



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 AM UTC

PDB ID : 1FNP / pdb_00001fnp
Title : CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CENTER PRO L209-> PHE FROM THE PHOTOSYNTHETIC PURPLE BACTERIUM RHODOBACTER SPHAEROIDES
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Deposited on : 2000-08-23
Resolution : 2.60 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

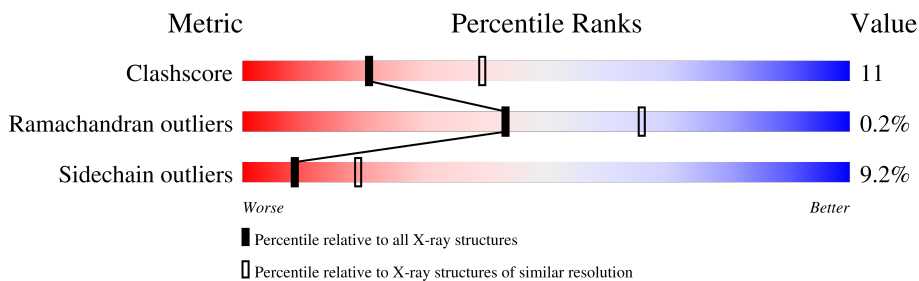
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	
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	304	X	-	-	-
4	BCL	M	801	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7256 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 REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2236	1511	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	209	PHE	PRO	engineered mutation	UNP P02954

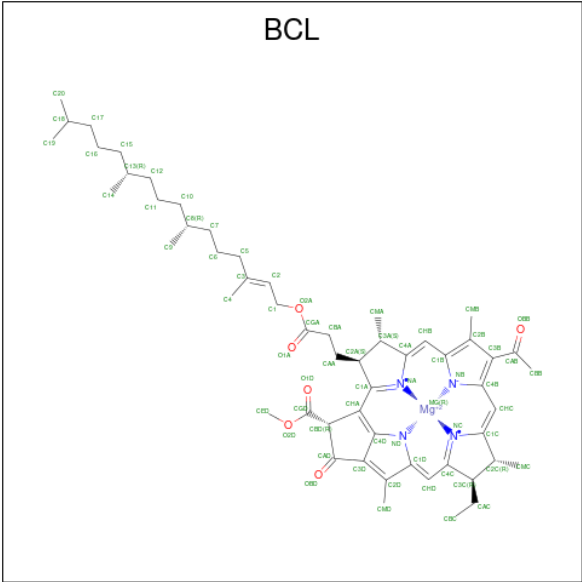
- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2399	1600	393	396	10			

- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

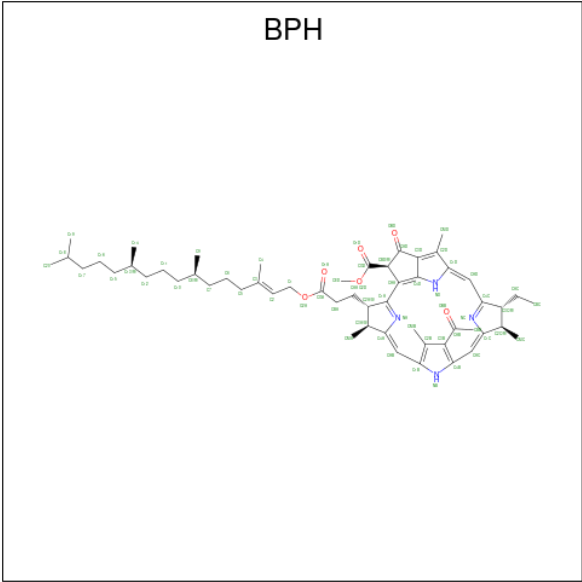
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



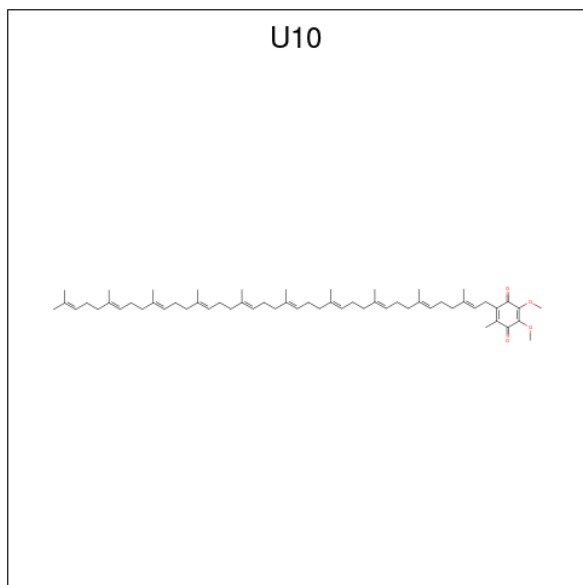
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



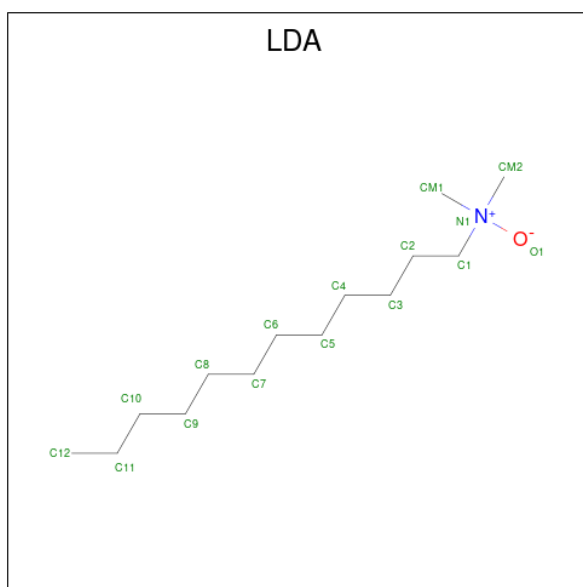
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

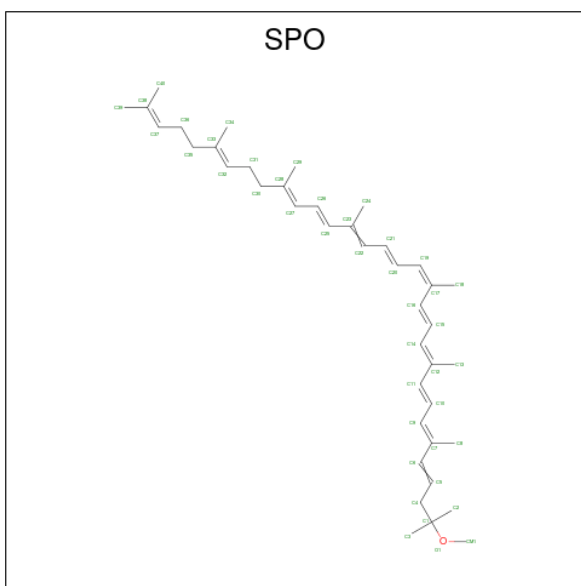
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 11 is water.

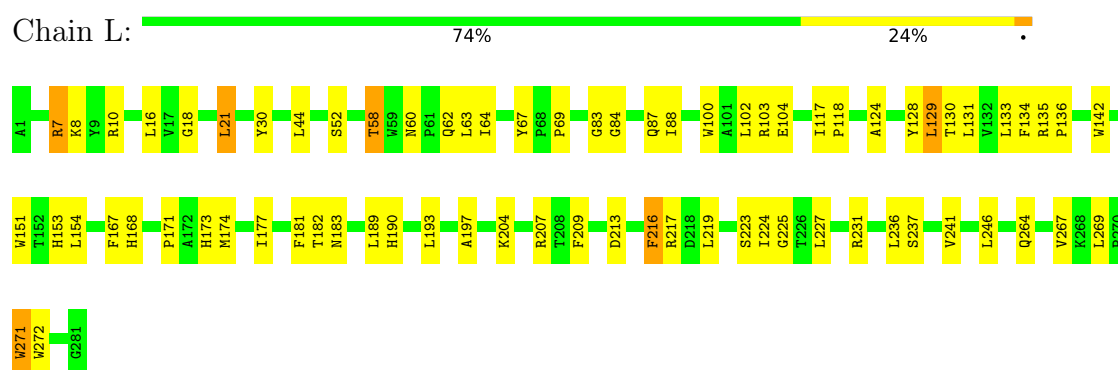
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	38	Total 38	O 38	0	0
11	M	39	Total 39	O 39	0	0
11	H	65	Total 65	O 65	0	0

3 Residue-property plots

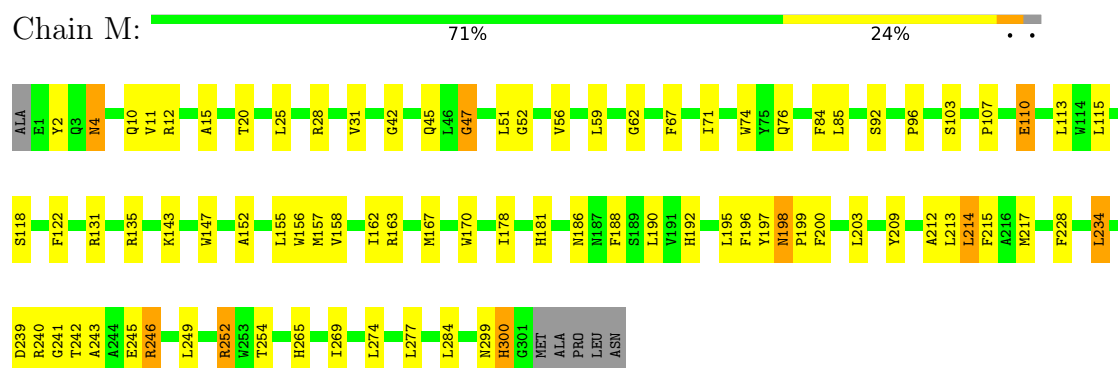
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: REACTION CENTER PROTEIN M CHAIN



• Molecule 3: REACTION CENTER PROTEIN H CHAIN



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	141.75Å 141.75Å 187.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.2 (50.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.216 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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: U10, BPH, PO4, SPO, LDA, BCL, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.56	1/2324 (0.0%)	0.76	0/3179
2	M	0.54	1/2491 (0.0%)	0.78	0/3400
3	H	0.49	0/1877	0.80	2/2553 (0.1%)
All	All	0.53	2/6692 (0.0%)	0.78	2/9132 (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	L	0	1
2	M	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	153	HIS	ND1-CE1	5.07	1.37	1.32
2	M	265	HIS	ND1-CE1	5.05	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	83	ARG	CA-C-N	5.33	125.09	119.76
3	H	83	ARG	C-N-CA	5.33	125.09	119.76

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	10	ARG	Sidechain
2	M	197	TYR	Sidechain
2	M	252	ARG	Sidechain
2	M	47	GLY	Peptide

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	2236	0	2189	55	0
2	M	2399	0	2306	62	0
3	H	1829	0	1836	35	0
4	L	132	0	148	12	0
4	M	132	0	148	12	0
5	L	65	0	76	8	0
5	M	65	0	76	11	0
6	L	48	0	63	6	0
6	M	48	0	63	4	0
7	H	32	0	62	2	0
7	L	16	0	31	0	0
7	M	64	0	124	1	0
8	M	1	0	0	0	0
9	M	5	0	0	1	0
10	M	42	0	60	1	0
11	H	65	0	0	4	0
11	L	38	0	0	6	0
11	M	39	0	0	0	0
All	All	7256	0	7182	158	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 11.

All (158) 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)
4:L:304:BCL:HHC	4:L:304:BCL:HBB2	1.42	1.02
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:801:BCL:HBB2	4:M:801:BCL:HHC	1.49	0.92
2:M:152:ALA:HB2	5:M:401:BPH:HAC1	1.54	0.90
3:H:194:GLN:HE21	3:H:194:GLN:H	1.21	0.85
4:L:302:BCL:CBB	4:L:302:BCL:HHC	2.10	0.82
11:L:731:HOH:O	2:M:217:MET:SD	2.39	0.81
11:L:706:HOH:O	2:M:252:ARG:HD3	1.82	0.79
4:M:802:BCL:HHC	4:M:802:BCL:CBB	2.15	0.77
4:M:802:BCL:HHC	4:M:802:BCL:HBB3	1.67	0.77
5:L:402:BPH:HBB2	2:M:209:TYR:HB3	1.68	0.76
1:L:223:SER:HA	6:L:502:U10:H1M1	1.67	0.75
4:M:801:BCL:HHC	4:M:801:BCL:CBB	2.17	0.73
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.71	0.72
2:M:196:PHE:CZ	4:M:802:BCL:HBB2	2.26	0.71
1:L:167:PHE:HB3	4:L:302:BCL:HMC3	1.72	0.71
2:M:45:GLN:HE21	2:M:47:GLY:HA3	1.56	0.71
1:L:241:VAL:HG21	5:L:402:BPH:HAC2	1.70	0.70
2:M:214:LEU:HD23	2:M:217:MET:HE3	1.72	0.70
2:M:196:PHE:HZ	4:M:802:BCL:HBB2	1.56	0.69
4:L:304:BCL:HHC	4:L:304:BCL:CBB	2.20	0.68
4:M:801:BCL:HBB3	4:M:802:BCL:H41	1.76	0.66
1:L:30:TYR:O	1:L:103:ARG:NH2	2.29	0.66
1:L:209:PHE:CE2	3:H:173:GLU:HG3	2.30	0.66
4:L:302:BCL:HHC	4:L:302:BCL:HBB2	1.77	0.66
3:H:94:GLU:HG3	11:H:744:HOH:O	1.95	0.65
1:L:131:LEU:HD11	4:L:302:BCL:HED3	1.79	0.65
2:M:242:THR:O	2:M:246:ARG:HG2	1.96	0.65
1:L:190:HIS:HD1	6:L:502:U10:H4M1	1.62	0.64
1:L:168:HIS:NE2	4:L:302:BCL:HBB2	2.14	0.63
2:M:198:ASN:C	2:M:198:ASN:HD22	2.06	0.62
5:M:401:BPH:HBB3	5:M:401:BPH:HHC	1.80	0.62
3:H:148:PRO:O	3:H:151:LEU:HB2	1.99	0.62
2:M:118:SER:HB3	10:M:600:SPO:H311	1.82	0.62
1:L:197:ALA:HB1	2:M:234:LEU:HD21	1.82	0.61
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.18	0.61
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.82	0.60
5:L:402:BPH:HBB3	5:L:402:BPH:CHC	2.28	0.60
3:H:14:SER:HA	3:H:17:ILE:HG22	1.82	0.59
4:L:302:BCL:H52	4:L:304:BCL:HBB3	1.83	0.59
2:M:20:THR:HG23	2:M:25:LEU:HD21	1.84	0.58
3:H:37:ARG:NH1	3:H:60:LYS:O	2.35	0.58
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:241:GLY:CA	3:H:117:ARG:HD2	2.34	0.58
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.86	0.58
4:L:302:BCL:HHC	4:L:302:BCL:HBB3	1.84	0.57
2:M:228:PHE:HB2	2:M:243:ALA:HB2	1.86	0.57
2:M:178:ILE:HG23	4:M:801:BCL:HED1	1.87	0.57
1:L:103:ARG:HG3	11:L:711:HOH:O	2.04	0.57
2:M:156:TRP:HB2	4:M:802:BCL:H62	1.85	0.57
1:L:171:PRO:HA	1:L:174:MET:HG3	1.86	0.56
1:L:271:TRP:H	1:L:271:TRP:CD1	2.22	0.56
6:M:501:U10:H202	7:H:702:LDA:H121	1.86	0.56
1:L:7:ARG:NH2	3:H:98:HIS:CD2	2.74	0.56
1:L:103:ARG:NH1	2:M:254:THR:O	2.39	0.56
3:H:173:GLU:HG2	11:H:750:HOH:O	2.05	0.56
2:M:242:THR:OG1	2:M:246:ARG:HD3	2.05	0.55
4:M:801:BCL:HBB3	4:M:802:BCL:C4	2.37	0.55
1:L:124:ALA:HB2	5:L:402:BPH:HAC1	1.89	0.54
1:L:62:GLN:HE21	1:L:151:TRP:HE1	1.53	0.54
2:M:10:GLN:HB2	3:H:144:ALA:HB3	1.90	0.53
9:M:800:PO4:O3	7:M:704:LDA:HM23	2.08	0.53
2:M:217:MET:HE1	6:M:501:U10:H161	1.90	0.53
2:M:62:GLY:HA3	5:M:401:BPH:H6C1	1.91	0.53
2:M:239:ASP:O	3:H:117:ARG:NH2	2.42	0.53
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.43	0.53
1:L:197:ALA:CB	2:M:234:LEU:HD21	2.39	0.52
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.91	0.52
2:M:147:TRP:HA	2:M:147:TRP:CE3	2.45	0.52
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.74	0.52
2:M:76:GLN:HE22	2:M:92:SER:H	1.58	0.51
3:H:70:ARG:NH1	3:H:121:PRO:O	2.42	0.51
2:M:107:PRO:HG2	2:M:110:GLU:HB2	1.92	0.51
3:H:34:GLU:O	3:H:37:ARG:HG3	2.11	0.51
2:M:84:PHE:HD2	2:M:85:LEU:HD12	1.76	0.50
2:M:96:PRO:HG2	2:M:170:TRP:HB2	1.94	0.50
3:H:32:GLN:NE2	7:H:702:LDA:H22	2.27	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:31:VAL:HG13	2:M:47:GLY:HA2	1.94	0.50
2:M:147:TRP:HA	2:M:147:TRP:HE3	1.77	0.50
1:L:69:PRO:HD3	1:L:83:GLY:O	2.12	0.49
5:L:402:BPH:HMC3	2:M:212:ALA:HB3	1.93	0.49
5:L:402:BPH:HMC3	2:M:212:ALA:CB	2.43	0.49
2:M:198:ASN:HD22	2:M:200:PHE:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.31	0.49
1:L:190:HIS:HA	6:L:502:U10:H4M1	1.95	0.49
1:L:231:ARG:HD3	2:M:4:ASN:O	2.13	0.49
1:L:227:LEU:O	1:L:231:ARG:HG3	2.13	0.48
2:M:198:ASN:ND2	2:M:200:PHE:H	2.11	0.48
2:M:241:GLY:HA2	3:H:117:ARG:HD2	1.94	0.48
2:M:2:TYR:CZ	2:M:4:ASN:HA	2.49	0.48
3:H:156:CYS:HB3	3:H:206:ASN:O	2.14	0.48
5:M:401:BPH:H7C1	5:M:401:BPH:H4C1	1.96	0.47
1:L:131:LEU:HD11	4:L:302:BCL:CED	2.44	0.47
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.96	0.47
2:M:234:LEU:HD12	2:M:234:LEU:HA	1.74	0.47
1:L:181:PHE:HB3	5:M:401:BPH:CBB	2.44	0.46
2:M:122:PHE:CE1	2:M:157:MET:HE1	2.50	0.46
5:L:402:BPH:HHC	5:L:402:BPH:CBB	2.30	0.46
1:L:129:LEU:O	1:L:133:LEU:HB3	2.15	0.46
2:M:240:ARG:HD3	2:M:245:GLU:HG2	1.99	0.45
1:L:18:GLY:O	1:L:21:LEU:HB2	2.16	0.45
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.85	0.45
2:M:45:GLN:HG2	2:M:47:GLY:H	1.82	0.45
2:M:158:VAL:HA	2:M:162:ILE:HB	1.97	0.45
2:M:15:ALA:HB1	2:M:31:VAL:HG21	1.99	0.45
3:H:121:PRO:HB3	3:H:225:VAL:O	2.16	0.45
3:H:70:ARG:HB3	3:H:118:ARG:HH12	1.80	0.45
2:M:214:LEU:HD23	2:M:217:MET:CE	2.45	0.44
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.99	0.44
1:L:130:THR:HA	1:L:134:PHE:HB2	1.99	0.44
2:M:217:MET:HE1	6:M:501:U10:C16	2.47	0.44
3:H:241:LEU:HB2	11:H:707:HOH:O	2.17	0.44
3:H:117:ARG:NH1	3:H:227:LEU:HD22	2.33	0.44
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.53	0.44
2:M:51:LEU:HD23	2:M:51:LEU:HA	1.85	0.43
3:H:134:MET:HB2	3:H:167:ILE:O	2.18	0.43
2:M:214:LEU:HA	2:M:217:MET:CE	2.48	0.43
3:H:194:GLN:HE21	3:H:194:GLN:N	2.03	0.43
1:L:60:ASN:O	1:L:64:ILE:HG13	2.17	0.43
2:M:62:GLY:CA	5:M:401:BPH:H6C1	2.48	0.43
1:L:225:GLY:H	6:L:502:U10:H3M2	1.84	0.43
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.00	0.43
1:L:58:THR:HG22	11:L:723:HOH:O	2.18	0.43
1:L:183:ASN:ND2	1:L:237:SER:OG	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:LEU:HD23	6:L:502:U10:H4M3	2.01	0.43
1:L:84:GLY:O	1:L:88:ILE:HG13	2.19	0.43
1:L:227:LEU:HD21	2:M:4:ASN:OD1	2.19	0.43
2:M:52:GLY:O	2:M:56:VAL:HG23	2.19	0.43
3:H:126:HIS:HB2	3:H:128:HIS:CD2	2.53	0.42
1:L:7:ARG:HH21	3:H:98:HIS:CG	2.38	0.42
1:L:224:ILE:HG13	2:M:42:GLY:HA3	2.02	0.42
4:L:304:BCL:CBB	4:L:304:BCL:CHC	2.90	0.42
2:M:163:ARG:O	2:M:167:MET:HG2	2.19	0.42
5:M:401:BPH:H6C2	5:M:401:BPH:H102	1.88	0.42
2:M:12:ARG:O	3:H:140:PHE:HA	2.20	0.42
3:H:11:ASP:HA	11:H:745:HOH:O	2.20	0.42
3:H:75:VAL:HA	3:H:76:PRO:C	2.45	0.42
1:L:128:TYR:HD1	4:L:304:BCL:HBB1	1.84	0.42
2:M:188:PHE:O	2:M:192:HIS:HD2	2.02	0.42
2:M:274:LEU:HD23	2:M:277:LEU:HD23	2.01	0.42
1:L:100:TRP:CZ2	6:M:501:U10:H251	2.55	0.41
1:L:189:LEU:HD13	1:L:216:PHE:HZ	1.84	0.41
2:M:113:LEU:HD23	2:M:113:LEU:HA	1.93	0.41
1:L:190:HIS:HD1	6:L:502:U10:C4M	2.32	0.41
2:M:186:ASN:HA	4:M:802:BCL:HBC3	2.03	0.41
5:M:401:BPH:H4C1	5:M:401:BPH:C7	2.48	0.41
2:M:4:ASN:ND2	3:H:194:GLN:HG3	2.35	0.41
2:M:198:ASN:HD22	2:M:199:PRO:N	2.19	0.41
3:H:181:VAL:O	3:H:188:THR:HA	2.21	0.41
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.04	0.41
2:M:67:PHE:O	2:M:71:ILE:HG12	2.21	0.41
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.37	0.40
4:M:801:BCL:O2A	5:M:401:BPH:HBB2	2.21	0.40
1:L:217:ARG:HD2	11:L:724:HOH:O	2.20	0.40
1:L:219:LEU:HD12	2:M:131:ARG:NH2	2.36	0.40
5:M:401:BPH:HBB3	5:M:401:BPH:CHC	2.50	0.40
1:L:67:TYR:HE1	11:L:722:HOH:O	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	269 (96%)	10 (4%)	0	100	100
2	M	299/307 (97%)	283 (95%)	14 (5%)	2 (1%)	18	38
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	816/848 (96%)	781 (96%)	33 (4%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	4	ASN
2	M	300	HIS

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%)	204 (93%)	16 (7%)	13	29
2	M	235/240 (98%)	210 (89%)	25 (11%)	6	14
3	H	195/208 (94%)	176 (90%)	19 (10%)	8	17
All	All	650/668 (97%)	590 (91%)	60 (9%)	8	19

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG

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Mol	Chain	Res	Type
1	L	16	LEU
1	L	21	LEU
1	L	44	LEU
1	L	52	SER
1	L	58	THR
1	L	63	LEU
1	L	102	LEU
1	L	129	LEU
1	L	154	LEU
1	L	204	LYS
1	L	207	ARG
1	L	213	ASP
1	L	216	PHE
1	L	246	LEU
1	L	271	TRP
2	M	11	VAL
2	M	28	ARG
2	M	59	LEU
2	M	74	TRP
2	M	103	SER
2	M	110	GLU
2	M	115	LEU
2	M	135	ARG
2	M	143	LYS
2	M	155	LEU
2	M	181	HIS
2	M	190	LEU
2	M	195	LEU
2	M	198	ASN
2	M	203	LEU
2	M	213	LEU
2	M	214	LEU
2	M	215	PHE
2	M	234	LEU
2	M	246	ARG
2	M	249	LEU
2	M	269	ILE
2	M	284	LEU
2	M	299	ASN
2	M	300	HIS
3	H	12	LEU
3	H	28	ILE

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Mol	Chain	Res	Type
3	H	70	ARG
3	H	72	THR
3	H	81	GLU
3	H	94	GLU
3	H	115	VAL
3	H	117	ARG
3	H	118	ARG
3	H	151	LEU
3	H	171	ILE
3	H	185	ASP
3	H	194	GLN
3	H	200	SER
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	231	ASP
3	H	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	173	HIS
1	L	183	ASN
2	M	24	ASN
2	M	43	ASN
2	M	45	GLN
2	M	76	GLN
2	M	192	HIS
2	M	198	ASN
3	H	32	GLN
3	H	52	ASN
3	H	98	HIS
3	H	128	HIS
3	H	194	GLN
3	H	206	ASN

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	M	401	-	59,70,70	1.77	12 (20%)	59,101,101	2.37	13 (22%)
6	U10	L	502	-	48,48,63	1.93	13 (27%)	60,61,79	1.40	6 (10%)
7	LDA	H	706	-	13,15,15	2.38	2 (15%)	14,17,17	0.52	0
4	BCL	M	802	2	69,74,74	1.35	7 (10%)	79,115,115	1.88	11 (13%)
7	LDA	H	702	-	13,15,15	2.78	2 (15%)	14,17,17	0.53	0
9	PO4	M	800	-	4,4,4	2.03	2 (50%)	6,6,6	0.96	0
10	SPO	M	600	-	41,41,41	3.02	18 (43%)	47,50,50	2.21	14 (29%)
7	LDA	M	707	-	13,15,15	2.37	2 (15%)	14,17,17	0.51	0
6	U10	M	501	-	48,48,63	2.15	17 (35%)	60,61,79	1.05	5 (8%)
4	BCL	L	304	1	69,74,74	1.49	8 (11%)	79,115,115	1.89	7 (8%)
4	BCL	L	302	1	69,74,74	1.36	9 (13%)	79,115,115	1.85	9 (11%)
7	LDA	M	703	-	13,15,15	2.77	2 (15%)	14,17,17	0.57	0
7	LDA	M	704	-	13,15,15	2.51	2 (15%)	14,17,17	0.51	0
5	BPH	L	402	-	59,70,70	1.69	9 (15%)	59,101,101	2.37	11 (18%)
7	LDA	L	705	-	13,15,15	2.60	2 (15%)	14,17,17	0.49	0
4	BCL	M	801	2	69,74,74	1.34	7 (10%)	79,115,115	1.89	10 (12%)
7	LDA	M	701	-	13,15,15	2.38	2 (15%)	14,17,17	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	M	401	-	-	13/37/105/105	0/5/6/6
6	U10	L	502	-	-	17/45/69/87	0/1/1/1
7	LDA	H	706	-	-	2/13/13/13	-
4	BCL	M	802	2	-	9/41/137/137	-
7	LDA	H	702	-	-	5/13/13/13	-
10	SPO	M	600	-	-	17/47/47/47	-
7	LDA	M	707	-	-	1/13/13/13	-
6	U10	M	501	-	-	8/45/69/87	0/1/1/1
4	BCL	L	304	1	1/1/21/25	6/41/137/137	-
4	BCL	L	302	1	-	7/41/137/137	-
7	LDA	M	703	-	-	6/13/13/13	-
7	LDA	M	704	-	-	2/13/13/13	-
5	BPH	L	402	-	-	8/37/105/105	0/5/6/6
7	LDA	L	705	-	-	0/13/13/13	-
4	BCL	M	801	2	1/1/21/25	11/41/137/137	-
7	LDA	M	701	-	-	1/13/13/13	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	600	SPO	C6-C5	8.30	1.55	1.32
7	M	701	LDA	O1-N1	-8.14	1.22	1.42
7	M	703	LDA	O1-N1	-7.93	1.22	1.42
7	H	702	LDA	O1-N1	-7.91	1.22	1.42
7	L	705	LDA	O1-N1	-7.88	1.22	1.42
10	M	600	SPO	C10-C11	7.72	1.54	1.34
7	M	704	LDA	O1-N1	-7.67	1.23	1.42
7	H	706	LDA	O1-N1	-7.40	1.24	1.42
10	M	600	SPO	C15-C16	7.31	1.53	1.34
7	M	707	LDA	O1-N1	-7.28	1.24	1.42
4	L	304	BCL	O2D-CGD	7.07	1.50	1.33
5	L	402	BPH	C1D-C2D	6.24	1.46	1.39
7	H	702	LDA	C1-N1	-6.14	1.45	1.51
6	M	501	U10	C7-C8	-6.06	1.41	1.50
7	M	703	LDA	C1-N1	-6.04	1.45	1.51
5	M	401	BPH	C1D-C2D	5.17	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	600	SPO	C26-C25	5.04	1.47	1.34
5	M	401	BPH	C3A-C2A	-5.00	1.50	1.54
10	M	600	SPO	C21-C20	4.98	1.49	1.36
7	L	705	LDA	C1-N1	-4.95	1.46	1.51
6	L	502	U10	O3-C3	4.93	1.48	1.36
4	L	304	BCL	O2A-CGA	4.88	1.47	1.33
4	M	802	BCL	MG-NA	4.84	2.17	2.06
4	M	801	BCL	MG-NA	4.78	2.17	2.06
5	L	402	BPH	C1B-C2B	4.76	1.44	1.39
7	M	704	LDA	C1-N1	-4.71	1.46	1.51
4	L	304	BCL	MG-ND	-4.56	1.96	2.05
4	L	302	BCL	O2D-CED	-4.51	1.35	1.45
6	M	501	U10	O3-C3	4.49	1.47	1.36
4	M	802	BCL	O2D-CGD	4.49	1.44	1.33
7	M	707	LDA	C1-N1	-4.37	1.47	1.51
6	L	502	U10	C7-C8	-4.37	1.43	1.50
5	L	402	BPH	C3A-C2A	-4.36	1.50	1.54
4	L	302	BCL	MG-NA	4.36	2.16	2.06
7	H	706	LDA	C1-N1	-4.25	1.47	1.51
4	M	801	BCL	O2A-CGA	4.22	1.45	1.33
5	M	401	BPH	C1B-C2B	4.16	1.44	1.39
5	M	401	BPH	C2C-C3C	-4.13	1.51	1.54
5	M	401	BPH	O2A-CGA	4.07	1.45	1.33
5	L	402	BPH	O2D-CGD	4.03	1.43	1.33
6	M	501	U10	O4-C4M	-3.97	1.36	1.45
4	L	302	BCL	O2D-CGD	3.81	1.42	1.33
4	M	801	BCL	O2D-CGD	3.72	1.42	1.33
5	M	401	BPH	O2D-CED	-3.64	1.37	1.45
6	M	501	U10	C27-C28	-3.62	1.39	1.50
10	M	600	SPO	O1-CM1	3.57	1.54	1.43
6	M	501	U10	O4-C4	3.54	1.45	1.36
4	M	802	BCL	C3B-C4B	3.48	1.48	1.41
6	L	502	U10	O4-C4	3.36	1.44	1.36
6	M	501	U10	C22-C23	-3.36	1.40	1.50
4	M	802	BCL	O2A-CGA	3.35	1.43	1.33
4	M	801	BCL	O2D-CED	-3.31	1.37	1.45
6	M	501	U10	C33-C34	3.20	1.40	1.33
4	M	802	BCL	O2D-CED	-3.17	1.38	1.45
10	M	600	SPO	C11-C12	-3.14	1.39	1.46
10	M	600	SPO	C25-C23	-3.11	1.39	1.46
4	M	801	BCL	C3B-C4B	3.10	1.47	1.41
10	M	600	SPO	C10-C9	3.09	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	402	BPH	O2D-CED	-3.08	1.38	1.45
5	M	401	BPH	O2D-CGD	3.07	1.40	1.33
6	L	502	U10	C33-C34	3.05	1.40	1.33
6	L	502	U10	C23-C24	3.05	1.40	1.33
6	M	501	U10	O3-C3M	-3.02	1.38	1.45
6	L	502	U10	C28-C29	2.98	1.39	1.33
6	L	502	U10	C13-C14	2.98	1.39	1.33
4	L	302	BCL	MG-ND	-2.96	1.99	2.05
5	M	401	BPH	C2-C3	2.92	1.39	1.33
5	L	402	BPH	C2-C3	2.92	1.39	1.33
4	L	304	BCL	MG-NA	2.89	2.13	2.06
4	L	302	BCL	C3B-C4B	2.88	1.46	1.41
4	L	302	BCL	C1-C2	-2.85	1.41	1.49
10	M	600	SPO	C32-C33	2.84	1.39	1.33
5	L	402	BPH	C3B-C4B	2.84	1.46	1.41
4	L	304	BCL	C1-C2	-2.81	1.41	1.49
10	M	600	SPO	C16-C17	-2.81	1.39	1.46
4	L	302	BCL	C2-C3	2.80	1.39	1.33
6	L	502	U10	C18-C19	2.79	1.39	1.33
6	L	502	U10	C8-C9	2.77	1.39	1.33
4	L	302	BCL	O2A-CGA	2.75	1.41	1.33
4	M	801	BCL	C2-C3	2.73	1.39	1.33
6	M	501	U10	C13-C14	2.73	1.39	1.33
10	M	600	SPO	C6-C7	-2.67	1.40	1.46
4	L	304	BCL	C3B-C4B	2.67	1.46	1.41
6	M	501	U10	C18-C19	2.65	1.39	1.33
4	L	304	BCL	C2-C3	2.64	1.39	1.33
10	M	600	SPO	C26-C27	2.64	1.51	1.43
9	M	800	PO4	P-O3	-2.62	1.47	1.54
10	M	600	SPO	C15-C14	2.60	1.51	1.43
4	M	801	BCL	MG-ND	-2.59	2.00	2.05
6	M	501	U10	C23-C24	2.54	1.38	1.33
10	M	600	SPO	C37-C38	2.54	1.40	1.32
6	L	502	U10	O4-C4M	-2.53	1.39	1.45
4	M	802	BCL	C1-C2	-2.52	1.42	1.49
6	M	501	U10	C38-C39	2.50	1.39	1.32
5	M	401	BPH	C3B-C4B	2.46	1.45	1.41
6	L	502	U10	C38-C39	2.46	1.39	1.32
7	M	701	LDA	C1-N1	-2.44	1.49	1.51
5	L	402	BPH	O2A-CGA	2.43	1.40	1.33
5	M	401	BPH	C3B-C2B	-2.42	1.35	1.39
4	M	802	BCL	C2-C3	2.42	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	U10	O3-C3M	-2.39	1.40	1.45
10	M	600	SPO	O1-C1	2.39	1.55	1.41
6	M	501	U10	C28-C29	2.38	1.38	1.33
6	M	501	U10	C8-C9	2.38	1.38	1.33
6	M	501	U10	C17-C18	-2.37	1.43	1.50
10	M	600	SPO	C8-C7	2.32	1.55	1.50
5	L	402	BPH	C3B-C2B	-2.21	1.35	1.39
9	M	800	PO4	P-O4	-2.18	1.48	1.54
5	M	401	BPH	CHA-CBD	2.18	1.54	1.51
5	M	401	BPH	C5-C3	2.17	1.55	1.51
6	M	501	U10	C36-C34	2.12	1.55	1.51
4	L	302	BCL	MG-NC	2.10	2.11	2.06
6	L	502	U10	O2-C2	-2.08	1.18	1.23
4	L	304	BCL	O2D-CED	-2.07	1.40	1.45
6	M	501	U10	C30-C29	2.07	1.55	1.50
10	M	600	SPO	C24-C23	2.06	1.55	1.50

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	O2D-CGD-CBD	12.17	124.32	110.95
5	M	401	BPH	O2D-CGD-CBD	11.71	123.82	110.95
4	L	304	BCL	C4A-NA-C1A	8.12	110.38	106.68
4	L	304	BCL	O2D-CGD-CBD	8.10	125.40	111.23
4	M	801	BCL	C4A-NA-C1A	8.01	110.33	106.68
4	M	802	BCL	C4A-NA-C1A	7.83	110.25	106.68
4	L	302	BCL	C4A-NA-C1A	7.70	110.19	106.68
4	M	801	BCL	O2D-CGD-CBD	7.41	124.18	111.23
5	M	401	BPH	O1D-CGD-CBD	-7.30	113.65	124.72
5	L	402	BPH	O1D-CGD-CBD	-7.18	113.84	124.72
4	L	302	BCL	C1C-NC-C4C	7.04	109.89	106.68
4	M	802	BCL	C1C-NC-C4C	7.00	109.87	106.68
4	L	302	BCL	O2D-CGD-CBD	6.95	123.37	111.23
4	M	802	BCL	O2D-CGD-CBD	6.64	122.84	111.23
4	M	801	BCL	C1C-NC-C4C	6.60	109.69	106.68
10	M	600	SPO	C15-C14-C12	-6.26	118.50	127.28
4	L	304	BCL	O1D-CGD-CBD	-5.81	113.05	124.52
5	M	401	BPH	C4D-CHA-CBD	-5.57	105.78	108.45
4	M	801	BCL	O1D-CGD-CBD	-5.47	113.74	124.52
5	L	402	BPH	C4D-CHA-CBD	-5.29	105.92	108.45
10	M	600	SPO	C26-C27-C28	-5.28	120.26	127.69
6	L	502	U10	C3M-O3-C3	5.18	134.69	116.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	802	BCL	O1D-CGD-CBD	-4.80	115.05	124.52
4	L	304	BCL	C1C-NC-C4C	4.73	108.84	106.68
10	M	600	SPO	C4-C5-C6	-4.45	118.67	124.91
10	M	600	SPO	C20-C19-C17	-4.33	121.20	127.28
4	L	302	BCL	O1D-CGD-CBD	-4.23	116.18	124.52
10	M	600	SPO	C20-C21-C22	-4.16	115.01	123.52
6	L	502	U10	C7-C6-C1	-4.15	117.78	124.89
6	L	502	U10	C7-C6-C5	4.09	123.27	118.52
10	M	600	SPO	C25-C23-C22	-4.03	112.67	119.01
5	M	401	BPH	O2A-CGA-CBA	3.71	123.14	111.83
4	L	302	BCL	O2A-CGA-CBA	3.63	122.90	111.83
5	L	402	BPH	OBD-CAD-CBD	-3.56	120.60	125.82
10	M	600	SPO	C15-C16-C17	-3.54	116.65	126.36
4	M	802	BCL	O2A-CGA-CBA	3.50	122.50	111.83
5	L	402	BPH	O2A-CGA-CBA	3.45	122.36	111.83
5	M	401	BPH	OBD-CAD-CBD	-3.26	121.05	125.82
5	M	401	BPH	OBB-CAB-C3B	3.23	125.39	119.99
4	L	304	BCL	O2A-CGA-CBA	3.13	121.37	111.83
4	M	801	BCL	O2A-CGA-CBA	3.09	121.27	111.83
10	M	600	SPO	C6-C7-C9	-3.05	114.21	119.01
5	M	401	BPH	C1B-NB-C4B	-2.96	104.50	108.82
10	M	600	SPO	C8-C7-C6	2.93	122.57	118.09
4	M	802	BCL	C1-C2-C3	2.89	130.93	126.20
5	L	402	BPH	C1B-NB-C4B	-2.85	104.66	108.82
4	M	801	BCL	C1-C2-C3	2.83	130.84	126.20
4	L	302	BCL	C1-C2-C3	2.74	130.69	126.20
10	M	600	SPO	C21-C22-C23	-2.73	123.45	127.28
5	L	402	BPH	O2A-CGA-O1A	-2.64	117.02	123.63
10	M	600	SPO	C10-C9-C7	-2.62	123.60	127.28
10	M	600	SPO	C24-C23-C25	2.59	122.05	118.09
6	M	501	U10	C7-C8-C9	2.57	131.26	126.83
5	L	402	BPH	C4D-ND-C1D	-2.57	105.80	108.87
4	L	302	BCL	O2A-CGA-O1A	-2.54	117.26	123.63
6	M	501	U10	C4M-O4-C4	2.48	125.18	116.47
5	M	401	BPH	C4D-ND-C1D	-2.47	105.91	108.87
6	L	502	U10	C4M-O4-C4	2.46	125.11	116.47
5	M	401	BPH	O2A-CGA-O1A	-2.45	117.49	123.63
5	M	401	BPH	CED-O2D-CGD	2.38	121.32	115.92
5	M	401	BPH	C1-C2-C3	2.38	130.09	126.20
5	M	401	BPH	CMD-C2D-C3D	2.36	129.40	124.68
4	M	802	BCL	CED-O2D-CGD	2.35	121.24	115.92
4	L	302	BCL	CED-O2D-CGD	2.32	121.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	802	BCL	CHB-C1B-NB	2.32	127.53	124.05
5	L	402	BPH	C3D-C4D-ND	2.31	110.67	107.71
5	L	402	BPH	C1-C2-C3	2.31	129.98	126.20
4	M	802	BCL	C4D-CHA-C1A	2.30	123.99	121.24
5	M	401	BPH	C3D-C4D-ND	2.24	110.57	107.71
4	L	304	BCL	CED-O2D-CGD	2.22	120.95	115.92
4	M	802	BCL	C3A-C2A-C1A	2.19	104.62	101.34
4	M	801	BCL	C4D-CHA-C1A	2.19	123.85	121.24
4	M	801	BCL	C2A-C1A-CHA	2.10	127.51	123.87
4	M	801	BCL	CHB-C1B-NB	2.09	127.19	124.05
6	M	501	U10	O3-C3-C2	-2.09	109.59	116.64
10	M	600	SPO	C13-C12-C11	2.09	121.28	118.09
6	M	501	U10	C27-C28-C29	2.08	132.38	127.62
5	L	402	BPH	OBB-CAB-C3B	2.07	123.44	119.99
6	M	501	U10	C3M-O3-C3	2.06	123.71	116.47
4	M	802	BCL	O2A-CGA-O1A	-2.05	118.50	123.63
6	L	502	U10	C6-C1-C2	2.03	120.77	119.17
4	L	302	BCL	C4D-CHA-C1A	2.02	123.65	121.24
6	L	502	U10	C22-C23-C24	2.02	132.24	127.62
10	M	600	SPO	C10-C11-C12	-2.01	120.85	126.36
4	L	304	BCL	CBC-CAC-C3C	2.01	117.68	113.41
4	M	801	BCL	O2A-CGA-O1A	-2.01	118.61	123.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	304	BCL	C13
4	M	801	BCL	C8

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	302	BCL	CBD-CGD-O2D-CED
4	L	302	BCL	O1D-CGD-O2D-CED
4	M	801	BCL	C4C-C3C-CAC-CBC
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	402	BPH	C2C-C3C-CAC-CBC
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
5	M	401	BPH	C4-C3-C5-C6
6	L	502	U10	C1-C6-C7-C8
6	L	502	U10	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	M	501	U10	C29-C31-C32-C33
7	M	703	LDA	C2-C1-N1-O1
7	M	703	LDA	C2-C1-N1-CM1
7	H	702	LDA	C2-C1-N1-O1
7	H	702	LDA	C2-C1-N1-CM1
7	H	702	LDA	N1-C1-C2-C3
10	M	600	SPO	C4-C1-O1-CM1
10	M	600	SPO	C36-C37-C38-C40
10	M	600	SPO	C36-C37-C38-C39
6	L	502	U10	C12-C11-C9-C10
6	L	502	U10	C15-C14-C16-C17
5	M	401	BPH	C2-C3-C5-C6
6	L	502	U10	C12-C11-C9-C8
6	L	502	U10	C13-C14-C16-C17
4	M	802	BCL	C3-C5-C6-C7
5	M	401	BPH	O1A-CGA-O2A-C1
5	M	401	BPH	CBA-CGA-O2A-C1
6	L	502	U10	C9-C11-C12-C13
6	L	502	U10	C29-C31-C32-C33
6	L	502	U10	C4-C3-O3-C3M
4	M	802	BCL	C13-C15-C16-C17
4	M	801	BCL	C15-C16-C17-C18
10	M	600	SPO	C21-C22-C23-C24
4	L	304	BCL	C10-C11-C12-C13
5	M	401	BPH	C10-C11-C12-C13
6	L	502	U10	C21-C22-C23-C24
10	M	600	SPO	C20-C21-C22-C23
7	M	703	LDA	C3-C4-C5-C6
7	M	701	LDA	C11-C10-C9-C8
4	M	801	BCL	C1A-C2A-CAA-CBA
4	M	801	BCL	C11-C12-C13-C15
4	M	801	BCL	C11-C12-C13-C14
6	L	502	U10	C14-C16-C17-C18
10	M	600	SPO	C34-C33-C35-C36
5	M	401	BPH	O2A-C1-C2-C3
7	H	702	LDA	C1-C2-C3-C4
4	M	801	BCL	CBA-CGA-O2A-C1
10	M	600	SPO	C2-C1-O1-CM1
10	M	600	SPO	C3-C1-O1-CM1
5	L	402	BPH	C4-C3-C5-C6
5	L	402	BPH	C14-C13-C15-C16
6	L	502	U10	C2-C3-O3-C3M

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Mol	Chain	Res	Type	Atoms
4	L	302	BCL	C2A-CAA-CBA-CGA
4	M	802	BCL	C11-C12-C13-C15
7	M	704	LDA	C4-C5-C6-C7
5	M	401	BPH	C3-C5-C6-C7
5	L	402	BPH	C2-C3-C5-C6
4	M	801	BCL	O1A-CGA-O2A-C1
4	L	302	BCL	C14-C13-C15-C16
4	L	304	BCL	C8-C10-C11-C12
10	M	600	SPO	C19-C20-C21-C22
4	L	302	BCL	C12-C13-C15-C16
4	M	801	BCL	C11-C10-C8-C7
10	M	600	SPO	C1-C4-C5-C6
4	M	802	BCL	C4-C3-C5-C6
6	M	501	U10	C30-C29-C31-C32
5	L	402	BPH	O2A-C1-C2-C3
7	M	707	LDA	C5-C6-C7-C8
7	M	703	LDA	C2-C3-C4-C5
7	H	706	LDA	C2-C3-C4-C5
6	L	502	U10	C20-C19-C21-C22
6	M	501	U10	C28-C29-C31-C32
7	M	703	LDA	C2-C1-N1-CM2
7	H	702	LDA	C2-C1-N1-CM2
10	M	600	SPO	C29-C28-C30-C31
4	L	304	BCL	CBA-CGA-O2A-C1
10	M	600	SPO	C24-C23-C25-C26
4	L	304	BCL	O1A-CGA-O2A-C1
4	M	802	BCL	C6-C7-C8-C10
5	M	401	BPH	C11-C10-C8-C7
4	L	302	BCL	C16-C17-C18-C20
4	M	801	BCL	C3A-C2A-CAA-CBA
10	M	600	SPO	C17-C19-C20-C21
4	M	802	BCL	C2-C3-C5-C6
6	L	502	U10	C18-C19-C21-C22
10	M	600	SPO	C27-C28-C30-C31
10	M	600	SPO	C32-C33-C35-C36
4	M	802	BCL	C6-C7-C8-C9
6	M	501	U10	C2-C3-O3-C3M
4	L	304	BCL	C4B-C3B-CAB-CBB
4	M	802	BCL	C11-C12-C13-C14
6	M	501	U10	C25-C24-C26-C27
10	M	600	SPO	C18-C17-C19-C20
4	M	802	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	M	401	BPH	C8-C10-C11-C12
10	M	600	SPO	C16-C17-C19-C20
7	M	703	LDA	C5-C6-C7-C8
6	M	501	U10	C23-C24-C26-C27
5	L	402	BPH	C8-C10-C11-C12
7	H	706	LDA	C6-C7-C8-C9
6	L	502	U10	C25-C24-C26-C27
4	L	304	BCL	C3A-C2A-CAA-CBA
6	L	502	U10	C11-C12-C13-C14
7	M	704	LDA	C7-C8-C9-C10
4	M	801	BCL	C11-C10-C8-C9
5	M	401	BPH	C11-C10-C8-C9
6	L	502	U10	C35-C34-C36-C37
4	M	801	BCL	C16-C17-C18-C20
5	L	402	BPH	C11-C12-C13-C15
5	M	401	BPH	C2-C1-O2A-CGA
6	M	501	U10	C24-C26-C27-C28
6	M	501	U10	C14-C16-C17-C18
4	L	302	BCL	CAD-CBD-CGD-O2D

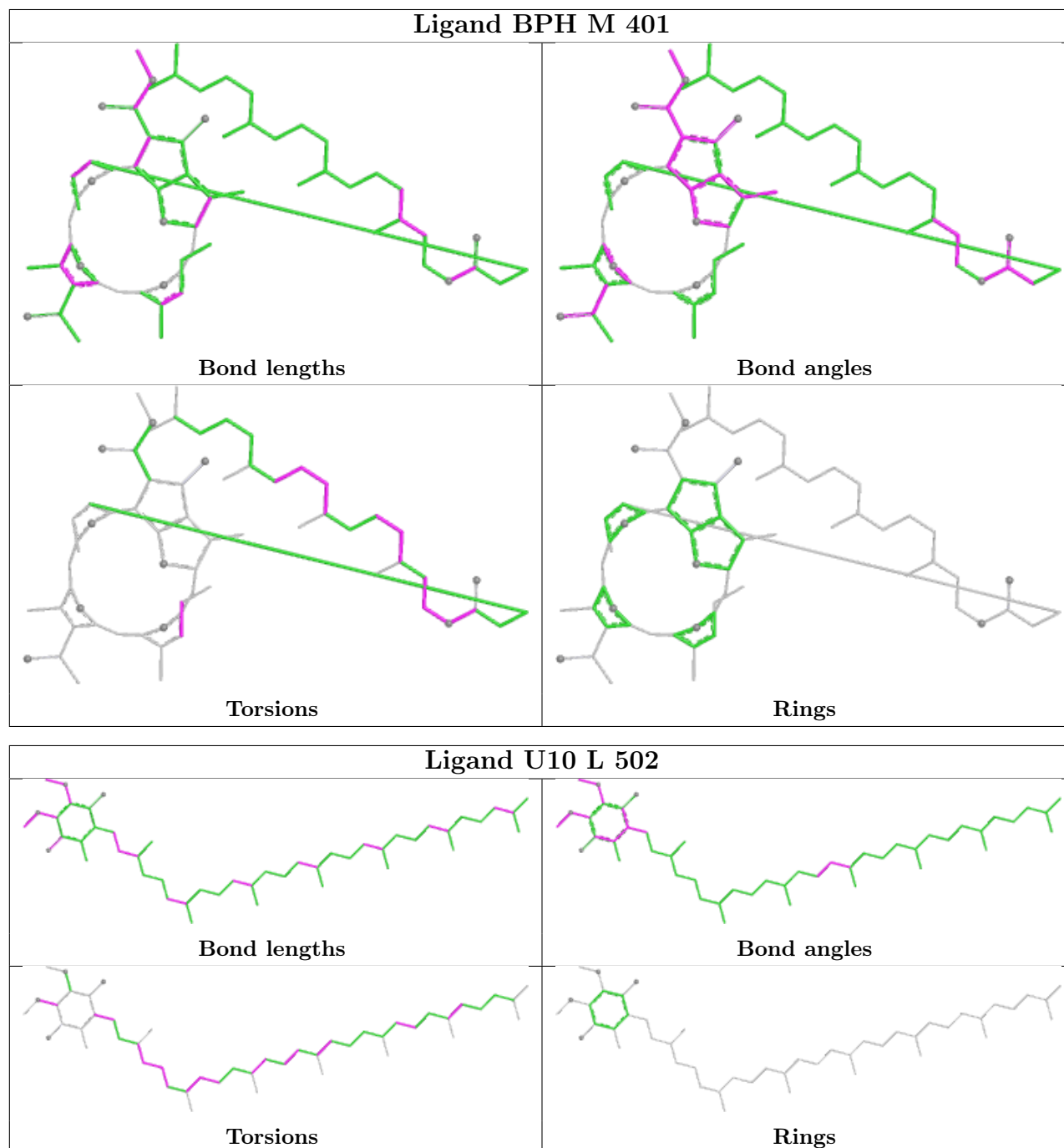
There are no ring outliers.

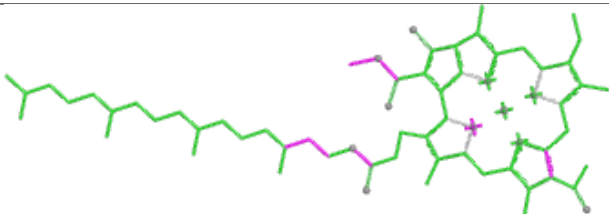
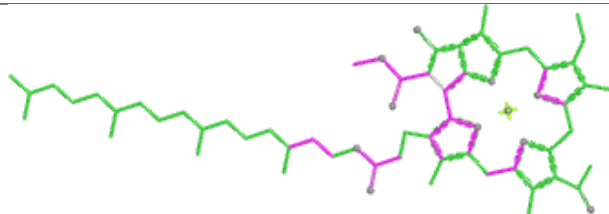
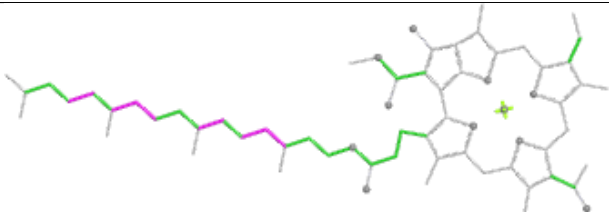
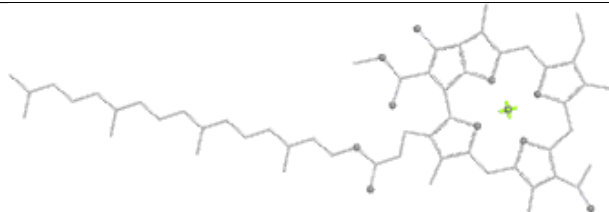
12 monomers are involved in 55 short contacts:

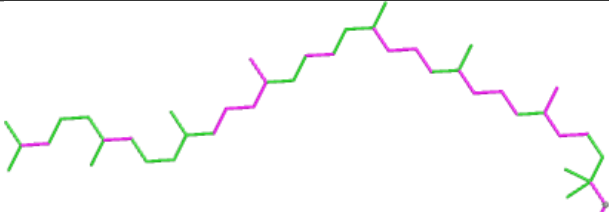
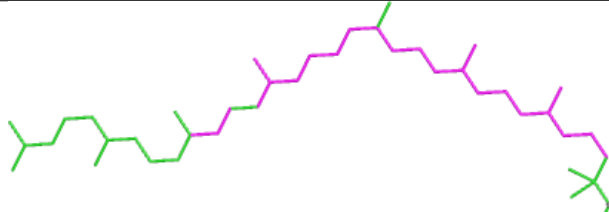
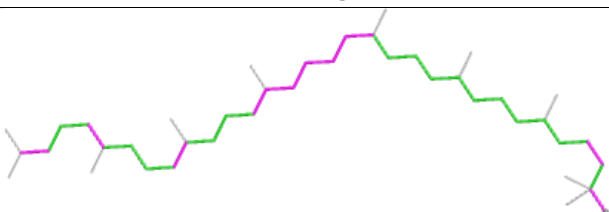
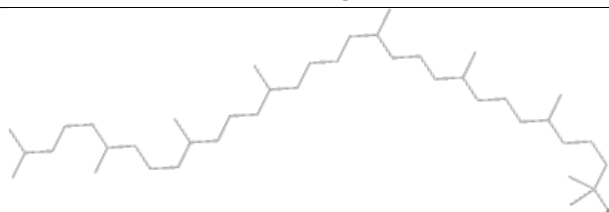
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	401	BPH	11	0
6	L	502	U10	6	0
4	M	802	BCL	8	0
7	H	702	LDA	2	0
9	M	800	PO4	1	0
10	M	600	SPO	1	0
6	M	501	U10	4	0
4	L	304	BCL	5	0
4	L	302	BCL	8	0
7	M	704	LDA	1	0
5	L	402	BPH	8	0
4	M	801	BCL	6	0

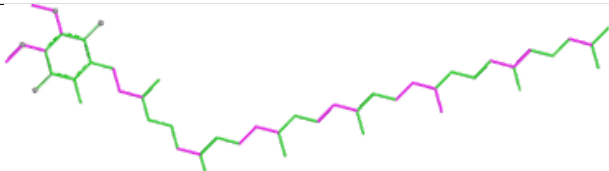
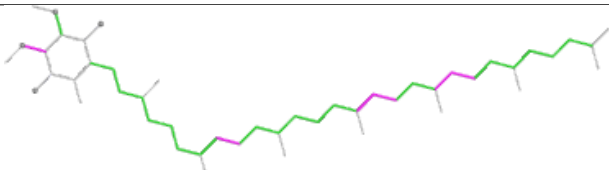
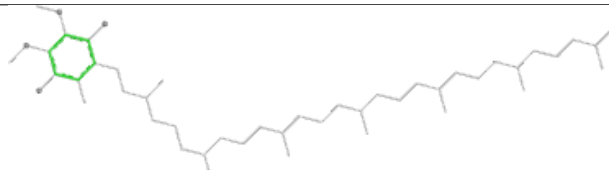
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

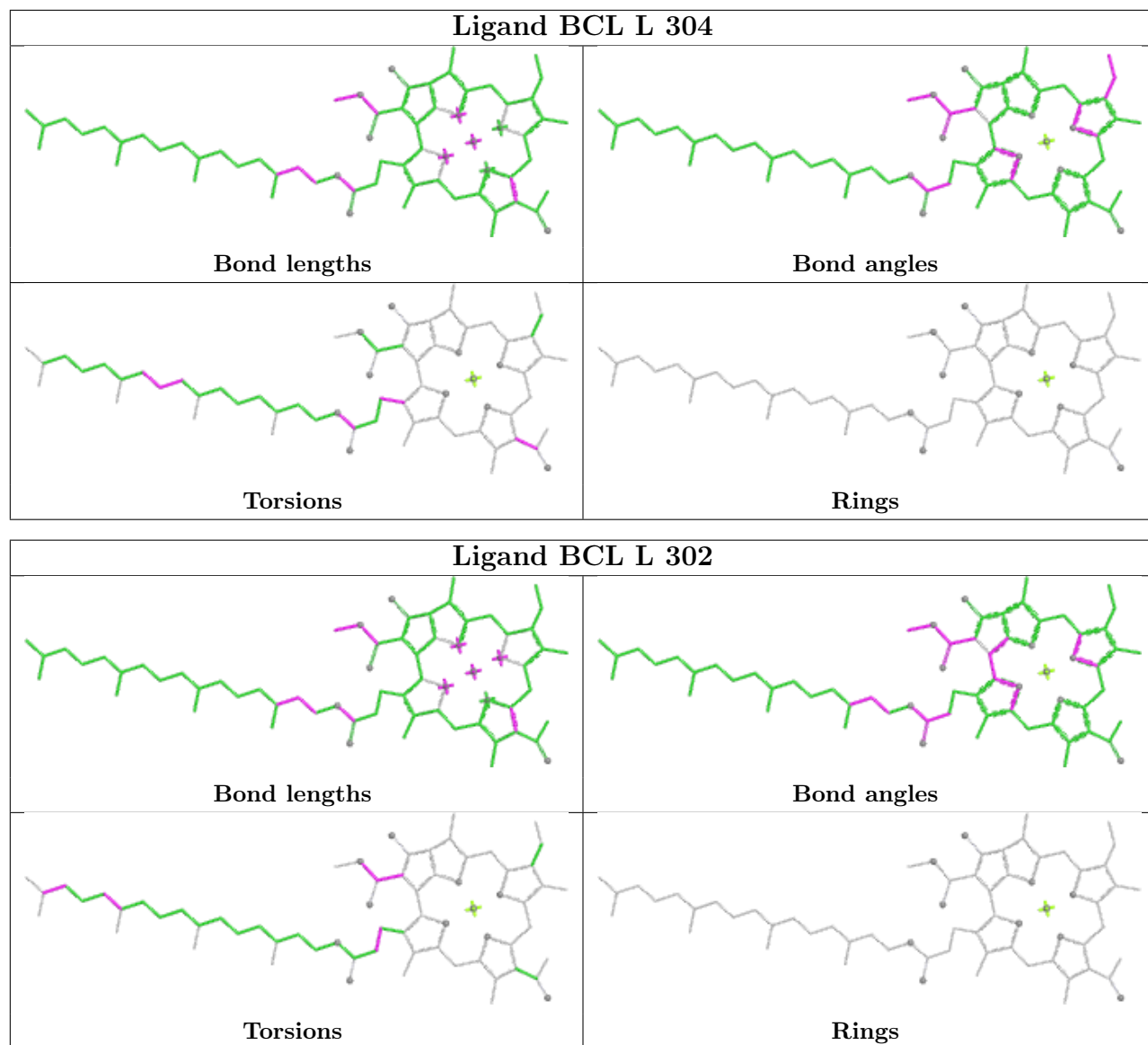
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

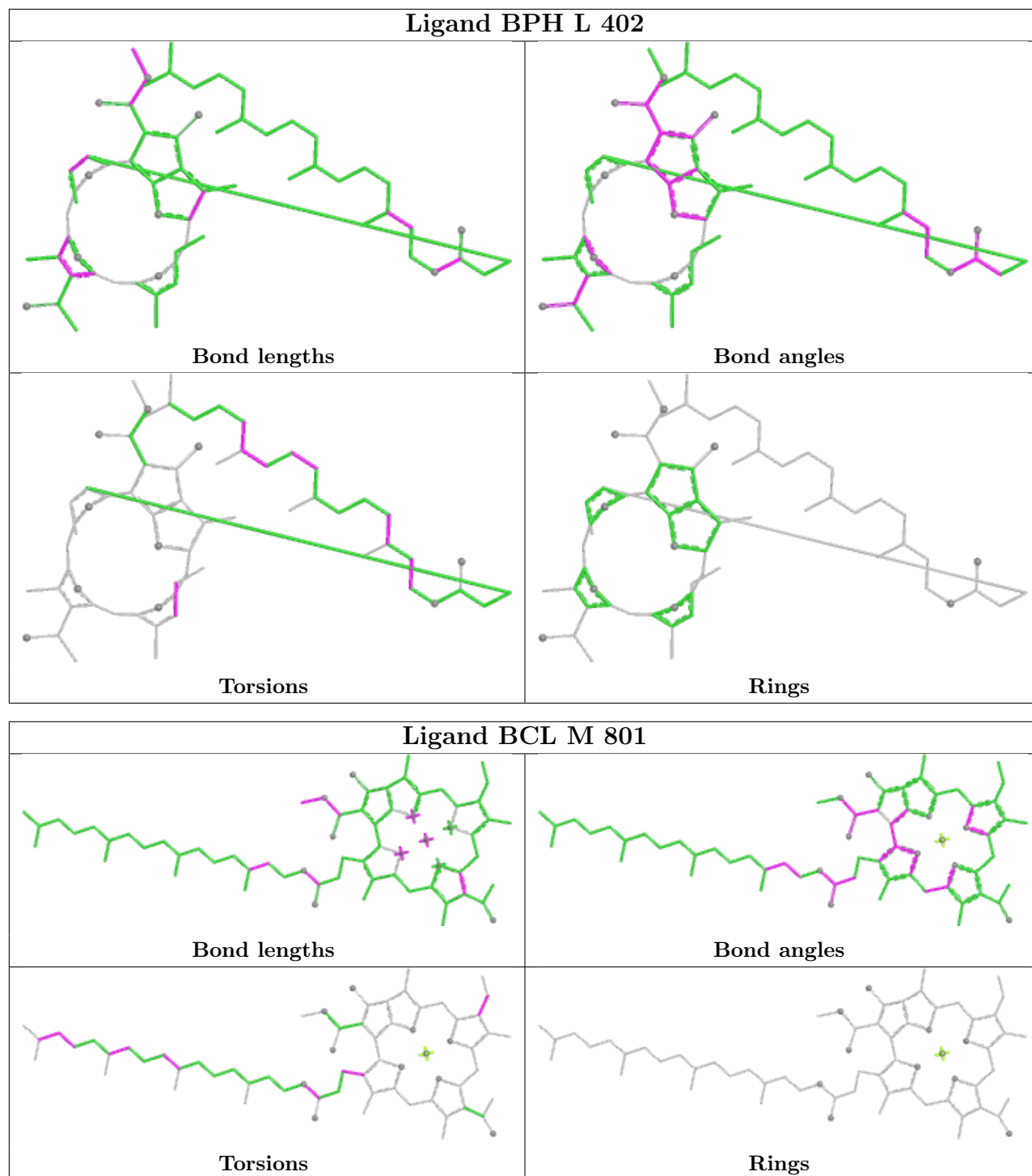


Ligand BCL M 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SPO M 600	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 M 501	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.