



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 1F6N / pdb_00001f6n
Title : CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CENTER PRO L209-> TYR FROM THE PHOTOSYNTHETIC PURPLE BACTERIUM RHODOBACTER SPHAEROIDES
Authors : Kuglstatter, A.; Ermler, U.; Michel, H.; Baciou, L.; Fritzsche, G.
Deposited on : 2000-06-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

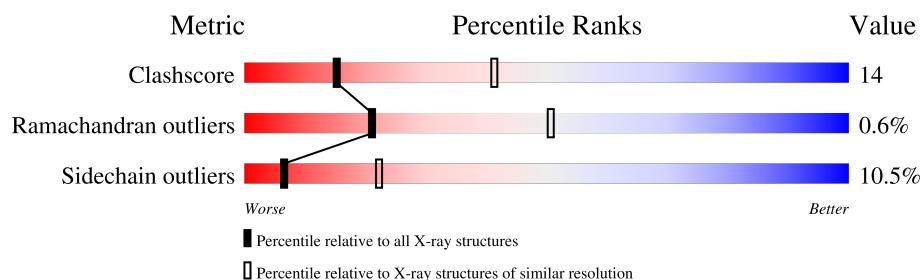
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	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	301	X	-	-	-
4	BCL	L	304	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7186 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
			2237	1511	355	363	8			

There is a discrepancy between the modelled and reference sequences:

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

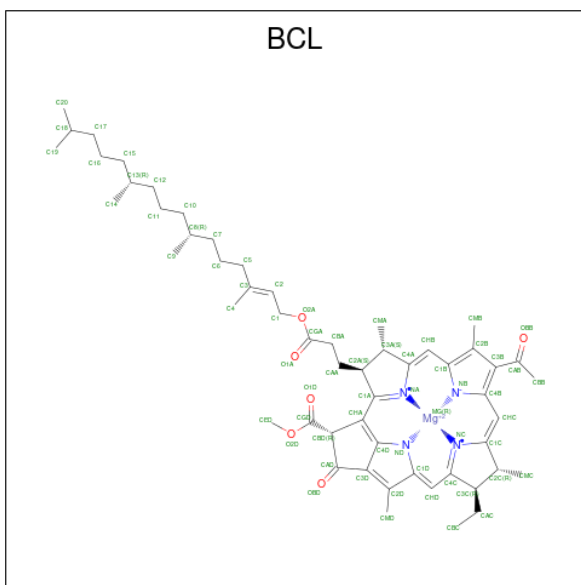
- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2404	1603	394	397	10			

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

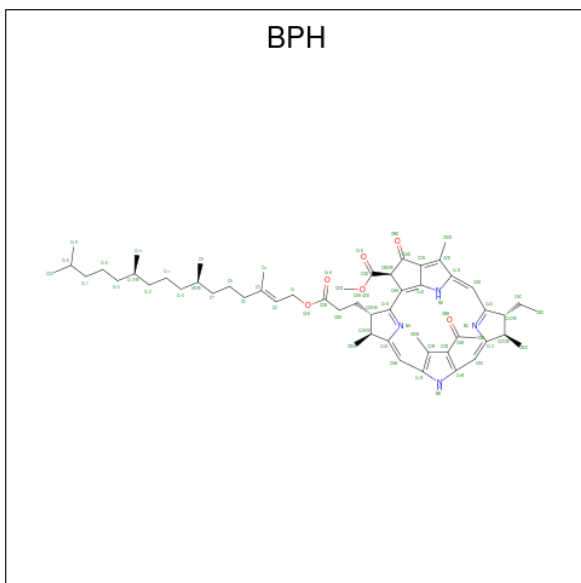
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



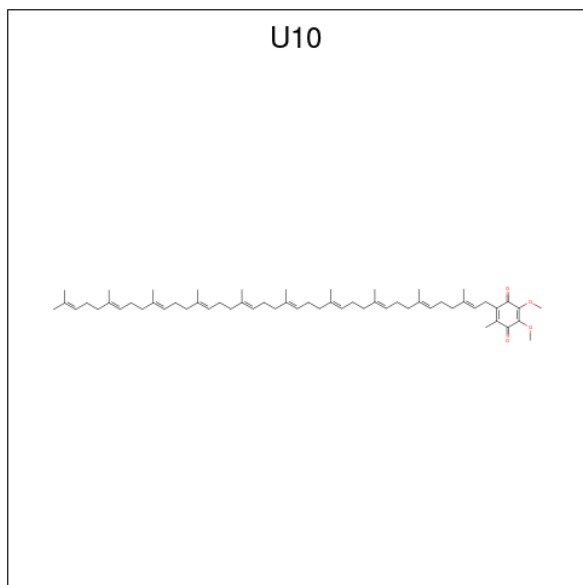
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



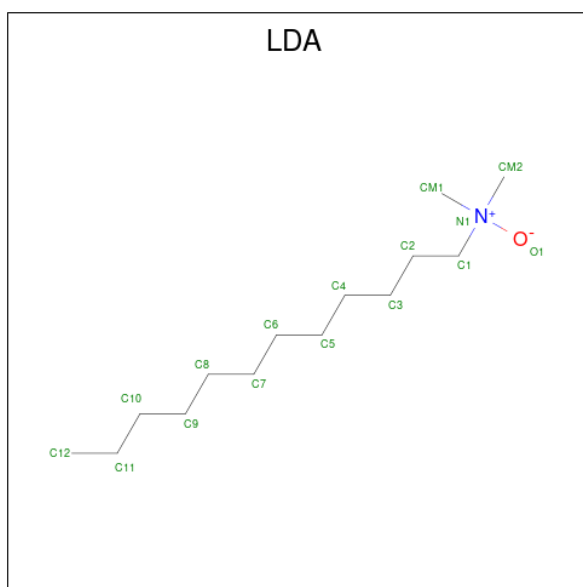
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



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: C₁₄H₃₁NO).



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	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).

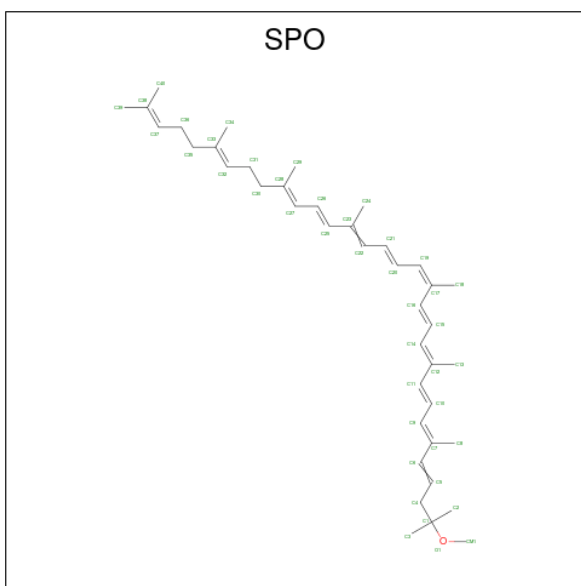
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- 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.

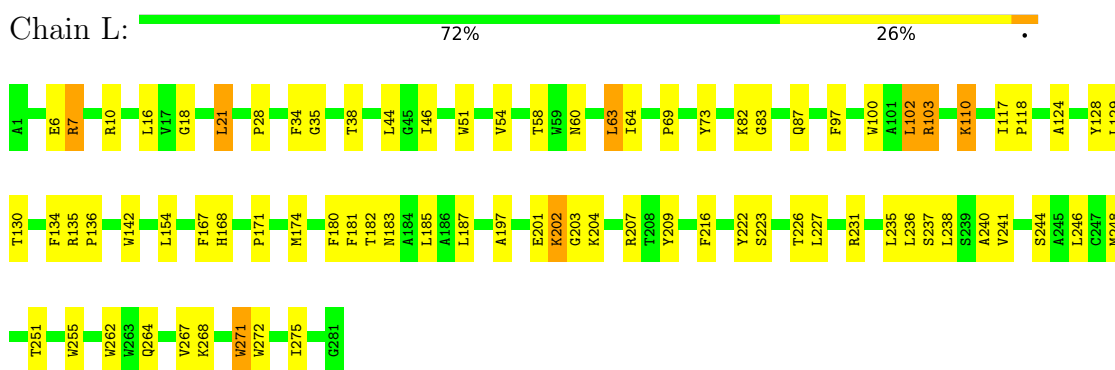
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	22	Total 22	O 22	0	0
11	M	27	Total 27	O 27	0	0
11	H	49	Total 49	O 49	0	0

3 Residue-property plots

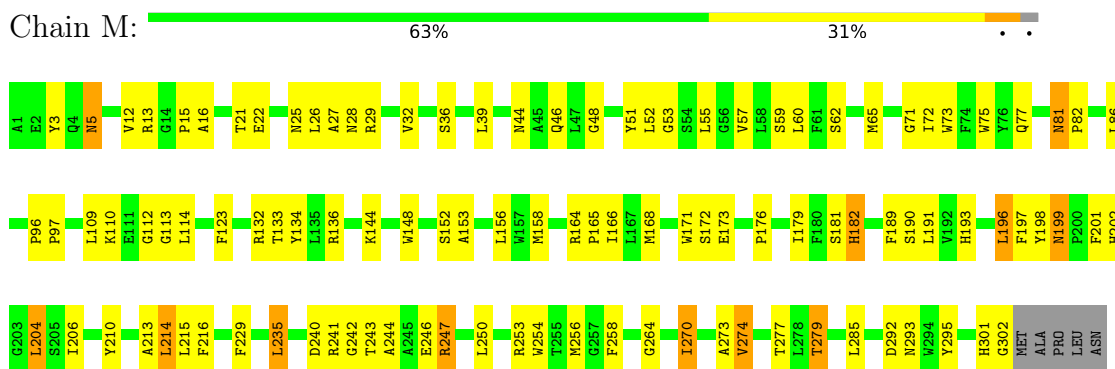
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

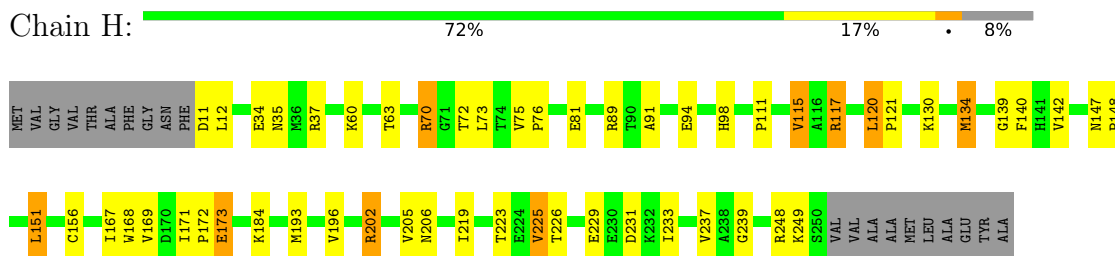
• Molecule 1: REACTION CENTER PROTEIN L CHAIN



• 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	141.53Å 141.53Å 187.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.1 (50.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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: SPO, FE, PO4, LDA, BCL, BPH, 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	0.56	0/2325	0.80	0/3181
2	M	0.56	0/2496	0.83	2/3407 (0.1%)
3	H	0.50	0/1877	0.85	0/2553
All	All	0.54	0/6698	0.83	2/9141 (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	3
2	M	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	81	ASN	CA-C-N	5.54	125.89	119.47
2	M	81	ASN	C-N-CA	5.54	125.89	119.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	103	ARG	Sidechain
1	L	216	PHE	Sidechain
1	L	73	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	M	198	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2237	0	2189	62	0
2	M	2404	0	2311	73	0
3	H	1829	0	1836	42	0
4	L	198	0	221	30	0
4	M	66	0	74	14	0
5	L	65	0	76	9	0
5	M	65	0	76	11	0
6	L	48	0	63	0	0
6	M	48	0	63	1	0
7	H	32	0	62	1	0
7	L	16	0	31	3	0
7	M	32	0	62	0	0
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	4	0
11	H	49	0	0	2	0
11	L	22	0	0	4	0
11	M	27	0	0	1	0
All	All	7186	0	7124	193	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 14.

All (193) 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:301:BCL:HBB2	4:L:301:BCL:HHC	1.40	1.02
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.42	1.01
4:L:302:BCL:HHC	4:L:302:BCL:HBB3	1.49	0.93
2:M:153:ALA:HB2	5:M:401:BPH:HAC1	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.59	0.83
4:L:302:BCL:HHC	4:L:302:BCL:CBB	2.10	0.81
4:L:304:BCL:HHC	4:L:304:BCL:HBB2	1.61	0.80
2:M:46:GLN:HE21	2:M:48:GLY:HA3	1.50	0.77
4:M:801:BCL:HBB2	4:M:801:BCL:HHC	1.65	0.76
4:M:801:BCL:HHC	4:M:801:BCL:CBB	2.14	0.76
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.68	0.75
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.69	0.75
1:L:271:TRP:H	1:L:271:TRP:CD1	2.05	0.74
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.68	0.73
1:L:202:LYS:HG3	1:L:203:GLY:H	1.55	0.72
11:L:704:HOH:O	2:M:253:ARG:HD3	1.89	0.72
1:L:124:ALA:HB2	5:L:402:BPH:HAC1	1.71	0.72
1:L:167:PHE:HB3	4:L:302:BCL:HMC3	1.72	0.71
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.09	0.71
2:M:243:THR:OG1	2:M:247:ARG:HD3	1.90	0.71
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.28	0.68
1:L:202:LYS:CG	1:L:203:GLY:H	2.07	0.68
3:H:233:ILE:O	3:H:237:VAL:HG12	1.94	0.66
5:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.77	0.66
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.77	0.66
4:L:301:BCL:H92	4:M:801:BCL:H192	1.78	0.65
2:M:256:MET:HE3	2:M:258:PHE:CE2	2.32	0.65
1:L:202:LYS:HG2	11:L:723:HOH:O	1.97	0.64
5:L:402:BPH:HBB3	5:L:402:BPH:CHC	2.25	0.64
1:L:231:ARG:HD3	2:M:5:ASN:O	1.98	0.63
5:M:401:BPH:HBB3	5:M:401:BPH:HHC	1.79	0.63
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.80	0.63
3:H:111:PRO:HB2	3:H:239:GLY:HA2	1.81	0.63
5:L:402:BPH:HHC	5:L:402:BPH:CBB	2.25	0.63
1:L:227:LEU:O	1:L:231:ARG:HG3	2.00	0.62
4:L:301:BCL:HHC	4:L:301:BCL:CBB	2.21	0.62
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.17	0.61
2:M:199:ASN:HD22	2:M:199:ASN:C	2.08	0.61
1:L:168:HIS:NE2	4:L:302:BCL:HBB2	2.15	0.61
3:H:156:CYS:HB3	3:H:206:ASN:O	2.01	0.59
1:L:241:VAL:HG21	5:L:402:BPH:HAC2	1.84	0.59
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.37	0.59
2:M:32:VAL:HG13	2:M:48:GLY:HA2	1.85	0.59
1:L:128:TYR:HD1	4:L:304:BCL:HBB1	1.67	0.59
7:L:703:LDA:HM21	11:H:747:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:70:ARG:HB2	11:H:746:HOH:O	2.02	0.58
1:L:18:GLY:O	1:L:21:LEU:HB2	2.04	0.58
2:M:243:THR:O	2:M:247:ARG:HG2	2.04	0.58
4:L:301:BCL:H71	5:M:401:BPH:HMB3	1.85	0.58
4:L:301:BCL:HED1	2:M:179:ILE:HG23	1.86	0.58
2:M:123:PHE:HE1	2:M:158:MET:HE1	1.67	0.58
2:M:172:SER:HB2	11:M:826:HOH:O	2.04	0.57
1:L:7:ARG:NH2	3:H:98:HIS:CD2	2.72	0.57
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.86	0.56
2:M:123:PHE:CE1	2:M:158:MET:HE1	2.39	0.56
2:M:13:ARG:O	3:H:140:PHE:HA	2.05	0.56
4:L:302:BCL:C1C	4:M:801:BCL:HBB3	2.36	0.56
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.88	0.55
3:H:115:VAL:HG22	3:H:117:ARG:HG2	1.89	0.55
1:L:202:LYS:HG3	1:L:203:GLY:N	2.21	0.55
1:L:130:THR:HA	1:L:134:PHE:HB2	1.89	0.55
2:M:153:ALA:CB	5:M:401:BPH:HAC1	2.32	0.55
1:L:6:GLU:HG2	1:L:10:ARG:HD2	1.87	0.55
2:M:25:ASN:HD21	2:M:27:ALA:HB3	1.70	0.55
1:L:69:PRO:HD3	1:L:83:GLY:O	2.07	0.55
2:M:197:PHE:HZ	4:M:801:BCL:HBB2	1.72	0.54
1:L:181:PHE:HB3	5:M:401:BPH:CBB	2.37	0.54
2:M:197:PHE:CZ	4:M:801:BCL:HBB2	2.42	0.54
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.76	0.54
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.42	0.54
3:H:202:ARG:HG2	3:H:202:ARG:NH2	2.22	0.54
1:L:35:GLY:O	1:L:38:THR:HG22	2.08	0.54
4:L:302:BCL:H52	4:L:304:BCL:HBB3	1.89	0.54
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.90	0.53
1:L:271:TRP:CD1	1:L:271:TRP:N	2.75	0.53
4:L:301:BCL:HBB3	4:M:801:BCL:H41	1.91	0.53
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.08	0.53
3:H:70:ARG:NH1	3:H:121:PRO:O	2.42	0.53
1:L:60:ASN:O	1:L:64:ILE:HG13	2.08	0.53
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.90	0.53
3:H:202:ARG:HG2	3:H:202:ARG:HH21	1.74	0.52
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.74	0.52
4:L:301:BCL:H72	4:M:801:BCL:H18	1.91	0.52
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.44	0.52
2:M:199:ASN:HD22	2:M:201:PHE:H	1.59	0.51
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:LYS:HG2	2:M:254:TRP:HZ3	1.75	0.51
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.93	0.51
3:H:142:VAL:HG21	3:H:147:ASN:CG	2.35	0.51
2:M:270:ILE:O	2:M:274:VAL:HB	2.11	0.51
1:L:209:TYR:CE2	3:H:173:GLU:HG3	2.46	0.51
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.93	0.51
1:L:209:TYR:CZ	3:H:173:GLU:HG3	2.45	0.50
2:M:190:SER:HB2	4:M:801:BCL:H3C	1.94	0.50
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.93	0.50
1:L:171:PRO:HA	1:L:174:MET:HG3	1.93	0.50
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.11	0.50
2:M:168:MET:HG3	2:M:173:GLU:HG3	1.93	0.49
2:M:240:ASP:O	3:H:117:ARG:NH2	2.45	0.49
1:L:197:ALA:CB	2:M:235:LEU:HD21	2.42	0.49
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.38	0.49
5:L:402:BPH:HMC3	2:M:213:ALA:CB	2.43	0.49
1:L:97:PHE:CE2	4:L:302:BCL:H121	2.48	0.49
3:H:34:GLU:O	3:H:37:ARG:HG3	2.13	0.48
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.95	0.48
2:M:15:PRO:HD3	3:H:139:GLY:HA3	1.95	0.48
5:L:402:BPH:HMC3	2:M:213:ALA:HB3	1.94	0.48
4:L:304:BCL:HBB2	4:L:304:BCL:CHC	2.38	0.48
2:M:134:TYR:CE2	2:M:144:LYS:HG3	2.49	0.47
7:L:703:LDA:H32	7:H:702:LDA:HM21	1.96	0.47
5:L:402:BPH:HMC2	2:M:214:LEU:N	2.28	0.47
2:M:51:TYR:O	2:M:132:ARG:NH1	2.48	0.47
1:L:223:SER:O	2:M:44:ASN:HB2	2.14	0.47
2:M:53:GLY:O	2:M:57:VAL:HG23	2.15	0.47
3:H:89:ARG:HD3	3:H:91:ALA:O	2.14	0.47
1:L:100:TRP:CH2	6:M:501:U10:H251	2.49	0.47
2:M:112:GLY:O	2:M:114:LEU:N	2.47	0.46
10:M:600:SPO:H5	10:M:600:SPO:HM13	1.96	0.46
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.81	0.46
2:M:25:ASN:HD22	2:M:28:ASN:ND2	2.14	0.46
3:H:75:VAL:HA	3:H:76:PRO:C	2.40	0.46
1:L:201:GLU:HB2	1:L:204:LYS:HD3	1.96	0.46
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.16	0.46
4:L:301:BCL:H41	4:L:301:BCL:H62	1.65	0.45
2:M:196:LEU:HD23	2:M:202:HIS:CD2	2.50	0.45
10:M:600:SPO:H131	10:M:600:SPO:H15	1.68	0.45
2:M:277:THR:HG21	5:M:401:BPH:HAC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:235:LEU:HA	2:M:235:LEU:HD12	1.71	0.45
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.52	0.45
1:L:51:TRP:O	1:L:54:VAL:HG22	2.17	0.45
5:M:401:BPH:HBA2	5:M:401:BPH:H3A	1.73	0.45
2:M:36:SER:HB3	2:M:39:LEU:HB2	1.99	0.45
5:M:401:BPH:H7C1	5:M:401:BPH:H4C1	1.99	0.45
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.99	0.44
2:M:81:ASN:HD22	2:M:82:PRO:HD2	1.83	0.44
1:L:128:TYR:CD1	4:L:304:BCL:HBB1	2.51	0.44
3:H:63:THR:HA	3:H:73:LEU:O	2.18	0.44
3:H:202:ARG:HH21	3:H:202:ARG:CG	2.30	0.44
3:H:169:VAL:HG23	3:H:171:ILE:HD12	1.99	0.44
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.99	0.44
1:L:187:LEU:HD23	2:M:273:ALA:HB2	2.00	0.44
2:M:189:PHE:O	2:M:193:HIS:HD2	2.01	0.44
1:L:28:PRO:HD3	7:L:703:LDA:O1	2.18	0.43
3:H:70:ARG:NH1	3:H:120:LEU:HB3	2.33	0.43
4:L:302:BCL:HBB3	4:M:801:BCL:HAC2	1.99	0.43
1:L:183:ASN:ND2	1:L:237:SER:OG	2.52	0.43
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.53	0.43
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.01	0.43
2:M:62:SER:HA	2:M:65:MET:HB2	2.01	0.43
3:H:120:LEU:HD22	3:H:120:LEU:N	2.33	0.43
3:H:130:LYS:NZ	3:H:172:PRO:HG2	2.34	0.43
4:L:302:BCL:NC	4:M:801:BCL:HBB3	2.33	0.43
3:H:34:GLU:OE2	3:H:37:ARG:NH2	2.52	0.43
1:L:103:ARG:HG3	11:L:709:HOH:O	2.19	0.43
4:L:301:BCL:HBC3	4:L:301:BCL:CHD	2.48	0.43
3:H:37:ARG:NH1	3:H:60:LYS:O	2.51	0.43
3:H:134:MET:HE2	3:H:167:ILE:HB	2.01	0.43
3:H:248:ARG:CZ	3:H:248:ARG:HB2	2.48	0.43
1:L:275:ILE:H	1:L:275:ILE:HD12	1.84	0.43
1:L:275:ILE:HD12	1:L:275:ILE:N	2.33	0.43
2:M:55:LEU:HD12	2:M:55:LEU:HA	1.90	0.42
5:M:401:BPH:HBB3	5:M:401:BPH:CHC	2.48	0.42
5:M:401:BPH:H4C1	5:M:401:BPH:C7	2.48	0.42
2:M:152:SER:CB	2:M:274:VAL:HG22	2.49	0.42
1:L:222:TYR:CG	1:L:223:SER:N	2.87	0.42
3:H:121:PRO:HB3	3:H:225:VAL:O	2.18	0.42
2:M:16:ALA:HB1	2:M:32:VAL:HG21	2.01	0.42
2:M:73:TRP:HE1	2:M:77:GLN:NE2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.50	0.42
1:L:248:MET:HG3	4:L:302:BCL:HED2	2.01	0.42
3:H:196:VAL:HG12	3:H:205:VAL:HG22	2.02	0.42
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.02	0.41
1:L:248:MET:CG	4:L:302:BCL:HED2	2.51	0.41
2:M:73:TRP:NE1	2:M:77:GLN:NE2	2.68	0.41
2:M:182:HIS:CE1	10:M:600:SPO:H181	2.55	0.41
1:L:10:ARG:NH1	11:L:712:HOH:O	2.52	0.41
1:L:187:LEU:HB2	2:M:216:PHE:CD2	2.55	0.41
2:M:71:GLY:HA3	10:M:600:SPO:H42	2.03	0.41
2:M:46:GLN:HG2	2:M:48:GLY:N	2.36	0.41
4:L:304:BCL:H91	4:L:304:BCL:H111	1.80	0.41
4:M:801:BCL:CBB	4:M:801:BCL:CHC	2.88	0.41
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.56	0.41
1:L:244:SER:OG	4:L:302:BCL:HMA2	2.21	0.41
4:L:301:BCL:HBB3	4:M:801:BCL:C4	2.51	0.41
2:M:96:PRO:HD3	2:M:176:PRO:HB3	2.02	0.41
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.56	0.41
1:L:7:ARG:HH21	3:H:98:HIS:CG	2.38	0.40
1:L:63:LEU:HD13	1:L:63:LEU:HA	1.93	0.40
4:L:301:BCL:H143	4:M:801:BCL:H171	2.03	0.40
4:L:304:BCL:OBD	2:M:206:ILE:HD12	2.21	0.40
1:L:209:TYR:CE1	1:L:226:THR:HG23	2.56	0.40
4:L:301:BCL:CBB	4:L:301:BCL:CHC	2.91	0.40
2:M:302:GLY:HA2	3:H:11:ASP:OD2	2.22	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%)	263 (94%)	15 (5%)	1 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	300/307 (98%)	283 (94%)	13 (4%)	4 (1%)	9	31
3	H	238/260 (92%)	228 (96%)	10 (4%)	0	100	100
All	All	817/848 (96%)	774 (95%)	38 (5%)	5 (1%)	21	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	113	GLY
2	M	301	HIS
1	L	202	LYS
2	M	5	ASN
2	M	22	GLU

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%)	200 (91%)	20 (9%)	9	28
2	M	235/240 (98%)	205 (87%)	30 (13%)	4	15
3	H	195/208 (94%)	177 (91%)	18 (9%)	8	27
All	All	650/668 (97%)	582 (90%)	68 (10%)	6	22

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	16	LEU
1	L	21	LEU
1	L	44	LEU
1	L	46	ILE
1	L	58	THR
1	L	63	LEU
1	L	82	LYS
1	L	102	LEU

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Mol	Chain	Res	Type
1	L	110	LYS
1	L	129	LEU
1	L	154	LEU
1	L	185	LEU
1	L	207	ARG
1	L	235	LEU
1	L	238	LEU
1	L	246	LEU
1	L	251	THR
1	L	268	LYS
1	L	271	TRP
2	M	12	VAL
2	M	29	ARG
2	M	52	LEU
2	M	59	SER
2	M	60	LEU
2	M	72	ILE
2	M	75	TRP
2	M	86	LEU
2	M	109	LEU
2	M	110	LYS
2	M	133	THR
2	M	136	ARG
2	M	156	LEU
2	M	166	ILE
2	M	181	SER
2	M	182	HIS
2	M	191	LEU
2	M	196	LEU
2	M	199	ASN
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	270	ILE
2	M	274	VAL
2	M	279	THR
2	M	285	LEU
2	M	292	ASP
3	H	12	LEU

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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	120	LEU
3	H	134	MET
3	H	151	LEU
3	H	173	GLU
3	H	184	LYS
3	H	193	MET
3	H	202	ARG
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	159	ASN
1	L	173	HIS
1	L	183	ASN
2	M	25	ASN
2	M	44	ASN
2	M	77	GLN
2	M	81	ASN
2	M	193	HIS
2	M	199	ASN
2	M	299	GLN
3	H	32	GLN
3	H	98	HIS
3	H	128	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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$
4	BCL	L	304	1	69,74,74	2.03	11 (15%)	79,115,115	3.33	17 (21%)
5	BPH	M	401	-	59,70,70	1.89	13 (22%)	59,101,101	2.39	14 (23%)
7	LDA	H	705	-	13,15,15	2.28	2 (15%)	14,17,17	0.46	0
6	U10	M	501	-	48,48,63	2.16	15 (31%)	60,61,79	1.03	4 (6%)
5	BPH	L	402	-	59,70,70	1.72	9 (15%)	59,101,101	2.38	11 (18%)
7	LDA	L	703	-	13,15,15	2.11	1 (7%)	14,17,17	0.59	0
7	LDA	H	702	-	13,15,15	2.87	2 (15%)	14,17,17	0.57	0
10	SPO	M	600	-	41,41,41	2.99	20 (48%)	47,50,50	2.33	14 (29%)
4	BCL	L	301	2	69,74,74	1.33	7 (10%)	79,115,115	1.89	9 (11%)
7	LDA	M	704	-	13,15,15	2.55	2 (15%)	14,17,17	0.54	0
4	BCL	M	801	2	69,74,74	1.25	7 (10%)	79,115,115	1.88	12 (15%)
6	U10	L	502	-	48,48,63	1.84	16 (33%)	60,61,79	1.15	6 (10%)
7	LDA	M	701	-	13,15,15	2.35	2 (15%)	14,17,17	0.48	0
9	PO4	M	800	-	4,4,4	1.99	1 (25%)	6,6,6	0.54	0
4	BCL	L	302	1	69,74,74	1.39	9 (13%)	79,115,115	1.75	8 (10%)

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
4	BCL	L	304	1	1/1/21/25	16/41/137/137	-
5	BPH	M	401	-	-	19/37/105/105	0/5/6/6
7	LDA	H	705	-	-	4/13/13/13	-
6	U10	M	501	-	-	4/45/69/87	0/1/1/1
5	BPH	L	402	-	-	7/37/105/105	0/5/6/6
7	LDA	L	703	-	-	2/13/13/13	-
7	LDA	H	702	-	-	5/13/13/13	-
10	SPO	M	600	-	-	19/47/47/47	-
4	BCL	L	301	2	1/1/21/25	9/41/137/137	-
7	LDA	M	704	-	-	1/13/13/13	-
4	BCL	M	801	2	-	7/41/137/137	-
6	U10	L	502	-	-	12/45/69/87	0/1/1/1
7	LDA	M	701	-	-	2/13/13/13	-
4	BCL	L	302	1	-	8/41/137/137	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	BCL	MG-NA	9.71	2.29	2.06
7	H	702	LDA	O1-N1	-8.54	1.21	1.42
10	M	600	SPO	C6-C5	8.06	1.54	1.32
10	M	600	SPO	C10-C11	7.89	1.55	1.34
7	M	701	LDA	O1-N1	-7.72	1.23	1.42
7	H	705	LDA	O1-N1	-7.71	1.23	1.42
7	M	704	LDA	O1-N1	-7.55	1.23	1.42
7	L	703	LDA	O1-N1	-7.46	1.23	1.42
10	M	600	SPO	C15-C16	6.48	1.51	1.34
4	L	304	BCL	O2D-CGD	6.39	1.48	1.33
6	M	501	U10	C7-C8	-6.39	1.40	1.50
4	L	302	BCL	O2D-CGD	5.94	1.47	1.33
6	M	501	U10	O3-C3	5.87	1.50	1.36
7	H	702	LDA	C1-N1	-5.85	1.45	1.51
5	L	402	BPH	C1D-C2D	5.72	1.45	1.39
5	L	402	BPH	C3A-C2A	-5.51	1.49	1.54
5	M	401	BPH	C3A-C2A	-5.24	1.50	1.54
7	M	704	LDA	C1-N1	-5.21	1.46	1.51
5	M	401	BPH	C1D-C2D	5.12	1.45	1.39
10	M	600	SPO	C26-C25	5.06	1.47	1.34
5	M	401	BPH	O2A-CGA	4.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	402	BPH	C1B-C2B	4.84	1.44	1.39
10	M	600	SPO	C21-C20	4.81	1.49	1.36
4	L	301	BCL	MG-NA	4.78	2.17	2.06
4	L	304	BCL	MG-ND	-4.60	1.96	2.05
4	M	801	BCL	MG-NA	4.60	2.17	2.06
5	M	401	BPH	C2C-C3C	-4.59	1.50	1.54
4	L	301	BCL	O2A-CGA	4.56	1.46	1.33
4	L	302	BCL	MG-NA	4.55	2.17	2.06
4	L	304	BCL	MG-NB	4.55	2.14	2.05
4	M	801	BCL	O2D-CGD	4.52	1.44	1.33
4	L	304	BCL	C3B-C4B	4.43	1.49	1.41
5	M	401	BPH	C1B-C2B	4.18	1.44	1.39
5	M	401	BPH	O2D-CGD	4.17	1.43	1.33
6	L	502	U10	O3-C3	3.96	1.46	1.36
5	L	402	BPH	O2D-CGD	3.92	1.42	1.33
6	M	501	U10	O4-C4	3.90	1.46	1.36
4	L	304	BCL	O2A-CGA	3.87	1.44	1.33
4	L	302	BCL	O2D-CED	-3.75	1.36	1.45
5	L	402	BPH	O2A-CGA	3.74	1.44	1.33
5	M	401	BPH	O2D-CED	-3.74	1.37	1.45
10	M	600	SPO	O1-CM1	3.63	1.54	1.43
6	M	501	U10	O4-C4M	-3.58	1.37	1.45
4	L	304	BCL	CHB-C1B	-3.36	1.31	1.39
7	M	701	LDA	C1-N1	-3.35	1.48	1.51
6	L	502	U10	O4-C4	3.29	1.44	1.36
10	M	600	SPO	C25-C23	-3.25	1.39	1.46
4	M	801	BCL	C3B-C4B	3.22	1.47	1.41
6	M	501	U10	O3-C3M	-3.22	1.38	1.45
6	L	502	U10	C18-C19	3.13	1.40	1.33
4	L	304	BCL	C2-C3	3.13	1.40	1.33
4	L	301	BCL	O2D-CED	-3.10	1.38	1.45
10	M	600	SPO	C11-C12	-3.09	1.39	1.46
6	M	501	U10	C13-C14	3.09	1.40	1.33
10	M	600	SPO	C31-C32	-3.08	1.41	1.50
6	L	502	U10	C23-C24	3.04	1.40	1.33
6	M	501	U10	C28-C29	3.04	1.40	1.33
10	M	600	SPO	C16-C17	-2.98	1.39	1.46
6	L	502	U10	O3-C3M	-2.98	1.38	1.45
6	M	501	U10	C33-C34	2.97	1.39	1.33
5	L	402	BPH	O2D-CED	-2.96	1.38	1.45
4	L	301	BCL	O2D-CGD	2.96	1.40	1.33
6	M	501	U10	C38-C39	2.96	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	BCL	C2-C3	2.94	1.39	1.33
4	L	304	BCL	C1B-NB	-2.93	1.34	1.37
6	L	502	U10	C28-C29	2.93	1.39	1.33
4	L	301	BCL	C3B-C4B	2.89	1.46	1.41
5	M	401	BPH	C2-C3	2.87	1.39	1.33
6	M	501	U10	C18-C19	2.83	1.39	1.33
6	L	502	U10	C13-C14	2.81	1.39	1.33
5	L	402	BPH	C2-C3	2.81	1.39	1.33
10	M	600	SPO	C10-C9	2.79	1.51	1.43
6	M	501	U10	C23-C24	2.79	1.39	1.33
4	L	302	BCL	C1-C2	-2.76	1.41	1.49
6	L	502	U10	C16-C14	2.76	1.57	1.51
6	L	502	U10	C33-C34	2.75	1.39	1.33
4	M	801	BCL	O2A-CGA	2.74	1.41	1.33
9	M	800	PO4	P-O3	-2.74	1.46	1.54
4	L	302	BCL	O2A-CGA	2.72	1.41	1.33
5	M	401	BPH	C3B-C4B	2.70	1.45	1.41
10	M	600	SPO	C6-C7	-2.67	1.40	1.46
10	M	600	SPO	C32-C33	2.66	1.39	1.33
7	H	705	LDA	C1-N1	-2.66	1.48	1.51
6	L	502	U10	C7-C8	-2.66	1.46	1.50
5	M	401	BPH	C3B-C2B	-2.64	1.35	1.39
4	L	304	BCL	CHB-C4A	-2.64	1.31	1.37
4	L	302	BCL	C3B-C4B	2.60	1.46	1.41
6	L	502	U10	C8-C9	2.60	1.39	1.33
10	M	600	SPO	C37-C38	2.58	1.40	1.32
4	M	801	BCL	MG-ND	-2.56	2.00	2.05
6	L	502	U10	C38-C39	2.56	1.40	1.32
4	L	301	BCL	MG-ND	-2.56	2.00	2.05
6	M	501	U10	C8-C9	2.55	1.38	1.33
4	M	801	BCL	O2D-CED	-2.55	1.39	1.45
6	L	502	U10	C20-C19	2.54	1.56	1.50
4	M	801	BCL	C2-C3	2.49	1.38	1.33
4	L	302	BCL	C2-C3	2.49	1.38	1.33
10	M	600	SPO	O1-C1	2.46	1.55	1.41
5	L	402	BPH	C3B-C2B	-2.44	1.35	1.39
5	L	402	BPH	C3B-C4B	2.43	1.45	1.41
6	L	502	U10	O4-C4M	-2.43	1.39	1.45
10	M	600	SPO	C8-C7	2.43	1.55	1.50
10	M	600	SPO	C15-C14	2.41	1.50	1.43
6	M	501	U10	C31-C29	2.34	1.56	1.51
10	M	600	SPO	C26-C27	2.33	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	401	BPH	CHA-CBD	2.26	1.54	1.51
6	M	501	U10	C15-C14	2.17	1.56	1.50
6	M	501	U10	C36-C34	2.15	1.55	1.51
5	M	401	BPH	C3D-C4D	2.13	1.44	1.41
10	M	600	SPO	C40-C38	2.13	1.56	1.50
5	M	401	BPH	C5-C3	2.12	1.55	1.51
4	L	304	BCL	C4B-NB	-2.11	1.35	1.37
4	L	302	BCL	MG-ND	-2.11	2.01	2.05
10	M	600	SPO	C39-C38	2.07	1.56	1.50
6	L	502	U10	C15-C14	2.05	1.55	1.50
4	L	302	BCL	C4-C3	2.03	1.55	1.50
6	L	502	U10	C27-C28	-2.00	1.44	1.50

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	CHB-C4A-NA	-15.84	101.53	124.40
4	L	304	BCL	CHB-C1B-NB	-13.71	103.48	124.05
5	L	402	BPH	O2D-CGD-CBD	12.37	124.53	110.95
5	M	401	BPH	O2D-CGD-CBD	11.71	123.82	110.95
4	L	304	BCL	C4A-NA-C1A	8.88	110.73	106.68
4	L	301	BCL	C4A-NA-C1A	8.15	110.40	106.68
4	L	302	BCL	C4A-NA-C1A	8.07	110.36	106.68
4	L	304	BCL	O2D-CGD-CBD	7.96	125.15	111.23
10	M	600	SPO	C15-C14-C12	-7.59	116.63	127.28
4	M	801	BCL	C4A-NA-C1A	7.42	110.06	106.68
5	M	401	BPH	O1D-CGD-CBD	-7.38	113.53	124.72
5	L	402	BPH	O1D-CGD-CBD	-7.31	113.64	124.72
4	L	301	BCL	O2D-CGD-CBD	7.24	123.89	111.23
4	L	304	BCL	C1C-NC-C4C	6.98	109.86	106.68
4	M	801	BCL	C1C-NC-C4C	6.94	109.85	106.68
4	L	302	BCL	C1C-NC-C4C	6.89	109.82	106.68
4	M	801	BCL	O2D-CGD-CBD	6.75	123.03	111.23
4	L	304	BCL	O1D-CGD-CBD	-6.23	112.22	124.52
4	L	301	BCL	C1C-NC-C4C	6.11	109.47	106.68
4	L	304	BCL	C1-C2-C3	5.69	135.52	126.20
5	M	401	BPH	C4D-CHA-CBD	-5.65	105.74	108.45
10	M	600	SPO	C26-C27-C28	-5.53	119.91	127.69
5	L	402	BPH	C4D-CHA-CBD	-5.47	105.83	108.45
4	L	301	BCL	O1D-CGD-CBD	-5.39	113.89	124.52
4	L	302	BCL	O2D-CGD-CBD	5.07	120.10	111.23
4	M	801	BCL	O1D-CGD-CBD	-5.01	114.64	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	600	SPO	C4-C5-C6	-4.93	117.99	124.91
4	L	304	BCL	CHB-C1B-C2B	4.75	141.22	127.43
4	L	304	BCL	O2A-CGA-CBA	4.45	125.40	111.83
10	M	600	SPO	C20-C19-C17	-4.43	121.07	127.28
4	L	304	BCL	C2A-C1A-CHA	4.39	131.49	123.87
4	L	301	BCL	C1-C2-C3	3.78	132.39	126.20
10	M	600	SPO	C20-C21-C22	-3.73	115.88	123.52
5	M	401	BPH	O2A-CGA-CBA	3.72	123.18	111.83
10	M	600	SPO	C15-C16-C17	-3.71	116.20	126.36
4	M	801	BCL	O2A-CGA-CBA	3.67	123.01	111.83
10	M	600	SPO	C25-C23-C22	-3.64	113.28	119.01
5	L	402	BPH	O2A-CGA-CBA	3.63	122.91	111.83
10	M	600	SPO	C21-C22-C23	-3.60	122.23	127.28
5	L	402	BPH	OBD-CAD-CBD	-3.44	120.77	125.82
4	L	302	BCL	O2A-CGA-CBA	3.41	122.22	111.83
4	L	302	BCL	O1D-CGD-CBD	-3.37	117.88	124.52
4	L	304	BCL	O2A-CGA-O1A	-3.28	115.43	123.63
10	M	600	SPO	C6-C7-C9	-3.23	113.92	119.01
5	M	401	BPH	OBD-CAD-CBD	-3.23	121.08	125.82
10	M	600	SPO	C8-C7-C6	3.19	122.96	118.09
4	L	304	BCL	CHA-C1A-NA	-3.15	119.26	126.39
4	L	302	BCL	CED-O2D-CGD	3.06	122.86	115.92
5	M	401	BPH	C1B-NB-C4B	-3.05	104.36	108.82
4	L	301	BCL	O2A-CGA-CBA	3.03	121.08	111.83
4	L	304	BCL	C2B-C1B-NB	3.03	113.47	110.33
6	M	501	U10	C7-C8-C9	2.93	131.88	126.83
4	L	304	BCL	CHC-C1C-NC	2.88	128.55	124.40
5	M	401	BPH	CED-O2D-CGD	2.87	122.42	115.92
5	L	402	BPH	C1B-NB-C4B	-2.75	104.81	108.82
5	M	401	BPH	CMD-C2D-C3D	2.69	130.06	124.68
4	M	801	BCL	C1-C2-C3	2.63	130.51	126.20
4	L	302	BCL	O2A-CGA-O1A	-2.60	117.11	123.63
5	M	401	BPH	OBB-CAB-C3B	2.60	124.33	119.99
6	L	502	U10	C3M-O3-C3	2.58	125.53	116.47
4	L	304	BCL	CED-O2D-CGD	2.53	121.65	115.92
5	M	401	BPH	O2A-CGA-O1A	-2.51	117.34	123.63
5	L	402	BPH	C1-C2-C3	2.51	130.31	126.20
4	L	304	BCL	CMB-C2B-C1B	2.48	129.19	125.42
4	L	304	BCL	CAB-C3B-C2B	2.43	132.79	127.74
5	M	401	BPH	C4D-ND-C1D	-2.42	105.97	108.87
4	M	801	BCL	C4D-CHA-C1A	2.42	124.13	121.24
5	L	402	BPH	C4D-ND-C1D	-2.41	105.98	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	O2A-CGA-O1A	-2.38	117.67	123.63
6	M	501	U10	C4M-O4-C4	2.33	124.66	116.47
4	M	801	BCL	CED-O2D-CGD	2.31	121.15	115.92
10	M	600	SPO	C10-C9-C7	-2.28	124.08	127.28
5	L	402	BPH	CED-O2D-CGD	2.27	121.07	115.92
4	M	801	BCL	O2A-CGA-O1A	-2.26	117.97	123.63
5	M	401	BPH	C1-C2-C3	2.26	129.90	126.20
4	M	801	BCL	CHB-C1B-NB	2.23	127.40	124.05
4	L	301	BCL	C2A-C1A-CHA	2.23	127.74	123.87
4	L	302	BCL	C1-C2-C3	2.21	129.82	126.20
6	L	502	U10	C7-C6-C1	-2.21	121.10	124.89
6	L	502	U10	C32-C33-C34	2.20	132.66	127.62
5	M	401	BPH	C3D-C4D-ND	2.20	110.53	107.71
10	M	600	SPO	C10-C11-C12	-2.17	120.40	126.36
5	L	402	BPH	C3D-C4D-ND	2.14	110.45	107.71
5	M	401	BPH	CMA-C3A-C4A	-2.13	110.01	114.61
6	L	502	U10	C7-C8-C9	2.13	130.49	126.83
6	L	502	U10	C6-C1-C2	2.13	120.85	119.17
4	M	801	BCL	CAC-C3C-C4C	-2.08	107.96	112.58
10	M	600	SPO	C13-C12-C11	2.08	121.26	118.09
4	L	301	BCL	CAC-C3C-C4C	-2.07	107.98	112.58
4	M	801	BCL	C3A-C2A-C1A	2.06	104.43	101.34
6	L	502	U10	C22-C23-C24	2.06	132.33	127.62
4	L	301	BCL	C4D-CHA-C1A	2.05	123.69	121.24
10	M	600	SPO	C24-C23-C25	2.04	121.20	118.09
6	M	501	U10	C12-C13-C14	2.03	132.27	127.62
6	M	501	U10	C6-C1-C2	2.01	120.76	119.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	301	BCL	C8
4	L	304	BCL	C13

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	BCL	CHA-CBD-CGD-O1D
4	L	301	BCL	CHA-CBD-CGD-O2D
4	L	304	BCL	CBD-CGD-O2D-CED
4	L	304	BCL	O2A-C1-C2-C3
4	L	304	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
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	M	501	U10	C24-C26-C27-C28
6	M	501	U10	C29-C31-C32-C33
7	L	703	LDA	C2-C1-N1-CM2
7	H	702	LDA	C2-C1-N1-O1
7	H	702	LDA	C2-C1-N1-CM1
7	H	702	LDA	C2-C1-N1-CM2
10	M	600	SPO	C4-C5-C6-C7
4	L	304	BCL	O1A-CGA-O2A-C1
4	L	304	BCL	CBA-CGA-O2A-C1
4	L	304	BCL	O1D-CGD-O2D-CED
5	M	401	BPH	C2-C3-C5-C6
5	M	401	BPH	CBA-CGA-O2A-C1
5	M	401	BPH	O1A-CGA-O2A-C1
10	M	600	SPO	C36-C37-C38-C40
4	L	301	BCL	C4-C3-C5-C6
4	L	301	BCL	C2-C3-C5-C6
6	L	502	U10	C29-C31-C32-C33
4	M	801	BCL	CBD-CGD-O2D-CED
5	M	401	BPH	CBD-CGD-O2D-CED
4	L	302	BCL	CBD-CGD-O2D-CED
10	M	600	SPO	C36-C37-C38-C39
4	L	301	BCL	C11-C12-C13-C14
10	M	600	SPO	C24-C23-C25-C26
4	L	302	BCL	C15-C16-C17-C18
10	M	600	SPO	C20-C21-C22-C23
6	L	502	U10	C19-C21-C22-C23
6	L	502	U10	C24-C26-C27-C28
4	L	304	BCL	C8-C10-C11-C12
4	M	801	BCL	C5-C6-C7-C8
5	L	402	BPH	C8-C10-C11-C12
10	M	600	SPO	C19-C20-C21-C22
5	L	402	BPH	C5-C6-C7-C8
4	L	301	BCL	C4B-C3B-CAB-CBB
4	L	304	BCL	C4B-C3B-CAB-CBB
10	M	600	SPO	C21-C22-C23-C24
5	M	401	BPH	O1D-CGD-O2D-CED
4	L	301	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	H	702	LDA	C3-C4-C5-C6
6	L	502	U10	C35-C34-C36-C37
10	M	600	SPO	C9-C10-C11-C12
6	L	502	U10	C33-C34-C36-C37
7	M	701	LDA	C1-C2-C3-C4
4	L	304	BCL	C1A-C2A-CAA-CBA
4	L	301	BCL	C11-C12-C13-C15
7	H	702	LDA	C2-C3-C4-C5
4	L	302	BCL	C2A-CAA-CBA-CGA
5	L	402	BPH	C14-C13-C15-C16
5	M	401	BPH	C10-C11-C12-C13
10	M	600	SPO	C4-C1-O1-CM1
5	M	401	BPH	C3-C5-C6-C7
4	L	302	BCL	O1D-CGD-O2D-CED
10	M	600	SPO	C2-C1-O1-CM1
10	M	600	SPO	C3-C1-O1-CM1
4	M	801	BCL	C15-C16-C17-C18
4	L	304	BCL	C11-C10-C8-C7
4	L	304	BCL	C4-C3-C5-C6
4	L	304	BCL	C2-C3-C5-C6
7	H	705	LDA	C4-C5-C6-C7
5	M	401	BPH	C11-C10-C8-C7
10	M	600	SPO	C1-C4-C5-C6
5	M	401	BPH	O2A-C1-C2-C3
4	L	301	BCL	C3-C5-C6-C7
7	H	705	LDA	C5-C6-C7-C8
5	L	402	BPH	C16-C17-C18-C19
5	M	401	BPH	C11-C10-C8-C9
7	H	705	LDA	C2-C3-C4-C5
7	H	705	LDA	C3-C4-C5-C6
6	L	502	U10	C25-C24-C26-C27
4	L	304	BCL	CAD-CBD-CGD-O2D
4	M	801	BCL	CAD-CBD-CGD-O2D
5	M	401	BPH	CAD-CBD-CGD-O2D
4	L	302	BCL	C16-C17-C18-C20
4	L	304	BCL	CAD-CBD-CGD-O1D
4	M	801	BCL	CAD-CBD-CGD-O1D
5	M	401	BPH	CAD-CBD-CGD-O1D
5	L	402	BPH	O2A-C1-C2-C3
10	M	600	SPO	C17-C19-C20-C21
5	M	401	BPH	C16-C17-C18-C20
4	M	801	BCL	O1D-CGD-O2D-CED

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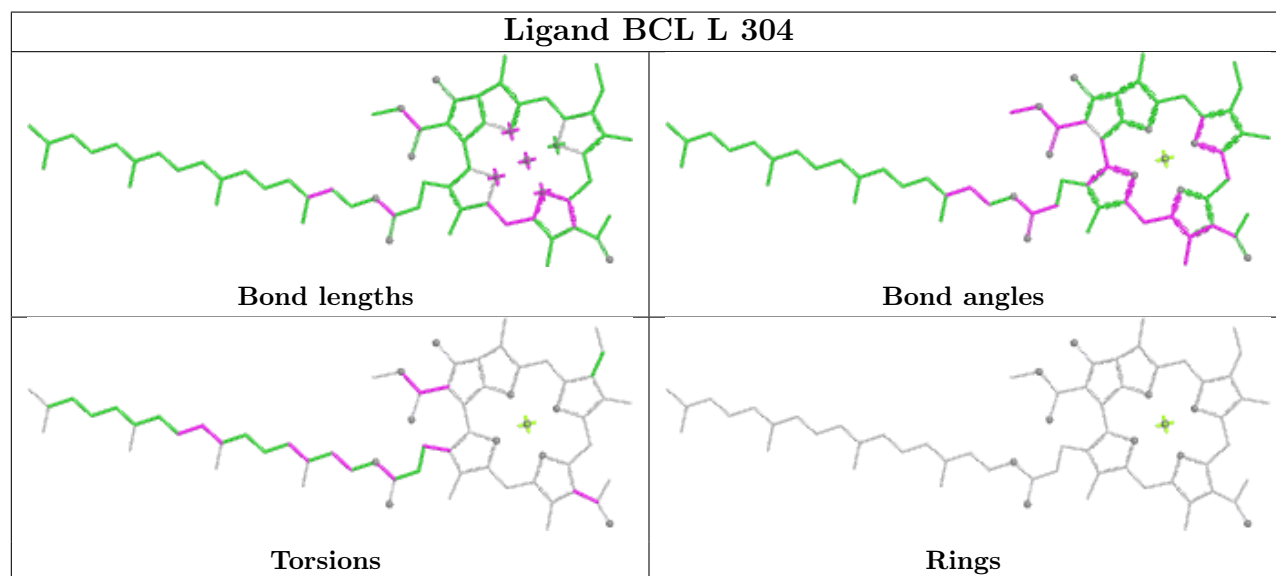
Mol	Chain	Res	Type	Atoms
6	L	502	U10	C23-C24-C26-C27
4	L	302	BCL	C16-C17-C18-C19
4	L	304	BCL	C3A-C2A-CAA-CBA
10	M	600	SPO	C18-C17-C19-C20
5	M	401	BPH	C16-C17-C18-C19
4	L	304	BCL	C2B-C3B-CAB-CBB
10	M	600	SPO	C27-C28-C30-C31
10	M	600	SPO	C16-C17-C19-C20
7	L	703	LDA	C1-C2-C3-C4
10	M	600	SPO	C34-C33-C35-C36
6	L	502	U10	C20-C19-C21-C22
6	L	502	U10	C30-C29-C31-C32
10	M	600	SPO	C29-C28-C30-C31
6	L	502	U10	C18-C19-C21-C22
6	L	502	U10	C28-C29-C31-C32
7	M	701	LDA	N1-C1-C2-C3
5	M	401	BPH	C5-C6-C7-C8
6	M	501	U10	C14-C16-C17-C18
6	M	501	U10	C5-C4-O4-C4M
4	M	801	BCL	C4-C3-C5-C6
4	L	302	BCL	C12-C13-C15-C16
7	M	704	LDA	C7-C8-C9-C10
6	L	502	U10	C36-C37-C38-C39
10	M	600	SPO	C32-C33-C35-C36
5	M	401	BPH	C2-C1-O2A-CGA
4	L	302	BCL	C5-C6-C7-C8

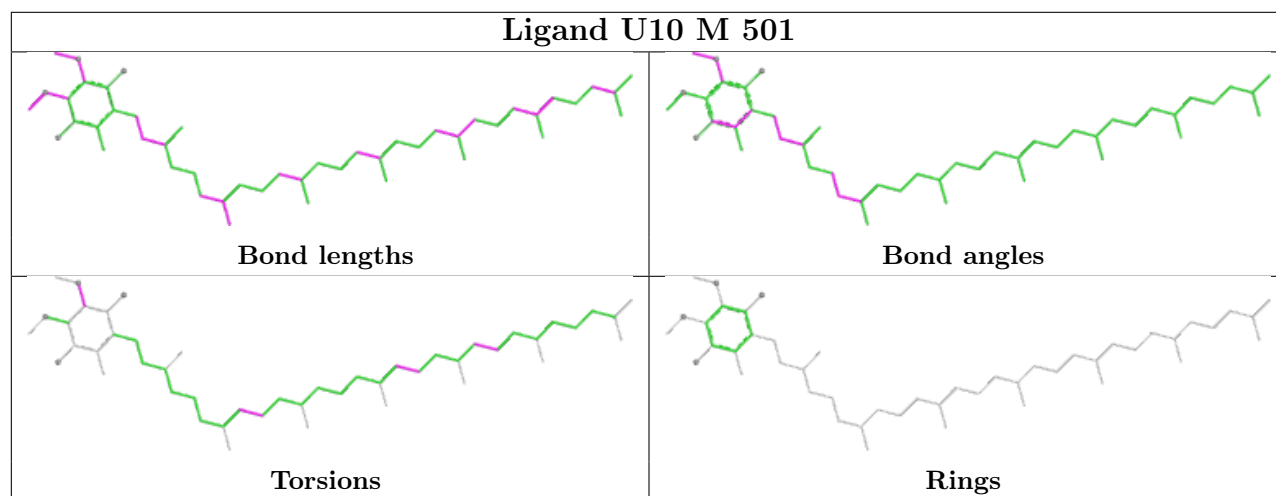
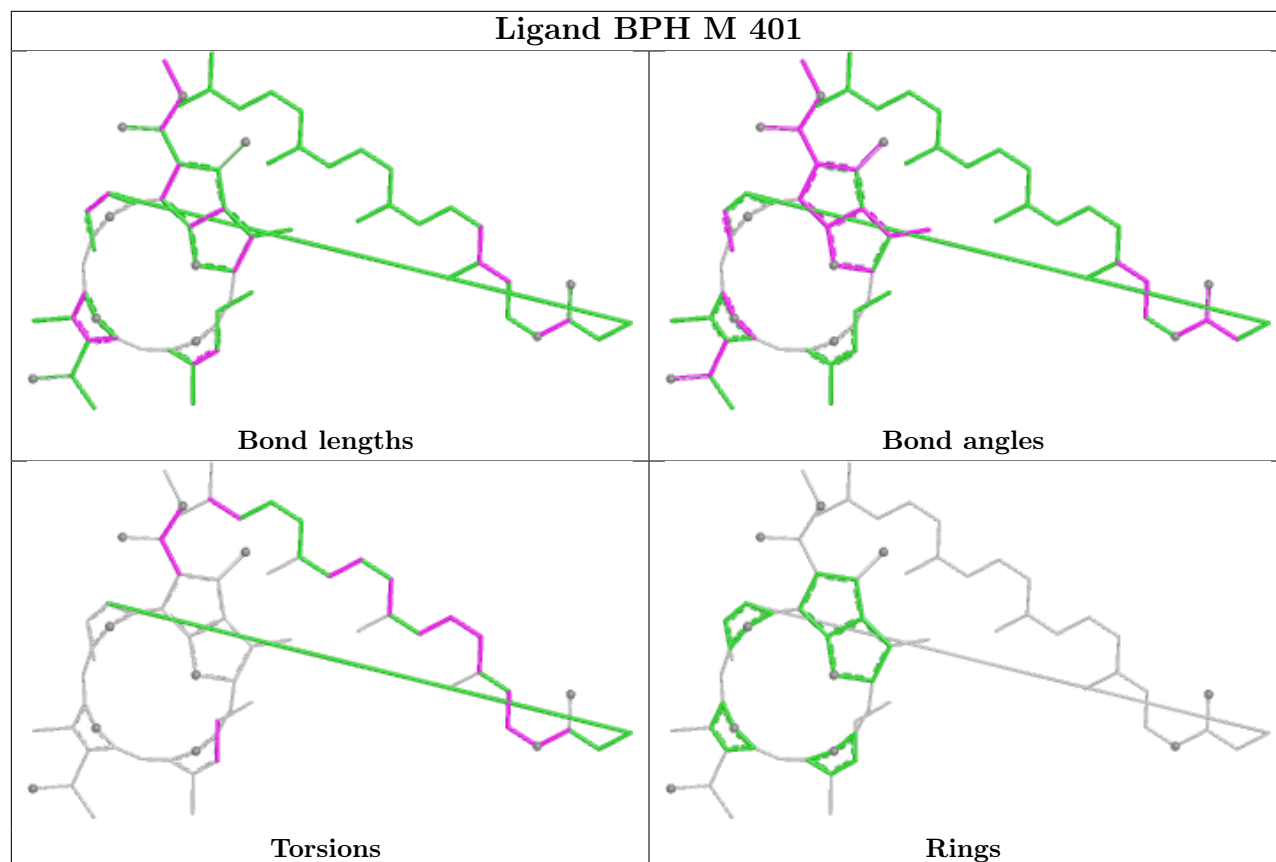
There are no ring outliers.

10 monomers are involved in 63 short contacts:

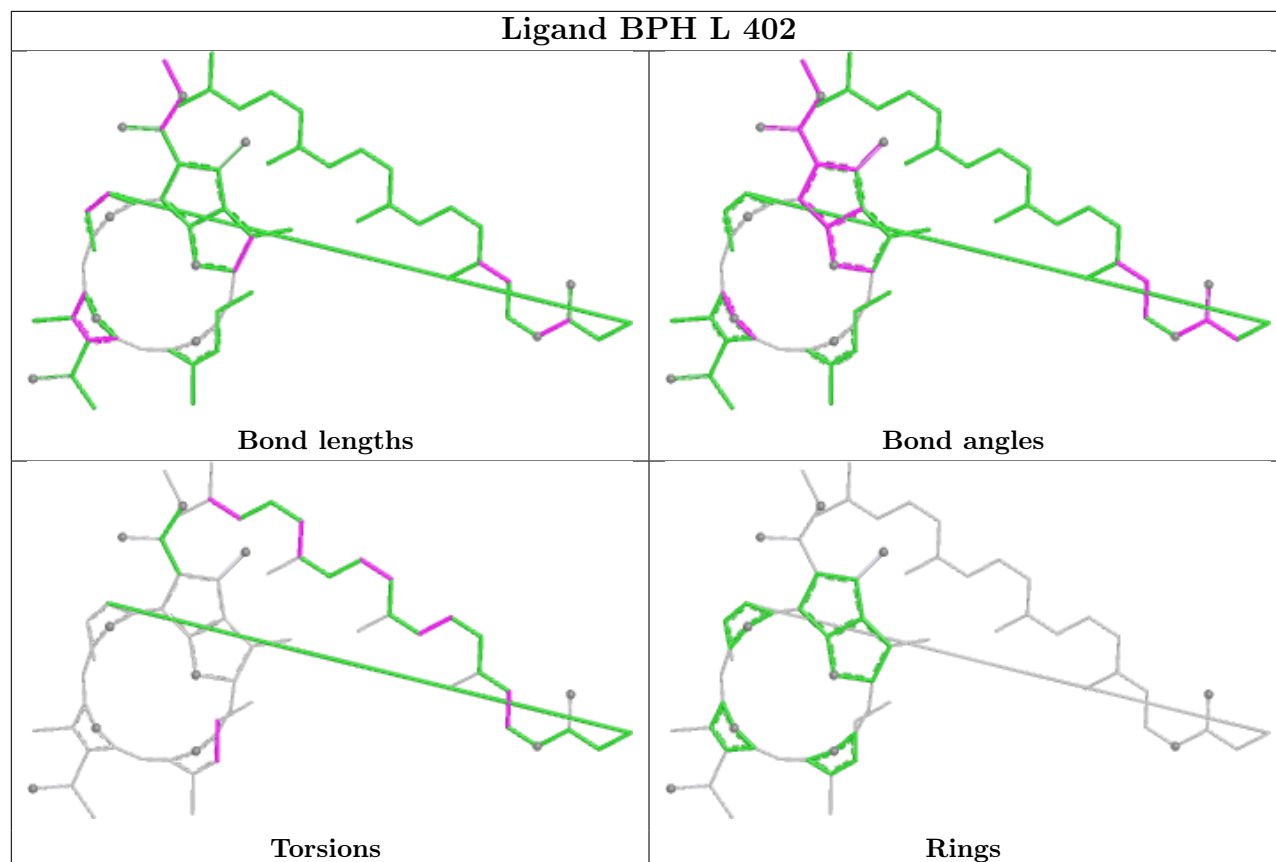
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	304	BCL	7	0
5	M	401	BPH	11	0
6	M	501	U10	1	0
5	L	402	BPH	9	0
7	L	703	LDA	3	0
7	H	702	LDA	1	0
10	M	600	SPO	4	0
4	L	301	BCL	12	0
4	M	801	BCL	14	0
4	L	302	BCL	12	0

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.

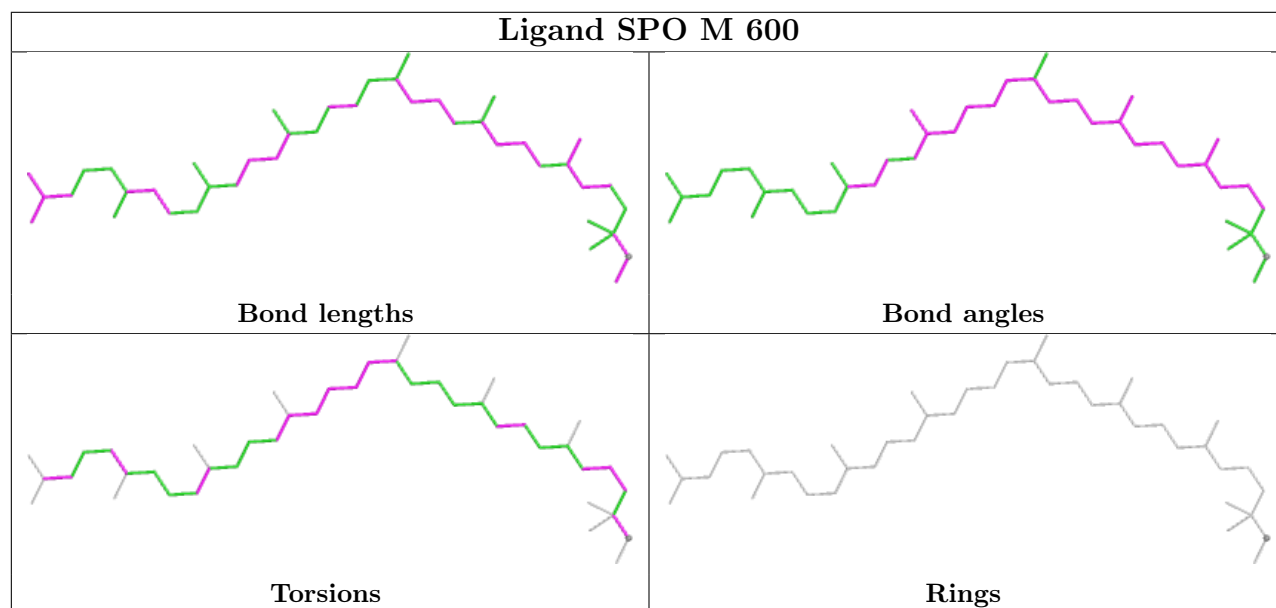


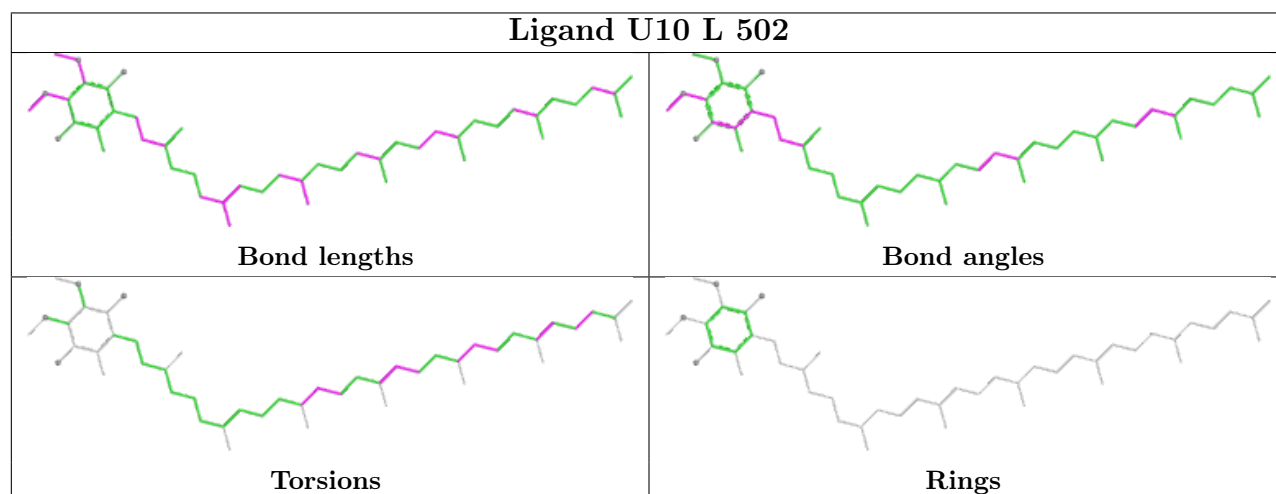
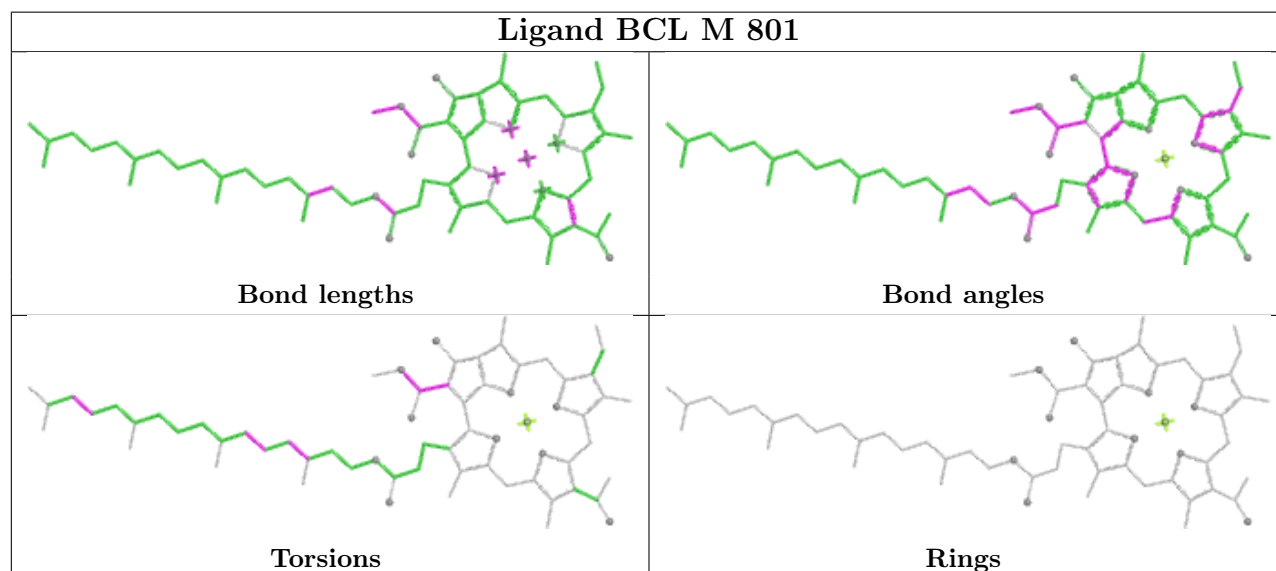
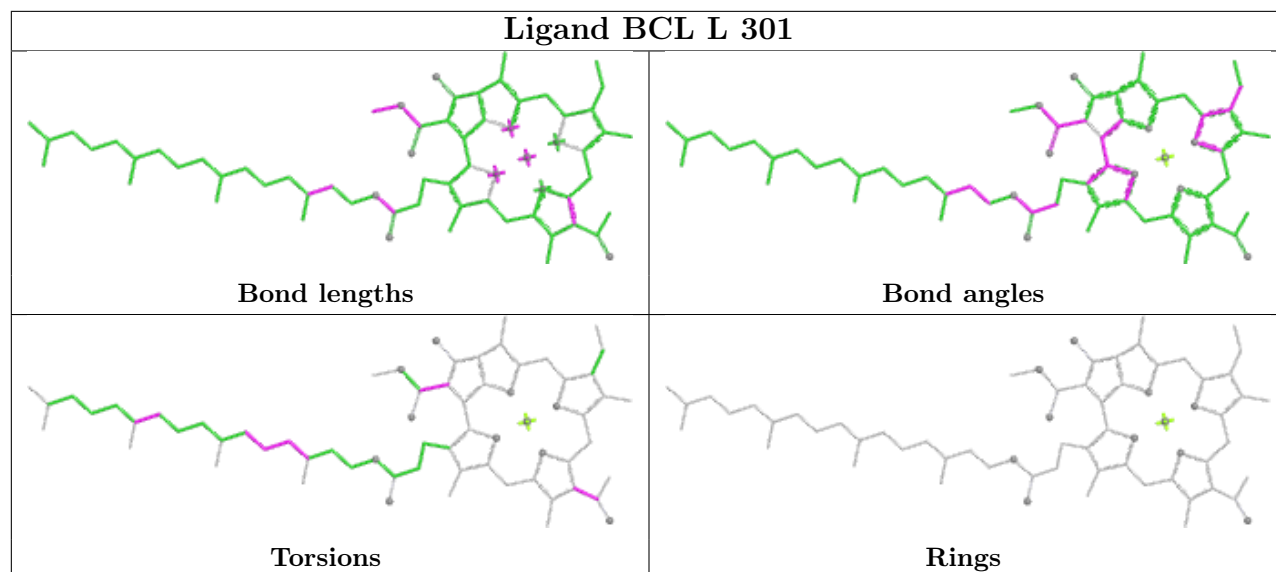


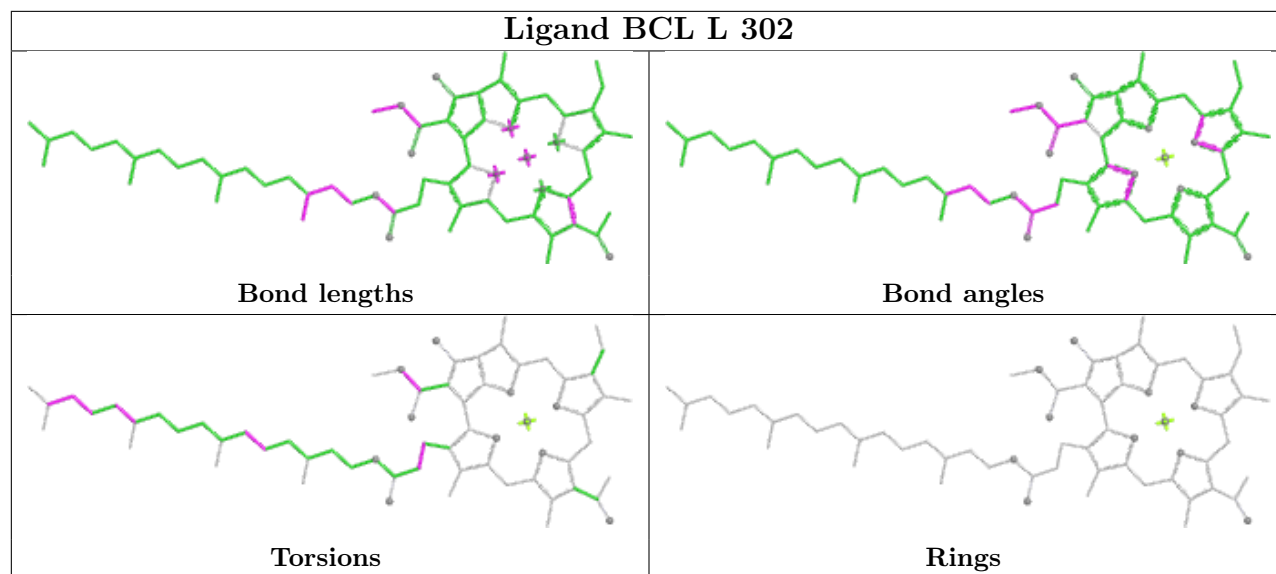
Ligand BPH L 402



Ligand SPO 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.