



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 PM UTC

PDB ID : 1MPS / pdb_00001mps
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

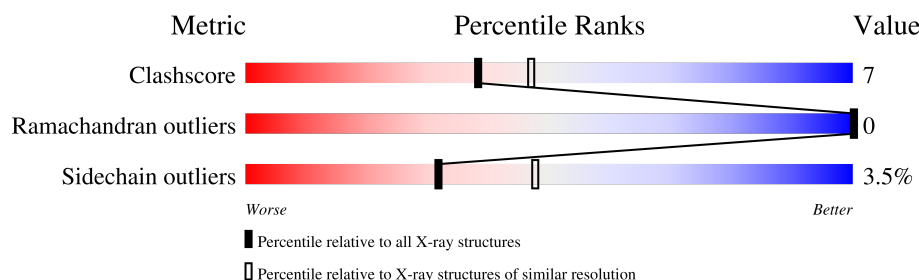
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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	L	281	83% 15% .
2	M	307	81% 15% . .
3	H	260	76% 16% 8%

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			

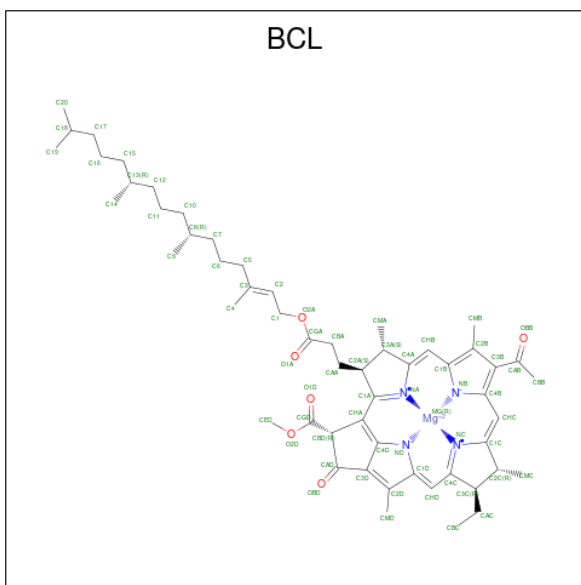
There are 2 discrepancies between the modelled and reference sequences:

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.

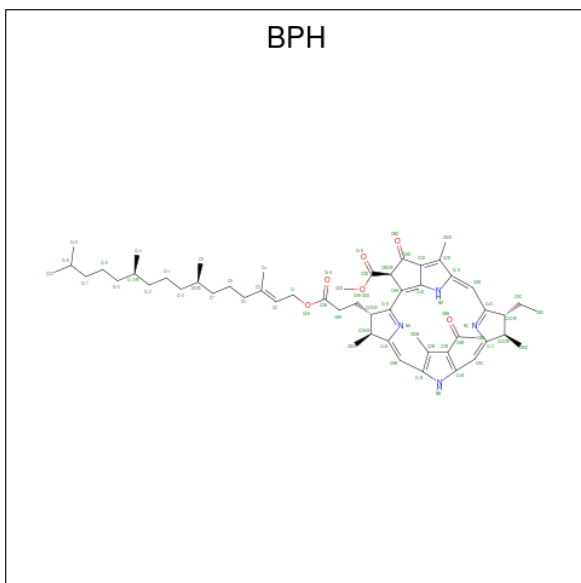
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



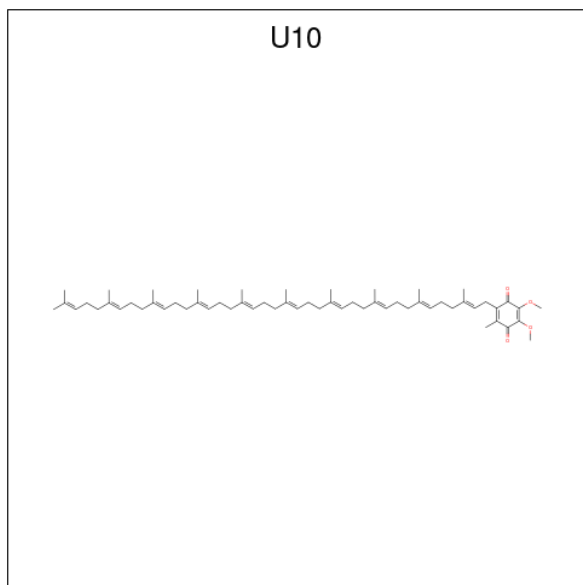
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	17	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

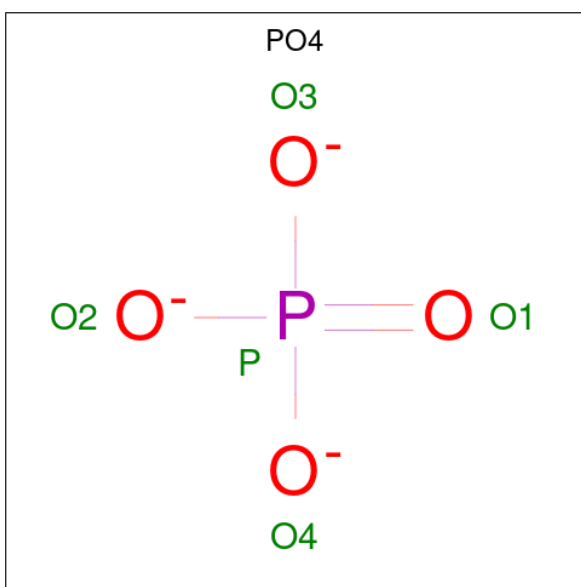


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	48	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

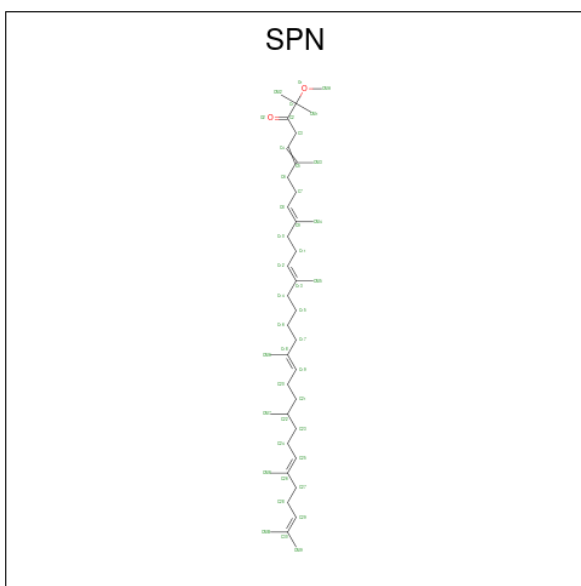
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



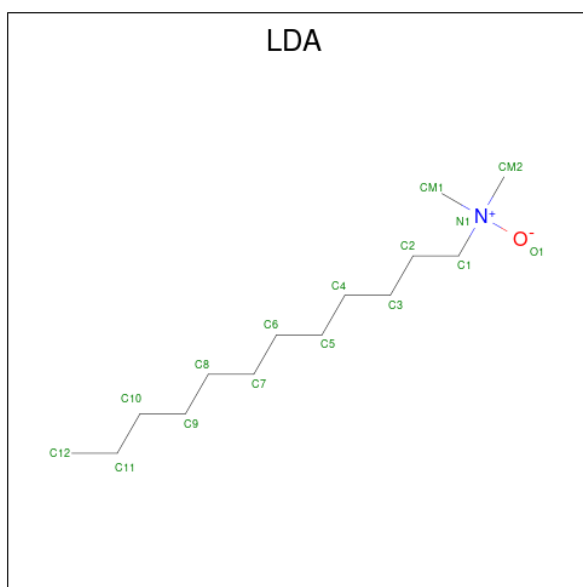
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is SPEROIDENONE (CCD ID: 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 (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 11 is water.

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

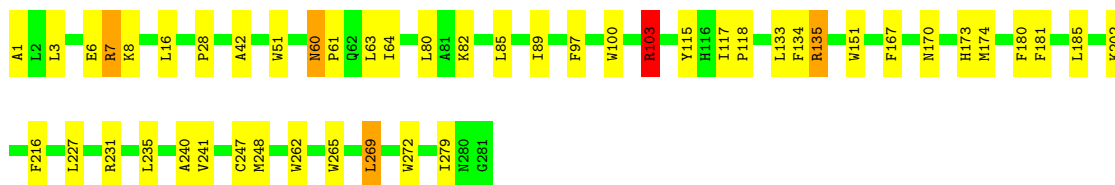
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

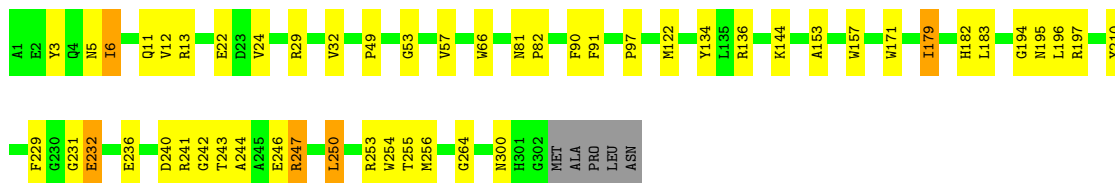
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L:  83% 15% .



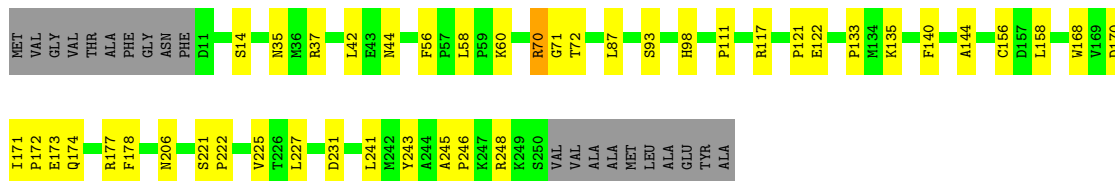
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain M:  81% 15% . .



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H:  76% 16% 8%



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, α , β , γ	141.90Å 141.90Å 187.90Å 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 ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, PO4, LDA, BPH, U10, SPN, BCL

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	0.50	0/2320	0.97	9/3175 (0.3%)
2	M	0.49	0/2498	0.90	3/3409 (0.1%)
3	H	0.47	0/1877	0.93	4/2553 (0.2%)
All	All	0.49	0/6695	0.94	16/9137 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6	GLU	N-CA-C	9.07	121.25	111.36
3	H	71	GLY	N-CA-C	6.56	118.03	111.21
3	H	44	ASN	N-CA-C	-6.09	101.50	110.52
3	H	243	TYR	N-CA-C	6.00	119.79	112.23
1	L	60	ASN	CA-C-N	5.89	126.04	119.32
1	L	60	ASN	C-N-CA	5.89	126.04	119.32
1	L	103	ARG	N-CA-C	-5.82	104.84	111.07
2	M	6	ILE	N-CA-C	-5.46	105.80	111.58
3	H	133	PRO	N-CA-C	-5.42	102.77	111.38
1	L	3	LEU	N-CA-C	-5.37	103.45	110.53
1	L	134	PHE	N-CA-C	5.34	116.79	111.07
1	L	269	LEU	CA-C-N	5.32	126.49	119.84
1	L	269	LEU	C-N-CA	5.32	126.49	119.84
1	L	7	ARG	N-CA-C	5.20	117.34	111.11
2	M	183	LEU	N-CA-C	-5.08	105.44	111.69
2	M	231	GLY	N-CA-C	5.07	119.88	113.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	35	0
2	M	2407	0	2325	41	0
3	H	1829	0	1836	26	0
4	L	132	0	148	5	0
4	M	132	0	148	4	0
5	L	130	0	152	15	0
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	96	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 (96) 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:HBB3	5:L:402:BPH:CHC	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:H:70:ARG:NH2	3:H:121:PRO:O	2.42	0.53
2:M:53:GLY:O	2:M:57:VAL:HG23	2.08	0.53
2:M:243:THR:OG1	2:M:247:ARG:HD2	2.09	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
3:H:241:LEU:HB2	11:H:296:HOH:O	2.10	0.51
1:L:174:MET:HE2	4:M:801:BCL:HED3	1.93	0.51
4:L:304:BCL:HHC	4:L:304:BCL:OBB	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
5:L:401:BPH:HBB3	5:L:401:BPH:CHC	2.41	0.49
2:M:24:VAL:HG11	2:M:29:ARG:NH2	2.27	0.49
4:M:802:BCL:HBB3	4:M:802:BCL:HMB1	1.93	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:OBB	4:L:302:BCL:HHC	2.14	0.46
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
1:L:231:ARG:HD2	2:M:6:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:TRP:CE2	9:M:600:SPN:HM73	2.52	0.45
3:H:173:GLU:O	3:H:174:GLN:C	2.58	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: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
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.52	0.44
2:M:247:ARG:NH2	3:H:111:PRO:O	2.51	0.43
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
2:M:136:ARG:NE	2:M:136:ARG:HA	2.34	0.42
1:L:82:LYS:HB3	1:L:82:LYS:HE2	1.86	0.42
1:L:103:ARG:NH2	2:M:255:THR:O	2.51	0.42
5:L:402:BPH:H142	5:L:402:BPH:H101	2.00	0.42
1:L:60:ASN:HB3	1:L:63:LEU:HD12	2.01	0.42
3:H:135:LYS:HB3	3:H:135:LYS:HE2	1.81	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: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
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
2:M:196:LEU:HD23	2:M:196:LEU:HA	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:302:BCL:HBB2	4:L:302:BCL:HMB3	2.03	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 [i](#)

5.3.1 Protein backbone [i](#)

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 [i](#)

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%)	212 (96%)	8 (4%)	31	46
2	M	236/240 (98%)	228 (97%)	8 (3%)	32	48
3	H	195/208 (94%)	188 (96%)	7 (4%)	31	46
All	All	651/668 (98%)	628 (96%)	23 (4%)	32	48

All (23) 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	202	LYS
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
2	M	12	VAL
2	M	22	GLU
2	M	179	ILE
2	M	182	HIS
2	M	232	GLU
2	M	247	ARG
2	M	250	LEU
2	M	300	ASN
3	H	14	SER
3	H	70	ARG
3	H	72	THR
3	H	93	SER
3	H	158	LEU
3	H	225	VAL
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	264	GLN
2	M	5	ASN
2	M	187	ASN
2	M	299	GLN
2	M	300	ASN
3	H	68	HIS
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
5	BPH	L	401	-	59,70,70	1.68	11 (18%)	59,101,101	2.48	12 (20%)
6	U10	L	502	-	48,48,63	1.84	12 (25%)	60,61,79	1.22	6 (10%)
10	LDA	M	702	-	13,15,15	2.36	2 (15%)	14,17,17	0.53	0
5	BPH	L	402	-	59,70,70	1.78	10 (16%)	59,101,101	2.33	14 (23%)
4	BCL	M	802	2	69,74,74	1.34	7 (10%)	79,115,115	2.00	14 (17%)
8	PO4	M	800	-	4,4,4	1.99	3 (75%)	6,6,6	0.79	0
10	LDA	M	701	-	13,15,15	2.95	2 (15%)	14,17,17	0.56	0
4	BCL	L	304	1	69,74,74	1.17	7 (10%)	79,115,115	1.93	9 (11%)
4	BCL	M	801	2	69,74,74	1.37	8 (11%)	79,115,115	2.01	14 (17%)
9	SPN	M	600	-	42,42,42	3.96	19 (45%)	50,52,52	2.10	19 (38%)
4	BCL	L	302	1	69,74,74	1.32	8 (11%)	79,115,115	1.84	13 (16%)
10	LDA	M	703	-	13,15,15	2.26	2 (15%)	14,17,17	0.54	0
6	U10	M	501	-	48,48,63	1.90	15 (31%)	60,61,79	1.01	3 (5%)

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
6	U10	L	502	-	-	14/45/69/87	0/1/1/1
10	LDA	M	702	-	-	0/13/13/13	-
5	BPH	L	402	-	1/1/18/22	7/37/105/105	0/5/6/6
4	BCL	M	802	2	1/1/21/25	1/41/137/137	-
4	BCL	L	302	1	1/1/21/25	0/41/137/137	-
10	LDA	M	701	-	-	0/13/13/13	-
4	BCL	L	304	1	-	2/41/137/137	-
4	BCL	M	801	2	-	1/41/137/137	-
9	SPN	M	600	-	-	13/50/51/51	-
5	BPH	L	401	-	2/2/18/22	0/37/105/105	0/5/6/6
10	LDA	M	703	-	-	3/13/13/13	-
6	U10	M	501	-	-	9/45/69/87	0/1/1/1

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C8-C9	8.93	1.53	1.33
9	M	600	SPN	C4-C5	8.85	1.53	1.33
9	M	600	SPN	C19-C18	8.65	1.53	1.33
9	M	600	SPN	C12-C13	8.62	1.52	1.33
10	M	701	LDA	O1-N1	-8.36	1.21	1.42
9	M	600	SPN	C3-C2	7.93	1.59	1.52
9	M	600	SPN	C3-C4	-7.15	1.39	1.50
10	M	703	LDA	O1-N1	-7.09	1.24	1.42
10	M	702	LDA	O1-N1	-6.96	1.25	1.42
10	M	701	LDA	C1-N1	-6.54	1.44	1.51
5	L	402	BPH	C1D-C2D	5.98	1.46	1.39
5	L	402	BPH	C3A-C2A	-5.95	1.49	1.54
9	M	600	SPN	C17-C18	-5.84	1.39	1.51
9	M	600	SPN	C14-C13	-5.81	1.39	1.51
9	M	600	SPN	C6-C5	-5.74	1.39	1.51
9	M	600	SPN	C10-C9	-5.35	1.40	1.51
5	L	401	BPH	C1D-C2D	5.11	1.45	1.39
4	L	302	BCL	O2D-CGD	5.08	1.45	1.33
4	M	802	BCL	MG-NA	4.94	2.18	2.06
10	M	702	LDA	C1-N1	-4.80	1.46	1.51
5	L	401	BPH	C2C-C3C	-4.66	1.50	1.54
4	M	801	BCL	MG-NA	4.64	2.17	2.06
6	L	502	U10	O3-C3	4.61	1.47	1.36
4	M	801	BCL	O2D-CED	-4.41	1.35	1.45
4	M	801	BCL	O2A-CGA	4.40	1.46	1.33
4	M	802	BCL	O2D-CED	-4.32	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	302	BCL	MG-NA	4.32	2.16	2.06
4	L	302	BCL	O2D-CED	-4.14	1.36	1.45
4	M	802	BCL	O2A-CGA	4.12	1.45	1.33
5	L	401	BPH	C1B-C2B	4.10	1.44	1.39
5	L	401	BPH	C3A-C2A	-4.09	1.51	1.54
6	M	501	U10	O3-C3	4.06	1.46	1.36
5	L	402	BPH	C1B-C2B	4.05	1.44	1.39
6	M	501	U10	O3-C3M	-3.99	1.36	1.45
4	L	304	BCL	O2D-CGD	3.95	1.42	1.33
10	M	703	LDA	C1-N1	-3.93	1.47	1.51
6	L	502	U10	O4-C4	3.91	1.46	1.36
4	L	304	BCL	MG-NA	3.83	2.15	2.06
5	L	402	BPH	C2C-C3C	-3.79	1.51	1.54
4	M	801	BCL	O2D-CGD	3.78	1.42	1.33
9	M	600	SPN	C20-C19	-3.77	1.39	1.50
9	M	600	SPN	C11-C12	-3.77	1.39	1.50
5	L	402	BPH	O2A-CGA	3.71	1.44	1.33
6	M	501	U10	O4-C4	3.68	1.45	1.36
9	M	600	SPN	C7-C8	-3.63	1.39	1.50
4	M	802	BCL	O2D-CGD	3.57	1.42	1.33
5	L	401	BPH	O2A-CGA	3.56	1.43	1.33
4	M	801	BCL	C3B-C4B	3.43	1.47	1.41
4	L	304	BCL	O2D-CED	-3.39	1.37	1.45
6	M	501	U10	O4-C4M	-3.26	1.38	1.45
9	M	600	SPN	O1-CMA	3.21	1.53	1.43
6	L	502	U10	O4-C4M	-3.14	1.38	1.45
5	L	401	BPH	O2D-CGD	3.11	1.40	1.33
5	L	402	BPH	O2D-CGD	3.09	1.40	1.33
6	M	501	U10	C33-C34	3.08	1.40	1.33
5	L	402	BPH	C2-C3	3.03	1.40	1.33
5	L	401	BPH	C2-C3	3.01	1.40	1.33
4	M	802	BCL	C2-C3	2.92	1.39	1.33
6	L	502	U10	C13-C14	2.91	1.39	1.33
6	L	502	U10	C28-C29	2.91	1.39	1.33
6	M	501	U10	C8-C9	2.89	1.39	1.33
6	M	501	U10	C23-C24	2.89	1.39	1.33
6	L	502	U10	C18-C19	2.89	1.39	1.33
6	L	502	U10	C23-C24	2.89	1.39	1.33
9	M	600	SPN	C25-C26	2.87	1.39	1.33
4	M	801	BCL	C2-C3	2.86	1.39	1.33
6	M	501	U10	C28-C29	2.86	1.39	1.33
6	L	502	U10	C8-C9	2.84	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	U10	C33-C34	2.84	1.39	1.33
5	L	402	BPH	C3B-C4B	2.80	1.46	1.41
6	M	501	U10	C13-C14	2.80	1.39	1.33
4	L	302	BCL	O2A-CGA	2.79	1.41	1.33
4	L	302	BCL	C3B-C4B	2.76	1.46	1.41
6	M	501	U10	C18-C19	2.74	1.39	1.33
6	M	501	U10	C7-C8	-2.72	1.46	1.50
4	L	302	BCL	C2-C3	2.71	1.39	1.33
5	L	401	BPH	C3B-C4B	2.71	1.45	1.41
4	L	304	BCL	C3B-C4B	2.71	1.46	1.41
5	L	401	BPH	O2D-CED	-2.68	1.39	1.45
6	L	502	U10	C7-C8	-2.68	1.46	1.50
9	M	600	SPN	C21-C22	-2.61	1.40	1.52
5	L	402	BPH	C3B-C2B	-2.60	1.35	1.39
8	M	800	PO4	P-O3	-2.55	1.47	1.54
4	M	802	BCL	C3B-C4B	2.53	1.46	1.41
4	L	304	BCL	O2A-CGA	2.51	1.40	1.33
4	L	304	BCL	C2-C3	2.51	1.38	1.33
9	M	600	SPN	C16-C15	-2.49	1.39	1.51
4	M	801	BCL	MG-ND	-2.45	2.00	2.05
4	M	802	BCL	MG-ND	-2.44	2.00	2.05
6	L	502	U10	O3-C3M	-2.41	1.39	1.45
6	L	502	U10	C38-C39	2.41	1.39	1.32
6	M	501	U10	C27-C28	-2.39	1.43	1.50
6	M	501	U10	C38-C39	2.35	1.39	1.32
9	M	600	SPN	C29-C30	2.27	1.39	1.32
5	L	402	BPH	O2D-CED	-2.26	1.40	1.45
5	L	401	BPH	C3B-C2B	-2.24	1.35	1.39
9	M	600	SPN	CM4-C9	2.22	1.56	1.50
4	L	304	BCL	C1-C2	-2.18	1.43	1.49
4	L	302	BCL	C4-C3	2.13	1.55	1.50
8	M	800	PO4	P-O4	-2.12	1.48	1.54
5	L	401	BPH	CHA-CBD	2.11	1.54	1.51
6	M	501	U10	C10-C9	2.07	1.55	1.50
8	M	800	PO4	P-O2	-2.06	1.48	1.54
6	M	501	U10	C17-C18	-2.06	1.44	1.50
4	L	302	BCL	C5-C3	2.03	1.55	1.51
4	M	801	BCL	CMD-C2D	2.03	1.54	1.50

All (104) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	401	BPH	O2D-CGD-CBD	12.80	125.01	110.95
5	L	402	BPH	O2D-CGD-CBD	11.33	123.40	110.95
4	M	802	BCL	C4A-NA-C1A	8.64	110.62	106.68
4	L	304	BCL	C4A-NA-C1A	8.02	110.34	106.68
4	M	801	BCL	C4A-NA-C1A	7.86	110.27	106.68
4	L	302	BCL	C4A-NA-C1A	7.77	110.22	106.68
4	L	304	BCL	O2D-CGD-CBD	7.31	124.01	111.23
4	M	801	BCL	C1C-NC-C4C	7.09	109.91	106.68
5	L	401	BPH	O1D-CGD-CBD	-6.99	114.12	124.72
4	M	802	BCL	C1C-NC-C4C	6.90	109.83	106.68
4	M	802	BCL	O2D-CGD-CBD	6.74	123.01	111.23
4	M	801	BCL	O2D-CGD-CBD	6.60	122.77	111.23
4	L	302	BCL	C1C-NC-C4C	6.59	109.69	106.68
5	L	402	BPH	O1D-CGD-CBD	-6.46	114.93	124.72
4	L	304	BCL	C1C-NC-C4C	6.44	109.62	106.68
5	L	401	BPH	C4D-CHA-CBD	-5.92	105.61	108.45
4	L	302	BCL	O2D-CGD-CBD	5.43	120.72	111.23
5	L	402	BPH	C4D-CHA-CBD	-5.33	105.90	108.45
4	L	304	BCL	O1D-CGD-CBD	-4.94	114.78	124.52
4	M	802	BCL	O1D-CGD-CBD	-4.73	115.19	124.52
4	M	801	BCL	O1D-CGD-CBD	-4.65	115.35	124.52
9	M	600	SPN	CM4-C9-C10	4.32	122.73	115.23
9	M	600	SPN	CM5-C13-C14	4.25	122.60	115.23
9	M	600	SPN	CM6-C18-C17	4.20	122.53	115.23
9	M	600	SPN	CM3-C5-C6	3.91	122.01	115.23
4	L	302	BCL	OBB-CAB-C3B	3.89	127.31	120.43
4	M	802	BCL	O2A-CGA-CBA	3.84	123.55	111.83
4	M	801	BCL	C1-C2-C3	3.83	132.47	126.20
5	L	401	BPH	OBB-CAB-C3B	3.80	126.33	119.99
4	M	801	BCL	O2A-CGA-CBA	3.80	123.41	111.83
9	M	600	SPN	CM7-C22-C21	3.78	124.76	111.27
4	M	801	BCL	OBB-CAB-C3B	3.73	127.02	120.43
5	L	402	BPH	O2A-CGA-CBA	3.52	122.56	111.83
6	L	502	U10	C3M-O3-C3	3.51	128.82	116.47
4	M	802	BCL	C1-C2-C3	3.40	131.77	126.20
9	M	600	SPN	C16-C17-C18	3.40	121.75	113.47
9	M	600	SPN	C15-C14-C13	3.37	121.69	113.47
9	M	600	SPN	C3-C4-C5	-3.36	121.04	126.83
4	L	302	BCL	O2A-CGA-CBA	3.29	121.88	111.83
4	L	304	BCL	CAB-C3B-C2B	3.27	134.54	127.74
4	M	802	BCL	CAB-C3B-C2B	3.27	134.53	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	O1D-CGD-CBD	-3.27	118.08	124.52
9	M	600	SPN	C11-C12-C13	-3.15	120.41	127.62
5	L	402	BPH	OBD-CAD-CBD	-3.13	121.23	125.82
4	M	801	BCL	CMB-C2B-C1B	-3.10	120.69	125.42
4	L	304	BCL	O2A-CGA-CBA	3.08	121.22	111.83
5	L	402	BPH	C1B-NB-C4B	-3.06	104.35	108.82
5	L	401	BPH	OBD-CAD-CBD	-3.02	121.39	125.82
6	L	502	U10	C7-C6-C1	-3.00	119.75	124.89
6	M	501	U10	C4M-O4-C4	2.99	126.99	116.47
6	L	502	U10	C4M-O4-C4	2.97	126.91	116.47
4	L	304	BCL	OBB-CAB-C3B	2.92	125.59	120.43
5	L	402	BPH	C1-C2-C3	2.91	130.96	126.20
4	L	302	BCL	C1-C2-C3	2.91	130.96	126.20
5	L	401	BPH	O2A-CGA-CBA	2.90	120.67	111.83
9	M	600	SPN	C20-C19-C18	-2.88	121.04	127.62
9	M	600	SPN	C7-C8-C9	-2.86	121.07	127.62
5	L	401	BPH	C1B-NB-C4B	-2.86	104.65	108.82
4	L	302	BCL	CAB-C3B-C2B	2.80	133.56	127.74
5	L	401	BPH	C1-C2-C3	2.78	130.76	126.20
5	L	401	BPH	C2D-C1D-ND	2.76	111.43	109.43
6	L	502	U10	C7-C8-C9	2.75	131.57	126.83
4	L	302	BCL	CBB-CAB-C3B	-2.69	114.72	120.40
5	L	401	BPH	CMD-C2D-C3D	2.68	130.03	124.68
4	M	802	BCL	CED-O2D-CGD	2.61	121.84	115.92
5	L	401	BPH	C4D-ND-C1D	-2.61	105.75	108.87
5	L	402	BPH	C4D-ND-C1D	-2.60	105.75	108.87
4	M	802	BCL	CBB-CAB-C3B	-2.56	115.00	120.40
4	M	801	BCL	CBB-CAB-C3B	-2.54	115.05	120.40
9	M	600	SPN	C17-C18-C19	-2.52	115.51	121.17
4	L	302	BCL	CED-O2D-CGD	2.52	121.62	115.92
9	M	600	SPN	C11-C10-C9	2.51	121.51	113.19
5	L	402	BPH	OBB-CAB-C3B	2.50	124.17	119.99
9	M	600	SPN	C7-C6-C5	2.50	121.46	113.19
4	L	304	BCL	CBB-CAB-C3B	-2.47	115.19	120.40
5	L	402	BPH	C3D-C4D-ND	2.45	110.84	107.71
6	M	501	U10	C7-C6-C1	-2.44	120.70	124.89
9	M	600	SPN	C10-C9-C8	-2.44	115.69	121.17
4	M	801	BCL	C2A-C1A-CHA	2.43	128.09	123.87
9	M	600	SPN	C14-C13-C12	-2.39	115.81	121.17
4	M	801	BCL	CAB-C3B-C2B	2.39	132.70	127.74
5	L	402	BPH	O2A-CGA-O1A	-2.35	117.75	123.63
9	M	600	SPN	C21-C20-C19	2.35	118.33	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502	U10	C7-C6-C5	2.33	121.22	118.52
5	L	402	BPH	C2B-C1B-NB	2.32	111.11	109.43
5	L	401	BPH	C3D-C4D-ND	2.31	110.66	107.71
6	M	501	U10	C7-C8-C9	2.29	130.78	126.83
4	M	801	BCL	O2A-CGA-O1A	-2.29	117.89	123.63
4	L	302	BCL	C1D-ND-C4D	-2.29	104.71	106.31
9	M	600	SPN	C4-C3-C2	2.28	122.34	111.68
9	M	600	SPN	C6-C5-C4	-2.27	116.06	121.17
4	M	802	BCL	O2A-CGA-O1A	-2.23	118.04	123.63
4	M	802	BCL	CAC-C3C-C4C	-2.17	107.77	112.58
4	L	302	BCL	O2A-CGA-O1A	-2.13	118.30	123.63
5	L	402	BPH	CMD-C2D-C3D	2.13	128.94	124.68
6	L	502	U10	C6-C1-C2	2.13	120.85	119.17
4	M	801	BCL	C4-C3-C5	-2.11	111.57	115.23
4	L	302	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
4	M	801	BCL	CHB-C1B-NB	2.08	127.17	124.05
4	M	802	BCL	C3A-C2A-C1A	2.08	104.45	101.34
4	M	802	BCL	C4D-CHA-C1A	2.05	123.69	121.24
5	L	402	BPH	CED-O2D-CGD	2.04	120.55	115.92
4	L	304	BCL	O2A-CGA-O1A	-2.03	118.54	123.63
4	M	802	BCL	C2A-C3A-C4A	2.02	105.14	101.87

All (5) chirality outliers are listed below:

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

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	502	U10	C5-C6-C7-C8
10	M	703	LDA	C2-C1-N1-O1
10	M	703	LDA	C2-C1-N1-CM1
9	M	600	SPN	CM3-C5-C6-C7
9	M	600	SPN	C14-C15-C16-C17
9	M	600	SPN	CM5-C13-C14-C15
9	M	600	SPN	C16-C17-C18-CM6
9	M	600	SPN	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
9	M	600	SPN	C12-C13-C14-C15
9	M	600	SPN	C16-C17-C18-C19
9	M	600	SPN	C11-C10-C9-CM4
9	M	600	SPN	C4-C5-C6-C7
6	L	502	U10	C4-C3-O3-C3M
9	M	600	SPN	C20-C21-C22-CM7
5	L	402	BPH	C4-C3-C5-C6
5	L	402	BPH	C2-C3-C5-C6
6	M	501	U10	C23-C24-C26-C27
5	L	402	BPH	O2A-C1-C2-C3
6	M	501	U10	C35-C34-C36-C37
9	M	600	SPN	C21-C22-C23-C24
6	M	501	U10	C25-C24-C26-C27
6	M	501	U10	C33-C34-C36-C37
4	M	801	BCL	C4C-C3C-CAC-CBC
6	L	502	U10	C1-C6-C7-C8
10	M	703	LDA	C2-C1-N1-CM2
5	L	402	BPH	C15-C16-C17-C18
6	L	502	U10	C2-C3-O3-C3M
4	L	304	BCL	CHA-CBD-CGD-O1D
4	L	304	BCL	CHA-CBD-CGD-O2D
6	L	502	U10	C12-C11-C9-C10
9	M	600	SPN	CM8-C26-C27-C28
6	M	501	U10	C5-C4-O4-C4M
6	M	501	U10	C30-C29-C31-C32
6	L	502	U10	C15-C14-C16-C17
6	L	502	U10	C25-C24-C26-C27
6	L	502	U10	C35-C34-C36-C37
6	L	502	U10	C12-C11-C9-C8
6	M	501	U10	C28-C29-C31-C32
9	M	600	SPN	C25-C26-C27-C28
6	M	501	U10	C14-C16-C17-C18
6	L	502	U10	C5-C4-O4-C4M
6	L	502	U10	C33-C34-C36-C37
5	L	402	BPH	CHA-CBD-CGD-O1D
5	L	402	BPH	C2C-C3C-CAC-CBC
6	L	502	U10	C20-C19-C21-C22
4	M	802	BCL	C13-C15-C16-C17
5	L	402	BPH	C6-C7-C8-C10
6	L	502	U10	C13-C14-C16-C17
6	M	501	U10	C29-C31-C32-C33
6	L	502	U10	C31-C32-C33-C34

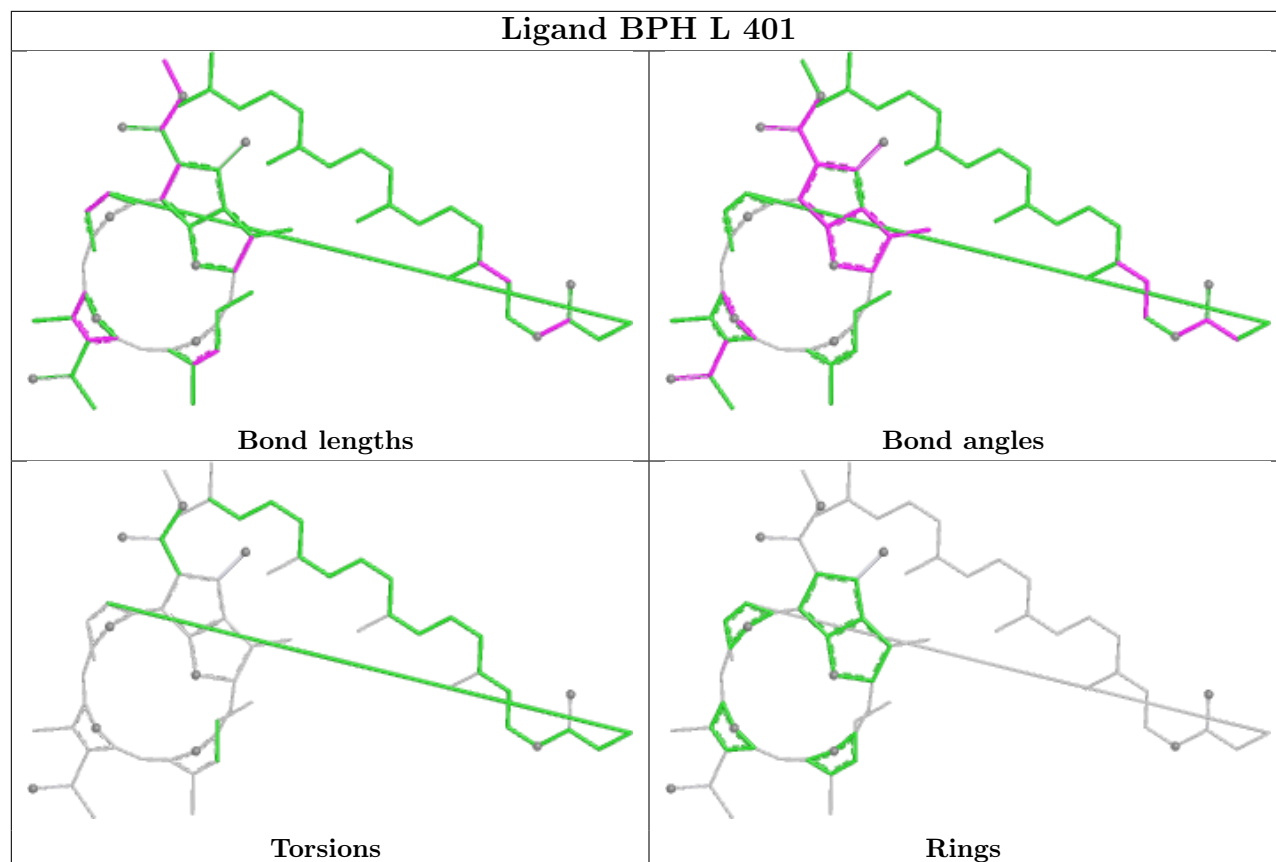
There are no ring outliers.

9 monomers are involved in 29 short contacts:

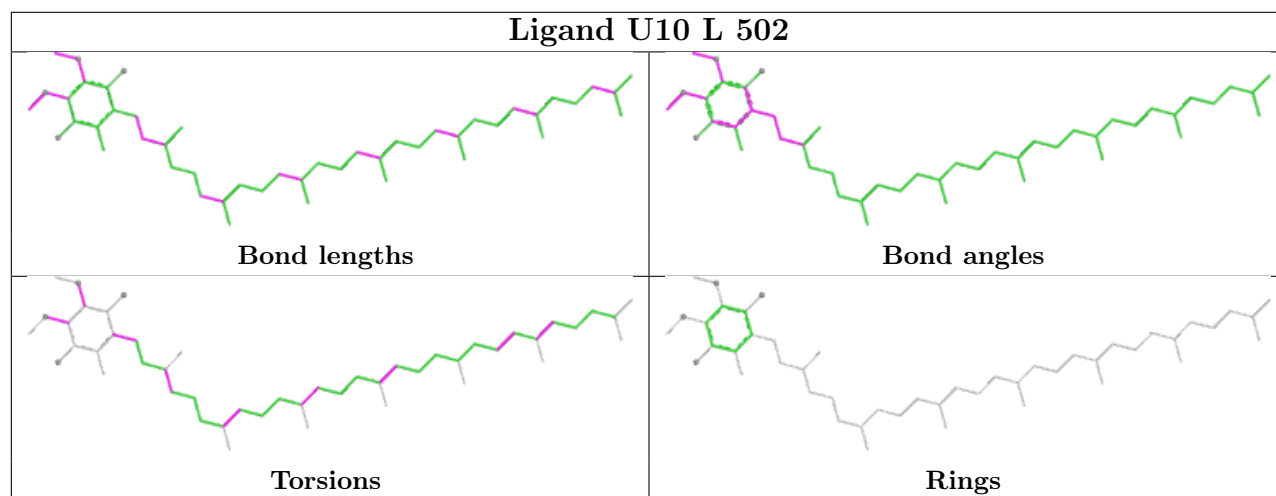
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	401	BPH	6	0
5	L	402	BPH	9	0
4	M	802	BCL	1	0
10	M	701	LDA	2	0
4	L	304	BCL	1	0
4	M	801	BCL	3	0
9	M	600	SPN	1	0
4	L	302	BCL	4	0
6	M	501	U10	3	0

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.

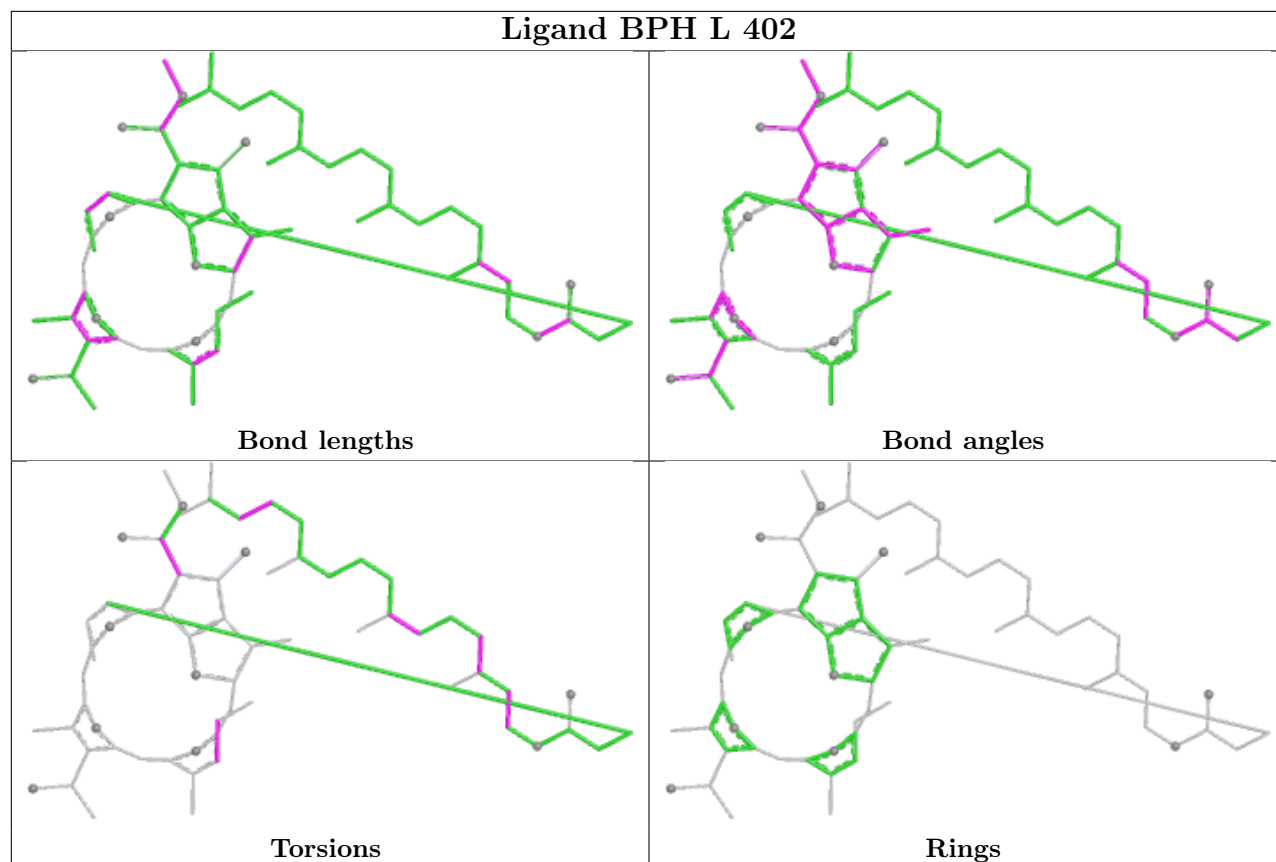
Ligand BPH L 401



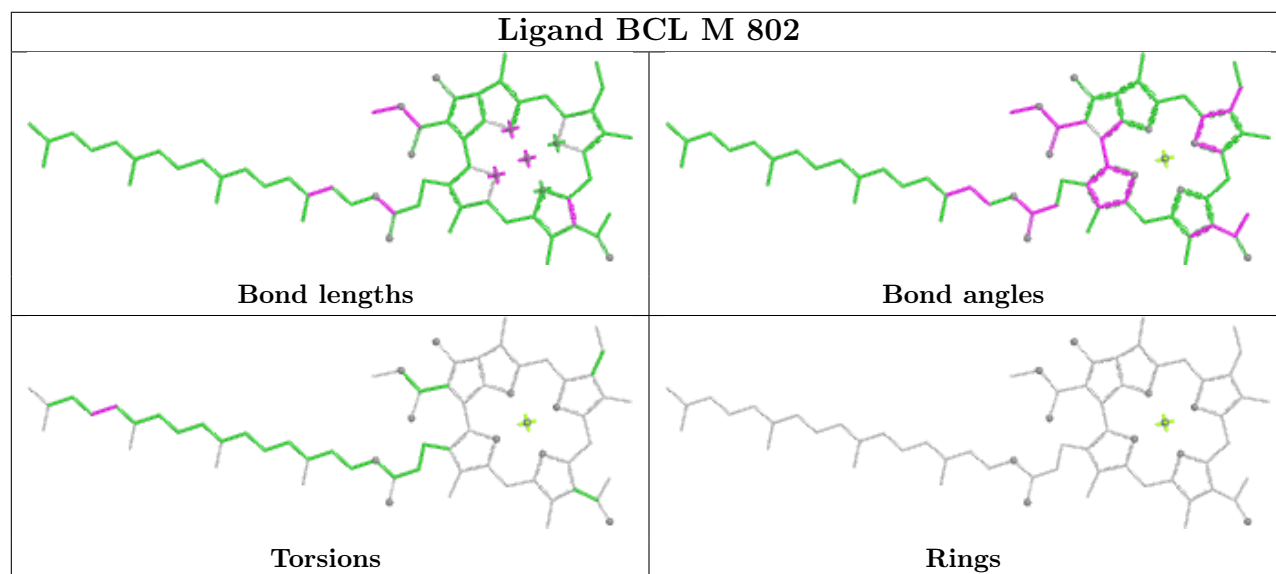
Ligand U10 L 502

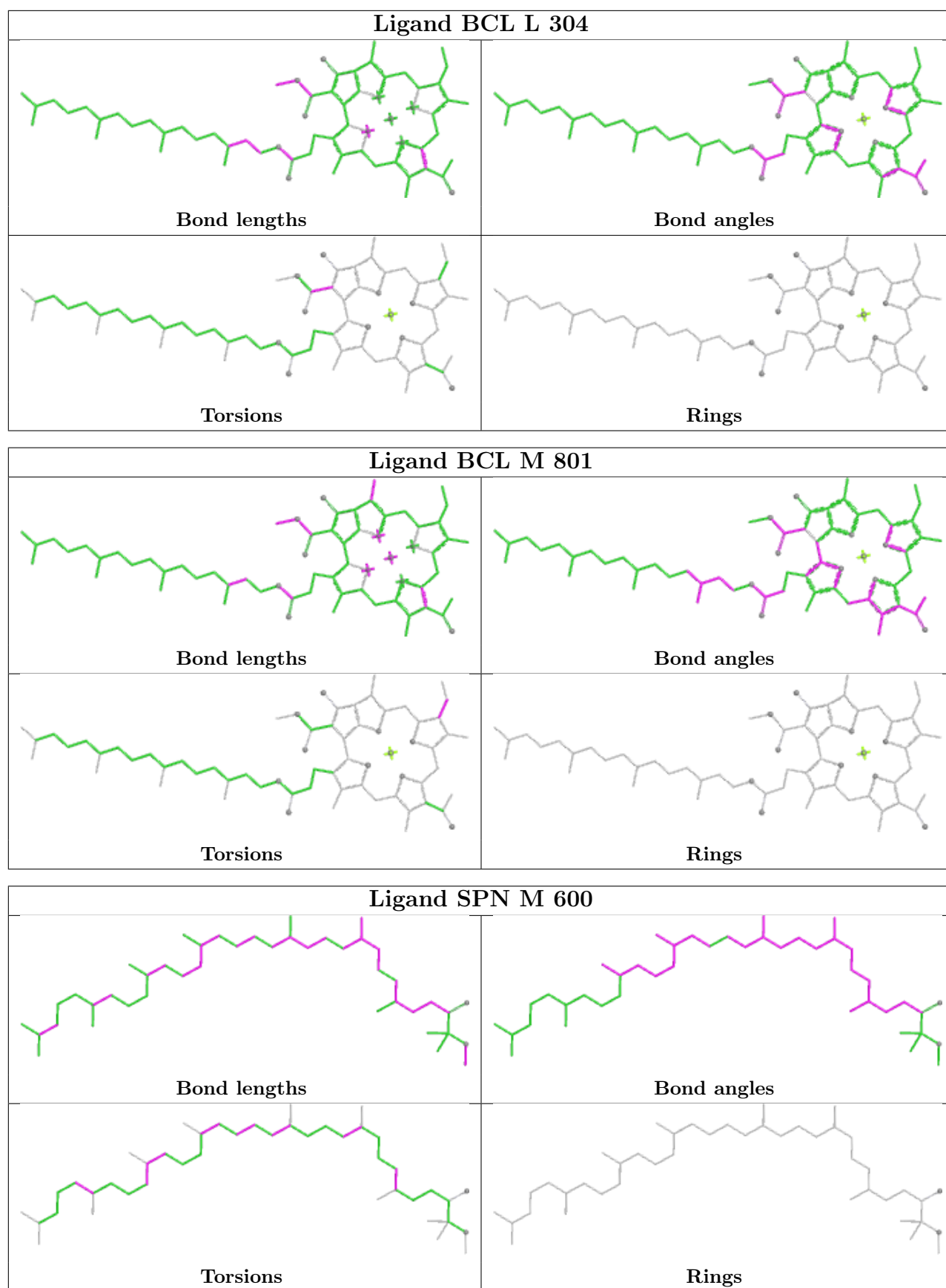


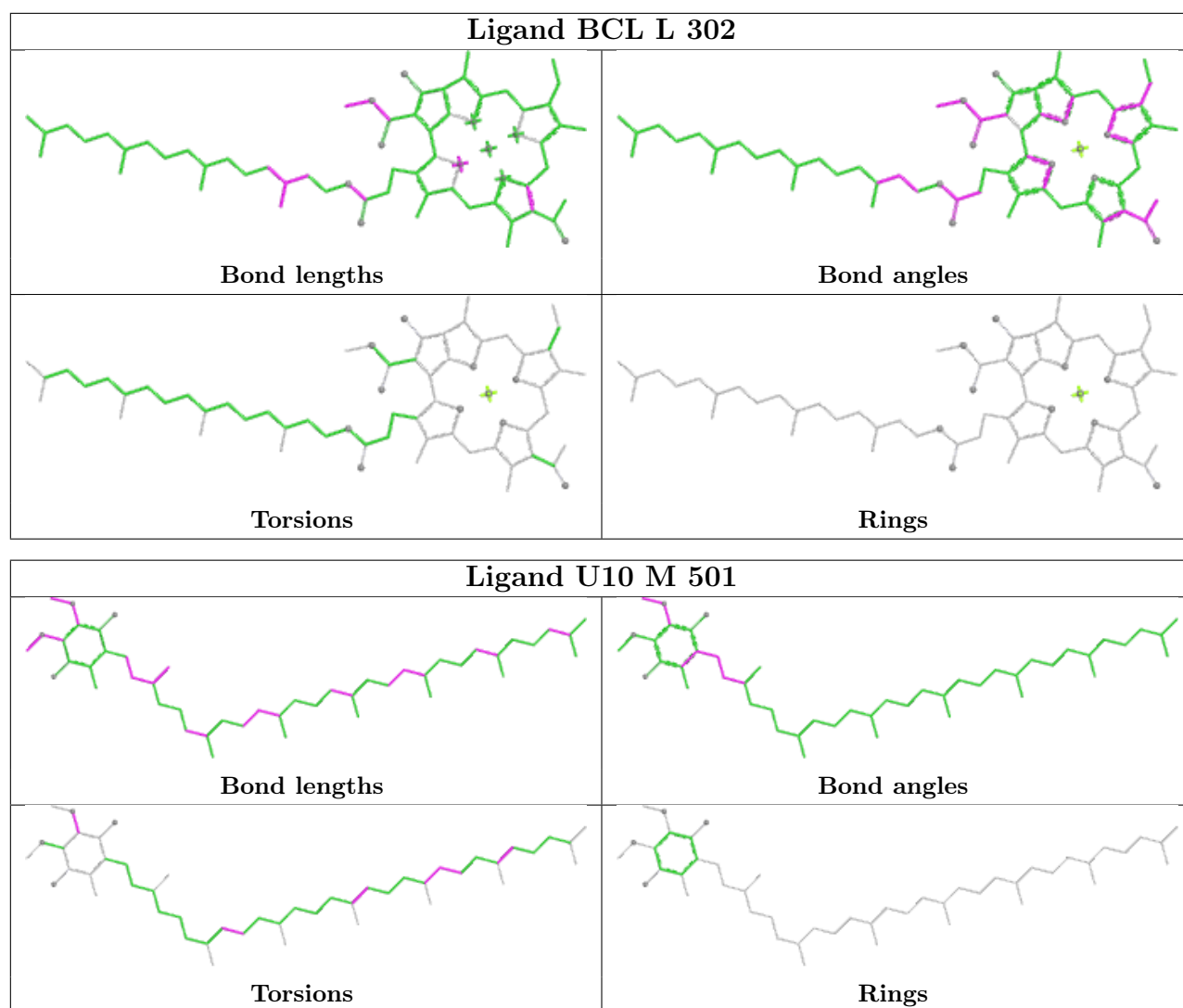
Ligand BPH L 402



Ligand BCL M 802







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.