



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:52 AM UTC

PDB ID : 1E6D / pdb_00001e6d
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH TRP M115 REPLACED WITH PHE (CHAIN M, WM115F) PHE M197 REPLACED WITH ARG (CHAIN M, FM197R)
Authors : Ridge, J.P.; Fyfe, P.K.; McAuley, K.E.; Van Brederode, M.E.; Robert, B.; Van Grondelle, R.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.
Deposited on : 2000-08-11
Resolution : 2.30 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

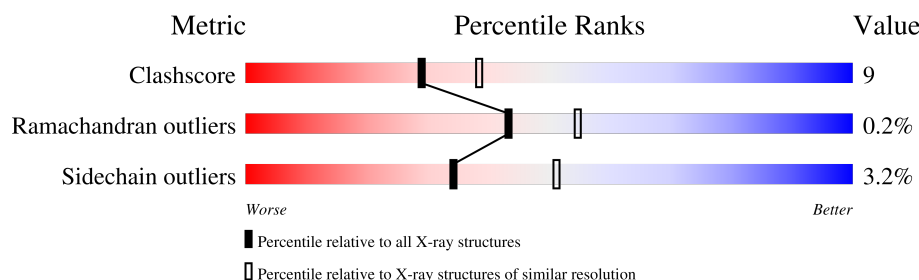
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	77% 13% 8%
2	L	281	80% 17%
3	M	307	77% 20%

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
10	PO4	M	1800	-	X	-	-
10	PO4	M	1801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1304	X	-	-	-
5	BCL	M	1301	X	-	-	-
6	BPH	M	1401	X	-	-	-
9	SPN	M	1600	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7334 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 H SUBUNIT.

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 L SUBUNIT.

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

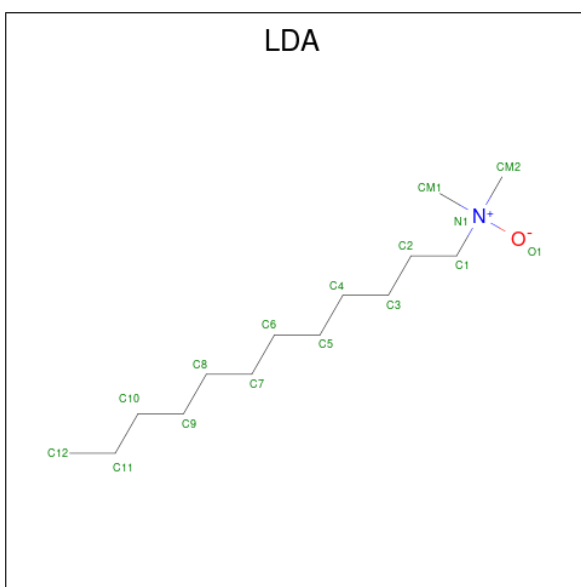
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2405	1602	396	397	10			

There are 2 discrepancies between the modelled and reference sequences:

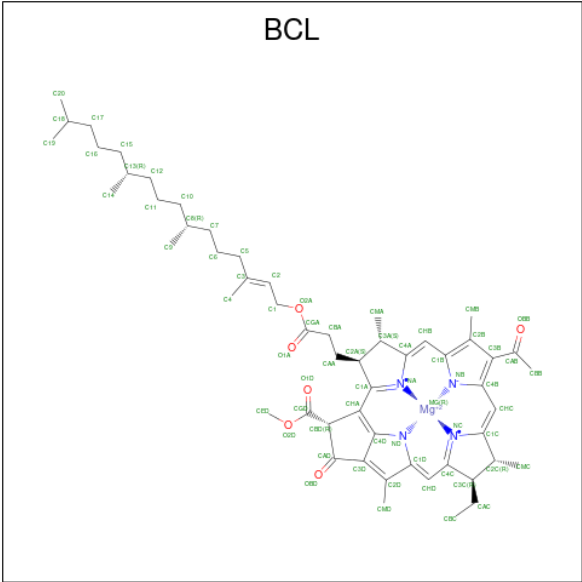
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	engineered mutation	UNP P02953
M	115	PHE	TRP	engineered mutation	UNP P02953

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



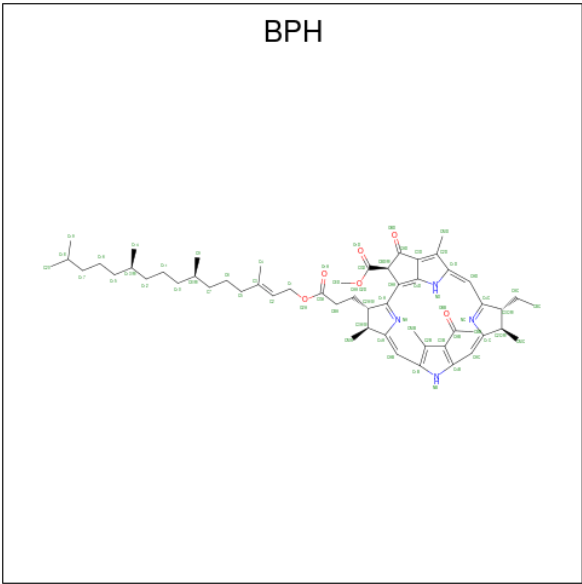
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



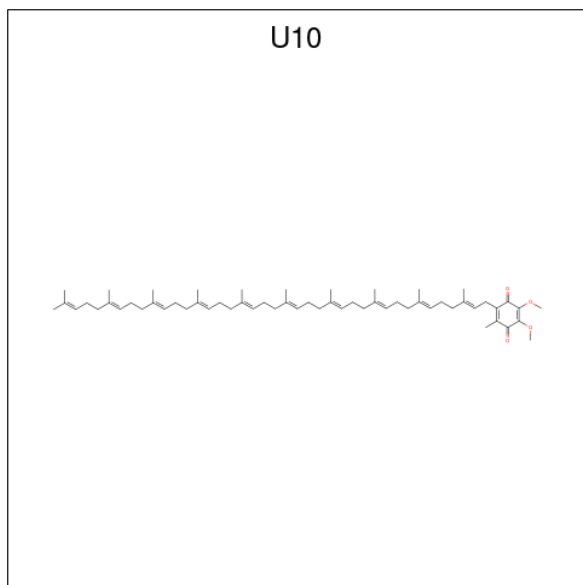
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

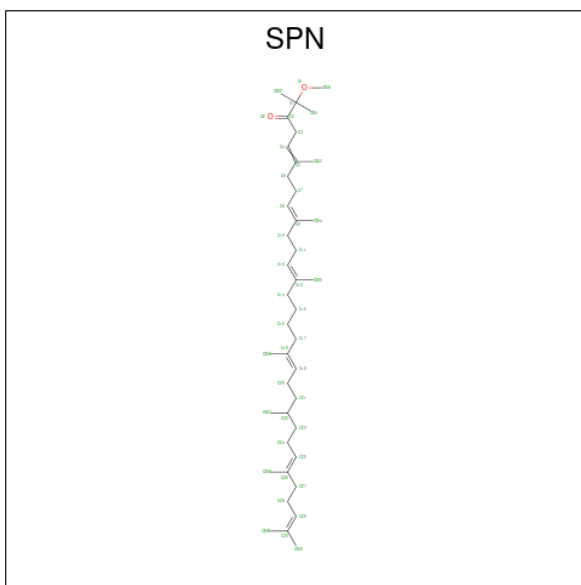


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

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

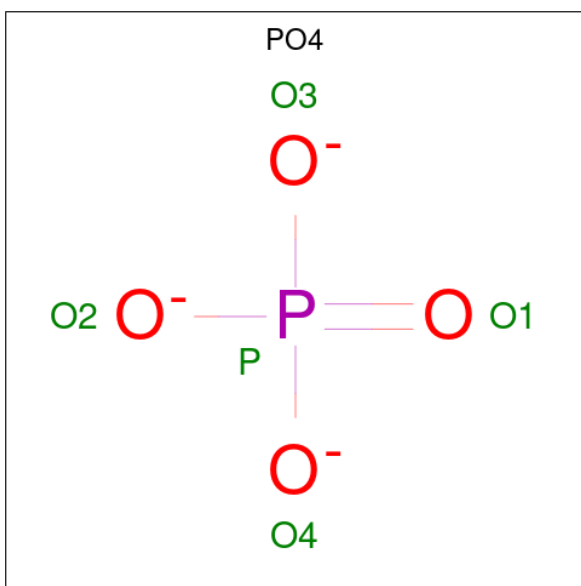
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	1	Total O 1 1	0	0
11	H	94	Total O 94 94	0	0
11	L	1	Total O 1 1	0	0
11	L	1	Total O 1 1	0	0
11	L	47	Total O 47 47	0	0
11	M	2	Total O 2 2	0	0
11	M	1	Total O 1 1	0	0
11	M	65	Total O 65 65	0	0

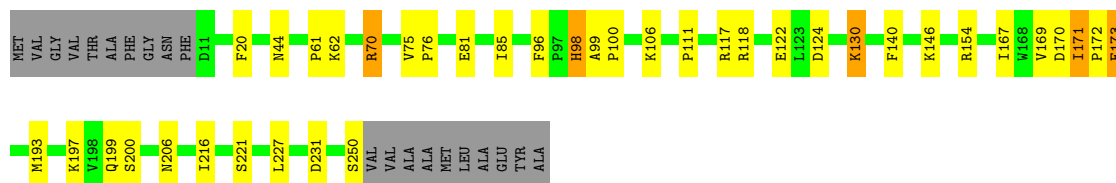
3 Residue-property plots

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.

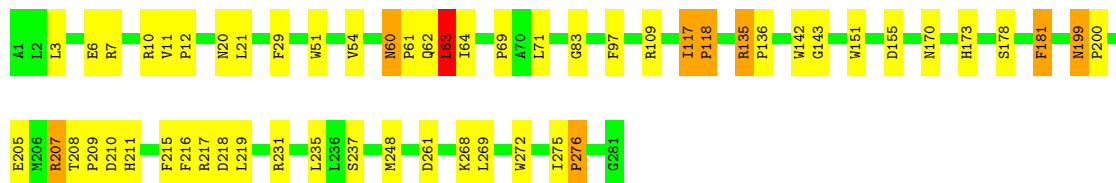
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H: 



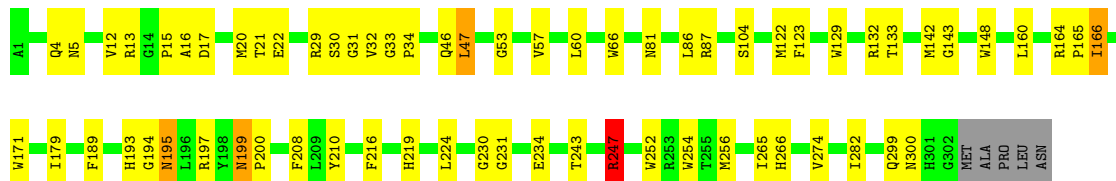
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L: 



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

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	141.20Å 141.20Å 187.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.40 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (26.40-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7334	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: PO4, BCL, U10, SPN, BPH, FE, LDA

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	0.93	0/1877	1.63	19/2553 (0.7%)
2	L	0.97	1/2320 (0.0%)	1.52	23/3175 (0.7%)
3	M	0.88	3/2495 (0.1%)	1.48	21/3404 (0.6%)
All	All	0.93	4/6692 (0.1%)	1.54	63/9132 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	254	TRP	NE1-CE2	-5.23	1.31	1.37
2	L	29	PHE	N-CA	-5.16	1.39	1.46
3	M	252	TRP	NE1-CE2	-5.09	1.31	1.37
3	M	219	HIS	CE1-NE2	-5.00	1.27	1.32

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	CD-NE-CZ	18.28	149.99	124.40
2	L	237	SER	CA-CB-OG	-7.96	95.19	111.10
1	H	98	HIS	CA-CB-CG	-7.27	106.53	113.80
1	H	173	GLU	CB-CG-CD	6.96	124.43	112.60
1	H	96	PHE	CA-CB-CG	-6.92	106.88	113.80
3	M	166	ILE	CB-CA-C	-6.88	103.16	111.97
2	L	6	GLU	N-CA-C	6.79	120.78	112.23
2	L	269	LEU	N-CA-C	-6.70	101.62	109.93
3	M	219	HIS	CA-CB-CG	-6.61	107.19	113.80
2	L	181	PHE	CA-CB-CG	6.49	120.29	113.80
2	L	63	LEU	N-CA-C	-6.47	106.01	114.04
2	L	135	ARG	CD-NE-CZ	6.36	133.30	124.40
3	M	234	GLU	N-CA-C	6.04	117.86	111.28
3	M	208	PHE	CA-CB-CG	-5.98	107.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	130	LYS	CB-CG-CD	5.95	124.99	111.30
3	M	231	GLY	N-CA-C	5.92	120.05	112.83
2	L	117	ILE	CA-C-N	5.86	125.55	119.05
2	L	117	ILE	C-N-CA	5.86	125.55	119.05
2	L	60	ASN	CA-C-N	5.79	125.47	119.05
2	L	60	ASN	C-N-CA	5.79	125.47	119.05
2	L	118	PRO	N-CA-CB	5.76	109.66	103.33
1	H	20	PHE	CA-CB-CG	-5.75	108.05	113.80
1	H	206	ASN	CA-CB-CG	-5.71	106.89	112.60
3	M	282	ILE	CA-C-N	5.63	126.23	119.98
3	M	282	ILE	C-N-CA	5.63	126.23	119.98
2	L	170	ASN	CA-C-N	5.55	125.38	119.28
2	L	170	ASN	C-N-CA	5.55	125.38	119.28
3	M	247	ARG	NE-CZ-NH2	5.52	124.17	119.20
3	M	46	GLN	N-CA-C	5.49	118.19	109.96
1	H	124	ASP	CA-CB-CG	5.38	117.98	112.60
2	L	276	PRO	N-CA-CB	5.35	108.01	103.35
1	H	167	ILE	CA-C-O	-5.35	114.69	120.36
2	L	173	HIS	CA-CB-CG	5.35	119.15	113.80
3	M	160	LEU	N-CA-C	5.33	117.08	111.28
2	L	199	ASN	OD1-CG-ND2	-5.31	117.29	122.60
3	M	123	PHE	CA-CB-CG	5.31	119.11	113.80
3	M	15	PRO	N-CA-CB	5.28	107.76	103.32
1	H	44	ASN	CA-C-O	-5.28	115.87	121.94
2	L	20	ASN	CA-C-N	5.25	127.64	120.54
2	L	20	ASN	C-N-CA	5.25	127.64	120.54
1	H	117	ARG	NE-CZ-NH2	5.24	123.91	119.20
3	M	81	ASN	CA-C-N	5.23	124.86	119.05
3	M	81	ASN	C-N-CA	5.23	124.86	119.05
3	M	31	GLY	N-CA-C	-5.23	103.56	112.51
1	H	216	ILE	CA-C-N	5.23	125.23	119.90
1	H	216	ILE	C-N-CA	5.23	125.23	119.90
2	L	29	PHE	N-CA-C	5.22	118.07	109.76
2	L	10	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	M	230	GLY	CA-C-N	5.21	125.86	120.03
3	M	230	GLY	C-N-CA	5.21	125.86	120.03
1	H	206	ASN	OD1-CG-ND2	5.20	127.80	122.60
2	L	3	LEU	N-CA-C	-5.18	103.20	110.50
1	H	154	ARG	NE-CZ-NH2	5.18	123.86	119.20
3	M	132	ARG	NE-CZ-NH2	5.12	123.80	119.20
3	M	266	HIS	CA-CB-CG	-5.11	108.69	113.80
2	L	83	GLY	N-CA-C	5.10	121.78	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	CG-CD-NE	5.08	123.17	112.00
1	H	171	ILE	CA-C-N	5.06	125.09	119.32
1	H	171	ILE	C-N-CA	5.06	125.09	119.32
3	M	143	GLY	N-CA-C	-5.04	106.09	112.54
1	H	250	SER	CA-C-O	-5.03	112.25	120.80
3	M	4	GLN	N-CA-C	5.02	119.40	113.28
2	L	109	ARG	NE-CZ-NH2	5.01	123.71	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	18	0
2	L	2232	0	2187	38	0
3	M	2405	0	2324	47	0
4	H	32	0	62	0	0
4	M	80	0	155	11	0
5	L	132	0	148	5	0
5	M	132	0	148	12	0
6	L	65	0	75	6	0
6	M	65	0	76	10	0
7	L	48	0	63	8	0
7	M	48	0	63	3	0
8	M	1	0	0	0	0
9	M	43	0	69	2	0
10	M	10	0	0	3	0
11	H	95	0	0	1	0
11	L	49	0	0	8	0
11	M	68	0	0	1	0
All	All	7334	0	7206	125	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 9.

All (125) 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)
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.38	1.06
3:M:243:THR:O	3:M:247:ARG:HG2	1.58	1.02
5:M:1303:BCL:H191	4:M:1706:LDA:H121	1.47	0.97
6:L:1402:BPH:HHC	6:L:1402:BPH:HBB3	1.51	0.93
4:M:1701:LDA:H91	4:M:1702:LDA:H121	1.54	0.88
7:L:1502:U10:H4M1	11:L:3004:HOH:O	1.75	0.85
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.59	0.83
5:M:1303:BCL:C19	4:M:1706:LDA:H121	2.14	0.77
3:M:243:THR:OG1	3:M:247:ARG:HD3	1.85	0.76
2:L:215:PHE:CB	3:M:142:MET:HE1	2.14	0.76
2:L:261:ASP:OD2	11:L:2047:HOH:O	2.05	0.73
2:L:231:ARG:HD3	3:M:5:ASN:O	1.89	0.72
3:M:199:ASN:HD22	3:M:199:ASN:C	1.98	0.71
3:M:189:PHE:O	3:M:193:HIS:HD2	1.73	0.71
1:H:197:LYS:HE2	1:H:199:GLN:HE21	1.55	0.70
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.72	0.70
4:M:1701:LDA:H91	4:M:1702:LDA:C12	2.21	0.70
3:M:148:TRP:CD1	4:M:1703:LDA:HM22	2.27	0.70
2:L:217:ARG:NH1	11:L:2037:HOH:O	2.24	0.70
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.28	0.68
7:L:1502:U10:H3M3	11:L:2041:HOH:O	1.96	0.66
6:L:1402:BPH:HBB3	6:L:1402:BPH:CHC	2.26	0.65
6:M:1401:BPH:HHC	6:M:1401:BPH:HBB3	1.80	0.64
5:M:1301:BCL:H141	9:M:1600:SPN:H101	1.79	0.64
1:H:146:LYS:NZ	1:H:200:SER:O	2.31	0.63
6:L:1402:BPH:HBB2	3:M:210:TYR:HB3	1.81	0.62
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.81	0.62
3:M:243:THR:O	3:M:247:ARG:CG	2.43	0.61
2:L:208:THR:HB	2:L:209:PRO:HD2	1.81	0.61
2:L:215:PHE:HB2	3:M:142:MET:CE	2.25	0.60
3:M:60:LEU:HA	6:M:1401:BPH:H4C2	1.84	0.60
4:M:1703:LDA:CM2	10:M:1801:PO4:O3	2.50	0.59
3:M:148:TRP:HD1	4:M:1703:LDA:HM22	1.65	0.59
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.85	0.58
5:L:1302:BCL:CBB	5:L:1302:BCL:HMB3	2.35	0.57
2:L:60:ASN:O	2:L:64:ILE:HG13	2.05	0.56
7:L:1502:U10:H3M1	11:L:2036:HOH:O	2.05	0.56
5:L:1302:BCL:HMB3	5:L:1302:BCL:HBB2	1.89	0.55
6:L:1402:BPH:HHC	6:L:1402:BPH:CBB	2.32	0.54
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.07	0.54
2:L:231:ARG:HG2	3:M:224:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:265:ILE:HG21	7:M:1501:U10:H3M2	1.90	0.54
1:H:118:ARG:HD2	11:H:2055:HOH:O	2.08	0.53
3:M:189:PHE:O	3:M:193:HIS:CD2	2.59	0.53
4:M:1703:LDA:HM11	10:M:1800:PO4:O4	2.10	0.52
2:L:60:ASN:OD1	2:L:61:PRO:HD2	2.10	0.52
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.91	0.52
3:M:32:VAL:HG12	3:M:33:GLY:O	2.09	0.52
2:L:181:PHE:CD2	6:M:1401:BPH:HBB1	2.45	0.52
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.46	0.51
2:L:215:PHE:CG	3:M:142:MET:HE1	2.46	0.50
2:L:207:ARG:HD2	2:L:207:ARG:N	2.26	0.50
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.50
5:M:1301:BCL:H102	5:M:1303:BCL:H202	1.93	0.50
7:L:1502:U10:C3M	11:L:2041:HOH:O	2.56	0.50
6:M:1401:BPH:HHD	6:M:1401:BPH:HBC3	1.93	0.50
7:L:1502:U10:H202	5:M:1301:BCL:H43	1.94	0.49
2:L:135:ARG:HD2	2:L:248:MET:O	2.12	0.49
1:H:173:GLU:HG2	11:L:2042:HOH:O	2.11	0.49
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.93	0.49
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.47	0.49
1:H:171:ILE:HB	1:H:172:PRO:CD	2.37	0.49
5:L:1304:BCL:OBB	5:L:1304:BCL:HHC	2.13	0.49
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.95	0.49
3:M:129:TRP:CH2	4:M:1706:LDA:H102	2.49	0.48
5:M:1301:BCL:C3B	9:M:1600:SPN:H152	2.43	0.48
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.29	0.48
2:L:181:PHE:HB3	6:M:1401:BPH:CBB	2.44	0.47
1:H:111:PRO:O	3:M:247:ARG:NH2	2.44	0.47
7:L:1502:U10:H322	7:L:1502:U10:H301	1.41	0.47
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.97	0.47
2:L:178:SER:HB3	7:L:1502:U10:H222	1.97	0.47
1:H:62:LYS:NZ	2:L:199:ASN:HD21	2.14	0.46
3:M:129:TRP:O	3:M:133:THR:HG23	2.16	0.46
6:L:1402:BPH:CHC	6:L:1402:BPH:CBB	2.91	0.46
1:H:140:PHE:HA	3:M:13:ARG:O	2.16	0.46
3:M:21:THR:O	3:M:22:GLU:C	2.57	0.46
6:M:1401:BPH:HBB3	6:M:1401:BPH:CHC	2.45	0.46
3:M:166:ILE:HD11	3:M:171:TRP:CH2	2.51	0.45
2:L:117:ILE:HB	2:L:118:PRO:HD3	1.98	0.45
6:M:1401:BPH:H192	6:M:1401:BPH:H161	1.61	0.45
5:M:1301:BCL:H152	5:M:1301:BCL:H111	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1706:LDA:H123	4:M:1706:LDA:H92	1.52	0.45
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.65	0.45
2:L:97:PHE:CE1	5:L:1302:BCL:H121	2.51	0.45
1:H:61:PRO:HA	1:H:76:PRO:HD2	2.00	0.44
5:M:1301:BCL:CBB	5:M:1301:BCL:HMB1	2.48	0.44
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.99	0.44
2:L:62:GLN:HB2	2:L:151:TRP:CD1	2.52	0.44
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.53	0.44
3:M:256:MET:CE	7:M:1501:U10:H102	2.47	0.44
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.52	0.43
3:M:247:ARG:HG2	3:M:247:ARG:H	1.54	0.43
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.43
3:M:265:ILE:HD12	3:M:265:ILE:HA	1.85	0.43
3:M:300:ASN:N	3:M:300:ASN:OD1	2.50	0.43
1:H:130:LYS:HE3	1:H:170:ASP:OD1	2.19	0.43
6:L:1402:BPH:HBA2	6:L:1402:BPH:H3A	1.85	0.43
6:M:1401:BPH:HH2	6:M:1401:BPH:CB2	2.49	0.43
3:M:34:PRO:O	3:M:47:LEU:HB2	2.18	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.43	0.43
7:L:1502:U10:H272	7:L:1502:U10:H251	1.43	0.42
5:L:1302:BCL:CBB	5:L:1302:BCL:CMB	2.97	0.42
3:M:199:ASN:HD22	3:M:200:PRO:N	2.15	0.42
2:L:155:ASP:OD1	3:M:197:ARG:NH1	2.37	0.42
2:L:51:TRP:O	2:L:54:VAL:HG22	2.20	0.42
3:M:53:GLY:O	3:M:57:VAL:HG23	2.20	0.42
7:M:1501:U10:H28	7:M:1501:U10:H322	1.73	0.41
2:L:205:GLU:OE2	11:L:2032:HOH:O	2.21	0.41
5:M:1301:BCL:H141	5:M:1301:BCL:H162	1.84	0.41
2:L:275:ILE:HA	2:L:276:PRO:HD3	1.91	0.41
4:M:1703:LDA:HM23	10:M:1801:PO4:P	2.61	0.41
3:M:17:ASP:OD2	11:M:2016:HOH:O	2.22	0.41
3:M:179:ILE:HG23	5:M:1301:BCL:HED1	2.01	0.41
3:M:16:ALA:HB1	3:M:32:VAL:HG21	2.03	0.41
3:M:164:ARG:N	3:M:165:PRO:HD2	2.35	0.41
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.38	0.41
2:L:11:VAL:HB	2:L:12:PRO:HD2	2.02	0.41
2:L:181:PHE:HB3	6:M:1401:BPH:HBB2	2.03	0.41
6:M:1401:BPH:HBC3	6:M:1401:BPH:CHD	2.50	0.41
5:M:1301:BCL:H101	5:M:1301:BCL:H61	1.68	0.41
2:L:63:LEU:HD12	2:L:63:LEU:HA	1.88	0.40
1:H:99:ALA:HA	1:H:100:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:194:GLY:O	3:M:195:ASN:CB	2.69	0.40
5:M:1301:BCL:H3A	5:M:1301:BCL:HBA1	1.92	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%)	233 (98%)	5 (2%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/307 (98%)	290 (97%)	8 (3%)	2 (1%)	18	23
All	All	817/848 (96%)	794 (97%)	21 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	30	SER
3	M	195	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	190 (97%)	5 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	220/220 (100%)	213 (97%)	7 (3%)	34	51
3	M	236/240 (98%)	227 (96%)	9 (4%)	29	44
All	All	651/668 (98%)	630 (97%)	21 (3%)	34	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	70	ARG
1	H	106	LYS
1	H	193	MET
1	H	221	SER
1	H	231	ASP
2	L	21	LEU
2	L	63	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	268	LYS
3	M	12	VAL
3	M	47	LEU
3	M	86	LEU
3	M	104	SER
3	M	199	ASN
3	M	216	PHE
3	M	247	ARG
3	M	274	VAL
3	M	299	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	206	ASN
2	L	183	ASN
2	L	199	ASN
2	L	280	ASN
3	M	28	ASN
3	M	187	ASN
3	M	193	HIS

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Mol	Chain	Res	Type
3	M	199	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	BCL	L	1304	2	69,74,74	1.47	11 (15%)	79,115,115	2.30	17 (21%)
6	BPH	M	1401	-	59,70,70	2.06	16 (27%)	59,101,101	3.05	18 (30%)
4	LDA	H	1707	-	13,15,15	2.25	2 (15%)	14,17,17	0.75	0
4	LDA	M	1706	-	13,15,15	2.58	2 (15%)	14,17,17	0.86	0
6	BPH	L	1402	-	59,70,70	2.22	15 (25%)	59,101,101	2.77	18 (30%)
10	PO4	M	1800	-	4,4,4	3.37	2 (50%)	6,6,6	1.96	2 (33%)
4	LDA	M	1705	-	13,15,15	2.41	2 (15%)	14,17,17	0.70	0
7	U10	L	1502	-	48,48,63	2.07	16 (33%)	60,61,79	1.67	10 (16%)
5	BCL	M	1303	3	69,74,74	1.45	10 (14%)	79,115,115	2.31	18 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PO4	M	1801	-	4,4,4	2.30	1 (25%)	6,6,6	1.35	0
7	U10	M	1501	-	48,48,63	1.93	15 (31%)	60,61,79	1.52	9 (15%)
9	SPN	M	1600	-	42,42,42	4.10	19 (45%)	50,52,52	2.33	18 (36%)
4	LDA	M	1702	-	13,15,15	2.67	2 (15%)	14,17,17	0.64	0
4	LDA	H	1704	-	13,15,15	2.78	2 (15%)	14,17,17	0.43	0
4	LDA	M	1701	-	13,15,15	2.70	2 (15%)	14,17,17	0.63	0
5	BCL	M	1301	3	69,74,74	1.47	9 (13%)	79,115,115	2.22	18 (22%)
4	LDA	M	1703	-	13,15,15	2.39	2 (15%)	14,17,17	0.67	0
5	BCL	L	1302	2	69,74,74	1.46	9 (13%)	79,115,115	2.38	21 (26%)

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	BCL	L	1304	2	1/1/21/25	7/41/137/137	-
6	BPH	M	1401	-	1/1/18/22	14/37/105/105	0/5/6/6
4	LDA	H	1707	-	-	4/13/13/13	-
4	LDA	M	1706	-	-	9/13/13/13	-
6	BPH	L	1402	-	-	5/37/105/105	0/5/6/6
4	LDA	M	1705	-	-	7/13/13/13	-
7	U10	L	1502	-	-	19/45/69/87	0/1/1/1
5	BCL	M	1303	3	-	3/41/137/137	-
7	U10	M	1501	-	-	8/45/69/87	0/1/1/1
9	SPN	M	1600	-	-	22/50/51/51	-
4	LDA	M	1702	-	-	6/13/13/13	-
4	LDA	H	1704	-	-	8/13/13/13	-
4	LDA	M	1701	-	-	2/13/13/13	-
5	BCL	M	1301	3	1/1/21/25	13/41/137/137	-
4	LDA	M	1703	-	-	6/13/13/13	-
5	BCL	L	1302	2	-	0/41/137/137	-

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1600	SPN	C8-C9	10.02	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1600	SPN	C3-C2	9.79	1.60	1.52
9	M	1600	SPN	C4-C5	9.29	1.54	1.33
9	M	1600	SPN	C12-C13	8.77	1.53	1.33
9	M	1600	SPN	C19-C18	8.34	1.52	1.33
4	M	1702	LDA	O1-N1	-8.23	1.22	1.42
4	M	1706	LDA	O1-N1	-8.04	1.22	1.42
6	M	1401	BPH	C2C-C3C	-7.96	1.47	1.54
6	L	1402	BPH	C2C-C3C	-7.59	1.48	1.54
4	M	1703	LDA	O1-N1	-7.46	1.23	1.42
4	H	1707	LDA	O1-N1	-7.45	1.23	1.42
4	M	1701	LDA	O1-N1	-7.43	1.23	1.42
4	H	1704	LDA	O1-N1	-7.39	1.24	1.42
4	M	1705	LDA	O1-N1	-7.33	1.24	1.42
4	H	1704	LDA	C1-N1	-6.71	1.44	1.51
6	L	1402	BPH	C3A-C2A	-6.27	1.49	1.54
10	M	1800	PO4	P-O1	6.25	1.65	1.50
4	M	1701	LDA	C1-N1	-6.23	1.45	1.51
9	M	1600	SPN	C10-C9	-6.23	1.38	1.51
5	L	1302	BCL	MG-NA	5.95	2.20	2.06
6	M	1401	BPH	C1D-C2D	5.79	1.45	1.39
9	M	1600	SPN	C3-C4	-5.65	1.41	1.50
9	M	1600	SPN	C14-C13	-5.60	1.39	1.51
7	L	1502	U10	C7-C8	-5.58	1.41	1.50
6	L	1402	BPH	O2D-CGD	5.44	1.46	1.33
9	M	1600	SPN	C6-C5	-5.42	1.40	1.51
5	M	1303	BCL	MG-NA	5.36	2.19	2.06
5	M	1303	BCL	O2D-CGD	5.32	1.46	1.33
9	M	1600	SPN	C17-C18	-5.23	1.40	1.51
5	L	1304	BCL	O2D-CGD	5.21	1.46	1.33
5	M	1301	BCL	O2D-CGD	5.11	1.45	1.33
5	L	1302	BCL	O2D-CGD	4.92	1.45	1.33
4	M	1702	LDA	C1-N1	-4.87	1.46	1.51
7	M	1501	U10	O3-C3	4.76	1.48	1.36
6	M	1401	BPH	C1B-C2B	4.64	1.44	1.39
4	M	1705	LDA	C1-N1	-4.54	1.46	1.51
4	M	1706	LDA	C1-N1	-4.48	1.46	1.51
5	M	1301	BCL	MG-NA	4.43	2.16	2.06
10	M	1801	PO4	P-O1	4.42	1.60	1.50
6	L	1402	BPH	C1D-C2D	4.41	1.44	1.39
6	L	1402	BPH	C1B-C2B	4.41	1.44	1.39
4	M	1703	LDA	C1-N1	-4.24	1.47	1.51
7	M	1501	U10	C33-C34	4.21	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1401	BPH	O2D-CGD	4.05	1.43	1.33
5	L	1304	BCL	MG-NA	4.01	2.15	2.06
7	L	1502	U10	O4-C4M	-3.92	1.36	1.45
7	L	1502	U10	O3-C3	3.86	1.46	1.36
7	M	1501	U10	C23-C24	3.81	1.41	1.33
9	M	1600	SPN	C25-C26	3.79	1.41	1.33
7	L	1502	U10	O4-C4	3.75	1.45	1.36
5	M	1301	BCL	O2A-CGA	3.65	1.44	1.33
6	L	1402	BPH	CBD-CGD	-3.63	1.47	1.52
5	L	1304	BCL	C2-C3	3.63	1.41	1.33
6	L	1402	BPH	CMA-C3A	3.62	1.59	1.53
5	M	1301	BCL	CMA-C3A	3.54	1.60	1.53
6	L	1402	BPH	O2A-CGA	3.54	1.43	1.33
9	M	1600	SPN	O1-CMA	3.51	1.54	1.43
5	M	1301	BCL	CAA-C2A	3.49	1.60	1.54
6	L	1402	BPH	O2D-CED	-3.48	1.37	1.45
7	L	1502	U10	C8-C9	3.40	1.40	1.33
7	M	1501	U10	O4-C4	3.40	1.45	1.36
6	M	1401	BPH	O2D-CED	-3.39	1.37	1.45
7	M	1501	U10	O3-C3M	-3.31	1.37	1.45
9	M	1600	SPN	C20-C19	-3.24	1.40	1.50
7	L	1502	U10	C18-C19	3.22	1.40	1.33
9	M	1600	SPN	C11-C12	-3.22	1.40	1.50
6	L	1402	BPH	CHA-CBD	3.21	1.55	1.51
7	L	1502	U10	C28-C29	3.20	1.40	1.33
9	M	1600	SPN	C7-C8	-3.20	1.40	1.50
6	M	1401	BPH	O2A-CGA	3.16	1.42	1.33
5	M	1301	BCL	C2-C3	3.07	1.40	1.33
7	M	1501	U10	C7-C8	-3.06	1.45	1.50
4	H	1707	LDA	C1-N1	-3.06	1.48	1.51
5	L	1302	BCL	C2-C3	3.03	1.40	1.33
6	M	1401	BPH	CBD-CGD	-2.98	1.48	1.52
7	M	1501	U10	C13-C14	2.92	1.39	1.33
5	M	1303	BCL	O2A-CGA	2.91	1.41	1.33
9	M	1600	SPN	C29-C30	2.88	1.41	1.32
7	L	1502	U10	C33-C34	2.83	1.39	1.33
9	M	1600	SPN	C21-C22	-2.83	1.38	1.52
5	L	1304	BCL	C3B-C4B	2.83	1.46	1.41
5	M	1301	BCL	C2C-C3C	-2.83	1.46	1.54
5	M	1303	BCL	C2-C3	2.83	1.39	1.33
7	M	1501	U10	C8-C9	2.80	1.39	1.33
7	L	1502	U10	O3-C3M	-2.79	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1501	U10	C31-C29	2.77	1.57	1.51
5	M	1303	BCL	O2D-CED	-2.75	1.39	1.45
6	L	1402	BPH	C3B-C2B	-2.72	1.35	1.39
5	L	1304	BCL	CAA-C2A	2.71	1.59	1.54
6	M	1401	BPH	CMA-C3A	2.70	1.58	1.53
6	L	1402	BPH	C2-C3	2.67	1.39	1.33
7	L	1502	U10	C38-C39	2.65	1.40	1.32
6	M	1401	BPH	CHA-CBD	2.64	1.54	1.51
7	M	1501	U10	C38-C39	2.64	1.40	1.32
9	M	1600	SPN	C16-C15	-2.63	1.38	1.51
5	M	1303	BCL	C2C-C3C	-2.59	1.47	1.54
5	L	1302	BCL	CBB-CAB	2.51	1.55	1.50
5	L	1302	BCL	C2C-C3C	-2.48	1.47	1.54
6	L	1402	BPH	CAC-C3C	-2.44	1.48	1.53
7	M	1501	U10	C18-C19	2.43	1.38	1.33
6	M	1401	BPH	C3D-C4D	2.43	1.44	1.41
10	M	1800	PO4	P-O3	-2.42	1.47	1.54
5	M	1303	BCL	C4-C3	2.39	1.56	1.50
5	M	1303	BCL	MG-NC	2.39	2.11	2.06
5	L	1302	BCL	MG-ND	-2.38	2.01	2.05
5	L	1302	BCL	O2A-CGA	2.36	1.40	1.33
7	L	1502	U10	C13-C14	2.35	1.38	1.33
7	M	1501	U10	C20-C19	2.35	1.56	1.50
6	L	1402	BPH	CAA-C2A	2.34	1.58	1.54
5	L	1304	BCL	O2A-CGA	2.31	1.40	1.33
5	L	1304	BCL	C3B-C2B	-2.31	1.34	1.42
7	L	1502	U10	C25-C24	2.30	1.56	1.50
5	M	1301	BCL	C3B-C4B	2.29	1.45	1.41
6	M	1401	BPH	CMC-C2C	-2.28	1.49	1.53
7	M	1501	U10	O4-C4M	-2.28	1.40	1.45
5	L	1302	BCL	O2D-CED	-2.22	1.40	1.45
7	L	1502	U10	C36-C34	2.21	1.55	1.51
5	L	1304	BCL	O1D-CGD	2.20	1.26	1.21
5	L	1302	BCL	C4-C3	2.19	1.56	1.50
5	L	1304	BCL	CAC-C3C	2.18	1.58	1.54
7	L	1502	U10	C15-C14	2.16	1.56	1.50
7	L	1502	U10	C23-C24	2.16	1.38	1.33
6	M	1401	BPH	O1D-CGD	2.15	1.26	1.21
6	M	1401	BPH	C2-C3	2.15	1.38	1.33
7	L	1502	U10	C16-C14	2.12	1.55	1.51
5	M	1303	BCL	C3B-C4B	2.10	1.45	1.41
7	M	1501	U10	C35-C34	2.10	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1402	BPH	C3D-CAD	-2.09	1.43	1.47
5	M	1301	BCL	CMB-C2B	2.08	1.55	1.50
5	L	1304	BCL	C2C-C3C	-2.06	1.48	1.54
5	M	1303	BCL	O1D-CGD	2.06	1.26	1.21
9	M	1600	SPN	CM5-C13	2.05	1.55	1.50
6	M	1401	BPH	OBB-CAB	2.05	1.28	1.22
6	M	1401	BPH	C3A-C2A	-2.04	1.53	1.54
7	M	1501	U10	C27-C28	-2.02	1.44	1.50
6	M	1401	BPH	C4D-ND	-2.01	1.35	1.38
5	L	1304	BCL	MG-ND	-2.00	2.01	2.05

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1401	BPH	O2D-CGD-CBD	17.47	130.15	110.95
6	L	1402	BPH	O2D-CGD-CBD	14.27	126.63	110.95
5	L	1302	BCL	C4A-NA-C1A	10.85	111.63	106.68
5	M	1303	BCL	C1C-NC-C4C	10.35	111.40	106.68
5	L	1302	BCL	C1C-NC-C4C	9.02	110.79	106.68
5	M	1303	BCL	C4A-NA-C1A	8.72	110.66	106.68
5	L	1304	BCL	O2D-CGD-CBD	8.47	126.04	111.23
5	M	1301	BCL	C1C-NC-C4C	7.79	110.23	106.68
5	M	1301	BCL	C4A-NA-C1A	7.72	110.20	106.68
5	L	1304	BCL	C4A-NA-C1A	7.07	109.90	106.68
6	M	1401	BPH	O1D-CGD-CBD	-6.83	114.37	124.72
5	L	1304	BCL	C1C-NC-C4C	6.52	109.65	106.68
5	M	1301	BCL	O2D-CGD-CBD	6.42	122.46	111.23
7	M	1501	U10	C27-C28-C29	6.31	142.07	127.62
5	L	1304	BCL	C1-O2A-CGA	6.04	131.27	116.65
5	M	1303	BCL	O2D-CGD-CBD	5.92	121.58	111.23
7	L	1502	U10	C4M-O4-C4	5.90	137.21	116.47
6	L	1402	BPH	O2D-CGD-O1D	-5.71	112.73	123.85
5	M	1301	BCL	O2A-CGA-CBA	5.64	129.02	111.83
5	L	1302	BCL	O2D-CGD-CBD	5.45	120.75	111.23
5	M	1303	BCL	CAC-C3C-C4C	-5.43	100.52	112.58
9	M	1600	SPN	C7-C8-C9	-5.29	115.50	127.62
6	L	1402	BPH	CMA-C3A-C4A	-5.25	103.30	114.61
9	M	1600	SPN	C10-C9-C8	-4.80	110.39	121.17
5	L	1304	BCL	O1D-CGD-CBD	-4.76	115.13	124.52
6	M	1401	BPH	O2D-CGD-O1D	-4.72	114.65	123.85
6	L	1402	BPH	CBC-CAC-C3C	4.71	123.05	113.78
9	M	1600	SPN	C3-C4-C5	-4.68	118.78	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1600	SPN	CM5-C13-C14	4.61	123.22	115.23
6	M	1401	BPH	C4D-CHA-CBD	-4.56	106.27	108.45
5	L	1302	BCL	CAC-C3C-C4C	-4.32	103.00	112.58
6	M	1401	BPH	C4C-C3C-C2C	4.32	106.94	102.84
9	M	1600	SPN	C6-C5-C4	-4.30	111.52	121.17
5	M	1301	BCL	O2D-CGD-O1D	-4.19	115.70	123.85
7	L	1502	U10	C7-C8-C9	4.16	134.00	126.83
7	M	1501	U10	C4M-O4-C4	4.16	131.09	116.47
5	M	1303	BCL	O2A-CGA-CBA	4.16	124.51	111.83
9	M	1600	SPN	CM4-C9-C10	4.15	122.43	115.23
5	M	1301	BCL	O2A-CGA-O1A	-4.13	113.31	123.63
6	L	1402	BPH	O2A-CGA-O1A	-4.05	113.49	123.63
6	L	1402	BPH	O2A-CGA-CBA	4.02	124.09	111.83
5	L	1302	BCL	OBB-CAB-C3B	3.99	127.49	120.43
5	L	1304	BCL	CAB-C3B-C2B	3.97	136.00	127.74
5	L	1302	BCL	O2A-CGA-CBA	3.94	123.84	111.83
5	L	1304	BCL	CAC-C3C-C4C	-3.90	103.92	112.58
6	M	1401	BPH	CMA-C3A-C4A	-3.89	106.22	114.61
5	M	1301	BCL	OBB-CAB-C3B	3.82	127.18	120.43
7	L	1502	U10	C12-C13-C14	3.81	136.34	127.62
5	M	1301	BCL	CAA-C2A-C3A	-3.77	102.81	113.00
9	M	1600	SPN	CM7-C22-C21	3.75	124.65	111.27
6	M	1401	BPH	CED-O2D-CGD	3.72	124.36	115.92
7	L	1502	U10	C8-C7-C6	3.62	120.99	112.08
9	M	1600	SPN	C17-C18-C19	-3.60	113.08	121.17
7	L	1502	U10	C32-C33-C34	3.60	135.87	127.62
6	L	1402	BPH	OBD-CAD-CBD	-3.57	120.58	125.82
10	M	1800	PO4	O2-P-O1	-3.53	98.47	110.95
5	L	1302	BCL	C1-O2A-CGA	3.51	125.15	116.65
9	M	1600	SPN	C20-C19-C18	-3.48	119.66	127.62
9	M	1600	SPN	CM3-C5-C6	3.45	121.22	115.23
6	L	1402	BPH	O1D-CGD-CBD	-3.44	119.50	124.72
5	L	1304	BCL	CAA-C2A-C3A	-3.44	103.72	113.00
5	L	1304	BCL	CHB-C1B-NB	3.42	129.19	124.05
5	L	1304	BCL	C4D-CHA-C1A	3.40	125.30	121.24
5	M	1303	BCL	O2D-CGD-O1D	-3.38	117.27	123.85
5	M	1303	BCL	CMD-C2D-C1D	3.38	130.68	124.73
5	L	1302	BCL	CAA-C2A-C3A	-3.37	103.88	113.00
9	M	1600	SPN	CM6-C18-C17	3.36	121.06	115.23
7	L	1502	U10	C22-C23-C24	3.36	135.31	127.62
6	M	1401	BPH	C1C-C2C-C3C	3.33	106.01	102.84
9	M	1600	SPN	C11-C12-C13	-3.30	120.06	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1402	BPH	C4C-C3C-C2C	3.24	105.92	102.84
5	L	1304	BCL	O2D-CGD-O1D	-3.23	117.56	123.85
6	L	1402	BPH	C1-C2-C3	3.21	131.45	126.20
7	M	1501	U10	C22-C23-C24	-3.20	120.30	127.62
6	L	1402	BPH	C4D-CHA-CBD	-3.20	106.92	108.45
5	M	1301	BCL	CMA-C3A-C2A	-3.15	101.79	113.98
5	L	1302	BCL	O2D-CGD-O1D	-3.15	117.72	123.85
9	M	1600	SPN	C14-C13-C12	-3.15	114.10	121.17
6	L	1402	BPH	C4A-C3A-C2A	3.15	105.83	102.84
5	L	1302	BCL	C2C-C3C-C4C	3.13	106.03	101.34
5	M	1303	BCL	O1D-CGD-CBD	-3.10	118.41	124.52
5	M	1301	BCL	C2C-C3C-C4C	2.96	105.77	101.34
5	L	1302	BCL	C1D-ND-C4D	-2.96	104.24	106.31
5	L	1302	BCL	OBB-CAB-CBB	-2.92	113.22	119.77
5	L	1302	BCL	O2A-CGA-O1A	-2.86	116.46	123.63
7	L	1502	U10	C3M-O3-C3	2.85	126.50	116.47
6	L	1402	BPH	C1C-C2C-C3C	2.83	105.53	102.84
5	L	1304	BCL	C2C-C3C-C4C	2.81	105.55	101.34
5	M	1301	BCL	CMB-C2B-C1B	-2.79	121.17	125.42
6	L	1402	BPH	C1B-NB-C4B	-2.79	104.75	108.82
5	M	1301	BCL	CHB-C1B-NB	2.77	128.21	124.05
5	M	1301	BCL	C3C-C2C-C1C	2.77	106.34	101.87
9	M	1600	SPN	C16-C15-C14	2.77	123.29	113.13
5	M	1301	BCL	CAC-C3C-C4C	-2.76	106.46	112.58
6	M	1401	BPH	CMC-C2C-C1C	2.72	120.47	114.61
7	L	1502	U10	C25-C24-C26	-2.72	110.50	115.23
7	L	1502	U10	C35-C34-C36	-2.72	110.51	115.23
5	M	1303	BCL	C3C-C2C-C1C	2.71	106.25	101.87
9	M	1600	SPN	C11-C10-C9	2.71	122.17	113.19
6	M	1401	BPH	OBD-CAD-CBD	-2.68	121.89	125.82
5	L	1304	BCL	O2A-CGA-CBA	2.63	119.86	111.83
6	L	1402	BPH	CMA-C3A-C2A	-2.62	104.00	114.13
6	M	1401	BPH	CMA-C3A-C2A	-2.61	104.05	114.13
5	L	1302	BCL	CMA-C3A-C2A	-2.61	103.90	113.98
6	M	1401	BPH	CAA-C2A-C3A	-2.59	106.00	113.00
5	M	1303	BCL	CHB-C1B-NB	2.56	127.90	124.05
5	M	1303	BCL	CHD-C1D-ND	-2.56	121.21	124.80
5	M	1303	BCL	C3A-C2A-C1A	2.54	105.15	101.34
5	M	1303	BCL	CAB-C3B-C2B	2.52	132.98	127.74
5	L	1304	BCL	CMB-C2B-C1B	-2.52	121.59	125.42
5	L	1304	BCL	C2A-C1A-CHA	2.50	128.20	123.87
5	L	1302	BCL	CED-O2D-CGD	2.45	121.47	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1600	SPN	C15-C14-C13	2.44	119.42	113.47
7	M	1501	U10	C3M-O3-C3	2.43	125.02	116.47
7	M	1501	U10	C7-C8-C9	2.42	130.99	126.83
5	M	1301	BCL	C1D-ND-C4D	-2.40	104.63	106.31
5	M	1303	BCL	O2A-CGA-O1A	-2.39	117.64	123.63
6	M	1401	BPH	C1-O2A-CGA	2.38	122.41	116.65
9	M	1600	SPN	C7-C6-C5	2.37	121.03	113.19
7	M	1501	U10	C30-C29-C28	2.35	129.65	123.63
6	M	1401	BPH	O2A-CGA-CBA	2.34	118.98	111.83
6	M	1401	BPH	C1B-NB-C4B	-2.34	105.40	108.82
6	L	1402	BPH	CAA-C2A-C3A	-2.34	106.67	113.00
6	M	1401	BPH	C1-C2-C3	2.33	130.01	126.20
7	L	1502	U10	C15-C14-C16	-2.32	111.20	115.23
5	M	1301	BCL	OBB-CAB-CBB	-2.31	114.59	119.77
6	L	1402	BPH	C4-C3-C5	-2.30	111.23	115.23
5	M	1303	BCL	CHC-C1C-NC	2.28	127.70	124.40
5	L	1302	BCL	C1-C2-C3	-2.27	122.48	126.20
6	M	1401	BPH	O2A-CGA-O1A	-2.27	117.95	123.63
5	L	1302	BCL	C3C-C2C-C1C	2.27	105.53	101.87
5	M	1301	BCL	CMA-C3A-C4A	-2.26	105.71	111.77
5	L	1304	BCL	OBB-CAB-C3B	2.25	124.41	120.43
5	L	1302	BCL	CHC-C1C-NC	2.25	127.64	124.40
10	M	1800	PO4	O3-P-O2	2.25	114.90	107.91
7	M	1501	U10	C15-C14-C16	-2.23	111.35	115.23
7	M	1501	U10	C30-C29-C31	-2.19	111.43	115.23
5	M	1303	BCL	C1D-ND-C4D	-2.17	104.79	106.31
5	M	1303	BCL	C7-C6-C5	-2.16	107.51	113.26
5	M	1301	BCL	CED-O2D-CGD	-2.15	111.04	115.92
7	M	1501	U10	C32-C33-C34	-2.11	122.80	127.62
5	M	1303	BCL	C2C-C3C-C4C	2.11	104.50	101.34
5	L	1304	BCL	C3A-C2A-C1A	2.06	104.42	101.34
9	M	1600	SPN	CM4-C9-C8	-2.06	118.34	123.63
5	L	1302	BCL	CHB-C1B-NB	2.05	127.12	124.05
6	M	1401	BPH	C4-C3-C5	-2.04	111.69	115.23
6	L	1402	BPH	OBD-CAD-C3D	2.03	131.06	127.89
5	L	1302	BCL	O2A-C1-C2	-2.02	100.32	108.11
5	L	1302	BCL	O1D-CGD-CBD	-2.02	120.53	124.52

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1304	BCL	C13

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

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1703	LDA	C2-C1-N1-O1
4	M	1703	LDA	C2-C1-N1-CM1
4	M	1705	LDA	N1-C1-C2-C3
4	M	1706	LDA	C2-C1-N1-O1
4	M	1706	LDA	C2-C1-N1-CM1
6	M	1401	BPH	C1-C2-C3-C4
6	M	1401	BPH	C1-C2-C3-C5
9	M	1600	SPN	CM2-C1-C2-O2
9	M	1600	SPN	CM2-C1-C2-C3
9	M	1600	SPN	C3-C4-C5-CM3
9	M	1600	SPN	CM3-C5-C6-C7
6	M	1401	BPH	C4-C3-C5-C6
7	L	1502	U10	C12-C11-C9-C10
7	L	1502	U10	C25-C24-C26-C27
7	L	1502	U10	C30-C29-C31-C32
9	M	1600	SPN	CM5-C13-C14-C15
9	M	1600	SPN	C16-C17-C18-CM6
7	L	1502	U10	C23-C24-C26-C27
9	M	1600	SPN	C14-C15-C16-C17
9	M	1600	SPN	C11-C10-C9-CM4
7	L	1502	U10	C28-C29-C31-C32
9	M	1600	SPN	C4-C5-C6-C7
9	M	1600	SPN	C11-C10-C9-C8
9	M	1600	SPN	C12-C13-C14-C15
9	M	1600	SPN	C16-C17-C18-C19
7	L	1502	U10	C29-C31-C32-C33
7	M	1501	U10	C29-C31-C32-C33
9	M	1600	SPN	C9-C10-C11-C12
7	L	1502	U10	C20-C19-C21-C22
6	M	1401	BPH	C2-C3-C5-C6
7	L	1502	U10	C18-C19-C21-C22
5	M	1301	BCL	C11-C10-C8-C9
9	M	1600	SPN	C20-C21-C22-CM7
5	M	1301	BCL	C11-C12-C13-C15
6	M	1401	BPH	C6-C7-C8-C10
7	L	1502	U10	C3-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
5	L	1304	BCL	C13-C15-C16-C17
5	M	1301	BCL	C10-C11-C12-C13
7	L	1502	U10	C12-C11-C9-C8
5	M	1301	BCL	C3-C5-C6-C7
5	M	1301	BCL	C13-C15-C16-C17
6	M	1401	BPH	C15-C16-C17-C18
9	M	1600	SPN	C24-C25-C26-CM8
4	M	1703	LDA	C1-C2-C3-C4
4	H	1704	LDA	C5-C6-C7-C8
4	M	1706	LDA	C7-C8-C9-C10
4	M	1701	LDA	C3-C4-C5-C6
4	H	1707	LDA	C2-C3-C4-C5
4	H	1707	LDA	C3-C4-C5-C6
4	M	1702	LDA	C5-C6-C7-C8
4	M	1706	LDA	C9-C10-C11-C12
5	M	1301	BCL	C16-C17-C18-C20
7	M	1501	U10	C30-C29-C31-C32
7	M	1501	U10	C28-C29-C31-C32
4	M	1706	LDA	C11-C10-C9-C8
5	M	1301	BCL	C6-C7-C8-C10
5	M	1301	BCL	C11-C12-C13-C14
6	L	1402	BPH	C14-C13-C15-C16
7	M	1501	U10	C25-C24-C26-C27
7	M	1501	U10	C23-C24-C26-C27
6	L	1402	BPH	C8-C10-C11-C12
4	M	1706	LDA	C6-C7-C8-C9
4	H	1704	LDA	C3-C4-C5-C6
4	M	1706	LDA	N1-C1-C2-C3
4	H	1704	LDA	C1-C2-C3-C4
5	M	1301	BCL	C16-C17-C18-C19
6	L	1402	BPH	C4-C3-C5-C6
6	M	1401	BPH	CBA-CGA-O2A-C1
4	M	1706	LDA	C4-C5-C6-C7
4	M	1706	LDA	C1-C2-C3-C4
4	M	1705	LDA	C2-C3-C4-C5
6	M	1401	BPH	C12-C13-C15-C16
9	M	1600	SPN	C21-C22-C23-C24
7	M	1501	U10	C34-C36-C37-C38
6	L	1402	BPH	C2-C3-C5-C6
6	M	1401	BPH	C16-C17-C18-C19
4	M	1702	LDA	C11-C10-C9-C8
6	M	1401	BPH	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	L	1304	BCL	C10-C11-C12-C13
4	H	1707	LDA	C7-C8-C9-C10
7	L	1502	U10	C1-C6-C7-C8
6	M	1401	BPH	C16-C17-C18-C20
4	M	1702	LDA	C4-C5-C6-C7
7	L	1502	U10	C14-C16-C17-C18
7	L	1502	U10	C5-C6-C7-C8
4	M	1703	LDA	C4-C5-C6-C7
4	H	1704	LDA	C11-C10-C9-C8
4	M	1702	LDA	C6-C7-C8-C9
6	M	1401	BPH	C10-C11-C12-C13
7	L	1502	U10	C21-C22-C23-C24
4	H	1704	LDA	C2-C1-N1-CM1
4	M	1703	LDA	C2-C1-N1-CM2
5	L	1304	BCL	O1D-CGD-O2D-CED
7	L	1502	U10	C5-C4-O4-C4M
5	M	1301	BCL	C11-C10-C8-C7
4	M	1702	LDA	C3-C4-C5-C6
5	L	1304	BCL	CHA-CBD-CGD-O2D
9	M	1600	SPN	CM2-C1-O1-CMA
4	M	1702	LDA	C2-C3-C4-C5
4	H	1704	LDA	N1-C1-C2-C3
4	H	1707	LDA	C9-C10-C11-C12
5	M	1301	BCL	C14-C13-C15-C16
6	M	1401	BPH	C14-C13-C15-C16
5	L	1304	BCL	C12-C13-C15-C16
4	M	1705	LDA	C9-C10-C11-C12
7	L	1502	U10	C35-C34-C36-C37
9	M	1600	SPN	C25-C26-C27-C28
4	H	1704	LDA	C2-C3-C4-C5
4	M	1703	LDA	C3-C4-C5-C6
6	M	1401	BPH	C6-C7-C8-C9
6	L	1402	BPH	O2A-C1-C2-C3
7	L	1502	U10	C33-C34-C36-C37
7	L	1502	U10	C15-C14-C16-C17
9	M	1600	SPN	C2-C3-C4-C5
4	M	1705	LDA	C11-C10-C9-C8
5	M	1303	BCL	C16-C17-C18-C19
4	M	1705	LDA	C1-C2-C3-C4
7	M	1501	U10	C14-C16-C17-C18
5	L	1304	BCL	C14-C13-C15-C16
5	M	1301	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	CAA-CBA-CGA-O2A
4	M	1705	LDA	C2-C1-N1-CM1
4	M	1705	LDA	C2-C1-N1-CM2
4	M	1701	LDA	C1-C2-C3-C4
9	M	1600	SPN	C6-C7-C8-C9
9	M	1600	SPN	C10-C11-C12-C13
7	L	1502	U10	C13-C14-C16-C17
9	M	1600	SPN	C18-C19-C20-C21
5	L	1304	BCL	C8-C10-C11-C12
4	H	1704	LDA	C2-C1-N1-O1
7	M	1501	U10	C26-C27-C28-C29
5	M	1301	BCL	C1-C2-C3-C4
5	M	1303	BCL	O1D-CGD-O2D-CED

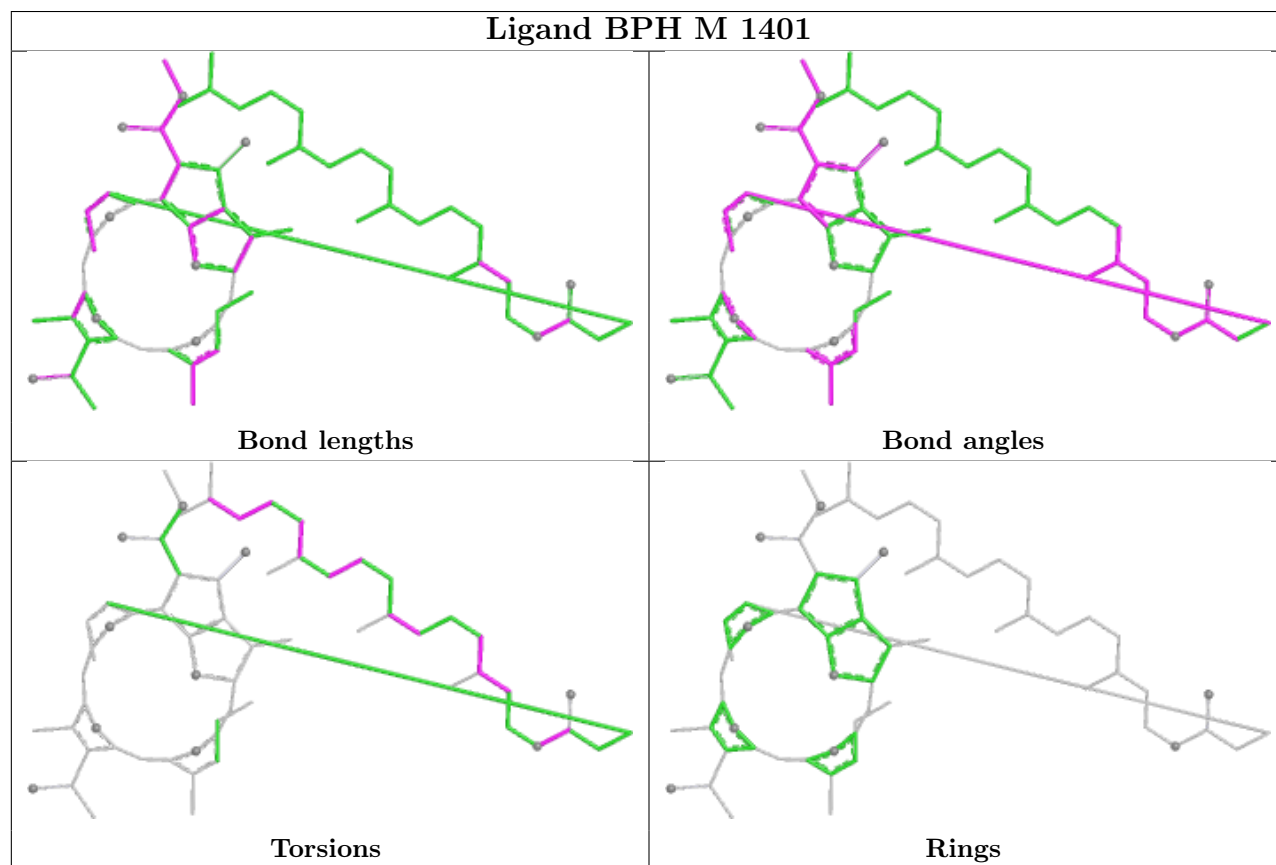
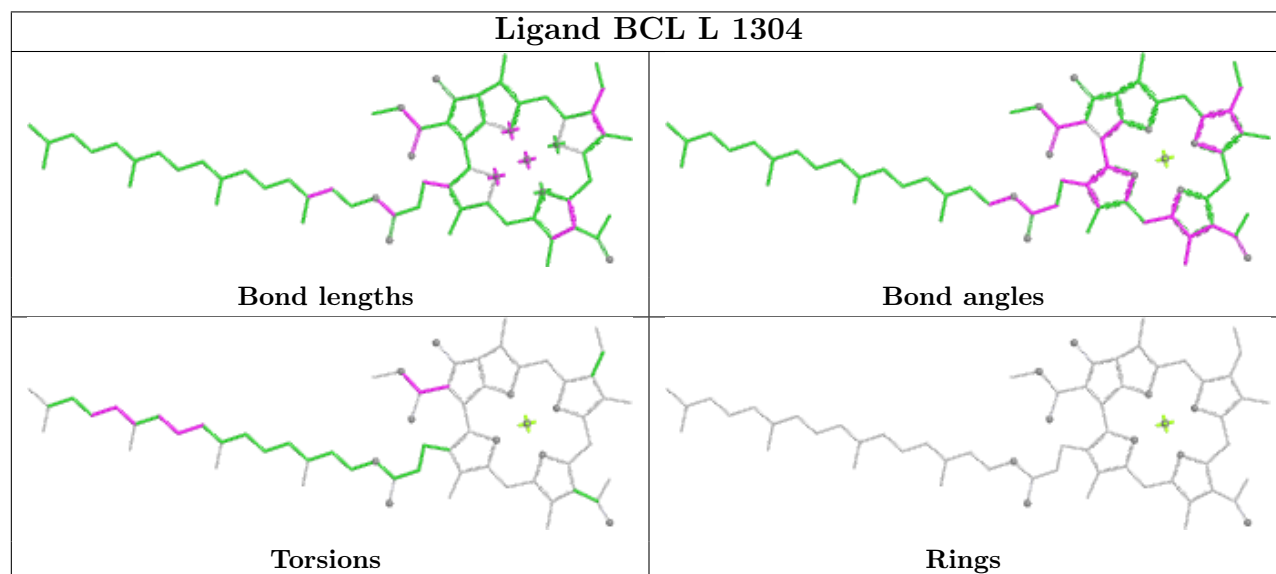
There are no ring outliers.

15 monomers are involved in 52 short contacts:

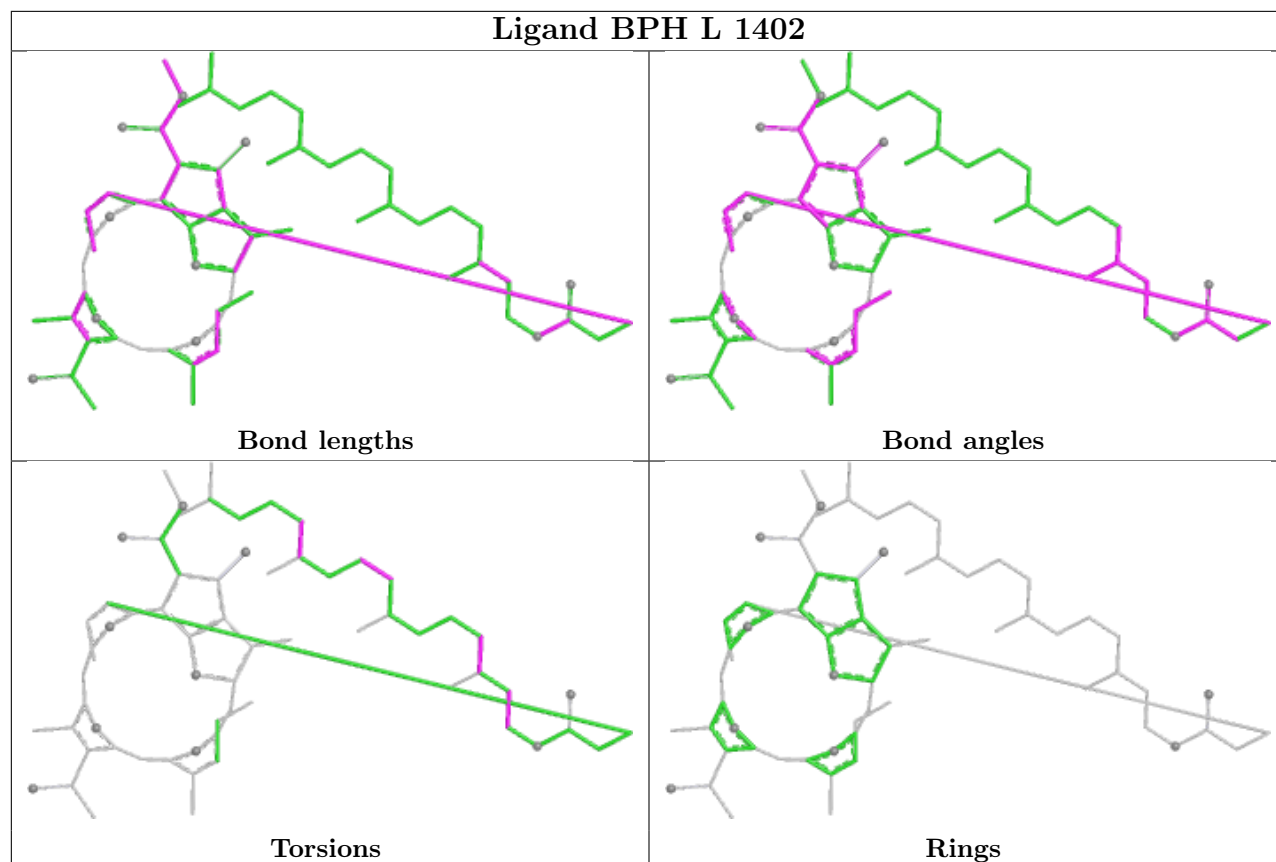
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1304	BCL	1	0
6	M	1401	BPH	10	0
4	M	1706	LDA	4	0
6	L	1402	BPH	6	0
10	M	1800	PO4	1	0
7	L	1502	U10	8	0
5	M	1303	BCL	3	0
10	M	1801	PO4	2	0
7	M	1501	U10	3	0
9	M	1600	SPN	2	0
4	M	1702	LDA	2	0
4	M	1701	LDA	2	0
5	M	1301	BCL	10	0
4	M	1703	LDA	5	0
5	L	1302	BCL	4	0

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

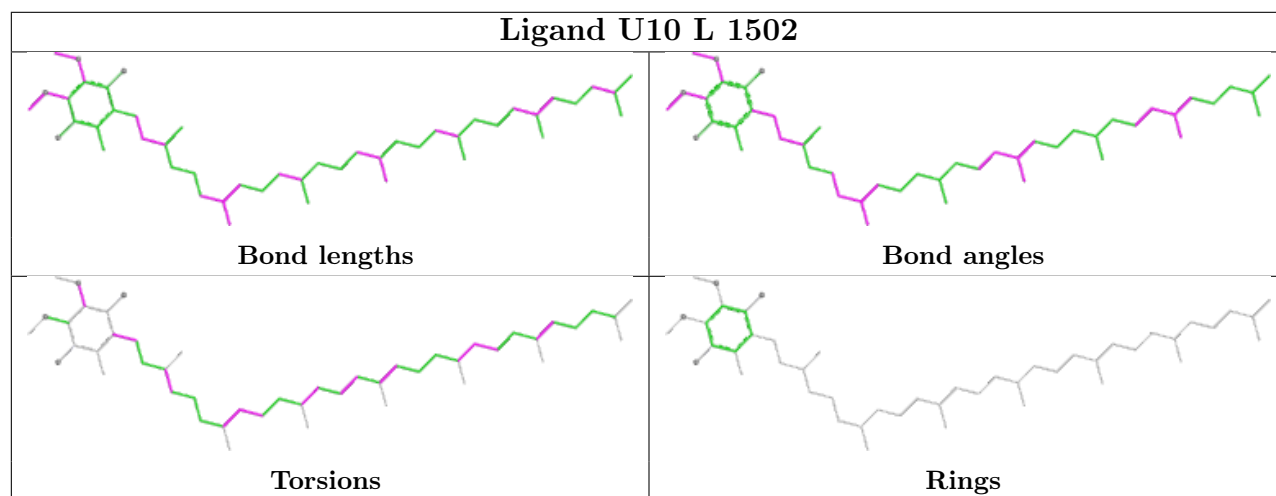
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

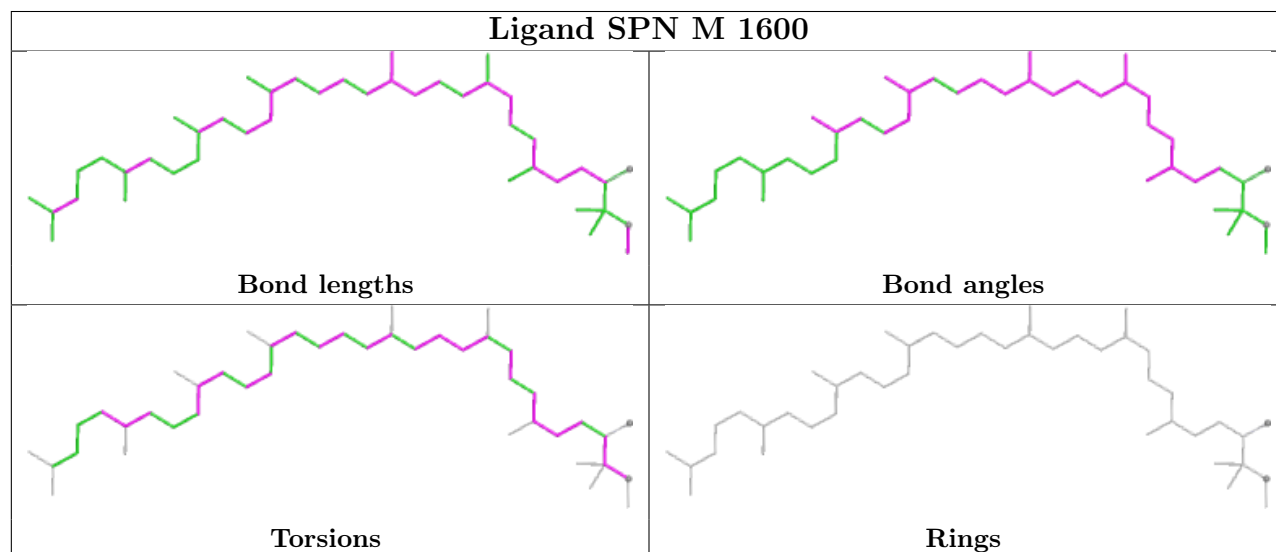
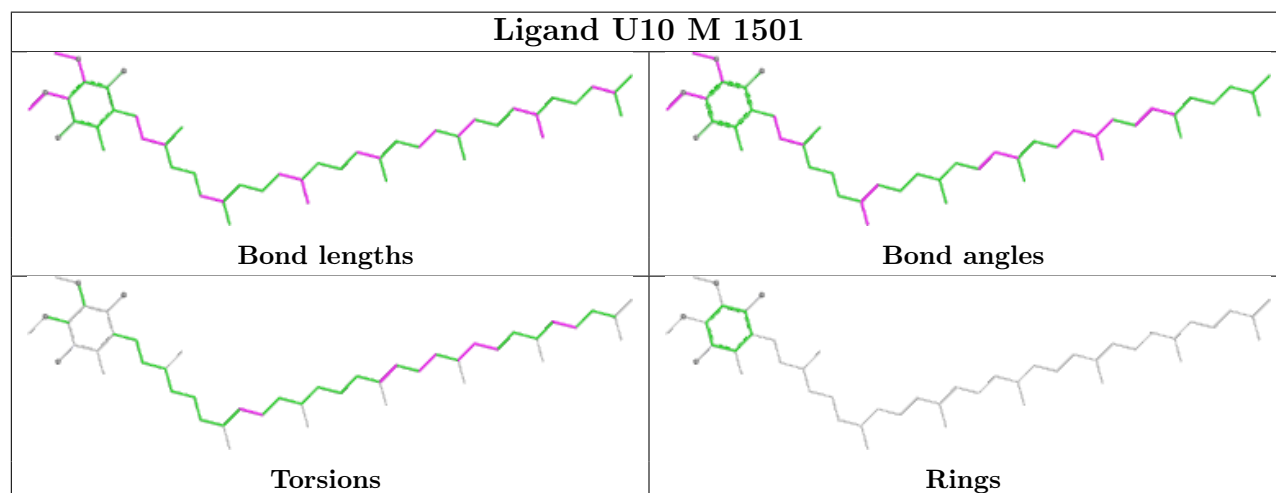
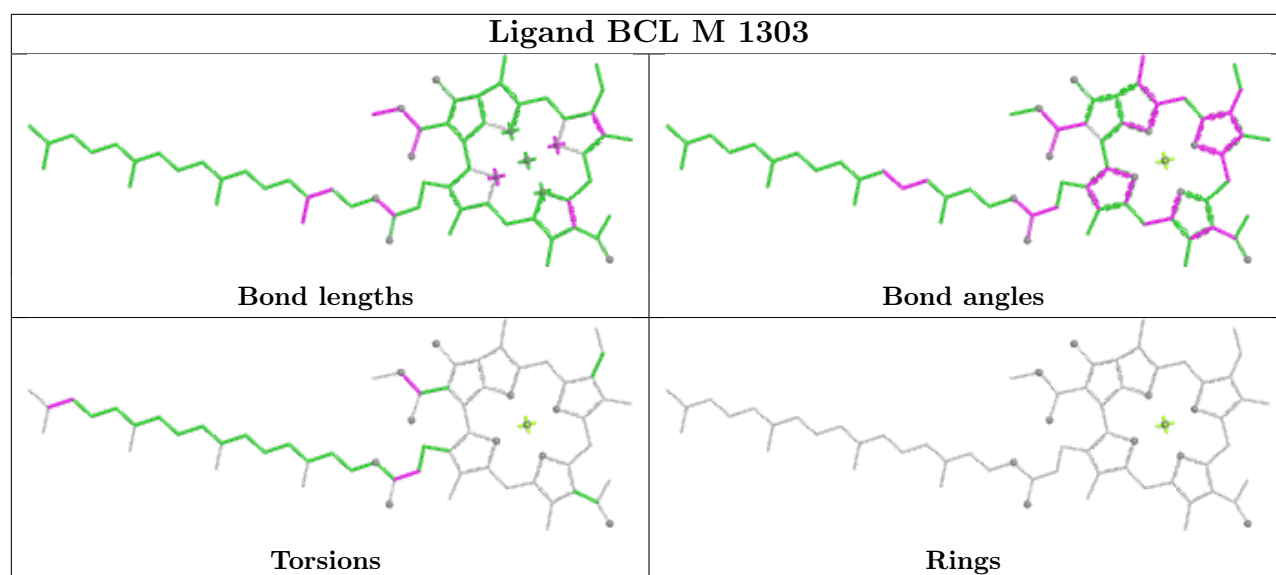


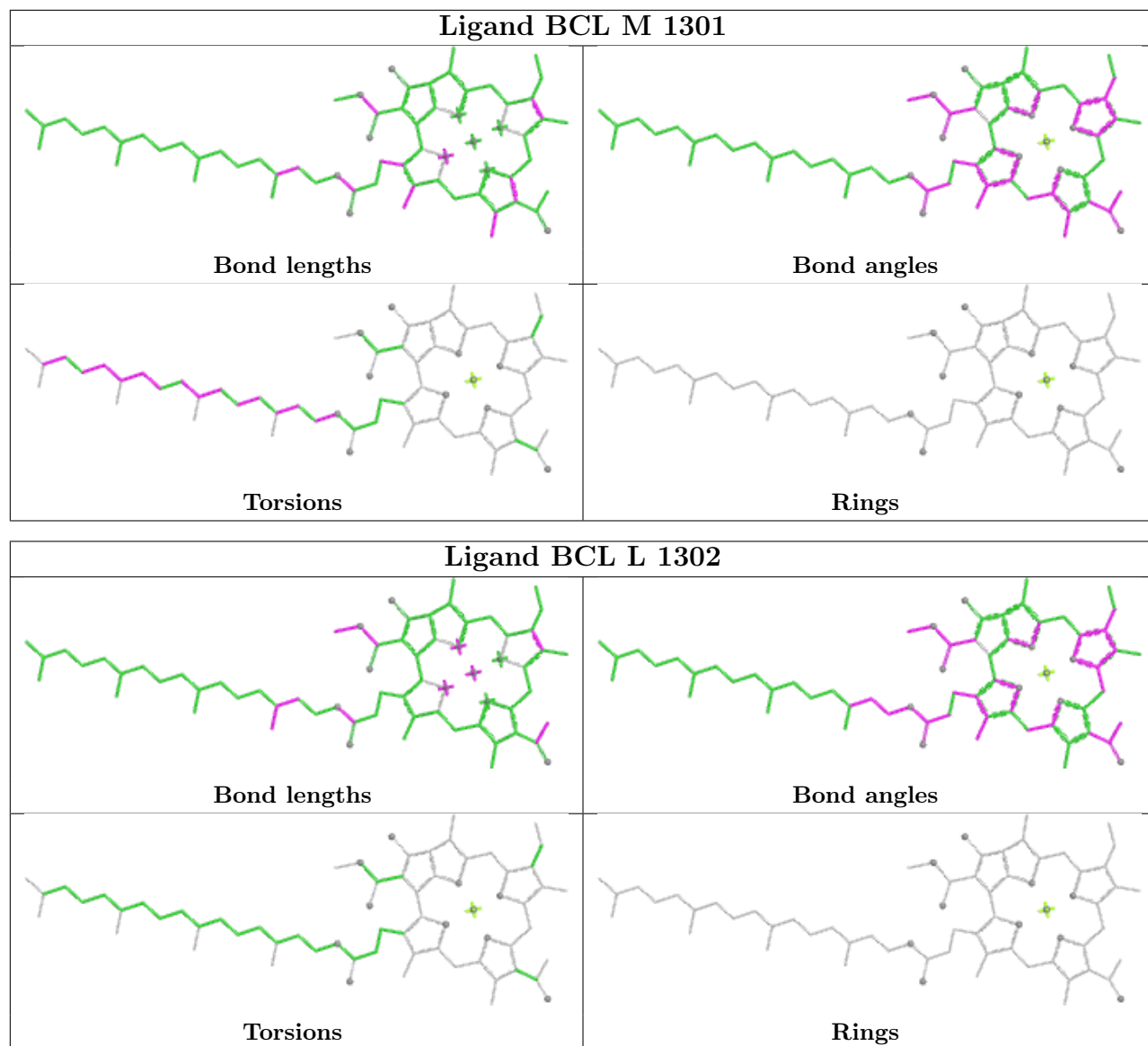
Ligand BPH L 1402



Ligand U10 L 1502







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.