



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:11 am BST

PDB ID : 1MPS  
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M 197 REPLACED WITH ARG AND TYR M 177 REPLACED WITH PHE (CHAIN M, Y177F, F197R)  
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Deposited on : 1998-03-09  
Resolution : 2.55 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)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
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

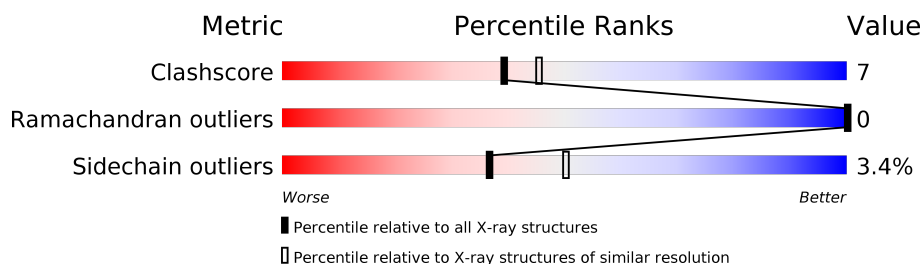
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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	L	281	
2	M	307	
3	H	260	

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
4	BCL	L	302	X	-	-	-
4	BCL	M	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BPH	L	401	X	-	-	-
5	BPH	L	402	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7155 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2407	1604	397	396	10			

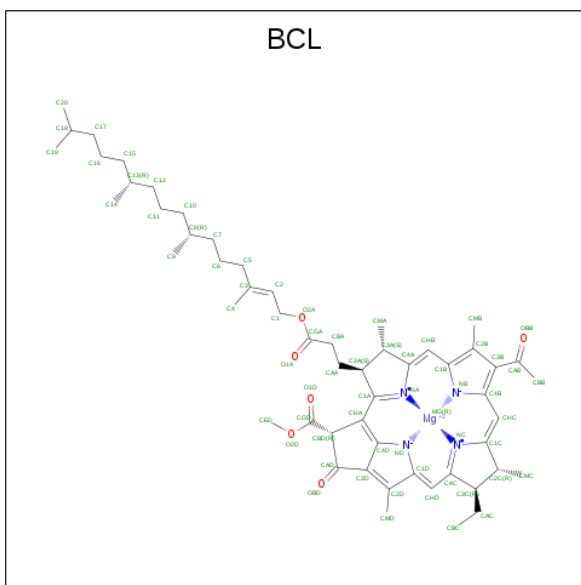
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	177	PHE	TYR	ENGINEERED MUTATION	UNP P02953
M	197	ARG	PHE	ENGINEERED MUTATION	UNP P02953

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

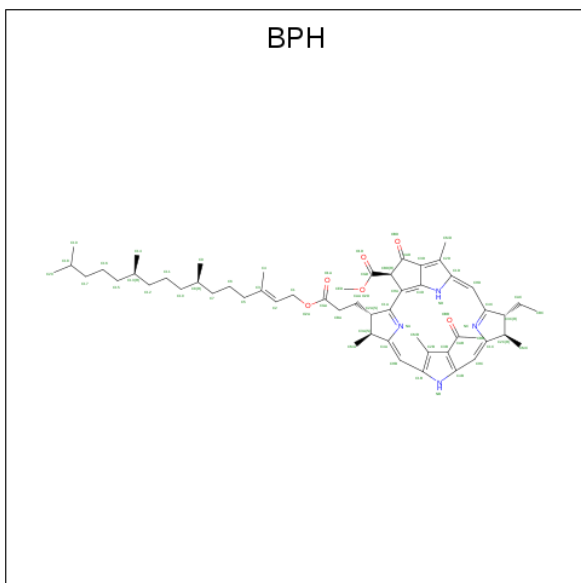
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



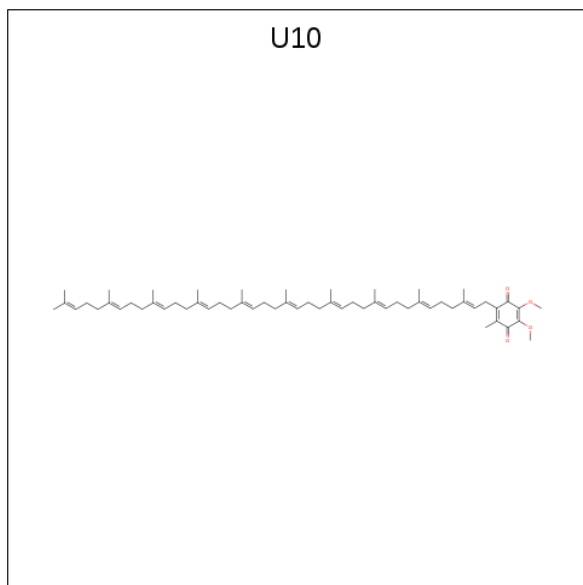
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	17	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $\text{C}_{55}\text{H}_{76}\text{N}_4\text{O}_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	17	0
			65	55	4	6		
5	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	48	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

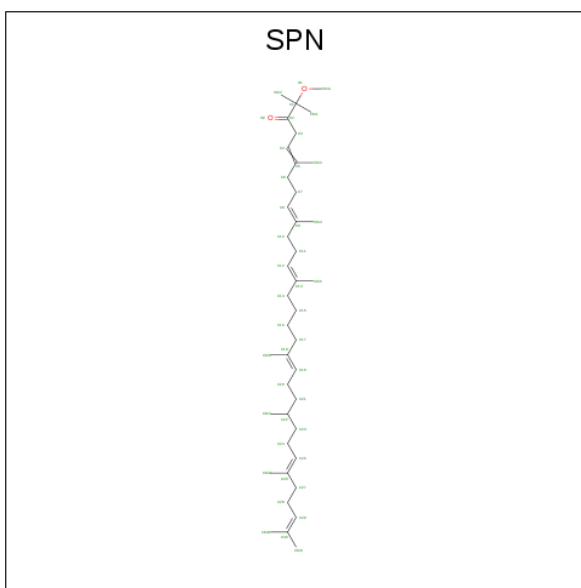
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



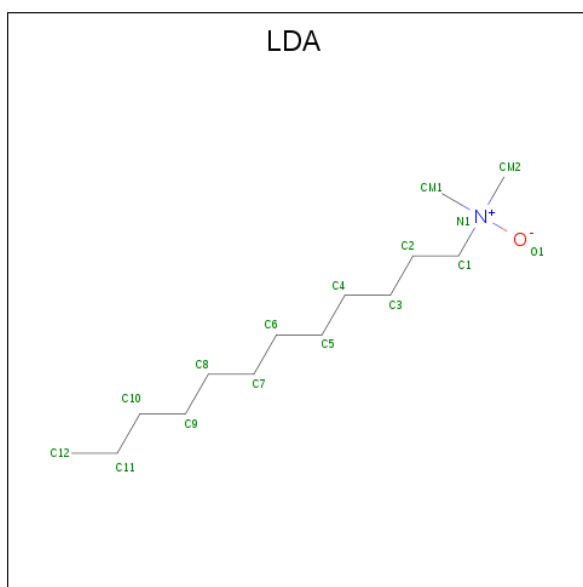
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula:  $C_{41}H_{70}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	11	0
			43	41	2		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C N O 16 14 1 1	0	0
10	M	1	Total C N O 16 14 1 1	0	0
10	M	1	Total C N O 16 14 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	28	Total O 28 28	0	0
11	M	35	Total O 35 35	0	0
11	H	37	Total O 37 37	0	0

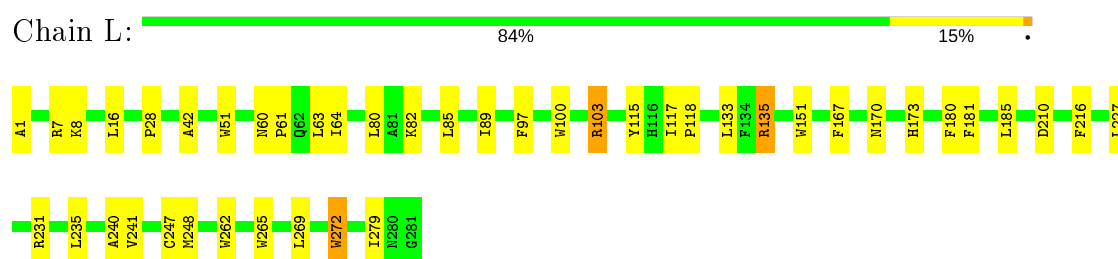


### 3 Residue-property plots [i](#)

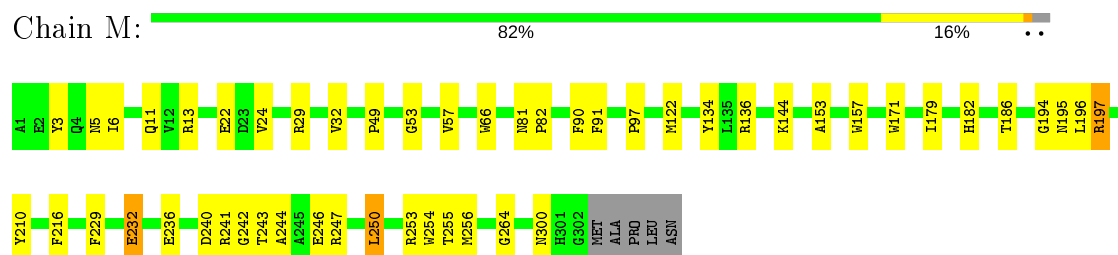
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

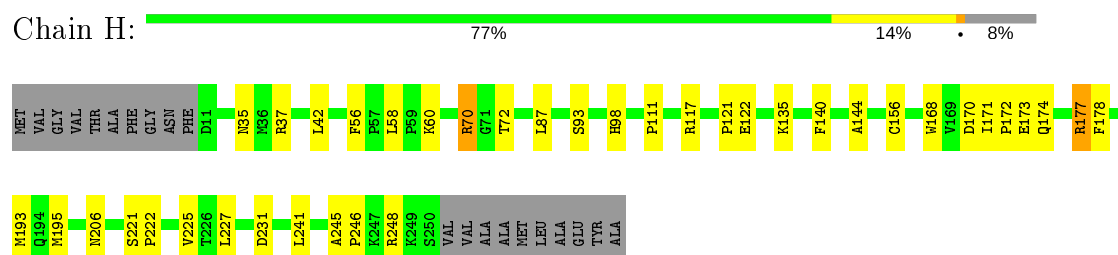
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.90 Å   141.90 Å   187.90 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	11.00 – 2.55	Depositor
% Data completeness (in resolution range)	76.5 (11.00-2.55)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.194 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	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: BCL, LDA, BPH, PO4, FE2, SPN, U10

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	L	0.41	0/2320	0.56	0/3175
2	M	0.40	0/2498	0.53	0/3409
3	H	0.37	0/1877	0.64	2/2553 (0.1%)
All	All	0.40	0/6695	0.57	2/9137 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	195	MET	CG-SD-CE	5.78	109.44	100.20
3	H	193	MET	CG-SD-CE	5.30	108.69	100.20

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	L	2232	0	2187	34	0
2	M	2407	0	2325	42	0
3	H	1829	0	1836	26	0
4	L	132	0	148	9	0
4	M	132	0	148	8	0
5	L	130	0	152	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	48	0	63	0	0
6	M	48	0	63	3	0
7	M	1	0	0	0	0
8	M	5	0	0	0	0
9	M	43	0	69	1	0
10	M	48	0	93	2	0
11	H	37	0	0	3	0
11	L	28	0	0	1	0
11	M	35	0	0	1	0
All	All	7155	0	7084	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:241:VAL:HG21	5:L:402:BPH:HAC2	1.61	0.83
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.65	0.78
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.68	0.76
5:L:401:BPH:HHC	5:L:401:BPH:HBB3	1.67	0.76
2:M:253:ARG:HD3	11:M:829:HOH:O	1.88	0.73
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.23	0.69
5:L:401:BPH:HAC1	2:M:153:ALA:HB2	1.76	0.68
1:L:103:ARG:HG2	11:L:507:HOH:O	2.01	0.60
5:L:402:BPH:CHC	5:L:402:BPH:HBB3	2.31	0.59
1:L:151:TRP:HE3	2:M:197:ARG:HH21	1.50	0.59
5:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.83	0.58
1:L:167:PHE:HB3	4:L:302:BCL:HMC3	1.85	0.58
1:L:181:PHE:CD2	5:L:401:BPH:HBB1	2.39	0.58
1:L:135:ARG:HD3	1:L:248:MET:O	2.04	0.58
1:L:115:TYR:O	1:L:118:PRO:HD2	2.04	0.57
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.35	0.56
3:H:170:ASP:HB2	3:H:177:ARG:HD2	1.87	0.56
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.87	0.56
4:M:802:BCL:HBB3	4:M:802:BCL:HMB1	1.87	0.55
5:L:402:BPH:CBB	2:M:210:TYR:HB3	2.36	0.55
2:M:13:ARG:O	3:H:140:PHE:HA	2.07	0.55
2:M:240:ASP:O	3:H:117:ARG:NH1	2.40	0.54
1:L:97:PHE:CE1	4:L:302:BCL:H121	2.43	0.54
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:70:ARG:NH2	3:H:121:PRO:O	2.42	0.53
4:M:801:BCL:CBB	4:M:801:BCL:HMB1	2.38	0.53
2:M:243:THR:OG1	2:M:247:ARG:HD2	2.09	0.53
2:M:53:GLY:O	2:M:57:VAL:HG23	2.08	0.53
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.91	0.52
3:H:177:ARG:NH1	11:H:295:HOH:O	2.40	0.52
6:M:501:U10:H202	10:M:701:LDA:H121	1.91	0.52
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.10	0.52
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.92	0.52
1:L:42:ALA:HA	5:L:402:BPH:H9C3	1.91	0.52
4:M:802:BCL:HMB1	4:M:802:BCL:CBB	2.40	0.51
3:H:241:LEU:HB2	11:H:296:HOH:O	2.10	0.51
4:L:304:BCL:OBB	4:L:304:BCL:HHC	2.11	0.50
2:M:194:GLY:O	2:M:195:ASN:HB3	2.10	0.50
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.93	0.50
4:L:304:BCL:CBB	4:L:304:BCL:HMB1	2.41	0.50
5:L:401:BPH:CHC	5:L:401:BPH:HBB3	2.41	0.49
2:M:24:VAL:HG11	2:M:29:ARG:NH2	2.27	0.49
2:M:24:VAL:HG11	2:M:29:ARG:HH21	1.77	0.48
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.95	0.48
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.94	0.48
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.48	0.47
1:L:100:TRP:HZ3	6:M:501:U10:H362	1.78	0.47
1:L:181:PHE:HB3	5:L:401:BPH:CBB	2.45	0.47
2:M:90:PHE:CD1	2:M:179:ILE:HD13	2.50	0.47
2:M:179:ILE:HG13	4:M:801:BCL:HED1	1.97	0.47
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.98	0.46
4:L:302:BCL:HHC	4:L:302:BCL:OBB	2.14	0.46
4:L:304:BCL:HMB1	4:L:304:BCL:HBB2	1.97	0.45
2:M:256:MET:CE	6:M:501:U10:H102	2.46	0.45
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.98	0.45
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.99	0.45
2:M:157:TRP:CE2	9:M:600:SPN:HM73	2.52	0.45
1:L:231:ARG:HD2	2:M:6:ILE:O	2.17	0.45
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.53	0.44
3:H:37:ARG:NH2	3:H:60:LYS:O	2.50	0.44
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.52	0.44
1:L:60:ASN:O	1:L:64:ILE:HG13	2.17	0.44
1:L:227:LEU:HD13	2:M:232:GLU:HG2	2.00	0.44
2:M:247:ARG:NH2	3:H:111:PRO:O	2.51	0.43
4:L:304:BCL:HMD2	4:M:802:BCL:HBB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.36	0.43
10:M:701:LDA:H52	3:H:56:PHE:CE2	2.53	0.43
1:L:28:PRO:O	2:M:254:TRP:HA	2.18	0.43
1:L:28:PRO:HB2	2:M:253:ARG:HG3	2.00	0.43
4:M:801:BCL:OBB	4:M:801:BCL:HHC	2.19	0.43
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.54	0.43
4:M:801:BCL:HBB2	4:M:801:BCL:HMB1	2.00	0.43
2:M:136:ARG:NE	2:M:136:ARG:HA	2.34	0.42
4:L:302:BCL:HMB1	4:L:302:BCL:HBB3	2.00	0.42
1:L:82:LYS:HE2	1:L:82:LYS:HB3	1.86	0.42
5:L:402:BPH:H101	5:L:402:BPH:H142	2.00	0.42
1:L:103:ARG:NH2	2:M:255:THR:O	2.51	0.42
3:H:135:LYS:HB3	3:H:135:LYS:HE2	1.81	0.42
1:L:60:ASN:HB3	1:L:63:LEU:HD12	2.01	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
1:L:51:TRP:CH2	1:L:80:LEU:HD13	2.55	0.42
2:M:97:PRO:HG2	2:M:171:TRP:HB2	2.02	0.41
2:M:236:GLU:HB3	11:H:292:HOH:O	2.20	0.41
3:H:221:SER:HA	3:H:222:PRO:HD3	1.94	0.41
2:M:250:LEU:HD12	2:M:250:LEU:HA	1.90	0.41
3:H:58:LEU:HD12	3:H:58:LEU:HA	1.91	0.41
5:L:402:BPH:HBB1	2:M:210:TYR:CD2	2.56	0.41
1:L:185:LEU:HD13	5:L:401:BPH:ND	2.36	0.41
5:L:402:BPH:HBC3	5:L:402:BPH:HHD	2.03	0.41
2:M:81:ASN:HA	2:M:82:PRO:HD2	1.90	0.41
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.96	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.21	0.41
2:M:196:LEU:HD23	2:M:196:LEU:HA	1.86	0.41
2:M:186:THR:HG23	4:M:802:BCL:HMD2	2.03	0.41
3:H:245:ALA:N	3:H:246:PRO:HD2	2.36	0.41
1:L:231:ARG:HD3	2:M:5:ASN:O	2.20	0.40
1:L:279:ILE:HG21	2:M:91:PHE:HB3	2.02	0.40
3:H:156:CYS:HB2	3:H:248:ARG:HG3	2.04	0.40
3:H:173:GLU:O	3:H:174:GLN:C	2.58	0.40
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.85	0.40
2:M:241:ARG:HD3	2:M:246:GLU:HG2	2.04	0.40
1:L:262:TRP:O	1:L:265:TRP:HD1	2.04	0.40
2:M:134:TYR:CE2	2:M:144:LYS:HG3	2.56	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	L	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	300/307 (98%)	288 (96%)	12 (4%)	0	100	100
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/848 (96%)	784 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	L	220/220 (100%)	211 (96%)	9 (4%)	30	41
2	M	236/240 (98%)	229 (97%)	7 (3%)	41	55
3	H	195/208 (94%)	189 (97%)	6 (3%)	40	54
All	All	651/668 (98%)	629 (97%)	22 (3%)	37	50

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	16	LEU
1	L	103	ARG
1	L	133	LEU
1	L	135	ARG
1	L	210	ASP

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Mol	Chain	Res	Type
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	272	TRP
2	M	22	GLU
2	M	182	HIS
2	M	197	ARG
2	M	216	PHE
2	M	232	GLU
2	M	250	LEU
2	M	300	ASN
3	H	70	ARG
3	H	72	THR
3	H	93	SER
3	H	177	ARG
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	183	ASN
1	L	264	GLN
2	M	299	GLN
2	M	300	ASN
3	H	98	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
10	LDA	M	703	-	12,15,15	2.16	1 (8%)	14,17,17	0.55	0
4	BCL	M	801	2	58,74,74	1.53	7 (12%)	69,115,115	2.26	16 (23%)
10	LDA	M	702	-	12,15,15	2.12	1 (8%)	14,17,17	0.53	0
4	BCL	L	304	1	58,74,74	1.34	8 (13%)	69,115,115	2.20	13 (18%)
4	BCL	M	802	2	58,74,74	1.51	7 (12%)	69,115,115	2.23	17 (24%)
10	LDA	M	701	-	12,15,15	2.53	1 (8%)	14,17,17	0.57	0
5	BPH	L	402	-	64,70,70	1.13	4 (6%)	76,101,101	1.63	16 (21%)
9	SPN	M	600	-	40,42,42	3.77	18 (45%)	50,52,52	2.15	20 (40%)
4	BCL	L	302	1	58,74,74	1.52	9 (15%)	69,115,115	2.06	16 (23%)
6	U10	L	502	-	48,48,63	1.80	12 (25%)	58,61,79	1.17	5 (8%)
8	PO4	M	800	-	4,4,4	1.93	2 (50%)	6,6,6	0.76	0
6	U10	M	501	-	48,48,63	1.86	13 (27%)	58,61,79	1.00	2 (3%)
5	BPH	L	401	-	64,70,70	1.09	4 (6%)	76,101,101	1.70	13 (17%)

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
10	LDA	M	703	-	-	3/13/13/13	-
4	BCL	M	801	2	-	2/37/137/137	-
10	LDA	M	702	-	-	0/13/13/13	-
4	BCL	L	304	1	-	1/37/137/137	-
4	BCL	M	802	2	1/1/21/25	2/37/137/137	-
10	LDA	M	701	-	-	0/13/13/13	-
4	BCL	L	302	1	1/1/21/25	1/37/137/137	-
9	SPN	M	600	-	-	13/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	L	402	-	1/1/18/22	10/54/105/105	0/5/6/6
6	U10	L	502	-	-	13/45/69/87	0/1/1/1
6	U10	M	501	-	-	9/45/69/87	0/1/1/1
5	BPH	L	401	-	2/2/18/22	8/54/105/105	0/5/6/6

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-8.76	1.21	1.42
9	M	600	SPN	C8-C9	8.60	1.53	1.33
9	M	600	SPN	C4-C5	8.52	1.53	1.33
9	M	600	SPN	C19-C18	8.34	1.53	1.33
9	M	600	SPN	C12-C13	8.30	1.52	1.33
9	M	600	SPN	C3-C4	-7.83	1.39	1.50
10	M	703	LDA	O1-N1	-7.43	1.24	1.42
10	M	702	LDA	O1-N1	-7.30	1.25	1.42
9	M	600	SPN	C17-C18	-5.79	1.39	1.51
9	M	600	SPN	C14-C13	-5.76	1.39	1.51
9	M	600	SPN	C6-C5	-5.69	1.39	1.51
9	M	600	SPN	C10-C9	-5.31	1.40	1.51
4	L	302	BCL	O2D-CGD	5.13	1.45	1.33
4	M	802	BCL	MG-NA	4.94	2.18	2.06
4	M	801	BCL	MG-NA	4.64	2.17	2.06
6	L	502	U10	O3-C3	4.51	1.47	1.36
4	M	801	BCL	O2A-CGA	4.39	1.46	1.33
4	L	302	BCL	MG-NA	4.32	2.16	2.06
4	M	801	BCL	O2D-CED	-4.18	1.35	1.45
4	M	802	BCL	O2A-CGA	4.11	1.45	1.33
4	M	802	BCL	O2D-CED	-4.10	1.35	1.45
4	M	802	BCL	C1B-NB	4.03	1.38	1.35
4	M	801	BCL	C1B-NB	4.03	1.38	1.35
4	L	304	BCL	O2D-CGD	3.99	1.42	1.33
6	M	501	U10	O3-C3	3.97	1.46	1.36
4	L	302	BCL	O2D-CED	-3.93	1.36	1.45
4	L	304	BCL	MG-NA	3.83	2.15	2.06
4	M	801	BCL	O2D-CGD	3.82	1.42	1.33
6	L	502	U10	O4-C4	3.82	1.46	1.36
4	L	302	BCL	C4B-NB	3.79	1.38	1.35
6	M	501	U10	O3-C3M	-3.79	1.36	1.45
5	L	402	BPH	O2A-CGA	3.70	1.44	1.33
4	M	802	BCL	O2D-CGD	3.61	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	801	BCL	C4B-NB	3.61	1.38	1.35
6	M	501	U10	O4-C4	3.59	1.45	1.36
5	L	401	BPH	O2A-CGA	3.56	1.43	1.33
4	L	304	BCL	C4B-NB	3.55	1.38	1.35
9	M	600	SPN	C20-C19	-3.49	1.39	1.50
9	M	600	SPN	C11-C12	-3.48	1.39	1.50
4	M	802	BCL	C4B-NB	3.41	1.38	1.35
4	L	304	BCL	C1B-NB	3.38	1.38	1.35
9	M	600	SPN	C7-C8	-3.36	1.39	1.50
4	L	304	BCL	O2D-CED	-3.22	1.37	1.45
9	M	600	SPN	O1-CMA	3.21	1.53	1.43
5	L	401	BPH	O2D-CGD	3.15	1.40	1.33
5	L	402	BPH	O2D-CGD	3.13	1.40	1.33
6	M	501	U10	O4-C4M	-3.10	1.38	1.45
4	L	302	BCL	C1B-NB	3.04	1.37	1.35
6	M	501	U10	C7-C8	-3.02	1.46	1.50
6	M	501	U10	C33-C34	2.99	1.40	1.33
6	L	502	U10	O4-C4M	-2.98	1.38	1.45
6	L	502	U10	C7-C8	-2.97	1.46	1.50
5	L	402	BPH	C2-C3	2.94	1.40	1.33
5	L	401	BPH	C2-C3	2.92	1.40	1.33
4	M	802	BCL	C2-C3	2.84	1.39	1.33
6	L	502	U10	C13-C14	2.83	1.39	1.33
6	L	502	U10	C28-C29	2.82	1.39	1.33
6	M	501	U10	C8-C9	2.81	1.39	1.33
6	M	501	U10	C23-C24	2.81	1.39	1.33
6	L	502	U10	C18-C19	2.81	1.39	1.33
6	L	502	U10	C23-C24	2.80	1.39	1.33
4	L	302	BCL	O2A-CGA	2.79	1.41	1.33
9	M	600	SPN	C25-C26	2.78	1.39	1.33
4	M	801	BCL	C2-C3	2.78	1.39	1.33
6	M	501	U10	C28-C29	2.78	1.39	1.33
6	L	502	U10	C8-C9	2.76	1.39	1.33
6	L	502	U10	C33-C34	2.76	1.39	1.33
6	M	501	U10	C13-C14	2.72	1.39	1.33
6	M	501	U10	C18-C19	2.66	1.39	1.33
4	L	302	BCL	C2-C3	2.64	1.39	1.33
5	L	401	BPH	O2D-CED	-2.55	1.39	1.45
6	L	502	U10	C38-C39	2.54	1.39	1.32
4	L	304	BCL	O2A-CGA	2.51	1.40	1.33
6	M	501	U10	C38-C39	2.49	1.39	1.32
8	M	800	PO4	P-O3	-2.46	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	BCL	C2-C3	2.44	1.38	1.33
9	M	600	SPN	C29-C30	2.40	1.39	1.32
9	M	600	SPN	C21-C22	-2.40	1.40	1.52
6	L	502	U10	O3-C3M	-2.30	1.39	1.45
6	M	501	U10	C27-C28	-2.20	1.43	1.50
9	M	600	SPN	C16-C15	-2.17	1.39	1.51
5	L	402	BPH	O2D-CED	-2.15	1.40	1.45
9	M	600	SPN	CM4-C9	2.12	1.56	1.50
8	M	800	PO4	P-O4	-2.04	1.48	1.54
4	L	304	BCL	C1-C2	-2.04	1.43	1.49
4	L	302	BCL	C4-C3	2.03	1.55	1.50
4	L	302	BCL	C5-C3	2.02	1.55	1.51

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	802	BCL	C4A-NA-C1A	8.71	110.62	106.71
4	L	304	BCL	C4A-NA-C1A	8.08	110.34	106.71
4	M	801	BCL	C4A-NA-C1A	7.92	110.27	106.71
4	L	302	BCL	C4A-NA-C1A	7.82	110.22	106.71
5	L	401	BPH	O2D-CGD-CBD	7.73	125.01	111.27
4	L	304	BCL	O2D-CGD-CBD	7.17	124.01	111.27
4	M	801	BCL	C1C-NC-C4C	7.13	109.91	106.71
4	M	802	BCL	C1C-NC-C4C	6.94	109.83	106.71
5	L	402	BPH	O2D-CGD-CBD	6.83	123.40	111.27
4	L	302	BCL	C1C-NC-C4C	6.63	109.69	106.71
4	M	802	BCL	O2D-CGD-CBD	6.61	123.01	111.27
4	L	304	BCL	C1C-NC-C4C	6.47	109.62	106.71
4	M	801	BCL	O2D-CGD-CBD	6.47	122.77	111.27
4	L	302	BCL	O2D-CGD-CBD	5.32	120.72	111.27
5	L	401	BPH	O1D-CGD-CBD	-5.07	114.12	124.48
4	M	801	BCL	CMB-C2B-C1B	-5.06	120.69	128.46
4	M	802	BCL	C4B-C3B-CAB	-4.86	117.74	127.13
4	L	304	BCL	O1D-CGD-CBD	-4.74	114.78	124.48
5	L	402	BPH	O1D-CGD-CBD	-4.67	114.93	124.48
4	M	802	BCL	O1D-CGD-CBD	-4.54	115.19	124.48
4	L	304	BCL	C4B-C3B-CAB	-4.51	118.41	127.13
4	M	801	BCL	O1D-CGD-CBD	-4.46	115.35	124.48
9	M	600	SPN	CM4-C9-C10	4.43	122.73	115.27
9	M	600	SPN	CM5-C13-C14	4.36	122.60	115.27
9	M	600	SPN	CM6-C18-C17	4.31	122.53	115.27
4	L	302	BCL	OBB-CAB-C3B	4.12	127.31	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	C4D-C3D-CAD	-4.07	106.20	108.47
9	M	600	SPN	CM3-C5-C6	4.01	122.01	115.27
4	M	801	BCL	OB B-CAB-C3B	3.96	127.02	119.99
4	L	304	BCL	CMB-C2B-C1B	-3.94	122.41	128.46
4	L	302	BCL	C4B-C3B-CAB	-3.87	119.66	127.13
4	L	302	BCL	CMB-C2B-C1B	-3.75	122.70	128.46
9	M	600	SPN	CM7-C22-C21	3.72	124.76	111.29
4	M	801	BCL	C1-C2-C3	3.72	132.47	126.04
4	M	802	BCL	O2A-CGA-CBA	3.71	123.55	111.91
4	M	801	BCL	CMB-C2B-C3B	3.68	131.57	124.68
4	M	801	BCL	O2A-CGA-CBA	3.66	123.41	111.91
4	M	801	BCL	C4B-C3B-CAB	-3.49	120.38	127.13
6	L	502	U10	C3M-O3-C3	3.49	128.82	116.47
9	M	600	SPN	C3-C4-C5	-3.46	121.04	126.79
5	L	402	BPH	O2A-CGA-CBA	3.39	122.56	111.91
4	M	802	BCL	C4D-C3D-CAD	-3.38	106.58	108.47
4	M	802	BCL	CMB-C2B-C1B	-3.38	123.27	128.46
4	M	802	BCL	C1-C2-C3	3.31	131.77	126.04
5	L	402	BPH	OBD-CAD-CBD	-3.27	121.23	125.89
4	L	304	BCL	CMD-C2D-C3D	3.25	130.76	124.68
4	M	802	BCL	OBD-CAD-CBD	-3.22	121.29	125.89
5	L	401	BPH	OB B-CAB-C3B	3.20	126.33	120.41
4	L	302	BCL	O2A-CGA-CBA	3.18	121.88	111.91
9	M	600	SPN	C16-C17-C18	3.16	121.75	113.45
4	L	304	BCL	OB B-CAB-C3B	3.16	125.59	119.99
5	L	401	BPH	OBD-CAD-CBD	-3.15	121.39	125.89
5	L	401	BPH	C4A-NA-C1A	3.15	110.69	108.14
9	M	600	SPN	C15-C14-C13	3.14	121.69	113.45
4	L	302	BCL	O1D-CGD-CBD	-3.13	118.08	124.48
4	L	304	BCL	OBD-CAD-CBD	-3.05	121.54	125.89
9	M	600	SPN	C11-C12-C13	-3.01	120.41	127.66
4	L	302	BCL	OBD-CAD-CBD	-3.01	121.60	125.89
6	M	501	U10	C4M-O4-C4	2.97	126.99	116.47
4	L	304	BCL	O2A-CGA-CBA	2.97	121.22	111.91
6	L	502	U10	C4M-O4-C4	2.95	126.91	116.47
4	M	801	BCL	C4D-C3D-CAD	-2.95	106.83	108.47
4	M	801	BCL	OBD-CAD-CBD	-2.91	121.73	125.89
6	L	502	U10	C7-C8-C9	2.87	131.57	126.79
5	L	401	BPH	CMD-C2D-C3D	2.86	130.03	124.68
4	L	304	BCL	CMB-C2B-C3B	2.85	130.02	124.68
5	L	402	BPH	C1-C2-C3	2.84	130.96	126.04
4	L	302	BCL	C1-C2-C3	2.84	130.96	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	401	BPH	O2A-CGA-CBA	2.79	120.67	111.91
9	M	600	SPN	C17-C18-C19	-2.77	115.51	121.12
9	M	600	SPN	C20-C19-C18	-2.75	121.04	127.66
9	M	600	SPN	C7-C8-C9	-2.74	121.07	127.66
5	L	401	BPH	C1-C2-C3	2.73	130.76	126.04
4	L	302	BCL	CMB-C2B-C3B	2.72	129.76	124.68
4	L	302	BCL	C4D-C3D-CAD	-2.70	106.96	108.47
4	M	801	BCL	CMD-C2D-C3D	2.69	129.72	124.68
9	M	600	SPN	C10-C9-C8	-2.68	115.69	121.12
5	L	402	BPH	C4D-CHA-C1A	-2.68	123.90	130.51
9	M	600	SPN	C14-C13-C12	-2.62	115.81	121.12
4	M	802	BCL	CED-O2D-CGD	2.61	121.84	115.94
9	M	600	SPN	C11-C10-C9	2.59	121.51	112.98
9	M	600	SPN	C7-C6-C5	2.58	121.46	112.98
5	L	401	BPH	C4D-CHA-C1A	-2.58	124.16	130.51
5	L	401	BPH	C3A-C4A-NA	-2.56	108.69	113.05
4	L	302	BCL	CED-O2D-CGD	2.51	121.62	115.94
9	M	600	SPN	C6-C5-C4	-2.50	116.06	121.12
5	L	401	BPH	CBB-CAB-C3B	-2.50	115.10	120.43
4	M	801	BCL	C2A-C1A-CHA	2.42	128.09	123.86
4	M	802	BCL	CMB-C2B-C3B	2.41	129.19	124.68
5	L	401	BPH	C3A-C4A-CHB	2.40	125.97	121.83
6	M	501	U10	C7-C8-C9	2.40	130.78	126.79
5	L	402	BPH	O2A-CGA-O1A	-2.31	117.75	123.59
9	M	600	SPN	C21-C20-C19	2.31	118.33	112.23
9	M	600	SPN	C4-C3-C2	2.29	122.34	111.34
5	L	402	BPH	CMD-C2D-C3D	2.28	128.94	124.68
6	L	502	U10	C7-C6-C5	2.28	121.22	118.48
5	L	402	BPH	C4A-NA-C1A	2.27	109.97	108.14
4	M	801	BCL	O2A-CGA-O1A	-2.26	117.89	123.59
4	L	302	BCL	CMD-C2D-C3D	2.25	128.89	124.68
5	L	401	BPH	C2A-C1A-NA	-2.24	109.29	111.86
4	M	802	BCL	O2A-CGA-O1A	-2.20	118.04	123.59
4	M	801	BCL	C4-C3-C5	-2.20	111.57	115.27
5	L	402	BPH	C3A-C4A-CHB	2.18	125.58	121.83
4	M	802	BCL	CAC-C3C-C4C	-2.17	107.77	112.58
6	L	502	U10	C6-C1-C2	2.11	120.85	119.18
4	L	302	BCL	O2A-CGA-O1A	-2.10	118.30	123.59
4	L	302	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
4	M	802	BCL	CMD-C2D-C3D	2.08	128.57	124.68
5	L	402	BPH	C3A-C4A-NA	-2.08	109.50	113.05
4	M	802	BCL	C3A-C2A-C1A	2.08	104.45	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	CBB-CAB-C3B	-2.07	116.00	120.43
9	M	600	SPN	C6-C7-C8	2.05	118.62	111.88
5	L	402	BPH	CED-O2D-CGD	2.04	120.55	115.94
5	L	402	BPH	OB B-CAB-C3B	2.04	124.17	120.41
5	L	402	BPH	C3A-C2A-C1A	2.04	104.08	101.64
4	M	802	BCL	C2A-C3A-C4A	2.02	105.14	101.87
5	L	402	BPH	C2C-C3C-C4C	2.02	104.37	101.34
4	L	304	BCL	O2A-CGA-O1A	-2.00	118.54	123.59

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	802	BCL	C13
5	L	402	BPH	C8
4	L	302	BCL	C13
5	L	401	BPH	C8
5	L	401	BPH	C13

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	M	703	LDA	C2-C1-N1-O1
10	M	703	LDA	C2-C1-N1-CM1
5	L	402	BPH	C4B-C3B-CAB-CBB
5	L	402	BPH	C4B-C3B-CAB-OB B
5	L	402	BPH	O2A-C1-C2-C3
9	M	600	SPN	CM3-C5-C6-C7
6	L	502	U10	C5-C6-C7-C8
5	L	401	BPH	C4B-C3B-CAB-CBB
5	L	401	BPH	C4B-C3B-CAB-OB B
9	M	600	SPN	C14-C15-C16-C17
9	M	600	SPN	C11-C10-C9-CM4
9	M	600	SPN	CM5-C13-C14-C15
9	M	600	SPN	C16-C17-C18-CM6
9	M	600	SPN	C4-C5-C6-C7
9	M	600	SPN	C11-C10-C9-C8
9	M	600	SPN	C12-C13-C14-C15
9	M	600	SPN	C16-C17-C18-C19
6	L	502	U10	C4-C3-O3-C3M
5	L	402	BPH	C4-C3-C5-C6
5	L	402	BPH	C2-C3-C5-C6
5	L	402	BPH	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
6	M	501	U10	C23-C24-C26-C27
6	M	501	U10	C25-C24-C26-C27
9	M	600	SPN	C20-C21-C22-CM7
6	L	502	U10	C1-C6-C7-C8
6	M	501	U10	C35-C34-C36-C37
6	M	501	U10	C33-C34-C36-C37
4	M	801	BCL	C4C-C3C-CAC-CBC
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	401	BPH	C4C-C3C-CAC-CBC
9	M	600	SPN	C21-C22-C23-C24
5	L	401	BPH	C2B-C3B-CAB-CBB
4	L	302	BCL	CAD-CBD-CGD-O2D
10	M	703	LDA	C2-C1-N1-CM2
6	L	502	U10	C2-C3-O3-C3M
5	L	402	BPH	C15-C16-C17-C18
5	L	401	BPH	C2B-C3B-CAB-OB
6	M	501	U10	C14-C16-C17-C18
9	M	600	SPN	CM8-C26-C27-C28
6	L	502	U10	C12-C11-C9-C10
6	L	502	U10	C5-C4-O4-C4M
6	M	501	U10	C5-C4-O4-C4M
6	L	502	U10	C15-C14-C16-C17
5	L	402	BPH	C2C-C3C-CAC-CBC
6	L	502	U10	C25-C24-C26-C27
6	M	501	U10	C30-C29-C31-C32
6	L	502	U10	C35-C34-C36-C37
9	M	600	SPN	C25-C26-C27-C28
6	L	502	U10	C12-C11-C9-C8
6	M	501	U10	C28-C29-C31-C32
4	M	801	BCL	CAD-CBD-CGD-O2D
6	L	502	U10	C33-C34-C36-C37
4	M	802	BCL	O2A-C1-C2-C3
5	L	401	BPH	O2A-C1-C2-C3
4	L	304	BCL	CHA-CBD-CGD-O2D
5	L	402	BPH	CHA-CBD-CGD-O2D
5	L	401	BPH	CHA-CBD-CGD-O2D
4	M	802	BCL	C13-C15-C16-C17
6	M	501	U10	C29-C31-C32-C33
6	L	502	U10	C31-C32-C33-C34
6	L	502	U10	C20-C19-C21-C22
5	L	401	BPH	C2C-C3C-CAC-CBC

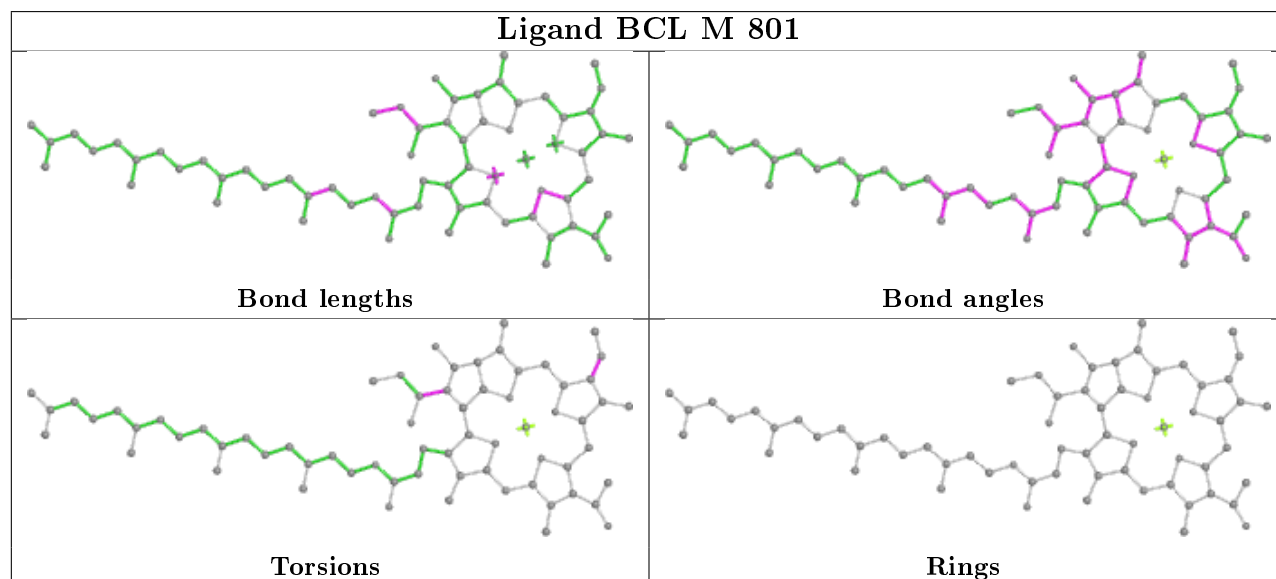
There are no ring outliers.

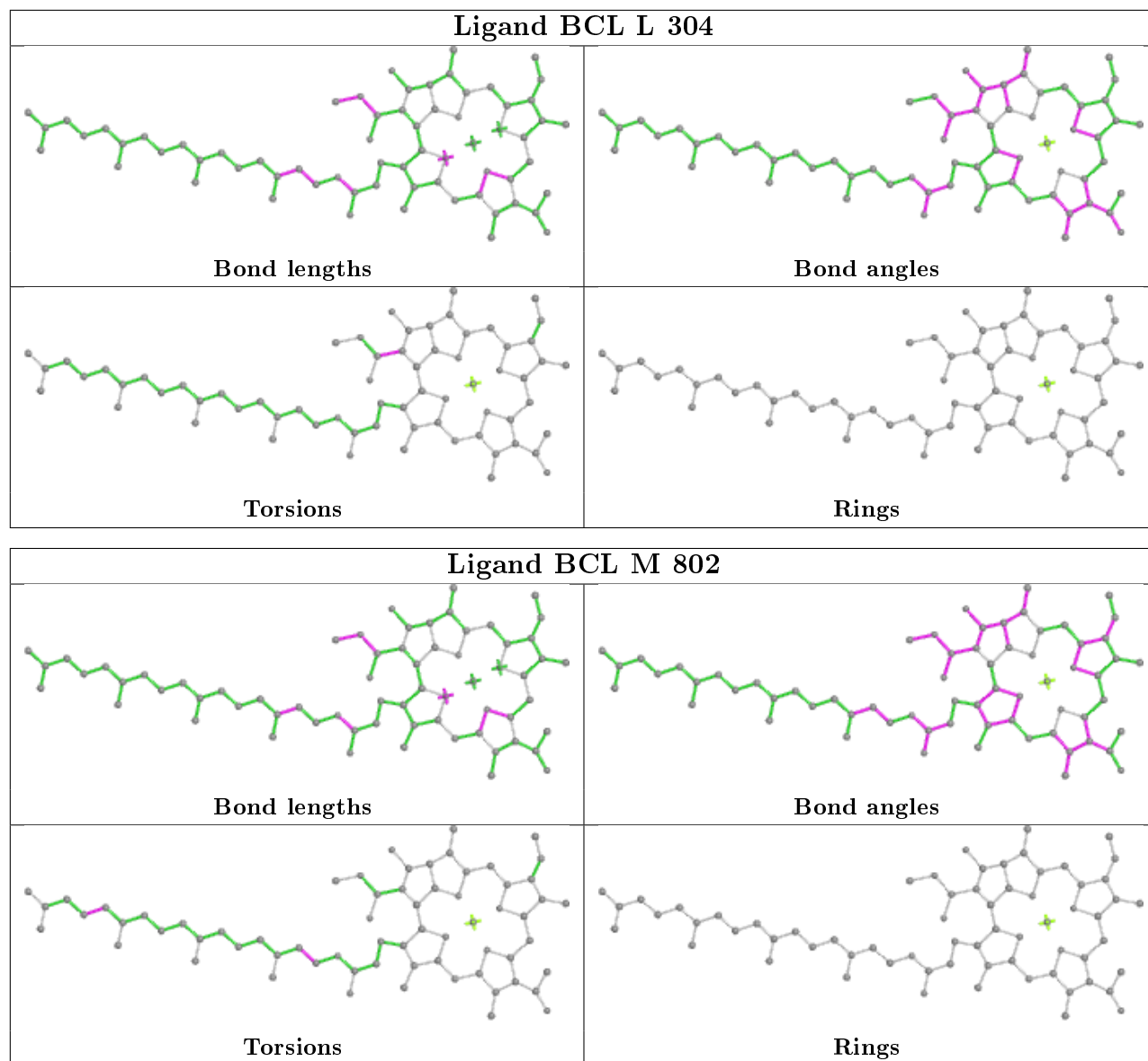


9 monomers are involved in 36 short contacts:

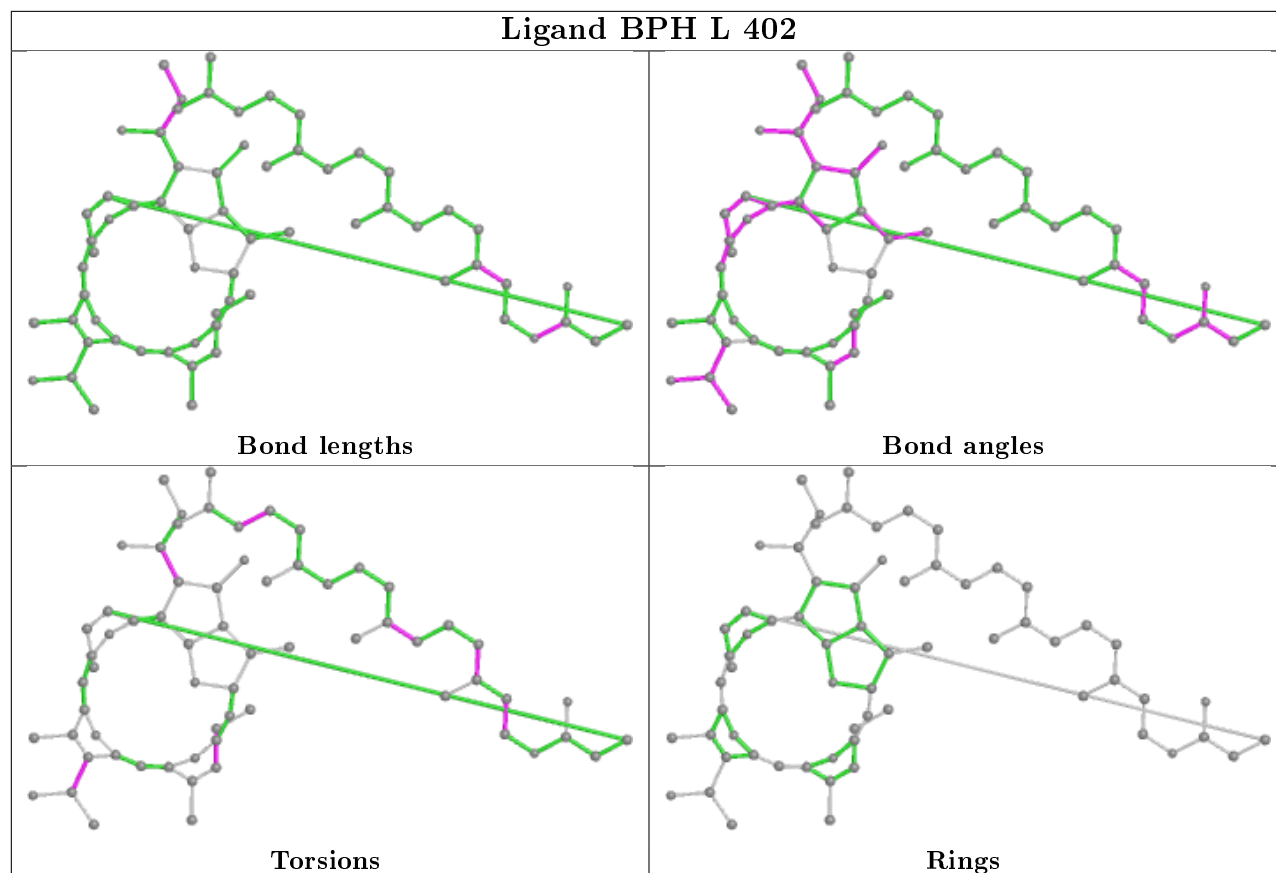
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	801	BCL	4	0
4	L	304	BCL	4	0
4	M	802	BCL	4	0
10	M	701	LDA	2	0
5	L	402	BPH	9	0
9	M	600	SPN	1	0
4	L	302	BCL	5	0
6	M	501	U10	3	0
5	L	401	BPH	6	0

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.

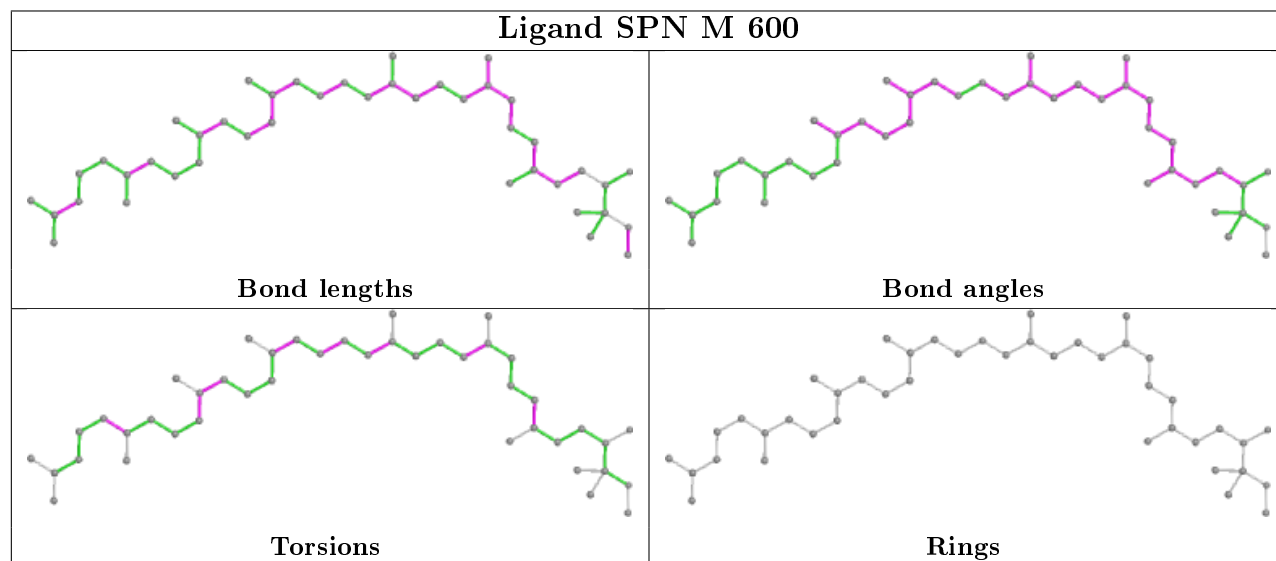


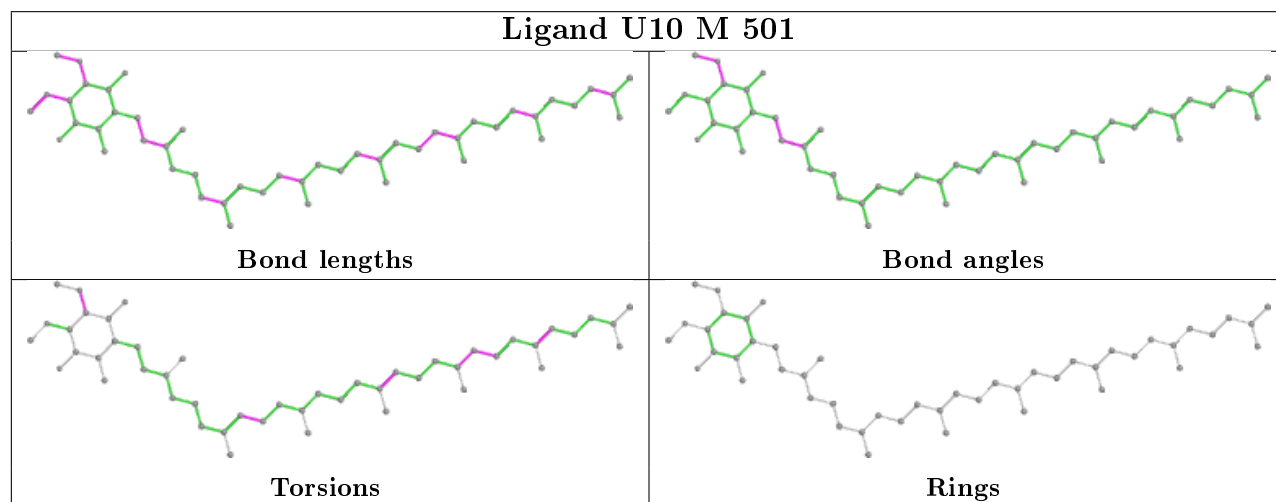
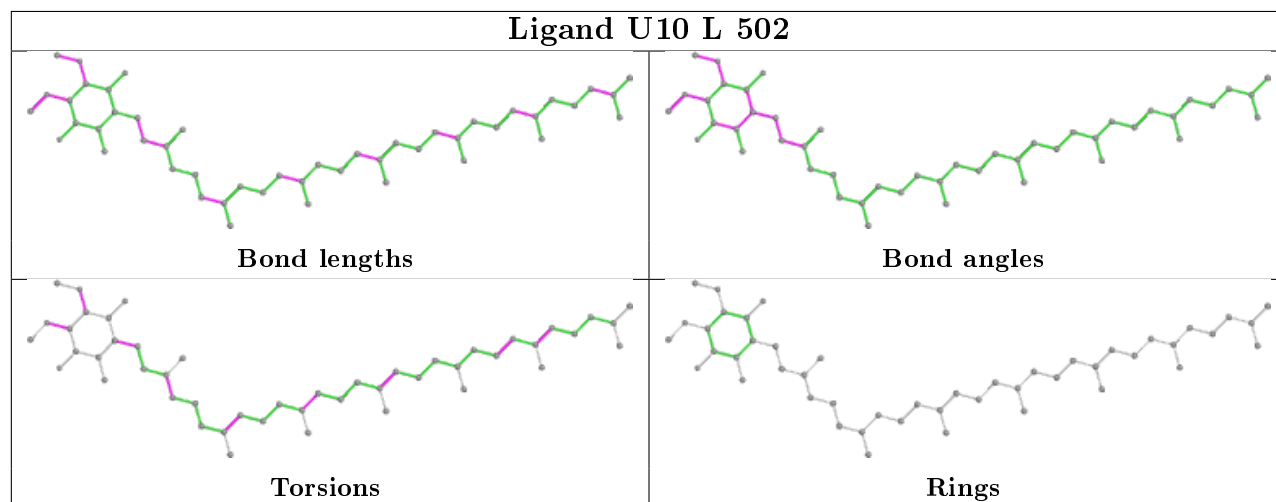
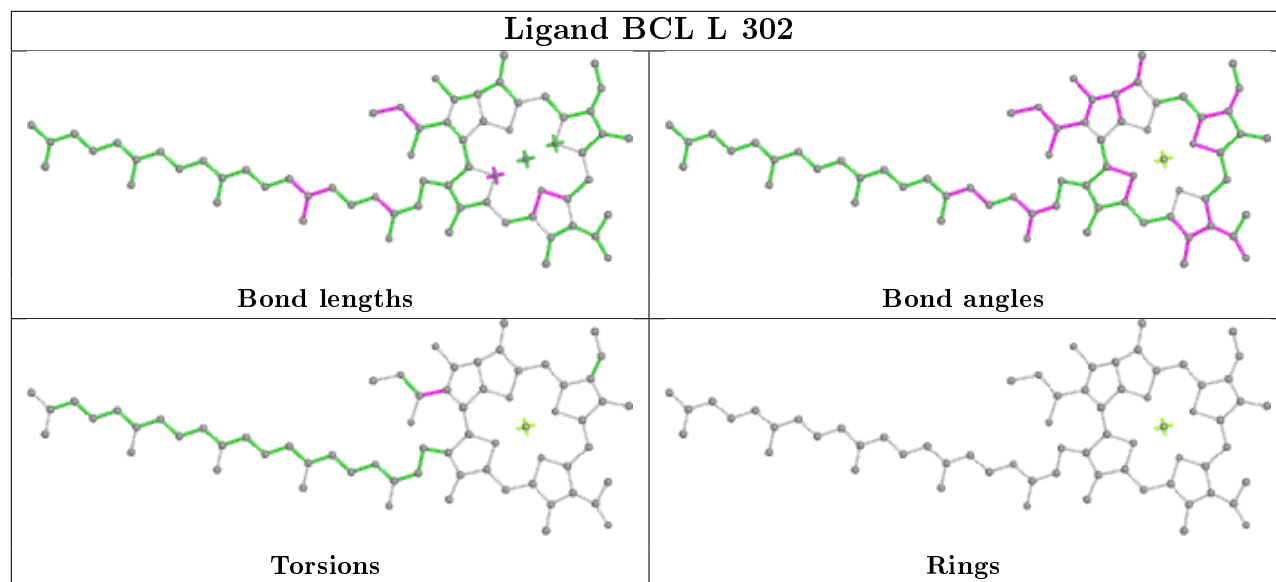


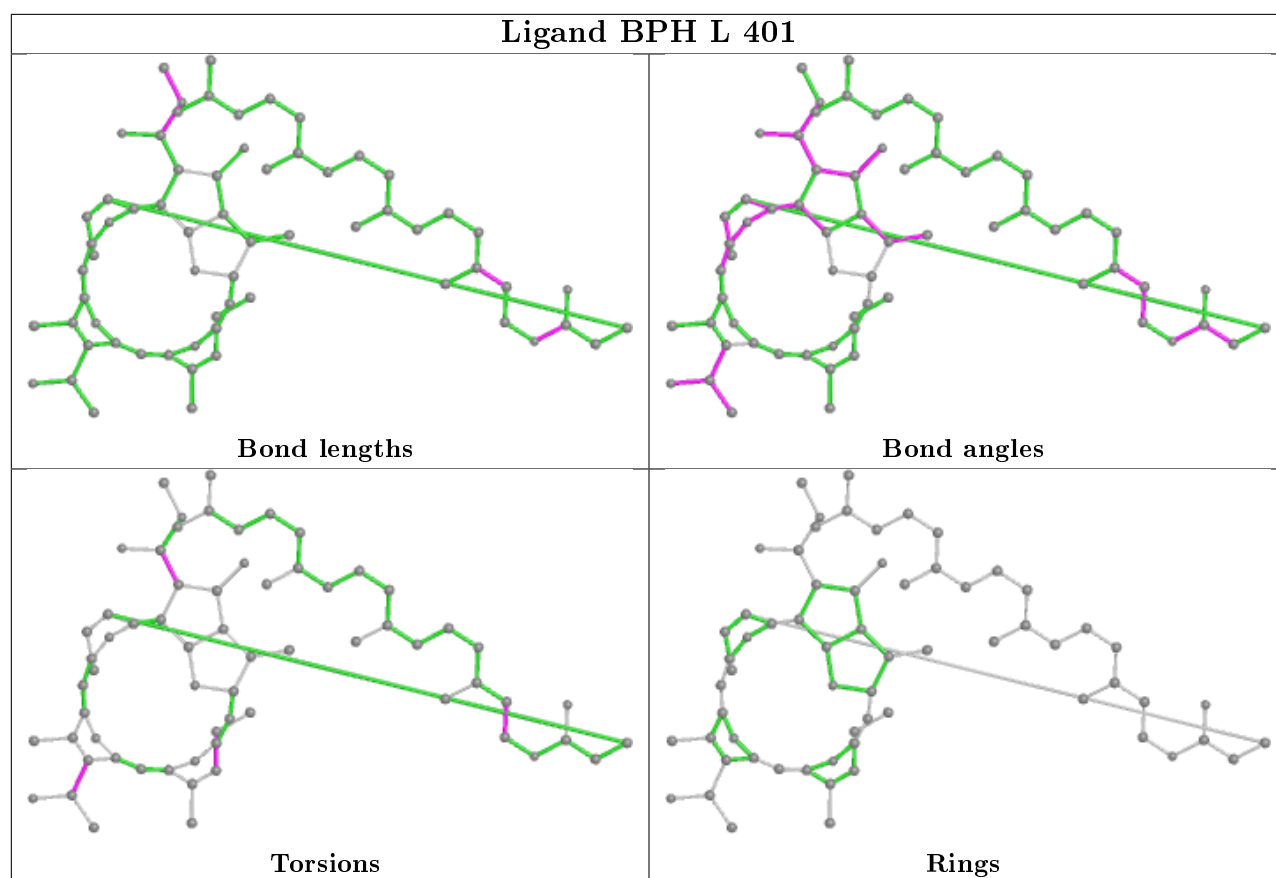
## Ligand BPH L 402



## Ligand SPN M 600







## 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.