



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:42 AM UTC

PDB ID : 1QOV / pdb_00001qov
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ALA M260
REPLACED WITH TRP (CHAIN M, A260W)
Authors : McAuley, K.E.; Fyfe, P.K.; Ridge, J.P.; Isaacs, N.W.; Cogdell, R.J.; Jones,
M.R.
Deposited on : 1999-11-17
Resolution : 2.10 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)
Xtrriage (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

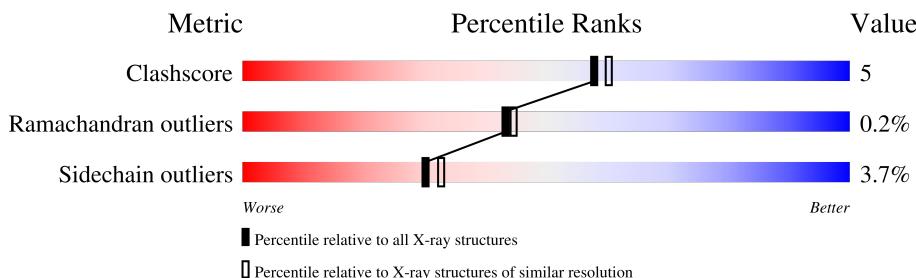
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	H	260	78% 12% • 8%
2	L	281	89% 10% •
3	M	307	85% 12% • •

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	M	1301	X	-	-	-
6	BPH	M	1401	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7312 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	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	1	0
			2235	1509	355	363	8			

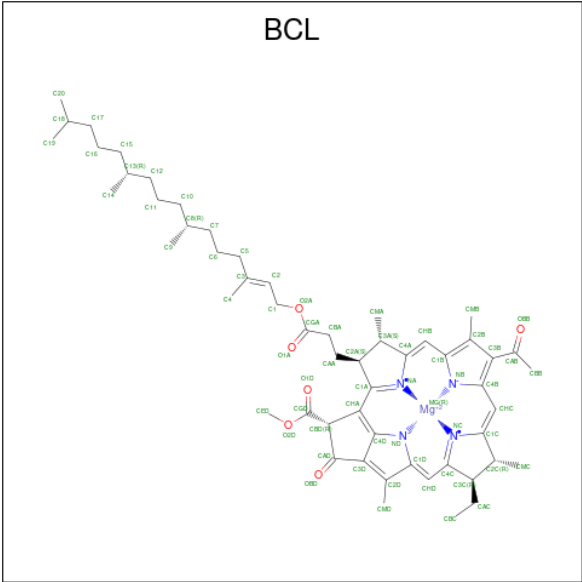
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	2	0
			2430	1622	401	397	10			

There is a discrepancy between the modelled and reference sequences:

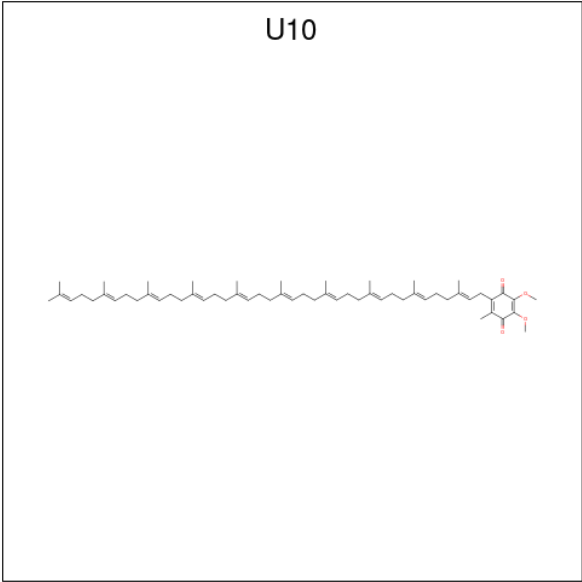
Chain	Residue	Modelled	Actual	Comment	Reference
M	260	TRP	ALA	engineered mutation	UNP P02953

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



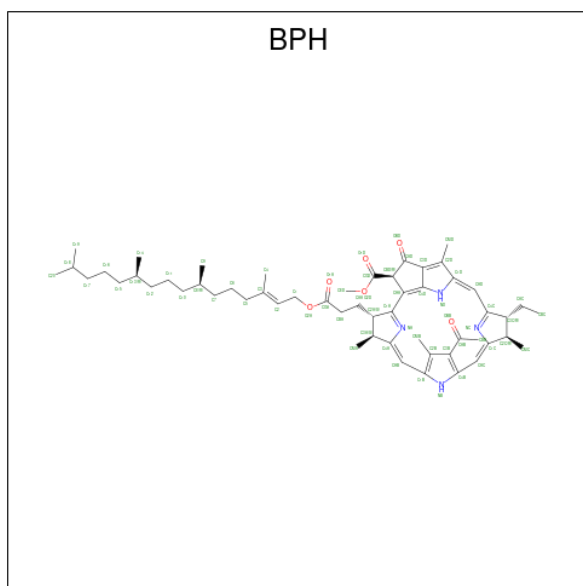
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



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

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

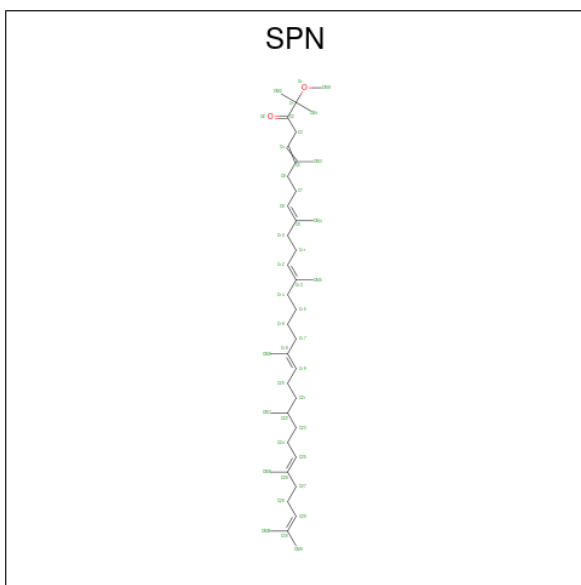


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	10	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

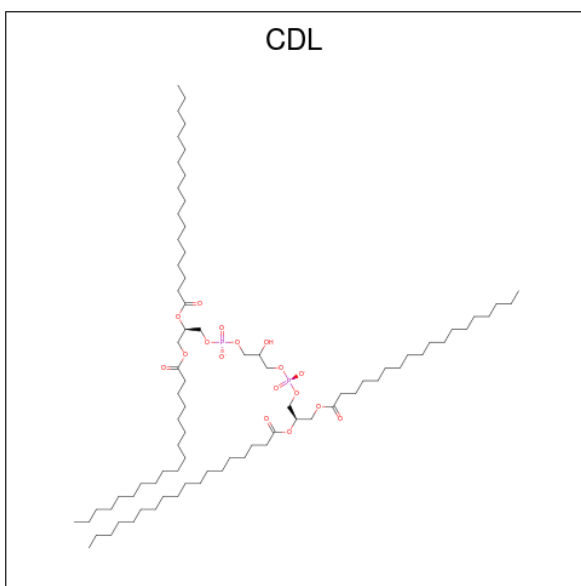
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 9 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total 1	Cl 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	118	Total 118	O 118	0	0
11	L	59	Total 59	O 59	0	0
11	M	73	Total 73	O 73	0	0

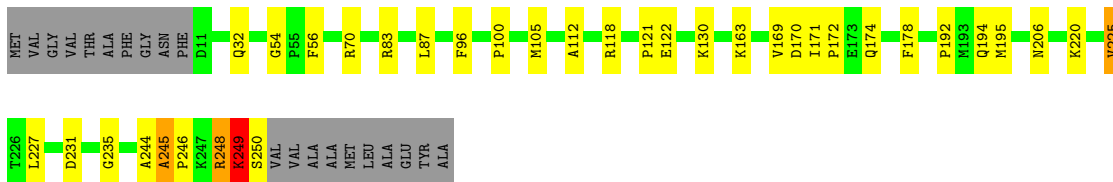
3 Residue-property plots

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: PHOTOSYNTHETIC REACTION CENTER

Chain H: 



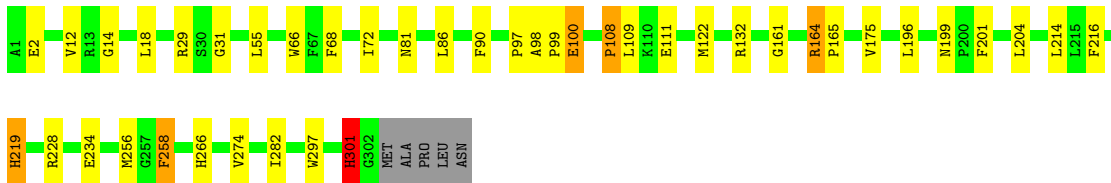
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L: 



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M: 



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	142.05Å 142.05Å 186.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.6 (30.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7312	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: SPN, CL, BCL, CDL, U10, FE2, BPH

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	H	0.78	0/1877	1.53	18/2553 (0.7%)
2	L	0.83	0/2326	1.46	20/3183 (0.6%)
3	M	0.74	0/2533	1.39	22/3457 (0.6%)
All	All	0.78	0/6736	1.45	60/9193 (0.7%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	ARG	CD-NE-CZ	13.48	143.28	124.40
1	H	248	ARG	CD-NE-CZ	11.66	140.72	124.40
3	M	258	PHE	CA-CB-CG	9.87	123.67	113.80
2	L	216	PHE	CA-CB-CG	-9.27	104.53	113.80
2	L	207	ARG	CD-NE-CZ	8.31	136.03	124.40
1	H	225	VAL	CB-CA-C	-8.22	97.83	110.50
2	L	38	THR	N-CA-CB	7.86	121.67	110.12
2	L	170	ASN	CA-C-N	7.27	127.12	119.05
2	L	170	ASN	C-N-CA	7.27	127.12	119.05
2	L	34	PHE	CA-CB-CG	-7.23	106.57	113.80
2	L	217	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	H	225	VAL	N-CA-CB	6.37	121.89	111.44
2	L	60	ASN	CA-C-N	6.36	126.57	119.32
2	L	60	ASN	C-N-CA	6.36	126.57	119.32
2	L	135	ARG	CA-C-N	6.24	125.73	119.24
2	L	135	ARG	C-N-CA	6.24	125.73	119.24
2	L	243	PHE	CA-CB-CG	-6.04	107.76	113.80
3	M	31	GLY	N-CA-C	-6.03	103.37	112.60
1	H	249	LYS	N-CA-C	6.01	120.18	112.12
3	M	266	HIS	CA-CB-CG	-5.99	107.81	113.80
3	M	29	ARG	CD-NE-CZ	5.89	132.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	81	ASN	CA-C-N	5.89	125.76	119.28
3	M	81	ASN	C-N-CA	5.89	125.76	119.28
1	H	121	PRO	N-CA-CB	5.88	108.80	103.33
2	L	173	HIS	CA-CB-CG	5.87	119.67	113.80
2	L	1	ALA	CA-C-O	-5.84	110.86	120.80
1	H	248	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	H	70	ARG	NH1-CZ-NH2	5.69	126.69	119.30
2	L	79	PRO	N-CA-CB	5.68	108.30	103.35
1	H	178	PHE	CA-CB-CG	5.56	119.36	113.80
2	L	163	THR	CA-CB-OG1	-5.49	101.37	109.60
1	H	174	GLN	OE1-CD-NE2	-5.47	117.12	122.60
1	H	244	ALA	N-CA-C	-5.47	106.11	112.89
3	M	199	ASN	CA-C-N	5.44	125.26	119.28
3	M	199	ASN	C-N-CA	5.44	125.26	119.28
3	M	109	LEU	N-CA-C	5.43	116.88	111.07
1	H	96	PHE	CA-C-N	5.41	125.71	119.92
1	H	96	PHE	C-N-CA	5.41	125.71	119.92
3	M	108	PRO	N-CA-CB	5.32	108.39	103.39
1	H	54	GLY	CA-C-N	5.31	125.01	119.64
1	H	54	GLY	C-N-CA	5.31	125.01	119.64
3	M	199	ASN	CA-CB-CG	5.28	117.88	112.60
3	M	164	ARG	CA-C-N	5.26	124.71	119.24
3	M	164	ARG	C-N-CA	5.26	124.71	119.24
3	M	282	ILE	CA-C-N	5.25	125.80	119.98
3	M	282	ILE	C-N-CA	5.25	125.80	119.98
2	L	146	PHE	CA-CB-CG	5.24	119.04	113.80
1	H	118	ARG	CD-NE-CZ	5.24	131.73	124.40
3	M	234	GLU	N-CA-C	5.21	116.96	111.28
2	L	199	ASN	OD1-CG-ND2	-5.20	117.40	122.60
3	M	97	PRO	N-CA-CB	5.20	107.87	103.35
3	M	301	HIS	CA-CB-CG	5.15	118.95	113.80
1	H	96	PHE	CA-CB-CG	-5.13	108.67	113.80
1	H	192	PRO	N-CA-CB	5.13	107.89	103.27
3	M	14	GLY	CA-C-N	5.10	125.02	119.76
3	M	14	GLY	C-N-CA	5.10	125.02	119.76
2	L	228	GLY	CA-C-O	-5.06	115.84	120.80
3	M	219	HIS	CA-CB-CG	-5.06	108.74	113.80
3	M	201	PHE	CA-CB-CG	-5.05	108.75	113.80
2	L	217	ARG	NE-CZ-NH2	5.02	123.72	119.20

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	H	1829	0	1836	17	0
2	L	2235	0	2192	10	0
3	M	2430	0	2344	19	0
4	L	198	0	222	7	0
4	M	66	0	71	6	0
5	L	48	0	62	10	0
6	M	130	0	145	3	0
7	M	1	0	0	0	0
8	M	43	0	69	2	0
9	M	81	0	106	0	0
10	M	1	0	0	1	0
11	H	118	0	0	2	0
11	L	59	0	0	0	0
11	M	73	0	0	0	0
All	All	7312	0	7047	64	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 5.

All (64) 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)
5:L:1502:U10:H38	5:L:1502:U10:H301	1.29	1.07
5:L:1502:U10:H38	5:L:1502:U10:C30	1.80	0.94
5:L:1502:U10:H301	5:L:1502:U10:C38	2.03	0.87
5:L:1502:U10:H371	4:M:1301:BCL:HED2	1.63	0.80
5:L:1502:U10:H351	3:M:90:PHE:HE2	1.54	0.71
5:L:1502:U10:C30	5:L:1502:U10:C38	2.66	0.69
3:M:108:PRO:HG2	3:M:111:GLU:HG3	1.77	0.66
1:H:195:MET:HE3	3:M:228:ARG:HB3	1.81	0.63
2:L:271:TRP:H	2:L:271:TRP:CD1	2.16	0.63
1:H:220:LYS:HE3	11:H:2107:HOH:O	1.99	0.62
1:H:194:GLN:O	1:H:195:MET:HE2	2.01	0.61
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.37	0.60
2:L:208:THR:HB	2:L:209:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1502:U10:H351	3:M:90:PHE:CE2	2.38	0.58
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.86	0.58
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.85	0.57
4:L:1303:BCL:HMB1	4:L:1303:BCL:HBB3	1.86	0.57
4:M:1301:BCL:HBB2	4:M:1301:BCL:HMB3	1.88	0.56
3:M:164:ARG:N	3:M:165:PRO:CD	2.68	0.55
5:L:1502:U10:C29	5:L:1502:U10:C41	2.67	0.54
1:H:249:LYS:O	1:H:250:SER:C	2.50	0.54
3:M:175:VAL:HG11	8:M:1600:SPN:H161	1.91	0.52
6:M:1402:BPH:HBB3	6:M:1402:BPH:HMB1	1.90	0.52
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.93	0.51
4:L:1303:BCL:HMB1	4:L:1303:BCL:CBB	2.42	0.50
1:H:206:ASN:HD21	1:H:248:ARG:HD2	1.76	0.49
1:H:245:ALA:HB3	1:H:246:PRO:HD3	1.95	0.49
5:L:1502:U10:C38	5:L:1502:U10:C33	2.66	0.49
3:M:219:HIS:HA	10:M:1900:CL:CL	2.50	0.49
3:M:256:MET:HE3	3:M:258:PHE:CG	2.47	0.49
5:L:1502:U10:H371	4:M:1301:BCL:CED	2.39	0.48
3:M:214:LEU:HD13	6:M:1402:BPH:ND	2.29	0.48
3:M:98:ALA:HB1	3:M:99:PRO:HD2	1.96	0.48
2:L:34:PHE:O	2:L:38:THR:HG23	2.13	0.47
3:M:161:GLY:HA3	8:M:1600:SPN:H201	1.97	0.47
1:H:32:GLN:HG2	1:H:56:PHE:CZ	2.50	0.46
2:L:219:LEU:HD12	3:M:132[B]:ARG:NH1	2.31	0.46
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.50	0.46
4:L:1304:BCL:HMB3	4:L:1304:BCL:HBB2	1.98	0.45
1:H:112:ALA:HA	1:H:235:GLY:O	2.17	0.45
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.52	0.45
4:M:1301:BCL:H151	4:M:1301:BCL:H112	1.67	0.45
4:L:1303:BCL:OBB	4:L:1303:BCL:HHC	2.17	0.44
1:H:171:ILE:HB	1:H:172:PRO:CD	2.48	0.44
1:H:32:GLN:NE2	11:H:2004:HOH:O	2.50	0.43
2:L:271:TRP:CD1	2:L:271:TRP:N	2.85	0.43
3:M:68:PHE:O	3:M:72:ILE:HG12	2.18	0.43
2:L:38:THR:HG22	2:L:99:SER:HB3	1.98	0.43
4:L:1304:BCL:HBA1	4:L:1304:BCL:C4A	2.49	0.42
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.20	0.42
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.42
4:L:1302:BCL:CBB	4:L:1302:BCL:HMB3	2.49	0.41
2:L:272:TRP:HA	2:L:275:ILE:HG13	2.02	0.41
3:M:297:TRP:O	3:M:301:HIS:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1301:BCL:OBB	4:M:1301:BCL:HHC	2.21	0.41
4:L:1302:BCL:HHC	4:L:1302:BCL:OBB	2.21	0.41
4:M:1301:BCL:HMB3	4:M:1301:BCL:CBB	2.49	0.41
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.03	0.41
1:H:195:MET:HE1	3:M:228:ARG:CZ	2.51	0.41
2:L:38:THR:HG22	2:L:99:SER:CB	2.51	0.41
1:H:169:VAL:HG23	1:H:171:ILE:HD13	2.03	0.41
6:M:1402:BPH:HBA2	6:M:1402:BPH:H3A	1.92	0.41
3:M:256:MET:HE3	3:M:258:PHE:CB	2.51	0.40
3:M:100:GLU:H	3:M:100:GLU:HG3	1.70	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	H	238/260 (92%)	235 (99%)	2 (1%)	1 (0%)	30	28
2	L	280/281 (100%)	275 (98%)	5 (2%)	0	100	100
3	M	302/307 (98%)	292 (97%)	9 (3%)	1 (0%)	36	36
All	All	820/848 (97%)	802 (98%)	16 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
1	H	245	ALA

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	H	195/208 (94%)	190 (97%)	5 (3%)	40	46
2	L	221/220 (100%)	212 (96%)	9 (4%)	27	29
3	M	239/241 (99%)	229 (96%)	10 (4%)	26	28
All	All	655/669 (98%)	631 (96%)	24 (4%)	30	33

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	105	MET
1	H	163	LYS
1	H	225	VAL
1	H	231	ASP
1	H	249	LYS
2	L	21	LEU
2	L	38	THR
2	L	54	VAL
2	L	72	GLU
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	267	VAL
2	L	271	TRP
3	M	2	GLU
3	M	12	VAL
3	M	18	LEU
3	M	55	LEU
3	M	86	LEU
3	M	100	GLU
3	M	196	LEU
3	M	204	LEU
3	M	216	PHE
3	M	274	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	H	68	HIS
1	H	199	GLN
1	H	206	ASN
2	L	258	GLN
3	M	188	ASN
3	M	299	GLN

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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	1304	2	69,74,74	1.48	15 (21%)	79,115,115	1.88	20 (25%)
4	BCL	L	1302	2	69,74,74	1.51	12 (17%)	79,115,115	2.23	15 (18%)
6	BPH	M	1401	-	59,70,70	2.13	14 (23%)	59,101,101	2.86	23 (38%)
8	SPN	M	1600	-	42,42,42	4.04	20 (47%)	50,52,52	2.50	16 (32%)
6	BPH	M	1402	-	59,70,70	2.07	16 (27%)	59,101,101	2.57	17 (28%)
9	CDL	M	1800	-	80,80,99	0.47	0	86,92,111	0.94	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	U10	L	1502	-	48,48,63	1.82	13 (27%)	60,61,79	2.81	17 (28%)
4	BCL	L	1303	3	69,74,74	1.53	10 (14%)	79,115,115	2.44	18 (22%)
4	BCL	M	1301	3	69,74,74	1.39	12 (17%)	79,115,115	2.26	23 (29%)

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	1304	2	-	8/41/137/137	-
4	BCL	L	1302	2	-	6/41/137/137	-
6	BPH	M	1401	-	2/2/18/22	12/37/105/105	0/5/6/6
8	SPN	M	1600	-	-	19/50/51/51	-
6	BPH	M	1402	-	-	4/37/105/105	0/5/6/6
4	BCL	M	1301	3	2/2/21/25	13/41/137/137	-
9	CDL	M	1800	-	-	30/91/91/110	-
5	U10	L	1502	-	-	10/45/69/87	0/1/1/1
4	BCL	L	1303	3	-	3/41/137/137	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1600	SPN	C3-C2	9.65	1.60	1.52
8	M	1600	SPN	C4-C5	9.22	1.54	1.33
8	M	1600	SPN	C19-C18	9.11	1.54	1.33
8	M	1600	SPN	C8-C9	8.80	1.53	1.33
8	M	1600	SPN	C12-C13	8.48	1.52	1.33
6	M	1401	BPH	C2C-C3C	-7.87	1.47	1.54
4	L	1302	BCL	MG-NA	6.41	2.21	2.06
6	M	1402	BPH	C2C-C3C	-6.37	1.49	1.54
6	M	1402	BPH	C1D-C2D	6.23	1.46	1.39
8	M	1600	SPN	C17-C18	-5.97	1.39	1.51
8	M	1600	SPN	C3-C4	-5.93	1.41	1.50
6	M	1402	BPH	C3A-C2A	-5.93	1.49	1.54
4	L	1303	BCL	MG-NA	5.90	2.20	2.06
8	M	1600	SPN	C10-C9	-5.90	1.39	1.51
6	M	1401	BPH	C1D-C2D	5.90	1.46	1.39
6	M	1401	BPH	C11-C10	-5.62	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1600	SPN	C14-C13	-5.37	1.40	1.51
8	M	1600	SPN	C6-C5	-5.24	1.40	1.51
4	L	1304	BCL	O2D-CGD	5.18	1.46	1.33
6	M	1401	BPH	C1B-C2B	5.01	1.45	1.39
4	L	1303	BCL	O2D-CGD	4.82	1.45	1.33
6	M	1402	BPH	C1B-C2B	4.76	1.44	1.39
4	M	1301	BCL	O2D-CGD	4.73	1.44	1.33
5	L	1502	U10	O4-C4	4.52	1.47	1.36
4	M	1301	BCL	MG-NA	4.49	2.16	2.06
4	L	1304	BCL	MG-NA	4.39	2.16	2.06
4	L	1302	BCL	O2D-CGD	4.10	1.43	1.33
6	M	1401	BPH	O2A-CGA	3.88	1.44	1.33
6	M	1402	BPH	O2D-CGD	3.80	1.42	1.33
6	M	1401	BPH	O2D-CGD	3.78	1.42	1.33
8	M	1600	SPN	C20-C19	-3.77	1.39	1.50
4	M	1301	BCL	O2A-CGA	3.72	1.44	1.33
5	L	1502	U10	C13-C14	3.53	1.41	1.33
6	M	1402	BPH	O2A-CGA	3.45	1.43	1.33
5	L	1502	U10	C7-C8	-3.43	1.45	1.50
8	M	1600	SPN	C25-C26	3.41	1.40	1.33
8	M	1600	SPN	C7-C8	-3.34	1.40	1.50
4	L	1303	BCL	C2-C3	3.34	1.40	1.33
4	L	1303	BCL	MG-NC	3.33	2.14	2.06
6	M	1402	BPH	C3B-C2B	-3.31	1.34	1.39
8	M	1600	SPN	C11-C12	-3.31	1.40	1.50
4	L	1303	BCL	O2A-CGA	3.30	1.43	1.33
5	L	1502	U10	O3-C3	3.30	1.44	1.36
5	L	1502	U10	C23-C24	3.15	1.40	1.33
5	L	1502	U10	O3-C3M	-3.15	1.38	1.45
4	L	1302	BCL	O2A-CGA	3.14	1.42	1.33
4	L	1302	BCL	C2-C3	3.13	1.40	1.33
6	M	1401	BPH	O2D-CED	-3.01	1.38	1.45
4	L	1304	BCL	C2C-C3C	-3.01	1.46	1.54
6	M	1402	BPH	CHA-CBD	2.97	1.55	1.51
8	M	1600	SPN	O1-CMA	2.96	1.52	1.43
4	L	1302	BCL	C4-C3	2.93	1.57	1.50
8	M	1600	SPN	C29-C30	2.92	1.41	1.32
5	L	1502	U10	C32-C33	-2.92	1.41	1.50
4	L	1302	BCL	MG-ND	-2.84	2.00	2.05
5	L	1502	U10	C8-C9	2.82	1.39	1.33
8	M	1600	SPN	C21-C22	-2.81	1.39	1.52
6	M	1401	BPH	CHA-CBD	2.79	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1303	BCL	MG-ND	-2.77	2.00	2.05
4	M	1301	BCL	CAA-C2A	2.75	1.59	1.54
4	L	1304	BCL	O2A-CGA	2.72	1.41	1.33
5	L	1502	U10	C18-C19	2.70	1.39	1.33
6	M	1401	BPH	C3B-C2B	-2.70	1.35	1.39
4	L	1304	BCL	CAA-C2A	2.62	1.58	1.54
4	L	1304	BCL	CMB-C2B	2.61	1.56	1.50
4	L	1304	BCL	CMC-C2C	2.61	1.58	1.53
6	M	1402	BPH	O2D-CED	-2.59	1.39	1.45
6	M	1402	BPH	C2-C3	2.59	1.39	1.33
4	L	1304	BCL	C2-C3	2.57	1.39	1.33
6	M	1401	BPH	C2-C3	2.54	1.38	1.33
4	M	1301	BCL	C3B-C4B	2.53	1.46	1.41
8	M	1600	SPN	C16-C15	-2.51	1.39	1.51
5	L	1502	U10	C38-C39	2.48	1.39	1.32
6	M	1401	BPH	C4D-ND	-2.46	1.34	1.38
4	M	1301	BCL	CMA-C3A	2.45	1.58	1.53
4	L	1303	BCL	O2D-CED	-2.44	1.39	1.45
4	L	1302	BCL	C3B-C4B	2.44	1.45	1.41
4	M	1301	BCL	C2C-C3C	-2.43	1.47	1.54
4	M	1301	BCL	C2-C3	2.41	1.38	1.33
4	L	1304	BCL	MG-ND	-2.39	2.01	2.05
4	L	1304	BCL	O1D-CGD	2.35	1.27	1.21
6	M	1402	BPH	O1D-CGD	2.34	1.27	1.21
6	M	1402	BPH	CAA-C2A	2.33	1.58	1.54
4	M	1301	BCL	CMB-C2B	2.32	1.55	1.50
4	L	1302	BCL	C2C-C3C	-2.29	1.48	1.54
4	L	1302	BCL	MG-NC	2.24	2.11	2.06
4	L	1302	BCL	CMA-C3A	2.21	1.57	1.53
4	L	1304	BCL	C3B-C2B	-2.21	1.35	1.42
4	L	1303	BCL	CMB-C2B	2.19	1.55	1.50
5	L	1502	U10	C27-C28	-2.16	1.43	1.50
5	L	1502	U10	C28-C29	2.16	1.38	1.33
4	L	1304	BCL	O2D-CED	-2.15	1.40	1.45
6	M	1401	BPH	C3D-C2D	-2.15	1.36	1.39
4	L	1303	BCL	C4-C3	2.13	1.55	1.50
4	L	1302	BCL	CMB-C2B	2.13	1.55	1.50
4	M	1301	BCL	C3B-C2B	-2.12	1.35	1.42
6	M	1401	BPH	C1A-C2A	2.12	1.54	1.51
6	M	1402	BPH	C3D-C4D	2.11	1.44	1.41
6	M	1402	BPH	C3B-C4B	2.10	1.44	1.41
6	M	1401	BPH	CAA-C2A	2.09	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1304	BCL	C3B-C4B	2.08	1.45	1.41
6	M	1402	BPH	C4-C3	2.06	1.55	1.50
4	L	1304	BCL	CMA-C3A	2.05	1.57	1.53
4	L	1303	BCL	CMD-C2D	2.05	1.55	1.50
4	L	1302	BCL	O2D-CED	-2.05	1.40	1.45
4	L	1304	BCL	CAC-C3C	2.03	1.57	1.54
5	L	1502	U10	C15-C14	2.03	1.55	1.50
4	M	1301	BCL	C4-C3	2.02	1.55	1.50
8	M	1600	SPN	CM3-C5	2.02	1.55	1.50
8	M	1600	SPN	C27-C26	2.02	1.55	1.51
4	M	1301	BCL	O2D-CED	-2.01	1.40	1.45
6	M	1402	BPH	C5-C3	2.00	1.55	1.51

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1502	U10	C32-C33-C34	15.40	162.88	127.62
6	M	1401	BPH	O2D-CGD-CBD	13.86	126.18	110.95
6	M	1402	BPH	O2D-CGD-CBD	13.02	125.25	110.95
4	L	1303	BCL	C1C-NC-C4C	11.88	112.10	106.68
4	L	1303	BCL	C4A-NA-C1A	10.49	111.46	106.68
4	L	1302	BCL	C1C-NC-C4C	9.85	111.17	106.68
4	L	1302	BCL	C4A-NA-C1A	8.94	110.76	106.68
4	M	1301	BCL	C1-C2-C3	8.20	139.63	126.20
8	M	1600	SPN	CM6-C18-C17	6.80	127.03	115.23
5	L	1502	U10	C27-C28-C29	6.73	143.03	127.62
4	L	1304	BCL	C4A-NA-C1A	6.53	109.66	106.68
5	L	1502	U10	C3M-O3-C3	6.42	139.02	116.47
4	L	1303	BCL	O2D-CGD-CBD	6.24	122.15	111.23
4	L	1304	BCL	O2D-CGD-CBD	6.24	122.14	111.23
8	M	1600	SPN	CM5-C13-C14	6.24	126.06	115.23
6	M	1401	BPH	C1-C2-C3	6.10	136.19	126.20
4	M	1301	BCL	C4-C3-C5	-5.74	105.26	115.23
4	M	1301	BCL	OBB-CAB-C3B	5.72	130.55	120.43
6	M	1402	BPH	O2A-CGA-O1A	-5.15	110.74	123.63
6	M	1402	BPH	CMA-C3A-C4A	-4.96	103.92	114.61
6	M	1401	BPH	C4D-CHA-CBD	-4.85	106.13	108.45
4	M	1301	BCL	O2A-CGA-CBA	4.77	126.39	111.83
4	M	1301	BCL	O2D-CGD-CBD	4.70	119.44	111.23
4	M	1301	BCL	O2A-CGA-O1A	-4.69	111.90	123.63
8	M	1600	SPN	C6-C5-C4	-4.65	110.74	121.17
4	L	1302	BCL	O2D-CGD-CBD	4.61	119.28	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1301	BCL	C4A-NA-C1A	4.57	108.77	106.68
6	M	1402	BPH	O2D-CGD-O1D	-4.56	114.98	123.85
4	L	1304	BCL	C1C-NC-C4C	4.53	108.75	106.68
6	M	1401	BPH	O1D-CGD-CBD	-4.52	117.88	124.72
8	M	1600	SPN	C3-C4-C5	-4.47	119.14	126.83
8	M	1600	SPN	C17-C18-C19	-4.43	111.23	121.17
8	M	1600	SPN	CM7-C22-C21	4.32	126.68	111.27
5	L	1502	U10	O5-C5-C6	-4.17	113.73	121.79
8	M	1600	SPN	C20-C19-C18	-4.16	118.11	127.62
6	M	1401	BPH	O2D-CGD-O1D	-4.08	115.91	123.85
4	M	1301	BCL	CAA-C2A-C3A	-4.05	102.07	113.00
6	M	1401	BPH	CBC-CAC-C3C	4.04	121.72	113.78
4	M	1301	BCL	C1C-NC-C4C	4.02	108.51	106.68
8	M	1600	SPN	C7-C8-C9	-3.97	118.53	127.62
6	M	1401	BPH	CMA-C3A-C4A	-3.96	106.08	114.61
8	M	1600	SPN	C11-C12-C13	-3.93	118.63	127.62
4	L	1302	BCL	O2D-CGD-O1D	-3.85	116.35	123.85
8	M	1600	SPN	CM4-C9-C10	3.82	121.85	115.23
6	M	1401	BPH	CED-O2D-CGD	3.81	124.55	115.92
4	L	1303	BCL	C1-C2-C3	-3.80	119.97	126.20
4	L	1302	BCL	O2A-CGA-O1A	-3.70	114.38	123.63
4	L	1302	BCL	CAC-C3C-C4C	-3.64	104.51	112.58
4	L	1302	BCL	OBB-CAB-CBB	-3.59	111.74	119.77
6	M	1402	BPH	OBD-CAD-CBD	-3.57	120.58	125.82
6	M	1402	BPH	O2A-CGA-CBA	3.56	122.70	111.83
6	M	1401	BPH	C11-C10-C8	3.55	127.78	115.97
4	L	1304	BCL	CHC-C1C-NC	3.53	129.50	124.40
4	M	1301	BCL	C5-C3-C2	3.51	129.04	121.17
8	M	1600	SPN	C10-C9-C8	-3.50	113.31	121.17
6	M	1401	BPH	C1C-C2C-C3C	3.49	106.16	102.84
4	L	1302	BCL	CHC-C1C-NC	3.43	129.35	124.40
5	L	1502	U10	O2-C2-C3	-3.42	113.79	121.03
4	L	1304	BCL	C1-O2A-CGA	3.41	124.90	116.65
6	M	1401	BPH	C6-C5-C3	3.39	121.74	113.47
5	L	1502	U10	C30-C29-C31	-3.39	109.34	115.23
4	L	1304	BCL	OBB-CAB-C3B	3.38	126.41	120.43
8	M	1600	SPN	C14-C13-C12	-3.38	113.59	121.17
6	M	1401	BPH	CAA-C2A-C3A	-3.36	103.91	113.00
4	L	1302	BCL	CMA-C3A-C2A	-3.34	101.08	113.98
4	L	1304	BCL	CHB-C1B-NB	3.32	129.02	124.05
8	M	1600	SPN	C16-C17-C18	3.31	121.53	113.47
4	L	1303	BCL	CMD-C2D-C1D	3.30	130.54	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1402	BPH	O1D-CGD-CBD	-3.30	119.72	124.72
4	L	1304	BCL	O2D-CGD-O1D	-3.29	117.45	123.85
4	L	1303	BCL	CHC-C1C-NC	3.25	129.09	124.40
4	M	1301	BCL	O2D-CGD-O1D	-3.24	117.55	123.85
6	M	1402	BPH	C4A-C3A-C2A	3.21	105.89	102.84
4	L	1303	BCL	O2A-CGA-CBA	3.16	121.47	111.83
6	M	1402	BPH	CAA-C2A-C3A	-3.16	104.46	113.00
4	L	1303	BCL	CAC-C3C-C4C	-3.11	105.67	112.58
4	M	1301	BCL	OBb-CAB-CBB	-3.06	112.93	119.77
6	M	1402	BPH	C1C-C2C-C3C	3.02	105.71	102.84
4	M	1301	BCL	C2C-C3C-C4C	3.01	105.85	101.34
4	L	1302	BCL	OBb-CAB-C3B	3.01	125.75	120.43
4	M	1301	BCL	CMA-C3A-C2A	-2.97	102.52	113.98
6	M	1401	BPH	O2A-CGA-O1A	-2.96	116.22	123.63
6	M	1401	BPH	C1B-NB-C4B	-2.95	104.52	108.82
9	M	1800	CDL	OB8-CB6-CB4	2.93	116.83	108.40
6	M	1401	BPH	C4C-C3C-C2C	2.92	105.62	102.84
5	L	1502	U10	C16-C14-C13	2.91	127.70	121.17
4	L	1302	BCL	C2C-C3C-C4C	2.89	105.67	101.34
4	L	1302	BCL	CAA-C2A-C3A	-2.81	105.42	113.00
4	L	1303	BCL	O1D-CGD-CBD	-2.76	119.08	124.52
6	M	1402	BPH	C1B-NB-C4B	-2.75	104.81	108.82
4	L	1303	BCL	O2D-CGD-O1D	-2.72	118.56	123.85
6	M	1402	BPH	CED-O2D-CGD	2.69	122.01	115.92
5	L	1502	U10	C20-C19-C21	-2.67	110.59	115.23
4	L	1304	BCL	O2A-CGA-CBA	2.63	119.85	111.83
9	M	1800	CDL	CB6-CB4-CB3	-2.63	105.66	111.78
4	L	1304	BCL	CAA-C2A-C3A	-2.62	105.92	113.00
4	M	1301	BCL	C4D-CHA-C1A	2.61	124.36	121.24
4	L	1303	BCL	CHD-C1D-ND	-2.58	121.17	124.80
4	L	1303	BCL	CHB-C1B-NB	2.53	127.84	124.05
4	L	1304	BCL	C3C-C2C-C1C	2.50	105.91	101.87
4	M	1301	BCL	CHB-C1B-NB	2.49	127.79	124.05
4	L	1304	BCL	OBb-CAB-CBB	-2.47	114.25	119.77
5	L	1502	U10	C6-C1-C2	2.45	121.11	119.17
6	M	1402	BPH	C4D-ND-C1D	-2.45	105.94	108.87
5	L	1502	U10	C1M-C1-C6	-2.43	120.46	124.45
8	M	1600	SPN	CM3-C5-C6	2.43	119.44	115.23
5	L	1502	U10	C1-C6-C5	-2.42	117.27	119.62
4	L	1303	BCL	C5-C3-C2	2.42	126.59	121.17
4	M	1301	BCL	CAB-C3B-C2B	2.41	132.75	127.74
5	L	1502	U10	C4-C3-C2	-2.40	116.28	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1304	BCL	CHB-C4A-NA	2.39	127.85	124.40
6	M	1402	BPH	C4-C3-C5	-2.38	111.10	115.23
4	L	1303	BCL	C3C-C2C-C1C	2.37	105.69	101.87
5	L	1502	U10	C17-C18-C19	2.30	132.90	127.62
6	M	1401	BPH	CMB-C2B-C3B	2.29	129.26	124.68
6	M	1401	BPH	C5-C3-C2	-2.28	116.06	121.17
4	L	1304	BCL	O1D-CGD-CBD	-2.26	120.06	124.52
4	M	1301	BCL	CHA-C1A-NA	-2.25	121.30	126.39
6	M	1401	BPH	CMD-C2D-C3D	2.24	129.17	124.68
9	M	1800	CDL	OA8-CA7-OA9	-2.24	118.02	123.63
9	M	1800	CDL	OB6-CB5-OB7	-2.22	118.52	123.70
8	M	1600	SPN	C15-C16-C17	2.21	121.26	113.13
6	M	1402	BPH	C4C-C3C-C2C	2.21	104.94	102.84
6	M	1401	BPH	OBD-CAD-CBD	-2.20	122.60	125.82
4	L	1303	BCL	O2A-CGA-O1A	-2.19	118.15	123.63
5	L	1502	U10	C7-C6-C5	-2.19	115.97	118.52
4	M	1301	BCL	O1D-CGD-CBD	-2.19	120.20	124.52
4	L	1304	BCL	CAB-C3B-C2B	2.15	132.21	127.74
4	L	1302	BCL	C2A-C3A-C4A	2.14	105.33	101.87
4	L	1303	BCL	C3A-C2A-C1A	2.13	104.53	101.34
4	L	1302	BCL	CMA-C3A-C4A	-2.13	106.05	111.77
8	M	1600	SPN	C7-C6-C5	2.13	120.23	113.19
6	M	1401	BPH	C7-C6-C5	-2.11	107.64	113.26
4	M	1301	BCL	C2B-C1B-NB	-2.11	108.14	110.33
5	L	1502	U10	C12-C13-C14	-2.10	122.82	127.62
4	L	1304	BCL	CMB-C2B-C1B	-2.09	122.23	125.42
4	L	1304	BCL	C2A-C3A-C4A	2.09	105.25	101.87
6	M	1402	BPH	CBC-CAC-C3C	2.09	117.88	113.78
5	L	1502	U10	O5-C5-C4	2.09	125.45	121.03
6	M	1401	BPH	C4-C3-C5	2.08	118.85	115.23
6	M	1401	BPH	CMA-C3A-C2A	-2.07	106.14	114.13
4	L	1304	BCL	CHB-C1B-C2B	-2.06	121.44	127.43
9	M	1800	CDL	CA6-CA4-CA3	-2.06	106.98	111.78
4	L	1304	BCL	O2A-CGA-O1A	-2.05	118.49	123.63
5	L	1502	U10	C31-C29-C28	2.05	125.78	121.17
6	M	1402	BPH	C3D-C4D-ND	2.05	110.34	107.71
4	M	1301	BCL	CMA-C3A-C4A	-2.05	106.27	111.77
4	L	1303	BCL	CHB-C1B-C2B	-2.04	121.50	127.43
4	L	1302	BCL	C3C-C2C-C1C	2.03	105.15	101.87
4	L	1303	BCL	CMC-C2C-C3C	-2.03	106.13	113.98
4	L	1304	BCL	CMA-C3A-C2A	-2.02	106.17	113.98
4	M	1301	BCL	C3C-C2C-C1C	2.02	105.13	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1401	BPH	C6-C7-C8	-2.02	109.25	115.97
4	M	1301	BCL	CHD-C1D-ND	-2.00	121.98	124.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1301	BCL	C8
4	M	1301	BCL	C13
6	M	1401	BPH	C8
6	M	1401	BPH	C13

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1301	BCL	C1-C2-C3-C4
5	L	1502	U10	C29-C31-C32-C33
5	L	1502	U10	C31-C32-C33-C34
6	M	1401	BPH	O2A-C1-C2-C3
6	M	1401	BPH	C1-C2-C3-C5
8	M	1600	SPN	C3-C4-C5-CM3
9	M	1800	CDL	CA3-OA5-PA1-OA2
9	M	1800	CDL	CA3-OA5-PA1-OA3
9	M	1800	CDL	CA3-OA5-PA1-OA4
6	M	1401	BPH	C4-C3-C5-C6
8	M	1600	SPN	C11-C10-C9-CM4
8	M	1600	SPN	C16-C17-C18-CM6
6	M	1401	BPH	C2-C3-C5-C6
8	M	1600	SPN	C14-C15-C16-C17
8	M	1600	SPN	C4-C5-C6-C7
8	M	1600	SPN	C11-C10-C9-C8
8	M	1600	SPN	C12-C13-C14-C15
8	M	1600	SPN	C16-C17-C18-C19
5	L	1502	U10	C24-C26-C27-C28
8	M	1600	SPN	CM5-C13-C14-C15
8	M	1600	SPN	C20-C21-C22-CM7
6	M	1401	BPH	C15-C16-C17-C18
4	L	1302	BCL	C15-C16-C17-C18
4	M	1301	BCL	C15-C16-C17-C18
9	M	1800	CDL	CB7-C71-C72-C73
4	L	1302	BCL	C13-C15-C16-C17
9	M	1800	CDL	C11-CA5-OA6-CA4
9	M	1800	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
6	M	1401	BPH	C5-C6-C7-C8
8	M	1600	SPN	C24-C25-C26-CM8
9	M	1800	CDL	C54-C55-C56-C57
9	M	1800	CDL	C79-C80-C81-C82
9	M	1800	CDL	C39-C40-C41-C42
4	L	1302	BCL	C14-C13-C15-C16
9	M	1800	CDL	C78-C79-C80-C81
4	M	1301	BCL	C4-C3-C5-C6
9	M	1800	CDL	C34-C35-C36-C37
5	L	1502	U10	C15-C14-C16-C17
5	L	1502	U10	C13-C14-C16-C17
6	M	1402	BPH	C8-C10-C11-C12
4	M	1301	BCL	C11-C12-C13-C15
4	M	1301	BCL	C12-C13-C15-C16
6	M	1401	BPH	C11-C12-C13-C15
6	M	1401	BPH	C12-C13-C15-C16
5	L	1502	U10	C33-C34-C36-C37
4	M	1301	BCL	C14-C13-C15-C16
6	M	1401	BPH	C6-C7-C8-C9
9	M	1800	CDL	OA5-CA3-CA4-OA6
9	M	1800	CDL	C36-C37-C38-C39
9	M	1800	CDL	C80-C81-C82-C83
4	L	1304	BCL	C13-C15-C16-C17
4	M	1301	BCL	C2-C3-C5-C6
9	M	1800	CDL	C52-C53-C54-C55
4	M	1301	BCL	C3-C5-C6-C7
9	M	1800	CDL	C21-C22-C23-C24
5	L	1502	U10	C35-C34-C36-C37
6	M	1402	BPH	C4-C3-C5-C6
8	M	1600	SPN	CM3-C5-C6-C7
4	M	1301	BCL	C11-C10-C8-C9
6	M	1401	BPH	C11-C12-C13-C14
8	M	1600	SPN	C21-C22-C23-C24
6	M	1402	BPH	C2-C3-C5-C6
6	M	1401	BPH	C1-C2-C3-C4
5	L	1502	U10	C20-C19-C21-C22
9	M	1800	CDL	C40-C41-C42-C43
9	M	1800	CDL	C11-C12-C13-C14
9	M	1800	CDL	C13-C14-C15-C16
9	M	1800	CDL	C19-C20-C21-C22
5	L	1502	U10	C18-C19-C21-C22
8	M	1600	SPN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
4	M	1301	BCL	C10-C11-C12-C13
6	M	1402	BPH	O2A-C1-C2-C3
9	M	1800	CDL	C81-C82-C83-C84
4	L	1303	BCL	C16-C17-C18-C19
4	L	1304	BCL	C15-C16-C17-C18
4	L	1304	BCL	C16-C17-C18-C19
9	M	1800	CDL	OA5-CA3-CA4-CA6
4	L	1302	BCL	C11-C12-C13-C15
4	L	1304	BCL	C16-C17-C18-C20
9	M	1800	CDL	CA3-CA4-CA6-OA8
9	M	1800	CDL	C55-C56-C57-C58
4	L	1304	BCL	CHA-CBD-CGD-O1D
4	M	1301	BCL	CHA-CBD-CGD-O1D
4	M	1301	BCL	C11-C12-C13-C14
9	M	1800	CDL	CA5-C11-C12-C13
9	M	1800	CDL	C33-C34-C35-C36
9	M	1800	CDL	C20-C21-C22-C23
4	L	1302	BCL	C12-C13-C15-C16
4	M	1301	BCL	C1-C2-C3-C5
5	L	1502	U10	C25-C24-C26-C27
8	M	1600	SPN	CM8-C26-C27-C28
4	L	1304	BCL	C4C-C3C-CAC-CBC
8	M	1600	SPN	C2-C3-C4-C5
4	L	1304	BCL	C14-C13-C15-C16
4	L	1303	BCL	C16-C17-C18-C20
6	M	1401	BPH	C13-C15-C16-C17
9	M	1800	CDL	C72-C71-CB7-OB8
9	M	1800	CDL	C51-C52-C53-C54
9	M	1800	CDL	C72-C71-CB7-OB9
8	M	1600	SPN	C10-C11-C12-C13
8	M	1600	SPN	C18-C19-C20-C21
8	M	1600	SPN	C6-C7-C8-C9
4	L	1302	BCL	CAD-CBD-CGD-O2D
4	L	1303	BCL	CAA-CBA-CGA-O2A
4	L	1304	BCL	C12-C13-C15-C16

There are no ring outliers.

7 monomers are involved in 26 short contacts:

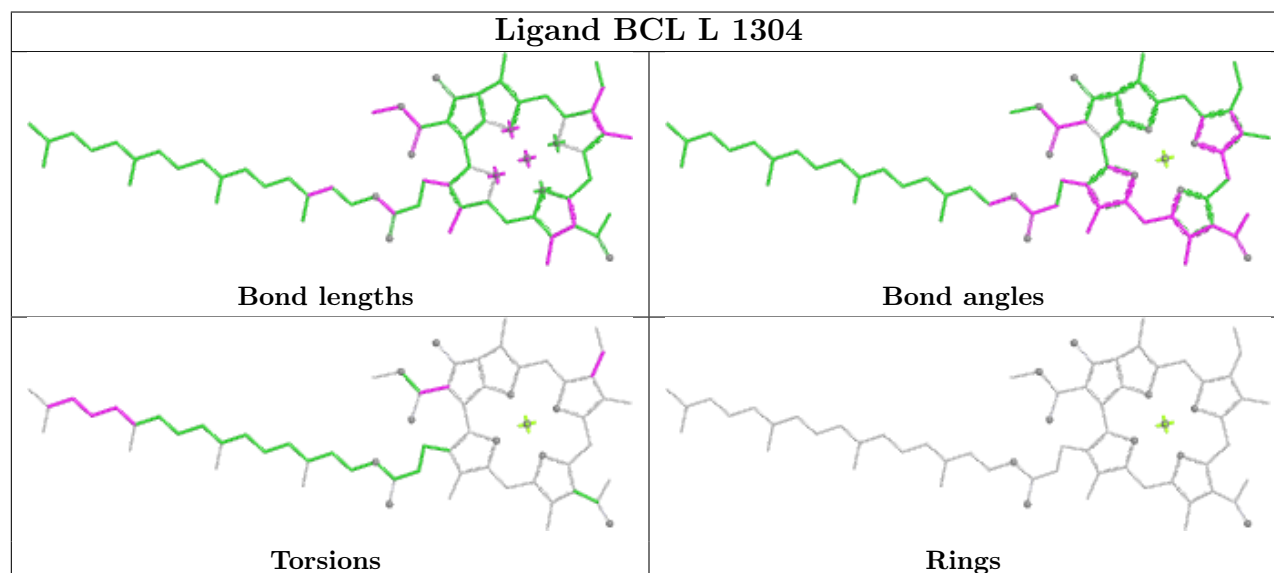
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1304	BCL	2	0
4	L	1302	BCL	2	0

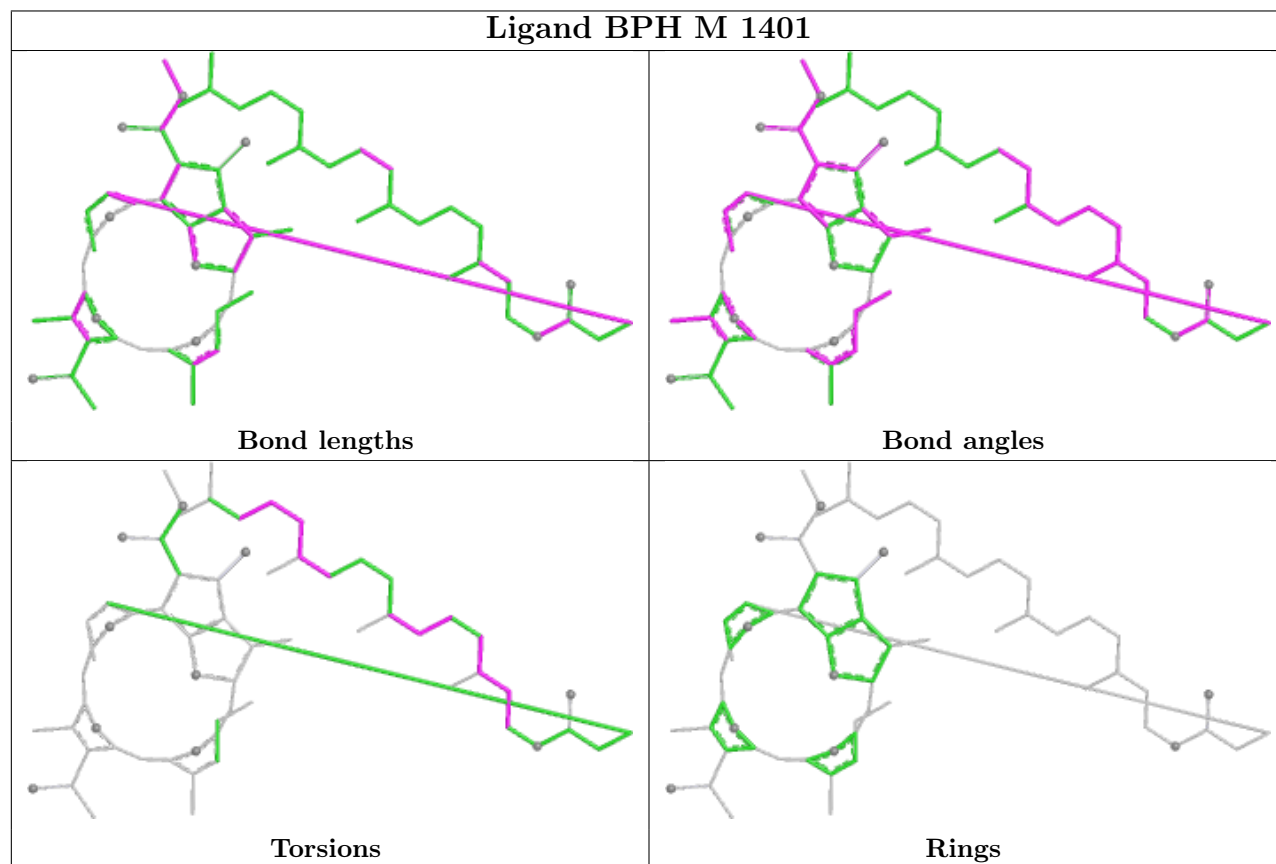
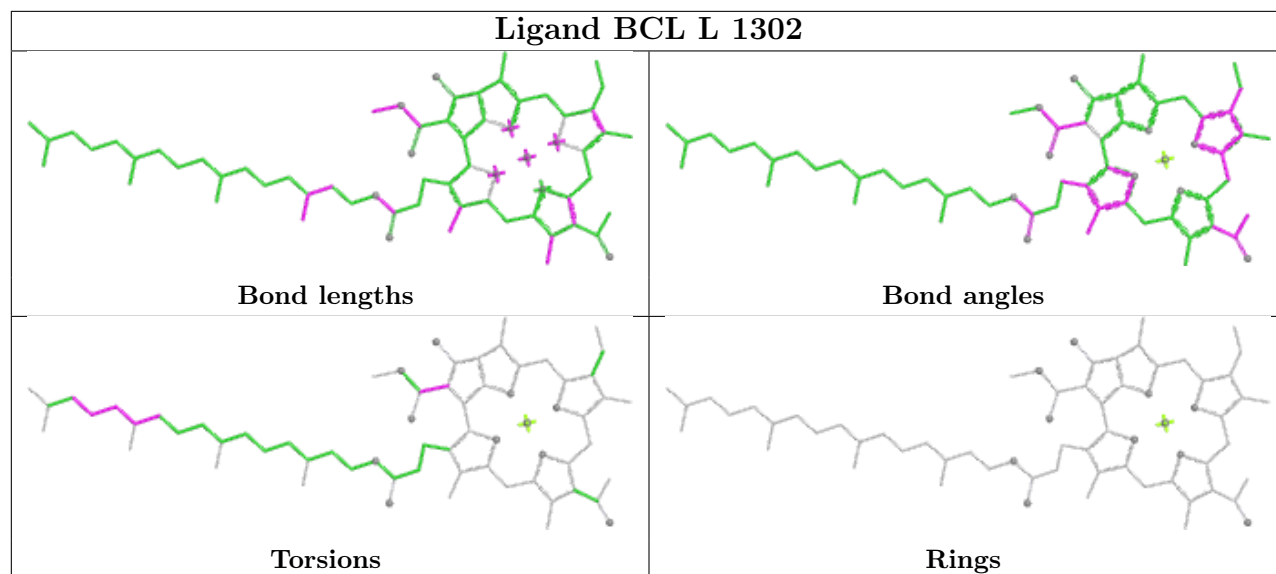
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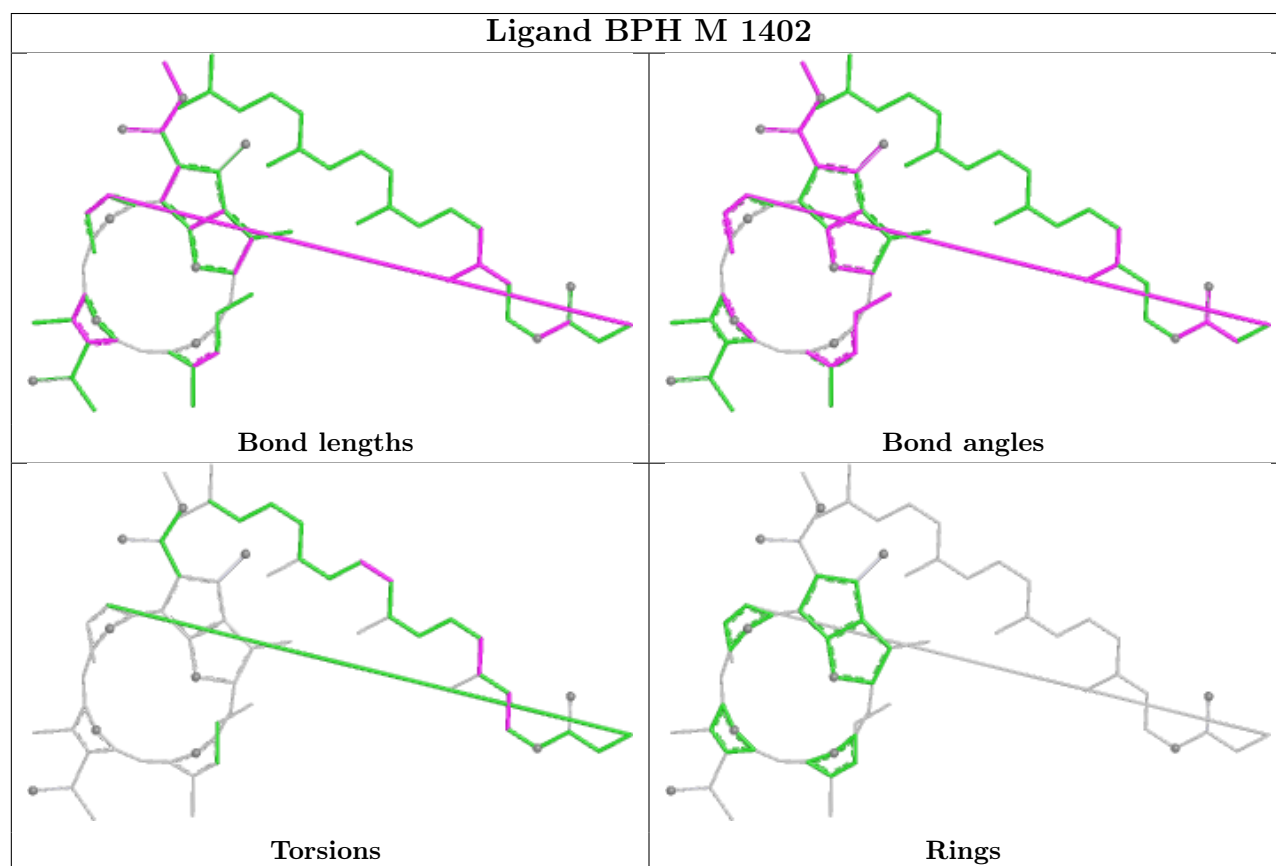
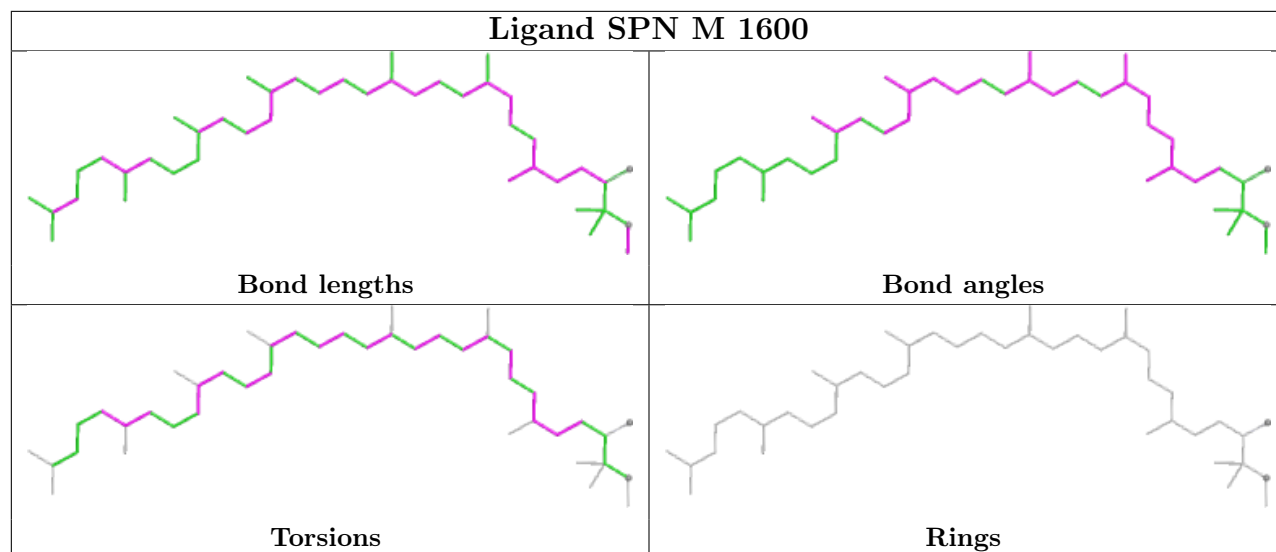
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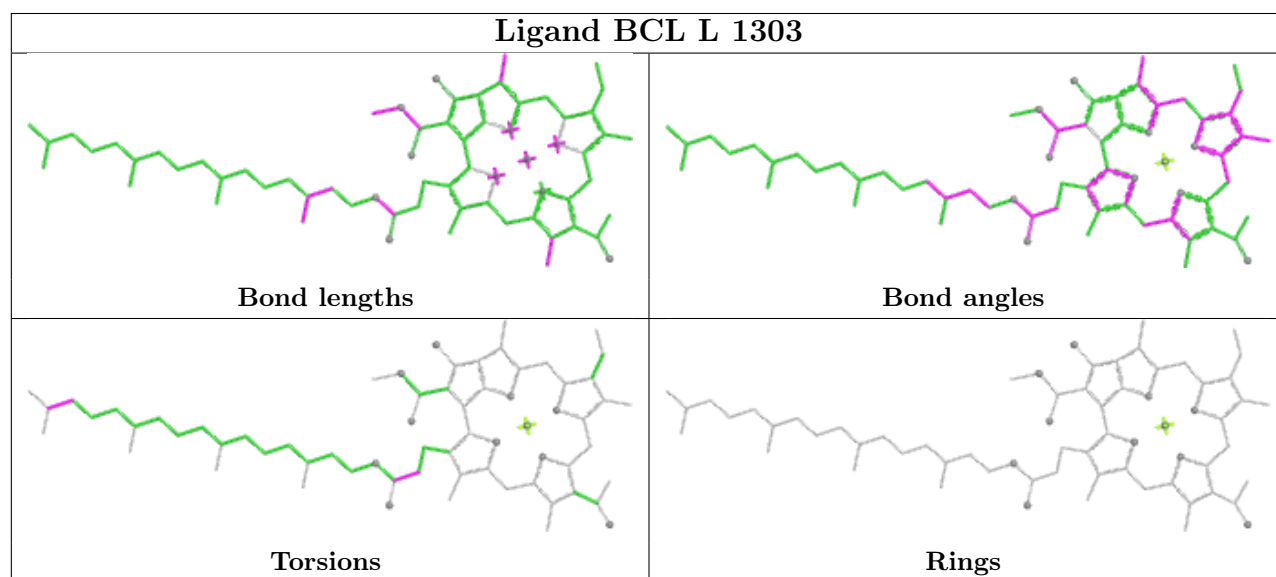
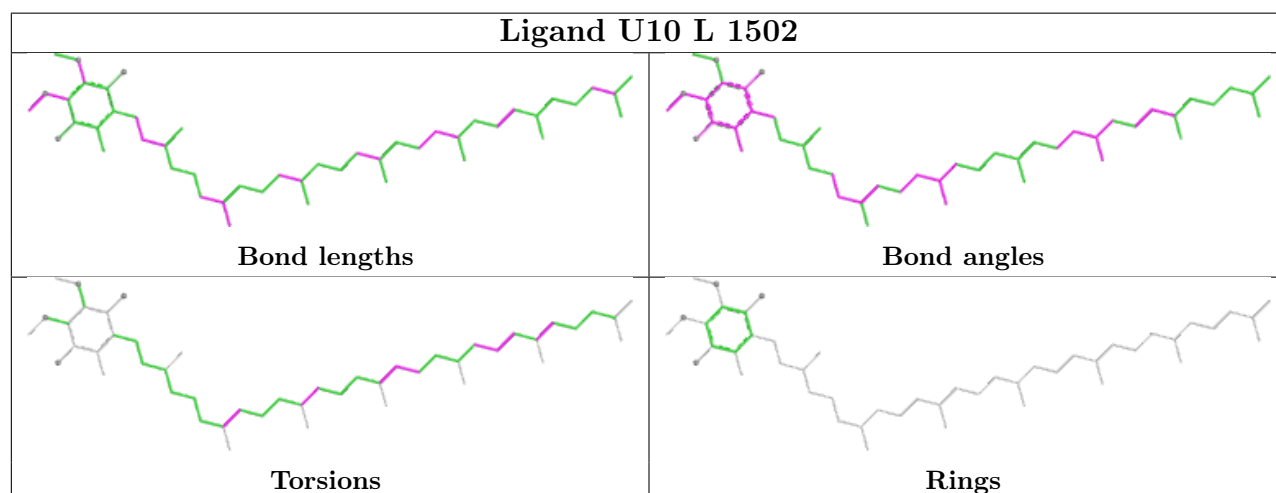
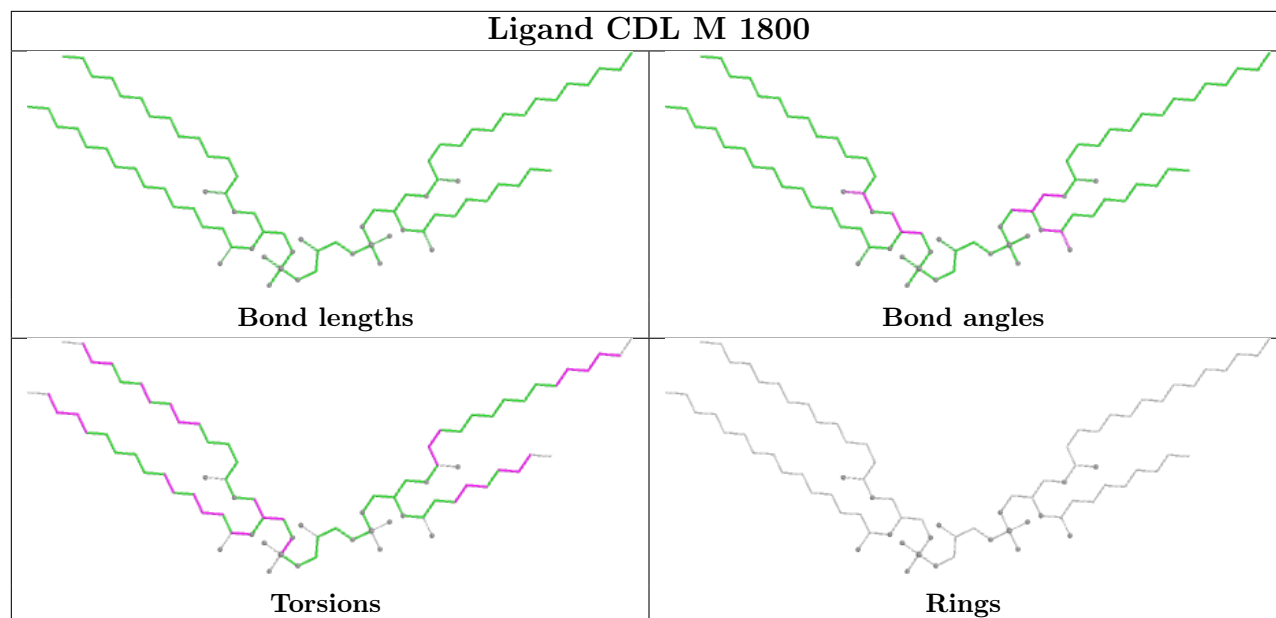
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1600	SPN	2	0
6	M	1402	BPH	3	0
5	L	1502	U10	10	0
4	L	1303	BCL	3	0
4	M	1301	BCL	6	0

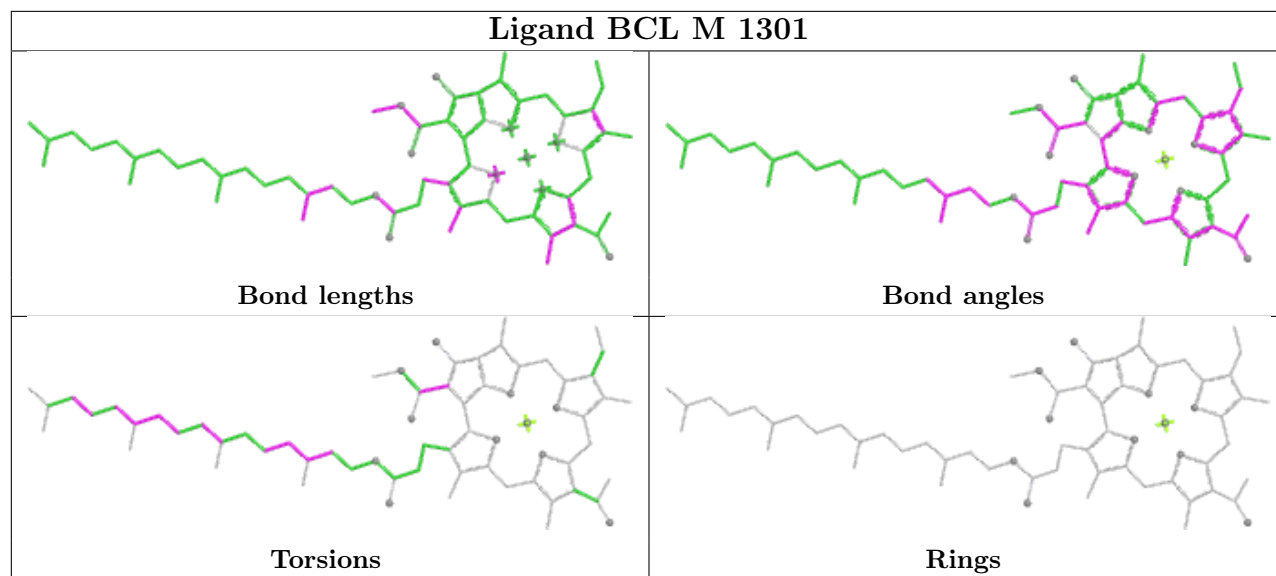
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.