Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2024 – 10:40 AM EST

PDB ID	:	2HG3
Title	:	Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with brominated phosphatidylcholine
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2006-06-26
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

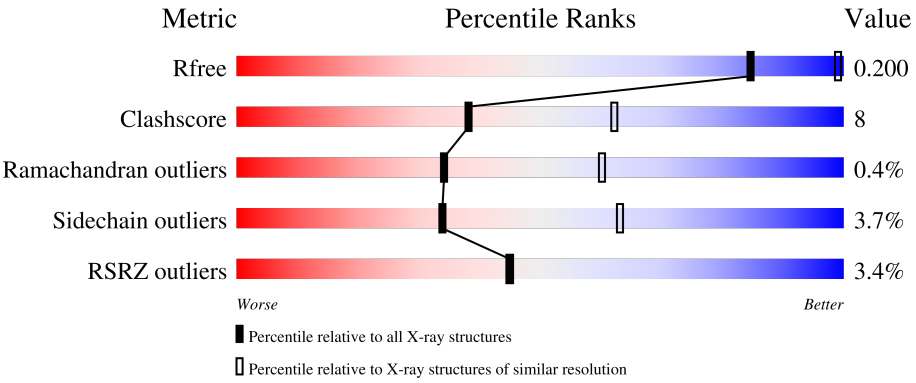
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 91% 9%
2	M	307	4% 84% 14%
3	H	260	2% 82% 9% 8%

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
13	PC9	M	801	-	-	-	X
13	PC9	M	802	-	-	-	X
4	PO4	L	702	-	X	-	-
4	PO4	M	703	-	-	X	-
7	U10	L	502	-	-	-	X
9	LDA	H	901	-	-	-	X
9	LDA	H	902	-	-	-	X
9	LDA	H	903	-	-	-	X
9	LDA	H	904	-	-	-	X
9	LDA	L	905	-	-	-	X
9	LDA	L	906	-	-	-	X
9	LDA	L	908	-	-	-	X
9	LDA	L	909	-	-	-	X
9	LDA	M	920	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7921 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
			Total	C	N	O	S			
1	L	281	2246	1516	357	365	8	0	4	0

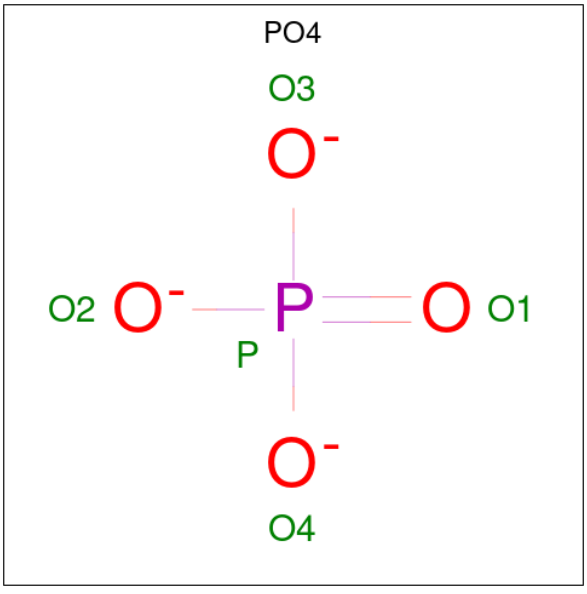
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2477	1654	405	407	11	0	14	0

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

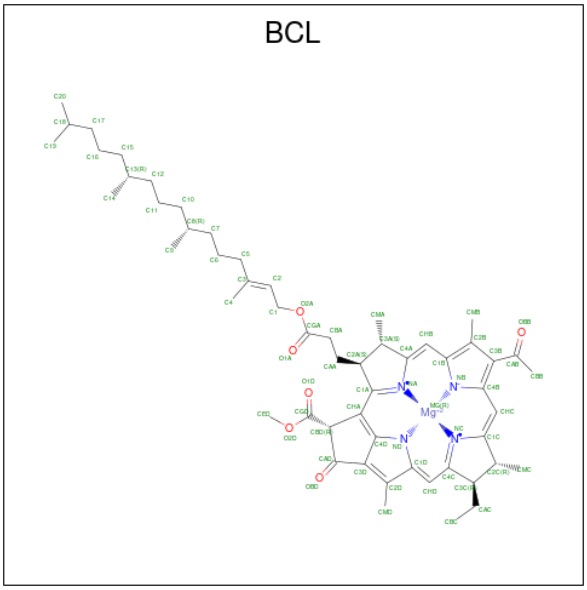
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	240	1851	1181	321	338	11	0	8	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



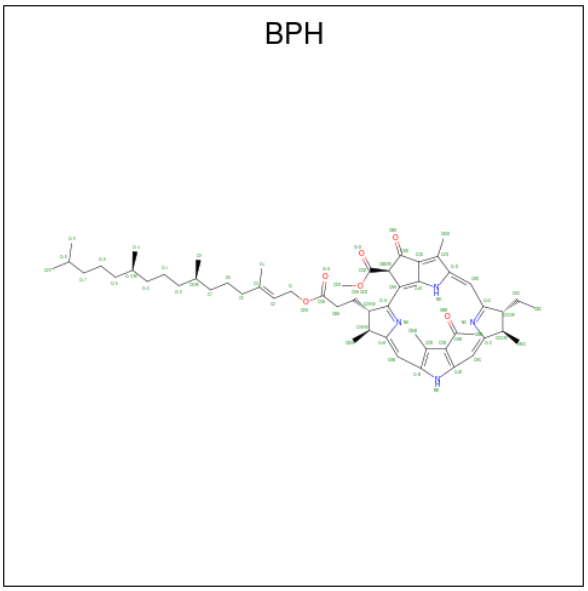
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



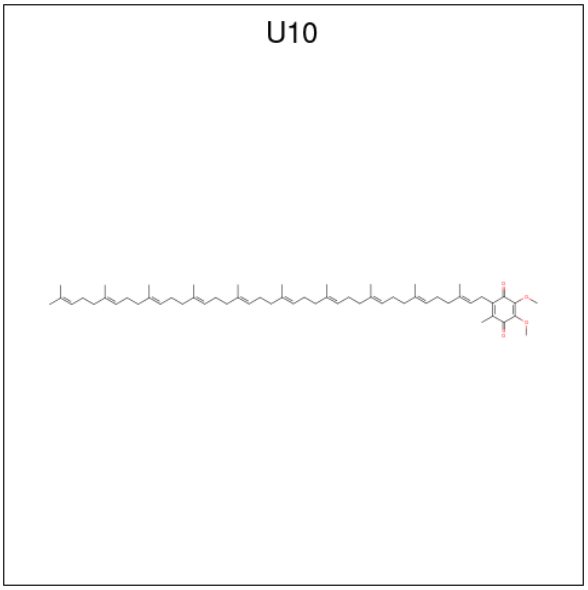
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



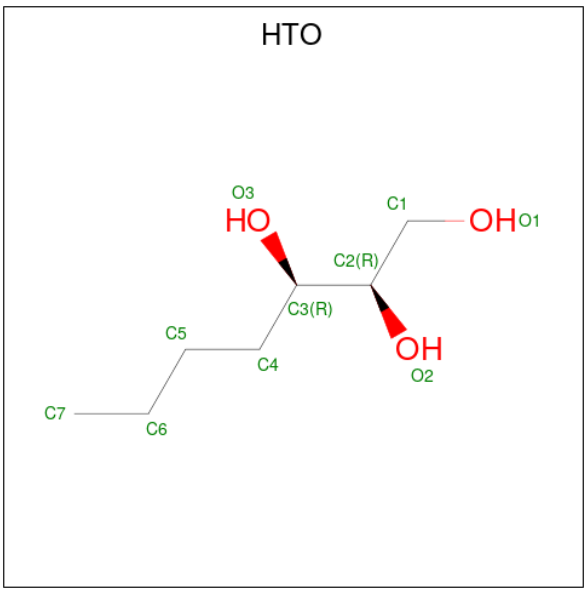
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



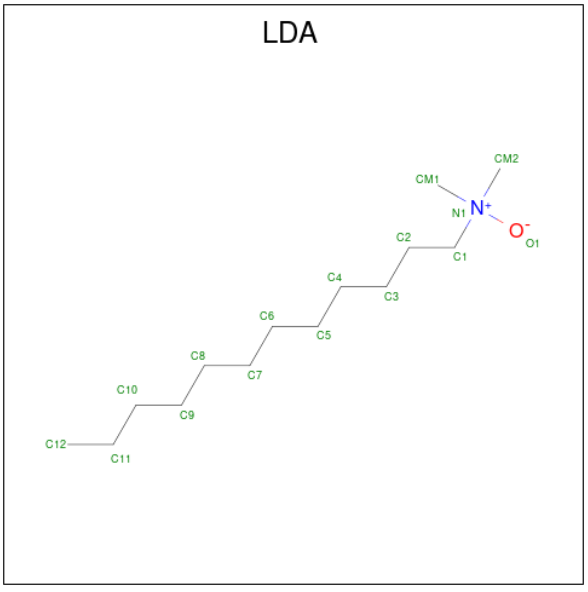
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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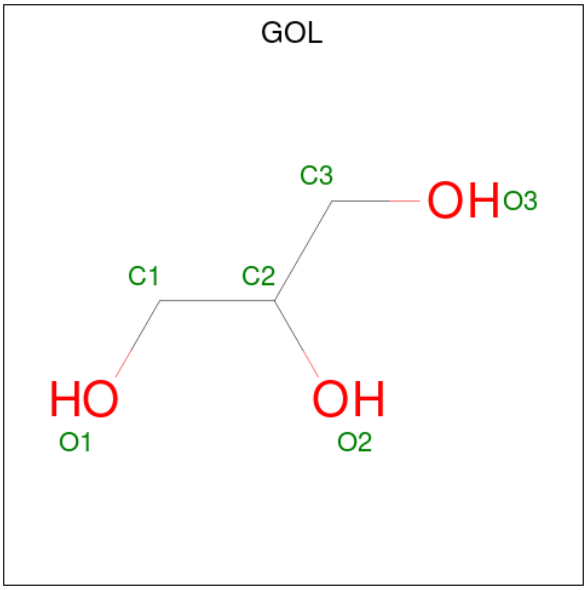
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1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

- 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			

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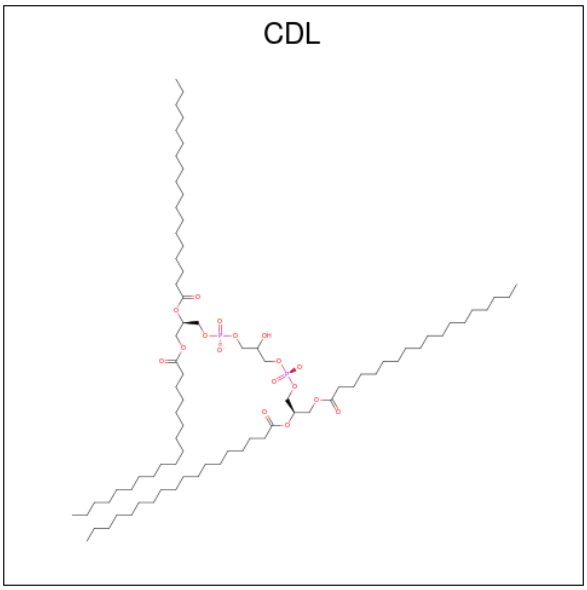
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total C O 6 3 3	0	0
10	H	1	Total C O 6 3 3	0	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

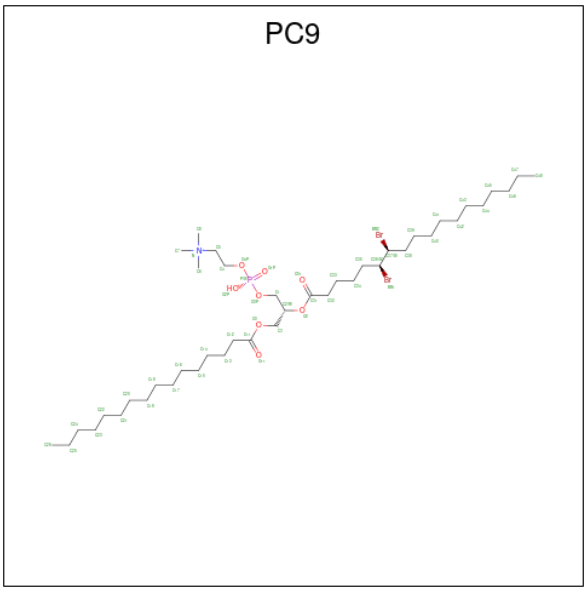
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 13 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC9) (formula: $C_{42}H_{83}Br_2NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	M	1	Total	Br	C	N	O	P	0	0
			54	2	42	1	8	1		
13	M	1	Total	Br	C	N	O	P	0	0
			54	2	42	1	8	1		

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

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

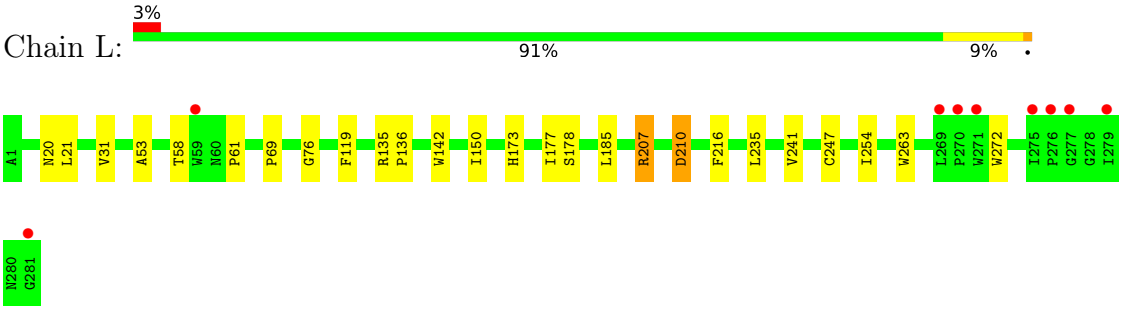
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	104	Total	O	0	0
			104	104		
15	M	141	Total	O	0	0
			141	141		
15	H	207	Total	O	0	0
			207	207		

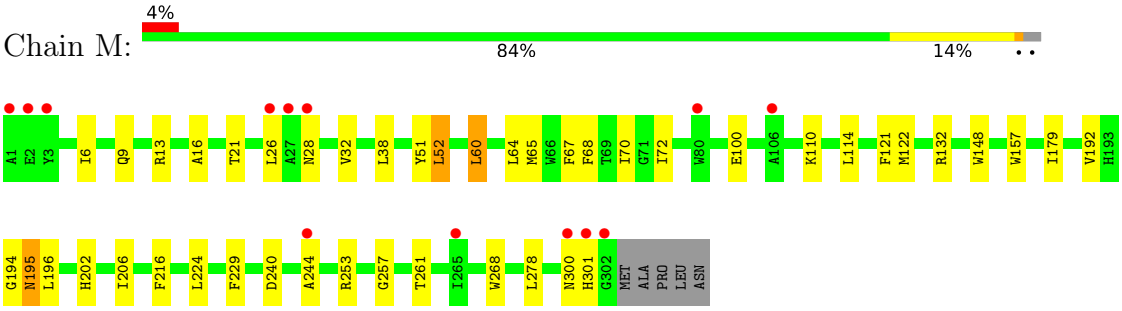
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

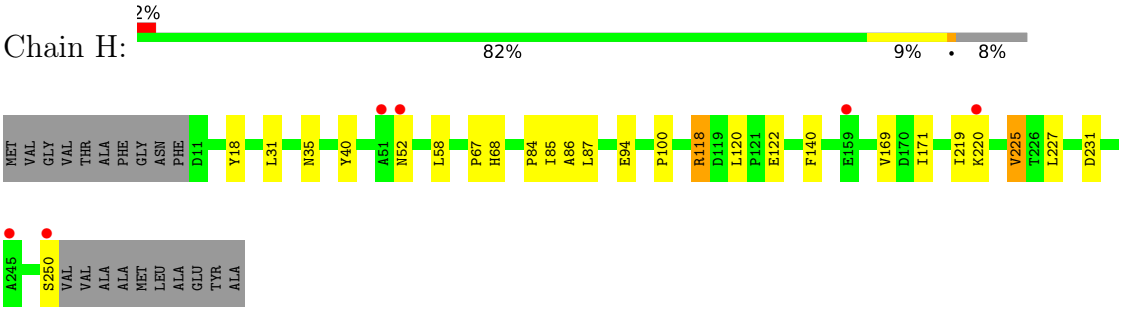
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.84Å 139.84Å 184.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.35 – 2.70 34.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.35-2.70) 99.7 (34.35-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.199 0.169 , 0.200	Depositor DCC
R_{free} test set	2852 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 78.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7921	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: U10, HTO, GOL, PC9, FE, BPH, PO4, LDA, K, CDL, BCL

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	0.85	0/2351	0.77	3/3217 (0.1%)
2	M	0.88	0/2628	0.79	1/3584 (0.0%)
3	H	0.96	2/1945 (0.1%)	0.83	0/2642
All	All	0.89	2/6924 (0.0%)	0.79	4/9443 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.36	1.61	1.51
3	H	94	GLU	CD-OE2	6.10	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	210	ASP	CB-CG-OD1	6.91	124.52	118.30
1	L	207	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	L	207	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	M	240	ASP	CB-CG-OD1	5.16	122.95	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	2246	0	2207	14	0
2	M	2477	0	2389	39	0
3	H	1851	0	1866	16	0
4	L	10	0	0	0	0
4	M	10	0	0	2	0
5	L	132	0	148	5	0
5	M	132	0	148	14	0
6	L	65	0	76	3	0
6	M	65	0	76	4	0
7	L	48	0	63	8	0
7	M	48	0	63	1	0
8	L	10	0	16	0	0
9	H	64	0	124	7	0
9	L	64	0	124	10	0
9	M	32	0	62	7	0
10	H	12	0	16	0	0
10	L	12	0	16	0	0
11	M	1	0	0	0	0
12	M	81	0	106	3	0
13	M	108	0	160	23	0
14	H	1	0	0	0	0
15	H	207	0	0	0	0
15	L	104	0	0	0	0
15	M	141	0	0	5	0
All	All	7921	0	7660	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (116) 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)
13:M:801:PC9:H261	9:H:903:LDA:H121	1.33	1.05
2:M:257:GLY:O	13:M:801:PC9:H32	1.64	0.98
5:M:311:BCL:H41	13:M:802:PC9:H441	1.45	0.97
3:H:118[B]:ARG:HD3	3:H:120:LEU:HD12	1.65	0.79
3:H:84:PRO:O	3:H:85:ILE:HD13	1.85	0.76
5:L:312:BCL:CBB	5:L:312:BCL:HMB1	2.18	0.74
12:M:800:CDL:HB4	12:M:800:CDL:HA61	1.66	0.74
2:M:122:MET:SD	9:M:920:LDA:H123	2.28	0.74
2:M:253[B]:ARG:NH2	13:M:801:PC9:O2	2.24	0.71
5:M:311:BCL:H41	13:M:802:PC9:C44	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:801:PC9:H141	13:M:801:PC9:H31	1.72	0.70
13:M:801:PC9:H261	9:H:903:LDA:C12	2.16	0.70
5:M:311:BCL:CBB	5:M:311:BCL:HMB1	2.22	0.69
7:L:502:U10:H303	5:M:311:BCL:C14	2.25	0.66
5:L:312:BCL:HMB1	5:L:312:BCL:HBB3	1.76	0.66
2:M:65[A]:MET:HE2	2:M:121:PHE:CZ	2.32	0.65
2:M:52:LEU:HD21	2:M:60[A]:LEU:HD21	1.78	0.65
2:M:70:ILE:HD13	9:M:920:LDA:HM22	1.78	0.65
13:M:801:PC9:C4	3:H:52:ASN:HD21	2.10	0.64
13:M:801:PC9:C26	9:H:903:LDA:H121	2.20	0.63
5:M:311:BCL:C4	13:M:802:PC9:H441	2.25	0.62
1:L:61:PRO:O	1:L:150:ILE:HD13	1.99	0.62
2:M:70:ILE:HG21	9:M:920:LDA:HM23	1.80	0.62
2:M:157:TRP:HE1	9:M:920:LDA:H122	1.65	0.61
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.84	0.59
13:M:802:PC9:H162	13:M:802:PC9:H121	1.84	0.59
3:H:118[B]:ARG:CD	3:H:120:LEU:HD12	2.31	0.59
5:M:313:BCL:H191	13:M:802:PC9:C26	2.33	0.58
1:L:178:SER:OG	7:L:502:U10:H302	2.03	0.58
5:M:311:BCL:HMB1	5:M:311:BCL:HBB2	1.86	0.58
12:M:800:CDL:HB4	12:M:800:CDL:CA6	2.33	0.58
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.85	0.57
6:M:401:BPH:HHD	6:M:401:BPH:CBC	2.35	0.57
5:L:314:BCL:HMB1	5:L:314:BCL:HBB2	1.86	0.56
9:L:906:LDA:HM22	9:L:908:LDA:H52	1.88	0.56
3:H:18:TYR:CD1	9:H:903:LDA:O1	2.59	0.55
7:L:502:U10:H303	5:M:311:BCL:H143	1.88	0.55
9:H:903:LDA:H62	9:H:904:LDA:CM2	2.37	0.55
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.42	0.55
2:M:301[A]:HIS:CE1	15:M:1031:HOH:O	2.60	0.54
6:L:402:BPH:HBB3	6:L:402:BPH:CMB	2.38	0.54
2:M:67[B]:PHE:HZ	5:M:313:BCL:H203	1.73	0.54
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.42	0.54
2:M:60[A]:LEU:HD12	6:M:401:BPH:H4C1	1.89	0.53
1:L:119:PHE:CD2	9:L:908:LDA:H111	2.42	0.53
2:M:65[A]:MET:HE3	2:M:121:PHE:CE2	2.44	0.53
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.92	0.52
2:M:110:LYS:NZ	15:M:1431:HOH:O	2.43	0.52
5:M:313:BCL:H191	13:M:802:PC9:H263	1.90	0.52
9:L:906:LDA:HM11	9:L:906:LDA:H32	1.91	0.51
13:M:801:PC9:H41	3:H:52:ASN:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:802:PC9:O11	13:M:802:PC9:H51	2.11	0.51
13:M:802:PC9:H412	13:M:802:PC9:H451	1.93	0.51
7:L:502:U10:H351	7:L:502:U10:H38	1.92	0.50
1:L:76:GLY:HA3	9:L:909:LDA:HM13	1.94	0.50
7:M:501:U10:H23	13:M:801:PC9:H191	1.94	0.50
9:H:903:LDA:H62	9:H:904:LDA:HM21	1.93	0.50
7:L:502:U10:H351	7:L:502:U10:C38	2.42	0.49
6:M:401:BPH:HHD	6:M:401:BPH:HBC2	1.94	0.49
9:L:906:LDA:CM2	9:L:908:LDA:H52	2.42	0.49
2:M:157:TRP:NE1	9:M:920:LDA:H122	2.26	0.49
2:M:65[A]:MET:CE	2:M:121:PHE:CE2	2.95	0.49
2:M:70:ILE:HD13	9:M:920:LDA:CM2	2.42	0.48
1:L:241:VAL:HG21	6:L:402:BPH:HAC1	1.95	0.48
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.96	0.48
4:M:703:PO4:O3	15:M:1448:HOH:O	2.20	0.48
9:M:920:LDA:H22	9:M:920:LDA:HM11	1.56	0.48
5:M:313:BCL:CBB	5:M:313:BCL:HMB1	2.43	0.47
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.95	0.47
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.95	0.47
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.47
1:L:263:TRP:HH2	7:L:502:U10:H352	1.80	0.46
13:M:801:PC9:O1P	13:M:801:PC9:H2	2.16	0.46
2:M:52:LEU:HD21	2:M:60[A]:LEU:CD2	2.46	0.46
13:M:801:PC9:H141	13:M:801:PC9:C3	2.42	0.46
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.98	0.46
13:M:802:PC9:H162	13:M:802:PC9:C12	2.46	0.45
2:M:6:ILE:CD1	2:M:224:LEU:HD13	2.46	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.16	0.45
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.52	0.45
5:M:311:BCL:HMB1	5:M:311:BCL:HBB3	1.98	0.45
5:L:312:BCL:CGA	5:L:314:BCL:HBC1	2.47	0.45
13:M:801:PC9:BR1	9:H:902:LDA:H102	2.72	0.44
9:L:908:LDA:HM11	9:L:908:LDA:C3	2.46	0.44
1:L:263:TRP:CH2	7:L:502:U10:H352	2.52	0.44
9:L:906:LDA:H22	9:L:906:LDA:HM21	1.71	0.44
2:M:68[A]:PHE:CE1	2:M:72:ILE:HD11	2.52	0.44
13:M:801:PC9:H222	13:M:801:PC9:H252	1.31	0.44
2:M:194:GLY:O	2:M:195:ASN:HB3	2.17	0.44
6:L:402:BPH:CMB	6:L:402:BPH:CBB	2.95	0.43
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.99	0.43
1:L:53:ALA:HB1	1:L:58:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:314:BCL:HMB1	5:L:314:BCL:CBB	2.49	0.43
6:M:401:BPH:CBC	6:M:401:BPH:CHD	2.95	0.43
2:M:229:PHE:HB2	2:M:244:ALA:HB2	2.00	0.43
2:M:65[A]:MET:CE	2:M:121:PHE:CZ	3.02	0.43
2:M:261:THR:HG23	3:H:35:ASN:O	2.19	0.42
4:M:703:PO4:P	15:M:1448:HOH:O	2.77	0.42
2:M:268:TRP:CE3	3:H:31:LEU:HD13	2.54	0.42
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.54	0.42
2:M:68[A]:PHE:O	2:M:72:ILE:HD13	2.18	0.42
2:M:253[B]:ARG:HH21	13:M:801:PC9:H12	1.85	0.42
1:L:216:PHE:CD2	7:L:502:U10:H102	2.55	0.42
2:M:301[A]:HIS:HE1	15:M:1031:HOH:O	1.99	0.42
9:L:908:LDA:C3	9:L:908:LDA:CM1	2.97	0.42
1:L:119:PHE:CE2	9:L:908:LDA:H111	2.55	0.42
2:M:179:ILE:HG23	5:M:311:BCL:HED1	2.02	0.42
2:M:6:ILE:HD13	2:M:224:LEU:HD13	2.02	0.41
1:L:76:GLY:CA	9:L:909:LDA:HM13	2.51	0.41
5:M:311:BCL:H61	5:M:313:BCL:H193	2.01	0.41
3:H:169:VAL:HG23	3:H:171:ILE:HD13	2.01	0.41
3:H:84:PRO:C	3:H:85:ILE:HD13	2.41	0.41
2:M:148:TRP:CD1	12:M:800:CDL:OB6	2.74	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	283/281 (101%)	272 (96%)	10 (4%)	1 (0%)	34	60
2	M	314/307 (102%)	298 (95%)	15 (5%)	1 (0%)	41	66
3	H	246/260 (95%)	240 (98%)	5 (2%)	1 (0%)	34	60
All	All	843/848 (99%)	810 (96%)	30 (4%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	86	ALA
1	L	31	VAL

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	224/220 (102%)	215 (96%)	9 (4%)	31	60
2	M	250/240 (104%)	239 (96%)	11 (4%)	28	56
3	H	203/208 (98%)	197 (97%)	6 (3%)	41	70
All	All	677/668 (101%)	651 (96%)	26 (4%)	34	62

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
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	254	ILE
1	L	272	TRP
2	M	38	LEU
2	M	52	LEU
2	M	60[A]	LEU
2	M	60[B]	LEU
2	M	100	GLU
2	M	114	LEU
2	M	132	ARG
2	M	192	VAL
2	M	196	LEU

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Mol	Chain	Res	Type
2	M	216	PHE
2	M	278	LEU
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP
3	H	250	SER

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

Mol	Chain	Res	Type
1	L	274	ASN
2	M	28	ASN
3	H	68	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	LDA	L	905	-	12,15,15	1.98	1 (8%)	14,17,17	0.41	0
9	LDA	L	906	-	12,15,15	1.70	1 (8%)	14,17,17	0.49	0
7	U10	M	501	-	48,48,63	1.08	2 (4%)	58,61,79	1.78	14 (24%)
9	LDA	M	920	-	12,15,15	1.76	1 (8%)	14,17,17	0.89	1 (7%)
5	BCL	L	314	1	64,74,74	1.00	4 (6%)	78,115,115	1.64	18 (23%)
12	CDL	M	800	-	80,80,99	1.30	4 (5%)	86,92,111	1.40	10 (11%)
9	LDA	L	909	-	12,15,15	2.03	1 (8%)	14,17,17	0.60	0
10	GOL	L	708	-	5,5,5	0.54	0	5,5,5	0.32	0
9	LDA	H	904	-	12,15,15	2.04	1 (8%)	14,17,17	0.49	0
4	PO4	M	703	-	4,4,4	0.82	0	6,6,6	0.45	0
6	BPH	M	401	-	51,70,70	1.13	4 (7%)	52,101,101	2.17	19 (36%)
4	PO4	L	701	-	4,4,4	0.94	0	6,6,6	0.68	0
5	BCL	M	313	2	64,74,74	1.47	6 (9%)	78,115,115	1.64	16 (20%)
7	U10	L	502	-	48,48,63	1.33	7 (14%)	58,61,79	1.83	16 (27%)
13	PC9	M	802	-	53,53,53	1.03	4 (7%)	59,63,63	1.44	6 (10%)
8	HTO	L	705	-	9,9,9	0.63	0	10,10,10	0.71	0
6	BPH	L	402	-	51,70,70	0.96	3 (5%)	52,101,101	1.59	6 (11%)
10	GOL	L	707	-	5,5,5	0.70	0	5,5,5	1.00	0
5	BCL	M	311	2	64,74,74	1.35	3 (4%)	78,115,115	1.76	21 (26%)
9	LDA	H	903	-	12,15,15	2.02	1 (8%)	14,17,17	0.53	0
10	GOL	H	709	-	5,5,5	0.54	0	5,5,5	0.22	0
9	LDA	L	908	-	12,15,15	1.92	1 (8%)	14,17,17	0.56	0
5	BCL	L	312	1	64,74,74	1.27	5 (7%)	78,115,115	1.28	8 (10%)
10	GOL	H	706	-	5,5,5	0.29	0	5,5,5	0.94	0
4	PO4	L	702	-	4,4,4	4.04	3 (75%)	6,6,6	1.25	1 (16%)
9	LDA	H	902	-	12,15,15	1.98	1 (8%)	14,17,17	0.55	0
4	PO4	M	704	-	4,4,4	1.91	1 (25%)	6,6,6	1.16	0
9	LDA	H	901	-	12,15,15	1.99	1 (8%)	14,17,17	0.56	0
9	LDA	M	907	-	12,15,15	1.92	1 (8%)	14,17,17	0.76	1 (7%)
13	PC9	M	801	-	53,53,53	1.12	6 (11%)	59,63,63	1.52	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LDA	L	905	-	-	7/13/13/13	-
9	LDA	L	906	-	-	10/13/13/13	-
7	U10	M	501	-	-	6/45/69/87	0/1/1/1
9	LDA	M	920	-	-	5/13/13/13	-
5	BCL	L	314	1	-	5/37/137/137	-
12	CDL	M	800	-	-	40/91/91/110	-
9	LDA	L	909	-	-	9/13/13/13	-
10	GOL	L	708	-	-	4/4/4/4	-
9	LDA	H	904	-	-	4/13/13/13	-
6	BPH	M	401	-	-	14/37/105/105	0/5/6/6
5	BCL	M	313	2	-	5/37/137/137	-
7	U10	L	502	-	-	9/45/69/87	0/1/1/1
13	PC9	M	802	-	-	34/60/60/60	-
8	HTO	L	705	-	-	0/10/10/10	-
6	BPH	L	402	-	-	8/37/105/105	0/5/6/6
10	GOL	L	707	-	-	4/4/4/4	-
5	BCL	M	311	2	-	9/37/137/137	-
9	LDA	H	903	-	-	8/13/13/13	-
10	GOL	H	709	-	-	4/4/4/4	-
9	LDA	L	908	-	-	6/13/13/13	-
5	BCL	L	312	1	-	6/37/137/137	-
10	GOL	H	706	-	-	2/4/4/4	-
9	LDA	H	902	-	-	6/13/13/13	-
9	LDA	H	901	-	-	4/13/13/13	-
9	LDA	M	907	-	-	7/13/13/13	-
13	PC9	M	801	-	-	29/60/60/60	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	313	BCL	MG-NA	8.01	2.25	2.06
4	L	702	PO4	P-O1	7.05	1.67	1.50
9	H	904	LDA	O1-N1	-6.97	1.25	1.42
9	H	903	LDA	O1-N1	-6.92	1.26	1.42
9	H	901	LDA	O1-N1	-6.78	1.26	1.42
9	L	909	LDA	O1-N1	-6.71	1.26	1.42
9	L	905	LDA	O1-N1	-6.69	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	902	LDA	O1-N1	-6.68	1.26	1.42
9	L	908	LDA	O1-N1	-6.56	1.26	1.42
5	M	311	BCL	C1B-NB	6.28	1.40	1.35
9	M	907	LDA	O1-N1	-6.24	1.27	1.42
9	M	920	LDA	O1-N1	-5.93	1.28	1.42
9	L	906	LDA	O1-N1	-5.71	1.28	1.42
12	M	800	CDL	OA8-CA7	5.52	1.49	1.33
12	M	800	CDL	OB6-CB5	5.50	1.49	1.34
12	M	800	CDL	OA6-CA5	4.73	1.47	1.34
5	L	312	BCL	MG-NA	4.70	2.17	2.06
5	M	311	BCL	MG-NA	4.66	2.17	2.06
7	L	502	U10	O3-C3	4.45	1.47	1.36
12	M	800	CDL	OB8-CB7	4.25	1.45	1.33
5	L	312	BCL	C4B-NB	3.98	1.38	1.35
7	L	502	U10	O4-C4	3.89	1.46	1.36
6	L	402	BPH	C2C-C3C	3.89	1.58	1.54
4	M	704	PO4	P-O1	3.64	1.59	1.50
5	L	312	BCL	MG-NC	3.63	2.14	2.06
7	M	501	U10	O3-C3	3.47	1.45	1.36
6	M	401	BPH	C3A-C2A	-3.47	1.51	1.54
5	L	312	BCL	C1B-NB	3.40	1.38	1.35
5	M	313	BCL	C3C-C4C	-3.34	1.47	1.51
13	M	801	PC9	P-O1P	3.32	1.62	1.50
5	L	314	BCL	C1D-ND	3.19	1.41	1.37
4	L	702	PO4	P-O2	3.19	1.64	1.54
5	M	313	BCL	C4B-NB	3.17	1.38	1.35
6	M	401	BPH	OBD-CAD	-3.06	1.18	1.22
7	M	501	U10	O4-C4	3.05	1.44	1.36
13	M	802	PC9	P-O1P	2.97	1.61	1.50
13	M	801	PC9	C1-C2	2.85	1.59	1.50
13	M	802	PC9	O2-C2	-2.85	1.39	1.46
13	M	802	PC9	O3-C3	2.67	1.51	1.45
6	M	401	BPH	C2C-C3C	-2.66	1.52	1.54
7	L	502	U10	C28-C29	2.62	1.39	1.33
13	M	801	PC9	BR1-C36	-2.54	1.91	1.97
5	L	314	BCL	C4B-NB	2.47	1.37	1.35
5	M	313	BCL	CHD-C1D	2.44	1.43	1.38
13	M	801	PC9	O3-C3	2.43	1.50	1.45
7	L	502	U10	C26-C24	2.38	1.56	1.51
6	M	401	BPH	C5-C3	2.34	1.56	1.51
13	M	802	PC9	O3-C11	2.31	1.40	1.33
6	L	402	BPH	C4-C3	2.22	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	313	BCL	CBA-CGA	-2.21	1.44	1.50
13	M	801	PC9	O2-C2	2.18	1.52	1.46
5	L	314	BCL	MG-ND	-2.16	2.01	2.05
7	L	502	U10	C3-C2	-2.15	1.42	1.48
5	M	311	BCL	C1D-ND	2.15	1.40	1.37
4	L	702	PO4	P-O4	-2.14	1.48	1.54
7	L	502	U10	C13-C14	2.14	1.38	1.33
7	L	502	U10	C38-C39	2.13	1.38	1.32
6	L	402	BPH	C3A-C2A	-2.12	1.52	1.54
13	M	801	PC9	C32-C31	2.09	1.56	1.50
5	M	313	BCL	C4D-ND	-2.07	1.34	1.37
5	L	314	BCL	C4D-ND	-2.05	1.34	1.37
5	L	312	BCL	C5-C3	2.04	1.55	1.51

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	401	BPH	O2D-CGD-CBD	6.80	119.62	111.00
7	L	502	U10	C25-C24-C26	6.06	125.46	115.27
13	M	802	PC9	O2-C31-C32	5.97	124.38	111.50
12	M	800	CDL	OB6-CB5-C51	5.93	124.28	111.50
13	M	801	PC9	O2-C31-C32	5.37	123.06	111.50
5	M	313	BCL	C4D-CHA-C1A	5.33	127.74	121.25
5	M	311	BCL	C1-O2A-CGA	5.30	130.35	116.44
6	L	402	BPH	C1-C2-C3	-5.19	117.07	126.04
6	L	402	BPH	O2D-CGD-CBD	5.05	117.39	111.00
7	M	501	U10	C30-C29-C31	4.97	123.63	115.27
5	M	311	BCL	C5-C3-C2	4.62	130.46	121.12
6	M	401	BPH	OBD-CAD-CBD	-4.59	119.09	125.82
6	M	401	BPH	C1-C2-C3	-4.33	118.56	126.04
7	M	501	U10	C17-C18-C19	-4.32	117.25	127.66
6	M	401	BPH	CMA-C3A-C4A	-4.24	105.10	114.38
5	M	311	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
7	L	502	U10	C7-C8-C9	-4.19	119.81	126.79
5	L	314	BCL	CAA-C2A-C3A	-4.15	101.40	112.78
7	M	501	U10	C32-C33-C34	-4.08	117.82	127.66
6	M	401	BPH	CAC-C3C-C4C	4.08	122.85	113.73
12	M	800	CDL	OA6-CA5-C11	4.05	120.24	111.50
12	M	800	CDL	OB8-CB7-C71	4.03	124.57	111.91
5	L	314	BCL	CMB-C2B-C1B	-4.03	122.27	128.46
13	M	801	PC9	O2-C2-C1	4.00	122.88	108.40
5	M	311	BCL	C4D-CHA-C1A	3.88	125.98	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	313	BCL	CAC-C3C-C2C	-3.86	104.61	114.26
7	L	502	U10	C12-C13-C14	-3.78	118.56	127.66
5	M	313	BCL	C1D-ND-C4D	3.77	109.02	106.33
6	M	401	BPH	C1C-C2C-C3C	-3.76	99.26	102.84
12	M	800	CDL	OA8-CA7-C31	3.64	123.34	111.91
5	L	314	BCL	CAC-C3C-C2C	-3.57	105.33	114.26
13	M	802	PC9	C3-C2-C1	-3.55	103.39	111.79
6	M	401	BPH	C1-O2A-CGA	3.55	125.75	116.44
13	M	801	PC9	C2-O2-C31	-3.55	109.06	117.79
7	L	502	U10	C25-C24-C23	-3.52	114.65	123.68
7	M	501	U10	C26-C27-C28	-3.50	100.39	111.88
5	M	311	BCL	O2D-CGD-CBD	3.47	117.43	111.27
5	L	312	BCL	CHD-C1D-ND	-3.44	121.29	124.45
7	M	501	U10	C11-C9-C8	-3.42	114.19	121.12
7	L	502	U10	O2-C2-C3	-3.42	113.67	120.93
6	M	401	BPH	CMC-C2C-C1C	3.35	121.70	114.38
5	M	313	BCL	CHA-C1A-NA	-3.34	118.74	126.40
12	M	800	CDL	CA4-OA6-CA5	-3.27	109.73	117.79
5	M	313	BCL	CMB-C2B-C1B	-3.24	123.48	128.46
5	L	314	BCL	O2D-CGD-CBD	3.22	117.00	111.27
7	M	501	U10	C15-C14-C16	3.21	120.67	115.27
13	M	802	PC9	O3-C11-C12	3.20	121.95	111.91
12	M	800	CDL	OA6-CA5-OA7	-3.18	116.03	123.70
7	M	501	U10	C7-C6-C5	-3.17	114.67	118.48
13	M	801	PC9	O3-C3-C2	3.15	117.60	108.43
5	M	311	BCL	CHD-C1D-ND	-3.11	121.60	124.45
5	M	313	BCL	C1-C2-C3	-3.08	120.71	126.04
7	M	501	U10	C31-C29-C28	-3.07	114.90	121.12
5	M	313	BCL	CHD-C1D-ND	-3.07	121.64	124.45
7	L	502	U10	C3M-O3-C3	3.06	127.32	116.47
5	M	311	BCL	O2A-C1-C2	3.00	116.51	108.64
6	M	401	BPH	CAA-C2A-C3A	-2.98	104.62	112.78
5	L	312	BCL	CAA-C2A-C3A	-2.96	104.67	112.78
7	L	502	U10	C36-C34-C33	2.95	127.08	121.12
13	M	802	PC9	O2-C2-C3	-2.94	97.75	108.40
5	M	311	BCL	CMB-C2B-C3B	2.94	130.18	124.68
5	L	314	BCL	CAA-CBA-CGA	2.93	121.82	113.25
5	M	311	BCL	C6-C5-C3	-2.92	105.81	113.45
6	M	401	BPH	C7-C6-C5	2.89	121.21	113.36
6	L	402	BPH	O2D-CGD-O1D	-2.84	118.29	123.84
5	L	314	BCL	CMB-C2B-C3B	2.82	129.96	124.68
13	M	801	PC9	BR2-C37-C38	-2.82	103.99	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	311	BCL	OBB-CAB-C3B	2.80	124.96	119.99
5	L	314	BCL	C5-C3-C2	-2.78	115.48	121.12
7	M	501	U10	C26-C24-C23	-2.75	115.55	121.12
7	M	501	U10	C16-C14-C13	-2.75	115.56	121.12
6	M	401	BPH	C4-C3-C2	-2.72	116.71	123.68
5	L	314	BCL	CBC-CAC-C3C	2.70	119.47	113.47
6	M	401	BPH	C4C-C3C-C2C	2.69	105.40	102.84
5	M	311	BCL	C1-C2-C3	2.69	130.69	126.04
5	M	313	BCL	C4A-NA-C1A	2.66	107.90	106.71
5	M	313	BCL	C2A-C1A-CHA	2.65	128.50	123.86
5	M	313	BCL	C4D-C3D-CAD	-2.65	104.97	108.10
5	L	312	BCL	C1-O2A-CGA	2.63	123.34	116.44
5	L	312	BCL	CAA-C2A-C1A	-2.60	103.45	111.97
13	M	801	PC9	O2-C31-O31	-2.60	117.42	123.70
5	M	311	BCL	C4-C3-C5	-2.60	110.90	115.27
5	M	311	BCL	CAA-C2A-C3A	-2.57	105.73	112.78
5	L	312	BCL	CMD-C2D-C1D	2.56	129.23	124.71
5	M	311	BCL	CHA-C1A-NA	-2.54	120.59	126.40
13	M	802	PC9	O3-C3-C2	2.52	115.78	108.43
6	M	401	BPH	CMB-C2B-C3B	2.52	129.40	124.68
12	M	800	CDL	OB8-CB7-OB9	-2.51	117.27	123.59
12	M	800	CDL	OB8-CB6-CB4	2.47	115.62	108.43
6	M	401	BPH	O2D-CGD-O1D	-2.44	119.07	123.84
5	L	314	BCL	CAC-C3C-C4C	-2.44	107.18	112.58
7	M	501	U10	C35-C34-C36	2.42	119.35	115.27
13	M	802	PC9	BR2-C37-C36	-2.41	105.60	110.27
5	L	312	BCL	CHA-C1A-NA	-2.41	120.88	126.40
5	L	314	BCL	CHD-C1D-ND	-2.40	122.25	124.45
9	M	920	LDA	O1-N1-C1	2.39	115.13	109.27
5	L	314	BCL	C4D-CHA-C1A	2.38	124.15	121.25
7	L	502	U10	C12-C11-C9	-2.37	105.17	112.98
6	M	401	BPH	C5-C3-C2	2.36	125.89	121.12
5	L	314	BCL	C4-C3-C5	2.34	119.21	115.27
5	L	314	BCL	C2C-C3C-C4C	2.34	104.84	101.34
6	L	402	BPH	CAA-C2A-C3A	-2.34	106.38	112.78
13	M	801	PC9	C13-C12-C11	-2.33	105.13	113.62
7	L	502	U10	C22-C23-C24	-2.33	122.05	127.66
12	M	800	CDL	OB6-CB4-CB6	2.33	116.82	108.40
5	M	313	BCL	C1C-NC-C4C	2.32	107.75	106.71
7	M	501	U10	C10-C9-C11	2.32	119.17	115.27
5	L	312	BCL	C4-C3-C5	2.31	119.16	115.27
5	M	313	BCL	C4B-C3B-CAB	-2.28	122.73	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	311	BCL	C2C-C3C-C4C	2.27	104.74	101.34
5	M	313	BCL	CMC-C2C-C3C	-2.27	104.67	113.83
5	M	311	BCL	OBB-CAB-CBB	-2.26	115.08	120.17
5	L	314	BCL	OBB-CAB-C3B	2.26	124.00	119.99
7	L	502	U10	O4-C4-C5	2.24	124.14	116.56
6	M	401	BPH	CAA-CBA-CGA	2.24	119.80	113.25
13	M	801	PC9	BR1-C36-C37	-2.24	105.93	110.27
13	M	801	PC9	BR2-C37-C36	2.24	114.61	110.27
7	L	502	U10	C6-C1-C2	-2.23	117.42	119.18
5	L	314	BCL	CHA-C1A-NA	-2.23	121.29	126.40
12	M	800	CDL	OA8-CA7-OA9	-2.22	118.00	123.59
5	M	313	BCL	O2D-CGD-O1D	-2.20	119.53	123.84
6	L	402	BPH	OBD-CAD-CBD	-2.20	122.60	125.82
7	L	502	U10	C1M-C1-C6	-2.19	120.83	124.40
6	L	402	BPH	CAC-C3C-C4C	2.19	118.63	113.73
9	M	907	LDA	O1-N1-C1	2.17	114.60	109.27
4	L	702	PO4	O4-P-O1	-2.17	102.95	110.89
6	M	401	BPH	CMD-C2D-C3D	2.16	128.73	124.68
5	L	312	BCL	CHD-C1D-C2D	2.16	130.01	125.48
5	L	314	BCL	OBB-CAB-CBB	-2.14	115.35	120.17
7	L	502	U10	C35-C34-C33	-2.13	118.21	123.68
5	M	313	BCL	OBB-CAB-CBB	-2.13	115.38	120.17
7	M	501	U10	C22-C23-C24	-2.12	122.56	127.66
5	M	311	BCL	C1B-CHB-C4A	-2.11	125.93	130.12
5	M	311	BCL	CMA-C3A-C4A	-2.11	106.09	111.77
6	M	401	BPH	CMA-C3A-C2A	-2.10	105.52	113.99
7	L	502	U10	C36-C37-C38	2.10	118.80	111.88
5	L	314	BCL	C1D-ND-C4D	2.10	107.83	106.33
7	L	502	U10	O5-C5-C6	-2.07	117.92	121.55
5	M	311	BCL	CMA-C3A-C2A	-2.07	105.49	113.83
6	M	401	BPH	O1D-CGD-CBD	-2.06	121.31	124.74
5	L	314	BCL	O1D-CGD-CBD	-2.06	120.27	124.48
5	M	311	BCL	C4-C3-C2	-2.04	118.45	123.68
5	M	311	BCL	CAA-CBA-CGA	2.03	119.18	113.25
7	L	502	U10	O4-C4-C3	-2.02	116.02	123.64
5	M	313	BCL	O2A-C1-C2	2.01	113.91	108.64
7	M	501	U10	C41-C39-C40	2.00	119.03	114.60

There are no chirality outliers.

All (245) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	401	BPH	C4C-C3C-CAC-CBC
6	M	401	BPH	C2C-C3C-CAC-CBC
6	M	401	BPH	C2-C3-C5-C6
6	M	401	BPH	C4-C3-C5-C6
9	L	906	LDA	C2-C1-N1-O1
9	L	906	LDA	C2-C1-N1-CM2
9	L	906	LDA	N1-C1-C2-C3
9	L	908	LDA	N1-C1-C2-C3
9	L	909	LDA	N1-C1-C2-C3
9	H	902	LDA	C2-C1-N1-CM2
9	H	903	LDA	C2-C1-N1-O1
9	H	903	LDA	C2-C1-N1-CM1
9	H	903	LDA	C2-C1-N1-CM2
10	L	708	GOL	O1-C1-C2-C3
10	L	708	GOL	C1-C2-C3-O3
10	H	706	GOL	C1-C2-C3-O3
10	H	709	GOL	C1-C2-C3-O3
12	M	800	CDL	CA2-OA2-PA1-OA3
12	M	800	CDL	CA2-OA2-PA1-OA4
12	M	800	CDL	OB6-CB4-CB6-OB8
13	M	801	PC9	O31-C31-O2-C2
13	M	801	PC9	C4-O4P-P-O2P
13	M	801	PC9	O4P-C4-C5-N
13	M	802	PC9	C1-O3P-P-O2P
13	M	802	PC9	C4-O4P-P-O1P
13	M	802	PC9	O11-C11-O3-C3
13	M	802	PC9	C12-C11-O3-C3
13	M	801	PC9	O11-C11-O3-C3
5	M	311	BCL	C3-C5-C6-C7
13	M	801	PC9	C32-C31-O2-C2
13	M	801	PC9	C12-C11-O3-C3
9	L	906	LDA	C11-C10-C9-C8
13	M	802	PC9	C42-C43-C44-C45
13	M	801	PC9	C2-C1-O3P-P
9	L	908	LDA	C6-C7-C8-C9
13	M	801	PC9	C22-C23-C24-C25
12	M	800	CDL	C38-C39-C40-C41
5	M	311	BCL	C11-C12-C13-C14
6	M	401	BPH	C11-C10-C8-C9
12	M	800	CDL	CB7-C71-C72-C73
6	M	401	BPH	C15-C16-C17-C18
10	L	707	GOL	O2-C2-C3-O3
13	M	802	PC9	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	M	501	U10	C29-C31-C32-C33
5	M	311	BCL	C8-C10-C11-C12
12	M	800	CDL	CA2-OA2-PA1-OA5
12	M	800	CDL	CB2-OB2-PB2-OB5
12	M	800	CDL	CB3-OB5-PB2-OB2
13	M	801	PC9	C1-O3P-P-O4P
13	M	801	PC9	C4-O4P-P-O3P
13	M	801	PC9	C16-C17-C18-C19
9	M	907	LDA	C4-C5-C6-C7
13	M	802	PC9	C44-C45-C46-C47
13	M	801	PC9	C11-C12-C13-C14
9	M	907	LDA	C7-C8-C9-C10
9	H	903	LDA	C7-C8-C9-C10
13	M	802	PC9	C22-C23-C24-C25
9	L	909	LDA	C11-C10-C9-C8
9	H	903	LDA	C11-C10-C9-C8
13	M	801	PC9	C39-C40-C41-C42
9	L	905	LDA	C7-C8-C9-C10
13	M	801	PC9	C15-C16-C17-C18
10	L	707	GOL	O1-C1-C2-C3
10	L	707	GOL	C1-C2-C3-O3
13	M	802	PC9	C32-C31-O2-C2
9	L	905	LDA	C3-C4-C5-C6
9	M	920	LDA	C4-C5-C6-C7
12	M	800	CDL	C13-C14-C15-C16
12	M	800	CDL	C78-C79-C80-C81
5	M	313	BCL	C16-C17-C18-C19
12	M	800	CDL	C18-C19-C20-C21
13	M	801	PC9	C13-C14-C15-C16
13	M	801	PC9	C42-C43-C44-C45
13	M	802	PC9	C16-C17-C18-C19
13	M	802	PC9	O31-C31-O2-C2
9	H	901	LDA	C4-C5-C6-C7
10	L	707	GOL	O1-C1-C2-O2
10	L	708	GOL	O1-C1-C2-O2
13	M	802	PC9	C20-C21-C22-C23
13	M	802	PC9	C17-C18-C19-C20
9	L	905	LDA	C1-C2-C3-C4
5	M	313	BCL	C13-C15-C16-C17
9	L	908	LDA	C1-C2-C3-C4
13	M	801	PC9	C17-C18-C19-C20
12	M	800	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
9	M	920	LDA	C9-C10-C11-C12
6	M	401	BPH	C11-C10-C8-C7
7	L	502	U10	C13-C14-C16-C17
9	L	906	LDA	C5-C6-C7-C8
9	L	909	LDA	C5-C6-C7-C8
12	M	800	CDL	C19-C20-C21-C22
9	L	905	LDA	C4-C5-C6-C7
9	H	903	LDA	C5-C6-C7-C8
9	H	904	LDA	C5-C6-C7-C8
7	L	502	U10	C15-C14-C16-C17
9	H	903	LDA	C3-C4-C5-C6
9	L	906	LDA	C3-C4-C5-C6
13	M	802	PC9	C1-O3P-P-O4P
9	L	908	LDA	C11-C10-C9-C8
5	M	313	BCL	C16-C17-C18-C20
7	L	502	U10	C20-C19-C21-C22
7	L	502	U10	C18-C19-C21-C22
12	M	800	CDL	CB3-CB4-CB6-OB8
13	M	802	PC9	C19-C20-C21-C22
9	L	908	LDA	C9-C10-C11-C12
10	L	708	GOL	O2-C2-C3-O3
10	H	709	GOL	O2-C2-C3-O3
9	H	901	LDA	C6-C7-C8-C9
9	L	905	LDA	C9-C10-C11-C12
7	M	501	U10	C30-C29-C31-C32
13	M	801	PC9	C23-C24-C25-C26
13	M	802	PC9	C43-C44-C45-C46
12	M	800	CDL	C31-CA7-OA8-CA6
12	M	800	CDL	OB5-CB3-CB4-OB6
13	M	801	PC9	C4-C5-N-C8
12	M	800	CDL	C54-C55-C56-C57
6	M	401	BPH	C12-C13-C15-C16
7	M	501	U10	C28-C29-C31-C32
9	H	902	LDA	C1-C2-C3-C4
9	H	902	LDA	C9-C10-C11-C12
5	M	311	BCL	C13-C15-C16-C17
12	M	800	CDL	OA5-CA3-CA4-CA6
12	M	800	CDL	OB5-CB3-CB4-CB6
9	L	905	LDA	C5-C6-C7-C8
12	M	800	CDL	CA3-CA4-CA6-OA8
6	L	402	BPH	C2-C3-C5-C6
13	M	802	PC9	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
10	H	709	GOL	O1-C1-C2-O2
13	M	802	PC9	O3P-C1-C2-O2
13	M	802	PC9	C45-C46-C47-C48
5	M	311	BCL	C5-C6-C7-C8
6	M	401	BPH	C13-C15-C16-C17
9	M	920	LDA	C3-C4-C5-C6
12	M	800	CDL	C73-C74-C75-C76
7	M	501	U10	C24-C26-C27-C28
6	M	401	BPH	C14-C13-C15-C16
13	M	801	PC9	C4-C5-N-C7
12	M	800	CDL	OA7-CA5-OA6-CA4
12	M	800	CDL	OA9-CA7-OA8-CA6
5	L	314	BCL	C12-C13-C15-C16
6	M	401	BPH	C6-C7-C8-C10
13	M	802	PC9	C32-C33-C34-C35
12	M	800	CDL	C11-CA5-OA6-CA4
13	M	801	PC9	C4-C5-N-C6
9	M	907	LDA	C2-C3-C4-C5
13	M	802	PC9	C14-C15-C16-C17
5	M	311	BCL	CAD-CBD-CGD-O2D
6	M	401	BPH	CAD-CBD-CGD-O2D
6	L	402	BPH	C8-C10-C11-C12
12	M	800	CDL	OA5-CA3-CA4-OA6
13	M	801	PC9	O3P-C1-C2-O2
9	L	909	LDA	C2-C1-N1-CM1
9	L	909	LDA	C2-C1-N1-CM2
9	H	902	LDA	C2-C1-N1-CM1
13	M	802	PC9	C4-C5-N-C8
10	H	706	GOL	O2-C2-C3-O3
9	M	920	LDA	C1-C2-C3-C4
12	M	800	CDL	C34-C35-C36-C37
9	H	904	LDA	C6-C7-C8-C9
9	L	906	LDA	C7-C8-C9-C10
9	M	907	LDA	C11-C10-C9-C8
13	M	801	PC9	C32-C33-C34-C35
12	M	800	CDL	CB2-OB2-PB2-OB3
12	M	800	CDL	CB3-OB5-PB2-OB3
12	M	800	CDL	CB3-OB5-PB2-OB4
13	M	801	PC9	C1-O3P-P-O2P
13	M	801	PC9	C4-O4P-P-O1P
13	M	802	PC9	C1-O3P-P-O1P
13	M	802	PC9	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
13	M	802	PC9	C4-C5-N-C6
5	L	312	BCL	C3-C5-C6-C7
12	M	800	CDL	C77-C78-C79-C80
12	M	800	CDL	C55-C56-C57-C58
9	L	909	LDA	C2-C1-N1-O1
9	H	902	LDA	C2-C1-N1-O1
5	L	314	BCL	C3-C5-C6-C7
9	L	909	LDA	C2-C3-C4-C5
6	L	402	BPH	C4C-C3C-CAC-CBC
12	M	800	CDL	C15-C16-C17-C18
5	L	312	BCL	C4-C3-C5-C6
6	L	402	BPH	C4-C3-C5-C6
5	L	314	BCL	C14-C13-C15-C16
6	M	401	BPH	C6-C7-C8-C9
6	M	401	BPH	C11-C12-C13-C14
12	M	800	CDL	C31-C32-C33-C34
9	L	909	LDA	C7-C8-C9-C10
9	M	907	LDA	C1-C2-C3-C4
9	L	909	LDA	C9-C10-C11-C12
13	M	802	PC9	O3P-C1-C2-C3
9	M	907	LDA	C5-C6-C7-C8
12	M	800	CDL	C20-C21-C22-C23
13	M	802	PC9	C4-O4P-P-O3P
12	M	800	CDL	C14-C15-C16-C17
13	M	802	PC9	BR1-C36-C37-C38
7	L	502	U10	C34-C36-C37-C38
7	L	502	U10	C30-C29-C31-C32
5	M	311	BCL	C15-C16-C17-C18
13	M	802	PC9	C38-C39-C40-C41
5	M	313	BCL	CAA-CBA-CGA-O2A
9	L	905	LDA	C11-C10-C9-C8
7	M	501	U10	C5-C4-O4-C4M
9	L	906	LDA	C2-C3-C4-C5
6	L	402	BPH	O2A-C1-C2-C3
6	L	402	BPH	C2C-C3C-CAC-CBC
13	M	802	PC9	C35-C36-C37-BR2
9	H	902	LDA	C5-C6-C7-C8
5	L	312	BCL	C11-C10-C8-C9
5	L	314	BCL	C13-C15-C16-C17
13	M	801	PC9	C18-C19-C20-C21
7	L	502	U10	C12-C11-C9-C10
5	L	312	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	M	800	CDL	C11-C12-C13-C14
13	M	801	PC9	O3-C11-C12-C13
7	M	501	U10	C34-C36-C37-C38
5	L	312	BCL	C11-C10-C8-C7
7	L	502	U10	C28-C29-C31-C32
9	L	908	LDA	C7-C8-C9-C10
12	M	800	CDL	C52-C51-CB5-OB6
12	M	800	CDL	C72-C71-CB7-OB8
5	M	313	BCL	C14-C13-C15-C16
5	L	312	BCL	CAD-CBD-CGD-O2D
6	L	402	BPH	CAD-CBD-CGD-O2D
7	L	502	U10	C12-C11-C9-C8
5	L	314	BCL	CHA-CBD-CGD-O1D
9	L	906	LDA	C6-C7-C8-C9
9	H	904	LDA	C9-C10-C11-C12
13	M	801	PC9	O3P-C1-C2-C3
12	M	800	CDL	C52-C51-CB5-OB7
9	M	920	LDA	C7-C8-C9-C10
12	M	800	CDL	C72-C71-CB7-OB9
10	H	709	GOL	O1-C1-C2-C3
13	M	801	PC9	C19-C20-C21-C22
9	H	901	LDA	N1-C1-C2-C3
9	H	903	LDA	N1-C1-C2-C3
9	M	907	LDA	C9-C10-C11-C12
9	H	904	LDA	C2-C3-C4-C5
9	H	901	LDA	C1-C2-C3-C4
13	M	802	PC9	C41-C42-C43-C44
6	L	402	BPH	C14-C13-C15-C16
9	L	906	LDA	C1-C2-C3-C4
5	M	311	BCL	C10-C11-C12-C13
5	M	311	BCL	C11-C12-C13-C15
13	M	802	PC9	O11-C11-C12-C13
13	M	802	PC9	O3-C11-C12-C13
13	M	802	PC9	C13-C14-C15-C16

There are no ring outliers.

19 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	906	LDA	4	0
7	M	501	U10	1	0
9	M	920	LDA	7	0

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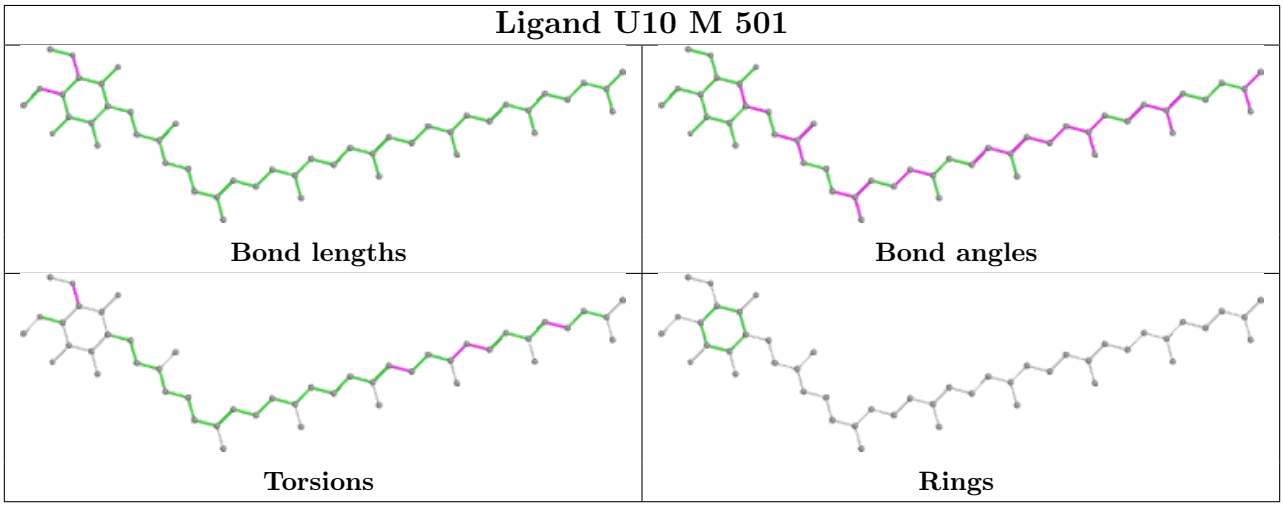
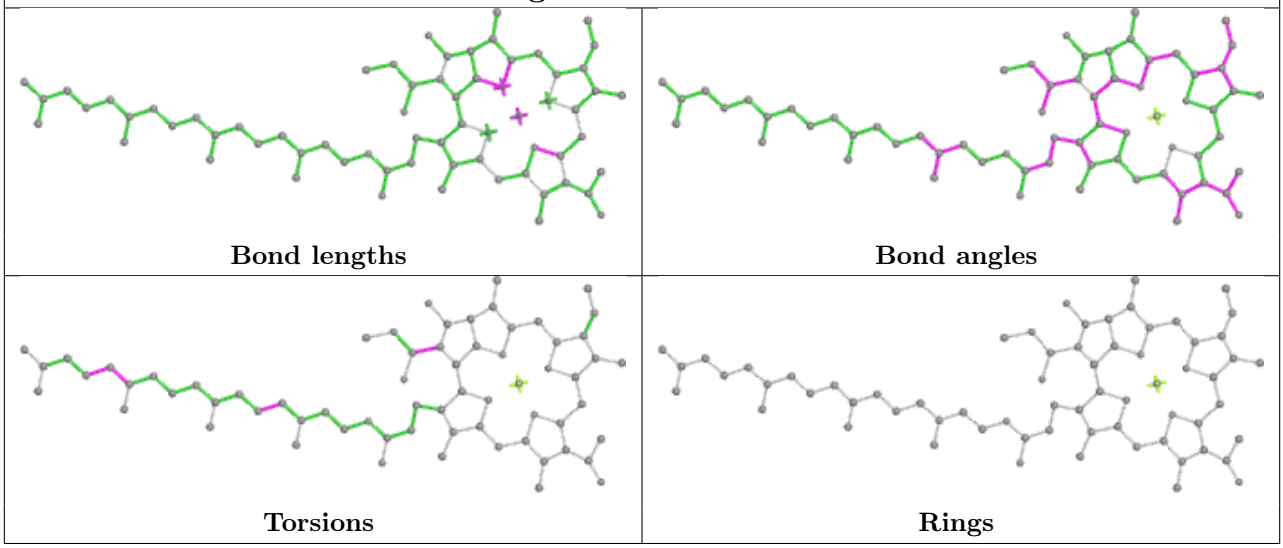
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	314	BCL	3	0
12	M	800	CDL	3	0
9	L	909	LDA	2	0
9	H	904	LDA	2	0
4	M	703	PO4	2	0
6	M	401	BPH	4	0
5	M	313	BCL	5	0
7	L	502	U10	8	0
13	M	802	PC9	9	0
6	L	402	BPH	3	0
5	M	311	BCL	10	0
9	H	903	LDA	6	0
9	L	908	LDA	6	0
5	L	312	BCL	3	0
9	H	902	LDA	1	0
13	M	801	PC9	14	0

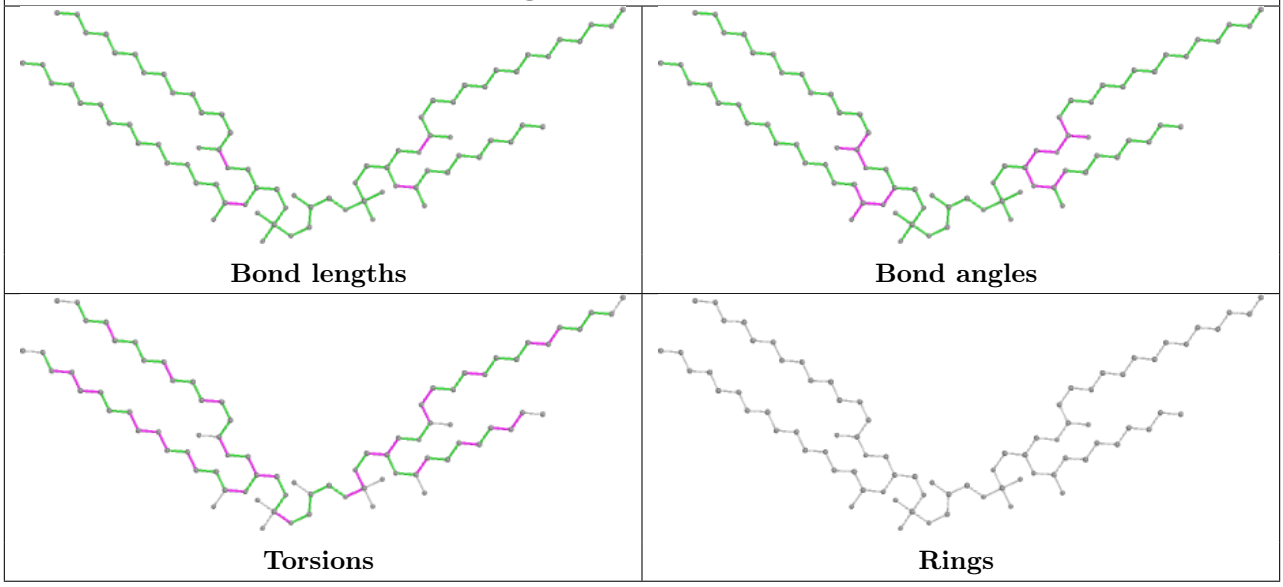
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



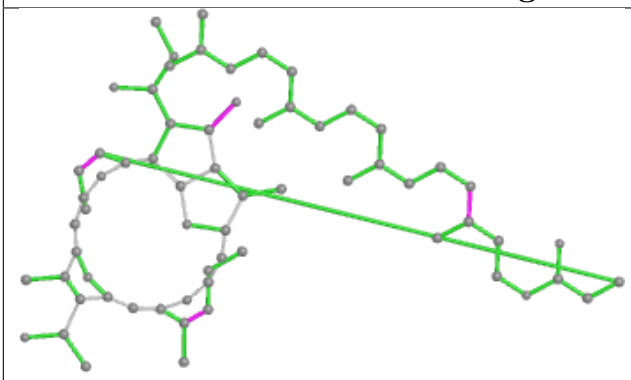
Ligand BCL L 314



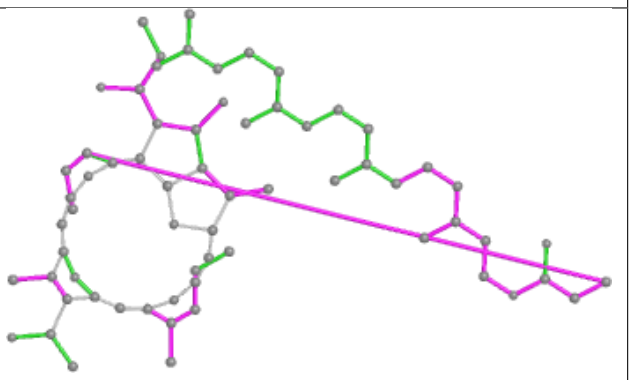
Ligand CDL M 800



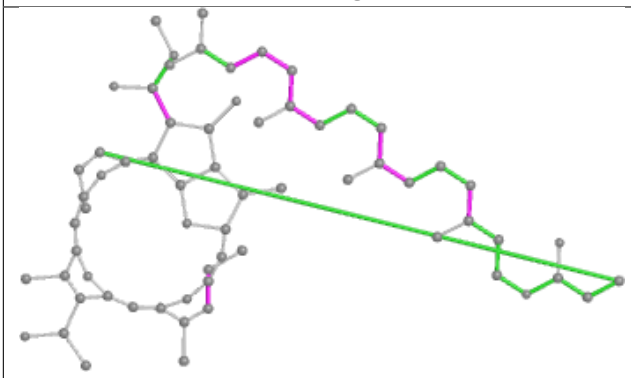
Ligand BPH M 401



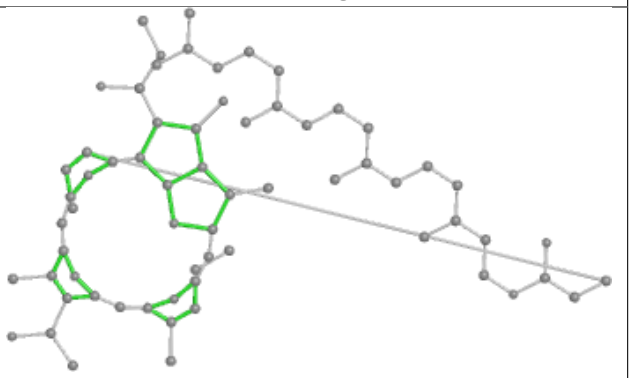
Bond lengths



Bond angles

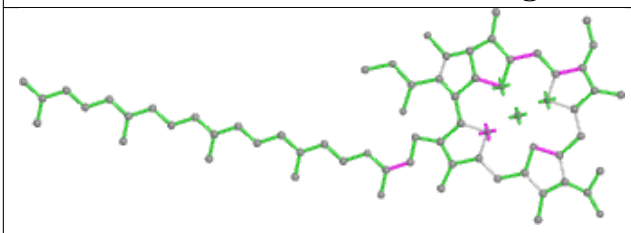


Torsions

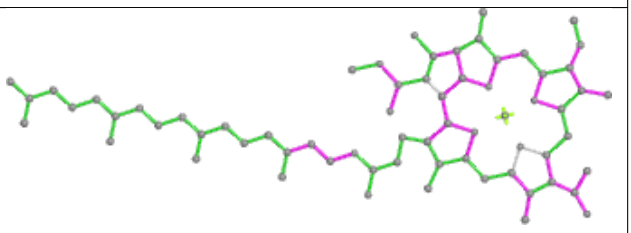


Rings

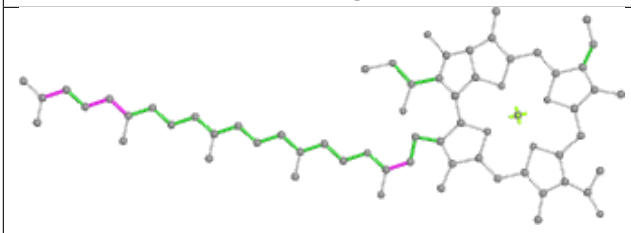
Ligand BCL M 313



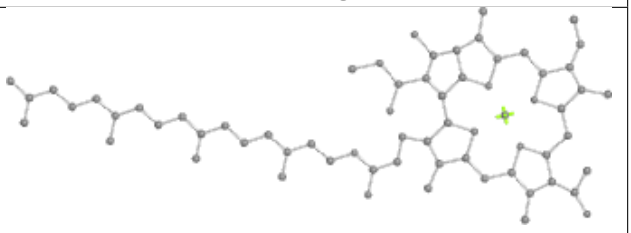
Bond lengths



Bond angles

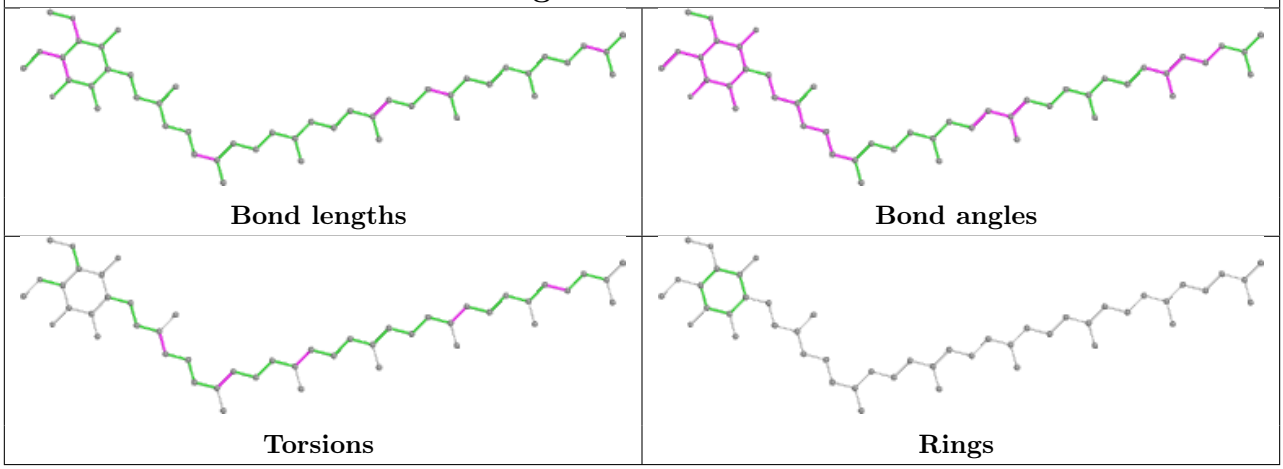


Torsions

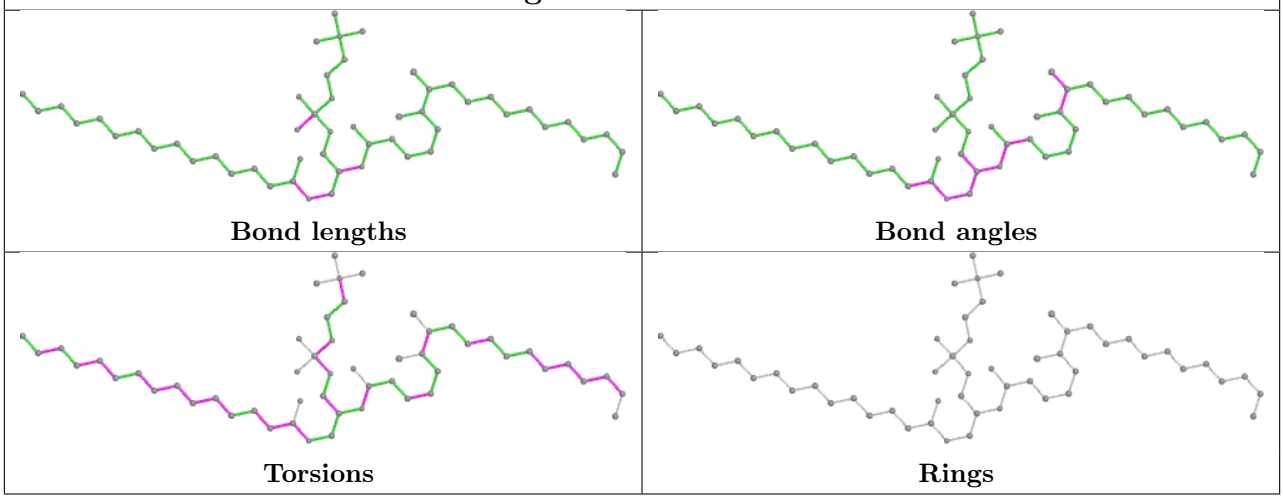


Rings

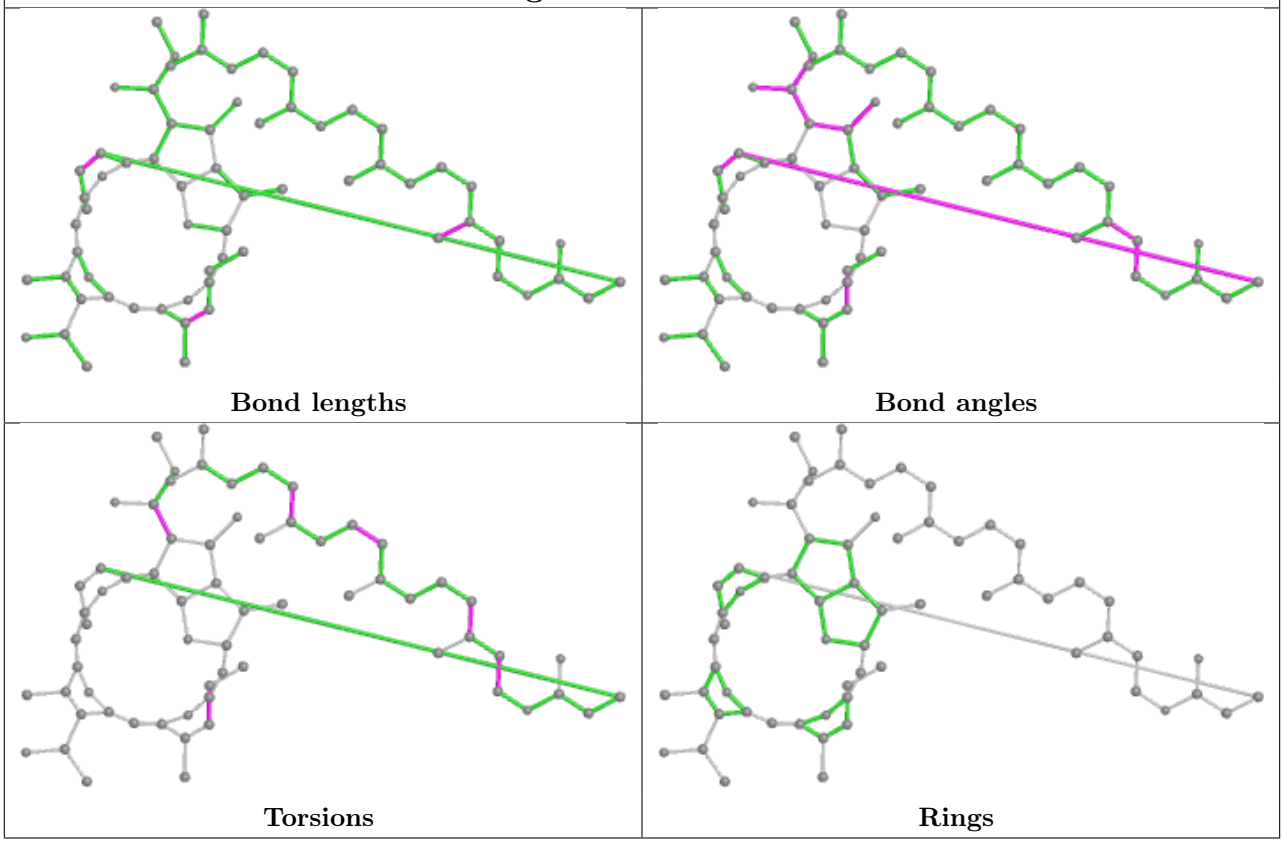
Ligand U10 L 502



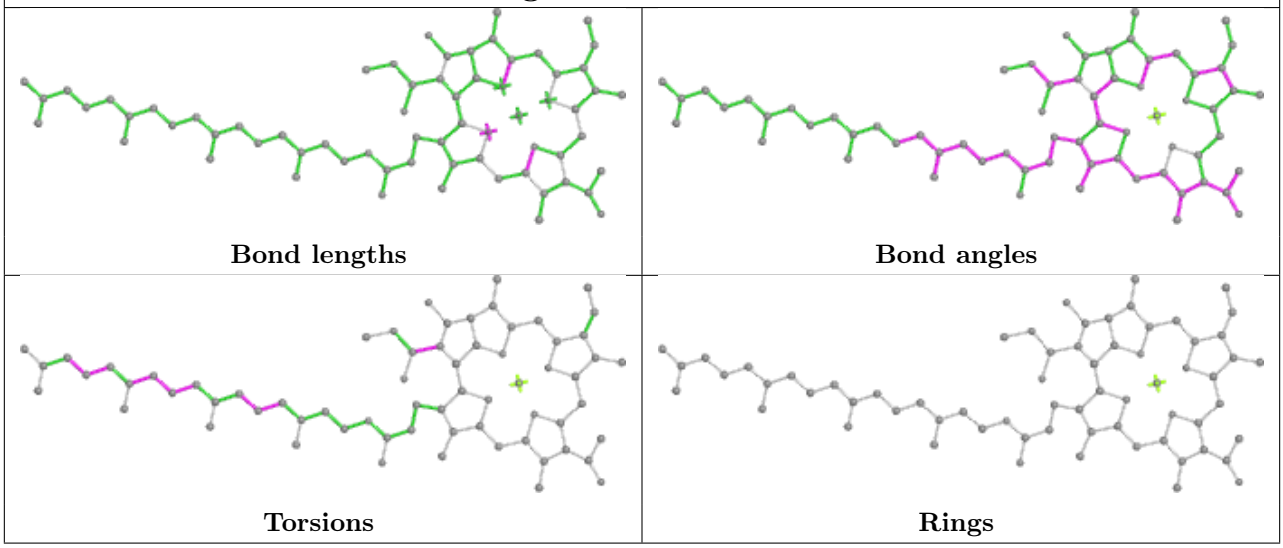
Ligand PC9 M 802



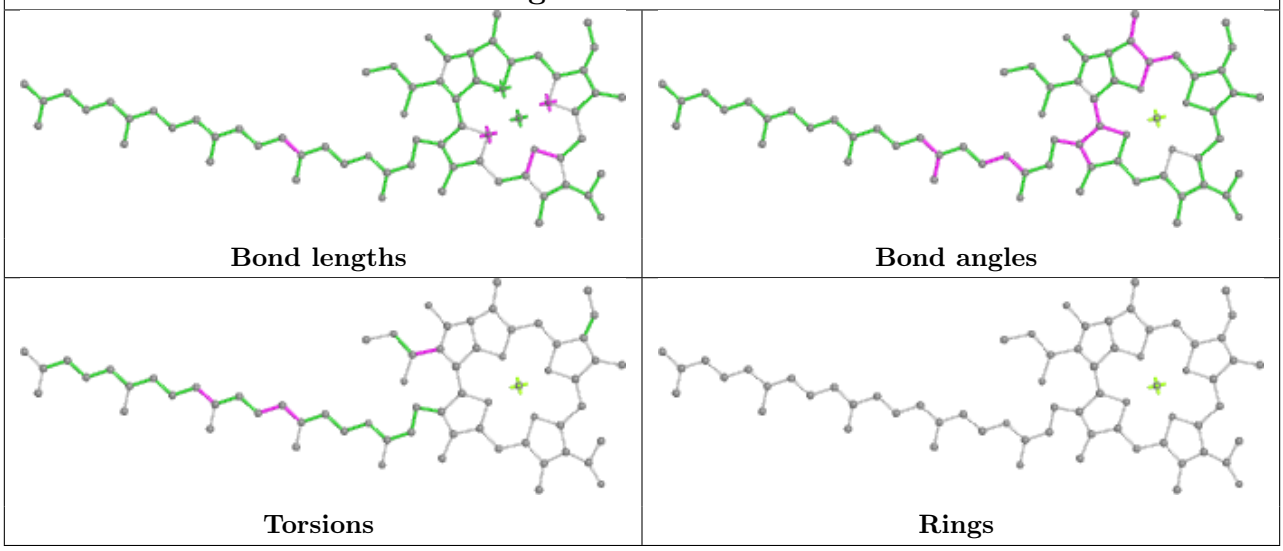
Ligand BPH L 402



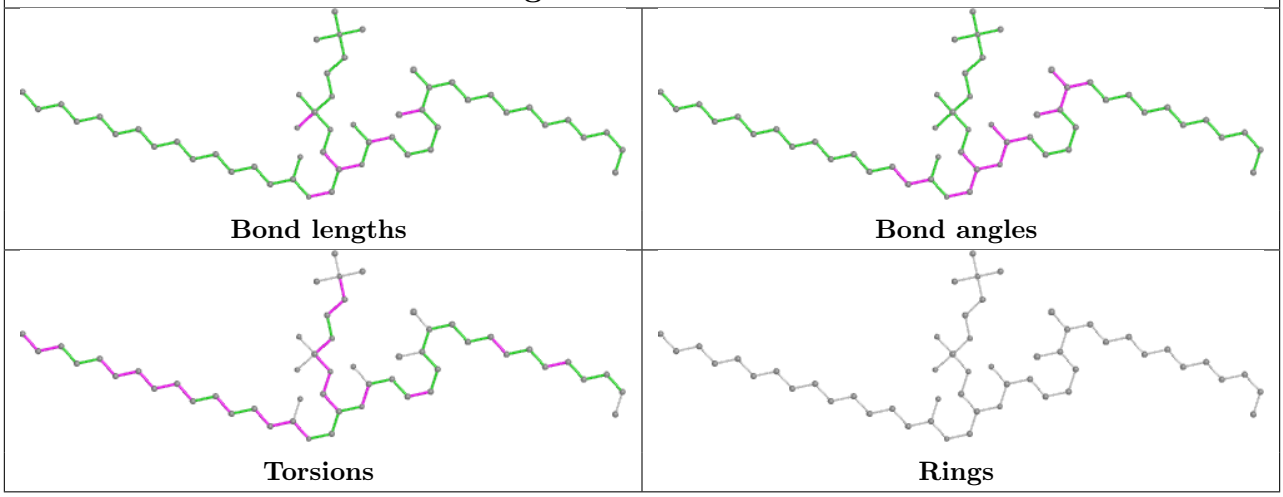
Ligand BCL M 311



Ligand BCL L 312



Ligand PC9 M 801



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, 95^{th} 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%)	-0.45	9 (3%) 47 48	42, 51, 63, 72	0
2	M	302/307 (98%)	-0.15	13 (4%) 35 33	40, 51, 61, 88	1 (0%)
3	H	240/260 (92%)	-0.29	6 (2%) 57 59	39, 51, 59, 83	0
All	All	823/848 (97%)	-0.30	28 (3%) 45 45	39, 51, 62, 88	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.7
1	L	271	TRP	4.2
2	M	1	ALA	3.8
1	L	270	PRO	3.6
1	L	269	LEU	3.1
1	L	275	ILE	3.1
2	M	2[A]	GLU	3.1
2	M	302	GLY	3.1
1	L	276[A]	PRO	2.8
1	L	281	GLY	2.8
1	L	59	TRP	2.7
2	M	301[A]	HIS	2.7
3	H	51	ALA	2.7
2	M	80	TRP	2.6
3	H	52	ASN	2.5
1	L	277	GLY	2.5
1	L	279	ILE	2.4
3	H	245	ALA	2.4
2	M	27	ALA	2.4
2	M	300[A]	ASN	2.4
2	M	3	TYR	2.3
3	H	220	LYS	2.3
3	H	159	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	26	LEU	2.2
2	M	244	ALA	2.1
2	M	265	ILE	2.1
2	M	106	ALA	2.0
2	M	28	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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
9	LDA	L	905	16/16	0.26	1.20	61,66,70,71	16
9	LDA	L	909	16/16	0.50	0.45	50,54,71,73	16
9	LDA	H	903	16/16	0.54	0.47	49,55,63,63	16
9	LDA	H	902	16/16	0.56	0.59	64,66,72,72	16
9	LDA	H	901	16/16	0.57	0.49	52,55,66,66	16
9	LDA	M	920	16/16	0.66	0.70	49,53,65,66	16
13	PC9	M	802	54/54	0.66	0.52	42,54,70,73	54
13	PC9	M	801	54/54	0.71	0.48	30,52,79,80	54
10	GOL	H	709	6/6	0.71	0.23	50,51,52,53	6
9	LDA	L	906	16/16	0.72	0.45	51,55,69,70	16
7	U10	L	502	48/63	0.73	0.45	37,56,66,67	48
12	CDL	M	800	81/100	0.74	0.37	50,69,80,87	81
9	LDA	L	908	16/16	0.75	0.44	51,59,72,73	16
4	PO4	M	703	5/5	0.75	0.38	64,65,66,67	5
9	LDA	H	904	16/16	0.80	0.44	60,62,66,66	16
9	LDA	M	907	16/16	0.81	0.30	60,64,70,71	16
10	GOL	L	707	6/6	0.85	0.28	58,61,62,66	6
8	HTO	L	705	10/10	0.88	0.41	56,60,62,65	10

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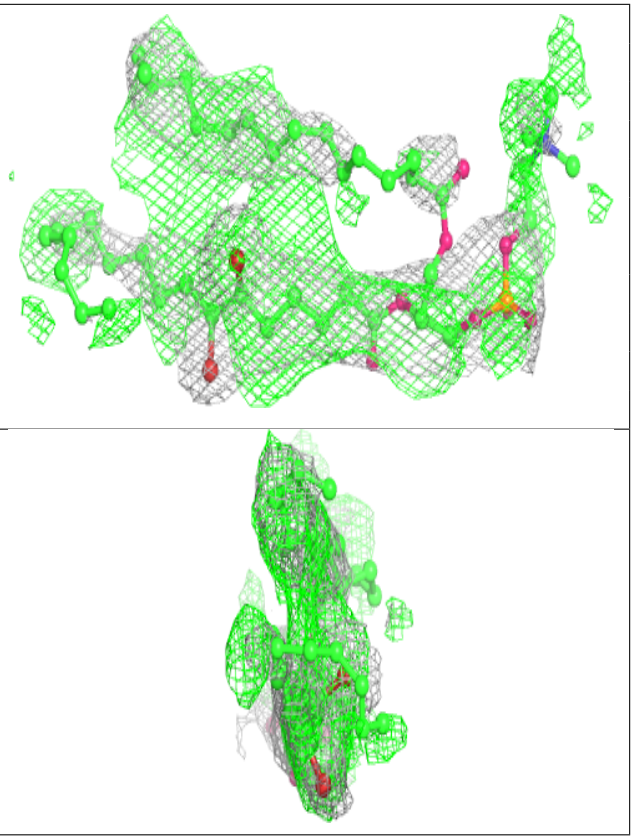
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	L	701	5/5	0.88	0.32	65,65,66,67	5
6	BPH	M	401	65/65	0.90	0.20	44,52,96,97	0
7	U10	M	501	48/63	0.91	0.22	46,54,80,83	0
4	PO4	L	702	5/5	0.93	0.16	64,65,66,68	5
10	GOL	L	708	6/6	0.95	0.27	49,57,59,60	0
10	GOL	H	706	6/6	0.95	0.45	59,62,63,65	6
5	BCL	M	311	66/66	0.96	0.21	41,51,103,104	0
4	PO4	M	704	5/5	0.96	0.19	54,54,56,58	5
5	BCL	L	312	66/66	0.97	0.12	40,48,55,59	0
5	BCL	M	313	66/66	0.97	0.14	41,48,72,80	0
6	BPH	L	402	65/65	0.97	0.12	42,49,55,56	0
5	BCL	L	314	66/66	0.98	0.11	38,46,66,73	0
14	K	H	700	1/1	0.98	0.13	52,52,52,52	0
11	FE	M	500	1/1	1.00	0.14	52,52,52,52	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.

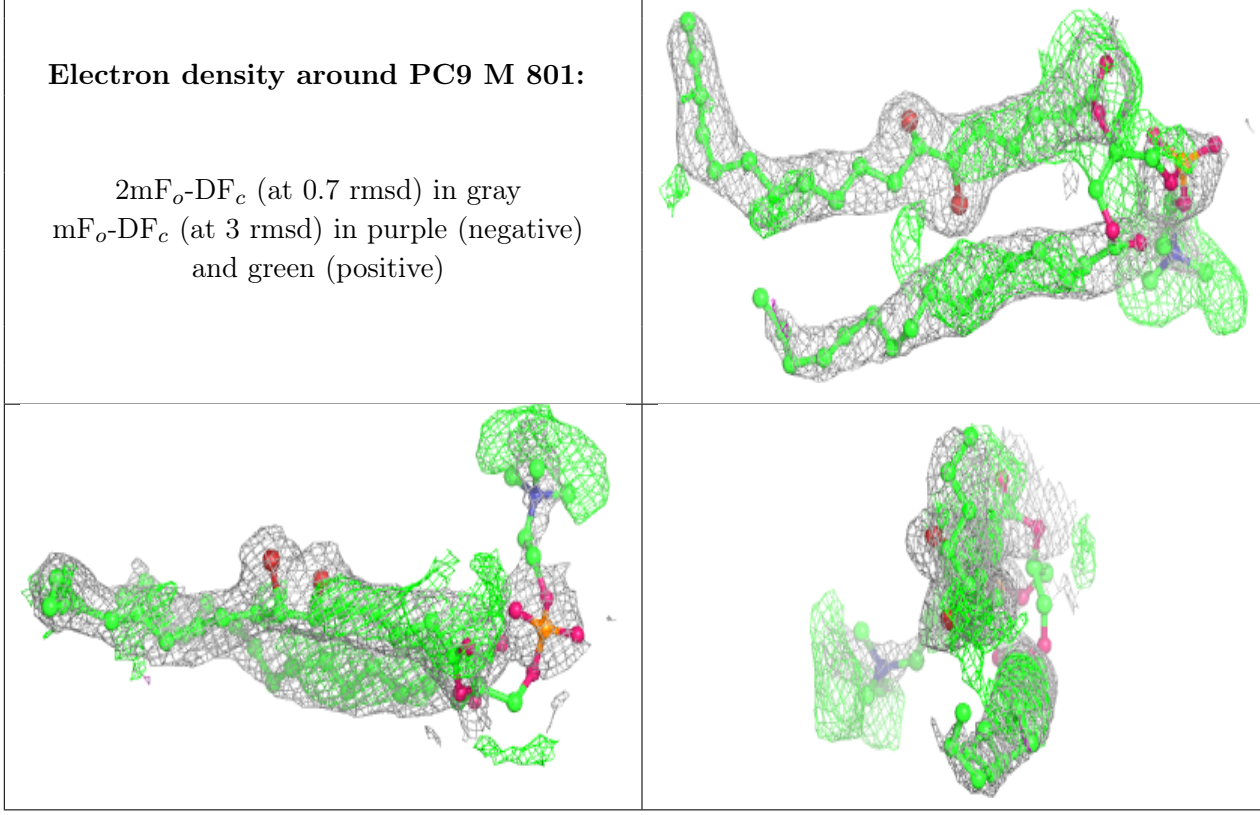
Electron density around PC9 M 802:

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



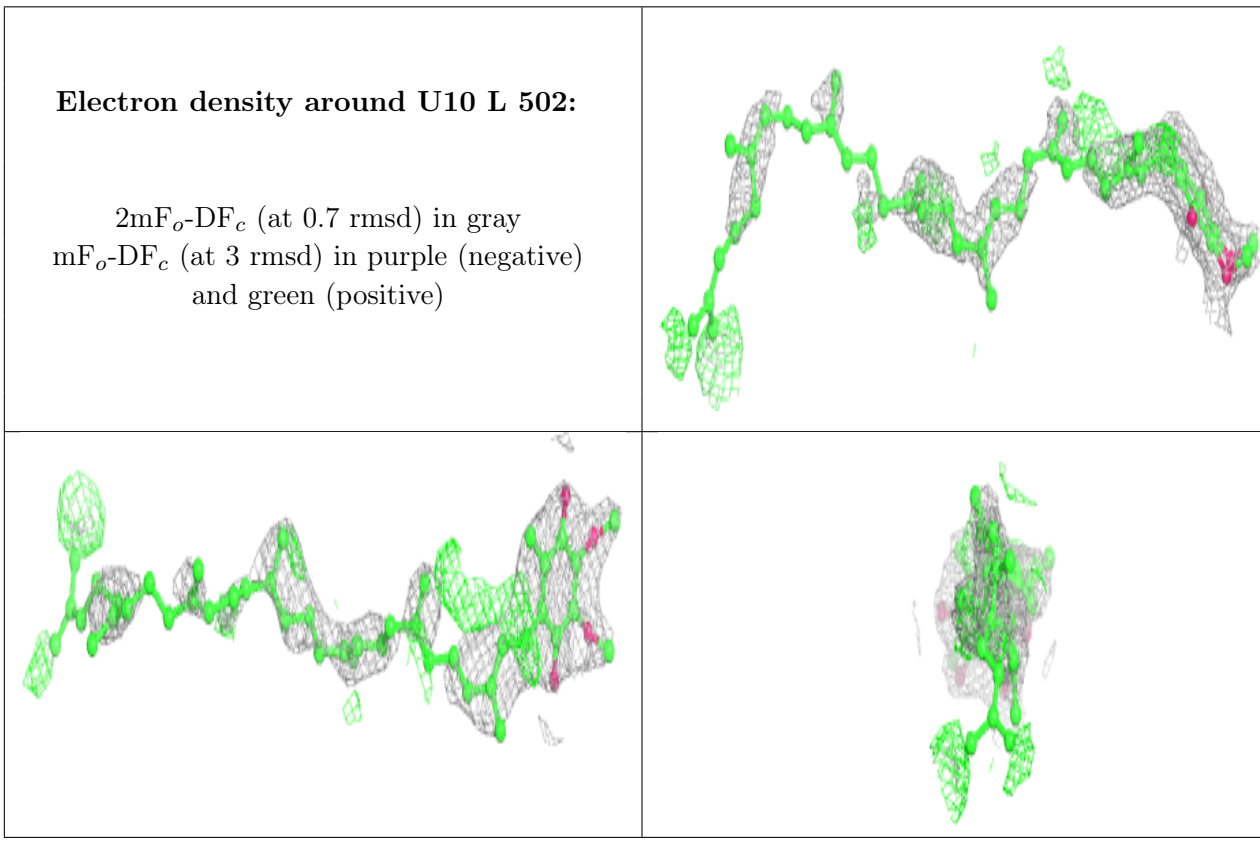
Electron density around PC9 M 801:

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



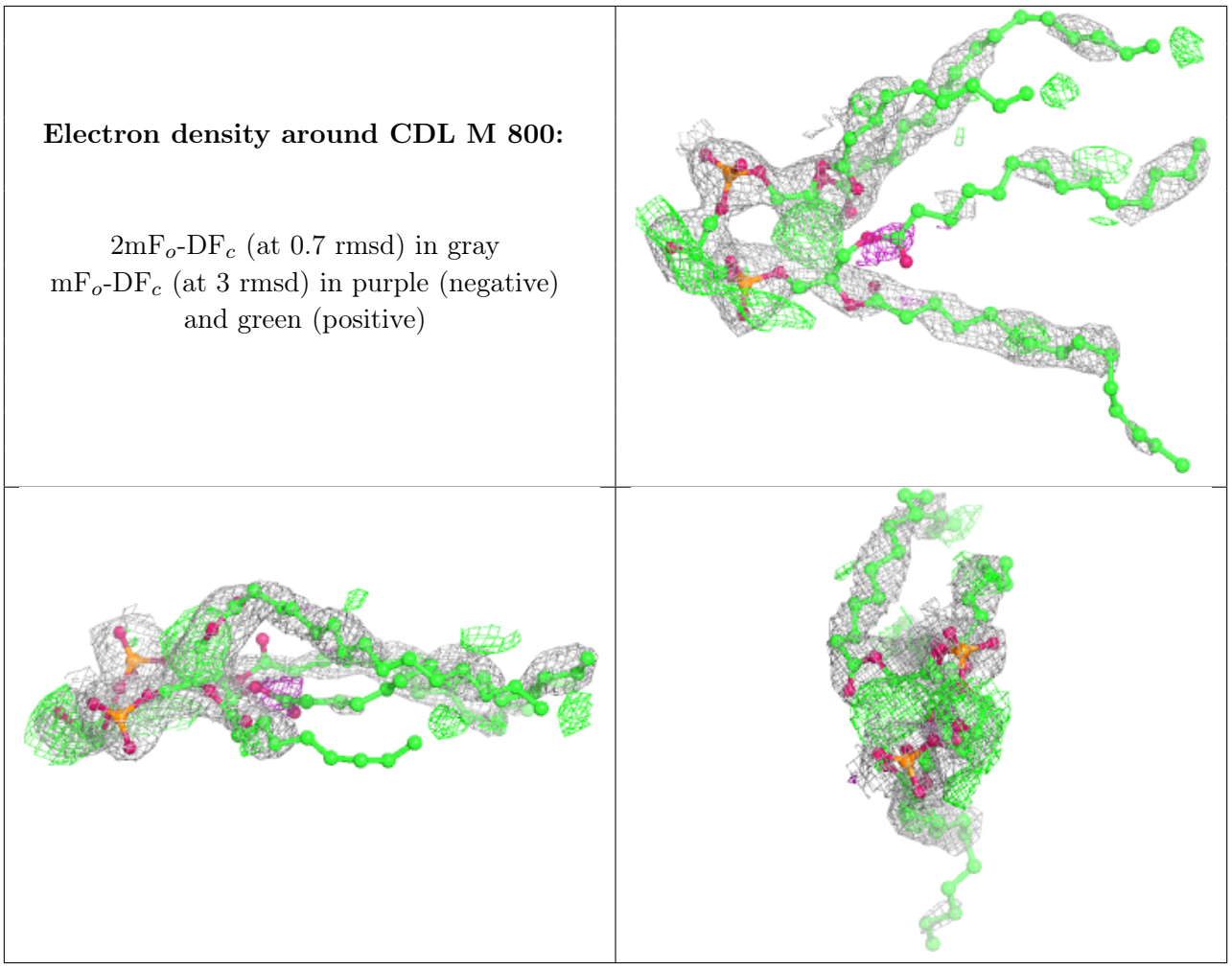
Electron density around U10 L 502:

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



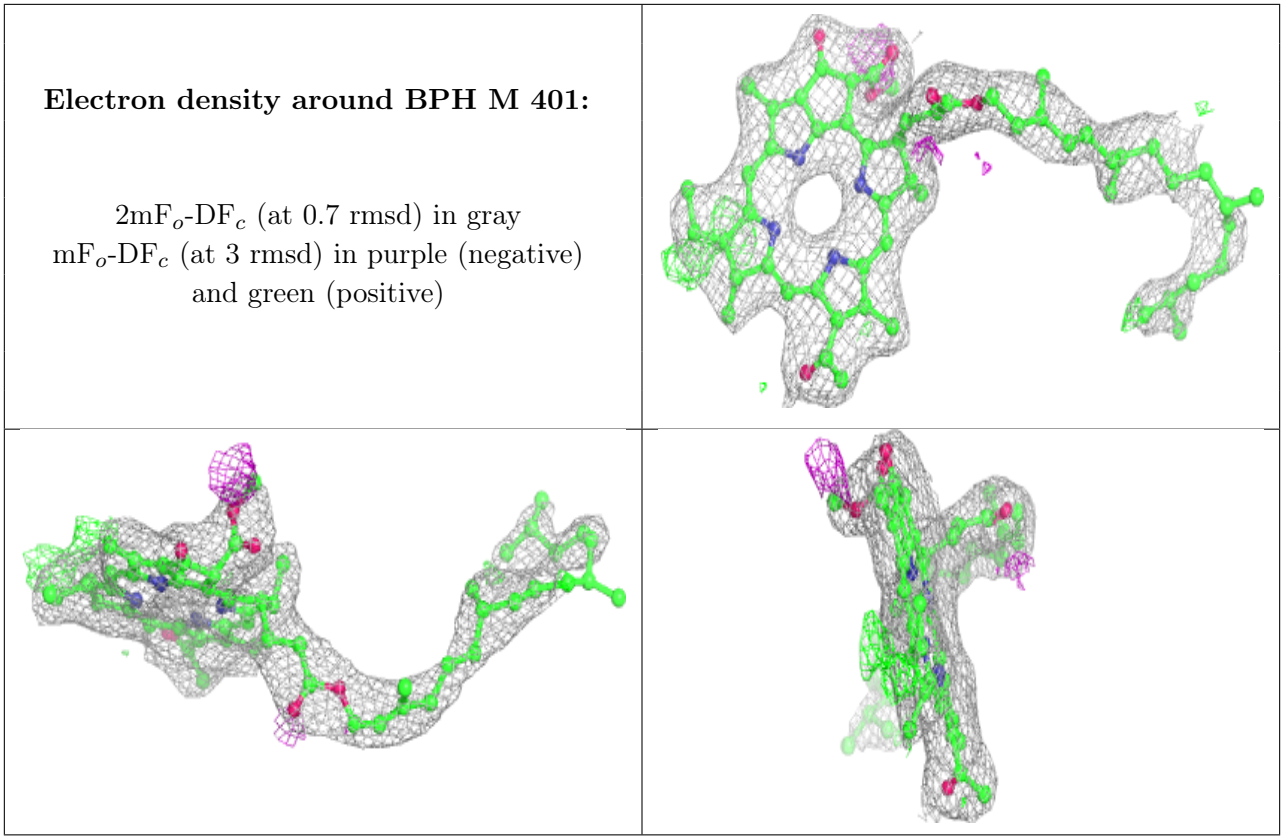
Electron density around CDL M 800:

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



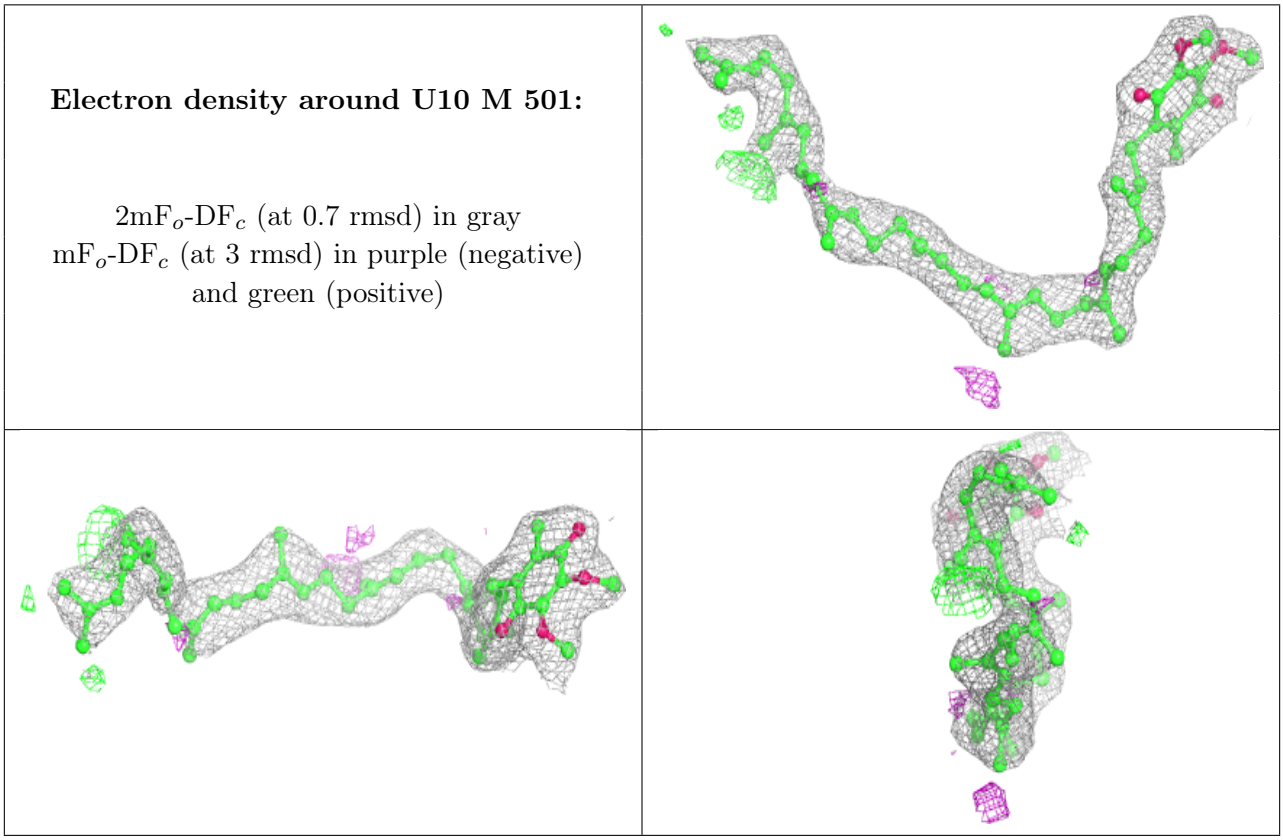
Electron density around BPH M 401:

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



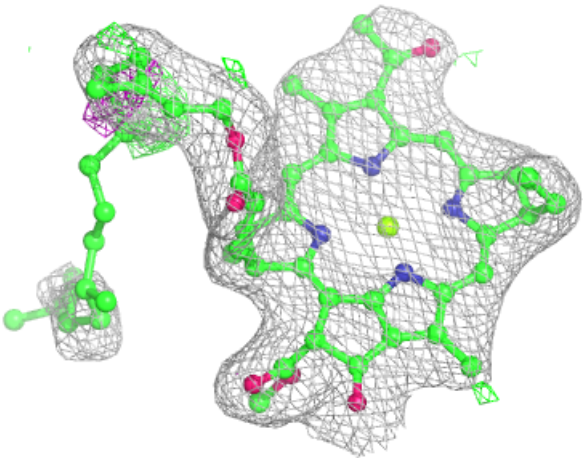
Electron density around U10 M 501:

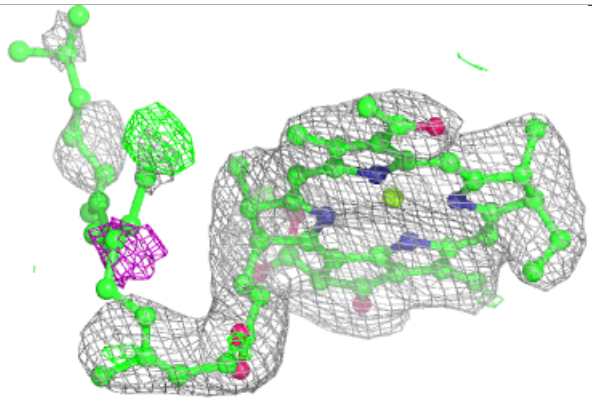
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

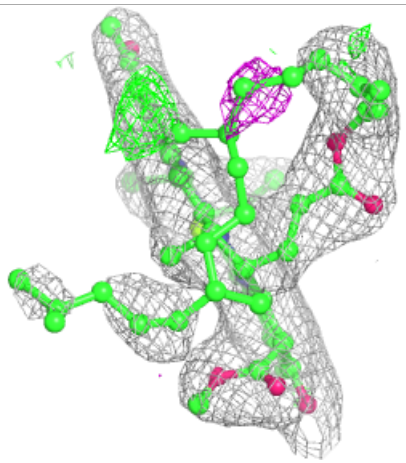


Electron density around BCL M 311:

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

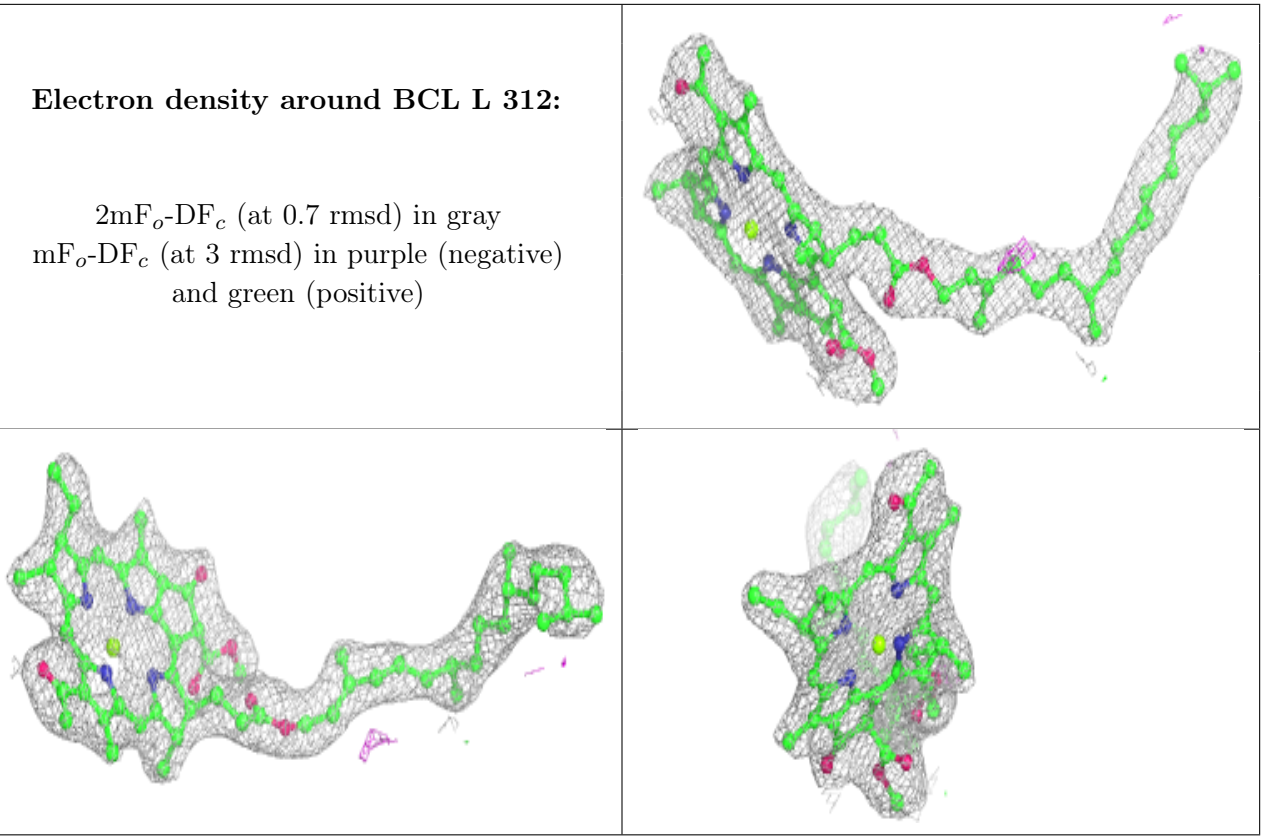






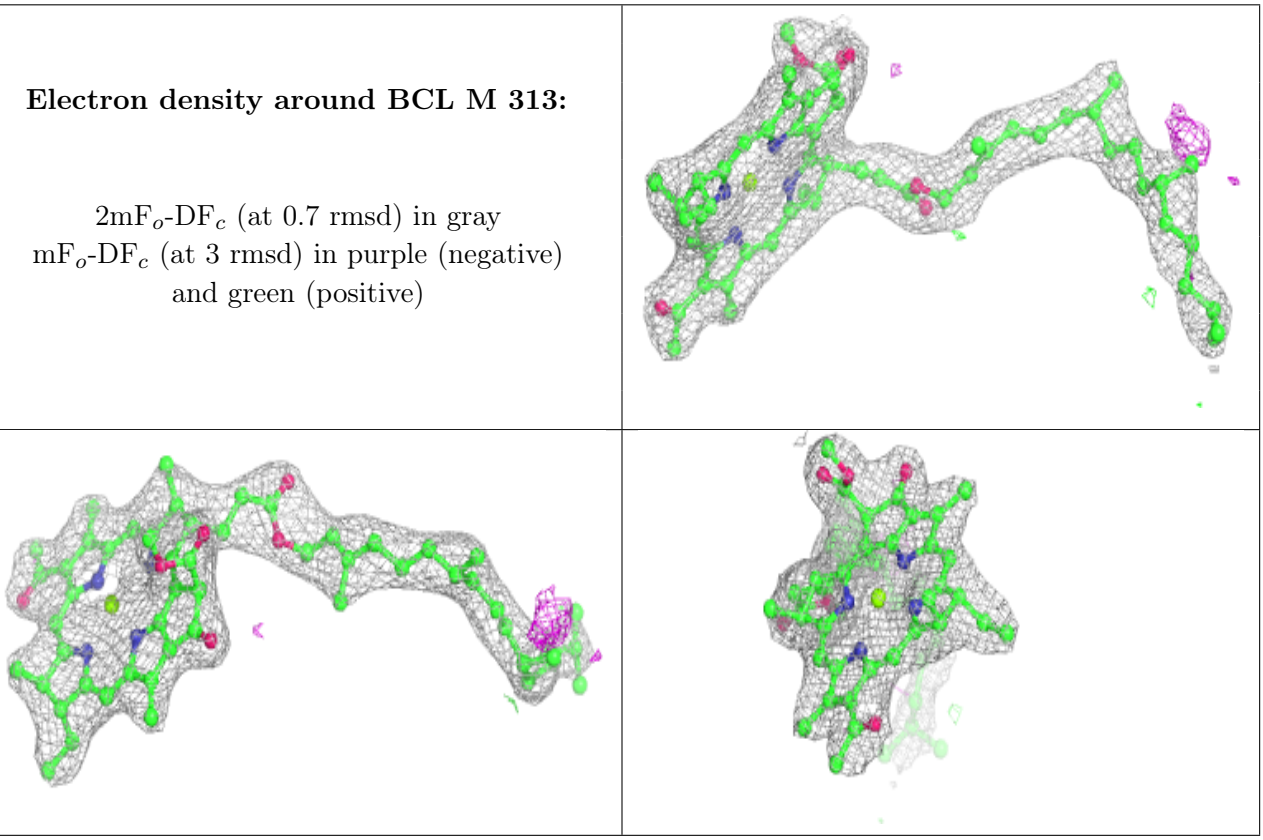
Electron density around BCL L 312:

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



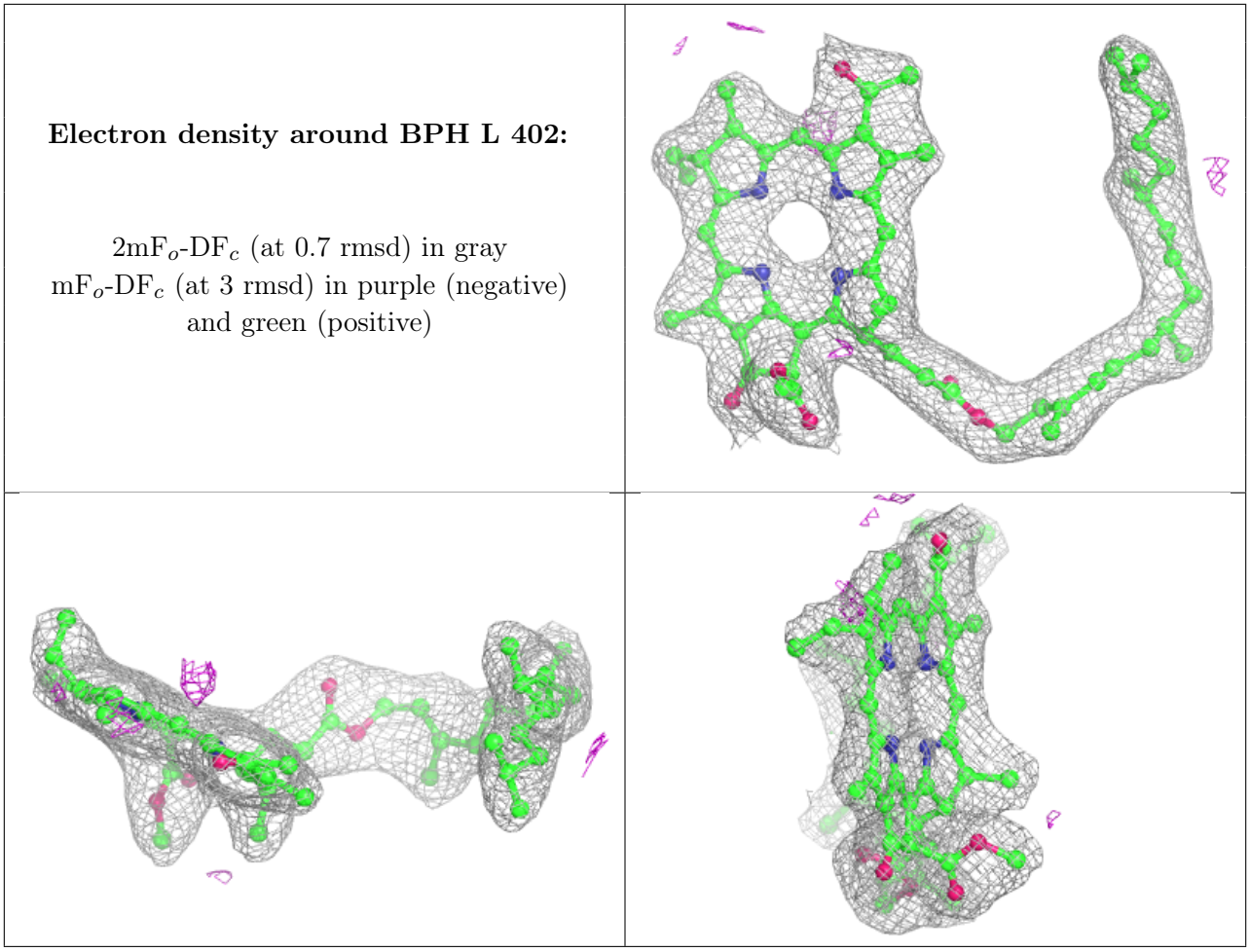
Electron density around BCL M 313:

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



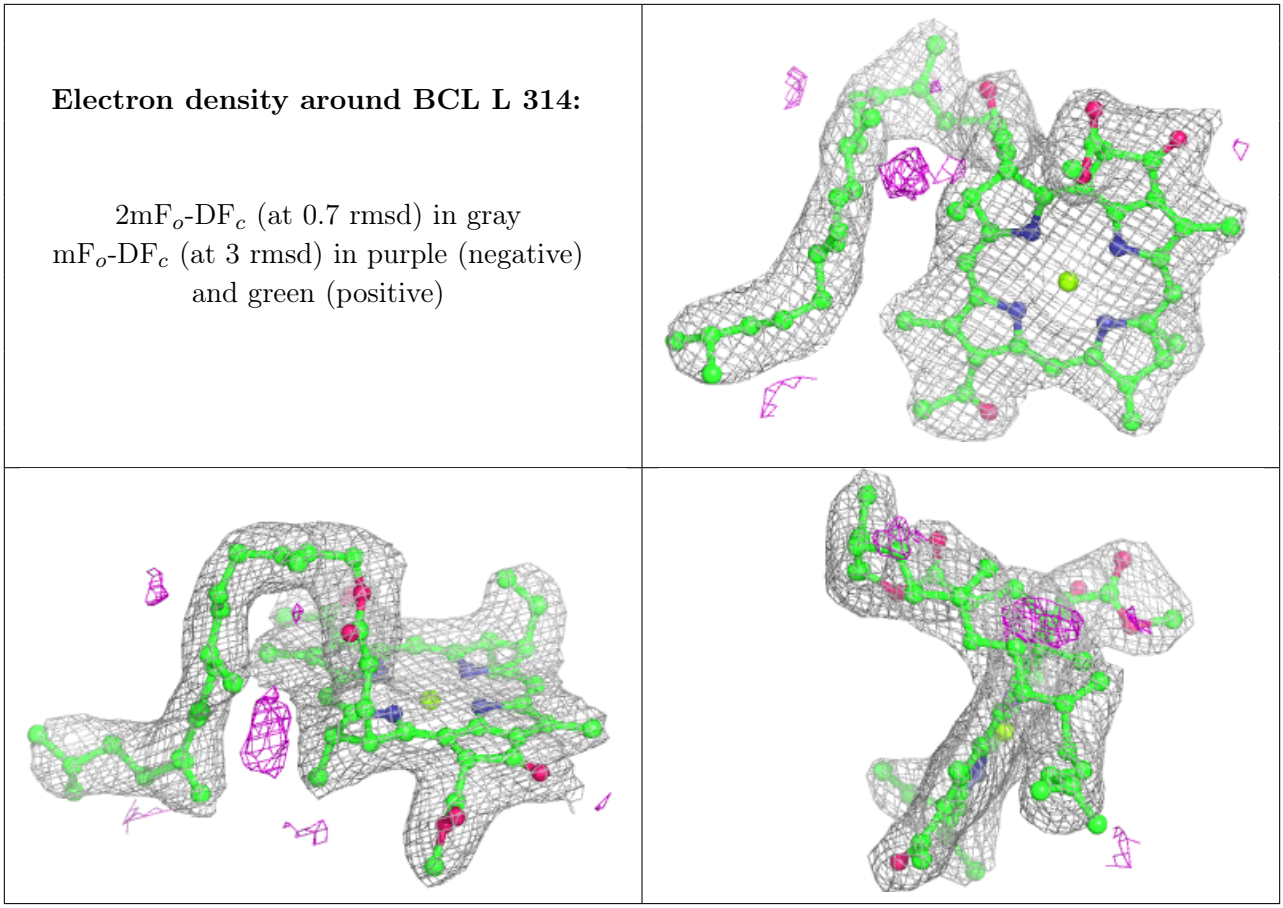
Electron density around BPH L 402:

$2mF_o$-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 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.