



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:33 am BST

PDB ID : 3V3Z
Title : I(L177)H mutant structure of photosynthetic reaction center from Rhodospirillum rubrum
Authors : Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Shuvalov, V.A.
Deposited on : 2011-12-14
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

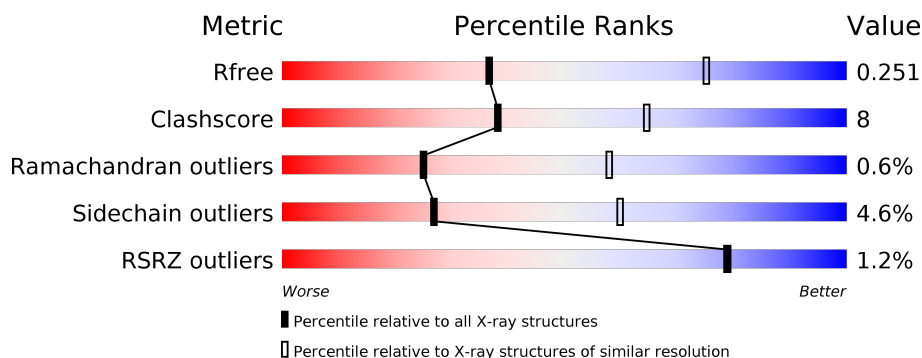
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	241	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 87% 12% </div> </div>
2	L	281	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 2% <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 81% 17% </div> </div>
3	M	302	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 85%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 85% 14% </div> </div>

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	BPH	L	402	X	-	-	-
10	BPH	M	401	X	-	-	-
11	U10	L	502	-	-	-	X
4	LDA	H	704	-	-	-	X
4	LDA	M	703	-	-	-	X
7	DIO	H	251	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7216 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	0
			1840	1178	315	338	9			

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2235	1508	357	362	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	177	HIS	ILE	ENGINEERED MUTATION	UNP P0C0Y8
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

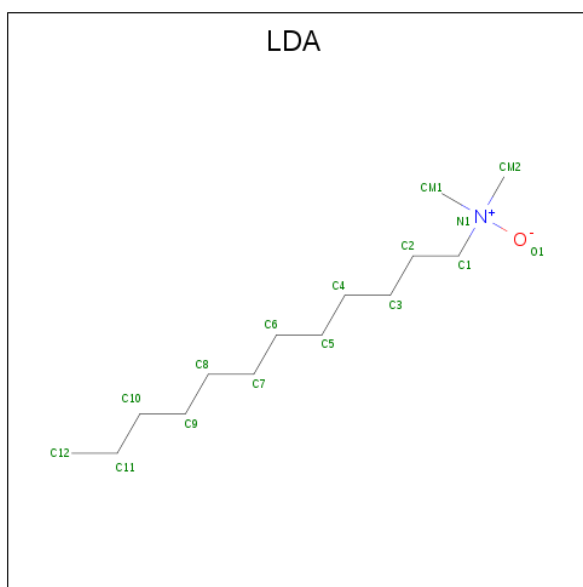
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There is a discrepancy between the modelled and reference sequences:

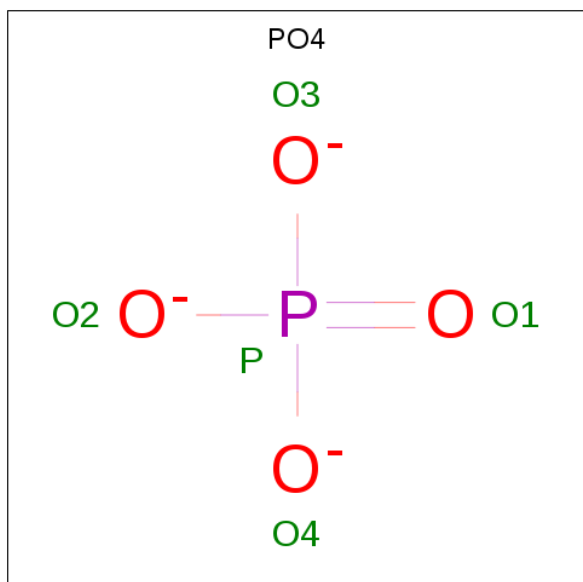
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



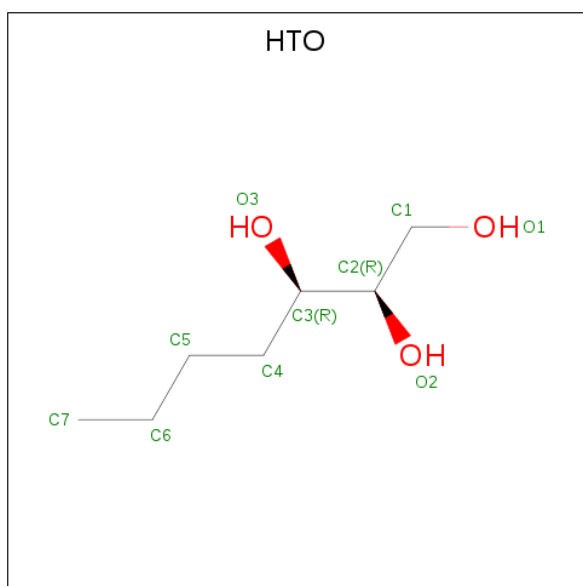
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



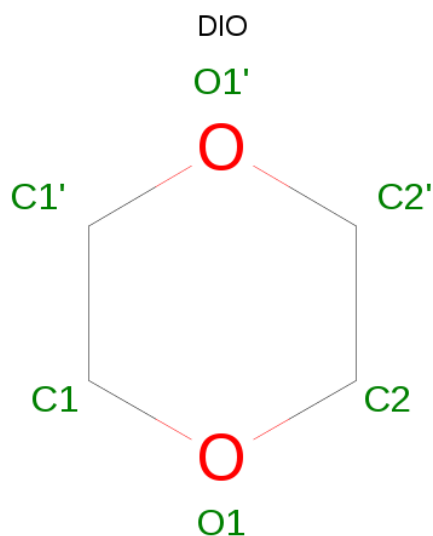
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0

- Molecule 6 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 10 7 3	0	0
6	H	1	Total C O 10 7 3	0	0
6	L	1	Total C O 10 7 3	0	0

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).

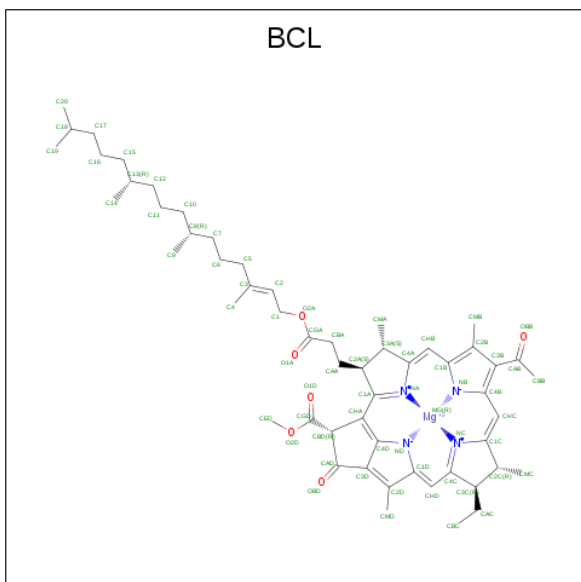


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 6 4 2	0	0
7	L	1	Total C O 6 4 2	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

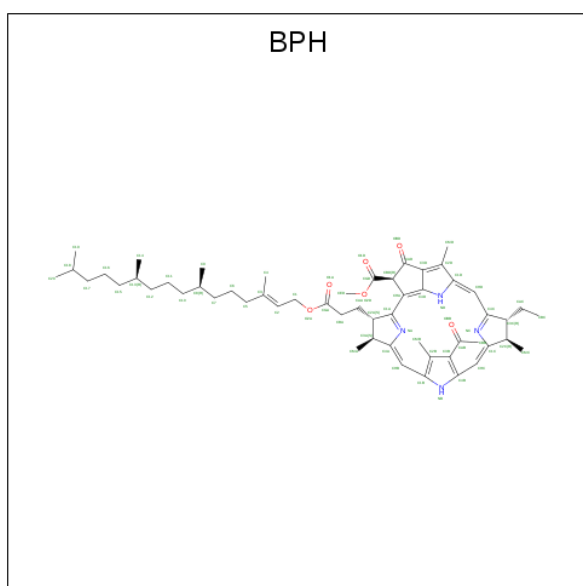
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total K 1 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $\text{C}_{55}\text{H}_{74}\text{MgN}_4\text{O}_6$).



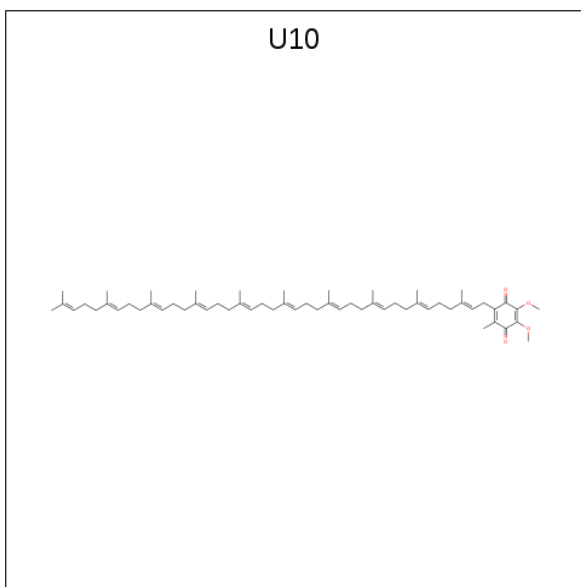
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

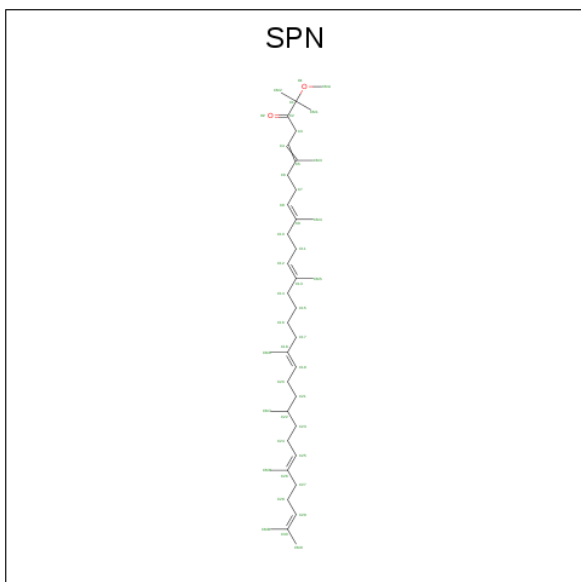


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			48	44	4		
11	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 13 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

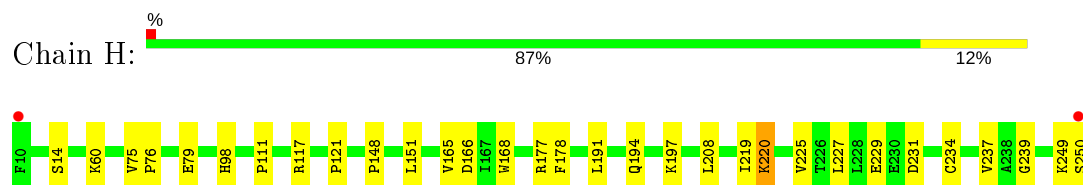
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	13	Total	O	0	0
			13	13		
15	L	19	Total	O	0	0
			19	19		
15	M	17	Total	O	0	0
			17	17		

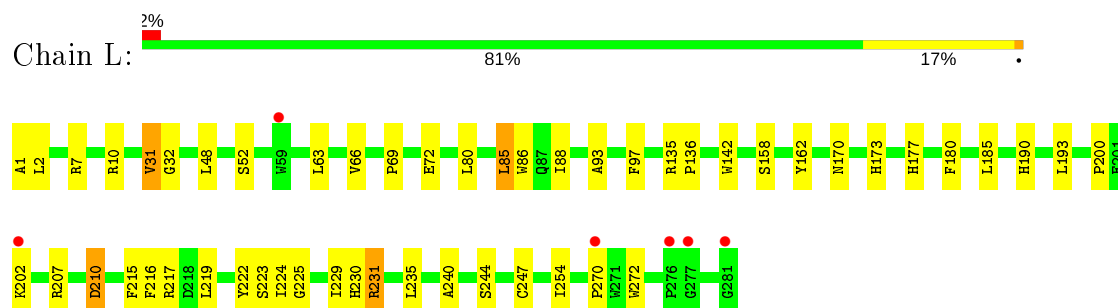
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

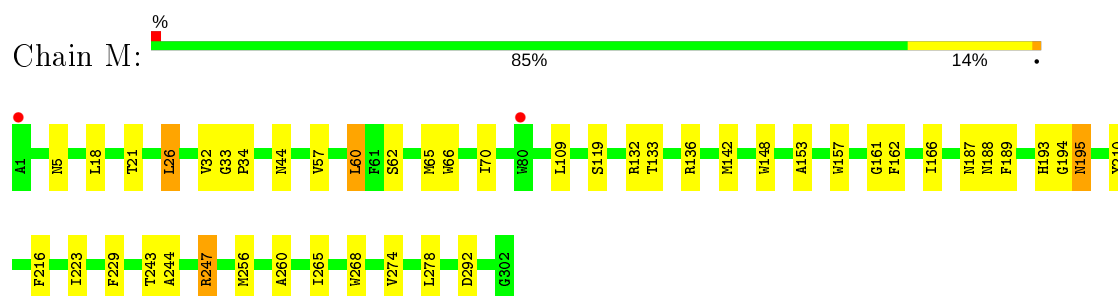
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.13Å 140.13Å 186.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.90 – 2.90 28.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.90-2.90) 96.6 (28.90-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.251 0.204 , 0.251	Depositor DCC
R_{free} test set	2286 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7216	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, DIO, CL, HTO, BPH, K, FE, SPN, U10, PO4

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	0.53	0/1889	0.62	0/2569
2	L	0.56	0/2324	0.59	0/3181
3	M	0.52	0/2501	0.60	1/3415 (0.0%)
All	All	0.54	0/6714	0.60	1/9165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	26	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

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	H	1840	0	1845	20	0
2	L	2235	0	2185	48	0
3	M	2409	0	2323	32	0
4	H	16	0	31	0	0
4	M	64	0	124	1	0
5	H	10	0	0	0	0
5	M	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	20	0	32	0	0
6	L	10	0	16	0	0
7	H	6	0	8	5	0
7	L	6	0	8	0	0
8	H	1	0	0	0	0
9	L	198	0	222	20	0
9	M	66	0	74	5	0
10	L	65	0	76	7	0
10	M	65	0	76	5	0
11	L	48	0	63	9	0
11	M	48	0	63	2	0
12	M	1	0	0	0	0
13	M	43	0	70	6	0
14	M	1	0	0	0	0
15	H	13	0	0	1	0
15	L	19	0	0	2	0
15	M	17	0	0	0	0
All	All	7216	0	7216	109	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 8.

All (109) 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:177:HIS:CD2	9:L:302:BCL:HMB3	1.62	1.34
2:L:177:HIS:NE2	9:L:302:BCL:CMB	1.92	1.33
2:L:177:HIS:NE2	9:L:302:BCL:HMB3	1.52	1.16
2:L:177:HIS:NE2	9:L:302:BCL:HMB1	1.81	0.95
2:L:177:HIS:CD2	9:L:302:BCL:CMB	2.42	0.93
9:L:304:BCL:HMB1	9:L:304:BCL:HBB2	1.53	0.88
10:L:402:BPH:HHB	10:L:402:BPH:HBB3	1.57	0.85
9:L:304:BCL:HMB1	9:L:304:BCL:CBB	2.10	0.82
1:H:177:ARG:HD3	7:H:251:DIO:H2'1	1.67	0.77
2:L:225:GLY:H	11:L:502:U10:H3M3	1.55	0.72
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.71	0.72
3:M:161:GLY:HA3	13:M:600:SPN:H201	1.73	0.71
10:L:402:BPH:HBB2	3:M:210:TYR:HB3	1.73	0.71
2:L:177:HIS:NE2	9:L:302:BCL:C2B	2.54	0.70
9:L:301:BCL:CAB	13:M:600:SPN:H162	2.22	0.70
3:M:189:PHE:O	3:M:193:HIS:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:ARG:HD3	7:H:251:DIO:C2'	2.22	0.69
9:M:303:BCL:HBB3	9:M:303:BCL:HMB1	1.75	0.69
10:M:401:BPH:HHC	10:M:401:BPH:HBB3	1.79	0.65
2:L:52:SER:HB2	2:L:85:LEU:HD12	1.78	0.65
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.78	0.64
2:L:177:HIS:CD2	9:L:302:BCL:C2B	2.81	0.64
3:M:243:THR:O	3:M:247:ARG:HG2	1.99	0.63
3:M:162:PHE:O	3:M:166:ILE:HG12	1.99	0.63
2:L:224:ILE:H	11:L:502:U10:C2	2.12	0.63
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.81	0.62
2:L:223:SER:HA	11:L:502:U10:O2	2.00	0.62
2:L:177:HIS:CE1	9:L:301:BCL:HMD2	2.35	0.61
9:L:301:BCL:CBB	9:L:301:BCL:HMB1	2.31	0.60
2:L:177:HIS:CE1	9:L:302:BCL:HBB3	2.36	0.60
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.84	0.59
3:M:157:TRP:HB2	9:M:303:BCL:H62	1.85	0.59
1:H:219:ILE:HG21	1:H:225:VAL:HG23	1.86	0.58
2:L:219:LEU:HA	3:M:132:ARG:HH12	1.68	0.58
9:L:301:BCL:HBB3	9:L:301:BCL:HMB1	1.89	0.55
2:L:97:PHE:CE1	9:L:302:BCL:H121	2.41	0.55
3:M:260:ALA:O	11:M:501:U10:H4M3	2.06	0.55
2:L:225:GLY:N	11:L:502:U10:H3M3	2.21	0.54
2:L:229:ILE:HD13	11:L:502:U10:C5	2.37	0.54
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.43	0.54
3:M:60:LEU:HA	10:M:401:BPH:H4C2	1.90	0.53
2:L:170:ASN:HB3	2:L:173:HIS:HB3	1.89	0.53
2:L:217:ARG:NH1	15:L:293:HOH:O	2.42	0.52
1:H:121:PRO:HB3	1:H:225:VAL:O	2.10	0.52
2:L:231:ARG:HD3	3:M:5:ASN:O	2.10	0.52
3:M:256:MET:CE	11:M:501:U10:H102	2.41	0.51
2:L:52:SER:HB2	2:L:85:LEU:CD1	2.39	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.93	0.51
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.28	0.51
9:L:301:BCL:OBB	13:M:600:SPN:H162	2.10	0.50
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.46	0.50
2:L:190:HIS:HA	11:L:502:U10:H4M3	1.94	0.50
1:H:79:GLU:HG2	15:H:256:HOH:O	2.11	0.50
1:H:177:ARG:HH11	7:H:251:DIO:H22	1.75	0.49
10:L:402:BPH:HHC	10:L:402:BPH:CBB	2.35	0.49
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.94	0.49
1:H:208:LEU:HD11	1:H:237:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:LYS:HG3	1:H:229:GLU:OE2	2.13	0.49
3:M:189:PHE:O	3:M:193:HIS:CD2	2.62	0.48
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.95	0.47
9:L:302:BCL:HMB1	9:L:302:BCL:CBB	2.43	0.47
2:L:190:HIS:HD1	11:L:502:U10:H4M1	1.79	0.47
9:M:303:BCL:HAA2	9:M:303:BCL:HBD	1.95	0.47
10:L:402:BPH:CHD	10:L:402:BPH:HBC2	2.44	0.47
3:M:119:SER:CB	13:M:600:SPN:HM82	2.45	0.47
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.97	0.46
2:L:52:SER:CB	2:L:85:LEU:HD12	2.45	0.46
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.98	0.46
2:L:2:LEU:HD21	2:L:10:ARG:CZ	2.46	0.45
10:L:402:BPH:HBC2	10:L:402:BPH:HHD	1.98	0.45
1:H:194:GLN:HE22	7:H:251:DIO:C2	2.29	0.44
1:H:117:ARG:NH1	1:H:227:LEU:HD22	2.32	0.44
2:L:222:TYR:CG	2:L:223:SER:N	2.85	0.44
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.65	0.44
1:H:208:LEU:HD21	1:H:237:VAL:HA	1.99	0.44
2:L:1:ALA:O	2:L:2:LEU:HD23	2.17	0.44
2:L:219:LEU:O	3:M:132:ARG:NH1	2.47	0.44
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.50	0.44
3:M:32:VAL:HG12	3:M:33:GLY:O	2.18	0.44
3:M:148:TRP:CE3	4:M:703:LDA:H82	2.53	0.43
3:M:194:GLY:O	3:M:195:ASN:HB3	2.17	0.43
9:L:302:BCL:HBB2	9:L:302:BCL:HMB1	2.00	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.43
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.53	0.43
3:M:157:TRP:CE2	13:M:600:SPN:HM73	2.53	0.43
2:L:66:VAL:O	2:L:86:TRP:HD1	2.02	0.43
15:L:292:HOH:O	3:M:136:ARG:HD3	2.18	0.43
9:M:303:BCL:CBB	9:M:303:BCL:HMB1	2.47	0.42
3:M:62:SER:HA	3:M:65:MET:HB2	2.01	0.42
1:H:234:CYS:SG	7:H:251:DIO:H1'1	2.59	0.42
3:M:119:SER:HB3	13:M:600:SPN:HM82	2.00	0.42
2:L:244:SER:C	9:L:302:BCL:HED3	2.39	0.42
2:L:31:VAL:HG12	2:L:32:GLY:N	2.35	0.42
2:L:223:SER:O	3:M:44:ASN:HB2	2.20	0.42
1:H:249:LYS:O	1:H:250:SER:HB3	2.20	0.41
2:L:210:ASP:OD1	2:L:210:ASP:N	2.53	0.41
3:M:265:ILE:O	3:M:268:TRP:HB2	2.21	0.41
10:M:401:BPH:H6C1	10:M:401:BPH:H4C1	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:TRP:NE1	3:M:70:ILE:HD11	2.35	0.41
2:L:185:LEU:HD12	10:M:401:BPH:C1D	2.51	0.41
2:L:93:ALA:HA	10:L:402:BPH:H9C2	2.03	0.40
9:M:303:BCL:HBC2	9:M:303:BCL:H2C	1.73	0.40
10:L:402:BPH:HBB1	3:M:210:TYR:CD2	2.57	0.40
2:L:48:LEU:HD11	2:L:88:ILE:HG21	2.04	0.40
11:L:502:U10:C8	11:L:502:U10:H1M1	2.50	0.40
2:L:193:LEU:CD2	11:L:502:U10:H4M2	2.51	0.40
3:M:153:ALA:HB2	10:M:401:BPH:HBC2	2.03	0.40
1:H:165:VAL:O	1:H:166:ASP:HB2	2.21	0.40
2:L:177:HIS:NE2	9:L:302:BCL:HBB3	2.35	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	239/241 (99%)	222 (93%)	17 (7%)	0	100	100
2	L	279/281 (99%)	251 (90%)	25 (9%)	3 (1%)	14	42
3	M	300/302 (99%)	277 (92%)	21 (7%)	2 (1%)	22	54
All	All	818/824 (99%)	750 (92%)	63 (8%)	5 (1%)	25	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	80	LEU
3	M	34	PRO
3	M	195	ASN
2	L	270	PRO
2	L	31	VAL

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	196/196 (100%)	190 (97%)	6 (3%)	40	74
2	L	220/220 (100%)	206 (94%)	14 (6%)	17	45
3	M	236/236 (100%)	226 (96%)	10 (4%)	30	63
All	All	652/652 (100%)	622 (95%)	30 (5%)	27	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	60	LYS
1	H	191	LEU
1	H	197	LYS
1	H	220	LYS
1	H	231	ASP
2	L	63	LEU
2	L	72	GLU
2	L	85	LEU
2	L	158	SER
2	L	200	PRO
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	231	ARG
2	L	235	LEU
2	L	247	CYS
2	L	254	ILE
2	L	272	TRP
3	M	18	LEU
3	M	57	VAL
3	M	60	LEU
3	M	109	LEU
3	M	188	ASN
3	M	216	PHE

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Mol	Chain	Res	Type
3	M	247	ARG
3	M	274	VAL
3	M	278	LEU
3	M	292	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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
9	BCL	L	301	-	58,74,74	1.42	3 (5%)	69,115,115	1.49	11 (15%)
9	BCL	M	303	-	58,74,74	1.30	3 (5%)	69,115,115	1.50	12 (17%)
4	LDA	M	701	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
11	U10	L	502	-	48,48,63	2.86	14 (29%)	58,61,79	1.71	17 (29%)
5	PO4	M	800	-	4,4,4	1.02	0	6,6,6	0.53	0
5	PO4	M	802	-	4,4,4	0.90	0	6,6,6	0.33	0
6	HTO	L	282	-	9,9,9	0.50	0	10,10,10	0.57	0
6	HTO	H	3	-	9,9,9	0.48	0	10,10,10	0.53	0
7	DIO	L	283	-	6,6,6	0.63	0	6,6,6	0.73	0
11	U10	M	501	-	48,48,63	2.76	12 (25%)	58,61,79	1.59	13 (22%)
5	PO4	M	801	-	4,4,4	0.91	0	6,6,6	0.39	0
10	BPH	M	401	-	64,70,70	1.41	8 (12%)	76,101,101	1.48	13 (17%)
9	BCL	L	304	-	58,74,74	1.39	4 (6%)	69,115,115	1.58	15 (21%)
4	LDA	M	702	-	12,15,15	1.96	1 (8%)	14,17,17	0.47	0
9	BCL	L	302	-	58,74,74	1.24	4 (6%)	69,115,115	1.61	15 (21%)
10	BPH	L	402	-	64,70,70	1.39	7 (10%)	76,101,101	1.37	10 (13%)
4	LDA	M	705	-	12,15,15	2.10	1 (8%)	14,17,17	0.33	0
7	DIO	H	251	-	6,6,6	0.45	0	6,6,6	1.05	0
13	SPN	M	600	-	40,42,42	0.64	0	50,52,52	1.45	5 (10%)
4	LDA	M	703	-	12,15,15	2.06	1 (8%)	14,17,17	0.59	0
5	PO4	H	803	-	4,4,4	0.84	0	6,6,6	0.54	0
6	HTO	H	2	-	9,9,9	0.32	0	10,10,10	0.62	0
5	PO4	H	804	-	4,4,4	0.92	0	6,6,6	0.41	0
4	LDA	H	704	-	12,15,15	2.06	1 (8%)	14,17,17	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	L	301	-	-	14/37/137/137	-
9	BCL	M	303	-	-	12/37/137/137	-
4	LDA	M	701	-	-	9/13/13/13	-
10	BPH	M	401	-	2/2/18/22	17/54/105/105	0/5/6/6
13	SPN	M	600	-	-	15/50/51/51	-
11	U10	L	502	-	-	21/45/69/87	0/1/1/1
9	BCL	L	304	-	-	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HTO	H	3	-	-	3/10/10/10	-
7	DIO	L	283	-	-	-	0/1/1/1
4	LDA	H	704	-	-	8/13/13/13	-
4	LDA	M	702	-	-	7/13/13/13	-
4	LDA	M	703	-	-	8/13/13/13	-
11	U10	M	501	-	-	11/45/69/87	0/1/1/1
7	DIO	H	251	-	-	-	0/1/1/1
6	HTO	H	2	-	-	10/10/10/10	-
9	BCL	L	302	-	-	10/37/137/137	-
6	HTO	L	282	-	-	0/10/10/10	-
10	BPH	L	402	-	2/2/18/22	18/54/105/105	0/5/6/6
4	LDA	M	705	-	-	7/13/13/13	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	705	LDA	O1-N1	-7.11	1.25	1.42
11	L	502	U10	C8-C9	7.04	1.49	1.33
4	M	703	LDA	O1-N1	-7.03	1.25	1.42
4	H	704	LDA	O1-N1	-7.01	1.25	1.42
4	M	701	LDA	O1-N1	-6.92	1.26	1.42
11	L	502	U10	C33-C34	6.79	1.49	1.33
9	L	301	BCL	C1B-NB	6.78	1.41	1.35
11	L	502	U10	C23-C24	6.78	1.49	1.33
11	L	502	U10	C13-C14	6.76	1.49	1.33
11	M	501	U10	C13-C14	6.67	1.49	1.33
4	M	702	LDA	O1-N1	-6.67	1.26	1.42
9	L	304	BCL	C4B-NB	6.67	1.41	1.35
11	M	501	U10	C33-C34	6.61	1.48	1.33
11	M	501	U10	C18-C19	6.58	1.48	1.33
11	L	502	U10	C28-C29	6.46	1.48	1.33
11	M	501	U10	C23-C24	6.41	1.48	1.33
11	M	501	U10	C28-C29	6.41	1.48	1.33
9	L	301	BCL	C4B-NB	6.18	1.40	1.35
11	L	502	U10	C18-C19	6.17	1.47	1.33
9	M	303	BCL	C1B-NB	5.97	1.40	1.35
9	L	302	BCL	C4B-NB	5.92	1.40	1.35
11	M	501	U10	C8-C9	5.90	1.47	1.33
9	M	303	BCL	C4B-NB	5.76	1.40	1.35
11	L	502	U10	C38-C39	5.59	1.48	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	501	U10	C38-C39	5.59	1.48	1.32
9	L	304	BCL	C1B-NB	5.49	1.40	1.35
9	L	302	BCL	C1B-NB	5.44	1.40	1.35
10	L	402	BPH	CHD-C4C	5.12	1.51	1.38
11	M	501	U10	O4-C4	-5.06	1.24	1.36
10	M	401	BPH	CHA-C1A	5.05	1.49	1.38
10	L	402	BPH	CHA-C1A	4.85	1.48	1.38
10	M	401	BPH	CHD-C4C	4.58	1.49	1.38
11	L	502	U10	O3-C3	-4.52	1.25	1.36
11	M	501	U10	O3-C3	-4.41	1.26	1.36
11	L	502	U10	O4-C4	-4.24	1.26	1.36
10	M	401	BPH	C4C-NC	-3.65	1.29	1.37
10	L	402	BPH	C1B-C2B	-3.59	1.38	1.45
10	M	401	BPH	C1B-C2B	-3.50	1.38	1.45
11	L	502	U10	C6-C1	3.40	1.41	1.35
10	M	401	BPH	C1A-NA	-3.25	1.31	1.37
10	L	402	BPH	C1A-NA	-3.16	1.31	1.37
11	L	502	U10	C3-C2	-2.90	1.40	1.48
10	L	402	BPH	C4C-NC	-2.86	1.31	1.37
11	M	501	U10	C6-C1	2.75	1.40	1.35
11	M	501	U10	C3-C2	-2.72	1.41	1.48
11	L	502	U10	C7-C6	2.61	1.55	1.51
11	L	502	U10	C7-C8	2.44	1.54	1.50
11	L	502	U10	C4-C5	-2.43	1.41	1.48
9	L	302	BCL	CHD-C4C	-2.42	1.34	1.41
9	L	304	BCL	CHD-C4C	-2.40	1.34	1.41
11	M	501	U10	C4-C5	-2.30	1.42	1.48
10	M	401	BPH	C3D-C2D	-2.20	1.35	1.39
9	M	303	BCL	CHD-C4C	-2.16	1.35	1.41
9	L	301	BCL	C4B-CHC	-2.12	1.35	1.41
10	L	402	BPH	C3D-C2D	-2.11	1.35	1.39
10	M	401	BPH	CHB-C4A	-2.10	1.34	1.40
10	L	402	BPH	CHB-C1B	2.05	1.42	1.38
10	M	401	BPH	CHB-C1B	2.05	1.42	1.38
9	L	304	BCL	C4B-CHC	-2.04	1.35	1.41
9	L	302	BCL	C1D-C2D	-2.03	1.38	1.42

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	304	BCL	O2D-CGD-CBD	5.75	121.49	111.27
9	L	301	BCL	C1C-NC-C4C	4.87	108.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	301	BCL	O2D-CGD-CBD	4.74	119.70	111.27
10	M	401	BPH	C4D-C3D-CAD	-4.64	104.93	107.87
10	L	402	BPH	C4D-CHA-C1A	-4.58	119.22	130.51
11	L	502	U10	C30-C29-C31	4.50	122.84	115.27
10	M	401	BPH	C4D-CHA-C1A	-4.28	119.96	130.51
10	M	401	BPH	C1-C2-C3	4.28	133.44	126.04
11	L	502	U10	O5-C5-C4	-4.26	111.90	120.93
9	L	302	BCL	O2D-CGD-CBD	4.14	118.62	111.27
9	L	304	BCL	C1C-NC-C4C	4.13	108.56	106.71
9	M	303	BCL	O2D-CGD-CBD	4.06	118.49	111.27
9	L	304	BCL	CHD-C4C-NC	3.84	129.34	125.08
9	L	302	BCL	CMB-C2B-C1B	-3.68	122.81	128.46
10	L	402	BPH	OBB-CAB-C3B	3.66	127.19	120.41
13	M	600	SPN	CM5-C13-C14	3.66	121.43	115.27
11	M	501	U10	C35-C34-C36	3.65	121.41	115.27
9	M	303	BCL	CAA-C2A-C3A	-3.62	102.87	112.78
10	M	401	BPH	C1C-NC-C4C	-3.57	107.40	110.54
9	L	302	BCL	C1D-CHD-C4C	-3.56	120.63	125.88
11	M	501	U10	C15-C14-C16	3.44	121.06	115.27
13	M	600	SPN	CM3-C5-C6	3.44	121.06	115.27
13	M	600	SPN	CM4-C9-C10	3.42	121.02	115.27
13	M	600	SPN	CM6-C18-C17	3.34	120.89	115.27
10	L	402	BPH	C4D-C3D-CAD	-3.33	105.76	107.87
9	M	303	BCL	CHD-C4C-NC	3.23	128.66	125.08
11	L	502	U10	O2-C2-C3	-3.21	114.11	120.93
9	L	302	BCL	C11-C12-C13	-3.15	105.74	115.92
10	M	401	BPH	C6-C5-C3	3.13	121.67	113.45
9	M	303	BCL	CED-O2D-CGD	3.10	122.95	115.94
11	M	501	U10	C10-C9-C11	3.04	120.38	115.27
11	M	501	U10	C22-C23-C24	-2.98	120.47	127.66
11	M	501	U10	C7-C8-C9	-2.92	121.93	126.79
10	M	401	BPH	CMD-C2D-C3D	2.90	130.11	124.68
11	L	502	U10	C20-C19-C21	2.90	120.15	115.27
10	M	401	BPH	C5-C3-C2	2.89	126.96	121.12
9	L	301	BCL	O2A-CGA-CBA	2.88	120.96	111.91
11	L	502	U10	C35-C34-C36	2.88	120.11	115.27
9	L	304	BCL	O1D-CGD-CBD	-2.87	118.62	124.48
9	L	302	BCL	CHD-C4C-NC	2.86	128.26	125.08
9	L	302	BCL	O2A-CGA-CBA	2.84	120.82	111.91
9	M	303	BCL	O2A-CGA-CBA	2.83	120.77	111.91
11	M	501	U10	C27-C28-C29	-2.81	120.89	127.66
9	L	304	BCL	CHB-C4A-NA	2.79	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	600	SPN	C3-C4-C5	-2.79	122.14	126.79
9	L	302	BCL	CED-O2D-CGD	2.79	122.25	115.94
9	L	302	BCL	C4D-C3D-CAD	-2.75	106.93	108.47
11	M	501	U10	C30-C29-C31	2.75	119.89	115.27
9	L	301	BCL	C1-O2A-CGA	2.73	123.60	116.44
10	L	402	BPH	C6-C5-C3	2.73	120.61	113.45
11	L	502	U10	C17-C18-C19	-2.70	121.15	127.66
11	L	502	U10	C25-C24-C26	2.69	119.80	115.27
9	L	302	BCL	C1-O2A-CGA	2.66	123.42	116.44
10	L	402	BPH	C1B-NB-C4B	2.65	111.49	106.51
9	L	304	BCL	C1-O2A-CGA	2.61	123.29	116.44
11	L	502	U10	O5-C5-C6	-2.58	117.02	121.55
10	L	402	BPH	CHC-C1C-NC	2.58	128.27	125.20
11	L	502	U10	C30-C29-C28	-2.58	117.06	123.68
9	M	303	BCL	C1-O2A-CGA	2.58	123.20	116.44
9	L	301	BCL	O1D-CGD-CBD	-2.55	119.26	124.48
9	L	302	BCL	C4-C3-C5	2.54	119.55	115.27
9	M	303	BCL	C4-C3-C5	2.53	119.53	115.27
11	M	501	U10	C17-C18-C19	-2.53	121.56	127.66
9	L	301	BCL	C1B-CHB-C4A	-2.51	125.16	130.12
9	L	301	BCL	CHD-C4C-NC	2.49	127.84	125.08
9	L	302	BCL	C6-C7-C8	-2.48	107.91	115.92
10	M	401	BPH	OBB-CAB-C3B	2.48	124.99	120.41
11	L	502	U10	C1M-C1-C6	-2.44	120.41	124.40
10	M	401	BPH	C1B-NB-C4B	2.44	111.12	106.51
9	L	304	BCL	C4A-NA-C1A	2.43	107.80	106.71
11	L	502	U10	C15-C14-C16	2.43	119.35	115.27
10	L	402	BPH	C4-C3-C5	-2.38	111.27	115.27
9	L	304	BCL	CED-O2D-CGD	2.36	121.28	115.94
9	M	303	BCL	CHB-C4A-NA	2.35	127.76	124.51
9	M	303	BCL	C1C-NC-C4C	2.35	107.76	106.71
9	L	304	BCL	O2A-CGA-CBA	2.34	119.26	111.91
9	L	304	BCL	C4-C3-C5	2.33	119.19	115.27
11	M	501	U10	C32-C33-C34	-2.32	122.07	127.66
9	L	301	BCL	CAC-C3C-C2C	-2.32	108.46	114.26
11	L	502	U10	C6-C1-C2	2.30	121.00	119.18
10	L	402	BPH	C2B-C1B-NB	-2.26	106.38	109.79
9	L	301	BCL	C4-C3-C5	2.26	119.07	115.27
9	L	302	BCL	C1B-CHB-C4A	-2.25	125.65	130.12
11	M	501	U10	C3M-O3-C3	2.24	124.41	116.47
9	L	304	BCL	C1D-CHD-C4C	-2.24	122.58	125.88
9	L	302	BCL	C3C-C4C-CHD	-2.24	118.61	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	303	BCL	C1D-CHD-C4C	-2.24	122.58	125.88
11	M	501	U10	C41-C39-C40	2.24	119.54	114.60
9	L	304	BCL	C3C-C4C-CHD	-2.22	118.66	123.39
9	M	303	BCL	CGD-CBD-CAD	-2.21	103.56	110.73
9	L	302	BCL	C7-C6-C5	-2.19	107.41	113.36
10	L	402	BPH	CAC-C3C-C4C	2.17	118.25	112.67
9	L	302	BCL	CMB-C2B-C3B	2.16	128.71	124.68
11	L	502	U10	C3M-O3-C3	2.14	124.06	116.47
11	L	502	U10	C4M-O4-C4	2.13	124.03	116.47
9	L	304	BCL	C5-C3-C2	-2.13	116.80	121.12
11	L	502	U10	C35-C34-C33	-2.12	118.23	123.68
9	L	304	BCL	OBD-CAD-CBD	2.11	128.91	125.89
11	L	502	U10	C1-C6-C5	-2.11	117.60	119.58
11	L	502	U10	C27-C28-C29	-2.10	122.59	127.66
9	L	301	BCL	CHB-C4A-NA	2.10	127.42	124.51
11	M	501	U10	C6-C1-C2	2.10	120.84	119.18
10	L	402	BPH	OBB-CAB-CBB	-2.09	115.11	119.73
10	M	401	BPH	C2B-C1B-NB	-2.08	106.65	109.79
9	L	301	BCL	C1D-CHD-C4C	-2.06	122.84	125.88
10	M	401	BPH	C1-O2A-CGA	2.04	121.80	116.44
11	M	501	U10	C25-C24-C26	2.03	118.69	115.27
10	M	401	BPH	OBB-CAB-CBB	-2.03	115.23	119.73
9	M	303	BCL	C3C-C4C-CHD	-2.02	119.07	123.39
9	L	304	BCL	O2D-CGD-O1D	-2.02	119.89	123.84
10	M	401	BPH	C3A-C2A-C1A	-2.00	99.25	101.64

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	M	401	BPH	C8
10	M	401	BPH	C13
10	L	402	BPH	C8
10	L	402	BPH	C13

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	502	U10	C17-C18-C19-C20
11	L	502	U10	C17-C18-C19-C21
11	L	502	U10	C19-C21-C22-C23
11	L	502	U10	C24-C26-C27-C28
11	L	502	U10	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
11	L	502	U10	C27-C28-C29-C31
11	L	502	U10	C28-C29-C31-C32
11	L	502	U10	C30-C29-C31-C32
11	L	502	U10	C32-C33-C34-C35
11	L	502	U10	C32-C33-C34-C36
11	L	502	U10	C33-C34-C36-C37
11	L	502	U10	C35-C34-C36-C37
11	L	502	U10	C37-C38-C39-C40
10	M	401	BPH	C4B-C3B-CAB-CBB
10	M	401	BPH	C4B-C3B-CAB-OB
11	M	501	U10	C27-C28-C29-C30
11	M	501	U10	C27-C28-C29-C31
11	M	501	U10	C32-C33-C34-C35
11	M	501	U10	C37-C38-C39-C41
10	L	402	BPH	C4C-C3C-CAC-CBC
4	M	705	LDA	C2-C1-N1-CM2
13	M	600	SPN	O1-C1-C2-O2
4	M	703	LDA	C2-C1-N1-O1
4	M	703	LDA	C2-C1-N1-CM1
4	M	703	LDA	N1-C1-C2-C3
6	H	2	HTO	C1-C2-C3-O3
6	H	2	HTO	C1-C2-C3-C4
6	H	2	HTO	O2-C2-C3-O3
6	H	2	HTO	O2-C2-C3-C4
4	H	704	LDA	C2-C1-N1-O1
4	H	704	LDA	C2-C1-N1-CM2
11	L	502	U10	C37-C38-C39-C41
11	M	501	U10	C37-C38-C39-C40
9	L	302	BCL	CBD-CGD-O2D-CED
9	M	303	BCL	C3-C5-C6-C7
9	L	304	BCL	CBD-CGD-O2D-CED
11	M	501	U10	C32-C33-C34-C36
10	M	401	BPH	CBD-CGD-O2D-CED
13	M	600	SPN	C11-C10-C9-CM4
13	M	600	SPN	C16-C17-C18-CM6
13	M	600	SPN	C11-C10-C9-C8
13	M	600	SPN	C16-C17-C18-C19
9	L	301	BCL	O1A-CGA-O2A-C1
11	L	502	U10	C14-C16-C17-C18
11	L	502	U10	C29-C31-C32-C33
11	M	501	U10	C24-C26-C27-C28
9	L	301	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	M	303	BCL	CBD-CGD-O2D-CED
10	M	401	BPH	CBA-CGA-O2A-C1
9	L	302	BCL	C14-C13-C15-C16
10	L	402	BPH	C6-C7-C8-C9
10	L	402	BPH	C14-C13-C15-C16
10	M	401	BPH	O1A-CGA-O2A-C1
10	M	401	BPH	C10-C11-C12-C13
10	L	402	BPH	C11-C10-C8-C7
9	L	301	BCL	C8-C10-C11-C12
9	L	302	BCL	O1D-CGD-O2D-CED
9	L	301	BCL	C15-C16-C17-C18
4	M	702	LDA	C7-C8-C9-C10
9	L	304	BCL	O1D-CGD-O2D-CED
4	H	704	LDA	C2-C3-C4-C5
10	M	401	BPH	O1D-CGD-O2D-CED
4	H	704	LDA	C7-C8-C9-C10
10	L	402	BPH	C10-C11-C12-C13
9	L	301	BCL	C16-C17-C18-C19
9	L	304	BCL	C16-C17-C18-C20
4	H	704	LDA	C5-C6-C7-C8
6	H	2	HTO	C2-C3-C4-C5
9	L	301	BCL	C2A-CAA-CBA-CGA
4	M	702	LDA	C3-C4-C5-C6
9	M	303	BCL	C3A-C2A-CAA-CBA
10	M	401	BPH	C16-C17-C18-C19
10	M	401	BPH	C16-C17-C18-C20
4	M	705	LDA	C11-C10-C9-C8
10	L	402	BPH	C15-C16-C17-C18
11	M	501	U10	C23-C24-C26-C27
9	M	303	BCL	O1D-CGD-O2D-CED
9	L	301	BCL	C16-C17-C18-C20
9	L	304	BCL	C16-C17-C18-C19
4	M	705	LDA	C7-C8-C9-C10
4	H	704	LDA	C4-C5-C6-C7
4	M	703	LDA	C1-C2-C3-C4
4	M	703	LDA	C3-C4-C5-C6
4	H	704	LDA	C11-C10-C9-C8
9	L	302	BCL	C13-C15-C16-C17
4	M	705	LDA	C1-C2-C3-C4
9	L	302	BCL	C4-C3-C5-C6
11	M	501	U10	C25-C24-C26-C27
9	L	302	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
10	L	402	BPH	C5-C6-C7-C8
10	L	402	BPH	CBD-CGD-O2D-CED
11	L	502	U10	C7-C8-C9-C10
4	M	703	LDA	C6-C7-C8-C9
9	L	301	BCL	C10-C11-C12-C13
9	L	304	BCL	C13-C15-C16-C17
4	M	701	LDA	C1-C2-C3-C4
13	M	600	SPN	C14-C15-C16-C17
9	L	304	BCL	C1A-C2A-CAA-CBA
6	H	2	HTO	O1-C1-C2-O2
4	M	701	LDA	C5-C6-C7-C8
9	L	302	BCL	C2-C3-C5-C6
10	M	401	BPH	C2C-C3C-CAC-CBC
10	L	402	BPH	C2C-C3C-CAC-CBC
6	H	2	HTO	O3-C3-C4-C5
4	M	703	LDA	C4-C5-C6-C7
6	H	3	HTO	C4-C5-C6-C7
6	H	2	HTO	C4-C5-C6-C7
13	M	600	SPN	CM5-C13-C14-C15
11	L	502	U10	C5-C6-C7-C8
13	M	600	SPN	CM1-C1-O1-CMA
9	M	303	BCL	C6-C7-C8-C10
9	L	302	BCL	C11-C12-C13-C15
10	M	401	BPH	C12-C13-C15-C16
9	L	304	BCL	C11-C12-C13-C15
10	L	402	BPH	C6-C7-C8-C10
9	M	303	BCL	C6-C7-C8-C9
9	L	302	BCL	C11-C12-C13-C14
6	H	2	HTO	O1-C1-C2-C3
4	M	705	LDA	N1-C1-C2-C3
4	M	702	LDA	C5-C6-C7-C8
10	L	402	BPH	C8-C10-C11-C12
4	M	701	LDA	C11-C10-C9-C8
4	M	702	LDA	C2-C3-C4-C5
10	L	402	BPH	C13-C15-C16-C17
10	L	402	BPH	O1D-CGD-O2D-CED
9	L	304	BCL	C11-C10-C8-C9
9	M	303	BCL	C4C-C3C-CAC-CBC
9	L	301	BCL	C13-C15-C16-C17
9	L	302	BCL	C12-C13-C15-C16
9	L	304	BCL	C11-C10-C8-C7
13	M	600	SPN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
10	L	402	BPH	CAD-CBD-CGD-O2D
9	L	304	BCL	C10-C11-C12-C13
4	M	701	LDA	C2-C1-N1-CM1
4	M	701	LDA	C2-C1-N1-CM2
4	M	705	LDA	C2-C1-N1-CM1
4	M	703	LDA	C2-C1-N1-CM2
13	M	600	SPN	CM2-C1-O1-CMA
9	L	301	BCL	C6-C7-C8-C9
10	M	401	BPH	C14-C13-C15-C16
10	L	402	BPH	C11-C10-C8-C9
13	M	600	SPN	CM7-C22-C23-C24
6	H	2	HTO	C3-C4-C5-C6
9	M	303	BCL	C1A-C2A-CAA-CBA
13	M	600	SPN	C12-C13-C14-C15
4	M	702	LDA	C4-C5-C6-C7
4	M	705	LDA	C2-C1-N1-O1
9	L	301	BCL	C6-C7-C8-C10
9	L	301	BCL	C11-C12-C13-C15
9	M	303	BCL	C2C-C3C-CAC-CBC
9	M	303	BCL	C11-C12-C13-C15
6	H	3	HTO	O1-C1-C2-O2
4	M	702	LDA	C1-C2-C3-C4
10	L	402	BPH	O2A-C1-C2-C3
9	L	304	BCL	C11-C12-C13-C14
9	L	301	BCL	C3-C5-C6-C7
4	H	704	LDA	C1-C2-C3-C4
9	L	301	BCL	C11-C12-C13-C14
11	M	501	U10	C5-C4-O4-C4M
11	L	502	U10	C34-C36-C37-C38
10	M	401	BPH	C4-C3-C5-C6
9	M	303	BCL	C15-C16-C17-C18
13	M	600	SPN	CM2-C1-C2-C3
10	M	401	BPH	NC-C4C-CHD-C1D
4	M	701	LDA	C7-C8-C9-C10
4	M	701	LDA	C6-C7-C8-C9
10	L	402	BPH	C4B-C3B-CAB-CBB
10	L	402	BPH	C4B-C3B-CAB-OB
9	L	304	BCL	C15-C16-C17-C18
4	M	702	LDA	C9-C10-C11-C12
6	H	3	HTO	O1-C1-C2-C3
10	M	401	BPH	C2-C3-C5-C6
9	M	303	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
10	M	401	BPH	CAD-CBD-CGD-O2D
10	M	401	BPH	NB-C1B-CHB-C4A
11	L	502	U10	C5-C4-O4-C4M
9	L	304	BCL	CHA-CBD-CGD-O2D
13	M	600	SPN	C2-C1-O1-CMA
11	L	502	U10	C2-C3-O3-C3M
4	M	701	LDA	C9-C10-C11-C12
11	M	501	U10	C34-C36-C37-C38
4	M	701	LDA	C2-C1-N1-O1
13	M	600	SPN	CM2-C1-C2-O2
9	L	304	BCL	C3-C5-C6-C7

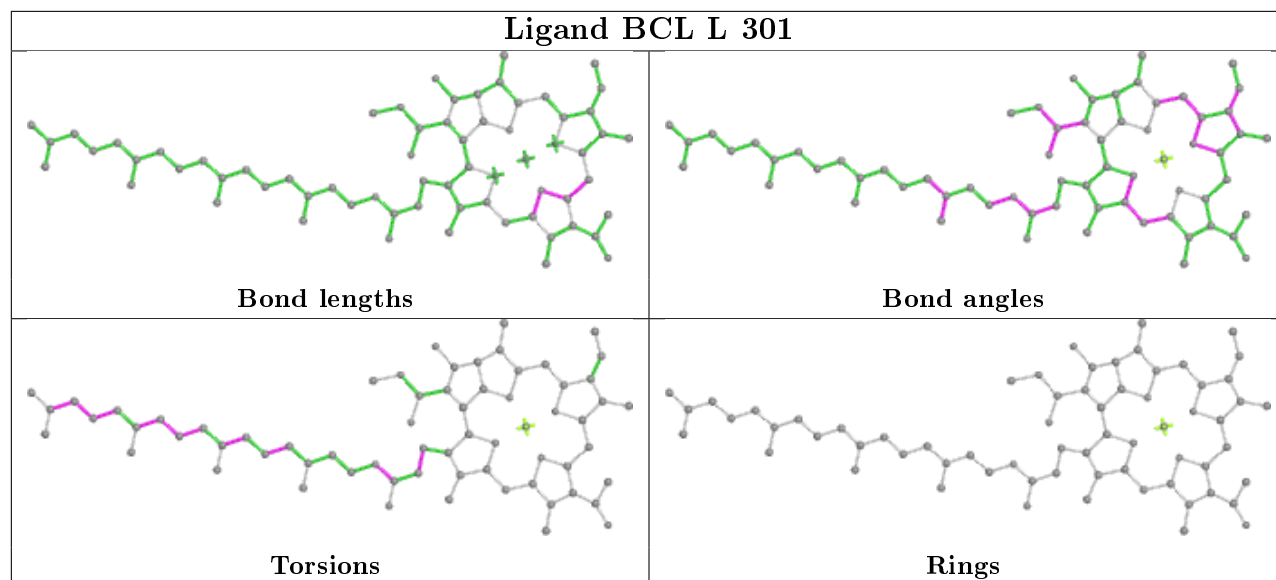
There are no ring outliers.

11 monomers are involved in 58 short contacts:

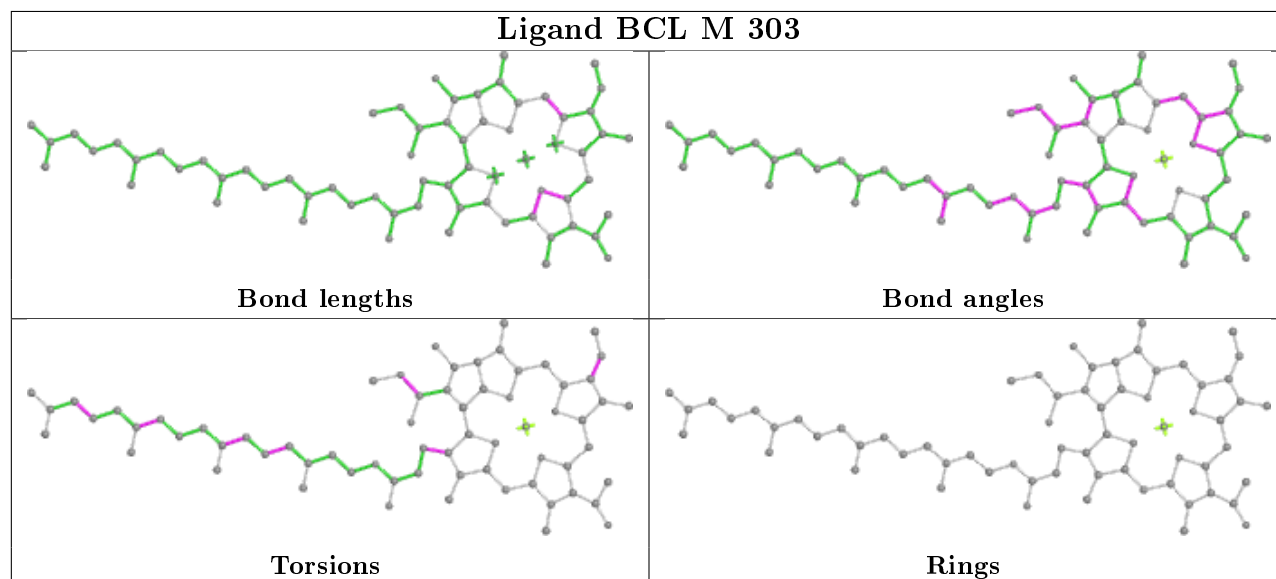
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	301	BCL	5	0
9	M	303	BCL	5	0
11	L	502	U10	9	0
11	M	501	U10	2	0
10	M	401	BPH	5	0
9	L	304	BCL	2	0
9	L	302	BCL	13	0
10	L	402	BPH	7	0
7	H	251	DIO	5	0
13	M	600	SPN	6	0
4	M	703	LDA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

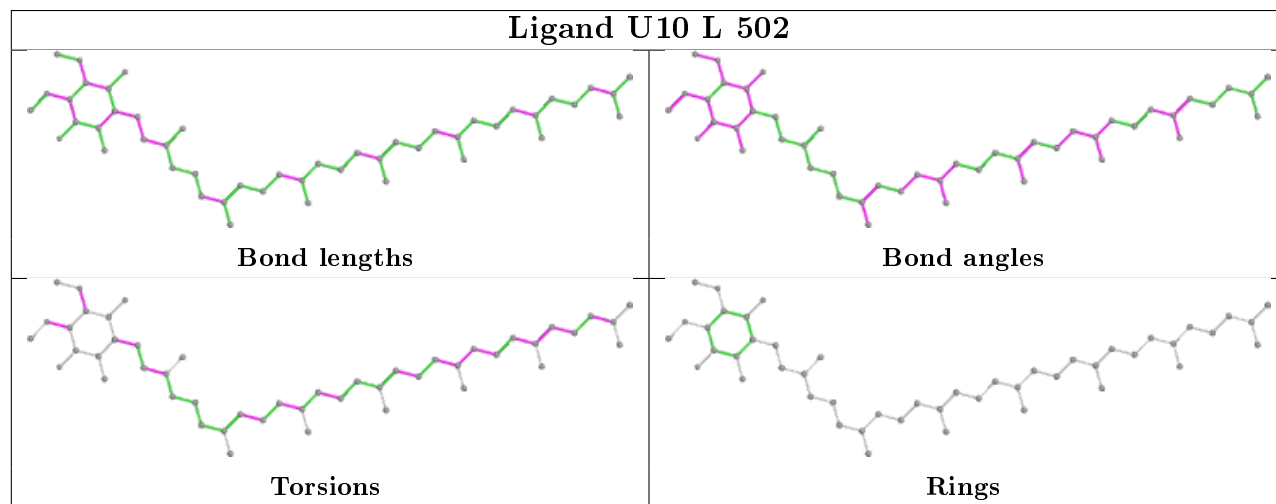
Ligand BCL L 301



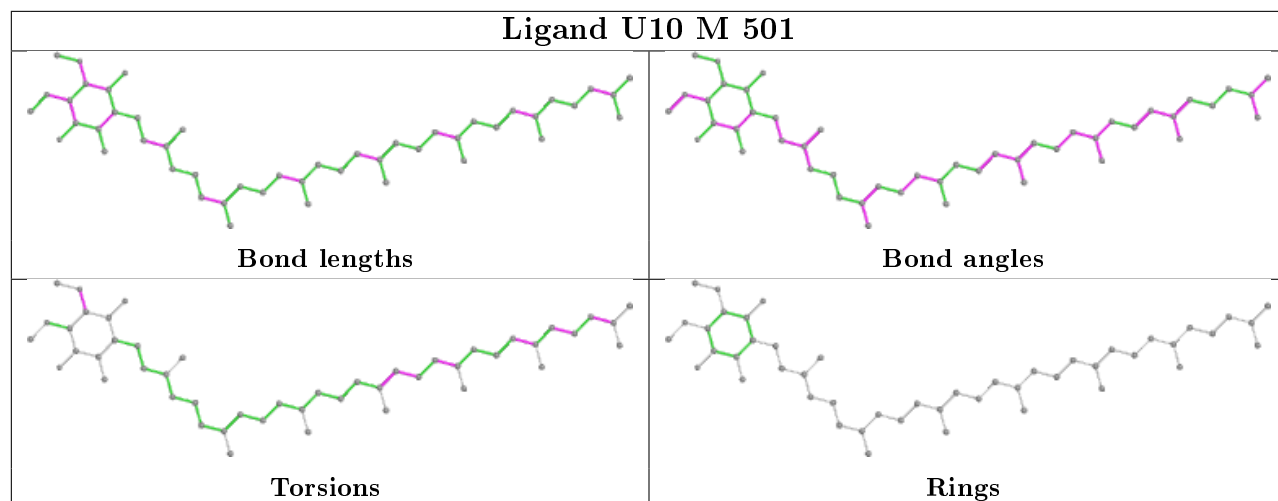
Ligand BCL M 303



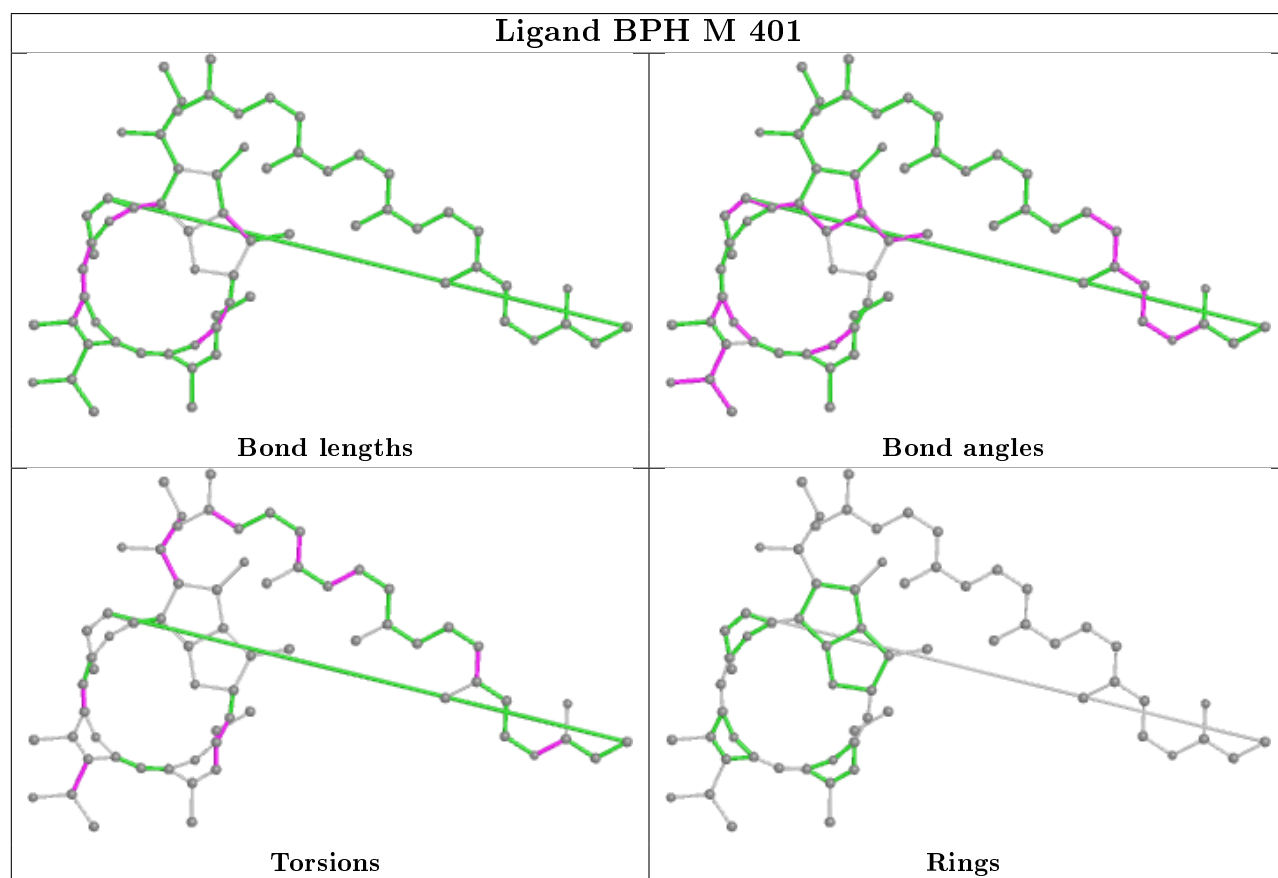
Ligand U10 L 502

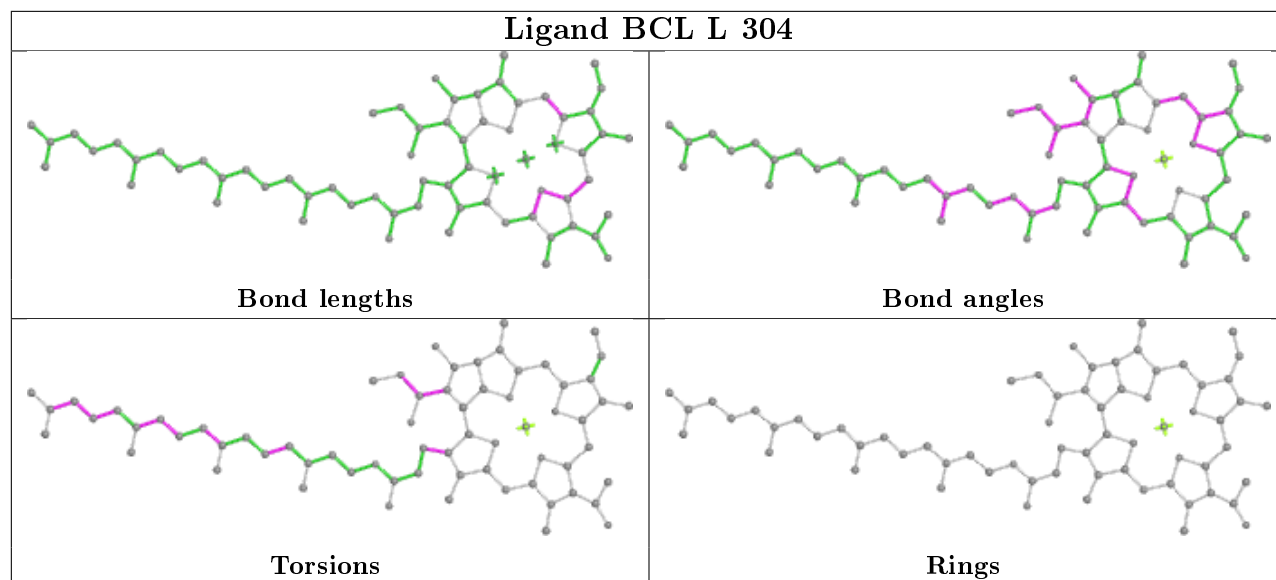
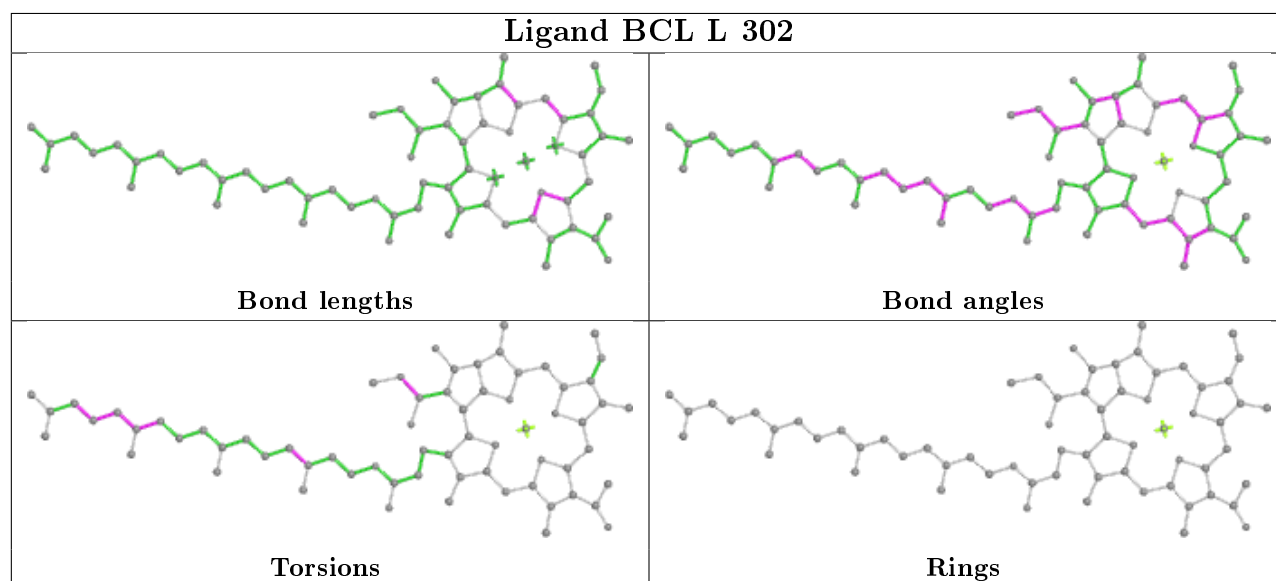


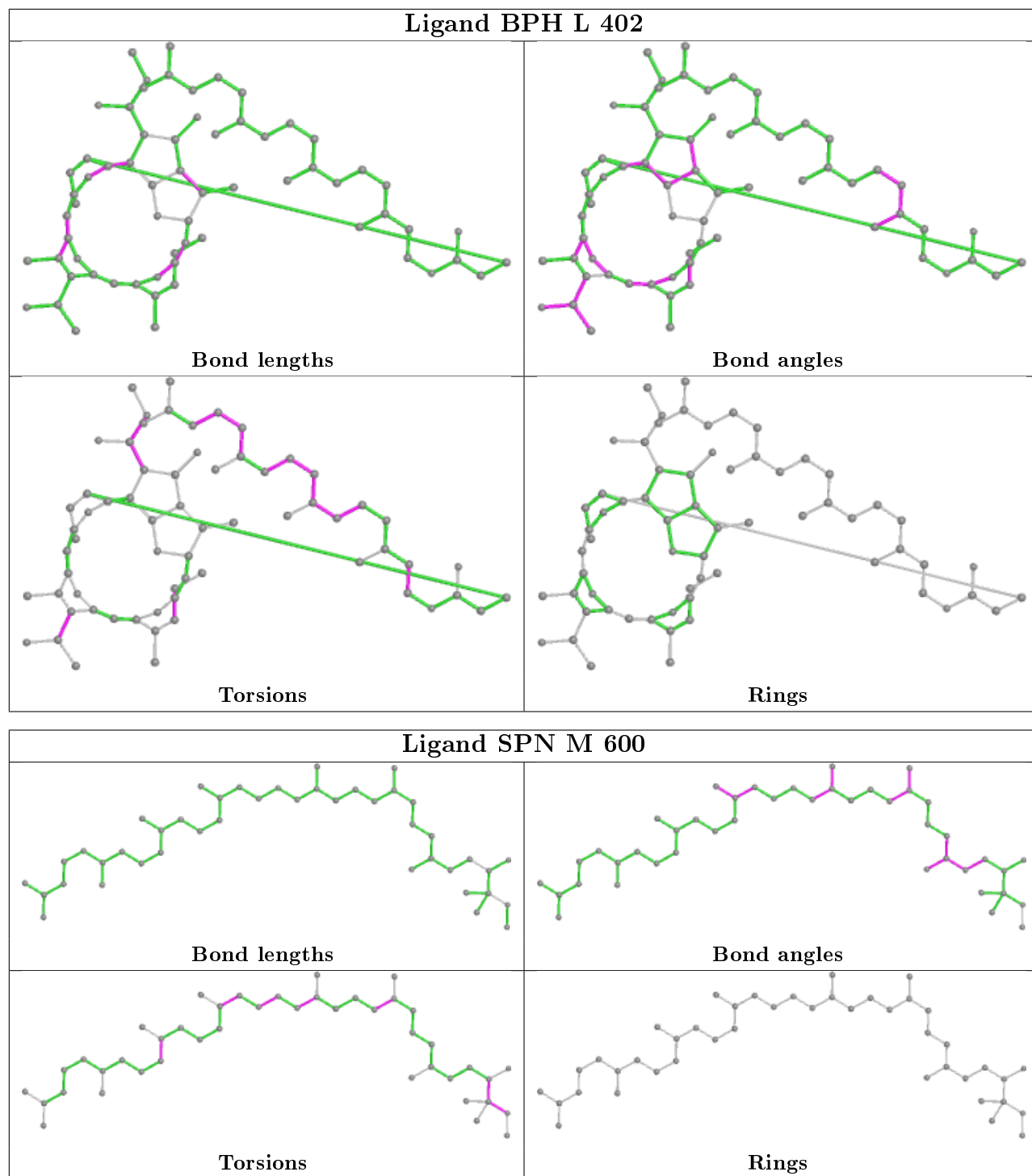
Ligand U10 M 501



Ligand BPH M 401



Ligand BCL L 304**Ligand BCL L 302**



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	241/241 (100%)	-0.39	2 (0%) 86 86	51, 65, 76, 101	0
2	L	281/281 (100%)	-0.45	6 (2%) 63 61	49, 65, 100, 106	0
3	M	302/302 (100%)	-0.46	2 (0%) 87 87	44, 67, 98, 101	0
All	All	824/824 (100%)	-0.44	10 (1%) 79 79	44, 66, 97, 106	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	5.1
1	H	10	PHE	4.0
2	L	59	TRP	3.5
3	M	80	TRP	3.2
3	M	1	ALA	3.2
2	L	281	GLY	2.9
2	L	277	GLY	2.6
2	L	202	LYS	2.5
2	L	270	PRO	2.5
2	L	276	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

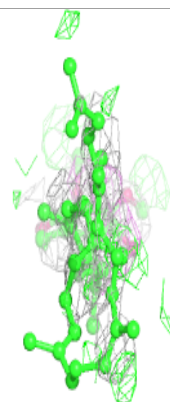
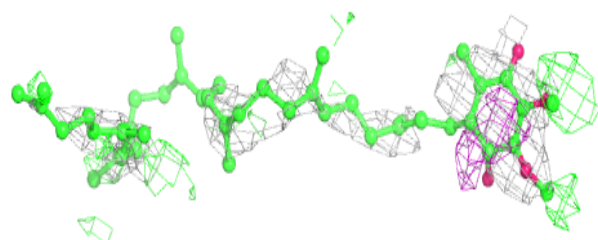
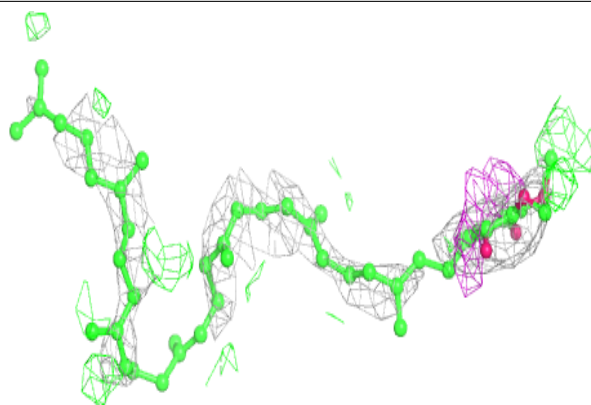
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	DIO	L	283	6/6	0.64	0.33	131,131,131,132	0
4	LDA	H	704	16/16	0.68	0.51	109,114,120,120	0
11	U10	L	502	48/63	0.69	0.51	128,135,140,140	0
4	LDA	M	703	16/16	0.70	0.50	98,102,107,108	0
6	HTO	H	3	10/10	0.74	0.34	113,114,114,115	0
4	LDA	M	702	16/16	0.79	0.39	96,109,120,121	0
5	PO4	H	804	5/5	0.81	0.25	123,123,123,123	0
6	HTO	H	2	10/10	0.82	0.31	134,136,136,136	0
5	PO4	H	803	5/5	0.86	0.20	124,124,124,124	0
6	HTO	L	282	10/10	0.86	0.33	97,98,99,100	0
5	PO4	M	801	5/5	0.87	0.27	140,140,140,140	0
4	LDA	M	701	16/16	0.88	0.23	77,85,88,88	0
13	SPN	M	600	43/43	0.89	0.23	65,76,86,87	0
10	BPH	M	401	65/65	0.89	0.22	63,73,107,107	0
4	LDA	M	705	16/16	0.89	0.48	83,90,100,101	0
5	PO4	M	802	5/5	0.90	0.15	110,110,111,111	0
11	U10	M	501	48/63	0.93	0.20	53,60,89,89	0
7	DIO	H	251	6/6	0.94	0.24	84,84,85,86	0
14	CL	M	304	1/1	0.94	0.06	83,83,83,83	0
8	K	H	1	1/1	0.95	0.08	64,64,64,64	0
9	BCL	L	301	66/66	0.95	0.21	62,71,111,113	0
9	BCL	L	302	66/66	0.97	0.17	45,61,64,65	0
10	BPH	L	402	65/65	0.97	0.16	48,56,66,66	0
9	BCL	M	303	66/66	0.97	0.15	57,60,71,76	0
5	PO4	M	800	5/5	0.98	0.08	67,67,68,69	0
9	BCL	L	304	66/66	0.98	0.12	37,42,64,66	0
12	FE	M	500	1/1	0.99	0.11	55,55,55,55	0

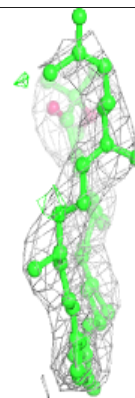
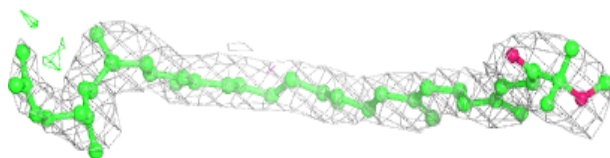
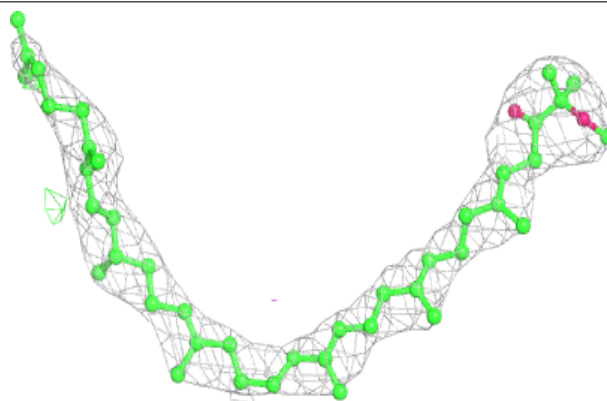
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around U10 L 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

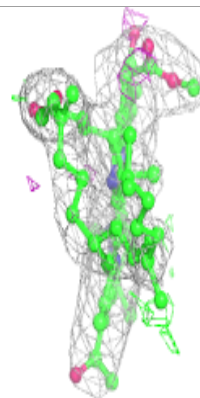
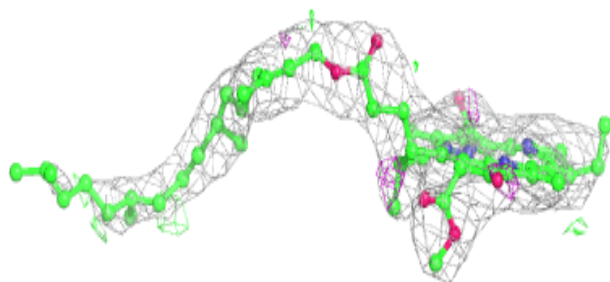
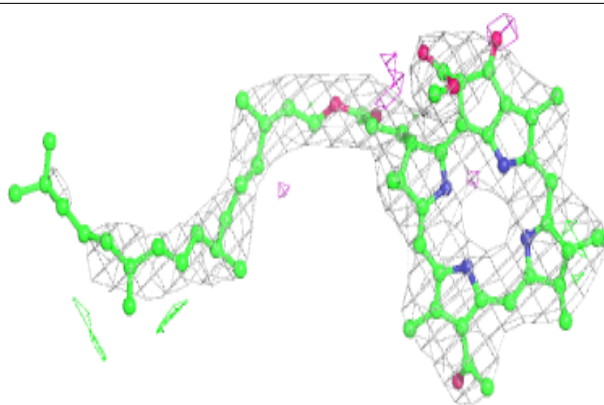
**Electron density around SPN M 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

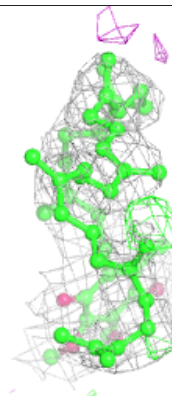
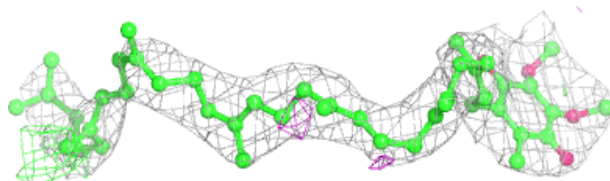
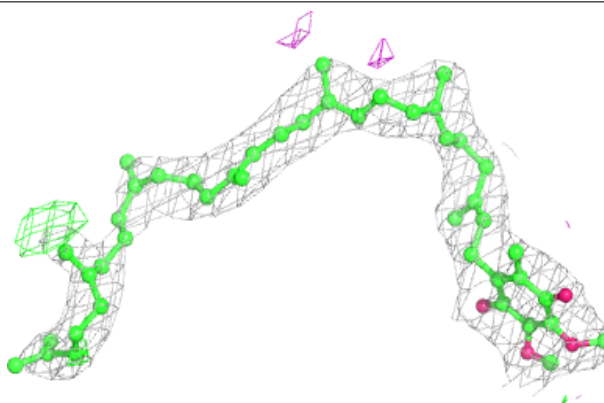


Electron density around BPH M 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

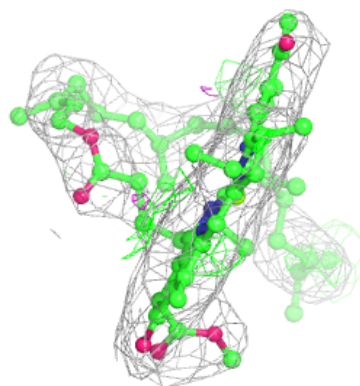
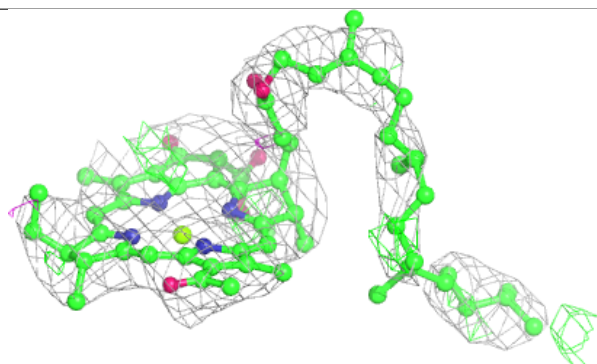
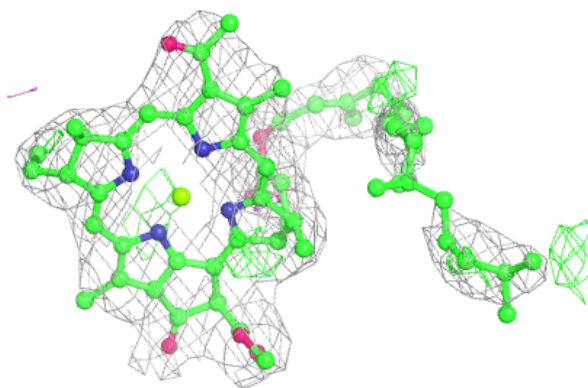
**Electron density around U10 M 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

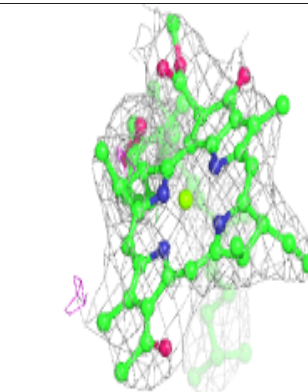
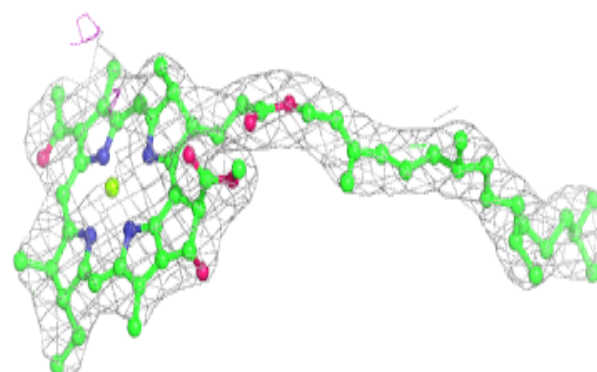
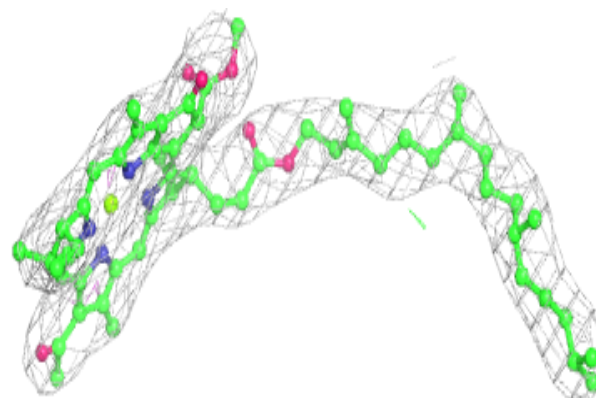


Electron density around BCL L 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

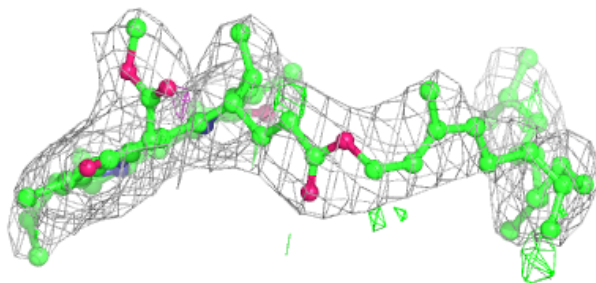
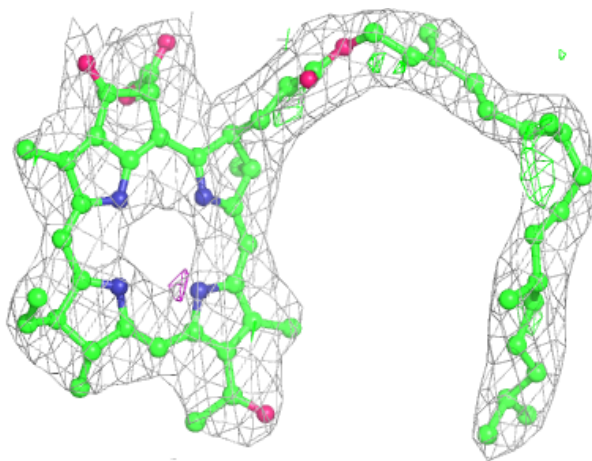
**Electron density around BCL L 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



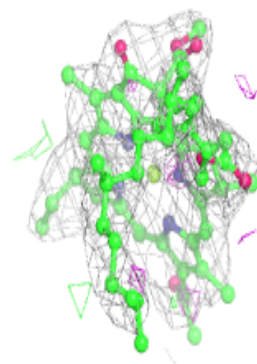
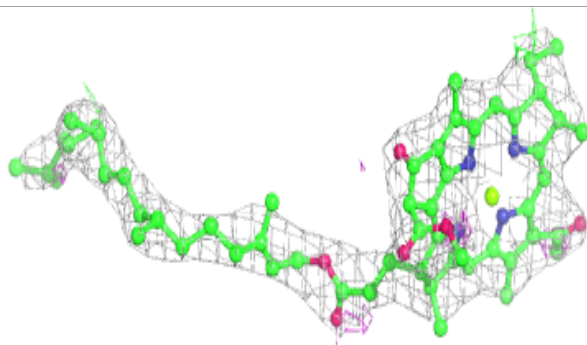
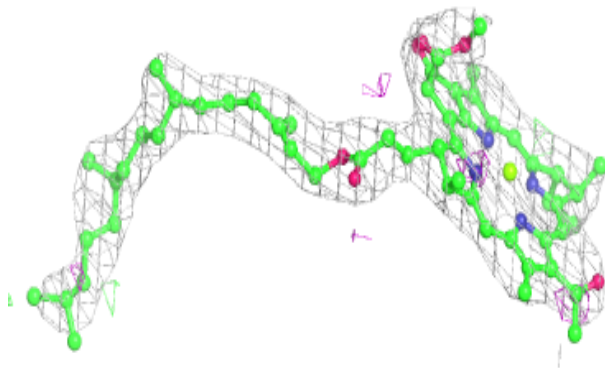
Electron density around BPH L 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

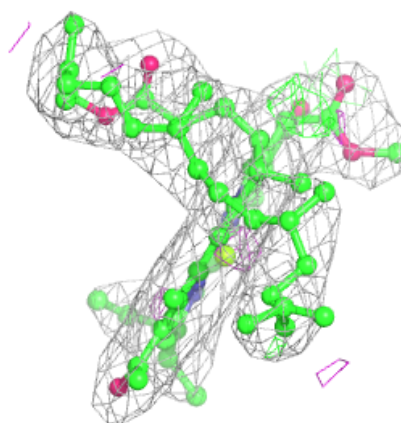
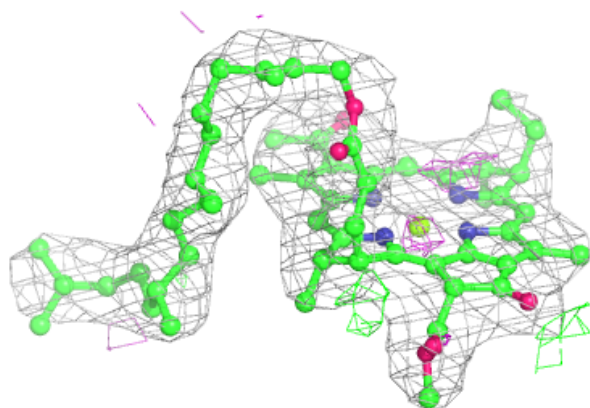
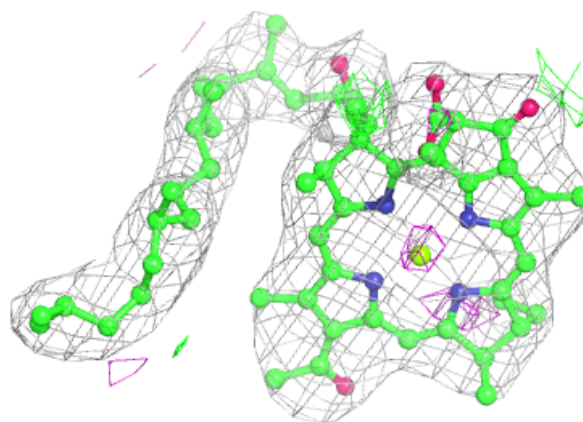


Electron density around BCL M 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCL L 304:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.