



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 12:24 am BST

PDB ID : 3I4D
Title : Photosynthetic reaction center from rhodobacter sphaeroides 2.4.1
Authors : Fujii, R.; Adachi, S.; Roszak, A.W.; Gardiner, A.T.; Cogdell, R.J.; Isaacs, N.W.; Koshihara, S.; Hashimoto, H.
Deposited on : 2009-07-01
Resolution : 2.01 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

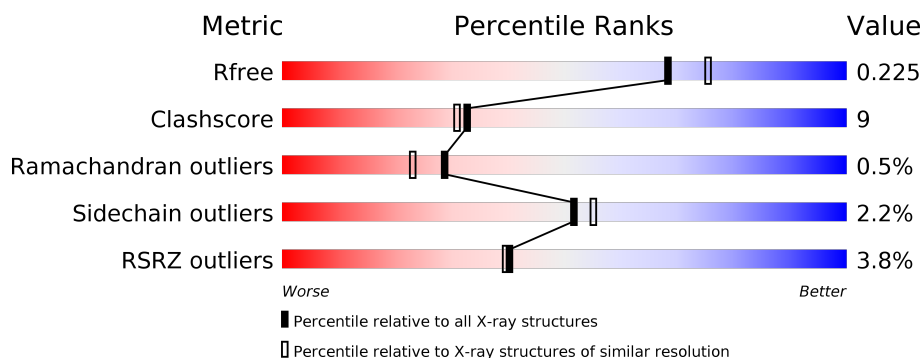
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>
2	M	307	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>••</div> </div> </div>
3	H	260	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>•</div> <div>8%</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	GOL	L	727	-	-	-	X
10	GOL	L	732	-	-	-	X
10	GOL	L	733	-	-	-	X
10	GOL	L	734	-	-	-	X
10	GOL	M	740	-	-	-	X
10	GOL	M	741	-	-	X	-
12	HTO	H	752	-	-	-	X
13	LDA	H	906	-	-	-	X
13	LDA	H	910	-	-	-	X
13	LDA	L	902	-	-	-	X
13	LDA	L	904	-	-	-	X
13	LDA	L	908	-	-	-	X
13	LDA	L	914	-	-	-	X
13	LDA	L	915	-	-	-	X
13	LDA	L	919	-	-	-	X
13	LDA	L	921	-	-	X	-
13	LDA	M	903	-	-	-	X
13	LDA	M	916	-	-	-	X
13	LDA	M	918	-	-	-	X
18	CDL	M	800	-	-	-	X
7	UQ1	L	503	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 8406 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	2	0
			2246	1516	358	364	8			

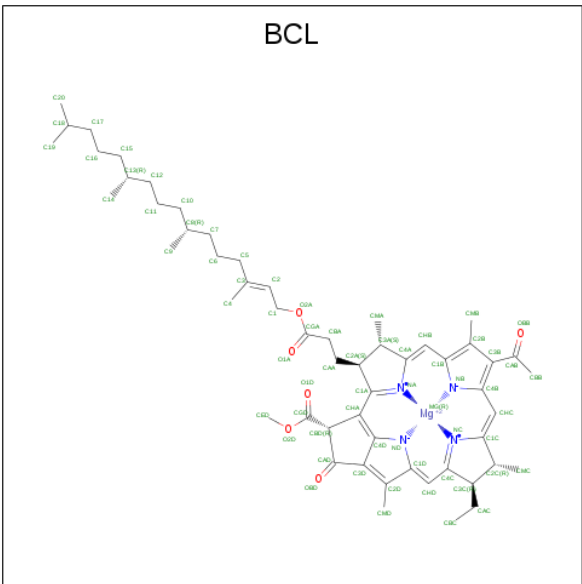
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	5	0
			2451	1635	402	402	12			

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

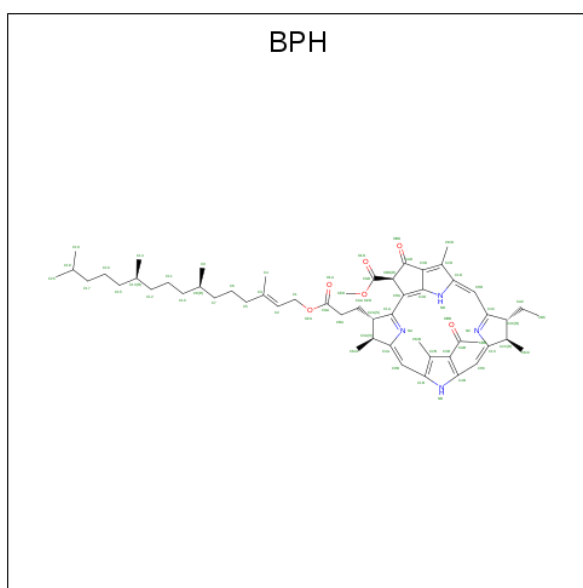
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	6	0
			1876	1199	324	343	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



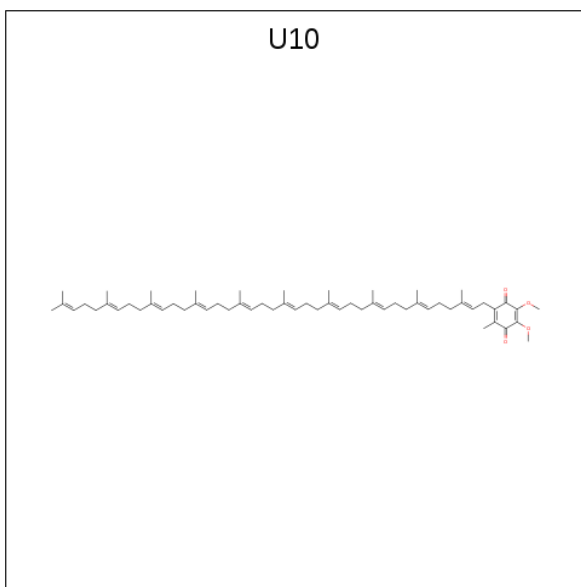
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



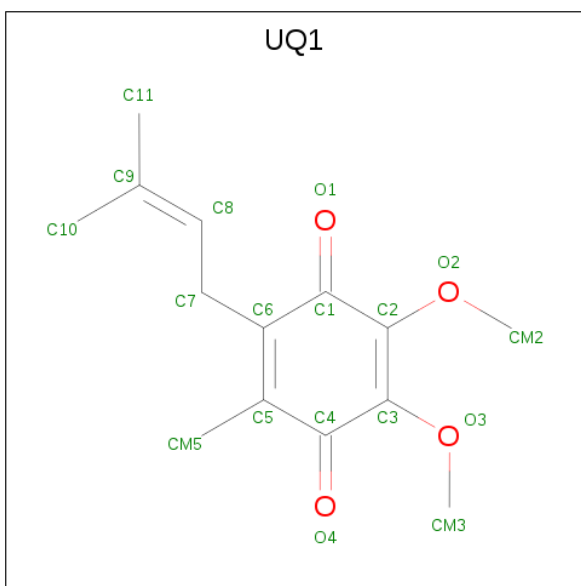
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	1
			84	80	4		
6	M	1	Total	C	O	0	1
			94	90	4		

- Molecule 7 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



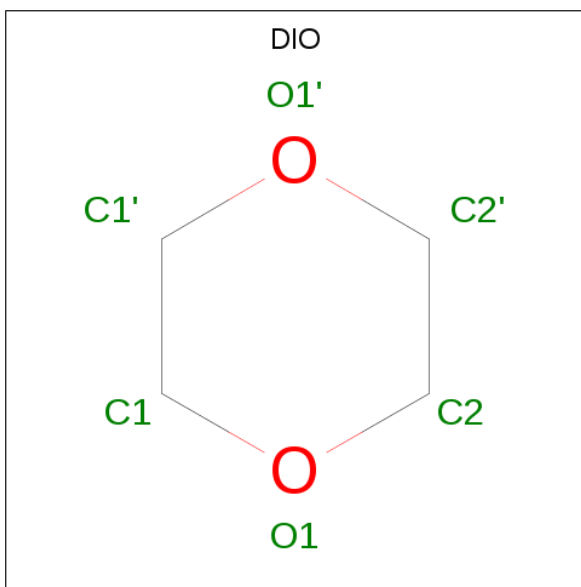
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



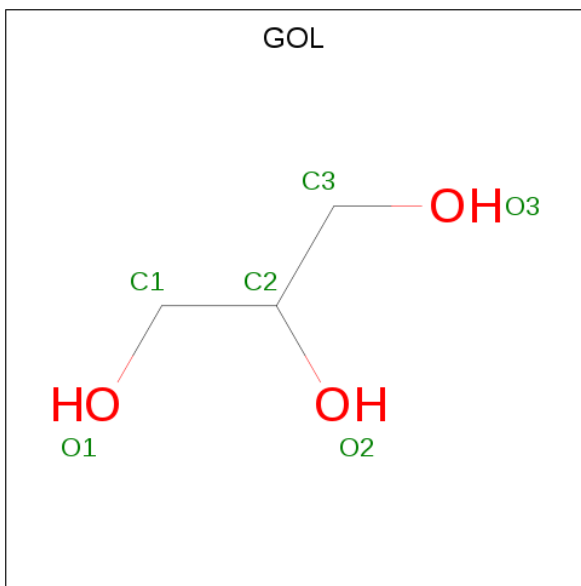
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	O	P	0	0
			5	4	1		
8	L	1	Total	O	P	0	0
			5	4	1		
8	L	1	Total	O	P	0	0
			5	4	1		
8	L	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		
8	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

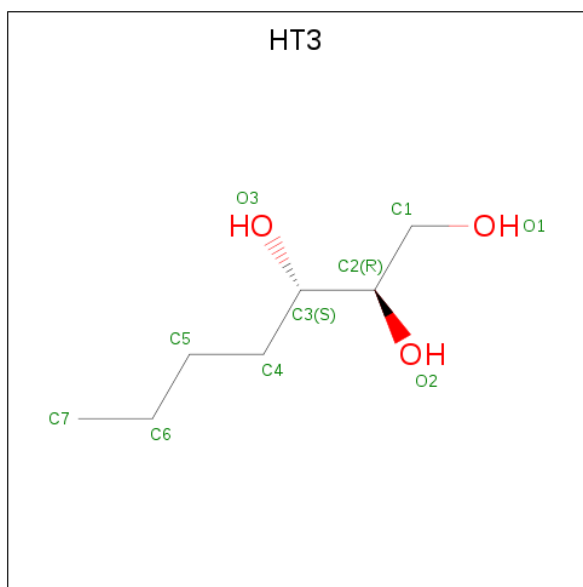
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10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

Continued on next page...

Continued from previous page...

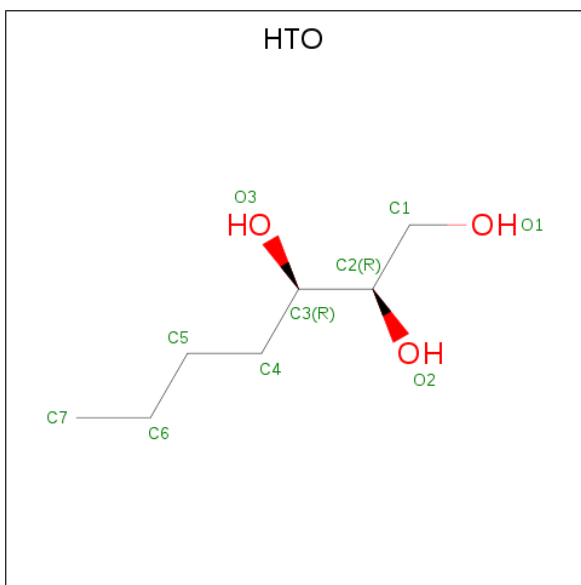
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is (2R,3S)-heptane-1,2,3-triol (three-letter code: HT3) (formula: C₇H₁₆O₃).



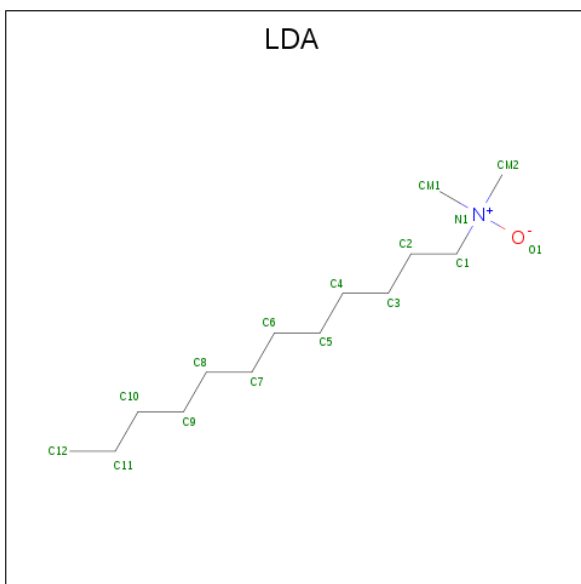
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 12 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	L	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

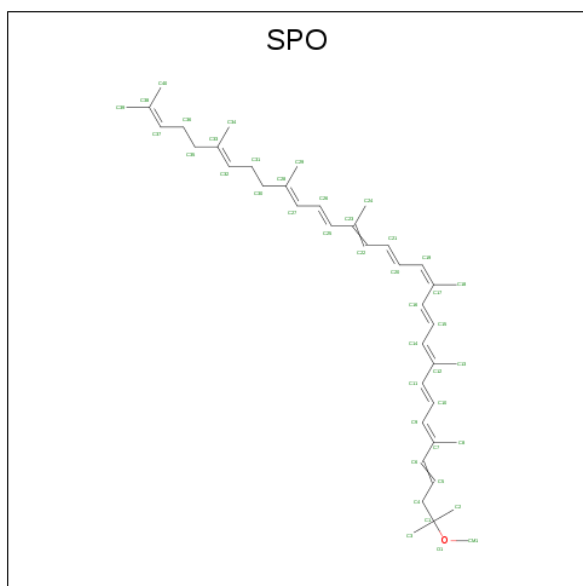
Continued from previous page...

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

- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 15 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total C O 42 41 1	0	0

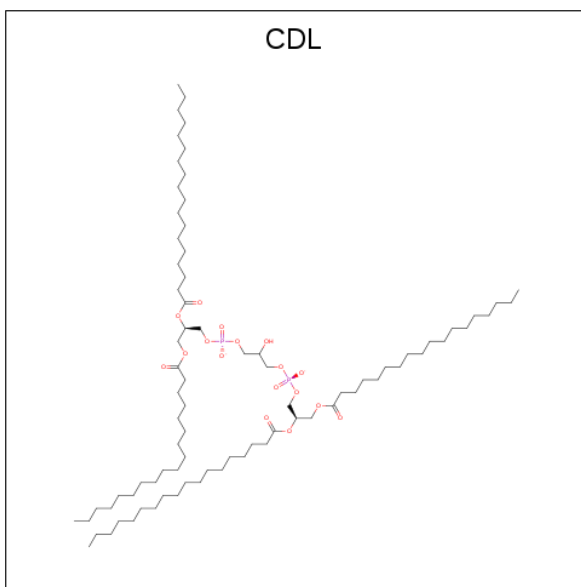
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total K 1 1	0	0
16	M	1	Total K 1 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

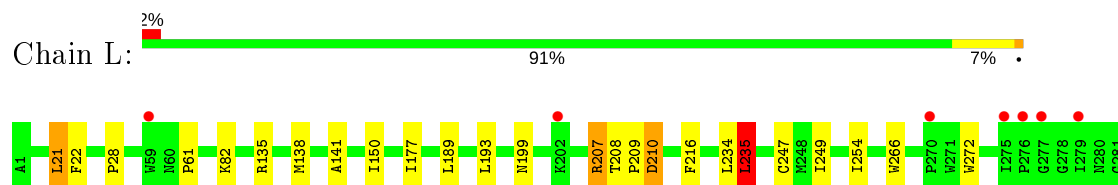
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	145	Total	O	0	0
			145	145		
19	M	150	Total	O	0	0
			150	150		
19	H	258	Total	O	0	0
			258	258		

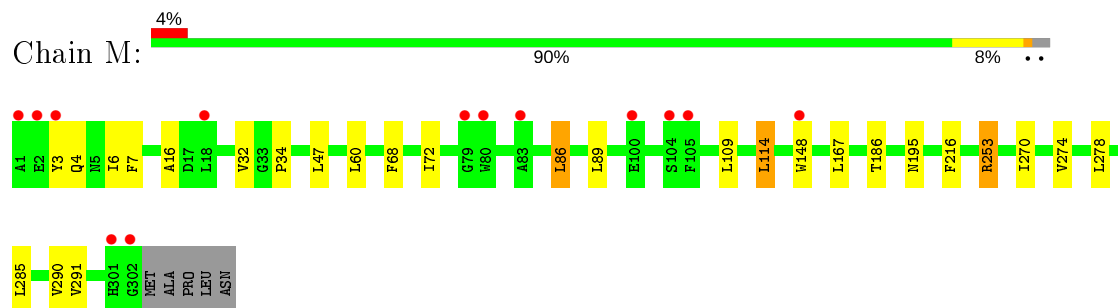
3 Residue-property plots [i](#)

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.

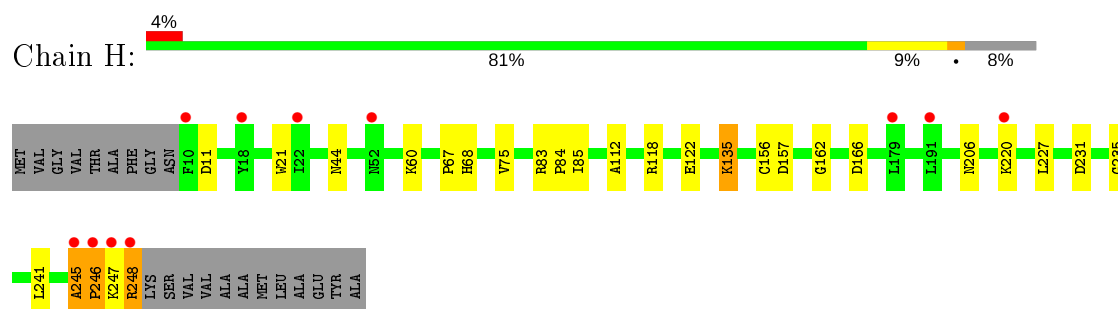
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.80Å 138.80Å 184.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.25 – 2.01 30.25 – 2.01	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.25-2.01) 90.9 (30.25-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.207 0.206 , 0.225	Depositor DCC
R_{free} test set	6134 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, GOL, LDA, DIO, CL, CDL, BPH, K, HTO, HT3, FE, SPO, UQ1, 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	0.94	0/2334	0.78	4/3194 (0.1%)
2	M	0.89	1/2543 (0.0%)	0.79	2/3469 (0.1%)
3	H	0.96	0/1925	0.86	5/2616 (0.2%)
All	All	0.93	1/6802 (0.0%)	0.81	11/9279 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	274	VAL	CB-CG2	-5.07	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	118[A]	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	H	118[B]	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	L	235	LEU	CA-CB-CG	5.83	128.72	115.30
3	H	83	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	L	135	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	L	210	ASP	CB-CG-OD1	5.29	123.06	118.30
2	M	253[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	M	253[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	H	135[A]	LYS	CD-CE-NZ	5.07	123.36	111.70
3	H	135[B]	LYS	CD-CE-NZ	5.07	123.36	111.70
1	L	207	ARG	NE-CZ-NH1	-5.03	117.78	120.30

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	2246	0	2203	28	0
2	M	2451	0	2369	27	0
3	H	1876	0	1882	19	0
4	L	132	0	148	5	0
4	M	132	0	148	12	0
5	L	65	0	75	0	0
5	M	65	0	76	4	0
6	L	84	0	70	14	0
6	M	94	0	102	7	0
7	L	18	0	18	13	0
8	H	5	0	0	0	0
8	L	20	0	0	1	0
8	M	10	0	0	1	0
9	L	6	0	8	0	0
10	H	54	0	72	4	0
10	L	72	0	96	3	0
10	M	30	0	40	6	0
11	L	10	0	16	0	0
12	H	10	0	16	3	0
12	L	10	0	16	0	0
13	H	64	0	124	9	0
13	L	176	0	341	27	0
13	M	96	0	186	6	0
14	M	1	0	0	0	0
15	M	42	0	60	1	0
16	H	1	0	0	0	0
16	M	1	0	0	0	0
17	M	1	0	0	0	0
18	M	81	0	106	9	0
19	H	258	0	0	1	0
19	L	145	0	0	2	0
19	M	150	0	0	1	0
All	All	8406	0	8172	138	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 (138) 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)
6:L:502[B]:U10:H502	2:M:86:LEU:HD11	1.25	1.14
6:L:502[B]:U10:C50	2:M:86:LEU:HD11	1.89	1.02
10:M:740:GOL:O1	10:M:742:GOL:O3	1.83	0.96
1:L:235:LEU:HA	13:L:921:LDA:HM21	1.47	0.94
2:M:253[A]:ARG:NH2	19:M:415:HOH:O	2.04	0.89
10:L:724:GOL:H2	3:H:241:LEU:HD13	1.56	0.88
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.54	0.86
1:L:235:LEU:HD23	13:L:921:LDA:HM11	1.58	0.84
6:M:501[B]:U10:H501	6:M:501[B]:U10:C53	2.09	0.82
4:M:601:BCL:C7	4:M:601:BCL:H41	2.07	0.82
1:L:235:LEU:HA	13:L:921:LDA:CM2	2.10	0.81
6:M:501[B]:U10:H501	6:M:501[B]:U10:H53	1.62	0.81
13:H:906:LDA:HM23	13:H:910:LDA:O1	1.82	0.80
4:M:601:BCL:H72	4:M:601:BCL:H41	1.63	0.78
10:H:739:GOL:H2	12:H:752:HTO:H72	1.64	0.77
4:M:601:BCL:CBB	4:M:601:BCL:HMB1	2.15	0.77
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.69	0.74
7:L:503:UQ1:H102	13:L:920:LDA:H121	1.71	0.73
10:H:739:GOL:H2	12:H:752:HTO:C7	2.18	0.73
13:H:906:LDA:CM2	13:H:910:LDA:O1	2.38	0.72
7:L:503:UQ1:HM53	2:M:89:LEU:HD23	1.72	0.72
13:M:903:LDA:H91	13:H:901:LDA:H121	1.72	0.72
4:M:601:BCL:HBB2	4:M:601:BCL:HMB1	1.73	0.70
6:L:502[B]:U10:H502	2:M:86:LEU:CD1	2.15	0.69
1:L:235:LEU:CA	13:L:921:LDA:CM2	2.72	0.67
3:H:162:GLY:HA2	12:H:752:HTO:H2	1.77	0.67
1:L:82[A]:LYS:NZ	19:L:448:HOH:O	2.28	0.66
13:H:909:LDA:H123	13:H:910:LDA:H111	1.77	0.65
1:L:28:PRO:HG3	13:L:902:LDA:HM21	1.79	0.64
1:L:61:PRO:O	1:L:150:ILE:HD12	1.97	0.64
7:L:503:UQ1:CM5	2:M:89:LEU:HD23	2.28	0.64
13:L:921:LDA:O1	2:M:6:ILE:HD12	2.00	0.62
13:L:905:LDA:H122	13:L:917:LDA:HM11	1.82	0.61
13:L:905:LDA:H122	13:L:917:LDA:CM1	2.30	0.61
4:L:602:BCL:HMB1	4:L:602:BCL:HBB3	1.83	0.60
4:L:604:BCL:HMB1	4:L:604:BCL:HBB2	1.84	0.60
7:L:503:UQ1:H102	13:L:920:LDA:C12	2.31	0.60
2:M:278[B]:LEU:HD11	18:M:800:CDL:H811	1.83	0.59
7:L:503:UQ1:CM2	7:L:503:UQ1:O1	2.49	0.59
3:H:135[A]:LYS:HE3	3:H:166:ASP:OD2	2.03	0.58
6:L:502[B]:U10:H402	15:M:600:SPO:H133	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:60:LEU:HD23	5:M:401:BPH:H4C1	1.85	0.57
2:M:34:PRO:HG2	2:M:47[A]:LEU:HD12	1.86	0.57
7:L:503:UQ1:HM22	7:L:503:UQ1:O1	2.03	0.57
3:H:246:PRO:HA	3:H:247:LYS:O	2.05	0.56
7:L:503:UQ1:C10	13:L:920:LDA:C12	2.83	0.56
1:L:141:ALA:HB2	8:L:708:PO4:O4	2.05	0.55
1:L:28:PRO:HD3	13:L:902:LDA:HM21	1.88	0.55
6:M:501[B]:U10:C50	6:M:501[B]:U10:C53	2.84	0.55
3:H:245:ALA:CB	3:H:246:PRO:HD3	2.30	0.55
4:L:602:BCL:HMB1	4:L:602:BCL:CBB	2.37	0.55
4:M:603:BCL:HMB1	4:M:603:BCL:CBB	2.36	0.55
2:M:290:VAL:HG12	2:M:291:VAL:HG23	1.89	0.54
6:L:502[A]:U10:H502	4:M:603:BCL:H171	1.90	0.53
7:L:503:UQ1:HM51	7:L:503:UQ1:C8	2.39	0.53
13:M:903:LDA:H82	13:H:910:LDA:H123	1.90	0.53
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.44	0.53
2:M:68:PHE:O	2:M:72:ILE:HG12	2.09	0.53
2:M:278[A]:LEU:CD2	18:M:800:CDL:H791	2.38	0.53
6:M:501[B]:U10:H371	6:M:501[B]:U10:H312	1.91	0.53
1:L:28:PRO:CD	13:L:902:LDA:HM21	2.40	0.52
1:L:235:LEU:CA	13:L:921:LDA:HM23	2.39	0.52
1:L:235:LEU:HB2	13:L:921:LDA:HM23	1.92	0.52
2:M:278[A]:LEU:HD21	18:M:800:CDL:H791	1.92	0.51
6:M:501[B]:U10:C50	6:M:501[B]:U10:H53	2.37	0.51
7:L:503:UQ1:O4	7:L:503:UQ1:CM3	2.59	0.50
1:L:28:PRO:CG	13:L:902:LDA:HM21	2.42	0.50
1:L:235:LEU:CA	13:L:921:LDA:HM21	2.31	0.49
4:M:601:BCL:HBB3	4:M:601:BCL:HMB1	1.93	0.49
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.48	0.48
1:L:266:TRP:CD1	7:L:503:UQ1:HM33	2.48	0.48
4:L:604:BCL:CBB	4:L:604:BCL:HMB1	2.43	0.48
13:H:909:LDA:H123	13:H:910:LDA:C11	2.43	0.48
1:L:21:LEU:HD13	1:L:22:PHE:CZ	2.48	0.48
1:L:177:ILE:HG12	4:L:602:BCL:HMB3	1.96	0.48
6:M:501[B]:U10:H472	6:M:501[B]:U10:H451	1.60	0.47
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.96	0.47
2:M:270:ILE:HD13	18:M:800:CDL:H712	1.97	0.47
5:M:401:BPH:CBC	5:M:401:BPH:HHD	2.45	0.47
2:M:186:THR:HG23	4:M:603:BCL:HMD2	1.95	0.47
4:M:603:BCL:H201	13:M:918:LDA:H111	1.97	0.46
13:H:906:LDA:HM21	13:H:910:LDA:O1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:LEU:HG	13:L:921:LDA:HM22	1.97	0.46
4:M:603:BCL:HMB1	4:M:603:BCL:HBB3	1.96	0.46
2:M:278[B]:LEU:CD1	18:M:800:CDL:H811	2.46	0.46
1:L:199:ASN:HB3	18:M:800:CDL:CA2	2.46	0.46
1:L:235:LEU:HD23	13:L:921:LDA:CM1	2.38	0.46
6:L:502[A]:U10:C38	7:L:503:UQ1:H112	2.46	0.46
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.98	0.45
10:L:728:GOL:HO3	10:L:733:GOL:HO1	1.61	0.45
3:H:247:LYS:HA	3:H:248:ARG:HA	1.81	0.45
1:L:208:THR:HB	1:L:209:PRO:HD2	1.99	0.45
3:H:44:ASN:HD21	10:H:729:GOL:H32	1.82	0.45
2:M:4:GLN:H	10:M:741:GOL:C1	2.29	0.44
13:M:903:LDA:C9	13:H:901:LDA:H121	2.45	0.44
1:L:199:ASN:HB3	18:M:800:CDL:HA21	2.00	0.44
3:H:75:VAL:HG12	10:H:738:GOL:H11	1.99	0.44
2:M:4:GLN:H	10:M:741:GOL:H12	1.83	0.44
1:L:138:MET:SD	1:L:249:ILE:HD11	2.58	0.44
10:L:728:GOL:O3	10:L:733:GOL:O1	2.31	0.43
4:M:603:BCL:HBD	4:M:603:BCL:HAA2	1.99	0.43
3:H:112:ALA:HA	3:H:235:GLY:O	2.19	0.43
1:L:254:ILE:HG21	1:L:254:ILE:HD13	1.72	0.43
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.54	0.43
2:M:3:TYR:CD1	10:M:741:GOL:H12	2.54	0.43
13:L:914:LDA:H122	13:L:919:LDA:H52	2.00	0.43
8:M:707:PO4:O1	10:M:740:GOL:O2	2.37	0.43
3:H:156:CYS:HB3	3:H:206[A]:ASN:O	2.19	0.42
2:M:278[B]:LEU:HD11	18:M:800:CDL:C81	2.49	0.42
2:M:109:LEU:HD22	2:M:114:LEU:HD13	2.01	0.42
1:L:189:LEU:HD23	5:M:401:BPH:HMD2	2.01	0.42
3:H:157:ASP:N	3:H:157:ASP:OD1	2.52	0.42
3:H:246:PRO:HA	3:H:247:LYS:C	2.39	0.42
3:H:135[A]:LYS:CE	3:H:166:ASP:OD2	2.66	0.42
6:L:502[A]:U10:C43	5:M:401:BPH:H201	2.49	0.42
7:L:503:UQ1:C10	13:L:920:LDA:H121	2.44	0.42
6:L:502[B]:U10:H421	6:L:502[B]:U10:H401	1.80	0.42
3:H:84:PRO:O	3:H:85:ILE:HD13	2.20	0.41
6:M:501[A]:U10:H412	6:M:501[A]:U10:H371	1.92	0.41
2:M:278[B]:LEU:CD1	18:M:800:CDL:C81	2.98	0.41
3:H:21:TRP:CD2	13:H:906:LDA:HM22	2.55	0.41
6:L:502[A]:U10:H372	7:L:503:UQ1:C11	2.50	0.41
2:M:7:PHE:H	10:M:741:GOL:H32	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:601:BCL:C7	4:M:601:BCL:C4	2.90	0.41
13:M:903:LDA:HM12	19:H:280:HOH:O	2.20	0.41
13:L:915:LDA:HM21	13:M:918:LDA:O1	2.22	0.40
1:L:235:LEU:N	13:L:921:LDA:HM23	2.36	0.40
3:H:245:ALA:HB3	3:H:246:PRO:CD	2.39	0.40
13:L:908:LDA:HM22	19:L:447:HOH:O	2.20	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	281/281 (100%)	276 (98%)	5 (2%)	0	100	100
2	M	305/307 (99%)	299 (98%)	5 (2%)	1 (0%)	41	37
3	H	243/260 (94%)	238 (98%)	2 (1%)	3 (1%)	13	7
All	All	829/848 (98%)	813 (98%)	12 (1%)	4 (0%)	29	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	195	ASN
3	H	246	PRO
3	H	11	ASP

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	222/220 (101%)	215 (97%)	7 (3%)	39	38
2	M	241/240 (100%)	238 (99%)	3 (1%)	71	76
3	H	200/208 (96%)	195 (98%)	5 (2%)	47	49
All	All	663/668 (99%)	648 (98%)	15 (2%)	52	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	272	TRP
2	M	86	LEU
2	M	114	LEU
2	M	216	PHE
3	H	60	LYS
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	231	ASP
3	H	248	ARG

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	28	ASN
3	H	44	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 75 ligands modelled in this entry, 4 are monoatomic - leaving 71 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$
13	LDA	L	920	-	12,15,15	2.02	1 (8%)	14,17,17	0.52	0
10	GOL	H	729	-	5,5,5	0.35	0	5,5,5	0.47	0
13	LDA	M	907	-	12,15,15	1.98	1 (8%)	14,17,17	0.86	0
8	PO4	H	709	-	4,4,4	0.93	0	6,6,6	0.94	0
13	LDA	L	915	-	12,15,15	1.91	1 (8%)	14,17,17	0.50	0
15	SPO	M	600	-	40,41,41	1.02	2 (5%)	47,50,50	1.58	10 (21%)
13	LDA	L	902	-	12,15,15	2.01	1 (8%)	14,17,17	0.77	1 (7%)
10	GOL	M	737	-	5,5,5	0.34	0	5,5,5	0.37	0
4	BCL	M	601	-	58,74,74	1.33	4 (6%)	69,115,115	1.90	17 (24%)
10	GOL	L	723	-	5,5,5	0.47	0	5,5,5	0.83	0
6	U10	L	502[B]	-	63,63,63	2.25	23 (36%)	76,79,79	1.49	16 (21%)
13	LDA	L	917	-	12,15,15	1.94	1 (8%)	14,17,17	0.57	0
6	U10	M	501[B]	-	63,63,63	2.23	24 (38%)	76,79,79	1.36	9 (11%)
10	GOL	M	740	-	5,5,5	0.52	0	5,5,5	0.19	0
13	LDA	M	918	-	12,15,15	2.08	1 (8%)	14,17,17	0.70	0
13	LDA	L	921	-	12,15,15	2.21	1 (8%)	14,17,17	0.81	1 (7%)
6	U10	L	502[A]	-	63,63,63	2.26	22 (34%)	76,79,79	1.65	17 (22%)
10	GOL	H	745	-	5,5,5	0.42	0	5,5,5	0.45	0
13	LDA	L	904	-	12,15,15	2.09	1 (8%)	14,17,17	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	L	728	-	5,5,5	0.40	0	5,5,5	0.21	0
13	LDA	H	909	-	12,15,15	2.09	1 (8%)	14,17,17	0.48	0
8	PO4	L	705	-	4,4,4	0.90	0	6,6,6	1.09	0
10	GOL	L	732	-	5,5,5	0.41	0	5,5,5	0.39	0
8	PO4	L	703	-	4,4,4	1.16	1 (25%)	6,6,6	1.08	0
13	LDA	H	906	-	12,15,15	2.05	1 (8%)	14,17,17	0.37	0
10	GOL	H	739	-	5,5,5	0.46	0	5,5,5	0.33	0
10	GOL	H	743	-	5,5,5	0.60	0	5,5,5	0.82	0
10	GOL	L	724	-	5,5,5	0.57	0	5,5,5	0.40	0
18	CDL	M	800	-	80,80,99	1.16	4 (5%)	86,92,111	1.23	7 (8%)
10	GOL	L	744	-	5,5,5	0.66	0	5,5,5	0.55	0
10	GOL	H	736	-	5,5,5	0.41	0	5,5,5	0.26	0
7	UQ1	L	503	-	18,18,18	2.30	7 (38%)	22,25,25	2.03	5 (22%)
8	PO4	L	708	-	4,4,4	1.02	0	6,6,6	0.53	0
10	GOL	L	730	-	5,5,5	0.46	0	5,5,5	0.62	0
13	LDA	L	905	-	12,15,15	2.01	1 (8%)	14,17,17	0.44	0
9	DIO	L	711	-	6,6,6	0.43	0	6,6,6	0.71	0
10	GOL	H	721	-	5,5,5	0.15	0	5,5,5	0.88	0
11	HT3	L	751	-	9,9,9	0.97	1 (11%)	10,10,10	1.66	3 (30%)
4	BCL	M	603	-	58,74,74	1.29	5 (8%)	69,115,115	1.68	15 (21%)
5	BPH	L	402	-	64,70,70	0.81	0	76,101,101	1.48	15 (19%)
10	GOL	H	746	-	5,5,5	0.59	0	5,5,5	0.55	0
10	GOL	M	726	-	5,5,5	0.54	0	5,5,5	0.51	0
13	LDA	M	911	-	12,15,15	2.01	1 (8%)	14,17,17	0.54	0
13	LDA	H	910	-	12,15,15	1.96	1 (8%)	14,17,17	0.80	0
10	GOL	M	741	-	5,5,5	0.51	0	5,5,5	1.49	1 (20%)
10	GOL	L	727	-	5,5,5	0.47	0	5,5,5	0.66	0
8	PO4	L	706	-	4,4,4	0.94	0	6,6,6	1.08	0
10	GOL	L	734	-	5,5,5	0.23	0	5,5,5	0.50	0
6	U10	M	501[A]	-	63,63,63	2.20	26 (41%)	76,79,79	1.60	13 (17%)
4	BCL	L	604	-	58,74,74	1.26	3 (5%)	69,115,115	1.75	18 (26%)
10	GOL	M	742	-	5,5,5	0.49	0	5,5,5	0.59	0
10	GOL	H	738	-	5,5,5	0.38	0	5,5,5	0.23	0
13	LDA	L	914	-	12,15,15	1.89	1 (8%)	14,17,17	0.69	0
13	LDA	H	901	-	12,15,15	2.09	1 (8%)	14,17,17	0.46	0
10	GOL	L	725	-	5,5,5	0.44	0	5,5,5	1.03	0
10	GOL	L	731	-	5,5,5	0.74	0	5,5,5	0.71	0
13	LDA	L	908	-	12,15,15	1.94	1 (8%)	14,17,17	0.59	0
13	LDA	M	916	-	12,15,15	1.98	1 (8%)	14,17,17	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LDA	M	903	-	12,15,15	2.34	1 (8%)	14,17,17	1.22	1 (7%)
13	LDA	M	912	-	12,15,15	1.97	1 (8%)	14,17,17	0.53	0
4	BCL	L	602	-	58,74,74	1.36	4 (6%)	69,115,115	1.43	12 (17%)
8	PO4	M	707	-	4,4,4	1.01	0	6,6,6	1.12	0
10	GOL	L	733	-	5,5,5	0.42	0	5,5,5	0.66	0
13	LDA	L	913	-	12,15,15	1.97	1 (8%)	14,17,17	0.40	0
10	GOL	L	722	-	5,5,5	0.42	0	5,5,5	0.69	0
10	GOL	H	735	-	5,5,5	0.59	0	5,5,5	0.62	0
8	PO4	M	704	-	4,4,4	0.92	0	6,6,6	1.20	1 (16%)
5	BPH	M	401	-	64,70,70	0.82	1 (1%)	76,101,101	1.72	14 (18%)
12	HTO	H	752	-	9,9,9	0.48	0	10,10,10	1.37	1 (10%)
13	LDA	L	919	-	12,15,15	2.05	1 (8%)	14,17,17	0.69	0
12	HTO	L	753	-	9,9,9	0.54	0	10,10,10	1.64	2 (20%)

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
13	LDA	L	920	-	-	3/13/13/13	-
10	GOL	H	729	-	-	2/4/4/4	-
13	LDA	M	907	-	-	5/13/13/13	-
13	LDA	L	915	-	-	2/13/13/13	-
15	SPO	M	600	-	-	3/47/47/47	-
13	LDA	L	902	-	-	6/13/13/13	-
10	GOL	M	737	-	-	2/4/4/4	-
4	BCL	M	601	-	-	16/37/137/137	-
10	GOL	L	723	-	-	2/4/4/4	-
6	U10	L	502[B]	-	-	17/63/87/87	0/1/1/1
13	LDA	L	917	-	-	9/13/13/13	-
6	U10	M	501[B]	-	-	11/63/87/87	0/1/1/1
10	GOL	M	740	-	-	4/4/4/4	-
13	LDA	M	918	-	-	5/13/13/13	-
13	LDA	L	921	-	-	9/13/13/13	-
6	U10	L	502[A]	-	-	14/63/87/87	0/1/1/1
10	GOL	H	745	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LDA	L	904	-	-	7/13/13/13	-
10	GOL	L	728	-	-	0/4/4/4	-
13	LDA	H	909	-	-	6/13/13/13	-
10	GOL	L	732	-	-	2/4/4/4	-
13	LDA	H	906	-	-	6/13/13/13	-
10	GOL	H	739	-	-	2/4/4/4	-
10	GOL	H	743	-	-	0/4/4/4	-
10	GOL	L	724	-	-	4/4/4/4	-
18	CDL	M	800	-	-	38/91/91/110	-
10	GOL	L	744	-	-	2/4/4/4	-
7	UQ1	L	503	-	-	4/9/33/33	0/1/1/1
5	BPH	L	402	-	-	5/54/105/105	0/5/6/6
10	GOL	L	730	-	-	2/4/4/4	-
13	LDA	L	905	-	-	4/13/13/13	-
9	DIO	L	711	-	-	-	0/1/1/1
10	GOL	H	721	-	-	1/4/4/4	-
11	HT3	L	751	-	-	5/10/10/10	-
10	GOL	H	735	-	-	2/4/4/4	-
5	BPH	M	401	-	-	14/54/105/105	0/5/6/6
10	GOL	H	746	-	-	4/4/4/4	-
10	GOL	M	726	-	-	3/4/4/4	-
13	LDA	M	911	-	-	5/13/13/13	-
10	GOL	M	741	-	-	1/4/4/4	-
10	GOL	L	727	-	-	4/4/4/4	-
10	GOL	L	734	-	-	2/4/4/4	-
6	U10	M	501[A]	-	-	12/63/87/87	0/1/1/1
4	BCL	L	604	-	-	3/37/137/137	-
10	GOL	M	742	-	-	2/4/4/4	-
10	GOL	H	738	-	-	2/4/4/4	-
13	LDA	L	914	-	-	6/13/13/13	-
13	LDA	H	901	-	-	5/13/13/13	-
10	GOL	L	725	-	-	3/4/4/4	-
10	GOL	L	731	-	-	0/4/4/4	-
13	LDA	L	908	-	-	8/13/13/13	-
13	LDA	M	916	-	-	7/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LDA	M	903	-	-	5/13/13/13	-
13	LDA	M	912	-	-	8/13/13/13	-
4	BCL	L	602	-	-	2/37/137/137	-
10	GOL	L	733	-	-	4/4/4/4	-
13	LDA	L	913	-	-	10/13/13/13	-
10	GOL	L	722	-	-	2/4/4/4	-
4	BCL	M	603	-	-	1/37/137/137	-
13	LDA	H	910	-	-	8/13/13/13	-
10	GOL	H	736	-	-	2/4/4/4	-
12	HTO	H	752	-	-	2/10/10/10	-
13	LDA	L	919	-	-	4/13/13/13	-
12	HTO	L	753	-	-	5/10/10/10	-

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502[B]	U10	C7-C8	-8.67	1.38	1.50
6	L	502[A]	U10	C7-C8	-8.67	1.38	1.50
13	L	921	LDA	O1-N1	-7.52	1.24	1.42
13	M	903	LDA	O1-N1	-7.16	1.25	1.42
13	H	901	LDA	O1-N1	-7.14	1.25	1.42
13	M	918	LDA	O1-N1	-7.13	1.25	1.42
13	H	909	LDA	O1-N1	-7.12	1.25	1.42
13	L	919	LDA	O1-N1	-7.06	1.25	1.42
13	H	906	LDA	O1-N1	-7.00	1.25	1.42
13	M	911	LDA	O1-N1	-6.91	1.26	1.42
13	L	904	LDA	O1-N1	-6.89	1.26	1.42
13	L	920	LDA	O1-N1	-6.89	1.26	1.42
13	L	902	LDA	O1-N1	-6.86	1.26	1.42
13	L	905	LDA	O1-N1	-6.84	1.26	1.42
13	L	913	LDA	O1-N1	-6.74	1.26	1.42
13	M	907	LDA	O1-N1	-6.72	1.26	1.42
13	M	916	LDA	O1-N1	-6.69	1.26	1.42
13	H	910	LDA	O1-N1	-6.68	1.26	1.42
13	M	912	LDA	O1-N1	-6.68	1.26	1.42
13	L	917	LDA	O1-N1	-6.64	1.26	1.42
7	L	503	UQ1	C7-C8	-6.57	1.41	1.50
13	L	908	LDA	O1-N1	-6.56	1.26	1.42
13	L	915	LDA	O1-N1	-6.44	1.27	1.42
13	L	914	LDA	O1-N1	-6.33	1.27	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	602	BCL	MG-NA	5.81	2.20	2.06
6	M	501[B]	U10	C7-C8	-5.77	1.42	1.50
6	M	501[A]	U10	C7-C8	-5.77	1.42	1.50
4	M	603	BCL	MG-NA	5.49	2.19	2.06
6	M	501[B]	U10	O4-C4M	5.13	1.57	1.45
6	M	501[A]	U10	O4-C4M	5.13	1.57	1.45
4	L	604	BCL	C1B-NB	4.75	1.39	1.35
18	M	800	CDL	OB6-CB5	4.65	1.47	1.34
18	M	800	CDL	OA8-CA7	4.63	1.46	1.33
18	M	800	CDL	OA6-CA5	4.56	1.47	1.34
4	M	601	BCL	C4B-NB	4.56	1.39	1.35
4	L	604	BCL	C3C-C4C	-4.45	1.46	1.51
4	L	602	BCL	C4B-NB	4.35	1.39	1.35
4	M	601	BCL	C1B-NB	4.27	1.39	1.35
4	L	602	BCL	C1B-NB	4.22	1.39	1.35
6	M	501[A]	U10	C27-C28	-4.20	1.36	1.50
4	M	601	BCL	MG-NA	4.12	2.16	2.06
18	M	800	CDL	OB8-CB7	4.05	1.45	1.33
6	M	501[B]	U10	C27-C28	-3.89	1.37	1.50
6	M	501[B]	U10	C22-C23	-3.89	1.37	1.50
6	M	501[A]	U10	C22-C23	-3.89	1.37	1.50
6	L	502[A]	U10	C47-C48	-3.84	1.37	1.50
6	L	502[B]	U10	C27-C28	-3.64	1.38	1.50
6	L	502[A]	U10	C27-C28	-3.64	1.38	1.50
6	L	502[B]	U10	C28-C29	3.58	1.41	1.33
6	L	502[A]	U10	C28-C29	3.58	1.41	1.33
6	L	502[A]	U10	C52-C53	-3.56	1.38	1.50
6	M	501[B]	U10	C42-C43	-3.51	1.39	1.50
6	L	502[A]	U10	C42-C43	-3.50	1.39	1.50
6	L	502[B]	U10	C6-C1	3.49	1.41	1.35
6	L	502[A]	U10	C6-C1	3.49	1.41	1.35
6	M	501[B]	U10	C47-C48	-3.47	1.39	1.50
6	M	501[B]	U10	C37-C38	-3.43	1.39	1.50
4	L	604	BCL	MG-NA	3.43	2.14	2.06
6	M	501[B]	U10	C6-C1	3.41	1.41	1.35
6	M	501[A]	U10	C6-C1	3.41	1.41	1.35
15	M	600	SPO	C21-C22	3.40	1.54	1.43
6	M	501[A]	U10	C37-C38	-3.39	1.39	1.50
4	M	603	BCL	C3B-C2B	-3.39	1.33	1.39
7	L	503	UQ1	C3-C4	-3.32	1.39	1.48
6	L	502[B]	U10	C52-C53	-3.31	1.39	1.50
6	L	502[B]	U10	C3-C2	-3.30	1.39	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502[A]	U10	C3-C2	-3.30	1.39	1.48
6	L	502[B]	U10	C17-C18	-3.30	1.39	1.50
6	L	502[A]	U10	C17-C18	-3.30	1.39	1.50
6	L	502[B]	U10	C42-C43	-3.29	1.39	1.50
4	M	601	BCL	MG-NC	3.28	2.14	2.06
7	L	503	UQ1	C8-C9	3.27	1.41	1.32
6	M	501[B]	U10	C38-C39	3.25	1.40	1.33
6	M	501[B]	U10	C4-C5	-3.19	1.39	1.48
6	M	501[A]	U10	C4-C5	-3.19	1.39	1.48
6	M	501[B]	U10	C17-C18	-3.18	1.40	1.50
6	M	501[A]	U10	C17-C18	-3.18	1.40	1.50
6	M	501[B]	U10	C32-C33	-3.17	1.40	1.50
6	L	502[B]	U10	C13-C14	3.16	1.40	1.33
6	L	502[A]	U10	C13-C14	3.16	1.40	1.33
6	M	501[B]	U10	C36-C34	3.15	1.57	1.51
6	L	502[B]	U10	C37-C38	-3.13	1.40	1.50
6	L	502[B]	U10	C47-C48	-3.13	1.40	1.50
6	M	501[B]	U10	C52-C53	-3.13	1.40	1.50
6	M	501[A]	U10	C42-C43	-3.11	1.40	1.50
6	M	501[A]	U10	C47-C48	-3.04	1.40	1.50
6	L	502[B]	U10	C48-C49	3.00	1.40	1.33
6	M	501[A]	U10	C52-C53	-2.99	1.40	1.50
6	M	501[B]	U10	C43-C44	2.98	1.40	1.33
4	L	602	BCL	CMB-C2B	2.98	1.57	1.51
6	L	502[B]	U10	C22-C23	-2.97	1.40	1.50
6	L	502[A]	U10	C22-C23	-2.97	1.40	1.50
6	M	501[B]	U10	C12-C13	-2.96	1.40	1.50
6	M	501[A]	U10	C12-C13	-2.96	1.40	1.50
6	M	501[A]	U10	C48-C49	2.96	1.40	1.33
6	L	502[B]	U10	C38-C39	2.94	1.40	1.33
6	M	501[A]	U10	C33-C34	2.94	1.40	1.33
6	M	501[A]	U10	C32-C33	-2.94	1.40	1.50
6	M	501[A]	U10	C53-C54	2.94	1.40	1.32
6	L	502[A]	U10	C38-C39	2.94	1.40	1.33
6	L	502[A]	U10	C37-C38	-2.92	1.40	1.50
6	L	502[B]	U10	C33-C34	2.92	1.40	1.33
6	L	502[A]	U10	C33-C34	2.92	1.40	1.33
6	M	501[A]	U10	C43-C44	2.90	1.39	1.33
6	L	502[B]	U10	C23-C24	2.89	1.39	1.33
6	L	502[A]	U10	C23-C24	2.89	1.39	1.33
4	M	603	BCL	C4B-NB	2.88	1.37	1.35
6	L	502[B]	U10	C32-C33	-2.85	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502[A]	U10	C32-C33	-2.85	1.41	1.50
6	M	501[B]	U10	C33-C34	2.85	1.39	1.33
6	M	501[B]	U10	C18-C19	2.79	1.39	1.33
6	M	501[A]	U10	C18-C19	2.79	1.39	1.33
6	M	501[B]	U10	C48-C49	2.78	1.39	1.33
6	L	502[A]	U10	C53-C54	2.77	1.40	1.32
6	L	502[B]	U10	C18-C19	2.75	1.39	1.33
6	L	502[A]	U10	C18-C19	2.75	1.39	1.33
6	L	502[B]	U10	C43-C44	2.70	1.39	1.33
6	L	502[B]	U10	C53-C54	2.67	1.40	1.32
6	M	501[B]	U10	C8-C9	2.62	1.39	1.33
6	M	501[A]	U10	C8-C9	2.62	1.39	1.33
6	L	502[B]	U10	C12-C13	-2.56	1.42	1.50
6	L	502[A]	U10	C12-C13	-2.56	1.42	1.50
4	M	603	BCL	OBD-CAD	2.53	1.25	1.22
6	M	501[A]	U10	C35-C34	2.45	1.57	1.50
6	M	501[B]	U10	C53-C54	2.43	1.39	1.32
7	L	503	UQ1	C6-C5	2.43	1.39	1.35
7	L	503	UQ1	C2-C1	-2.36	1.42	1.48
7	L	503	UQ1	C7-C6	2.28	1.55	1.51
6	L	502[A]	U10	C43-C44	2.26	1.38	1.33
6	M	501[A]	U10	C46-C44	2.26	1.56	1.51
4	M	603	BCL	C2C-C3C	-2.24	1.48	1.54
6	L	502[B]	U10	C31-C29	2.22	1.55	1.51
6	L	502[A]	U10	C31-C29	2.22	1.55	1.51
15	M	600	SPO	C4-C5	2.21	1.53	1.50
5	M	401	BPH	C3C-C4C	2.21	1.54	1.50
6	M	501[A]	U10	C30-C29	2.21	1.56	1.50
6	L	502[B]	U10	C4-C5	-2.21	1.42	1.48
6	L	502[A]	U10	C4-C5	-2.21	1.42	1.48
6	M	501[B]	U10	C3-C2	-2.16	1.42	1.48
6	M	501[A]	U10	C3-C2	-2.16	1.42	1.48
8	L	703	PO4	P-O1	2.11	1.55	1.50
7	L	503	UQ1	C6-C1	-2.11	1.40	1.46
6	M	501[B]	U10	C13-C14	2.06	1.37	1.33
6	M	501[A]	U10	C13-C14	2.06	1.37	1.33
6	M	501[A]	U10	C38-C39	2.05	1.37	1.33
6	M	501[B]	U10	C21-C19	-2.03	1.47	1.51
6	M	501[A]	U10	C21-C19	-2.03	1.47	1.51
11	L	751	HT3	O3-C3	2.01	1.47	1.43

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502[A]	U10	C50-C49-C51	5.97	125.32	115.27
6	M	501[A]	U10	C30-C29-C31	5.55	124.61	115.27
4	M	601	BCL	OBD-CAD-CBD	-5.45	118.11	125.89
4	M	601	BCL	C5-C3-C2	5.25	131.75	121.12
4	M	601	BCL	C4D-C3D-CAD	-5.24	105.55	108.47
18	M	800	CDL	OA6-CA5-C11	5.20	122.72	111.50
6	L	502[B]	U10	C35-C34-C36	4.91	123.53	115.27
5	M	401	BPH	C1-C2-C3	-4.73	117.87	126.04
6	M	501[A]	U10	C31-C29-C28	-4.69	111.62	121.12
4	L	604	BCL	CMB-C2B-C1B	-4.68	121.28	128.46
7	L	503	UQ1	CM5-C5-C6	-4.63	116.85	124.40
5	M	401	BPH	CAC-C3C-C4C	4.56	124.39	112.67
4	M	601	BCL	C4-C3-C2	-4.53	112.06	123.68
4	M	603	BCL	C4A-NA-C1A	4.43	108.70	106.71
6	M	501[B]	U10	C30-C29-C31	4.31	122.51	115.27
5	L	402	BPH	C1C-NC-C4C	-4.29	106.77	110.54
5	M	401	BPH	O2D-CGD-CBD	4.21	118.75	111.27
7	L	503	UQ1	C6-C5-C4	4.20	122.50	119.18
4	M	603	BCL	C4D-C3D-CAD	-4.19	106.13	108.47
4	M	603	BCL	CMB-C2B-C1B	-4.18	122.04	128.46
7	L	503	UQ1	C7-C6-C1	4.17	123.50	118.48
6	L	502[A]	U10	C51-C49-C48	-4.09	112.84	121.12
4	M	601	BCL	CMB-C2B-C1B	-4.07	122.21	128.46
4	M	601	BCL	C1-C2-C3	4.02	132.99	126.04
5	M	401	BPH	C1C-NC-C4C	-4.02	107.01	110.54
4	L	602	BCL	C4D-C3D-CAD	-3.97	106.26	108.47
4	M	601	BCL	C1-O2A-CGA	3.94	126.77	116.44
4	L	604	BCL	CMB-C2B-C3B	3.79	131.76	124.68
5	L	402	BPH	CAC-C3C-C4C	3.68	122.13	112.67
4	L	604	BCL	CAC-C3C-C4C	-3.68	104.42	112.58
15	M	600	SPO	C20-C19-C17	-3.65	122.09	127.31
6	M	501[A]	U10	C35-C34-C36	3.64	121.40	115.27
4	L	602	BCL	CMB-C2B-C1B	-3.64	122.88	128.46
15	M	600	SPO	C5-C6-C7	-3.49	120.62	125.89
6	M	501[A]	U10	C26-C27-C28	-3.46	100.50	111.88
5	M	401	BPH	CAA-C2A-C1A	-3.45	103.40	112.33
6	M	501[B]	U10	C35-C34-C36	3.45	121.08	115.27
12	H	752	HTO	C5-C4-C3	-3.44	108.52	114.18
4	M	603	BCL	CAC-C3C-C2C	-3.42	105.70	114.26
15	M	600	SPO	C2-C1-C4	-3.42	105.60	110.86
4	L	604	BCL	CAC-C3C-C2C	-3.42	105.72	114.26
18	M	800	CDL	OB8-CB7-OB9	-3.40	115.01	123.59
18	M	800	CDL	OB6-CB5-C51	3.38	118.78	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	602	BCL	C4A-NA-C1A	3.36	108.22	106.71
4	L	604	BCL	C4B-C3B-CAB	-3.36	120.64	127.13
5	L	402	BPH	CAA-C2A-C3A	-3.33	103.65	112.78
6	M	501[B]	U10	C45-C44-C46	3.32	120.85	115.27
4	L	602	BCL	CMB-C2B-C3B	3.29	130.83	124.68
5	M	401	BPH	C3A-C2A-C1A	3.28	105.57	101.64
6	M	501[B]	U10	C15-C14-C16	3.27	120.78	115.27
6	M	501[A]	U10	C15-C14-C16	3.27	120.78	115.27
4	M	603	BCL	O2A-CGA-O1A	-3.24	115.42	123.59
18	M	800	CDL	CA4-OA6-CA5	-3.20	109.92	117.79
4	M	603	BCL	CMD-C2D-C3D	3.19	130.65	124.68
18	M	800	CDL	OA8-CA7-C31	3.16	121.83	111.91
5	M	401	BPH	C1-O2A-CGA	3.13	124.65	116.44
4	M	603	BCL	OBD-CAD-CBD	-3.13	121.43	125.89
5	L	402	BPH	C1B-NB-C4B	3.12	112.39	106.51
5	L	402	BPH	CMC-C2C-C1C	3.07	120.67	112.09
15	M	600	SPO	C21-C20-C19	3.07	129.76	123.47
7	L	503	UQ1	CM3-O3-C3	3.01	127.14	116.47
5	M	401	BPH	O2A-C1-C2	-3.01	100.74	108.64
18	M	800	CDL	OB8-CB7-C71	2.99	121.28	111.91
11	L	751	HT3	O2-C2-C3	2.98	115.85	109.72
6	M	501[A]	U10	C40-C39-C41	2.97	120.27	115.27
5	L	402	BPH	C1-C2-C3	-2.97	120.91	126.04
6	M	501[B]	U10	C50-C49-C51	2.96	120.25	115.27
6	M	501[A]	U10	C25-C24-C26	2.95	120.23	115.27
6	M	501[B]	U10	C22-C21-C19	-2.93	103.33	112.98
6	M	501[A]	U10	C22-C21-C19	-2.93	103.33	112.98
6	M	501[A]	U10	C27-C28-C29	2.93	134.72	127.66
6	L	502[B]	U10	C25-C24-C26	2.88	120.12	115.27
6	L	502[A]	U10	C25-C24-C26	2.88	120.12	115.27
5	M	401	BPH	O1D-CGD-CBD	-2.85	118.64	124.48
4	M	601	BCL	OBB-CAB-C3B	2.84	125.04	119.99
12	L	753	HTO	O1-C1-C2	-2.84	104.88	111.07
4	L	604	BCL	C2C-C3C-C4C	2.82	105.56	101.34
4	L	604	BCL	O2D-CGD-CBD	2.82	116.27	111.27
4	M	603	BCL	O2A-C1-C2	2.81	116.02	108.64
15	M	600	SPO	C25-C23-C22	-2.81	114.64	118.94
4	L	602	BCL	C4B-CHC-C1C	-2.77	124.64	130.12
4	L	604	BCL	C4A-NA-C1A	2.74	107.94	106.71
6	L	502[B]	U10	C30-C29-C28	-2.73	116.68	123.68
6	L	502[A]	U10	C30-C29-C28	-2.73	116.68	123.68
5	L	402	BPH	CMB-C2B-C1B	-2.71	120.89	125.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	CMA-C3A-C2A	-2.71	102.90	113.83
6	M	501[A]	U10	C45-C44-C46	2.69	119.80	115.27
4	L	604	BCL	OBD-CAD-CBD	-2.68	122.07	125.89
5	L	402	BPH	CMA-C3A-C2A	-2.67	103.04	113.83
6	L	502[B]	U10	C45-C44-C46	2.66	119.74	115.27
13	M	903	LDA	O1-N1-C1	2.65	115.77	109.27
4	M	603	BCL	CHA-C1A-NA	-2.64	120.35	126.40
6	L	502[A]	U10	C47-C46-C44	-2.63	104.32	112.98
5	M	401	BPH	CMB-C2B-C1B	-2.63	121.01	125.06
18	M	800	CDL	OA6-CA5-OA7	-2.62	117.36	123.70
7	L	503	UQ1	C5-C6-C1	-2.62	117.11	119.58
4	M	603	BCL	CMB-C2B-C3B	2.62	129.58	124.68
6	M	501[A]	U10	C50-C49-C51	2.61	119.66	115.27
5	M	401	BPH	CMC-C2C-C1C	2.60	119.36	112.09
4	L	602	BCL	C4B-C3B-CAB	-2.60	122.11	127.13
4	L	604	BCL	CAA-C2A-C3A	-2.59	105.67	112.78
4	L	604	BCL	OBD-CAD-C3D	2.59	132.29	127.98
15	M	600	SPO	C18-C17-C19	2.58	126.54	122.92
4	M	601	BCL	CMB-C2B-C3B	2.56	129.47	124.68
4	L	604	BCL	CHA-C1A-NA	-2.55	120.56	126.40
6	L	502[B]	U10	C30-C29-C31	2.55	119.56	115.27
6	L	502[A]	U10	C30-C29-C31	2.55	119.56	115.27
15	M	600	SPO	C24-C23-C22	2.54	126.49	122.92
4	L	602	BCL	CAA-C2A-C3A	-2.52	105.89	112.78
5	L	402	BPH	C4D-C3D-CAD	-2.51	106.28	107.87
6	M	501[A]	U10	C26-C24-C23	-2.51	116.05	121.12
15	M	600	SPO	C16-C17-C19	-2.50	115.11	118.94
5	M	401	BPH	CAA-C2A-C3A	-2.49	105.96	112.78
6	L	502[B]	U10	C27-C26-C24	-2.48	104.83	112.98
6	L	502[A]	U10	C27-C26-C24	-2.48	104.83	112.98
4	M	603	BCL	C1C-NC-C4C	2.46	107.81	106.71
6	L	502[A]	U10	C40-C39-C41	2.44	119.37	115.27
12	L	753	HTO	O2-C2-C1	-2.44	103.43	109.14
4	L	602	BCL	CAA-C2A-C1A	-2.42	104.04	111.97
6	L	502[A]	U10	C35-C34-C36	2.42	119.34	115.27
4	L	602	BCL	OBD-CAD-CBD	-2.41	122.46	125.89
6	L	502[B]	U10	O2-C2-C3	-2.41	115.82	120.93
6	L	502[A]	U10	O2-C2-C3	-2.41	115.82	120.93
11	L	751	HT3	O3-C3-C2	2.41	114.67	109.72
5	M	401	BPH	OBD-CAD-CBD	-2.40	122.47	125.89
13	L	921	LDA	CM1-N1-C1	2.38	115.24	110.23
6	M	501[B]	U10	C35-C34-C33	-2.38	117.56	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	501[B]	U10	C56-C54-C55	2.37	119.84	114.60
4	L	604	BCL	CMA-C3A-C2A	-2.36	104.30	113.83
6	L	502[B]	U10	C1M-C1-C6	-2.35	120.57	124.40
6	L	502[A]	U10	C1M-C1-C6	-2.35	120.57	124.40
4	M	601	BCL	C6-C5-C3	-2.35	107.30	113.45
4	M	601	BCL	OBD-CAD-C3D	2.34	131.87	127.98
5	L	402	BPH	CMB-C2B-C3B	2.34	132.99	127.61
10	M	741	GOL	O2-C2-C1	2.32	119.35	109.12
8	M	704	PO4	O4-P-O3	2.31	115.38	107.97
6	L	502[B]	U10	C3M-O3-C3	2.31	124.64	116.47
6	L	502[A]	U10	C3M-O3-C3	2.31	124.64	116.47
4	M	601	BCL	CAA-C2A-C3A	-2.28	106.53	112.78
6	L	502[A]	U10	C46-C47-C48	-2.28	104.39	111.88
13	L	902	LDA	CM2-N1-C1	2.28	115.02	110.23
5	L	402	BPH	CMD-C2D-C3D	2.28	128.94	124.68
6	M	501[B]	U10	C10-C9-C11	2.26	119.07	115.27
6	M	501[A]	U10	C10-C9-C11	2.26	119.07	115.27
6	L	502[B]	U10	C36-C34-C33	-2.24	116.58	121.12
4	L	602	BCL	CMA-C3A-C2A	-2.23	104.83	113.83
4	M	601	BCL	CHA-C1A-NA	-2.23	121.29	126.40
15	M	600	SPO	C27-C26-C25	-2.23	116.26	123.22
6	L	502[B]	U10	C40-C39-C38	-2.23	117.97	123.68
4	M	601	BCL	CAA-C2A-C1A	-2.22	104.69	111.97
4	L	604	BCL	CMC-C2C-C3C	-2.21	104.90	113.83
4	L	604	BCL	O1D-CGD-CBD	-2.20	119.98	124.48
4	L	602	BCL	C1-O2A-CGA	2.20	122.21	116.44
6	L	502[B]	U10	C22-C21-C19	2.19	120.18	112.98
6	L	502[A]	U10	C22-C21-C19	2.19	120.18	112.98
5	L	402	BPH	C7-C6-C5	-2.18	107.44	113.36
6	L	502[B]	U10	C17-C16-C14	2.18	120.14	112.98
6	L	502[A]	U10	C17-C16-C14	2.18	120.14	112.98
6	L	502[A]	U10	C56-C54-C55	2.16	119.37	114.60
6	L	502[B]	U10	C56-C54-C55	2.15	119.36	114.60
4	M	601	BCL	CMA-C3A-C4A	-2.14	106.02	111.77
4	L	604	BCL	CBC-CAC-C3C	2.14	118.23	113.47
4	M	603	BCL	C1-C2-C3	-2.14	122.35	126.04
4	L	604	BCL	C4-C3-C5	2.13	118.85	115.27
4	L	602	BCL	CHA-C1A-NA	-2.13	121.52	126.40
4	M	603	BCL	OBD-CAD-C3D	2.12	131.50	127.98
4	L	604	BCL	C2A-C1A-CHA	2.11	127.56	123.86
15	M	600	SPO	C34-C33-C35	2.11	118.82	115.27
5	L	402	BPH	OBD-CAD-CBD	-2.09	122.90	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	603	BCL	CAC-C3C-C4C	-2.06	108.00	112.58
4	M	603	BCL	C4B-C3B-CAB	-2.06	123.15	127.13
5	L	402	BPH	CHB-C4A-NA	-2.06	121.40	124.94
4	M	601	BCL	CMD-C2D-C3D	2.03	128.47	124.68
11	L	751	HT3	O2-C2-C1	-2.02	104.40	109.14
5	L	402	BPH	CAC-C3C-C2C	2.02	119.30	114.26
6	L	502[B]	U10	C7-C8-C9	-2.01	123.44	126.79
6	L	502[A]	U10	C7-C8-C9	-2.01	123.44	126.79
4	M	601	BCL	O1D-CGD-CBD	-2.01	120.38	124.48
6	L	502[B]	U10	C40-C39-C41	2.01	118.64	115.27

There are no chirality outliers.

All (338) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	L	920	LDA	N1-C1-C2-C3
10	L	730	GOL	O1-C1-C2-C3
10	M	737	GOL	O1-C1-C2-C3
4	M	601	BCL	C2-C3-C5-C6
4	M	601	BCL	C4-C3-C5-C6
10	L	723	GOL	C1-C2-C3-O3
6	L	502[B]	U10	C28-C29-C31-C32
6	L	502[B]	U10	C30-C29-C31-C32
6	L	502[B]	U10	C44-C46-C47-C48
13	L	917	LDA	C2-C1-N1-O1
13	L	917	LDA	C2-C1-N1-CM2
6	M	501[B]	U10	C34-C36-C37-C38
6	M	501[B]	U10	C44-C46-C47-C48
10	M	740	GOL	C1-C2-C3-O3
13	L	921	LDA	C2-C1-N1-O1
13	L	921	LDA	C2-C1-N1-CM1
13	L	921	LDA	N1-C1-C2-C3
6	L	502[A]	U10	C28-C29-C31-C32
6	L	502[A]	U10	C30-C29-C31-C32
6	L	502[A]	U10	C34-C36-C37-C38
6	L	502[A]	U10	C48-C49-C51-C52
6	L	502[A]	U10	C50-C49-C51-C52
10	H	745	GOL	C1-C2-C3-O3
10	H	745	GOL	O2-C2-C3-O3
13	H	909	LDA	C2-C1-N1-O1
13	H	909	LDA	C2-C1-N1-CM1
13	H	909	LDA	C2-C1-N1-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	904	LDA	N1-C1-C2-C3
10	H	735	GOL	O1-C1-C2-C3
10	H	739	GOL	O1-C1-C2-C3
10	L	724	GOL	C1-C2-C3-O3
18	M	800	CDL	CB2-C1-CA2-OA2
18	M	800	CDL	CB2-OB2-PB2-OB3
18	M	800	CDL	OB5-CB3-CB4-OB6
10	L	744	GOL	C1-C2-C3-O3
10	L	744	GOL	O2-C2-C3-O3
11	L	751	HT3	O1-C1-C2-O2
11	L	751	HT3	O3-C3-C4-C5
13	H	910	LDA	C2-C1-N1-CM1
13	H	910	LDA	C2-C1-N1-CM2
10	L	727	GOL	C1-C2-C3-O3
10	L	727	GOL	O2-C2-C3-O3
10	L	734	GOL	C1-C2-C3-O3
6	M	501[A]	U10	C24-C26-C27-C28
6	M	501[A]	U10	C38-C39-C41-C42
6	M	501[A]	U10	C40-C39-C41-C42
6	M	501[A]	U10	C49-C51-C52-C53
13	L	913	LDA	C2-C1-N1-O1
13	L	913	LDA	C2-C1-N1-CM2
13	M	903	LDA	C2-C1-N1-CM1
13	M	903	LDA	C2-C1-N1-CM2
10	H	736	GOL	O1-C1-C2-C3
13	M	912	LDA	C2-C1-N1-O1
13	M	912	LDA	C2-C1-N1-CM1
10	L	733	GOL	C1-C2-C3-O3
13	H	906	LDA	C2-C1-N1-CM1
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C4B-C3B-CAB-CBB
5	M	401	BPH	C11-C12-C13-C15
12	L	753	HTO	O1-C1-C2-O2
12	L	753	HTO	O1-C1-C2-C3
12	L	753	HTO	O3-C3-C4-C5
18	M	800	CDL	OB9-CB7-OB8-CB6
18	M	800	CDL	C71-CB7-OB8-CB6
6	L	502[B]	U10	C35-C34-C36-C37
6	M	501[B]	U10	C45-C44-C46-C47
6	M	501[A]	U10	C45-C44-C46-C47
6	L	502[B]	U10	C33-C34-C36-C37
6	M	501[B]	U10	C43-C44-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	M	501[A]	U10	C43-C44-C46-C47
6	L	502[B]	U10	C24-C26-C27-C28
6	L	502[B]	U10	C34-C36-C37-C38
6	L	502[A]	U10	C24-C26-C27-C28
6	L	502[A]	U10	C49-C51-C52-C53
10	L	723	GOL	O2-C2-C3-O3
10	H	745	GOL	O1-C1-C2-O2
10	H	739	GOL	O1-C1-C2-O2
10	L	734	GOL	O2-C2-C3-O3
10	L	733	GOL	O2-C2-C3-O3
18	M	800	CDL	CA5-C11-C12-C13
13	M	911	LDA	C11-C10-C9-C8
5	M	401	BPH	C10-C11-C12-C13
4	M	601	BCL	C6-C7-C8-C10
7	L	503	UQ1	C3-C2-O2-CM2
7	L	503	UQ1	C2-C3-O3-CM3
6	M	501[A]	U10	C29-C31-C32-C33
13	L	905	LDA	C5-C6-C7-C8
18	M	800	CDL	O1-C1-CA2-OA2
4	M	601	BCL	C5-C6-C7-C8
4	M	601	BCL	C8-C10-C11-C12
18	M	800	CDL	C11-CA5-OA6-CA4
4	M	601	BCL	C10-C11-C12-C13
18	M	800	CDL	OA7-CA5-OA6-CA4
6	L	502[B]	U10	C20-C19-C21-C22
6	L	502[A]	U10	C20-C19-C21-C22
18	M	800	CDL	C38-C39-C40-C41
13	H	910	LDA	C3-C4-C5-C6
13	L	914	LDA	C2-C3-C4-C5
13	H	910	LDA	C7-C8-C9-C10
13	M	916	LDA	C7-C8-C9-C10
13	L	913	LDA	C5-C6-C7-C8
18	M	800	CDL	C19-C20-C21-C22
13	L	913	LDA	C7-C8-C9-C10
13	L	904	LDA	C4-C5-C6-C7
5	M	401	BPH	C14-C13-C15-C16
13	L	917	LDA	C11-C10-C9-C8
18	M	800	CDL	C71-C72-C73-C74
13	L	908	LDA	C4-C5-C6-C7
13	M	911	LDA	C3-C4-C5-C6
13	M	918	LDA	C11-C10-C9-C8
13	H	910	LDA	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	H	729	GOL	C1-C2-C3-O3
10	M	740	GOL	O1-C1-C2-C3
10	H	745	GOL	O1-C1-C2-C3
10	M	742	GOL	C1-C2-C3-O3
10	L	724	GOL	O1-C1-C2-C3
10	H	746	GOL	C1-C2-C3-O3
10	L	722	GOL	C1-C2-C3-O3
10	L	727	GOL	O1-C1-C2-C3
10	H	738	GOL	O1-C1-C2-C3
10	L	725	GOL	O1-C1-C2-C3
10	L	725	GOL	C1-C2-C3-O3
13	L	915	LDA	C2-C3-C4-C5
13	L	904	LDA	C3-C4-C5-C6
13	L	902	LDA	C5-C6-C7-C8
4	M	601	BCL	C16-C17-C18-C20
13	L	904	LDA	C7-C8-C9-C10
13	L	921	LDA	C7-C8-C9-C10
13	L	908	LDA	C7-C8-C9-C10
18	M	800	CDL	CB3-CB4-CB6-OB8
5	L	402	BPH	C4-C3-C5-C6
6	M	501[B]	U10	C28-C29-C31-C32
13	L	908	LDA	C11-C10-C9-C8
10	H	729	GOL	O2-C2-C3-O3
10	L	730	GOL	O1-C1-C2-O2
10	M	737	GOL	O1-C1-C2-O2
10	M	740	GOL	O2-C2-C3-O3
10	H	735	GOL	O1-C1-C2-O2
10	L	724	GOL	O2-C2-C3-O3
10	L	722	GOL	O2-C2-C3-O3
13	L	913	LDA	C6-C7-C8-C9
13	M	916	LDA	C11-C10-C9-C8
13	M	903	LDA	C3-C4-C5-C6
13	L	913	LDA	C1-C2-C3-C4
13	L	917	LDA	C1-C2-C3-C4
4	M	601	BCL	C2-C1-O2A-CGA
13	L	902	LDA	C1-C2-C3-C4
13	H	909	LDA	C2-C3-C4-C5
13	M	912	LDA	C5-C6-C7-C8
13	H	909	LDA	C4-C5-C6-C7
13	L	917	LDA	C5-C6-C7-C8
13	H	901	LDA	C5-C6-C7-C8
5	L	402	BPH	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	M	800	CDL	C12-C13-C14-C15
18	M	800	CDL	C31-C32-C33-C34
13	H	906	LDA	C3-C4-C5-C6
4	M	601	BCL	C13-C15-C16-C17
13	H	901	LDA	C1-C2-C3-C4
6	M	501[B]	U10	C30-C29-C31-C32
6	L	502[B]	U10	C18-C19-C21-C22
6	L	502[A]	U10	C18-C19-C21-C22
13	M	916	LDA	C5-C6-C7-C8
4	M	601	BCL	C6-C7-C8-C9
18	M	800	CDL	C18-C19-C20-C21
13	M	912	LDA	C6-C7-C8-C9
4	M	601	BCL	C16-C17-C18-C19
13	L	921	LDA	C4-C5-C6-C7
13	L	908	LDA	C3-C4-C5-C6
13	M	916	LDA	C2-C3-C4-C5
13	L	914	LDA	C6-C7-C8-C9
13	M	907	LDA	C4-C5-C6-C7
18	M	800	CDL	C72-C73-C74-C75
18	M	800	CDL	C78-C79-C80-C81
5	M	401	BPH	C2C-C3C-CAC-CBC
13	H	901	LDA	C6-C7-C8-C9
13	M	912	LDA	C4-C5-C6-C7
13	L	905	LDA	C9-C10-C11-C12
15	M	600	SPO	C4-C1-O1-CM1
6	M	501[A]	U10	C34-C36-C37-C38
10	M	740	GOL	O1-C1-C2-O2
10	M	742	GOL	O2-C2-C3-O3
10	H	738	GOL	O1-C1-C2-O2
10	H	736	GOL	O1-C1-C2-O2
13	L	904	LDA	C1-C2-C3-C4
5	M	401	BPH	C2B-C3B-CAB-CBB
18	M	800	CDL	CB6-CB4-OB6-CB5
13	L	904	LDA	C9-C10-C11-C12
13	L	914	LDA	C9-C10-C11-C12
18	M	800	CDL	C11-C12-C13-C14
13	L	921	LDA	C11-C10-C9-C8
15	M	600	SPO	C3-C1-O1-CM1
6	M	501[A]	U10	C50-C49-C51-C52
5	M	401	BPH	C11-C12-C13-C14
13	L	920	LDA	C1-C2-C3-C4
10	M	741	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	902	LDA	N1-C1-C2-C3
13	H	910	LDA	N1-C1-C2-C3
13	L	914	LDA	N1-C1-C2-C3
13	M	918	LDA	C3-C4-C5-C6
13	M	918	LDA	C4-C5-C6-C7
18	M	800	CDL	C36-C37-C38-C39
13	M	911	LDA	C6-C7-C8-C9
18	M	800	CDL	OB5-CB3-CB4-CB6
6	L	502[B]	U10	C15-C14-C16-C17
6	L	502[A]	U10	C15-C14-C16-C17
6	M	501[A]	U10	C48-C49-C51-C52
13	H	906	LDA	C7-C8-C9-C10
13	L	921	LDA	C3-C4-C5-C6
11	L	751	HT3	O1-C1-C2-C3
13	L	913	LDA	C11-C10-C9-C8
13	M	907	LDA	C1-C2-C3-C4
10	H	746	GOL	O2-C2-C3-O3
7	L	503	UQ1	C4-C3-O3-CM3
13	M	916	LDA	C9-C10-C11-C12
13	L	902	LDA	C7-C8-C9-C10
6	M	501[B]	U10	C24-C26-C27-C28
6	M	501[B]	U10	C39-C41-C42-C43
18	M	800	CDL	C16-C17-C18-C19
18	M	800	CDL	C1-CB2-OB2-PB2
13	H	906	LDA	C6-C7-C8-C9
13	L	914	LDA	C5-C6-C7-C8
13	L	913	LDA	C9-C10-C11-C12
6	L	502[B]	U10	C13-C14-C16-C17
6	L	502[A]	U10	C13-C14-C16-C17
18	M	800	CDL	C40-C41-C42-C43
5	M	401	BPH	C4B-C3B-CAB-OBB
13	H	901	LDA	C2-C3-C4-C5
13	H	909	LDA	C7-C8-C9-C10
13	M	912	LDA	C2-C3-C4-C5
5	M	401	BPH	C2B-C3B-CAB-OBB
13	L	917	LDA	C3-C4-C5-C6
13	L	905	LDA	C3-C4-C5-C6
13	H	901	LDA	C3-C4-C5-C6
18	M	800	CDL	C53-C54-C55-C56
4	L	604	BCL	CAD-CBD-CGD-O2D
12	L	753	HTO	C3-C4-C5-C6
4	M	601	BCL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	921	LDA	C2-C1-N1-CM2
13	L	913	LDA	C2-C1-N1-CM1
13	L	908	LDA	C2-C1-N1-CM1
13	L	908	LDA	C2-C1-N1-CM2
13	M	912	LDA	C2-C1-N1-CM2
13	H	906	LDA	C2-C1-N1-CM2
10	L	732	GOL	O2-C2-C3-O3
10	H	746	GOL	O1-C1-C2-O2
10	M	726	GOL	O2-C2-C3-O3
10	L	727	GOL	O1-C1-C2-O2
13	L	919	LDA	C9-C10-C11-C12
6	M	501[B]	U10	C35-C34-C36-C37
18	M	800	CDL	C76-C77-C78-C79
6	M	501[B]	U10	C33-C34-C36-C37
13	M	916	LDA	C3-C4-C5-C6
13	H	910	LDA	C5-C6-C7-C8
5	M	401	BPH	C16-C17-C18-C19
18	M	800	CDL	OA5-CA3-CA4-CA6
13	H	910	LDA	C2-C1-N1-O1
13	M	903	LDA	C2-C1-N1-O1
13	M	907	LDA	C9-C10-C11-C12
13	L	919	LDA	C6-C7-C8-C9
4	M	601	BCL	C11-C12-C13-C15
18	M	800	CDL	CB7-C71-C72-C73
12	H	752	HTO	O3-C3-C4-C5
13	L	902	LDA	C4-C5-C6-C7
18	M	800	CDL	OB6-CB4-CB6-OB8
13	M	916	LDA	C6-C7-C8-C9
10	L	725	GOL	O2-C2-C3-O3
13	L	917	LDA	C6-C7-C8-C9
7	L	503	UQ1	C1-C2-O2-CM2
13	L	920	LDA	C2-C3-C4-C5
4	L	602	BCL	C2-C1-O2A-CGA
18	M	800	CDL	C32-C31-CA7-OA8
11	L	751	HT3	O2-C2-C3-O3
15	M	600	SPO	C2-C1-O1-CM1
18	M	800	CDL	CA2-OA2-PA1-OA5
18	M	800	CDL	CB2-OB2-PB2-OB5
4	M	601	BCL	C11-C10-C8-C9
4	M	601	BCL	C11-C12-C13-C14
13	M	918	LDA	C1-C2-C3-C4
13	M	912	LDA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	M	401	BPH	C16-C17-C18-C20
5	L	402	BPH	C8-C10-C11-C12
10	L	724	GOL	O1-C1-C2-O2
4	M	603	BCL	CAA-CBA-CGA-O2A
18	M	800	CDL	C15-C16-C17-C18
6	M	501[B]	U10	C5-C4-O4-C4M
6	M	501[A]	U10	C5-C4-O4-C4M
11	L	751	HT3	C1-C2-C3-O3
5	M	401	BPH	C12-C13-C15-C16
4	L	604	BCL	C13-C15-C16-C17
13	L	919	LDA	C5-C6-C7-C8
6	M	501[A]	U10	C25-C24-C26-C27
13	L	902	LDA	C11-C10-C9-C8
18	M	800	CDL	OA9-CA7-OA8-CA6
10	H	746	GOL	O1-C1-C2-C3
10	M	726	GOL	C1-C2-C3-O3
13	L	919	LDA	C2-C3-C4-C5
6	L	502[B]	U10	C40-C39-C41-C42
6	L	502[B]	U10	C25-C24-C26-C27
6	L	502[B]	U10	C45-C44-C46-C47
6	L	502[A]	U10	C25-C24-C26-C27
13	M	903	LDA	C2-C3-C4-C5
10	L	733	GOL	O1-C1-C2-O2
12	L	753	HTO	C4-C5-C6-C7
18	M	800	CDL	C31-CA7-OA8-CA6
4	M	601	BCL	CAD-CBD-CGD-O2D
4	L	602	BCL	CAD-CBD-CGD-O2D
5	M	401	BPH	CAD-CBD-CGD-O2D
13	L	915	LDA	C4-C5-C6-C7
6	L	502[B]	U10	C43-C44-C46-C47
13	M	911	LDA	C1-C2-C3-C4
13	L	921	LDA	C6-C7-C8-C9
13	L	908	LDA	C2-C3-C4-C5
18	M	800	CDL	C39-C40-C41-C42
5	L	402	BPH	O2A-C1-C2-C3
13	M	918	LDA	C9-C10-C11-C12
13	M	907	LDA	C2-C1-N1-CM2
13	L	917	LDA	C2-C1-N1-CM1
10	M	726	GOL	O1-C1-C2-O2
13	L	904	LDA	C5-C6-C7-C8
13	L	913	LDA	C3-C4-C5-C6
6	L	502[B]	U10	C49-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	H	752	HTO	C2-C3-C4-C5
6	L	502[B]	U10	C31-C32-C33-C34
6	L	502[A]	U10	C31-C32-C33-C34
6	L	502[A]	U10	C46-C47-C48-C49
10	L	732	GOL	C1-C2-C3-O3
10	L	733	GOL	O1-C1-C2-C3
13	L	905	LDA	C4-C5-C6-C7
13	M	911	LDA	C4-C5-C6-C7
18	M	800	CDL	CA2-OA2-PA1-OA4
5	L	402	BPH	C2B-C3B-CAB-OBB
13	M	907	LDA	C2-C1-N1-O1
13	L	908	LDA	C2-C1-N1-O1
13	H	906	LDA	C2-C1-N1-O1
10	H	721	GOL	O2-C2-C3-O3
4	L	604	BCL	C12-C13-C15-C16
13	L	914	LDA	C7-C8-C9-C10
13	L	917	LDA	C4-C5-C6-C7

There are no ring outliers.

39 monomers are involved in 108 short contacts:

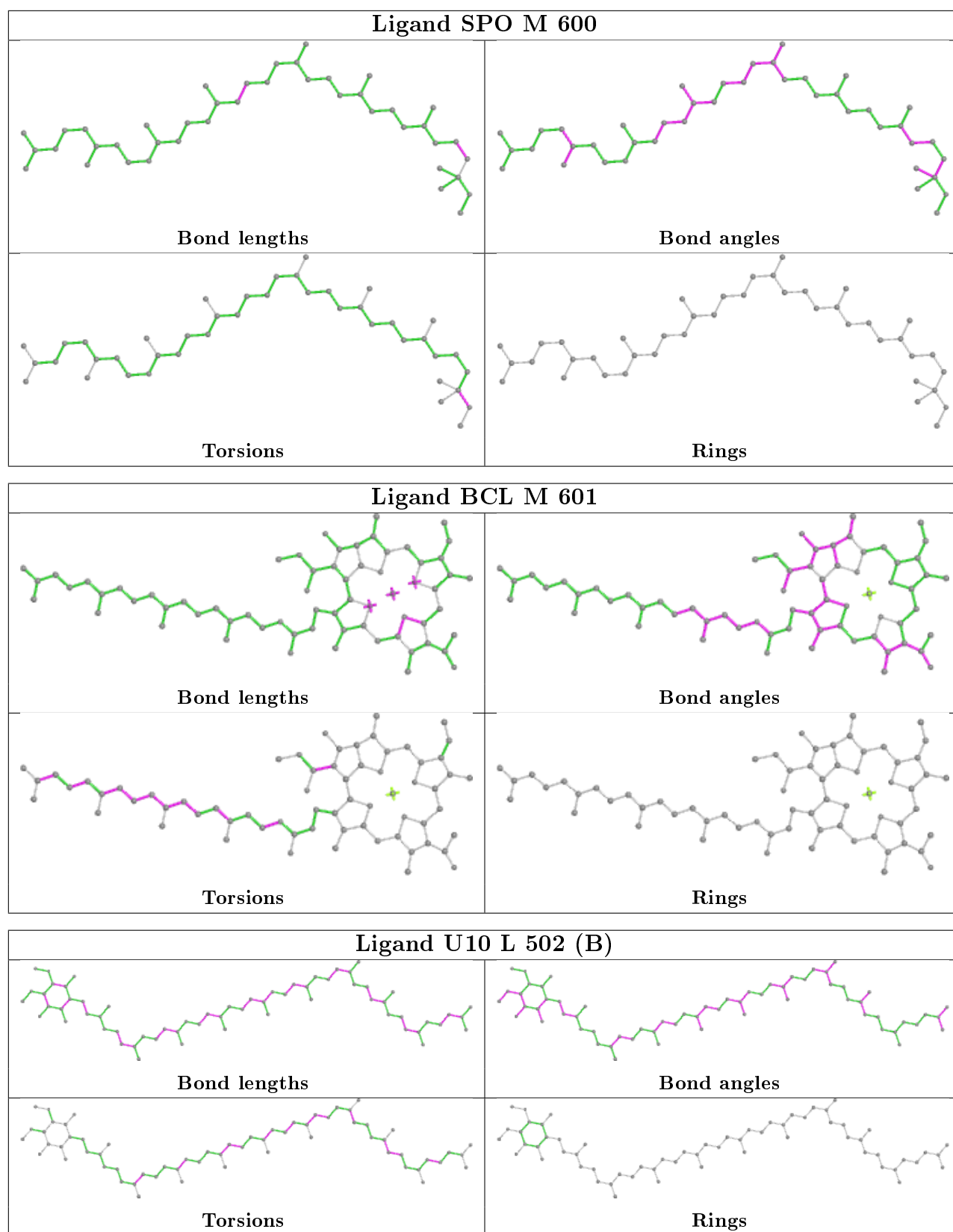
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	920	LDA	4	0
10	H	729	GOL	1	0
13	L	915	LDA	1	0
15	M	600	SPO	1	0
13	L	902	LDA	4	0
4	M	601	BCL	6	0
6	L	502[B]	U10	5	0
13	L	917	LDA	2	0
6	M	501[B]	U10	6	0
10	M	740	GOL	2	0
13	M	918	LDA	2	0
13	L	921	LDA	11	0
6	L	502[A]	U10	9	0
10	L	728	GOL	2	0
13	H	909	LDA	2	0
13	H	906	LDA	4	0
10	H	739	GOL	2	0
10	L	724	GOL	1	0
18	M	800	CDL	9	0
7	L	503	UQ1	13	0

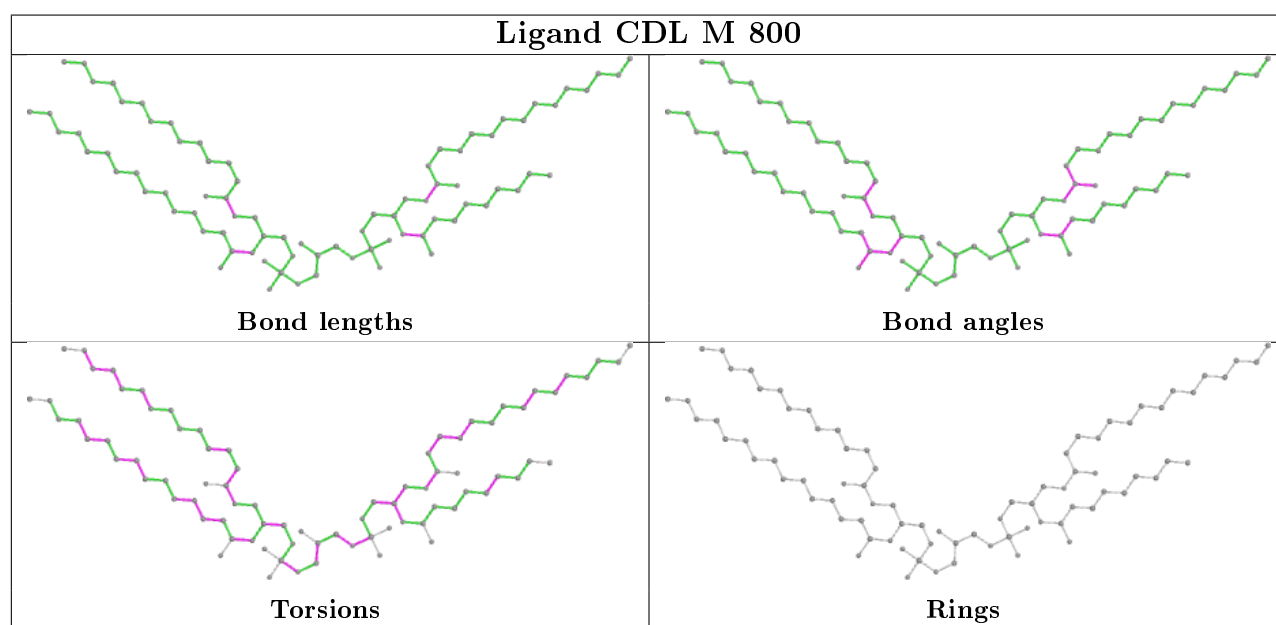
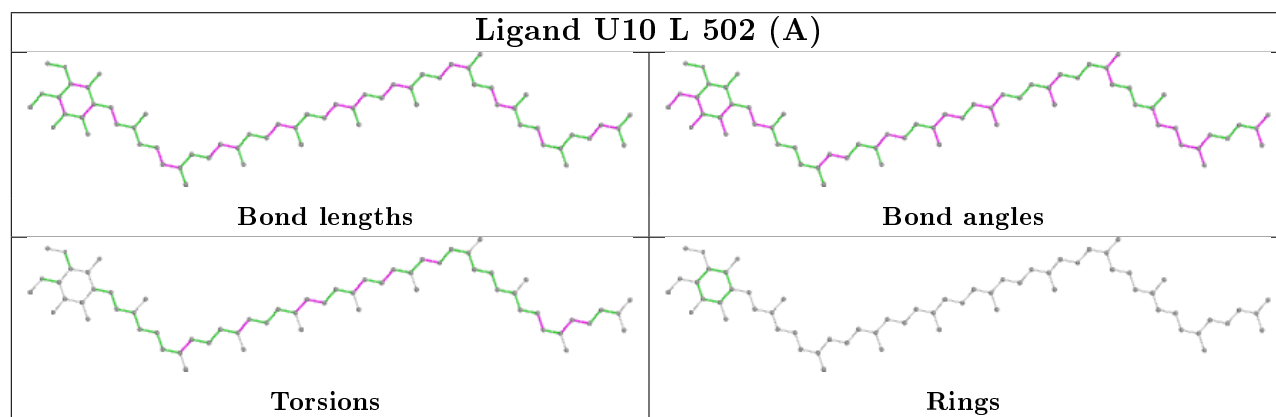
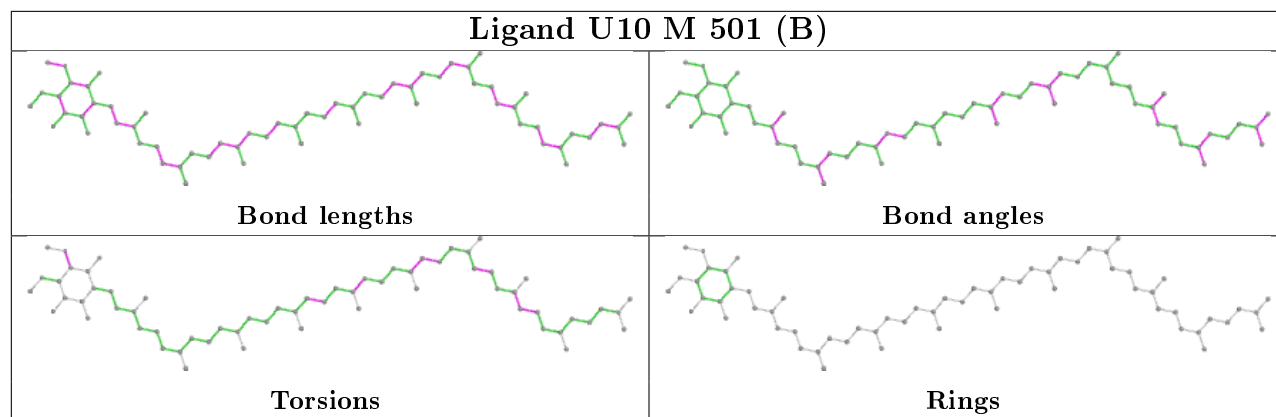
Continued on next page...

Continued from previous page...

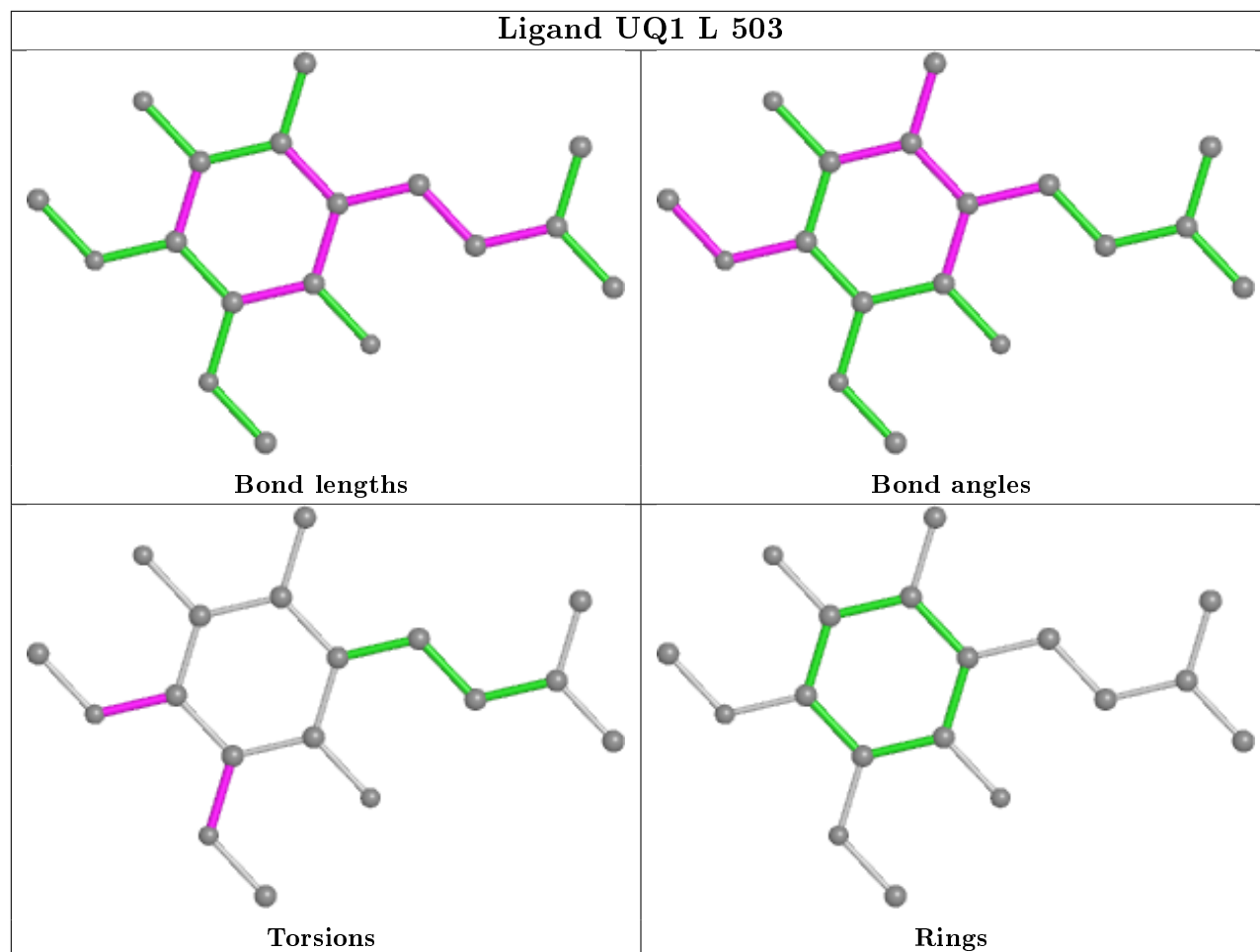
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	708	PO4	1	0
13	L	905	LDA	2	0
4	M	603	BCL	6	0
13	H	910	LDA	6	0
10	M	741	GOL	4	0
6	M	501[A]	U10	1	0
4	L	604	BCL	2	0
10	M	742	GOL	1	0
10	H	738	GOL	1	0
13	L	914	LDA	1	0
13	H	901	LDA	2	0
13	L	908	LDA	1	0
13	M	903	LDA	4	0
4	L	602	BCL	3	0
8	M	707	PO4	1	0
10	L	733	GOL	2	0
5	M	401	BPH	4	0
12	H	752	HTO	3	0
13	L	919	LDA	4	0

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

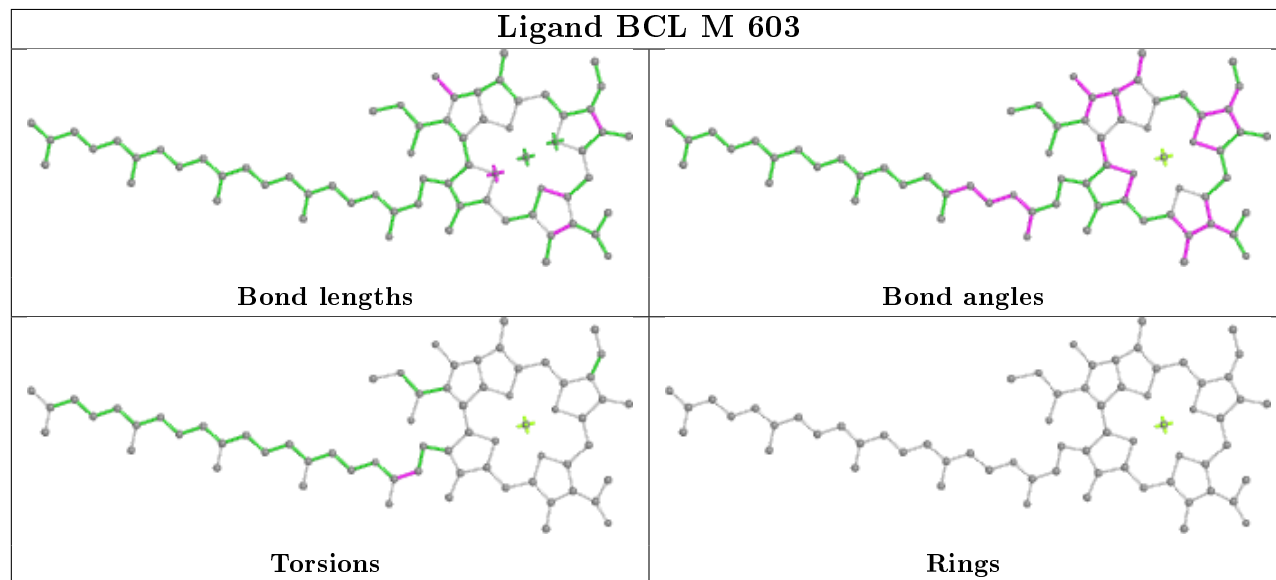




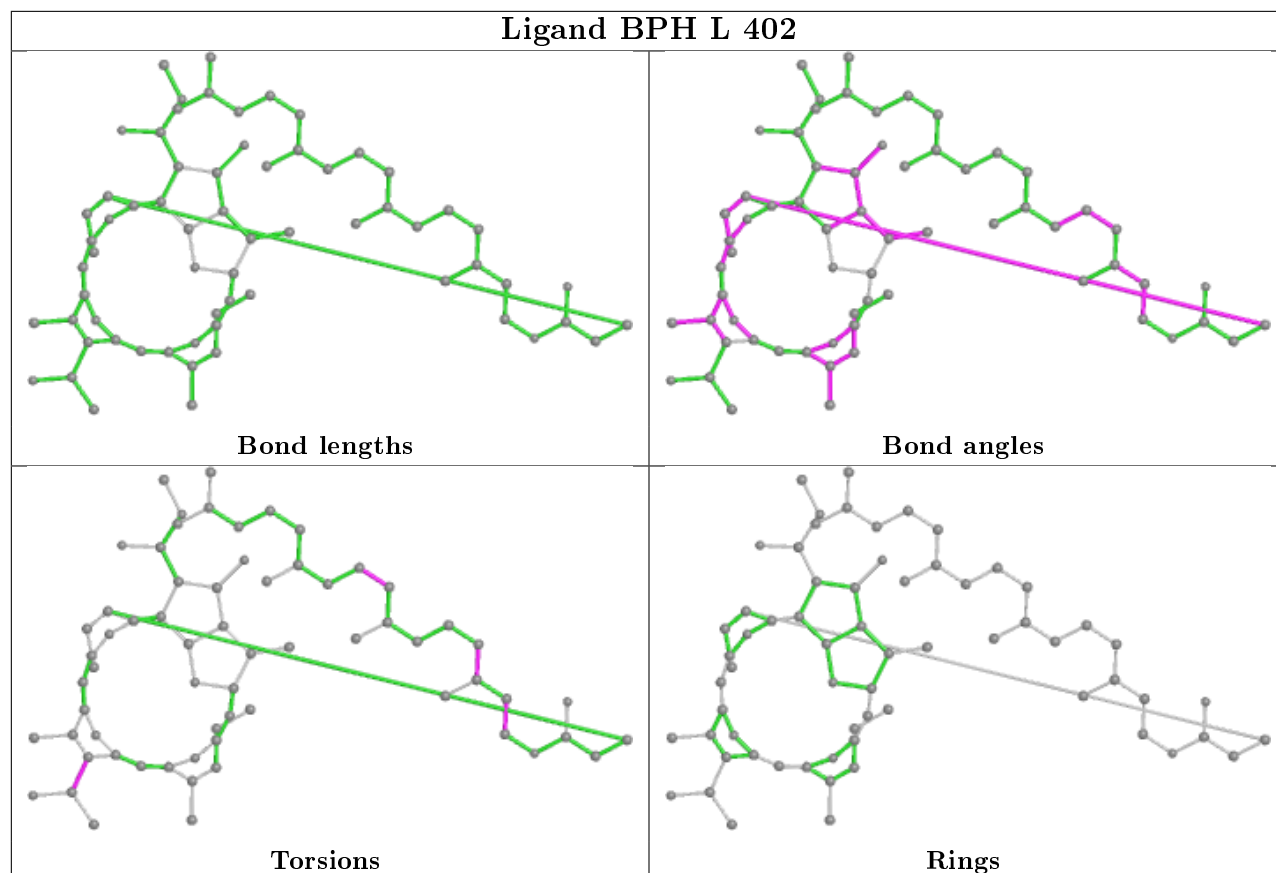
Ligand UQ1 L 503



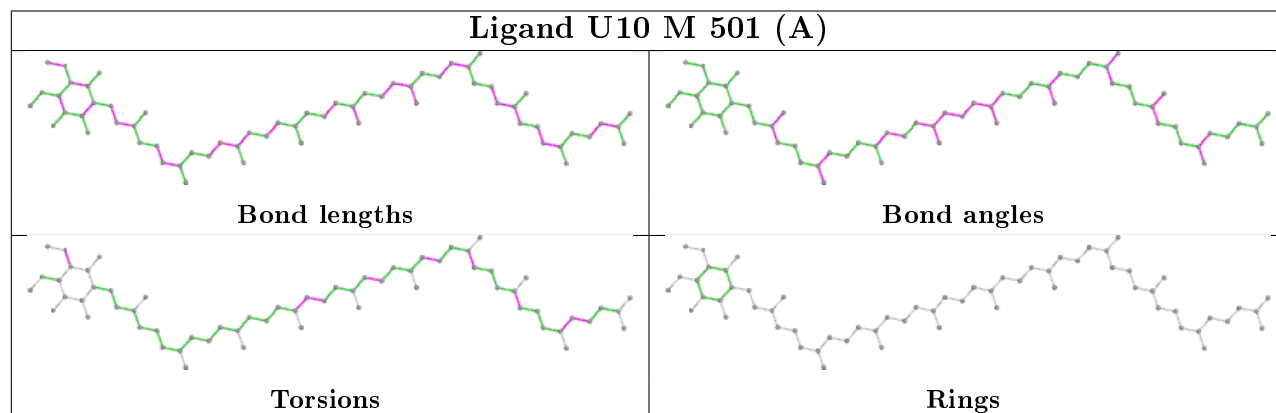
Ligand BCL M 603

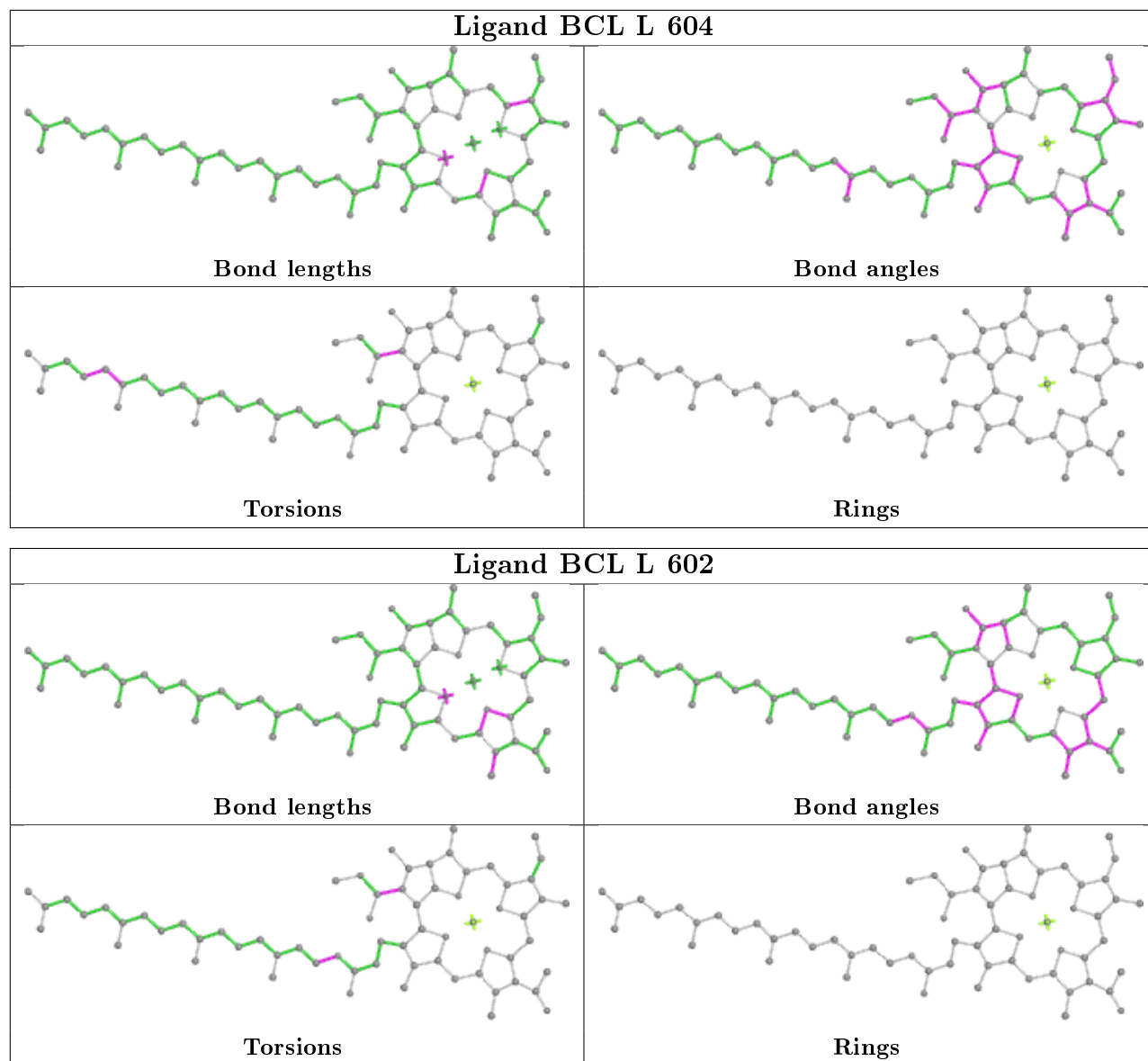


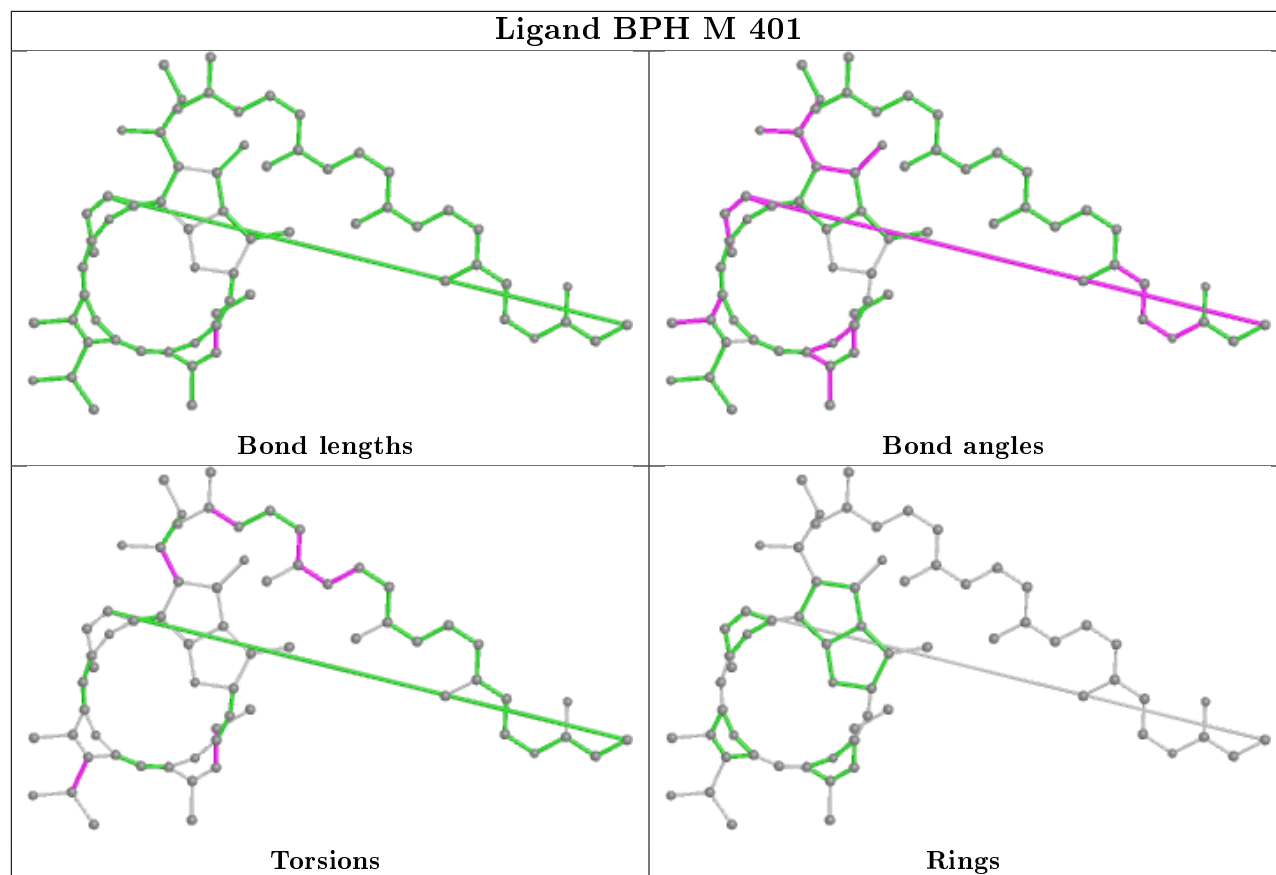
Ligand BPH L 402



Ligand U10 M 501 (A)







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%)	-0.41	7 (2%) 57 56	27, 35, 57, 81	0
2	M	302/307 (98%)	-0.22	13 (4%) 35 34	25, 40, 64, 83	0
3	H	239/260 (91%)	0.01	11 (4%) 32 31	31, 40, 52, 98	0
All	All	822/848 (96%)	-0.22	31 (3%) 40 39	25, 38, 60, 98	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	10	PHE	9.2
2	M	1	ALA	7.0
3	H	246	PRO	5.4
2	M	2	GLU	5.0
3	H	248	ARG	5.0
3	H	245	ALA	4.8
3	H	18	TYR	4.8
2	M	302	GLY	4.3
2	M	3	TYR	3.8
3	H	52	ASN	3.6
3	H	247	LYS	3.5
3	H	220[A]	LYS	3.5
1	L	59	TRP	3.3
1	L	277	GLY	3.1
1	L	279	ILE	3.1
2	M	105	PHE	3.0
2	M	301	HIS	2.8
1	L	270	PRO	2.6
2	M	83	ALA	2.4
3	H	22	ILE	2.4
2	M	100	GLU	2.3
2	M	18	LEU	2.3
1	L	275	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	79	GLY	2.2
2	M	80	TRP	2.2
1	L	202	LYS	2.1
3	H	191	LEU	2.1
2	M	104	SER	2.1
2	M	148	TRP	2.1
1	L	276	PRO	2.1
3	H	179	LEU	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
13	LDA	L	904	16/16	-0.06	0.73	43,50,83,85	16
13	LDA	L	908	16/16	0.04	0.53	44,54,87,88	16
13	LDA	H	910	16/16	0.11	0.63	39,55,79,88	16
13	LDA	M	918	16/16	0.19	0.64	42,57,77,85	16
13	LDA	L	920	16/16	0.32	0.35	47,70,102,104	16
13	LDA	M	916	16/16	0.36	0.41	47,56,79,89	16
13	LDA	L	914	16/16	0.41	0.45	41,54,82,85	16
13	LDA	M	903	16/16	0.44	0.76	46,52,73,82	16
13	LDA	L	917	16/16	0.49	0.33	34,52,77,82	16
13	LDA	L	913	16/16	0.50	0.34	46,55,81,82	16
13	LDA	H	906	16/16	0.50	0.63	48,57,68,72	16
10	GOL	H	745	6/6	0.51	0.31	60,60,61,61	6
10	GOL	L	727	6/6	0.51	0.47	55,56,60,60	6
13	LDA	L	919	16/16	0.51	0.71	46,58,86,93	16
11	HT3	L	751	10/10	0.52	0.27	53,56,58,58	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	LDA	L	902	16/16	0.53	0.51	42,56,83,83	16
7	UQ1	L	503	18/18	0.54	0.40	44,55,60,61	18
13	LDA	L	915	16/16	0.55	0.47	44,59,85,94	16
13	LDA	H	909	16/16	0.55	0.29	46,56,80,83	16
10	GOL	M	741	6/6	0.62	0.29	35,41,42,44	6
13	LDA	L	905	16/16	0.63	0.35	41,54,85,89	16
18	CDL	M	800	81/100	0.63	0.49	32,52,69,72	81
13	LDA	M	912	16/16	0.66	0.31	47,64,94,108	16
10	GOL	L	734	6/6	0.66	0.52	54,56,59,62	6
10	GOL	H	739	6/6	0.66	0.36	57,62,62,62	6
10	GOL	H	746	6/6	0.67	0.27	49,52,54,55	6
10	GOL	L	725	6/6	0.69	0.33	41,55,59,61	6
13	LDA	M	907	16/16	0.70	0.25	40,47,64,65	16
8	PO4	L	708	5/5	0.70	0.40	65,66,67,67	5
10	GOL	H	729	6/6	0.71	0.31	50,57,59,61	6
10	GOL	M	740	6/6	0.72	0.56	59,60,60,61	6
12	HTO	H	752	10/10	0.72	0.45	62,66,67,68	10
10	GOL	L	732	6/6	0.72	1.65	56,57,57,57	6
6	U10	L	502[B]	63/63	0.73	0.33	26,55,59,62	63
6	U10	L	502[A]	63/63	0.73	0.33	26,47,58,59	63
10	GOL	L	733	6/6	0.73	0.58	51,52,52,53	6
10	GOL	M	742	6/6	0.75	0.35	55,56,57,57	6
13	LDA	L	921	16/16	0.76	0.25	44,60,88,99	16
13	LDA	M	911	16/16	0.77	0.33	45,58,92,102	16
10	GOL	H	743	6/6	0.78	0.27	40,52,53,58	6
10	GOL	H	736	6/6	0.79	0.21	61,62,62,62	6
8	PO4	H	709	5/5	0.80	0.35	61,61,63,63	5
10	GOL	L	728	6/6	0.81	0.77	59,62,63,63	6
13	LDA	H	901	16/16	0.81	0.28	45,52,63,70	0
12	HTO	L	753	10/10	0.81	0.35	50,57,58,58	10
10	GOL	L	731	6/6	0.82	0.34	52,55,56,57	6
8	PO4	L	705	5/5	0.84	0.19	47,51,54,56	5
10	GOL	L	744	6/6	0.84	0.26	44,45,46,49	6
8	PO4	L	706	5/5	0.84	0.23	53,57,59,60	5
10	GOL	L	730	6/6	0.87	0.23	56,62,64,66	6
15	SPO	M	600	42/42	0.87	0.19	34,39,74,89	0
10	GOL	H	738	6/6	0.89	0.36	42,45,48,49	6
10	GOL	L	723	6/6	0.90	0.19	39,47,50,55	6
10	GOL	M	726	6/6	0.90	0.23	52,53,54,55	6
8	PO4	M	707	5/5	0.90	0.25	48,53,55,58	5
10	GOL	M	737	6/6	0.90	0.57	62,66,68,70	6
6	U10	M	501[A]	63/63	0.91	0.17	24,38,68,69	31

Continued on next page...

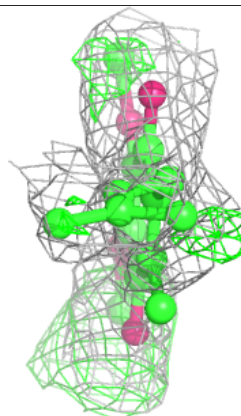
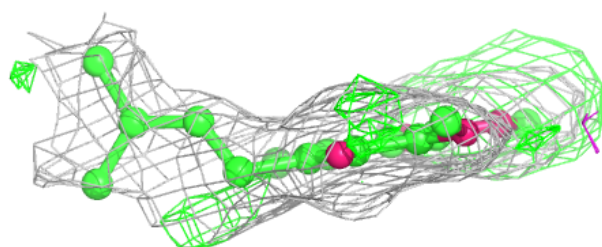
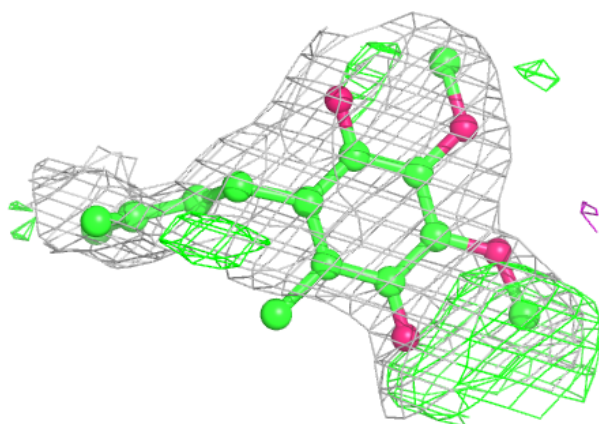
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	U10	M	501[B]	63/63	0.91	0.17	24,40,67,71	31
10	GOL	L	722	6/6	0.91	0.14	47,51,56,62	0
10	GOL	H	735	6/6	0.92	0.34	48,53,54,56	6
10	GOL	L	724	6/6	0.93	0.14	39,41,42,45	6
16	K	M	701	1/1	0.94	0.08	57,57,57,57	0
4	BCL	M	601	66/66	0.94	0.13	28,34,103,107	0
9	DIO	L	711	6/6	0.95	0.20	51,52,53,55	6
5	BPH	L	402	65/65	0.95	0.10	23,28,39,40	0
5	BPH	M	401	65/65	0.95	0.11	29,34,85,86	0
4	BCL	L	602	66/66	0.96	0.10	24,29,39,44	0
8	PO4	L	703	5/5	0.96	0.13	55,62,65,66	0
4	BCL	L	604	66/66	0.96	0.11	24,29,53,57	0
10	GOL	H	721	6/6	0.96	0.16	42,44,49,49	0
4	BCL	M	603	66/66	0.96	0.12	27,31,52,63	0
8	PO4	M	704	5/5	0.97	0.17	56,58,67,67	5
16	K	H	700	1/1	0.98	0.11	48,48,48,48	0
17	CL	M	702	1/1	0.98	0.10	47,47,47,47	0
14	FE	M	500	1/1	1.00	0.01	28,28,28,28	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.

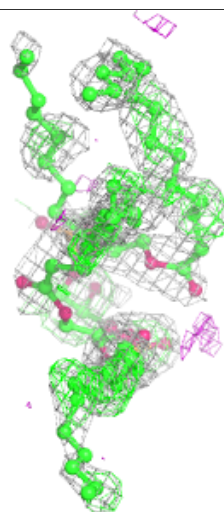
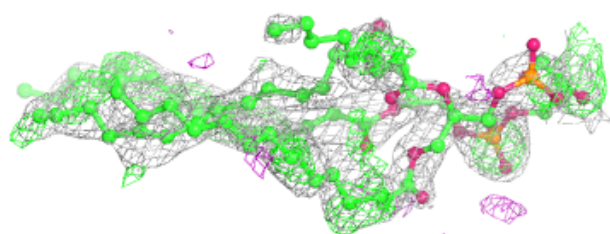
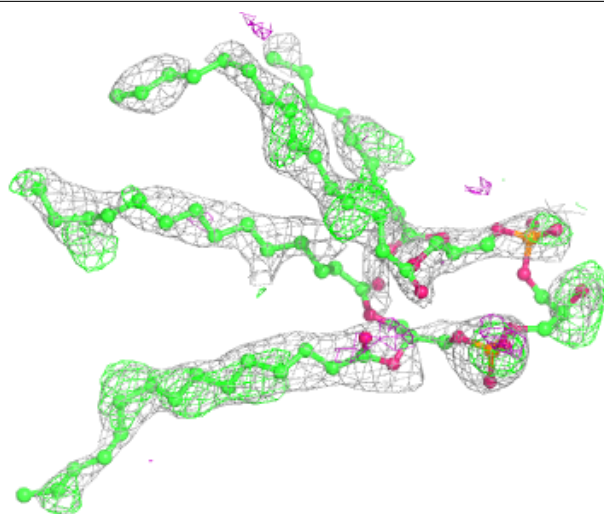
Electron density around UQ1 L 503:

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



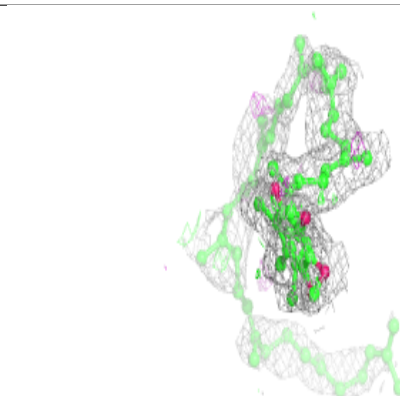
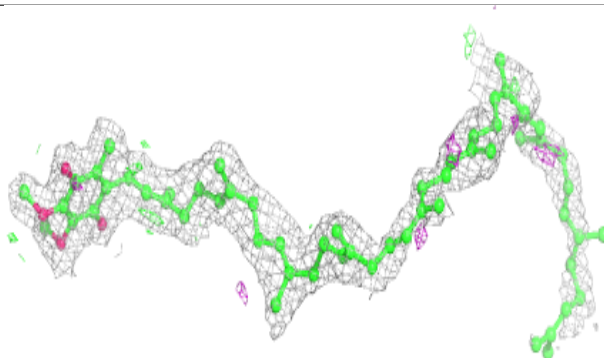
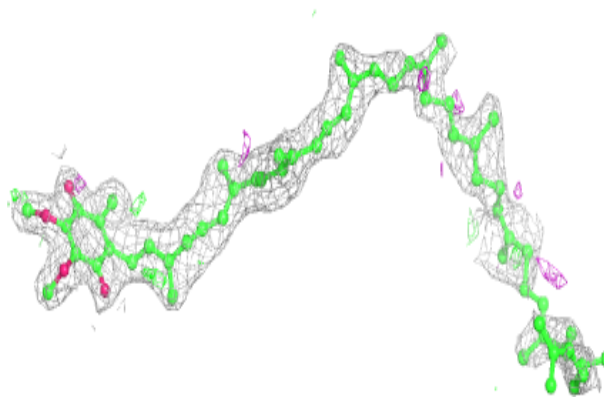
Electron density around CDL M 800:

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

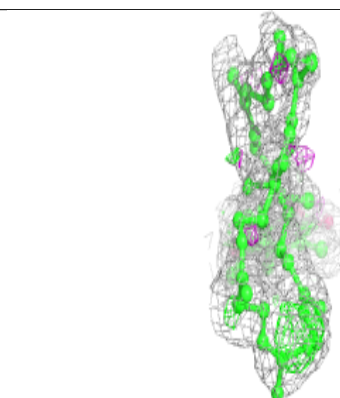
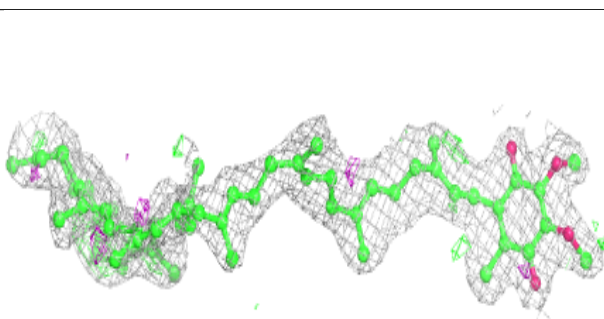
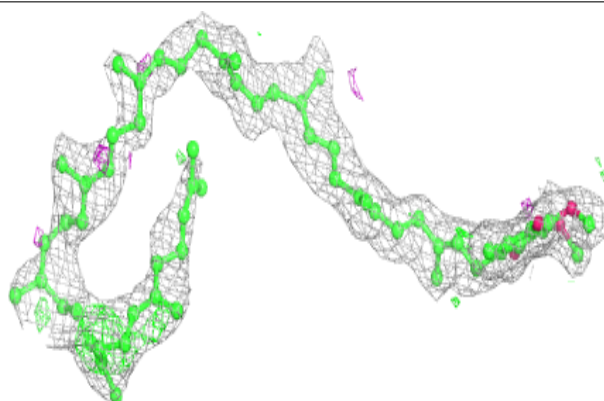


Electron density around U10 L 502 (B):

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

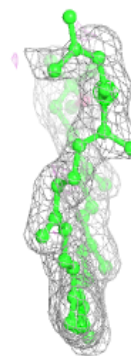
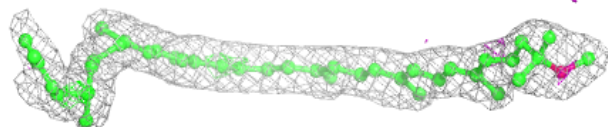
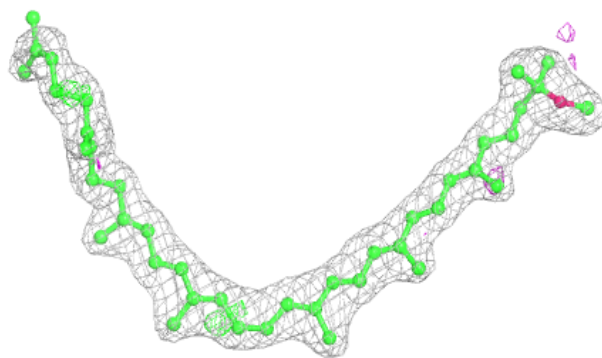
**Electron density around U10 L 502 (A):**

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

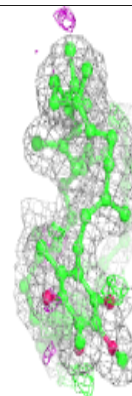
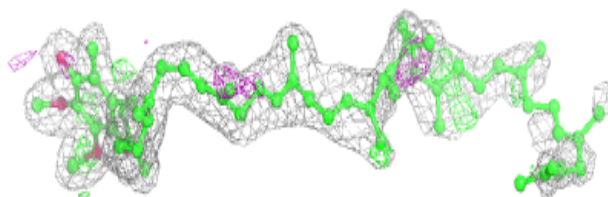
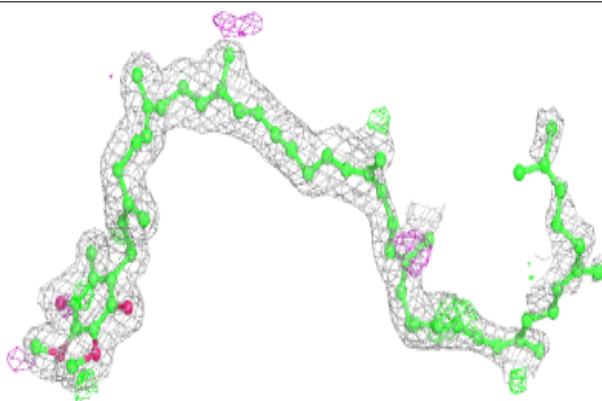


Electron density around SPO M 600:

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

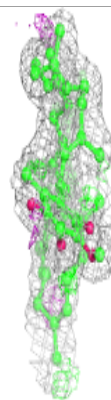
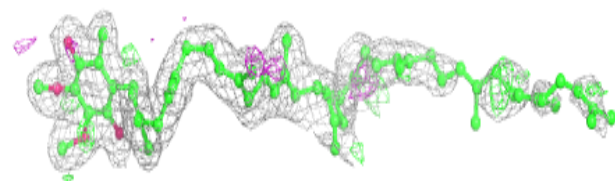
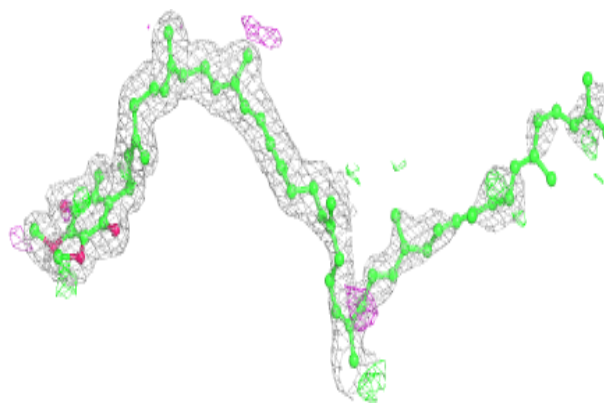
**Electron density around U10 M 501 (A):**

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

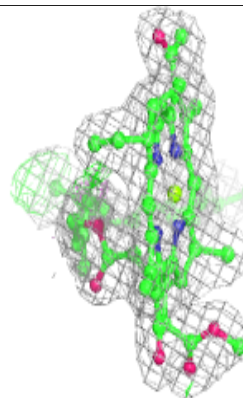
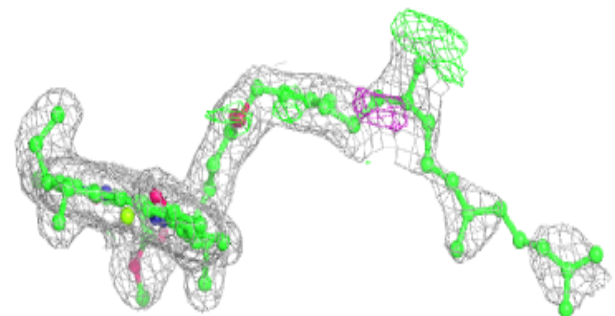
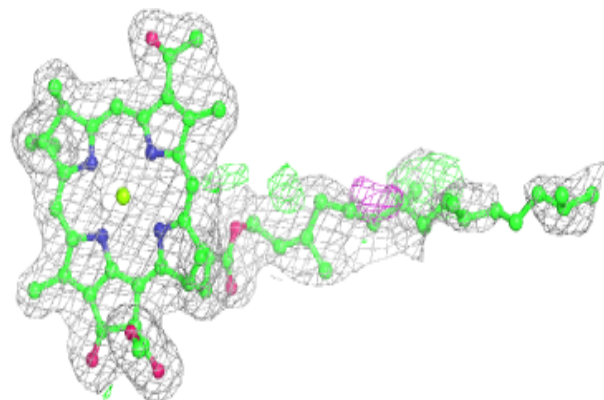


Electron density around U10 M 501 (B):

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

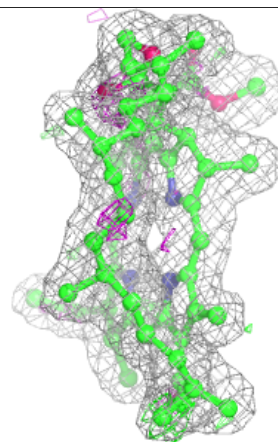
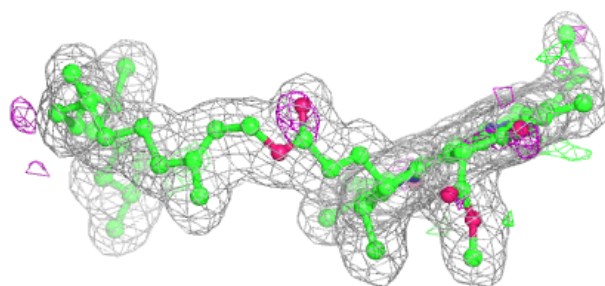
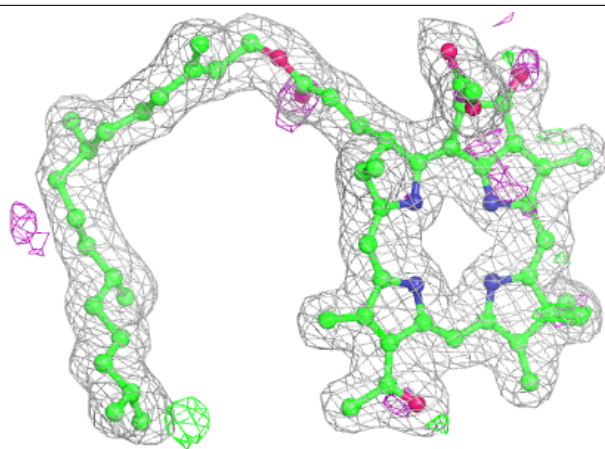
**Electron density around BCL M 601:**

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

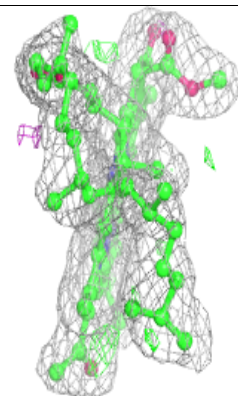
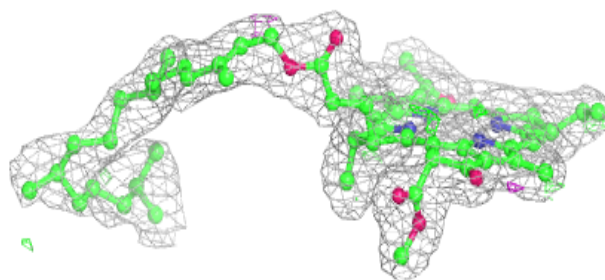
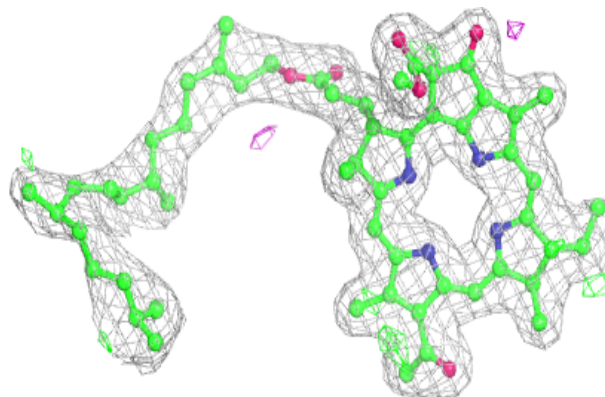


Electron density around BPH L 402:

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

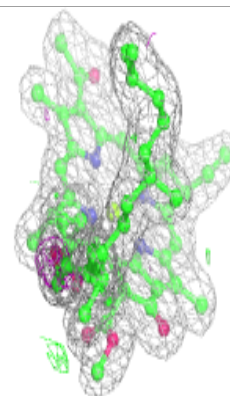
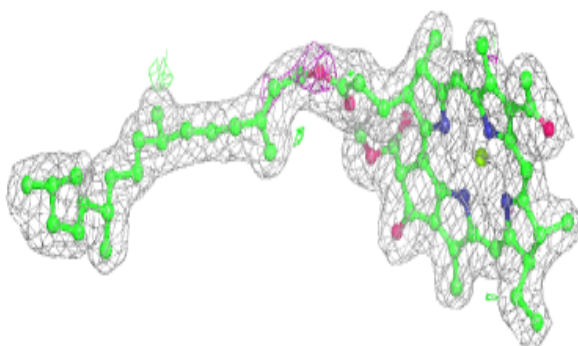
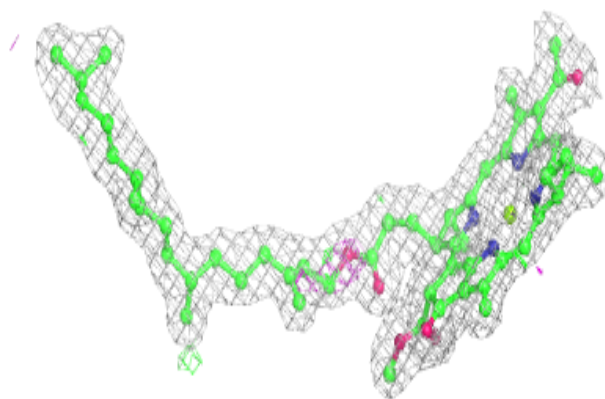
**Electron density around BPH M 401:**

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

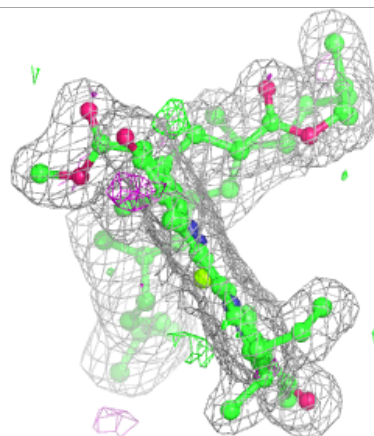
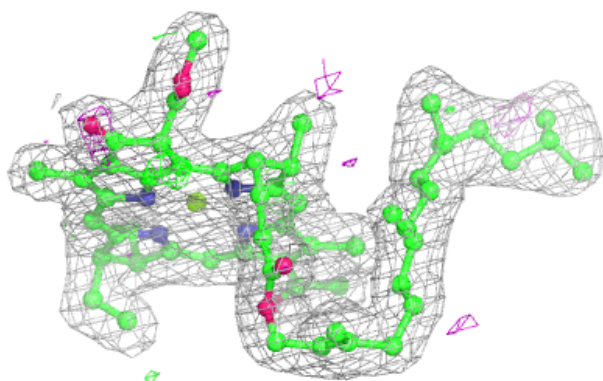
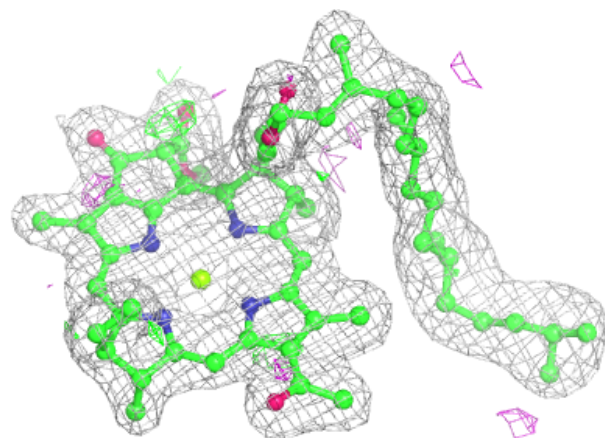


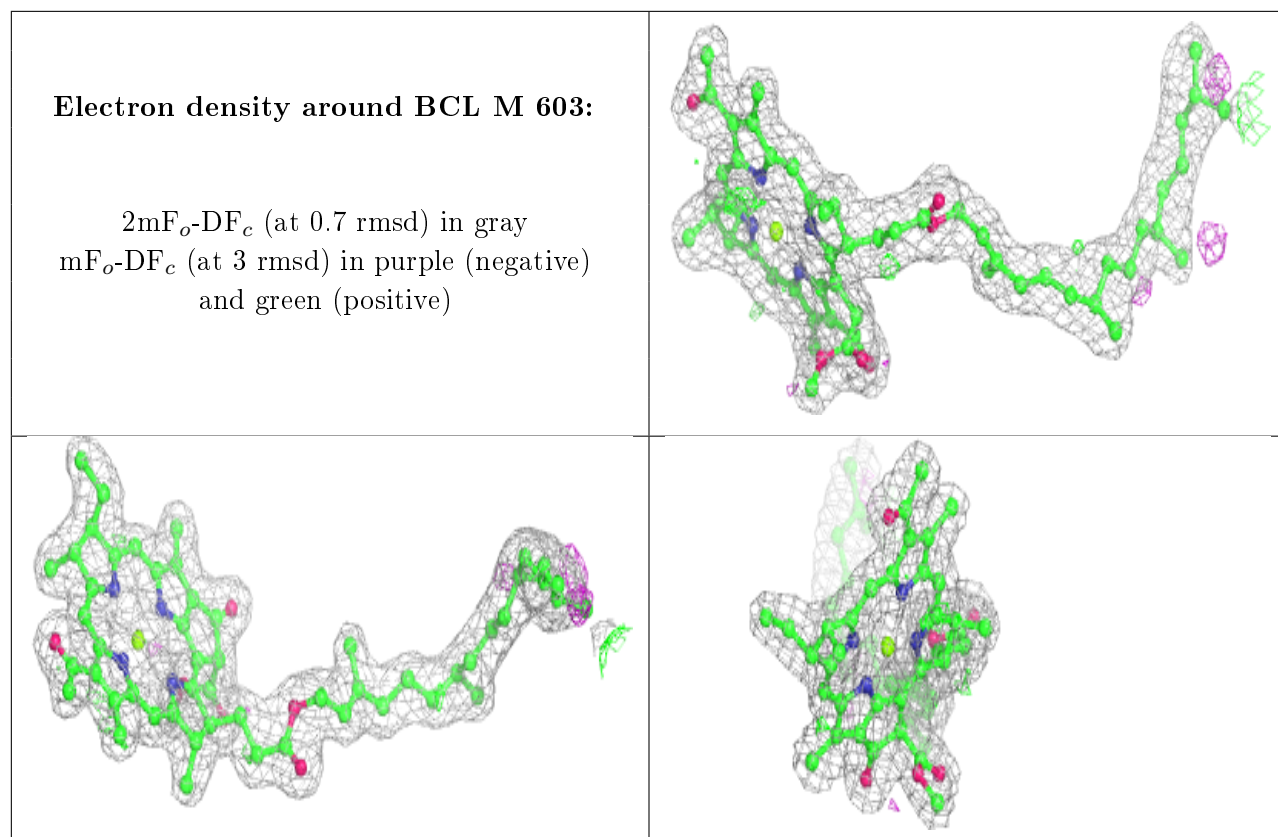
Electron density around BCL L 602:

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

**Electron density around BCL L 604:**

$2mF_o-DF_c$ (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.