3D-C2D	-7.13	1.36	1.55
8	L	400	BCB	C3B-C2B	-7.11	1.36	1.55
8	M	400	BCB	C3B-C2B	-6.94	1.37	1.55
8	L	400	BCB	C1A-CHA	-6.79	1.43	1.54
8	M	400	BCB	C3D-C2D	-6.72	1.37	1.55
8	M	401	BCB	C3D-C2D	-6.55	1.38	1.55
8	L	400	BCB	C4D-ND	-6.55	1.36	1.50
8	L	401	BCB	CHB-C4A	-6.47	1.38	1.52
8	M	401	BCB	C4D-ND	-6.40	1.36	1.50
8	L	400	BCB	CHB-C4A	-6.40	1.38	1.52
8	L	401	BCB	C4D-ND	-6.38	1.36	1.50
6	M	1324	LDA	O1-N1	-6.36	1.27	1.42
8	M	400	BCB	CHC-C1C	-6.13	1.38	1.52
8	L	400	BCB	C1D-ND	-6.10	1.37	1.50
8	M	401	BCB	C4B-NB	-6.03	1.37	1.50
8	M	400	BCB	C4D-ND	-5.91	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	BCB	CHB-C4A	-5.87	1.39	1.52
8	L	401	BCB	C1D-ND	-5.86	1.37	1.50
8	M	401	BCB	C3B-CAB	-5.85	1.45	1.52
8	M	401	BCB	C1B-NB	-5.83	1.38	1.50
8	M	400	BCB	C1D-ND	-5.80	1.38	1.50
8	M	401	BCB	C1D-ND	-5.66	1.38	1.50
8	M	400	BCB	CHB-C4A	-5.59	1.40	1.52
8	L	400	BCB	C4B-NB	-5.56	1.38	1.50
8	L	400	BCB	C1B-NB	-5.52	1.38	1.50
8	M	400	BCB	C1B-NB	-5.52	1.38	1.50
8	L	401	BCB	C4B-NB	-5.50	1.38	1.50
8	L	401	BCB	C1B-NB	-5.45	1.38	1.50
8	M	400	BCB	C4B-NB	-5.44	1.38	1.50
8	M	401	BCB	C2B-C1B	-5.26	1.43	1.53
8	L	400	BCB	C3B-CAB	-5.25	1.46	1.52
5	C	401	HEC	C3B-C2B	-5.24	1.35	1.40
8	M	401	BCB	CHC-C1C	-5.20	1.40	1.52
5	C	404	HEC	C3C-C2C	-5.18	1.35	1.40
8	L	401	BCB	C2B-C1B	-5.17	1.44	1.53
8	L	401	BCB	CHC-C1C	-5.16	1.41	1.52
5	C	404	HEC	C3B-C2B	-5.03	1.35	1.40
8	L	401	BCB	C3B-CAB	-5.03	1.46	1.52
8	L	400	BCB	CHC-C1C	-4.99	1.41	1.52
5	C	402	HEC	C3C-C2C	-4.98	1.35	1.40
8	L	400	BCB	C2B-C1B	-4.95	1.44	1.53
5	C	403	HEC	C3C-C2C	-4.78	1.35	1.40
8	L	400	BCB	C2D-C1D	-4.55	1.45	1.53
8	M	401	BCB	C2D-C1D	-4.52	1.45	1.53
8	M	400	BCB	C2B-C1B	-4.49	1.45	1.53
8	M	400	BCB	C3B-CAB	-4.36	1.47	1.52
8	L	401	BCB	C2D-C1D	-4.27	1.45	1.53
5	C	402	HEC	C3B-C2B	-4.26	1.36	1.40
5	C	403	HEC	C3B-C2B	-4.22	1.36	1.40
5	C	401	HEC	C3C-C2C	-4.12	1.36	1.40
8	M	400	BCB	O2A-CGA	4.02	1.45	1.33
9	L	402	BPB	C3B-C4B	3.98	1.46	1.41
8	L	400	BCB	C4C-C3C	-3.70	1.39	1.50
8	M	400	BCB	C3D-CAD	-3.56	1.44	1.51
8	M	400	BCB	C2D-C1D	-3.47	1.47	1.53
8	L	400	BCB	O2D-CED	-3.40	1.37	1.45
8	M	400	BCB	O2D-CED	-3.40	1.37	1.45
8	M	401	BCB	C4C-C3C	-3.39	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	502	MST	C2-S7	3.39	1.78	1.75
9	M	402	BPB	C3B-C4B	3.28	1.45	1.41
8	L	400	BCB	C3D-CAD	-3.26	1.45	1.51
8	L	401	BCB	C4C-C3C	-3.24	1.41	1.50
11	L	501	MQ9	C12-C13	-3.22	1.39	1.50
8	M	401	BCB	C3D-CAD	-3.21	1.45	1.51
9	M	402	BPB	O2D-CGD	3.20	1.41	1.33
8	L	401	BCB	C3D-CAD	-3.10	1.45	1.51
11	L	501	MQ9	C38-C39	3.09	1.40	1.33
11	L	501	MQ9	C43-C44	3.08	1.40	1.33
8	L	400	BCB	C1-C2	-3.06	1.40	1.49
9	L	402	BPB	O2D-CGD	3.06	1.40	1.33
9	M	402	BPB	O2D-CED	-3.03	1.38	1.45
8	L	401	BCB	O2D-CED	-3.01	1.38	1.45
8	M	401	BCB	C4A-C3A	-2.88	1.50	1.53
11	L	501	MQ9	C46-C44	2.82	1.57	1.51
11	L	501	MQ9	C48-C49	2.80	1.40	1.32
11	L	501	MQ9	C28-C29	2.76	1.39	1.33
11	L	501	MQ9	C50-C49	2.75	1.57	1.50
11	L	501	MQ9	C45-C44	2.73	1.57	1.50
8	L	401	BCB	C2-C3	2.67	1.39	1.33
8	M	401	BCB	CBD-CGD	2.66	1.56	1.52
8	M	401	BCB	C2A-C3A	-2.65	1.50	1.54
8	L	401	BCB	O2D-CGD	2.64	1.39	1.33
11	L	501	MQ9	C8-C9	2.64	1.39	1.33
8	M	400	BCB	C4C-C3C	-2.62	1.43	1.50
8	M	401	BCB	C2-C3	2.61	1.39	1.33
8	M	401	BCB	O2A-CGA	2.61	1.41	1.33
11	L	501	MQ9	C40-C39	2.57	1.57	1.50
5	C	402	HEC	CAD-C3D	2.54	1.55	1.52
8	L	400	BCB	O2D-CGD	2.54	1.39	1.33
9	M	402	BPB	C2-C3	2.53	1.39	1.33
11	L	501	MQ9	C32-C33	-2.52	1.42	1.50
9	L	402	BPB	C2-C3	2.52	1.39	1.33
11	L	501	MQ9	C33-C34	2.43	1.38	1.33
8	L	400	BCB	C2A-C3A	-2.42	1.50	1.54
11	L	501	MQ9	C13-C14	2.41	1.38	1.33
11	L	501	MQ9	C23-C24	2.40	1.38	1.33
8	L	401	BCB	C2A-C3A	-2.35	1.50	1.54
11	L	501	MQ9	C2-C3	-2.32	1.36	1.40
9	M	402	BPB	CAC-C3C	2.27	1.39	1.33
5	C	403	HEC	CAD-C3D	2.26	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	402	BPB	C3B-C2B	-2.26	1.35	1.39
8	M	401	BCB	C1A-C2A	-2.24	1.51	1.53
11	L	501	MQ9	C51-C49	2.24	1.56	1.50
13	M	600	NS5	C9-C10	2.23	1.55	1.51
11	L	501	MQ9	C7-C8	-2.17	1.47	1.50
11	L	501	MQ9	C18-C19	2.15	1.38	1.33
9	L	402	BPB	CAC-C3C	2.15	1.39	1.33
13	M	600	NS5	C30-C31	2.14	1.36	1.34
9	L	402	BPB	O2D-CED	-2.14	1.40	1.45
8	M	400	BCB	C2-C3	2.12	1.38	1.33
9	L	402	BPB	CMD-C2D	2.11	1.55	1.50
11	L	501	MQ9	C37-C38	-2.08	1.43	1.50
8	L	400	BCB	C2-C3	2.07	1.38	1.33
5	C	404	HEC	CAA-C2A	-2.06	1.48	1.52
9	L	402	BPB	C4C-C3C	-2.04	1.41	1.45
11	L	501	MQ9	C17-C18	-2.02	1.43	1.50
8	M	401	BCB	CAA-CBA	-2.01	1.46	1.52
11	L	501	MQ9	C22-C23	-2.01	1.43	1.50
8	M	400	BCB	C1-C2	-2.00	1.43	1.49

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	402	BPB	O2D-CGD-CBD	7.91	125.33	111.27
8	M	401	BCB	CMB-C2B-C3B	7.74	133.52	114.29
8	M	400	BCB	C1D-CHD-C4C	7.39	128.11	112.37
8	L	401	BCB	C1D-CHD-C4C	7.36	128.06	112.37
9	L	402	BPB	O2D-CGD-CBD	7.23	124.11	111.27
8	M	401	BCB	C1D-CHD-C4C	6.86	126.98	112.37
8	L	400	BCB	C1D-CHD-C4C	6.85	126.96	112.37
8	M	401	BCB	CMD-C2D-C3D	6.48	130.39	114.29
8	L	400	BCB	CMB-C2B-C3B	6.45	130.30	114.29
8	M	400	BCB	CBB-CAB-C3B	6.43	123.36	116.80
8	L	401	BCB	CMB-C2B-C3B	6.28	129.88	114.29
8	L	401	BCB	O2D-CGD-CBD	5.97	125.12	111.11
8	M	401	BCB	O2D-CGD-CBD	5.96	125.10	111.11
8	L	400	BCB	CMD-C2D-C3D	5.82	128.73	114.29
8	M	400	BCB	CMD-C2D-C3D	5.64	128.30	114.29
8	M	400	BCB	O2D-CGD-CBD	5.48	123.98	111.11
8	L	401	BCB	CMD-C2D-C3D	5.47	127.86	114.29
9	M	402	BPB	O1D-CGD-CBD	-5.29	113.66	124.48
11	L	501	MQ9	C37-C38-C39	5.23	140.25	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	401	BCB	O1D-CGD-CBD	-5.19	114.26	124.54
8	M	400	BCB	CMB-C2B-C3B	5.17	127.13	114.29
8	M	400	BCB	C4-C3-C5	5.12	123.88	115.27
9	L	402	BPB	C1-C2-C3	5.02	134.72	126.04
8	M	400	BCB	O1D-CGD-CBD	-5.00	114.64	124.54
9	L	402	BPB	O1D-CGD-CBD	-4.79	114.68	124.48
8	M	401	BCB	O1D-CGD-CBD	-4.53	115.57	124.54
9	L	402	BPB	CED-O2D-CGD	4.52	126.16	115.94
8	L	400	BCB	CHA-CBD-CGD	-4.44	104.97	115.02
8	M	400	BCB	CHA-CBD-CGD	-4.29	105.32	115.02
8	M	401	BCB	CHA-CBD-CGD	-4.16	105.61	115.02
5	C	403	HEC	CMB-C2B-C3B	4.15	130.70	125.82
9	L	402	BPB	CMB-C2B-C3B	4.09	132.33	124.68
12	L	502	MST	C2-N1-C6	-4.09	111.55	113.85
12	L	502	MST	C2-N3-C4	-4.08	111.56	113.85
8	M	401	BCB	O2A-CGA-CBA	3.87	124.05	111.91
8	M	401	BCB	OBB-CAB-C3B	3.86	125.59	121.52
8	L	401	BCB	CHA-CBD-CGD	-3.84	106.33	115.02
5	C	403	HEC	CMB-C2B-C1B	-3.83	122.58	128.46
8	L	400	BCB	O2D-CGD-CBD	3.81	120.06	111.11
8	L	400	BCB	O1D-CGD-CBD	-3.78	117.05	124.54
8	M	401	BCB	CHC-C4B-C3B	3.70	127.25	118.17
9	M	402	BPB	OBB-CAB-C3B	3.69	126.53	119.99
9	L	402	BPB	C4B-C3B-CAB	-3.60	119.38	127.19
9	L	402	BPB	C3C-C2C-C1C	3.57	105.58	100.72
8	L	400	BCB	CHC-C4B-C3B	3.43	126.57	118.17
5	C	404	HEC	CMB-C2B-C1B	-3.42	123.20	128.46
13	M	600	NS5	C19-C18-C17	3.41	130.46	123.47
8	L	401	BCB	CHC-C4B-C3B	3.29	126.24	118.17
9	M	402	BPB	C3C-C2C-C1C	3.26	105.16	100.72
9	M	402	BPB	C4B-C3B-CAB	-3.21	120.22	127.19
13	M	600	NS5	C16-C15-C14	-3.12	113.16	118.08
8	M	401	BCB	CHC-C1C-C2C	3.12	126.61	117.19
5	C	401	HEC	CMC-C2C-C1C	-3.12	123.67	128.46
8	M	400	BCB	CHC-C4B-C3B	3.10	125.77	118.17
8	L	401	BCB	CHC-C1C-C2C	3.08	126.49	117.19
11	L	501	MQ9	C22-C21-C19	-3.07	102.88	112.98
5	C	403	HEC	CMC-C2C-C1C	-2.99	123.86	128.46
11	L	501	MQ9	C42-C43-C44	2.98	134.83	127.66
5	C	401	HEC	CMC-C2C-C3C	2.98	129.32	125.82
8	M	400	BCB	C4-C3-C2	-2.97	116.05	123.68
8	M	401	BCB	OBD-CAD-CBD	-2.97	120.36	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	400	BCB	CHC-C1C-C2C	2.96	126.13	117.19
11	L	501	MQ9	C41-C39-C38	2.95	127.08	121.12
8	L	400	BCB	C4-C3-C5	2.94	120.22	115.27
8	L	400	BCB	O2A-CGA-CBA	2.93	121.12	111.91
5	C	402	HEC	CBA-CAA-C2A	-2.90	107.14	112.48
5	C	404	HEC	CMB-C2B-C3B	2.86	129.19	125.82
9	L	402	BPB	OBB-CAB-C3B	2.86	125.06	119.99
8	M	400	BCB	CHC-C1C-C2C	2.81	125.69	117.19
8	L	400	BCB	OBB-CAB-C3B	2.80	124.46	121.52
8	L	401	BCB	OBD-CAD-CBD	-2.79	120.79	127.49
5	C	403	HEC	CMC-C2C-C3C	2.76	129.06	125.82
8	L	400	BCB	OBD-CAD-CBD	-2.75	120.90	127.49
13	M	600	NS5	C18-C19-C20	2.70	129.00	123.47
8	M	401	BCB	O2A-CGA-O1A	-2.67	116.85	123.59
9	L	402	BPB	CBD-CHA-C4D	-2.67	105.54	108.54
8	M	400	BCB	C3B-C4B-NB	2.66	108.60	103.75
5	C	403	HEC	CMA-C3A-C2A	2.66	129.95	124.94
5	C	403	HEC	CMD-C2D-C1D	-2.62	124.44	128.46
8	L	400	BCB	O2A-CGA-O1A	-2.61	117.01	123.59
8	M	400	BCB	OBD-CAD-CBD	-2.59	121.27	127.49
11	L	501	MQ9	C40-C39-C41	-2.59	110.91	115.27
8	L	400	BCB	C3B-C4B-NB	2.57	108.44	103.75
9	M	402	BPB	CED-O2D-CGD	2.57	121.74	115.94
8	L	401	BCB	OBD-CAD-C3D	2.53	131.19	126.73
11	L	501	MQ9	C51-C49-C50	-2.53	109.01	114.60
8	M	400	BCB	C1-C2-C3	2.51	130.39	126.04
8	L	400	BCB	OBD-CAD-C3D	2.48	131.09	126.73
8	M	401	BCB	C3B-C4B-NB	2.47	108.27	103.75
8	L	400	BCB	C15-C13-C12	-2.47	99.16	112.13
8	L	401	BCB	C3B-C4B-NB	2.43	108.18	103.75
11	L	501	MQ9	C37-C36-C34	-2.42	105.03	112.98
9	M	402	BPB	C5-C3-C2	2.42	126.01	121.12
8	L	401	BCB	CBA-CAA-C2A	-2.41	112.45	115.72
8	L	401	BCB	CBB-CAB-C3B	2.39	119.24	116.80
8	M	401	BCB	OBB-CAB-CBB	-2.38	116.92	121.15
11	L	501	MQ9	C17-C18-C19	-2.38	121.94	127.66
9	M	402	BPB	CBD-CHA-C4D	-2.35	105.89	108.54
9	M	402	BPB	C4-C3-C5	-2.33	111.36	115.27
8	M	400	BCB	OBB-CAB-C3B	-2.31	119.08	121.52
8	M	401	BCB	O2D-CGD-O1D	-2.30	119.33	123.84
5	C	402	HEC	CMC-C2C-C1C	-2.30	124.93	128.46
8	L	401	BCB	C15-C13-C12	-2.29	100.08	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	400	BCB	CBA-CAA-C2A	-2.26	112.64	115.72
11	L	501	MQ9	C35-C34-C36	-2.25	111.49	115.27
8	M	400	BCB	OBB-CAB-CBB	-2.24	117.17	121.15
8	L	400	BCB	CED-O2D-CGD	2.23	120.99	115.94
9	M	402	BPB	CBD-CHA-C1A	2.20	130.36	126.84
8	M	400	BCB	OBD-CAD-C3D	2.20	130.60	126.73
8	M	400	BCB	O2A-CGA-CBA	2.18	118.74	111.91
5	C	401	HEC	CMB-C2B-C1B	-2.16	125.14	128.46
8	M	401	BCB	OBD-CAD-C3D	2.15	130.51	126.73
8	M	401	BCB	C1-C2-C3	-2.12	122.37	126.04
9	M	402	BPB	CBB-CAB-C3B	-2.12	114.05	120.34
11	L	501	MQ9	C22-C23-C24	2.12	132.76	127.66
11	L	501	MQ9	C15-C14-C16	-2.10	111.74	115.27
8	L	400	BCB	OBB-CAB-CBB	-2.09	117.44	121.15
5	C	404	HEC	CBD-CAD-C3D	-2.08	108.66	112.49
11	L	501	MQ9	C36-C37-C38	-2.05	105.14	111.88
13	M	600	NS5	C19-C20-C21	-2.03	124.41	127.31
9	M	402	BPB	C10-C8-C7	2.01	122.70	112.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	M	402	BPB	C8

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	402	BPB	O2A-C1-C2-C3
8	M	401	BCB	C2B-C3B-CAB-OBB
8	M	401	BCB	C2B-C3B-CAB-CBB
8	M	401	BCB	CAD-CBD-CGD-O1D
8	M	401	BCB	CAD-CBD-CGD-O2D
13	M	600	NS5	C6-C5-C7-C8
13	M	600	NS5	C20-C21-C23-C24
13	M	600	NS5	C22-C21-C23-C24
8	L	401	BCB	C2B-C3B-CAB-OBB
8	L	401	BCB	C2B-C3B-CAB-CBB
8	L	400	BCB	C2B-C3B-CAB-OBB
8	L	400	BCB	C2B-C3B-CAB-CBB
8	M	400	BCB	C4-C3-C5-C6
8	M	400	BCB	C2-C3-C5-C6
13	M	600	NS5	C10-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	L	501	MQ9	C46-C47-C48-C49
8	L	400	BCB	C4-C3-C5-C6
8	L	400	BCB	C2-C3-C5-C6
13	M	600	NS5	C7-C8-C9-C10
13	M	600	NS5	C13-C14-C15-C16
13	M	600	NS5	C17-C18-C19-C20
8	M	401	BCB	C15-C16-C17-C18
13	M	600	NS5	C13-C14-C15-C17
6	M	1325	LDA	C6-C7-C8-C9
6	L	1274	LDA	C3-C4-C5-C6
6	H	1259	LDA	C7-C8-C9-C10
11	L	501	MQ9	C45-C44-C46-C47
8	M	401	BCB	C11-C12-C13-C15
11	L	501	MQ9	C43-C44-C46-C47
6	H	1259	LDA	C6-C7-C8-C9
6	M	1325	LDA	C11-C10-C9-C8
8	M	400	BCB	C13-C15-C16-C17
8	M	400	BCB	C8-C10-C11-C12
13	M	600	NS5	C34-C35-C36-CM3
6	M	1324	LDA	C5-C6-C7-C8
6	H	1260	LDA	C5-C6-C7-C8
8	M	401	BCB	C2A-CAA-CBA-CGA
6	M	1326	LDA	C5-C6-C7-C8
6	H	1260	LDA	C7-C8-C9-C10
8	M	400	BCB	C4B-C3B-CAB-OB
8	M	400	BCB	C4B-C3B-CAB-CB
8	M	401	BCB	C11-C12-C13-C14
6	M	1324	LDA	C9-C10-C11-C12
6	H	1259	LDA	C2-C3-C4-C5
9	M	402	BPB	CAD-CBD-CGD-O2D
6	M	1324	LDA	C4-C5-C6-C7
8	L	400	BCB	C12-C13-C15-C16
8	L	400	BCB	C14-C13-C15-C16
9	L	402	BPB	C8-C10-C11-C12
8	L	400	BCB	CAD-CBD-CGD-O1D
6	H	1259	LDA	C5-C6-C7-C8
6	M	1325	LDA	C7-C8-C9-C10
6	H	1259	LDA	C1-C2-C3-C4
11	L	501	MQ9	C34-C36-C37-C38
8	M	400	BCB	C1A-C2A-CAA-CBA
8	L	400	BCB	C1A-C2A-CAA-CBA
8	L	401	BCB	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
6	H	1260	LDA	C1-C2-C3-C4
8	L	401	BCB	CHA-CBD-CGD-O2D
6	M	1326	LDA	C11-C10-C9-C8
8	L	401	BCB	C14-C13-C15-C16
9	L	402	BPB	CAD-CBD-CGD-O2D
8	L	401	BCB	CHA-CBD-CGD-O1D
13	M	600	NS5	C14-C15-C17-C18
8	L	400	BCB	CAD-CBD-CGD-O2D
13	M	600	NS5	C3-C4-C5-C7
6	L	1274	LDA	C2-C3-C4-C5
6	H	1260	LDA	C4-C5-C6-C7
9	M	402	BPB	C6-C7-C8-C10
6	L	1274	LDA	C6-C7-C8-C9

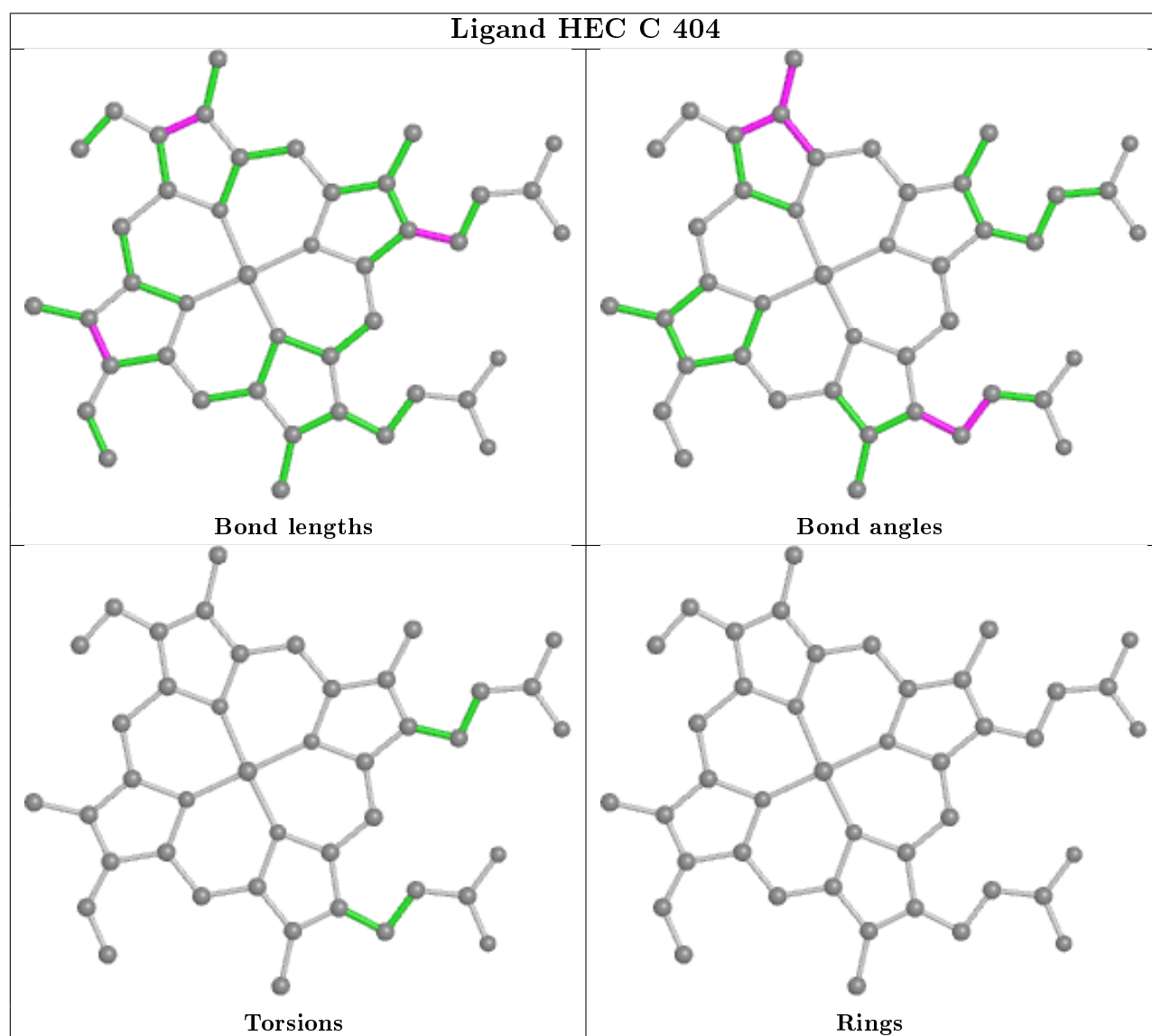
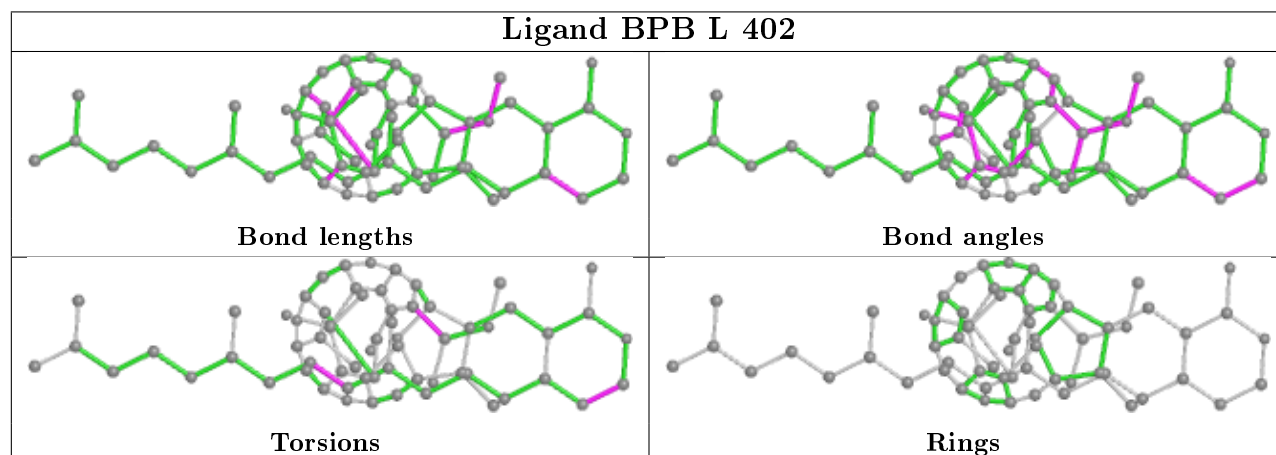
There are no ring outliers.

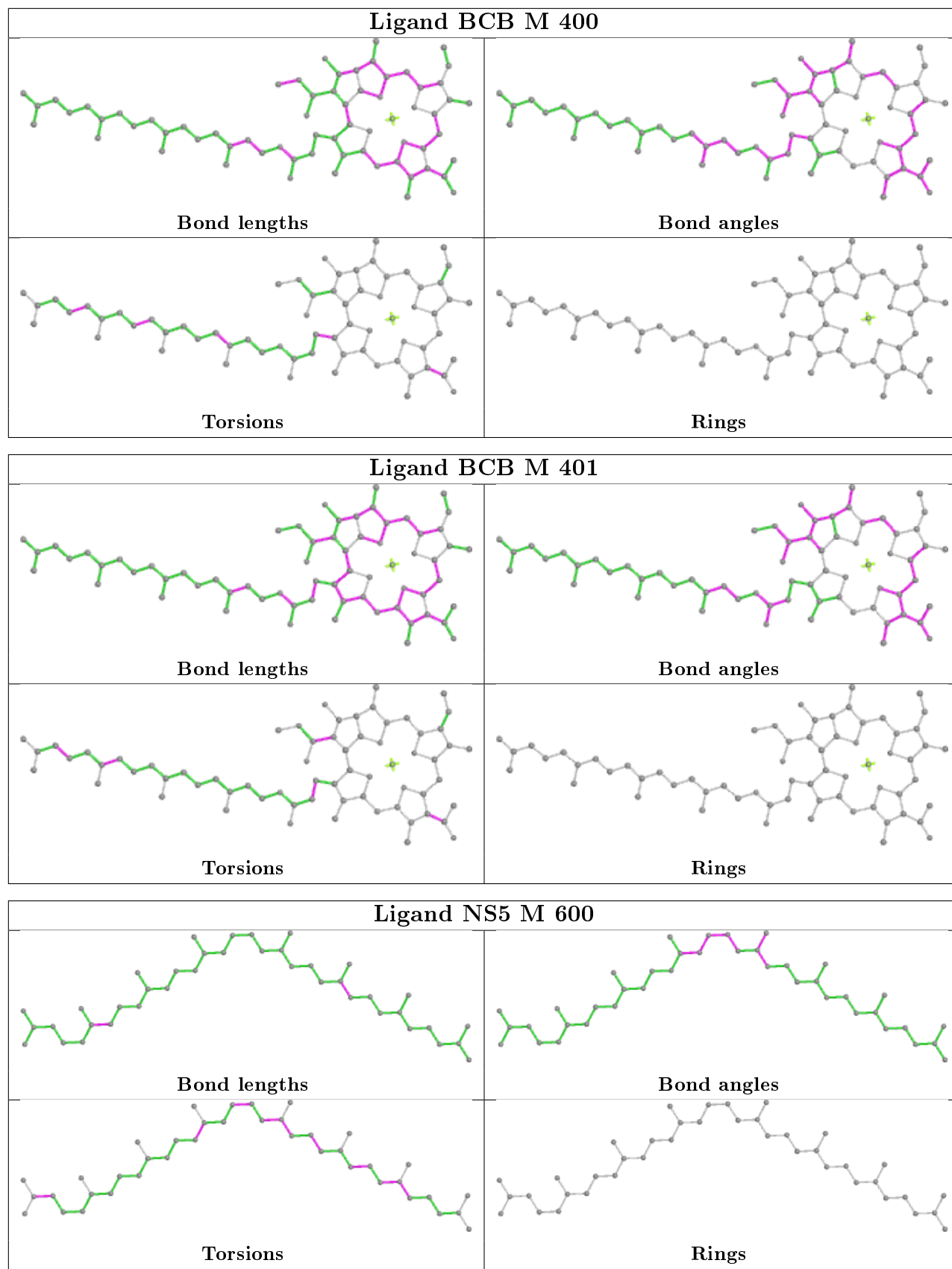
15 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	402	BPB	3	0
6	M	1326	LDA	1	0
7	M	1329	SO4	1	0
8	M	400	BCB	8	0
8	M	401	BCB	7	0
13	M	600	NS5	2	0
5	C	402	HEC	3	0
9	M	402	BPB	7	0
8	L	401	BCB	4	0
5	C	401	HEC	1	0
6	L	1274	LDA	4	0
6	H	1260	LDA	3	0
11	L	501	MQ9	1	0
6	M	1324	LDA	1	0
8	L	400	BCB	5	0

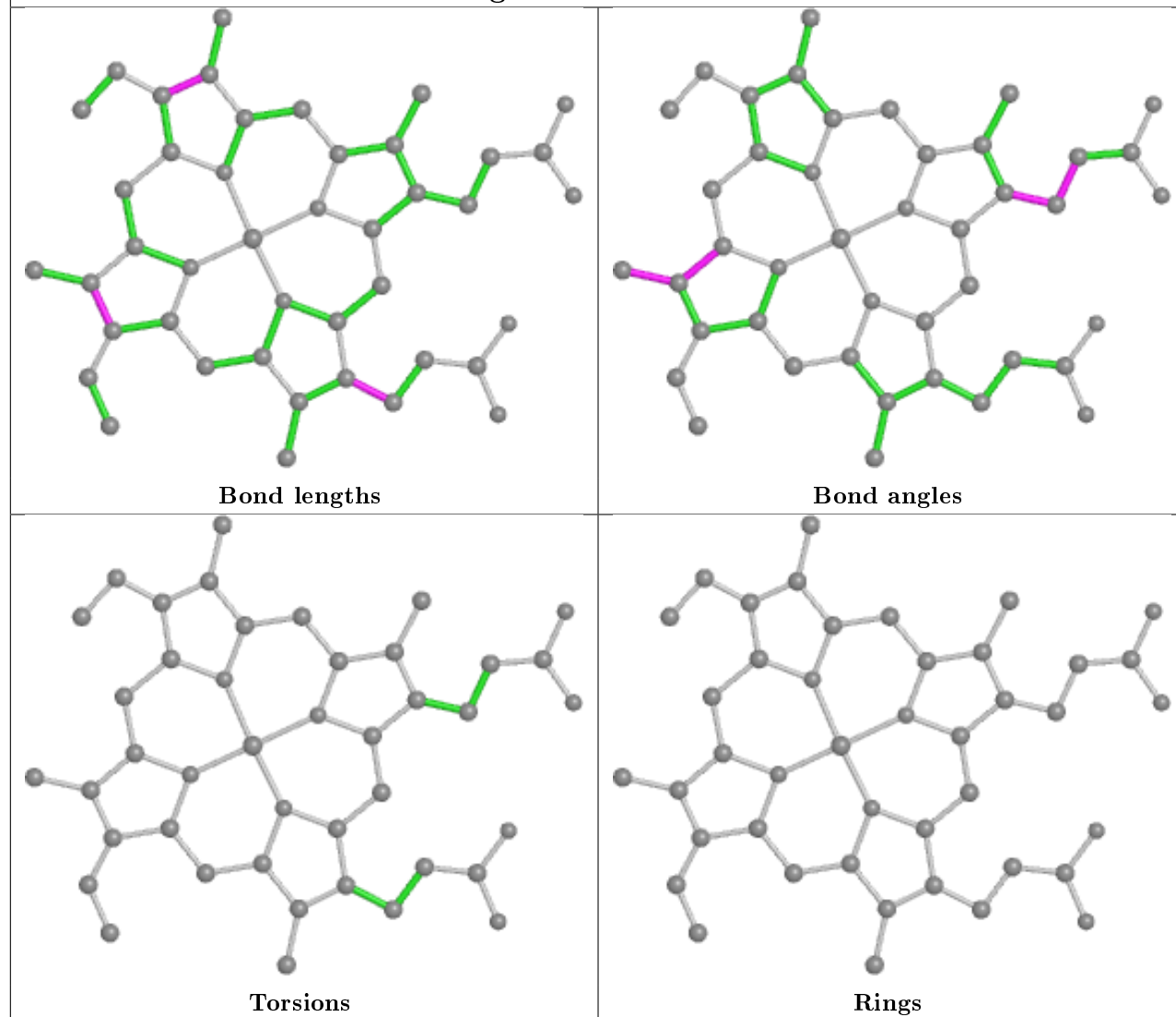
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

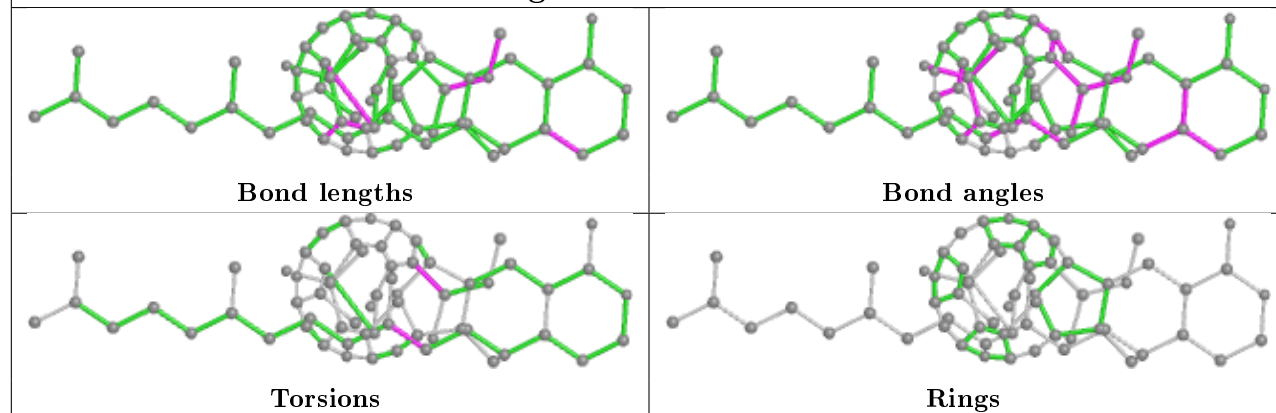




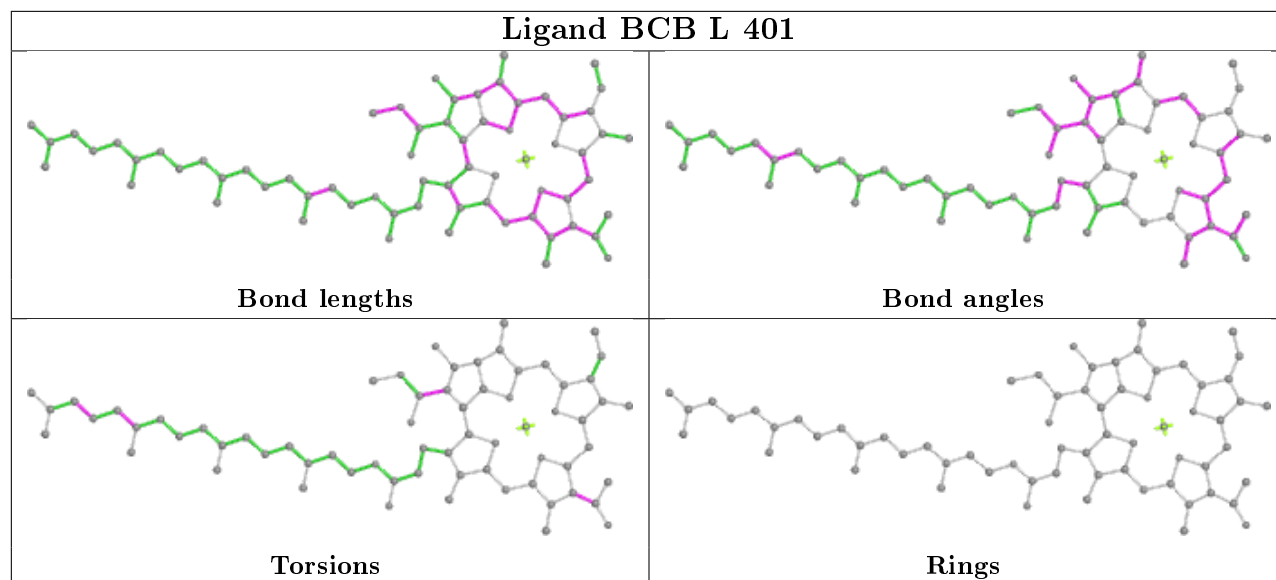
## Ligand HEC C 402



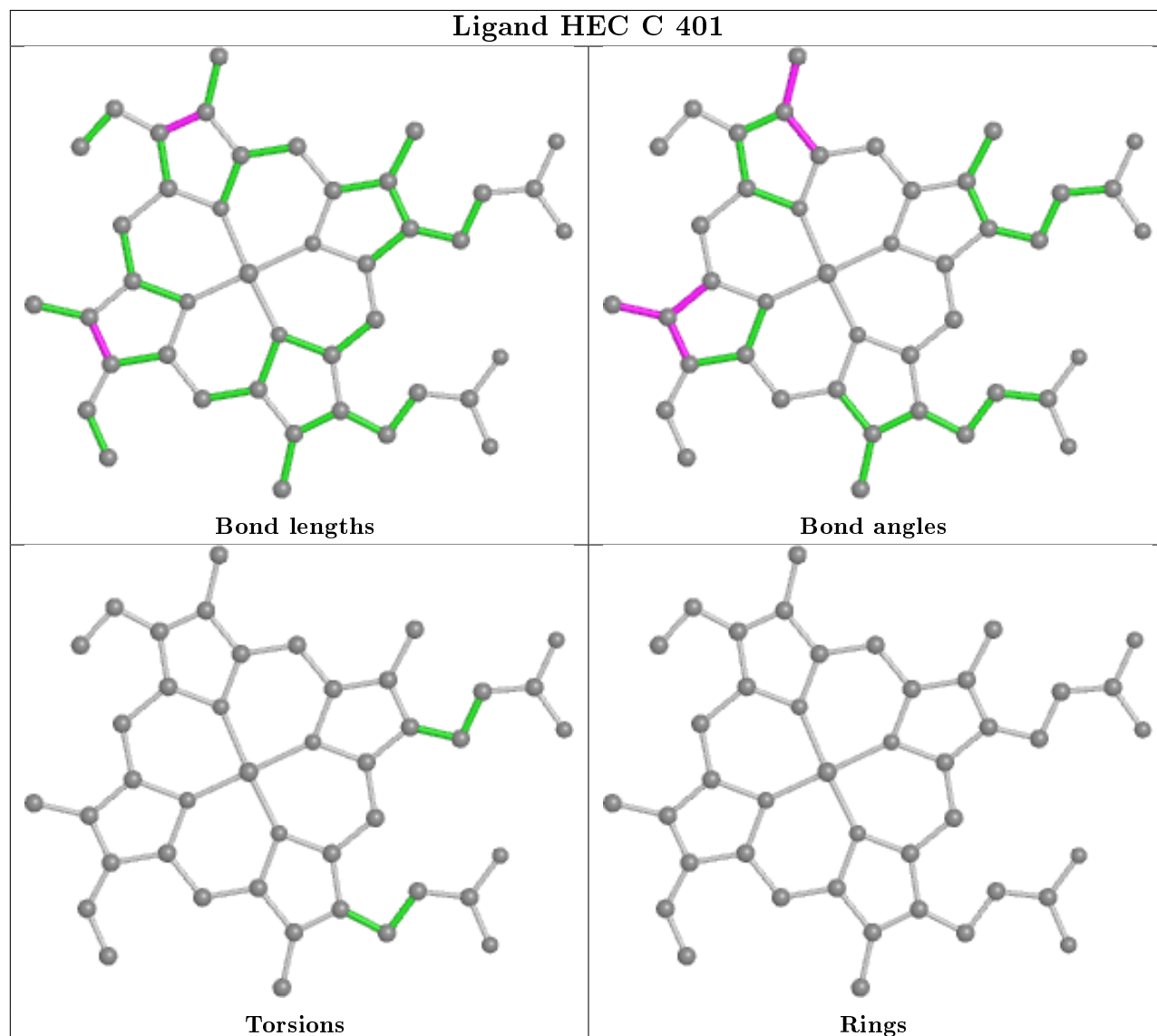
## Ligand BPB M 402



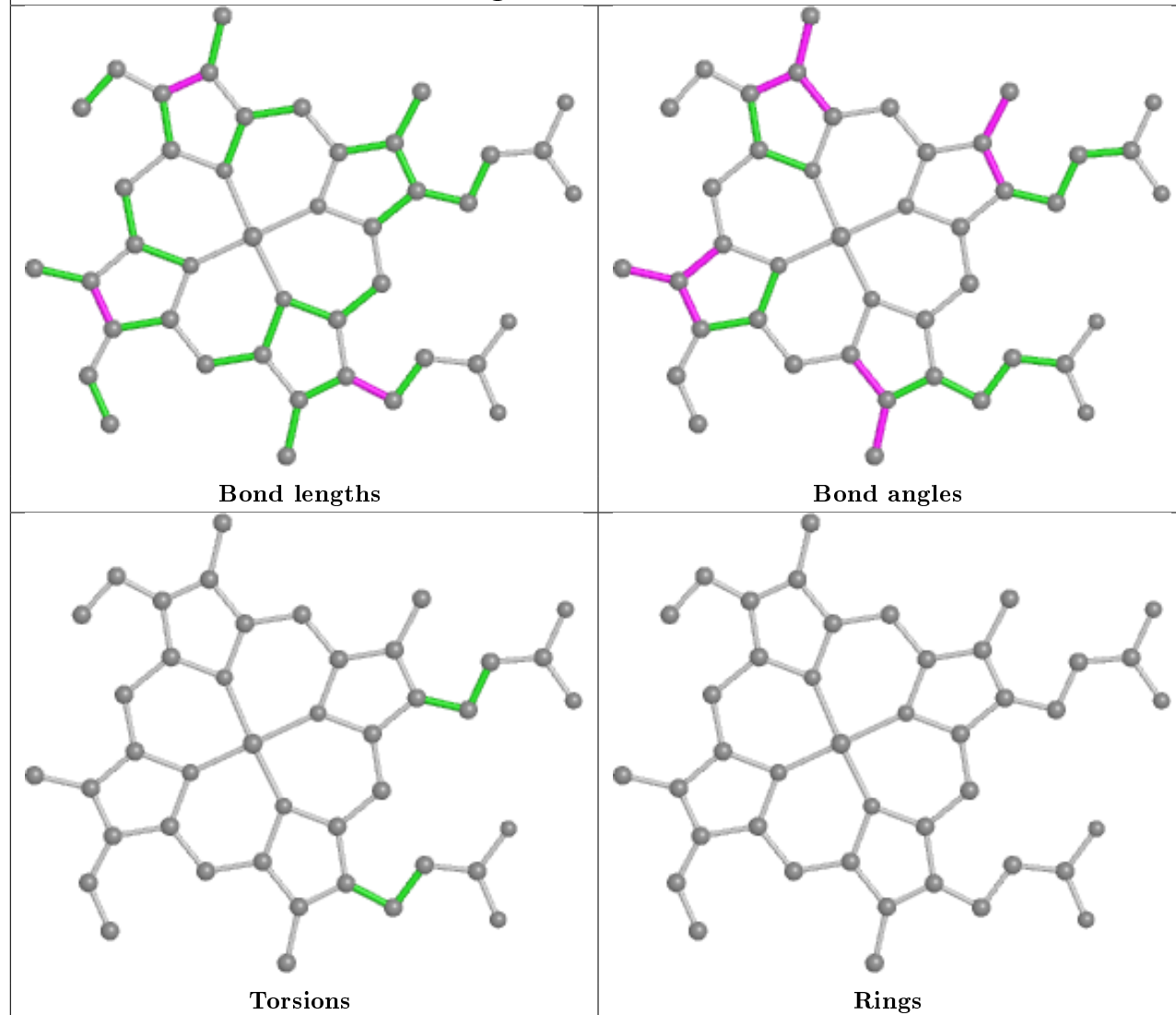
## Ligand BCB L 401



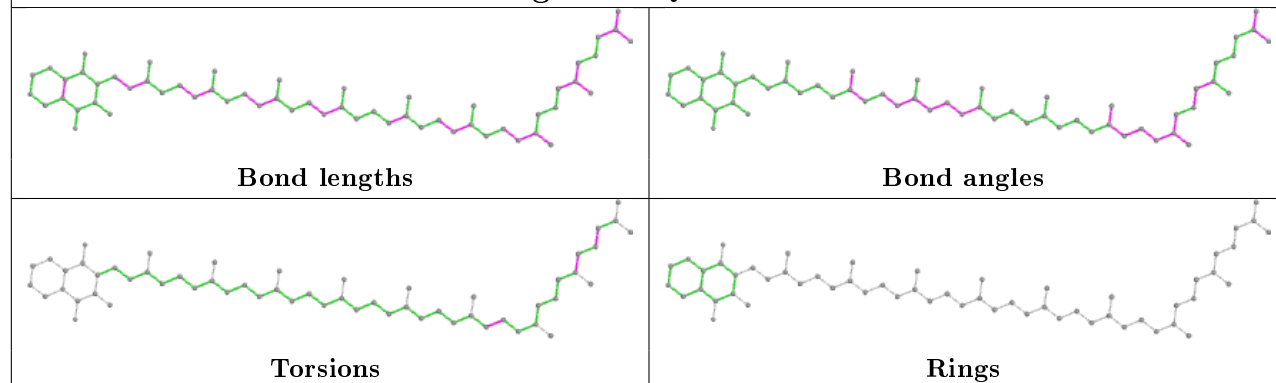
## Ligand HEC C 401

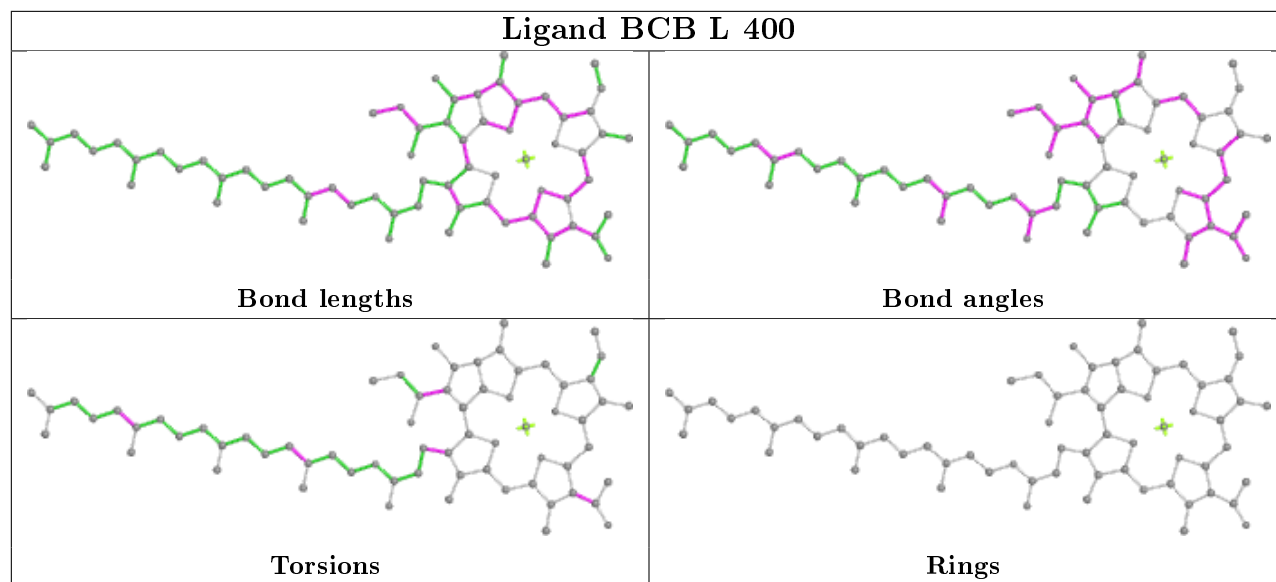


## Ligand HEC C 403



## Ligand MQ9 L 501





## 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 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.