



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:07 am BST

PDB ID : 2HG9
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with tetrabrominated phosphatidylcholine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-26
Resolution : 2.45 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

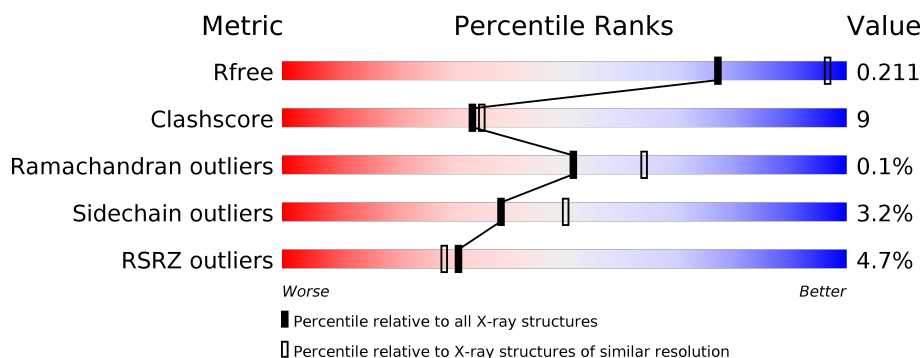
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	L	281	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	M	307	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> </div>
3	H	260	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div></div> </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	CDL	M	800	-	-	-	X
11	PCK	M	802	-	-	X	X
12	LDA	H	903	-	-	-	X
12	LDA	H	904	-	-	-	X
12	LDA	H	908	-	-	X	X
12	LDA	M	902	-	-	-	X
12	LDA	M	920	-	-	-	X
13	GOL	H	708	-	-	-	X
15	PC7	H	801	-	-	-	X
8	U10	L	502	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7843 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	3	0
			2237	1511	356	362	8			

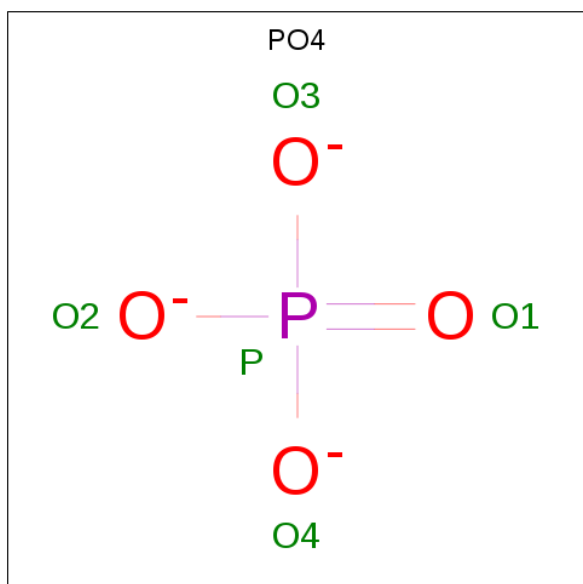
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	12	0
			2450	1631	402	406	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	9	0
			1862	1189	323	339	11			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

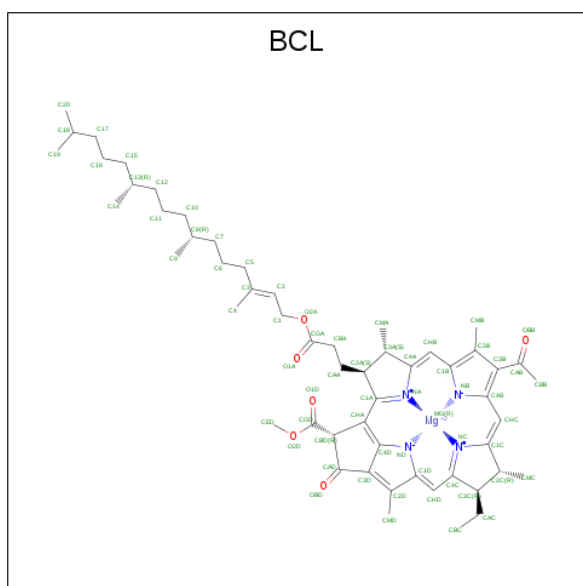


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

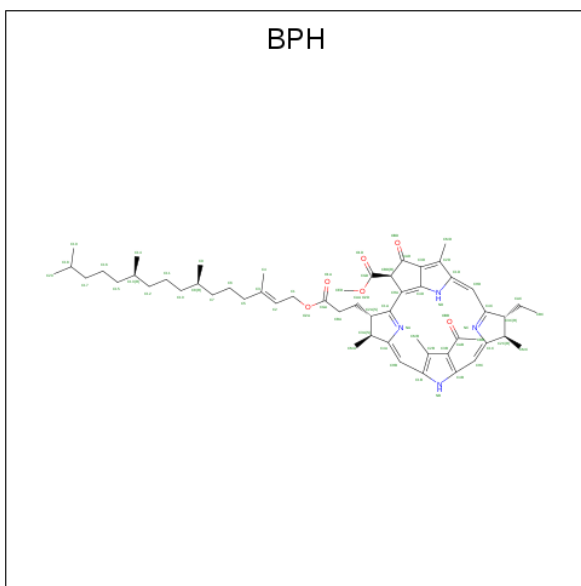
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Cl 1 1	0	0
5	M	1	Total Cl 1 1	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



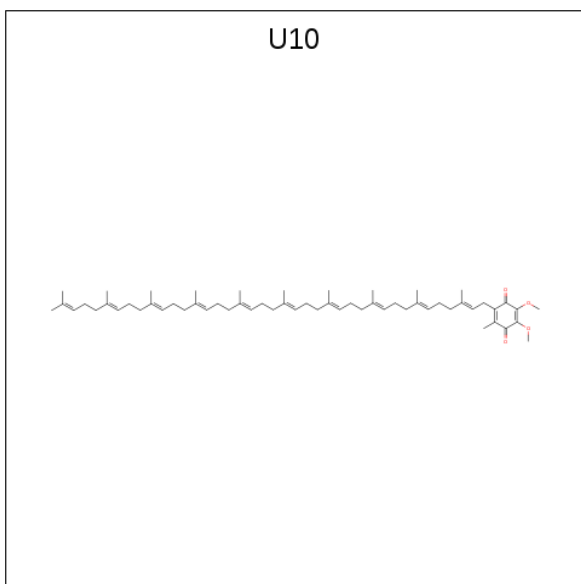
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

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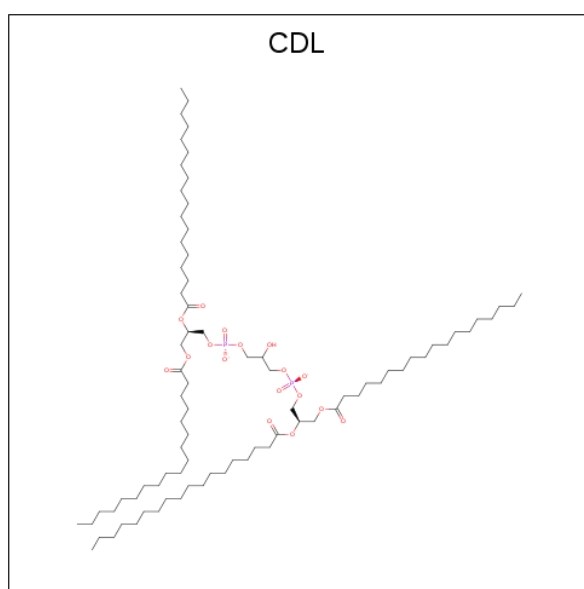
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

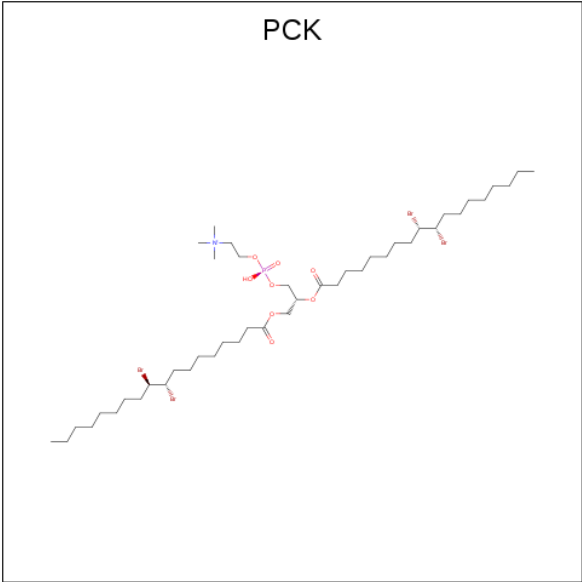
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	Fe		0	0
			1	1			

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



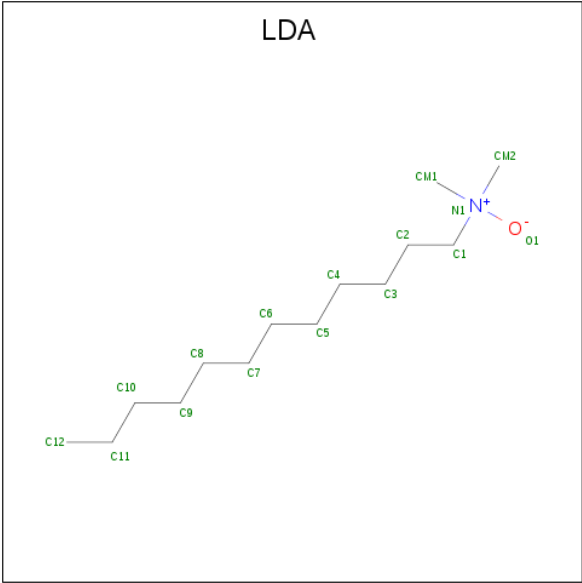
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is (7R,18S,19R)-18,19-DIBROMO-7-[[[(9S,10S)-9,10-DIBROMOOCTADECAN OYL]OXY]-4-HYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHE PTACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PCK) (formula: C₄₄H₈₅Br₄NO₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
11	M	1	58	4	44	1	8	1	0	0

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



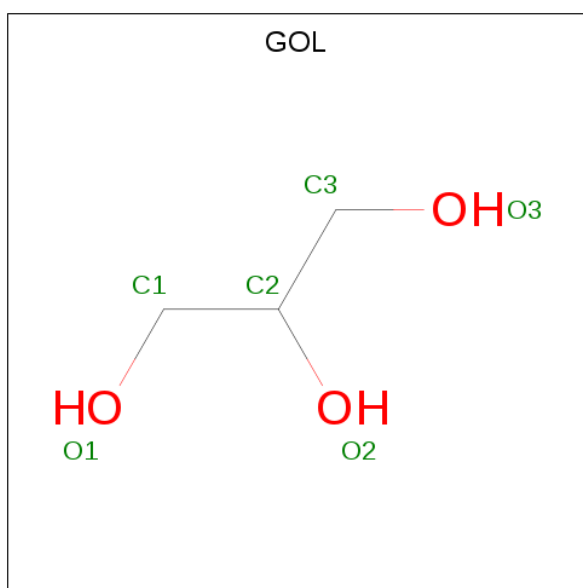
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	M	1	16	14	1	1	0	0
12	M	1	16	14	1	1	0	0

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

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

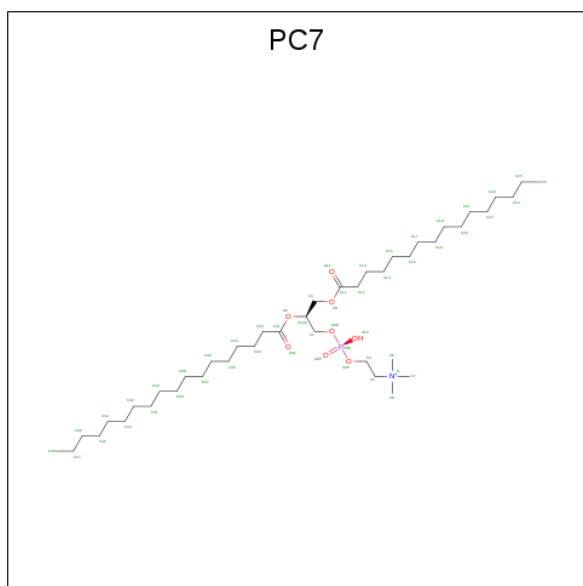


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			6	3	3		
13	M	1	Total	C	O	0	0
			6	3	3		
13	H	1	Total	C	O	0	0
			6	3	3		
13	H	1	Total	C	O	0	0
			6	3	3		
13	H	1	Total	C	O	0	0
			6	3	3		
13	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 15 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total C N O P 52 42 1 8 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	L	100	Total O 100 100	0	0
16	M	133	Total O 133 133	0	0
16	H	208	Total O 208 208	0	0

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.

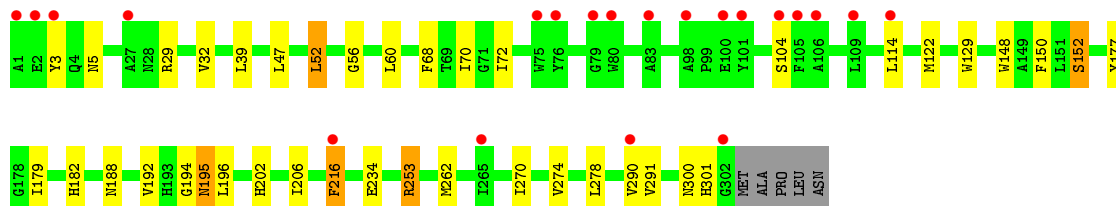
- Molecule 1: Reaction center protein L chain

Chain L: 




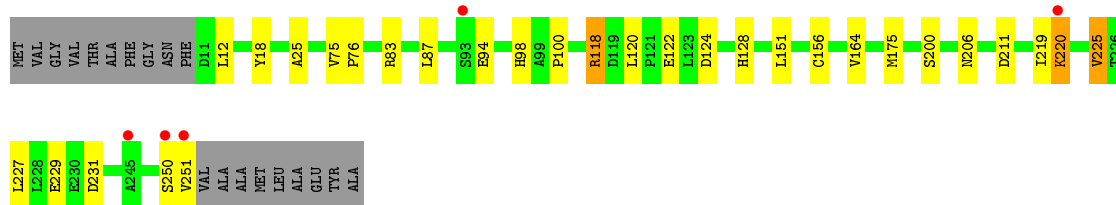
- Molecule 2: Reaction center protein M chain

Chain M: 



- Molecule 3: Reaction center protein H chain

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.55Å 139.55Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.36 – 2.45 39.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.36-2.45) 98.0 (39.36-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.209 0.183 , 0.211	Depositor DCC
R_{free} test set	3709 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7843	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CL, CDL, BPH, K, PC7, PCK, FE, 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	L	0.90	0/2342	0.73	1/3205 (0.0%)
2	M	0.90	1/2601 (0.0%)	0.80	3/3548 (0.1%)
3	H	0.95	3/1961 (0.2%)	0.84	4/2663 (0.2%)
All	All	0.92	4/6904 (0.1%)	0.79	8/9416 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.20	1.61	1.51
3	H	94	GLU	CB-CG	5.59	1.62	1.52
3	H	94	GLU	CD-OE2	5.30	1.31	1.25
2	M	152	SER	CB-OG	5.05	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	124	ASP	CB-CG-OD1	7.74	125.27	118.30
3	H	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	M	253[A]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	M	253[B]	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	H	83	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	M	29	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	L	210	ASP	CB-CG-OD1	5.37	123.13	118.30
3	H	211	ASP	CB-CG-OD1	5.19	122.97	118.30

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	L	2237	0	2202	10	0
2	M	2450	0	2370	38	0
3	H	1862	0	1884	21	0
4	H	5	0	0	0	0
4	L	5	0	0	0	0
4	M	10	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	1	0
6	L	132	0	148	8	0
6	M	132	0	148	20	0
7	L	65	0	75	3	0
7	M	65	0	76	4	0
8	L	48	0	63	4	0
8	M	48	0	63	1	0
9	M	1	0	0	0	0
10	M	81	0	106	2	0
11	M	58	0	80	24	0
12	H	64	0	124	19	0
12	M	48	0	93	9	0
13	H	24	0	32	2	0
13	M	12	0	16	0	0
14	H	1	0	0	0	0
15	H	52	0	84	6	0
16	H	208	0	0	0	0
16	L	100	0	0	0	0
16	M	133	0	0	7	0
All	All	7843	0	7564	128	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 (128) 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)
12:M:902:LDA:H121	12:H:908:LDA:H121	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47[A]:LEU:HD22	11:M:802:PCK:BR4	2.11	1.04
8:L:502:U10:H351	8:L:502:U10:H38	1.41	1.03
11:M:802:PCK:H252	11:M:802:PCK:H211	1.35	1.02
2:M:122:MET:SD	12:M:920:LDA:H122	2.01	1.01
6:M:311:BCL:H93	11:M:802:PCK:H482	1.42	1.00
2:M:188[B]:ASN:OD1	16:M:1416:HOH:O	1.80	0.98
2:M:47[B]:LEU:HD23	11:M:802:PCK:BR4	2.26	0.90
11:M:802:PCK:BR1	11:M:802:PCK:H442	2.30	0.87
11:M:802:PCK:H252	11:M:802:PCK:C21	2.08	0.83
12:M:902:LDA:H121	12:H:908:LDA:C12	2.08	0.82
11:M:802:PCK:H161	11:M:802:PCK:BR3	2.36	0.81
2:M:60[B]:LEU:HD23	7:M:401:BPH:H4C1	1.63	0.81
8:L:502:U10:H351	8:L:502:U10:C38	2.11	0.80
12:H:903:LDA:CM2	12:H:904:LDA:O1	2.30	0.80
6:M:313:BCL:H191	11:M:802:PCK:H262	1.64	0.80
12:H:903:LDA:HM22	12:H:904:LDA:H21	1.66	0.76
11:M:802:PCK:H211	11:M:802:PCK:C25	2.10	0.76
12:M:902:LDA:C12	12:H:908:LDA:H121	2.16	0.74
15:H:801:PC7:H451	12:H:901:LDA:H121	1.68	0.74
6:M:311:BCL:C7	6:M:311:BCL:H41	2.18	0.72
6:M:311:BCL:HBB2	6:M:311:BCL:HMB1	1.71	0.71
6:M:311:BCL:CBB	6:M:311:BCL:HMB1	2.22	0.70
2:M:47[A]:LEU:CD2	11:M:802:PCK:BR4	2.94	0.70
6:M:311:BCL:H102	6:M:311:BCL:H41	1.75	0.67
12:H:903:LDA:HM23	12:H:904:LDA:O1	1.93	0.67
15:H:801:PC7:H451	12:H:901:LDA:C12	2.23	0.66
11:M:802:PCK:BR1	11:M:802:PCK:C44	2.99	0.66
6:M:311:BCL:H92	11:M:802:PCK:H261	1.78	0.66
6:M:311:BCL:H41	6:M:311:BCL:H71	1.78	0.65
2:M:52:LEU:HD11	2:M:60[A]:LEU:CD2	2.26	0.64
2:M:253[B]:ARG:NH2	16:M:1251:HOH:O	2.31	0.64
2:M:301[A]:HIS:CE1	16:M:1031:HOH:O	2.51	0.63
3:H:220[A]:LYS:NZ	3:H:229:GLU:OE2	2.32	0.62
2:M:68:PHE:O	2:M:72:ILE:HD13	2.00	0.62
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.82	0.61
2:M:56:GLY:O	2:M:60[A]:LEU:HD13	2.00	0.61
15:H:801:PC7:H73	12:H:908:LDA:H122	1.82	0.61
2:M:179:ILE:HG23	6:M:311:BCL:HED1	1.83	0.61
6:L:312:BCL:HMB1	6:L:312:BCL:CBB	2.32	0.60
2:M:47[B]:LEU:CD2	11:M:802:PCK:BR4	3.02	0.60
2:M:262:MET:HA	2:M:262:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:70:ILE:HG21	12:M:920:LDA:HM13	1.84	0.58
6:M:311:BCL:C4	6:M:311:BCL:H71	2.34	0.57
6:M:311:BCL:H93	11:M:802:PCK:C48	2.27	0.57
6:L:314:BCL:HBB2	6:L:314:BCL:HMB1	1.85	0.56
1:L:201:GLU:OE2	1:L:204[B]:LYS:NZ	2.33	0.56
3:H:128[B]:HIS:ND1	13:H:708:GOL:H32	2.21	0.55
11:M:802:PCK:H271	11:M:802:PCK:BR1	2.61	0.55
6:M:313:BCL:HMB1	6:M:313:BCL:CBB	2.37	0.54
10:M:800:CDL:CA5	10:M:800:CDL:OA8	2.56	0.54
1:L:182:THR:OG1	6:M:311:BCL:H2	2.08	0.54
2:M:262:MET:HE3	2:M:262:MET:CA	2.38	0.53
2:M:39:LEU:HD23	12:M:907:LDA:H101	1.90	0.52
6:M:311:BCL:H92	11:M:802:PCK:C26	2.40	0.51
6:M:313:BCL:H191	11:M:802:PCK:C26	2.37	0.51
3:H:25:ALA:HB2	12:H:908:LDA:H61	1.92	0.51
3:H:18:TYR:CD1	12:H:908:LDA:HM23	2.46	0.51
6:L:314:BCL:HBB3	7:L:402:BPH:H141	1.92	0.50
6:L:312:BCL:CGA	6:L:314:BCL:HBC1	2.42	0.50
2:M:177:TYR:OH	12:M:920:LDA:H123	2.11	0.50
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.94	0.49
5:M:711:CL:CL	16:M:1177:HOH:O	2.57	0.49
6:M:311:BCL:C9	11:M:802:PCK:H461	2.42	0.49
12:H:904:LDA:H32	12:H:904:LDA:HM13	1.95	0.49
15:H:801:PC7:C7	12:H:908:LDA:H122	2.44	0.48
12:H:903:LDA:HM22	12:H:904:LDA:O1	2.13	0.48
2:M:150:PHE:N	7:M:401:BPH:HMD3	2.28	0.47
8:M:501:U10:H4M2	8:M:501:U10:O3	2.14	0.47
6:L:312:BCL:HMB1	6:L:312:BCL:HBB3	1.95	0.47
2:M:270:ILE:HD13	10:M:800:CDL:H711	1.97	0.47
3:H:18:TYR:HD1	12:H:908:LDA:HM23	1.80	0.47
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.50	0.47
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD21	1.96	0.46
7:L:402:BPH:HBB3	7:L:402:BPH:CMB	2.46	0.46
2:M:290:VAL:HG21	3:H:12:LEU:HD23	1.97	0.46
16:M:1078:HOH:O	3:H:175:MET:HE1	2.16	0.46
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.97	0.46
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.51	0.46
2:M:52:LEU:HD11	2:M:60[B]:LEU:HD12	1.97	0.46
6:M:313:BCL:HMB1	6:M:313:BCL:HBB3	1.96	0.46
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.51	0.46
2:M:152:SER:OG	2:M:278:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.99	0.45
2:M:68:PHE:CE1	2:M:72:ILE:HD11	2.51	0.45
2:M:234:GLU:OE2	2:M:262:MET:HE1	2.17	0.45
3:H:219:ILE:HG21	3:H:225:VAL:CG1	2.47	0.45
15:H:801:PC7:H41	15:H:801:PC7:H11	1.99	0.45
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.52	0.45
7:M:401:BPH:H4C3	11:M:802:PCK:BR2	2.73	0.44
3:H:25:ALA:HB2	12:H:908:LDA:C6	2.47	0.44
15:H:801:PC7:H11	15:H:801:PC7:C4	2.47	0.44
6:L:314:BCL:H202	7:L:402:BPH:H7C2	2.00	0.44
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD22	2.00	0.44
1:L:193:LEU:HD23	8:L:502:U10:C2	2.48	0.43
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.18	0.43
6:M:313:BCL:C20	11:M:802:PCK:H242	2.49	0.43
3:H:118[B]:ARG:NE	3:H:120:LEU:HD12	2.34	0.43
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.18	0.43
6:L:312:BCL:NA	6:M:313:BCL:HBB2	2.34	0.43
12:H:904:LDA:HM13	12:H:904:LDA:C3	2.48	0.43
2:M:188[A]:ASN:ND2	16:M:1416:HOH:O	2.49	0.43
3:H:87:LEU:HD23	3:H:100:PRO:HA	2.01	0.42
11:M:802:PCK:H252	11:M:802:PCK:C20	2.49	0.42
3:H:151:LEU:O	3:H:164:VAL:HG23	2.19	0.42
1:L:207:ARG:CG	1:L:211:HIS:CG	3.03	0.42
7:M:401:BPH:CMB	7:M:401:BPH:HBB3	2.48	0.42
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.55	0.42
6:L:314:BCL:CBB	6:L:314:BCL:HMB1	2.50	0.42
8:L:502:U10:C35	8:L:502:U10:C38	2.92	0.42
12:H:903:LDA:H102	12:H:904:LDA:H101	2.02	0.42
2:M:129:TRP:CH2	11:M:802:PCK:BR2	3.28	0.42
2:M:301[A]:HIS:HE1	16:M:1031:HOH:O	1.95	0.41
12:M:902:LDA:C11	12:H:908:LDA:H121	2.49	0.41
1:L:209:PRO:HA	1:L:212:GLU:OE1	2.20	0.41
1:L:80:LEU:O	1:L:85:LEU:HD12	2.20	0.41
6:M:313:BCL:H18	11:M:802:PCK:C24	2.51	0.41
2:M:290:VAL:HG12	2:M:291:VAL:HG23	2.03	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.40	0.41
3:H:118[B]:ARG:HE	3:H:120:LEU:HD12	1.86	0.41
3:H:128[B]:HIS:CE1	13:H:708:GOL:H32	2.55	0.41
11:M:802:PCK:H62	11:M:802:PCK:H41	1.83	0.41
12:M:902:LDA:H21	12:M:902:LDA:HM13	1.85	0.41
2:M:194:GLY:O	2:M:195:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:87:LEU:HD13	3:H:98:HIS:HB2	2.01	0.40
3:H:250:SER:O	3:H:251:VAL:HG23	2.21	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	L	282/281 (100%)	275 (98%)	7 (2%)	0	100	100
2	M	312/307 (102%)	300 (96%)	11 (4%)	1 (0%)	41	49
3	H	248/260 (95%)	245 (99%)	3 (1%)	0	100	100
All	All	842/848 (99%)	820 (97%)	21 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	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	L	223/220 (101%)	216 (97%)	7 (3%)	40	52
2	M	248/240 (103%)	239 (96%)	9 (4%)	35	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	205/208 (99%)	198 (97%)	7 (3%)	37	48
All	All	676/668 (101%)	653 (97%)	23 (3%)	39	48

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	247	CYS
1	L	272	TRP
2	M	32	VAL
2	M	52	LEU
2	M	104	SER
2	M	114	LEU
2	M	182	HIS
2	M	192	VAL
2	M	196	LEU
2	M	216	PHE
2	M	274	VAL
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	200	SER
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
3	H	68	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 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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$
12	LDA	M	920	-	12,15,15	2.03	1 (8%)	14,17,17	0.61	0
4	PO4	L	703	-	4,4,4	0.90	0	6,6,6	0.86	0
12	LDA	H	903	-	12,15,15	2.01	1 (8%)	14,17,17	0.50	0
6	BCL	L	312	1	58,74,74	1.31	3 (5%)	69,115,115	1.41	12 (17%)
12	LDA	H	908	-	12,15,15	2.02	1 (8%)	14,17,17	0.97	1 (7%)
10	CDL	M	800	-	80,80,99	1.18	4 (5%)	86,92,111	1.13	6 (6%)
13	GOL	H	708	-	5,5,5	0.27	0	5,5,5	0.50	0
8	U10	M	501	-	48,48,63	0.94	2 (4%)	58,61,79	1.58	13 (22%)
12	LDA	H	904	-	12,15,15	1.98	1 (8%)	14,17,17	0.74	0
7	BPH	M	401	-	64,70,70	0.89	2 (3%)	76,101,101	1.48	12 (15%)
13	GOL	M	710	-	5,5,5	0.42	0	5,5,5	0.43	0
12	LDA	M	907	-	12,15,15	2.04	1 (8%)	14,17,17	0.63	0
12	LDA	M	902	-	12,15,15	2.00	1 (8%)	14,17,17	0.81	0
13	GOL	M	707	-	5,5,5	0.49	0	5,5,5	0.30	0
6	BCL	M	311	2	58,74,74	1.27	4 (6%)	69,115,115	1.51	15 (21%)
4	PO4	M	702	-	4,4,4	0.82	0	6,6,6	1.07	0
13	GOL	H	706	-	5,5,5	0.35	0	5,5,5	1.03	0
6	BCL	L	314	1	58,74,74	1.01	2 (3%)	69,115,115	1.70	17 (24%)
8	U10	L	502	-	48,48,63	1.10	3 (6%)	58,61,79	1.77	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PC7	H	801	-	51,51,51	0.84	1 (1%)	57,59,59	0.92	3 (5%)
13	GOL	H	705	-	5,5,5	0.52	0	5,5,5	0.65	0
11	PCK	M	802	-	57,57,57	0.77	0	63,69,69	1.06	5 (7%)
6	BCL	M	313	2	58,74,74	1.38	3 (5%)	69,115,115	1.76	16 (23%)
13	GOL	H	709	-	5,5,5	0.43	0	5,5,5	0.42	0
7	BPH	L	402	-	64,70,70	0.86	2 (3%)	76,101,101	1.32	9 (11%)
4	PO4	H	704	-	4,4,4	0.79	0	6,6,6	0.84	0
12	LDA	H	901	-	12,15,15	2.02	1 (8%)	14,17,17	0.60	0
4	PO4	M	701	-	4,4,4	0.88	0	6,6,6	1.24	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
12	LDA	M	920	-	-	7/13/13/13	-
12	LDA	H	904	-	-	5/13/13/13	-
12	LDA	H	903	-	-	9/13/13/13	-
6	BCL	L	312	1	-	1/37/137/137	-
12	LDA	H	908	-	-	10/13/13/13	-
10	CDL	M	800	-	-	38/91/91/110	-
13	GOL	H	708	-	-	1/4/4/4	-
8	U10	M	501	-	-	5/45/69/87	0/1/1/1
7	BPH	M	401	-	-	15/54/105/105	0/5/6/6
13	GOL	M	710	-	-	4/4/4/4	-
12	LDA	M	907	-	-	6/13/13/13	-
12	LDA	M	902	-	-	2/13/13/13	-
13	GOL	M	707	-	-	3/4/4/4	-
6	BCL	M	311	2	-	10/37/137/137	-
13	GOL	H	706	-	-	2/4/4/4	-
6	BCL	L	314	1	-	2/37/137/137	-
8	U10	L	502	-	-	11/45/69/87	0/1/1/1
15	PC7	H	801	-	-	23/55/55/55	-
13	GOL	H	705	-	-	2/4/4/4	-
11	PCK	M	802	-	-	33/67/67/67	-
6	BCL	M	313	2	-	3/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GOL	H	709	-	-	2/4/4/4	-
7	BPH	L	402	-	-	7/54/105/105	0/5/6/6
12	LDA	H	901	-	-	6/13/13/13	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	901	LDA	O1-N1	-6.96	1.25	1.42
12	H	908	LDA	O1-N1	-6.95	1.25	1.42
12	M	907	LDA	O1-N1	-6.94	1.25	1.42
12	H	903	LDA	O1-N1	-6.86	1.26	1.42
12	M	902	LDA	O1-N1	-6.85	1.26	1.42
12	M	920	LDA	O1-N1	-6.85	1.26	1.42
12	H	904	LDA	O1-N1	-6.79	1.26	1.42
6	M	311	BCL	MG-NA	6.41	2.21	2.06
6	L	312	BCL	MG-NA	6.32	2.21	2.06
6	M	313	BCL	MG-NA	5.97	2.20	2.06
6	M	313	BCL	C4B-NB	5.10	1.39	1.35
10	M	800	CDL	OA6-CA5	4.75	1.47	1.34
10	M	800	CDL	OA8-CA7	4.66	1.47	1.33
10	M	800	CDL	OB6-CB5	4.60	1.47	1.34
10	M	800	CDL	OB8-CB7	4.26	1.45	1.33
8	L	502	U10	O3-C3	4.21	1.47	1.36
6	M	313	BCL	C3C-C4C	-3.73	1.46	1.51
6	L	312	BCL	C4B-NB	3.62	1.38	1.35
7	M	401	BPH	CHC-C1C	3.35	1.43	1.36
6	M	311	BCL	C1B-NB	3.31	1.38	1.35
6	L	312	BCL	C1B-NB	3.24	1.38	1.35
8	L	502	U10	O4-C4	3.17	1.44	1.36
6	L	314	BCL	C4B-NB	2.88	1.37	1.35
6	M	311	BCL	C4B-NB	2.82	1.37	1.35
8	M	501	U10	O3-C3	2.51	1.43	1.36
6	L	314	BCL	MG-NA	2.31	2.11	2.06
15	H	801	PC7	C1-C2	2.24	1.57	1.50
8	L	502	U10	C13-C14	2.22	1.38	1.33
8	M	501	U10	O4-C4	2.22	1.42	1.36
6	M	311	BCL	OBD-CAD	2.18	1.25	1.22
7	L	402	BPH	OBD-CAD	2.17	1.25	1.22
7	L	402	BPH	CHC-C1C	2.12	1.40	1.36
7	M	401	BPH	C3D-CAD	-2.08	1.43	1.47

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	800	CDL	OA6-CA5-C11	4.95	122.17	111.50
6	M	313	BCL	C4D-C3D-CAD	-4.75	105.82	108.47
10	M	800	CDL	OB6-CB5-C51	4.48	121.17	111.50
7	L	402	BPH	C1-C2-C3	-4.46	118.32	126.04
6	M	313	BCL	CMB-C2B-C1B	-4.44	121.64	128.46
7	M	401	BPH	CAC-C3C-C4C	4.19	123.44	112.67
8	L	502	U10	C30-C29-C31	4.16	122.27	115.27
8	M	501	U10	C32-C33-C34	-4.05	117.92	127.66
6	L	314	BCL	O2D-CGD-CBD	4.03	118.42	111.27
8	L	502	U10	C31-C29-C28	-4.00	113.02	121.12
6	L	314	BCL	CMB-C2B-C1B	-4.00	122.32	128.46
6	L	312	BCL	CMB-C2B-C1B	-3.98	122.34	128.46
8	M	501	U10	C30-C29-C31	3.85	121.74	115.27
6	M	311	BCL	C4-C3-C2	-3.73	114.11	123.68
6	L	314	BCL	CAC-C3C-C2C	-3.71	105.00	114.26
6	M	311	BCL	C1-O2A-CGA	3.70	126.15	116.44
7	M	401	BPH	O2D-CGD-CBD	3.53	117.55	111.27
6	M	313	BCL	C1-C2-C3	-3.47	120.04	126.04
8	M	501	U10	C31-C29-C28	-3.46	114.11	121.12
7	L	402	BPH	O2D-CGD-CBD	3.45	117.39	111.27
6	L	312	BCL	CAA-C2A-C3A	-3.42	103.41	112.78
8	L	502	U10	C1M-C1-C6	-3.42	118.82	124.40
8	L	502	U10	O2-C2-C3	-3.40	113.71	120.93
7	M	401	BPH	C1-C2-C3	-3.38	120.20	126.04
8	L	502	U10	C35-C34-C33	-3.34	115.11	123.68
6	M	313	BCL	CAC-C3C-C2C	-3.30	106.02	114.26
8	M	501	U10	C26-C27-C28	-3.29	101.06	111.88
15	H	801	PC7	O2-C31-C32	3.26	118.53	111.50
7	M	401	BPH	OBD-CAD-CBD	-3.24	121.27	125.89
7	M	401	BPH	C1-O2A-CGA	3.13	124.66	116.44
11	M	802	PCK	O3-C3-C2	3.12	117.53	108.43
8	L	502	U10	C7-C6-C5	-3.11	114.74	118.48
6	M	311	BCL	CHA-C1A-NA	-3.10	119.31	126.40
6	M	313	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	M	501	U10	C17-C18-C19	-3.07	120.28	127.66
6	L	314	BCL	CAA-C2A-C3A	-3.06	104.41	112.78
8	L	502	U10	C25-C24-C26	3.04	120.39	115.27
6	M	311	BCL	CMB-C2B-C1B	-3.04	123.79	128.46
6	M	313	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
6	M	313	BCL	O2D-CGD-O1D	-3.01	117.96	123.84
11	M	802	PCK	O2-C31-C32	2.99	117.95	111.50
6	L	314	BCL	CAA-CBA-CGA	2.98	121.95	113.25
6	L	314	BCL	OBB-CAB-C3B	2.97	125.26	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401	BPH	C4D-C3D-CAD	-2.96	105.99	107.87
7	L	402	BPH	C1C-NC-C4C	-2.96	107.94	110.54
7	L	402	BPH	O2D-CGD-O1D	-2.93	118.10	123.84
11	M	802	PCK	O3-C11-C12	2.92	121.09	111.91
12	H	908	LDA	CM1-N1-C1	2.91	116.35	110.23
6	L	314	BCL	CMD-C2D-C3D	2.90	130.10	124.68
6	L	312	BCL	CHA-C1A-NA	-2.88	119.80	126.40
6	L	312	BCL	C2C-C3C-C4C	2.87	105.63	101.34
6	M	311	BCL	C5-C3-C2	2.86	126.90	121.12
8	M	501	U10	C15-C14-C16	2.86	120.07	115.27
6	M	313	BCL	C4A-NA-C1A	2.84	107.98	106.71
7	L	402	BPH	CAC-C3C-C2C	2.81	121.28	114.26
6	L	314	BCL	OBB-CAB-CBB	-2.80	113.86	120.17
8	L	502	U10	C12-C13-C14	-2.77	120.99	127.66
6	L	312	BCL	CMB-C2B-C3B	2.75	129.81	124.68
7	M	401	BPH	CBB-CAB-C3B	-2.74	114.57	120.43
6	L	312	BCL	CBA-CAA-C2A	2.74	121.95	113.86
7	L	402	BPH	CAC-C3C-C4C	2.72	119.64	112.67
6	M	311	BCL	CMA-C3A-C4A	-2.71	104.48	111.77
6	L	314	BCL	CBC-CAC-C3C	2.70	119.48	113.47
6	M	311	BCL	CAA-C2A-C3A	-2.70	105.40	112.78
8	M	501	U10	C22-C23-C24	-2.69	121.17	127.66
6	M	313	BCL	C11-C10-C8	-2.67	107.29	115.92
10	M	800	CDL	OA8-CA7-C31	2.66	120.25	111.91
7	M	401	BPH	C1B-NB-C4B	2.65	111.51	106.51
6	M	313	BCL	CAC-C3C-C4C	-2.63	106.74	112.58
11	M	802	PCK	C18-C19-C20	-2.63	108.96	115.61
6	L	314	BCL	C5-C3-C2	-2.60	115.85	121.12
6	L	312	BCL	OBD-CAD-CBD	-2.60	122.18	125.89
7	L	402	BPH	O2A-CGA-O1A	-2.60	117.04	123.59
6	L	312	BCL	C1C-NC-C4C	2.56	107.86	106.71
6	L	314	BCL	CMB-C2B-C3B	2.55	129.46	124.68
6	M	313	BCL	C2C-C3C-C4C	2.54	105.15	101.34
8	M	501	U10	C6-C1-C2	2.54	121.19	119.18
6	L	312	BCL	C4B-C3B-CAB	-2.53	122.24	127.13
6	L	314	BCL	C4D-C3D-CAD	-2.49	107.08	108.47
6	M	311	BCL	CAA-CBA-CGA	2.48	120.51	113.25
15	H	801	PC7	C2-O2-C31	-2.47	111.70	117.79
8	M	501	U10	C7-C6-C5	-2.47	115.51	118.48
8	L	502	U10	C35-C34-C36	2.46	119.41	115.27
10	M	800	CDL	OA8-CA7-OA9	-2.45	117.42	123.59
6	M	313	BCL	CHC-C1C-NC	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	312	BCL	C4-C3-C5	2.39	119.29	115.27
7	M	401	BPH	CMD-C2D-C3D	2.38	129.13	124.68
10	M	800	CDL	OA6-CA5-OA7	-2.36	117.99	123.70
6	M	313	BCL	CMD-C2D-C3D	2.36	129.09	124.68
7	M	401	BPH	CAA-C2A-C3A	-2.34	106.37	112.78
6	M	311	BCL	OBB-CAB-C3B	2.34	124.14	119.99
8	M	501	U10	C25-C24-C26	2.33	119.20	115.27
6	L	312	BCL	CED-O2D-CGD	2.30	121.14	115.94
6	L	314	BCL	O1D-CGD-CBD	-2.29	119.80	124.48
6	M	311	BCL	CMB-C2B-C3B	2.26	128.91	124.68
7	M	401	BPH	CHD-C4C-NC	-2.25	122.53	125.20
7	M	401	BPH	CMA-C3A-C2A	-2.23	104.83	113.83
6	L	314	BCL	C4-C3-C5	2.22	119.01	115.27
6	M	311	BCL	C4-C3-C5	2.21	118.99	115.27
8	M	501	U10	C11-C9-C8	-2.21	116.65	121.12
8	L	502	U10	C3M-O3-C3	2.20	124.27	116.47
6	M	311	BCL	C2A-C1A-CHA	2.19	127.69	123.86
8	M	501	U10	C10-C9-C11	2.19	118.95	115.27
6	M	313	BCL	C4-C3-C5	2.16	118.91	115.27
15	H	801	PC7	O3-C11-C12	2.16	118.69	111.91
8	L	502	U10	C36-C34-C33	2.16	125.48	121.12
6	L	314	BCL	CAC-C3C-C4C	-2.15	107.80	112.58
8	L	502	U10	C15-C14-C13	-2.15	118.17	123.68
8	L	502	U10	C22-C23-C24	-2.14	122.52	127.66
6	M	313	BCL	O2A-C1-C2	2.14	114.25	108.64
10	M	800	CDL	CA6-OA8-CA7	2.13	125.02	117.12
6	M	311	BCL	C4B-C3B-CAB	-2.12	123.04	127.13
7	L	402	BPH	CMA-C3A-C2A	-2.11	105.33	113.83
6	L	314	BCL	CMC-C2C-C3C	-2.10	105.36	113.83
6	M	313	BCL	OBB-CAB-CBB	-2.08	115.50	120.17
8	M	501	U10	C41-C39-C40	2.06	119.16	114.60
6	M	311	BCL	CMA-C3A-C2A	-2.06	105.52	113.83
11	M	802	PCK	BR1-C19-C18	2.05	112.44	108.88
6	L	312	BCL	CAA-C2A-C1A	-2.04	105.28	111.97
6	L	314	BCL	CHA-C1A-NA	-2.03	121.74	126.40
8	L	502	U10	C21-C19-C18	-2.03	117.01	121.12
8	L	502	U10	O5-C5-C6	-2.02	118.00	121.55
6	M	311	BCL	OBD-CAD-CBD	-2.02	123.01	125.89
7	L	402	BPH	C6-C7-C8	-2.01	109.42	115.92

There are no chirality outliers.

All (207) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	920	LDA	C2-C1-N1-O1
12	M	920	LDA	C2-C1-N1-CM1
12	M	920	LDA	C2-C1-N1-CM2
12	H	903	LDA	C2-C1-N1-O1
12	H	903	LDA	C2-C1-N1-CM2
12	H	908	LDA	C2-C1-N1-O1
12	H	908	LDA	C2-C1-N1-CM1
12	H	908	LDA	N1-C1-C2-C3
10	M	800	CDL	CA2-OA2-PA1-OA3
10	M	800	CDL	CA2-OA2-PA1-OA4
10	M	800	CDL	CA2-OA2-PA1-OA5
12	H	904	LDA	N1-C1-C2-C3
7	M	401	BPH	C4C-C3C-CAC-CBC
7	M	401	BPH	C4B-C3B-CAB-CBB
7	M	401	BPH	C11-C10-C8-C9
13	M	710	GOL	O1-C1-C2-C3
13	M	710	GOL	C1-C2-C3-O3
13	M	707	GOL	O1-C1-C2-C3
8	L	502	U10	C28-C29-C31-C32
8	L	502	U10	C30-C29-C31-C32
15	H	801	PC7	O31-C31-O2-C2
15	H	801	PC7	C1-O3P-P-O1P
15	H	801	PC7	C1-O3P-P-O2P
15	H	801	PC7	C1-O3P-P-O4P
15	H	801	PC7	O4P-C4-C5-N
11	M	802	PCK	C40-C41-C42-C43
11	M	802	PCK	C32-C31-O2-C2
11	M	802	PCK	O3P-C1-C2-O2
11	M	802	PCK	C1-O3P-P-O1P
11	M	802	PCK	C4-O4P-P-O3P
11	M	802	PCK	C4-O4P-P-O2P
11	M	802	PCK	O4P-C4-C5-N
11	M	802	PCK	BR1-C19-C20-C21
11	M	802	PCK	BR2-C20-C21-C22
11	M	802	PCK	O31-C31-O2-C2
15	H	801	PC7	C32-C31-O2-C2
10	M	800	CDL	OA9-CA7-OA8-CA6
12	M	920	LDA	C7-C8-C9-C10
10	M	800	CDL	C31-CA7-OA8-CA6
6	M	311	BCL	C4-C3-C5-C6
6	M	311	BCL	C2-C3-C5-C6
8	L	502	U10	C24-C26-C27-C28
10	M	800	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
7	M	401	BPH	C13-C15-C16-C17
10	M	800	CDL	CA7-C31-C32-C33
11	M	802	PCK	C11-C12-C13-C14
11	M	802	PCK	C31-C32-C33-C34
8	M	501	U10	C29-C31-C32-C33
10	M	800	CDL	CB2-OB2-PB2-OB5
11	M	802	PCK	C1-O3P-P-O4P
15	H	801	PC7	C12-C11-O3-C3
10	M	800	CDL	C36-C37-C38-C39
12	H	908	LDA	C6-C7-C8-C9
10	M	800	CDL	C15-C16-C17-C18
10	M	800	CDL	C54-C55-C56-C57
11	M	802	PCK	C35-C36-C37-C38
10	M	800	CDL	C19-C20-C21-C22
12	H	901	LDA	C11-C10-C9-C8
12	H	908	LDA	C11-C10-C9-C8
10	M	800	CDL	C18-C19-C20-C21
15	H	801	PC7	O11-C11-O3-C3
11	M	802	PCK	C33-C34-C35-C36
13	H	709	GOL	O1-C1-C2-C3
11	M	802	PCK	C18-C19-C20-C21
12	H	908	LDA	C5-C6-C7-C8
11	M	802	PCK	C12-C13-C14-C15
12	H	908	LDA	C7-C8-C9-C10
10	M	800	CDL	C39-C40-C41-C42
7	L	402	BPH	C8-C10-C11-C12
12	M	920	LDA	C3-C4-C5-C6
7	L	402	BPH	C2-C3-C5-C6
15	H	801	PC7	C44-C45-C46-C47
13	M	710	GOL	O1-C1-C2-O2
13	M	710	GOL	O2-C2-C3-O3
13	M	707	GOL	O1-C1-C2-O2
13	H	709	GOL	O1-C1-C2-O2
12	M	907	LDA	C1-C2-C3-C4
11	M	802	PCK	C34-C35-C36-C37
6	M	311	BCL	C2-C1-O2A-CGA
12	H	901	LDA	C1-C2-C3-C4
8	L	502	U10	C15-C14-C16-C17
8	L	502	U10	C13-C14-C16-C17
10	M	800	CDL	OA7-CA5-OA6-CA4
15	H	801	PC7	C42-C43-C44-C45
15	H	801	PC7	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
10	M	800	CDL	C11-CA5-OA6-CA4
10	M	800	CDL	C51-CB5-OB6-CB4
10	M	800	CDL	C71-C72-C73-C74
10	M	800	CDL	OB7-CB5-OB6-CB4
11	M	802	PCK	C32-C33-C34-C35
11	M	802	PCK	O2-C2-C3-O3
10	M	800	CDL	C74-C75-C76-C77
7	L	402	BPH	C4-C3-C5-C6
15	H	801	PC7	C32-C33-C34-C35
12	H	903	LDA	C1-C2-C3-C4
6	M	313	BCL	C16-C17-C18-C19
10	M	800	CDL	OA5-CA3-CA4-CA6
11	M	802	PCK	O3P-C1-C2-C3
7	M	401	BPH	C2C-C3C-CAC-CBC
10	M	800	CDL	C34-C35-C36-C37
11	M	802	PCK	C1-C2-C3-O3
15	H	801	PC7	C14-C15-C16-C17
15	H	801	PC7	C33-C34-C35-C36
13	H	706	GOL	O2-C2-C3-O3
7	M	401	BPH	C2B-C3B-CAB-CBB
15	H	801	PC7	C1-C2-O2-C31
12	H	908	LDA	C4-C5-C6-C7
15	H	801	PC7	C17-C18-C19-C20
6	M	311	BCL	C12-C13-C15-C16
15	H	801	PC7	C11-C12-C13-C14
11	M	802	PCK	BR1-C19-C20-BR2
12	H	908	LDA	C1-C2-C3-C4
8	L	502	U10	C25-C24-C26-C27
6	M	311	BCL	C15-C16-C17-C18
12	H	904	LDA	C5-C6-C7-C8
15	H	801	PC7	C41-C42-C43-C44
15	H	801	PC7	C12-C13-C14-C15
12	H	904	LDA	C1-C2-C3-C4
10	M	800	CDL	OA5-CA3-CA4-OA6
11	M	802	PCK	C25-C26-C27-C28
10	M	800	CDL	OA6-CA4-CA6-OA8
15	H	801	PC7	O2-C2-C3-O3
10	M	800	CDL	C52-C53-C54-C55
6	M	313	BCL	C16-C17-C18-C20
6	M	311	BCL	C4C-C3C-CAC-CBC
11	M	802	PCK	C18-C19-C20-BR2
11	M	802	PCK	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
10	M	800	CDL	C35-C36-C37-C38
7	M	401	BPH	C11-C10-C8-C7
6	L	314	BCL	C12-C13-C15-C16
8	L	502	U10	C23-C24-C26-C27
7	M	401	BPH	C4B-C3B-CAB-OBB
12	H	903	LDA	C5-C6-C7-C8
7	M	401	BPH	C2B-C3B-CAB-OBB
15	H	801	PC7	C15-C16-C17-C18
7	M	401	BPH	CAD-CBD-CGD-O2D
6	M	311	BCL	CAD-CBD-CGD-O2D
7	L	402	BPH	CAD-CBD-CGD-O2D
8	M	501	U10	C30-C29-C31-C32
15	H	801	PC7	C1-C2-C3-O3
7	M	401	BPH	C10-C11-C12-C13
12	H	908	LDA	C2-C1-N1-CM2
7	M	401	BPH	CHA-CBD-CGD-O1D
12	M	907	LDA	C6-C7-C8-C9
13	H	705	GOL	O2-C2-C3-O3
12	M	902	LDA	C9-C10-C11-C12
8	M	501	U10	C28-C29-C31-C32
6	L	314	BCL	C14-C13-C15-C16
12	M	902	LDA	C2-C3-C4-C5
13	H	706	GOL	C1-C2-C3-O3
12	M	920	LDA	C5-C6-C7-C8
10	M	800	CDL	C81-C82-C83-C84
7	M	401	BPH	C3-C5-C6-C7
15	H	801	PC7	C2-C1-O3P-P
10	M	800	CDL	CB2-OB2-PB2-OB3
12	H	901	LDA	C9-C10-C11-C12
10	M	800	CDL	OB9-CB7-OB8-CB6
12	M	907	LDA	C7-C8-C9-C10
6	M	311	BCL	C11-C10-C8-C7
12	H	903	LDA	C4-C5-C6-C7
12	M	907	LDA	C5-C6-C7-C8
10	M	800	CDL	C72-C73-C74-C75
11	M	802	PCK	BR4-C40-C41-C42
10	M	800	CDL	C71-CB7-OB8-CB6
6	M	311	BCL	C14-C13-C15-C16
11	M	802	PCK	C15-C16-C17-C18
12	H	903	LDA	C7-C8-C9-C10
10	M	800	CDL	C32-C33-C34-C35
10	M	800	CDL	CA3-CA4-CA6-OA8

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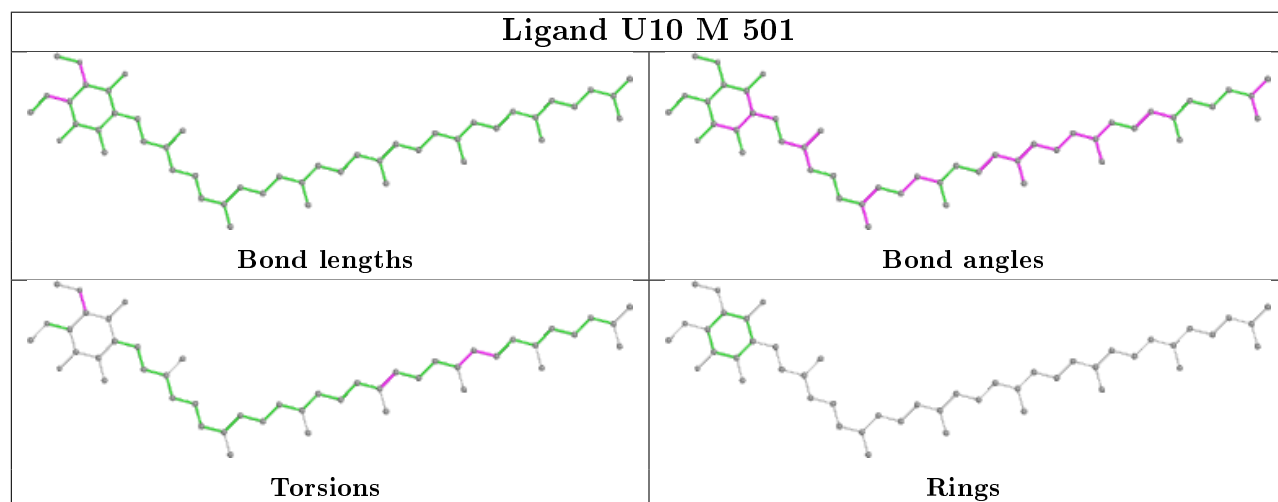
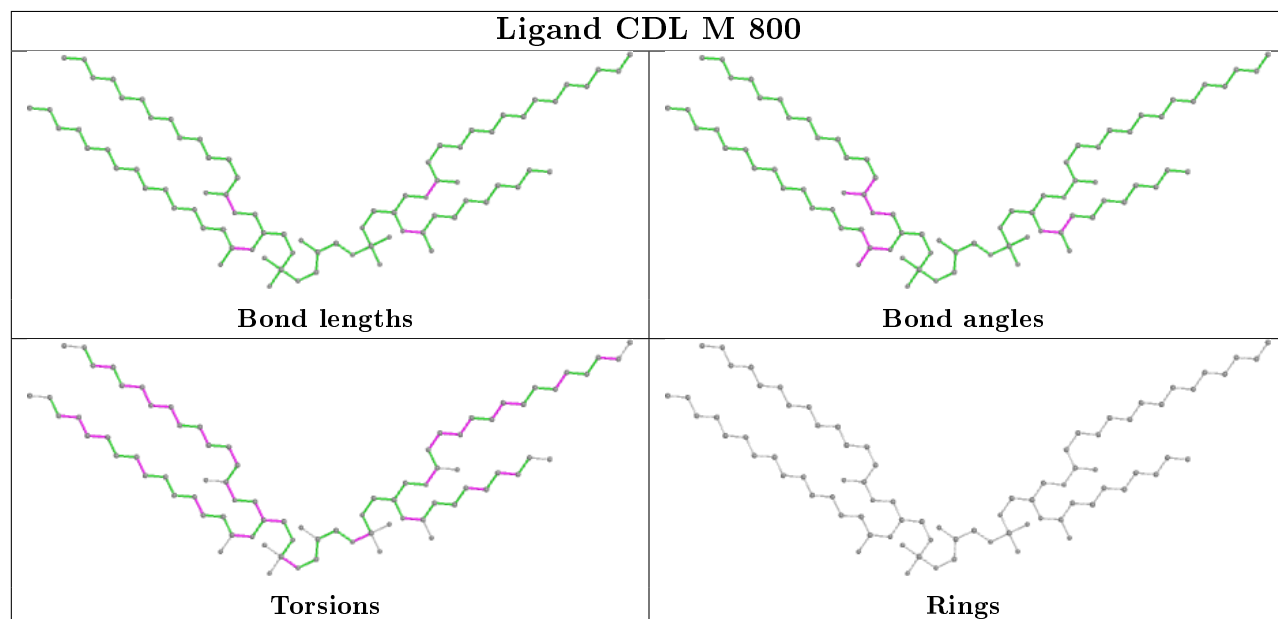
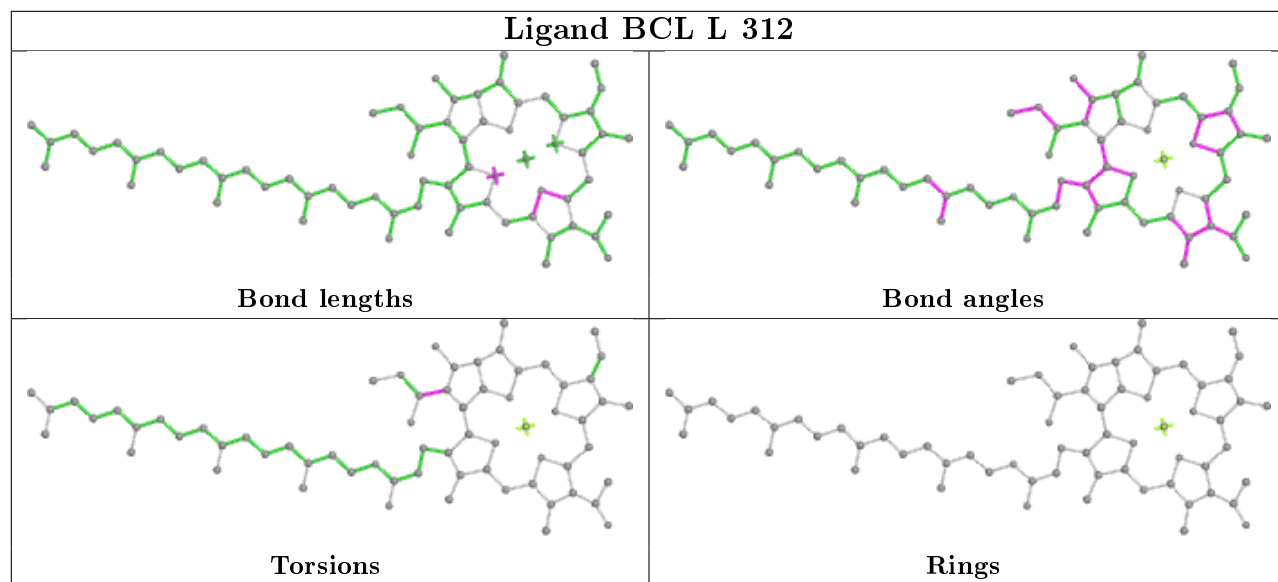
Mol	Chain	Res	Type	Atoms
12	M	907	LDA	C9-C10-C11-C12
11	M	802	PCK	C17-C18-C19-C20
10	M	800	CDL	C11-C12-C13-C14
12	H	901	LDA	C5-C6-C7-C8
8	L	502	U10	C20-C19-C21-C22
6	M	313	BCL	CAA-CBA-CGA-O2A
11	M	802	PCK	C17-C18-C19-BR1
12	H	903	LDA	C9-C10-C11-C12
8	M	501	U10	C5-C4-O4-C4M
7	L	402	BPH	C2B-C3B-CAB-OBB
7	L	402	BPH	O2A-C1-C2-C3
7	M	401	BPH	C6-C7-C8-C10
13	M	707	GOL	O2-C2-C3-O3
7	M	401	BPH	C16-C17-C18-C19
8	L	502	U10	C18-C19-C21-C22
10	M	800	CDL	C75-C76-C77-C78
7	L	402	BPH	C4B-C3B-CAB-OBB
6	M	311	BCL	C11-C10-C8-C9
6	L	312	BCL	CAD-CBD-CGD-O2D
10	M	800	CDL	C37-C38-C39-C40
12	H	903	LDA	C2-C1-N1-CM1
10	M	800	CDL	C20-C21-C22-C23
12	M	920	LDA	C9-C10-C11-C12
12	H	904	LDA	C9-C10-C11-C12
11	M	802	PCK	C45-C46-C47-C48
8	L	502	U10	C3-C4-O4-C4M
13	H	708	GOL	O1-C1-C2-C3
13	H	705	GOL	C1-C2-C3-O3
12	M	907	LDA	C11-C10-C9-C8
8	L	502	U10	C5-C4-O4-C4M
12	H	903	LDA	C2-C3-C4-C5
11	M	802	PCK	C5-C4-O4P-P
12	H	901	LDA	C2-C1-N1-O1
12	H	904	LDA	C3-C4-C5-C6
12	H	901	LDA	C6-C7-C8-C9
8	M	501	U10	C25-C24-C26-C27
11	M	802	PCK	C41-C42-C43-C44
10	M	800	CDL	C78-C79-C80-C81

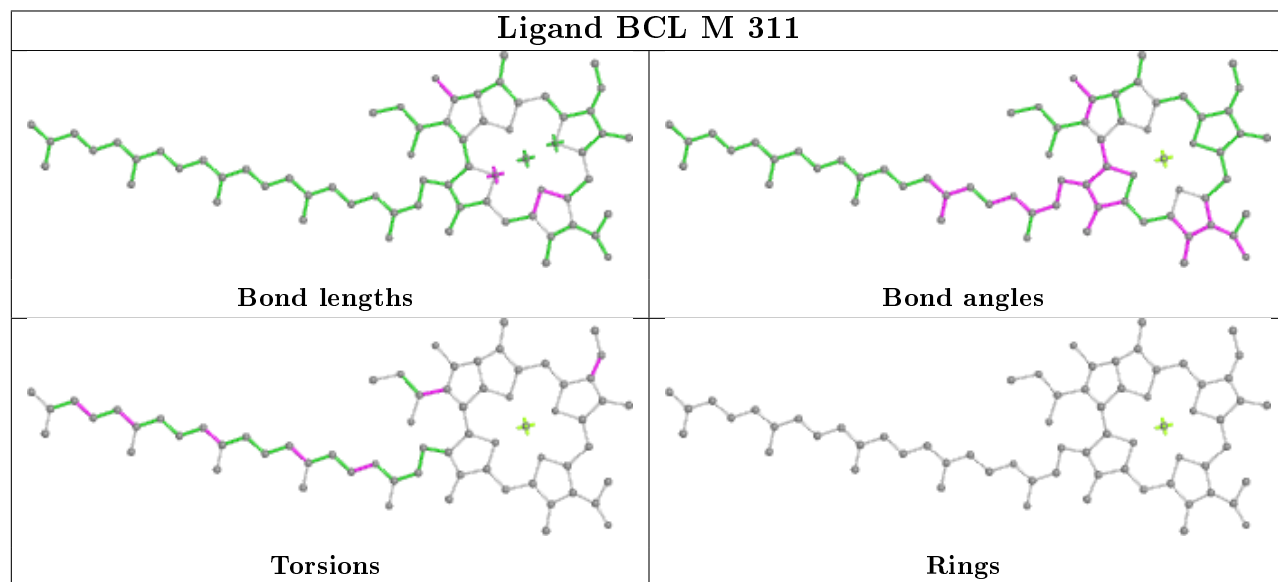
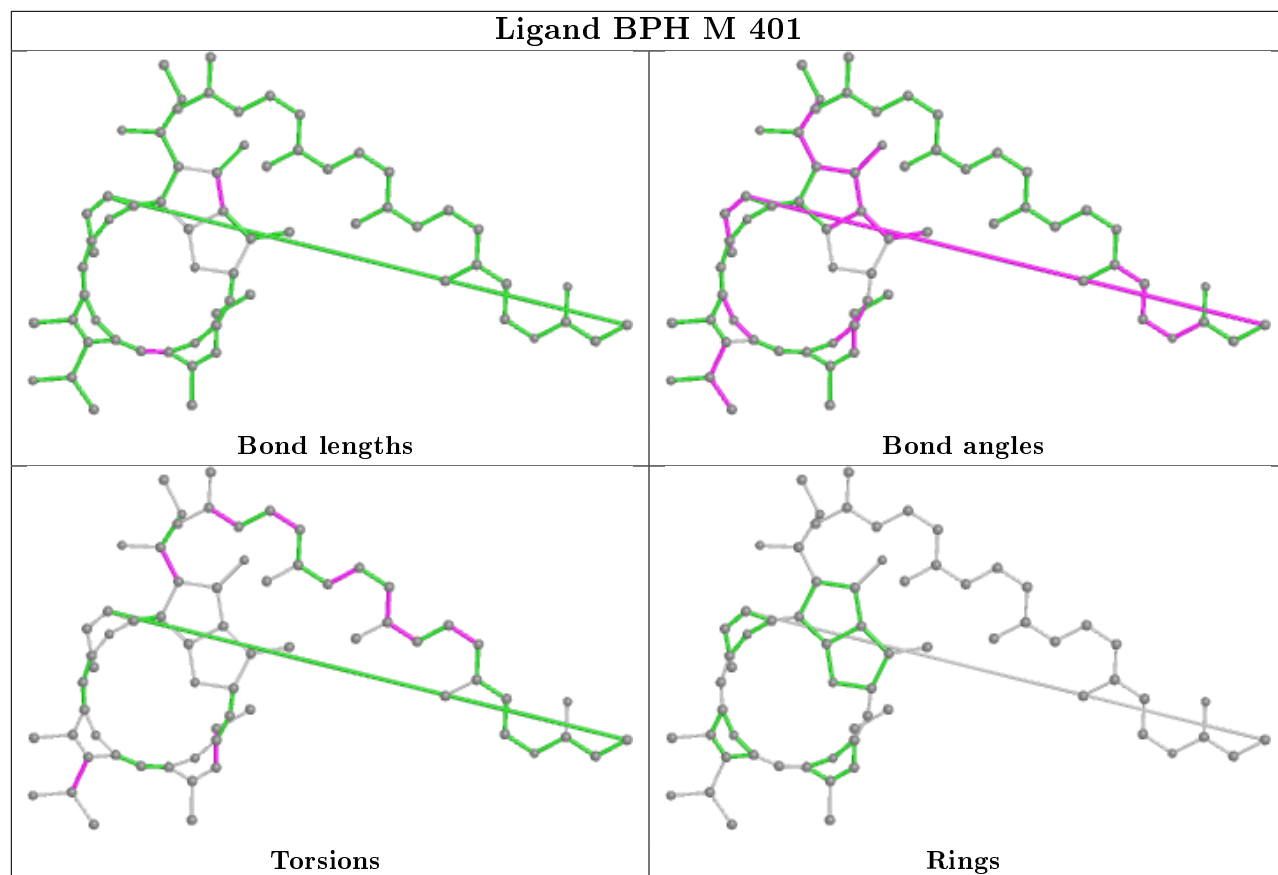
There are no ring outliers.

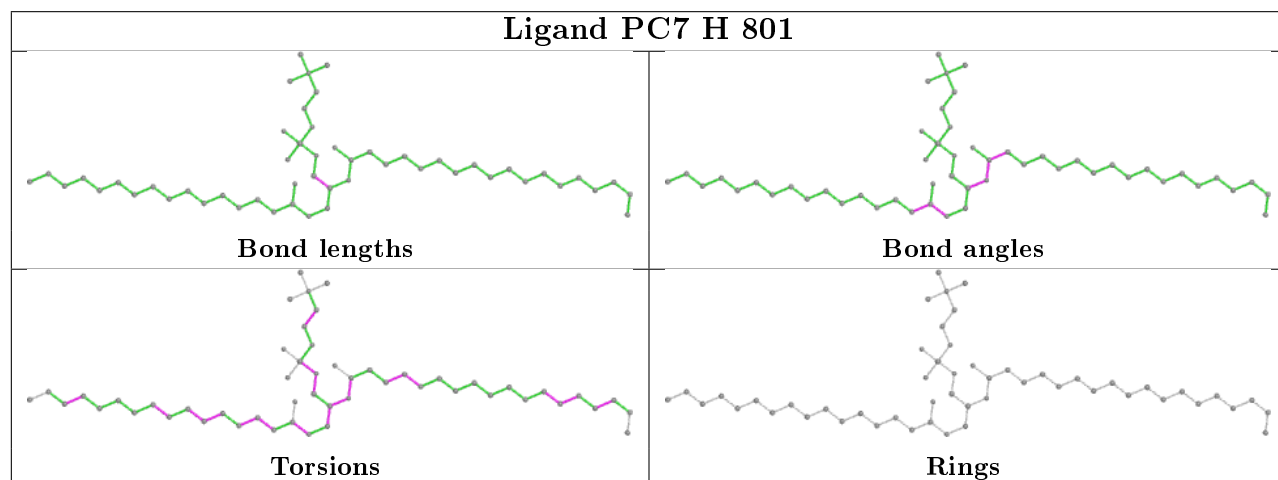
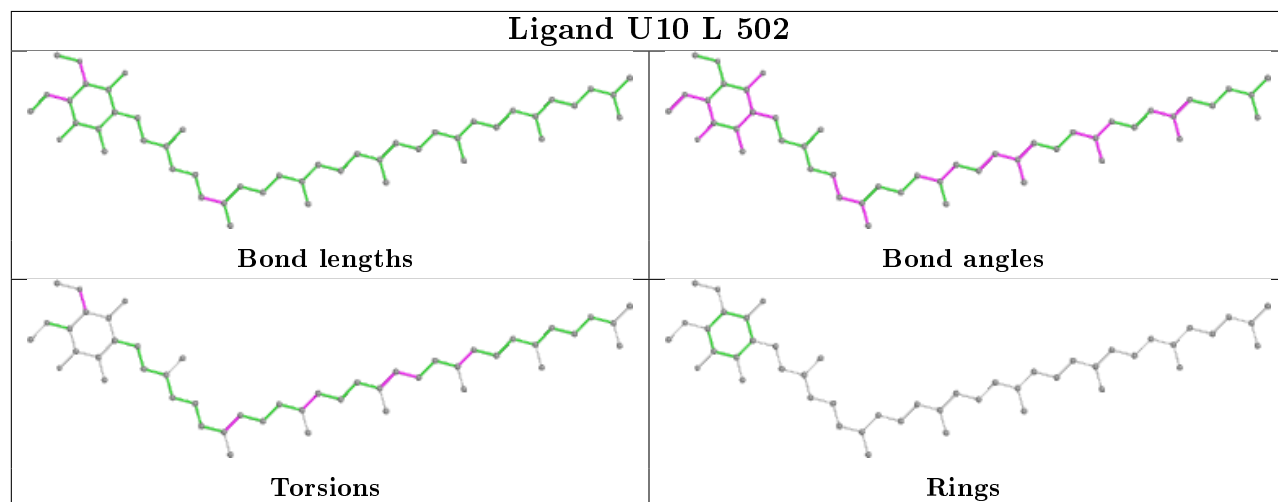
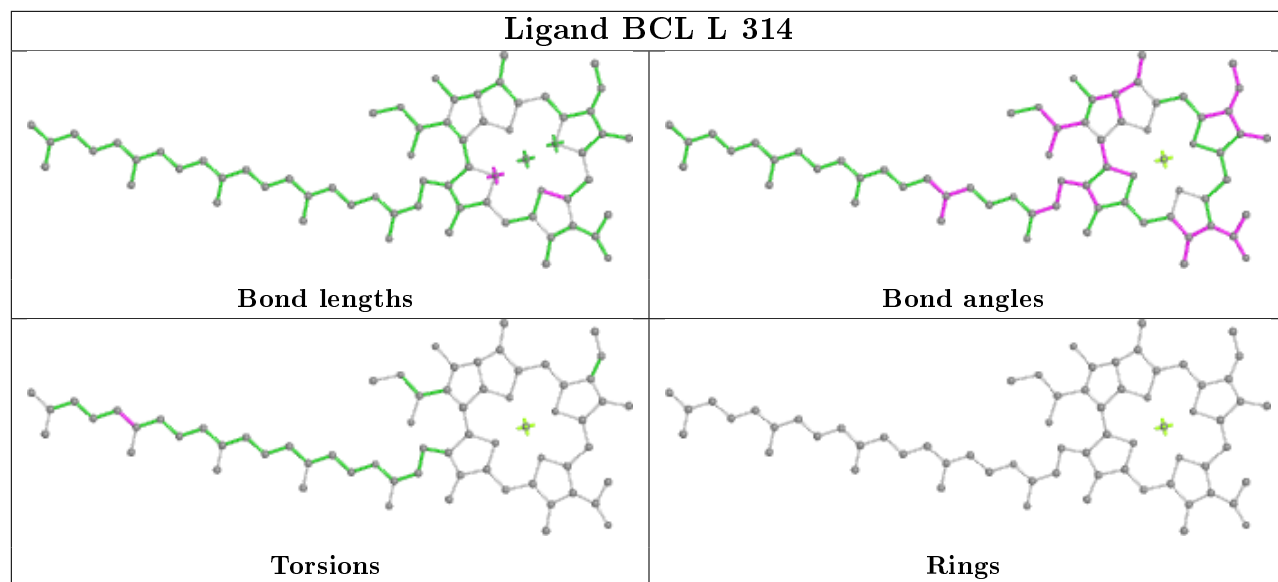
19 monomers are involved in 81 short contacts:

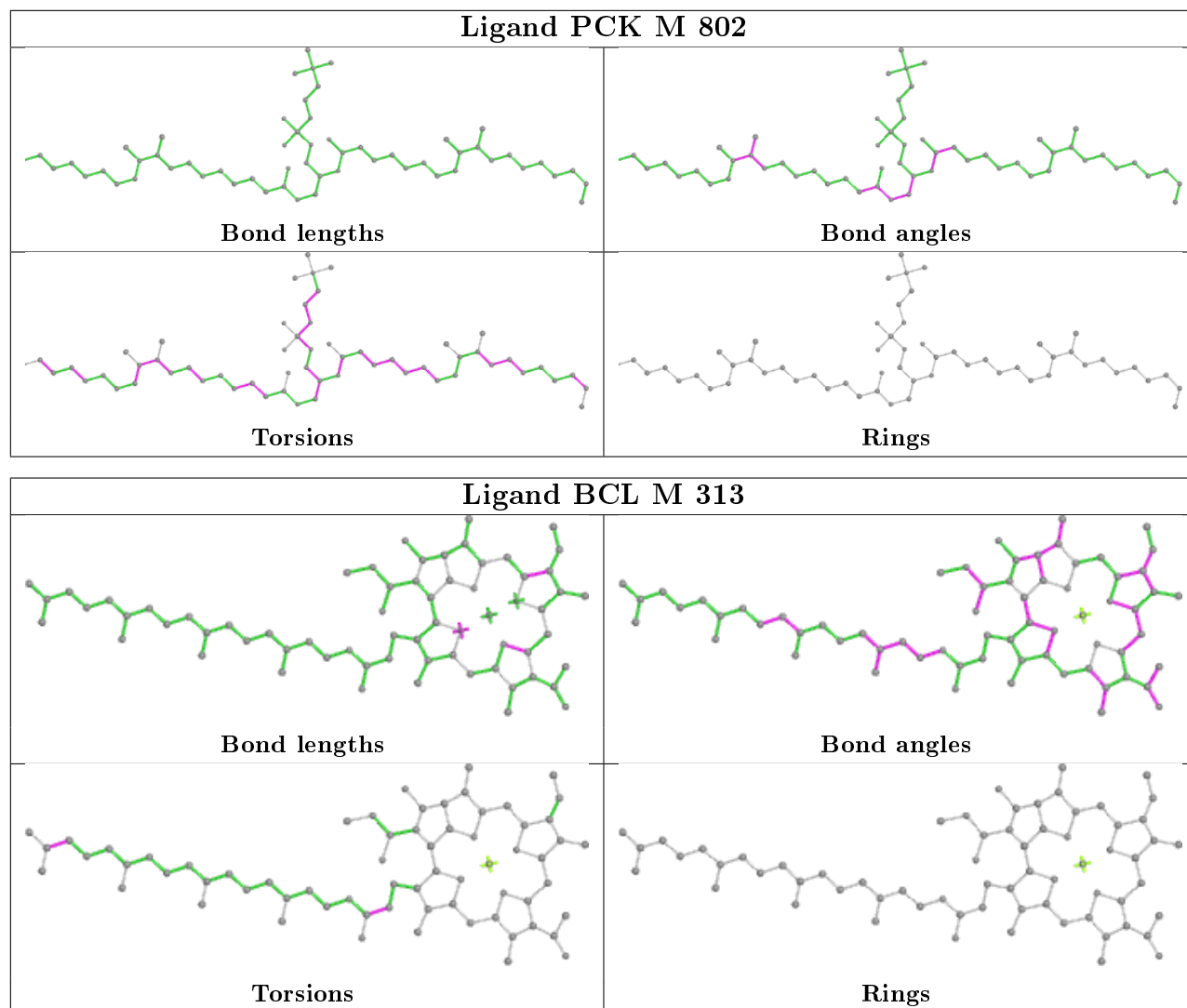
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	920	LDA	3	0
12	H	903	LDA	5	0
6	L	312	BCL	4	0
12	H	908	LDA	10	0
10	M	800	CDL	2	0
13	H	708	GOL	2	0
8	M	501	U10	1	0
12	H	904	LDA	7	0
7	M	401	BPH	4	0
12	M	907	LDA	1	0
12	M	902	LDA	5	0
6	M	311	BCL	13	0
6	L	314	BCL	5	0
8	L	502	U10	4	0
15	H	801	PC7	6	0
11	M	802	PCK	24	0
6	M	313	BCL	7	0
7	L	402	BPH	3	0
12	H	901	LDA	2	0

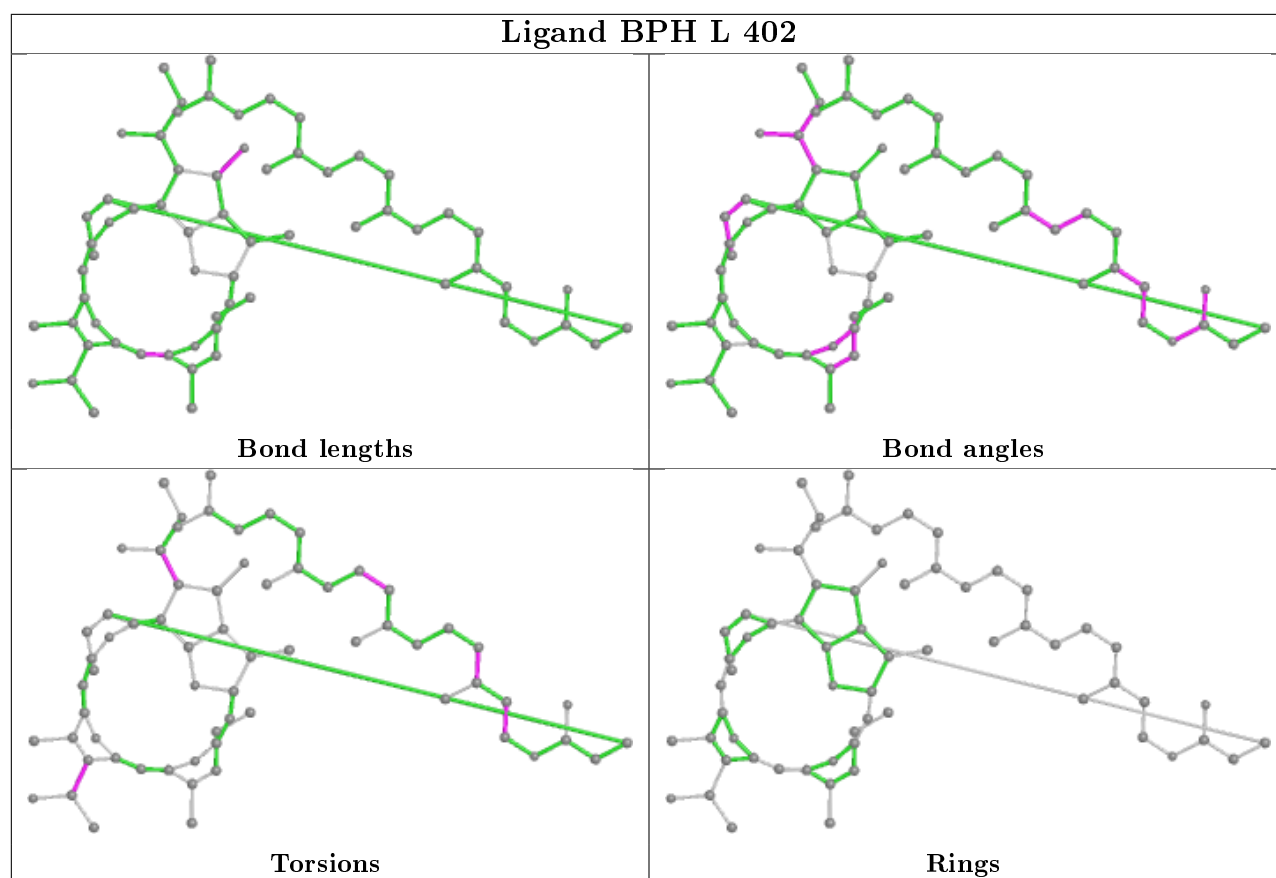
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	L	281/281 (100%)	-0.00	13 (4%) 32 30	43, 53, 66, 82	0
2	M	302/307 (98%)	0.18	21 (6%) 16 13	43, 53, 65, 89	0
3	H	241/260 (92%)	-0.24	5 (2%) 63 60	44, 53, 61, 95	0
All	All	824/848 (97%)	-0.00	39 (4%) 31 29	43, 53, 65, 95	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.3
3	H	251	VAL	8.6
2	M	2[A]	GLU	6.1
3	H	250	SER	6.0
1	L	277	GLY	4.7
1	L	270	PRO	4.5
2	M	114	LEU	3.9
2	M	302	GLY	3.8
1	L	268	LYS	3.4
2	M	100[A]	GLU	3.3
2	M	80	TRP	3.2
1	L	59	TRP	3.1
1	L	185	LEU	3.1
2	M	104	SER	3.0
2	M	75	TRP	2.9
1	L	80	LEU	2.9
2	M	106	ALA	2.9
2	M	98	ALA	2.8
3	H	220[A]	LYS	2.8
2	M	105	PHE	2.8
3	H	245	ALA	2.8
1	L	269	LEU	2.7
2	M	101	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	276[A]	PRO	2.6
2	M	3	TYR	2.6
1	L	202	LYS	2.5
1	L	281	GLY	2.5
2	M	109	LEU	2.4
1	L	279	ILE	2.4
2	M	216	PHE	2.4
1	L	278	GLY	2.3
2	M	27	ALA	2.3
1	L	271	TRP	2.2
2	M	290	VAL	2.2
2	M	83	ALA	2.2
2	M	79	GLY	2.1
2	M	76	TYR	2.1
3	H	93	SER	2.0
2	M	265	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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
11	PCK	M	802	58/58	0.22	0.74	60,69,82,84	58
12	LDA	H	904	16/16	0.37	0.63	53,54,58,58	16
15	PC7	H	801	52/52	0.44	0.68	24,60,69,69	52
12	LDA	H	908	16/16	0.45	0.61	45,51,61,61	16
12	LDA	H	903	16/16	0.47	0.44	56,61,64,65	16
12	LDA	M	920	16/16	0.62	0.80	42,46,59,59	16
10	CDL	M	800	81/100	0.63	0.51	43,67,79,82	81

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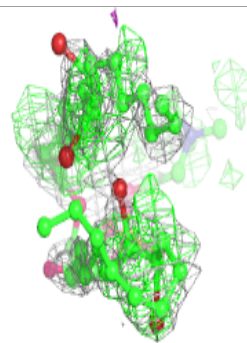
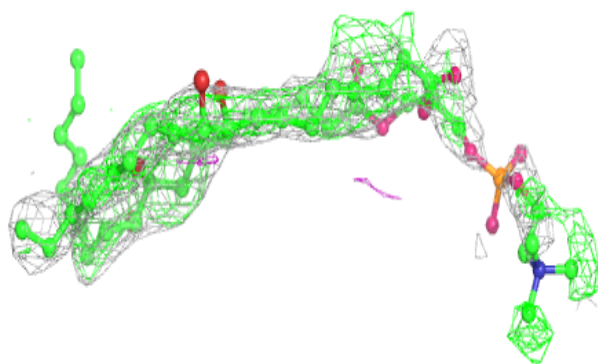
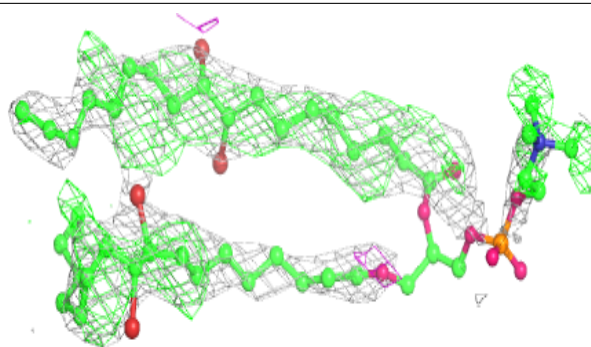
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	GOL	M	710	6/6	0.63	0.33	55,57,58,60	6
12	LDA	M	907	16/16	0.66	0.39	56,59,65,66	16
13	GOL	H	708	6/6	0.72	1.10	47,49,50,52	6
12	LDA	M	902	16/16	0.72	0.62	59,64,67,68	16
5	CL	L	712	1/1	0.72	0.35	66,66,66,66	1
8	U10	L	502	48/63	0.73	0.55	40,55,73,75	48
4	PO4	L	703	5/5	0.73	0.33	61,61,62,65	5
13	GOL	M	707	6/6	0.75	0.23	49,50,52,52	6
12	LDA	H	901	16/16	0.85	0.29	61,63,66,68	16
13	GOL	H	705	6/6	0.87	0.41	48,58,59,61	6
4	PO4	H	704	5/5	0.87	0.30	71,73,74,75	5
13	GOL	H	706	6/6	0.87	0.26	71,72,73,74	6
5	CL	M	711	1/1	0.88	0.24	74,74,74,74	1
13	GOL	H	709	6/6	0.88	0.19	55,56,57,58	6
7	BPH	M	401	65/65	0.88	0.23	45,55,106,107	0
8	U10	M	501	48/63	0.89	0.24	49,61,81,84	0
14	K	H	700	1/1	0.93	0.11	57,57,57,57	0
4	PO4	M	702	5/5	0.94	0.12	53,53,54,55	5
6	BCL	M	311	66/66	0.94	0.22	46,54,119,120	0
6	BCL	L	312	66/66	0.96	0.16	42,50,63,67	0
7	BPH	L	402	65/65	0.96	0.15	40,52,60,61	0
6	BCL	M	313	66/66	0.96	0.19	42,50,79,87	0
4	PO4	M	701	5/5	0.96	0.14	57,58,62,62	5
6	BCL	L	314	66/66	0.97	0.15	41,48,67,71	0
9	FE	M	500	1/1	0.99	0.17	51,51,51,51	0

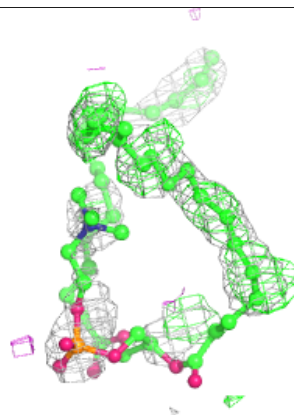
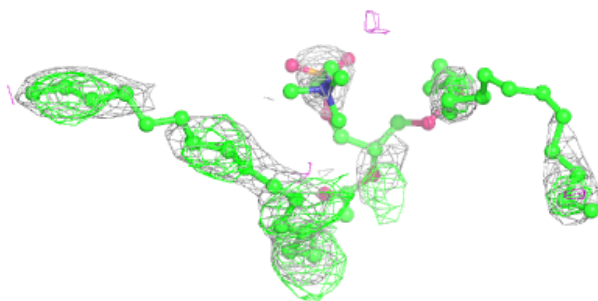
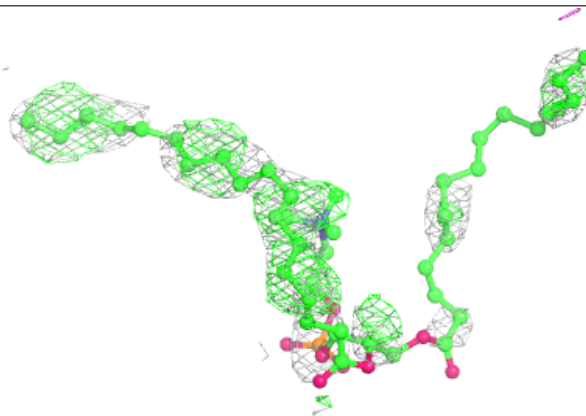
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCK M 802:

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

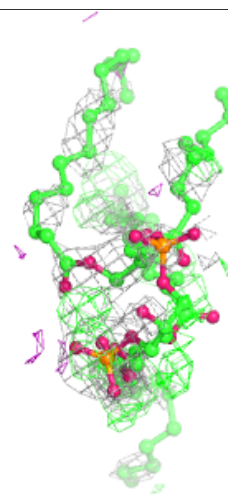
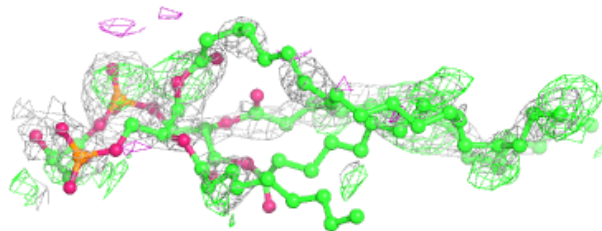
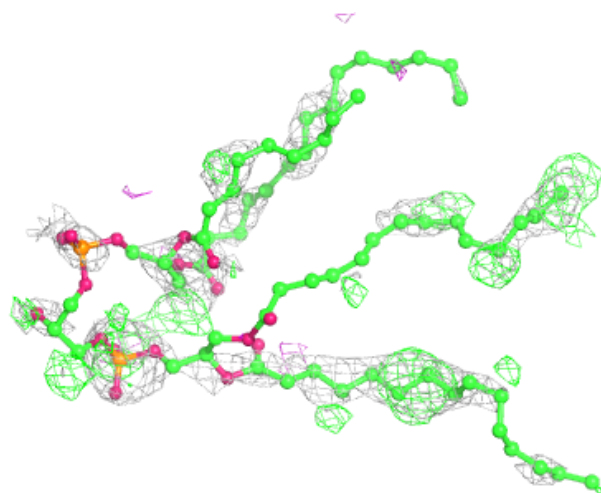
**Electron density around PC7 H 801:**

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



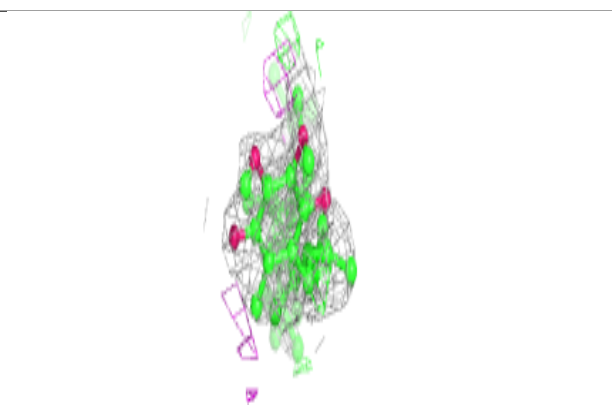
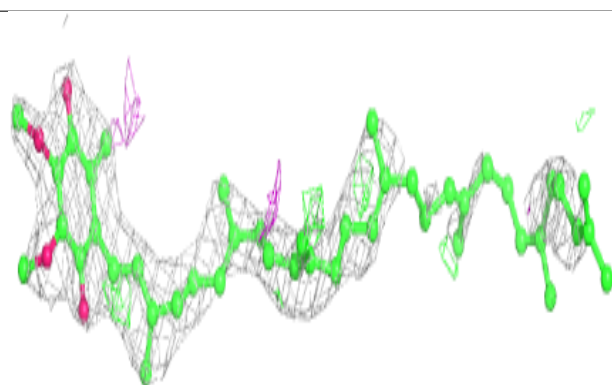
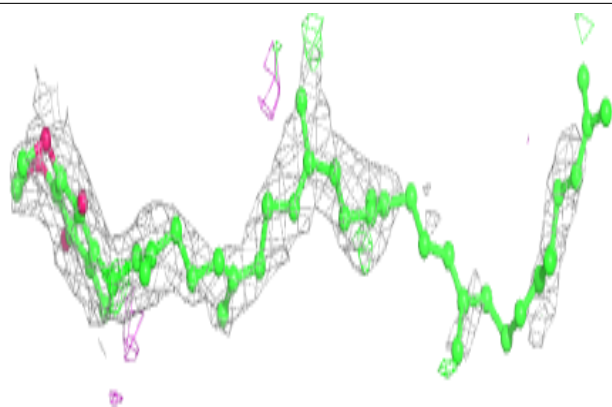
Electron density around CDL M 800:

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

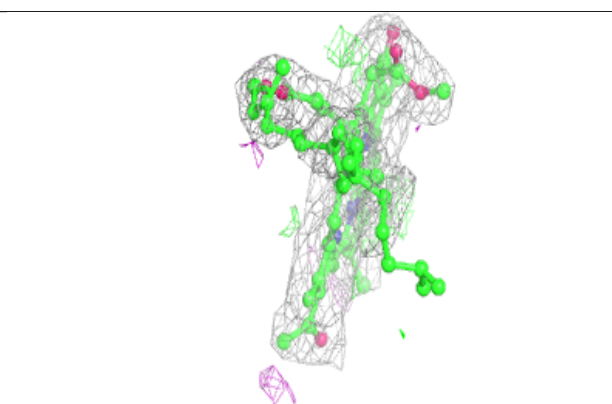
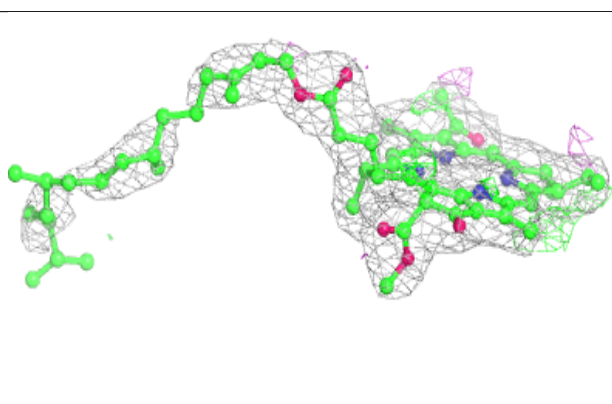
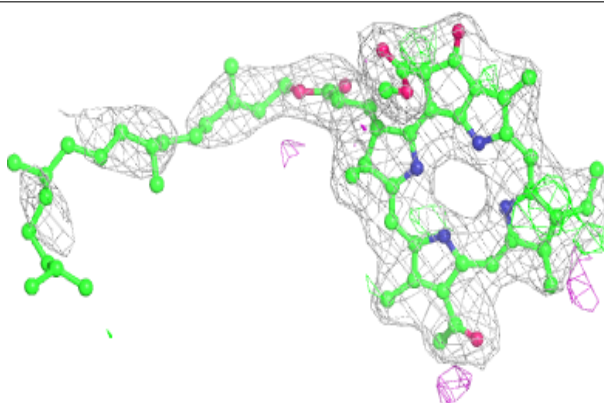


Electron density around U10 L 502:

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

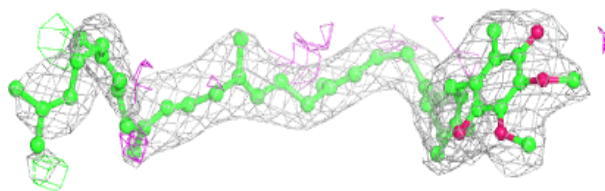
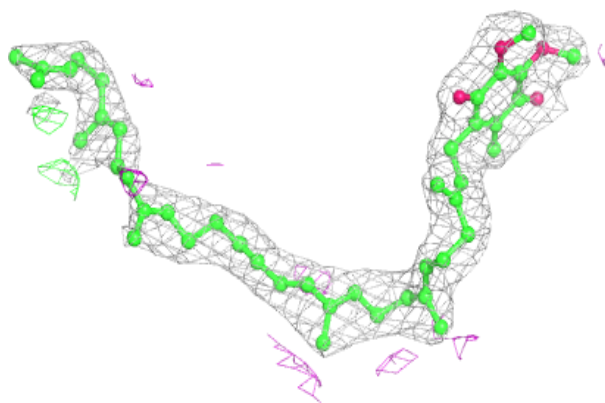
**Electron density around BPH M 401:**

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

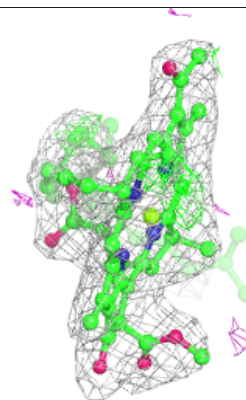
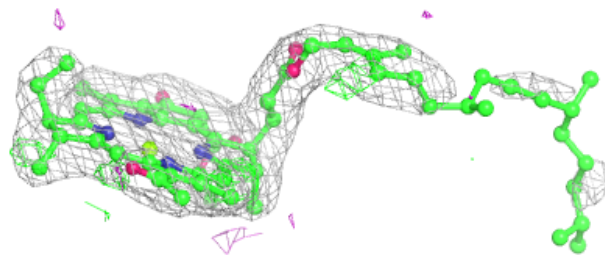
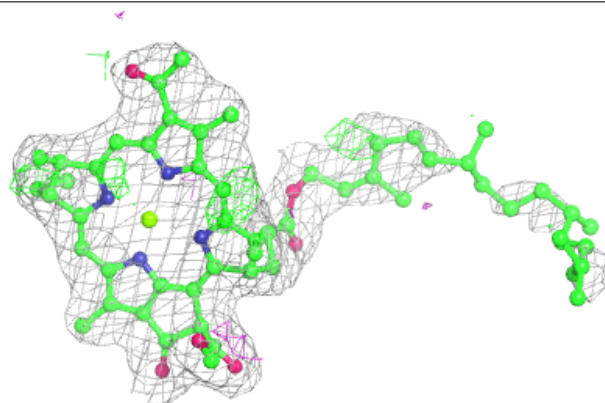


Electron density around U10 M 501:

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

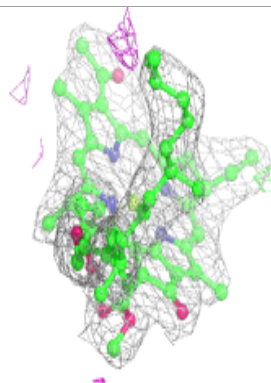
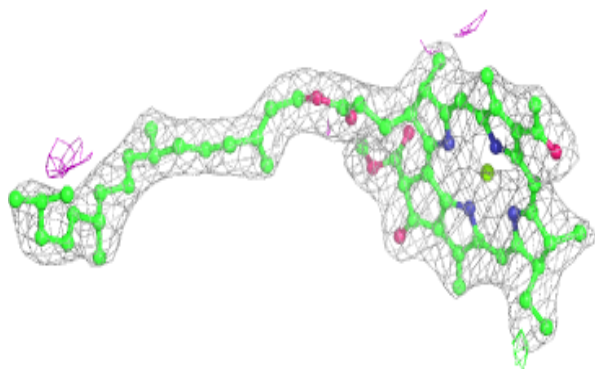
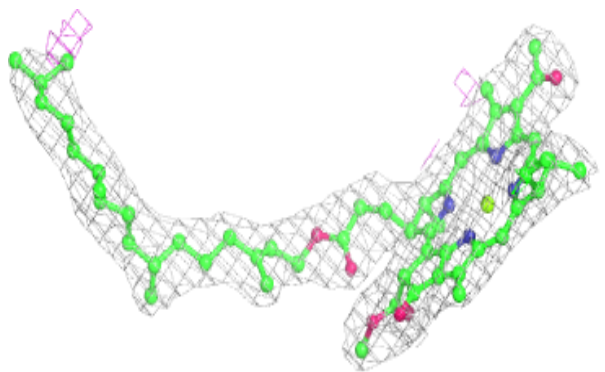
**Electron density around BCL M 311:**

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

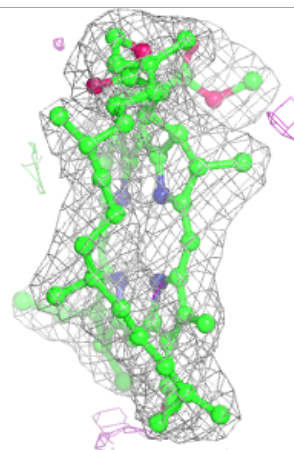
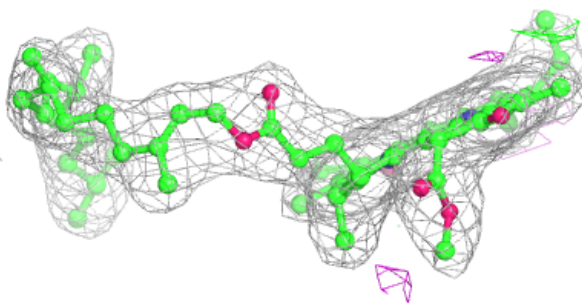
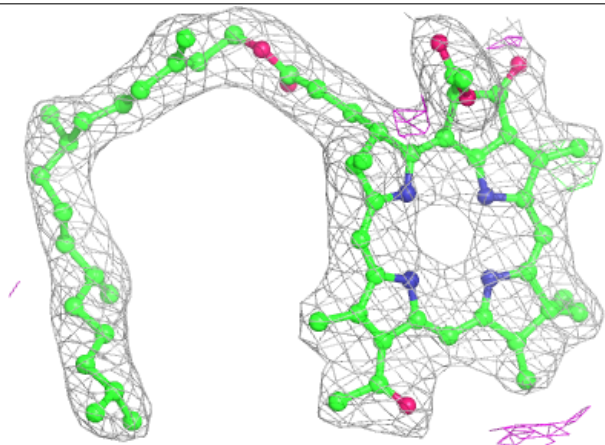


Electron density around BCL L 312:

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

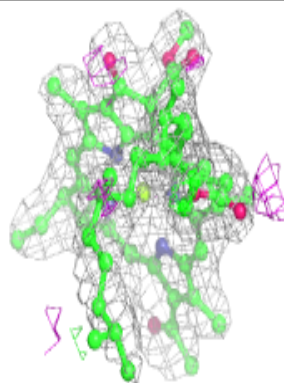
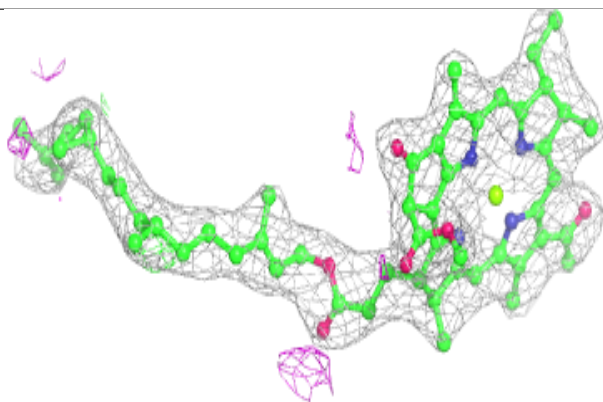
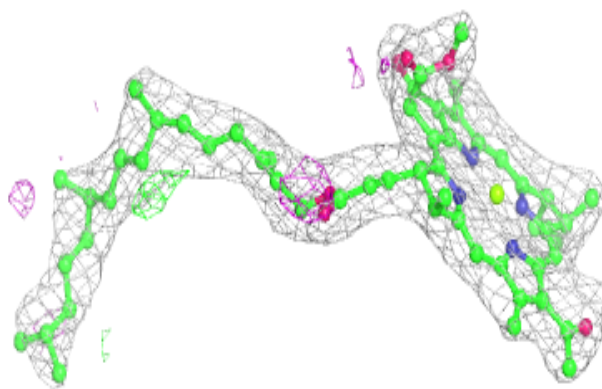
**Electron density around BPH L 402:**

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



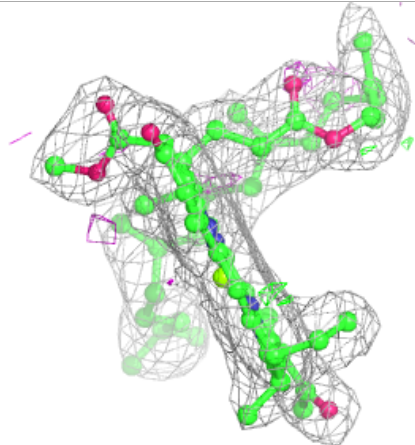
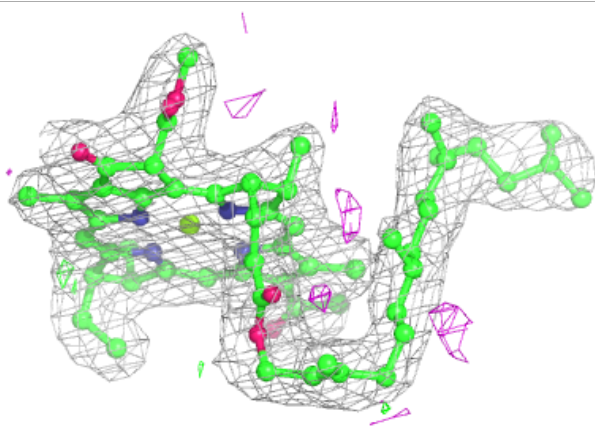
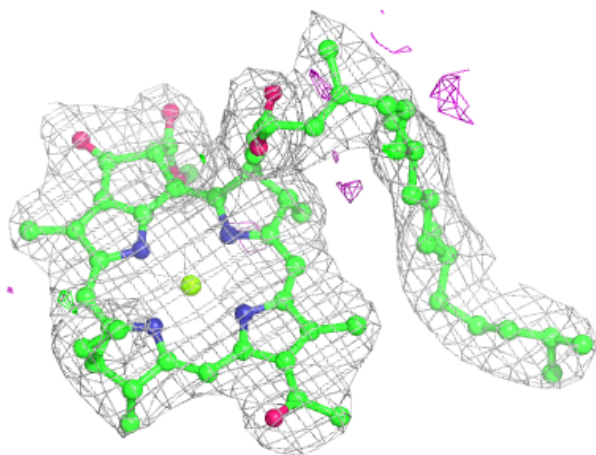
Electron density around BCL M 313:

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



Electron density around BCL L 314:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.