Full wwPDB X-ray Structure Validation Report (i)

Feb 8, 2024 – 11:17 AM EST

PDB ID	:	2HH1
Title	:	Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylcholine
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2006-06-27
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

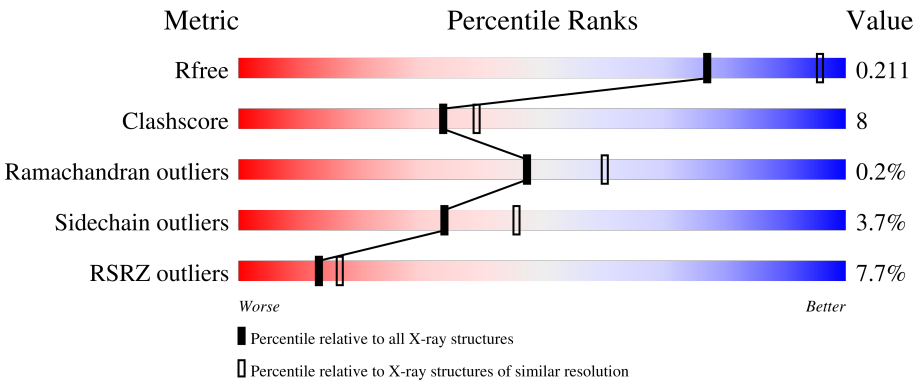
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	9% 89% 10% •
2	M	307	10% 83% 14% • •
3	H	260	3% 85% 7% • 6%

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
14	PC7	H	801	-	-	-	X
15	GOL	H	708	-	-	-	X
7	U10	L	502	-	-	-	X
8	PC9	L	802	-	-	X	X
9	LDA	H	903	-	-	-	X
9	LDA	H	904	-	-	-	X
9	LDA	H	905	-	-	-	X
9	LDA	L	902	-	-	-	X
9	LDA	M	907	-	-	-	X
9	LDA	M	920	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7923 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	2234	1508	355	363	8	0	2	0

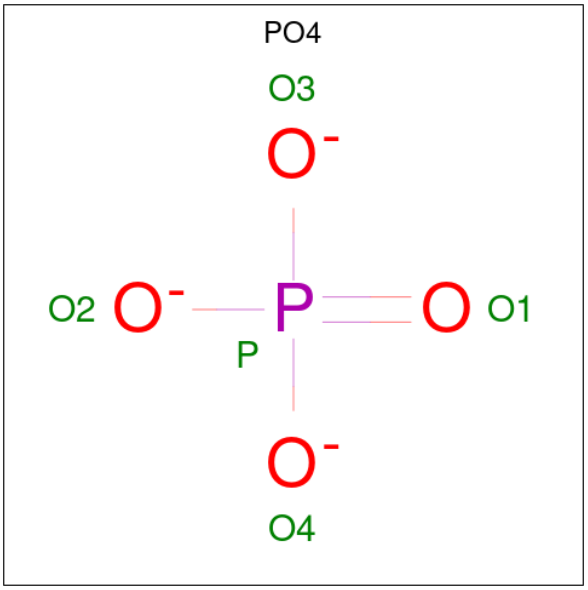
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2466	1643	403	409	11	0	9	0

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

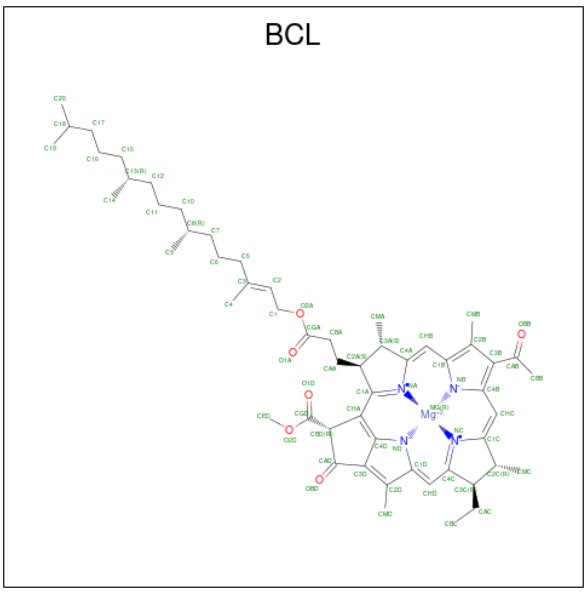
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	244	1891	1207	328	346	10	0	9	0

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



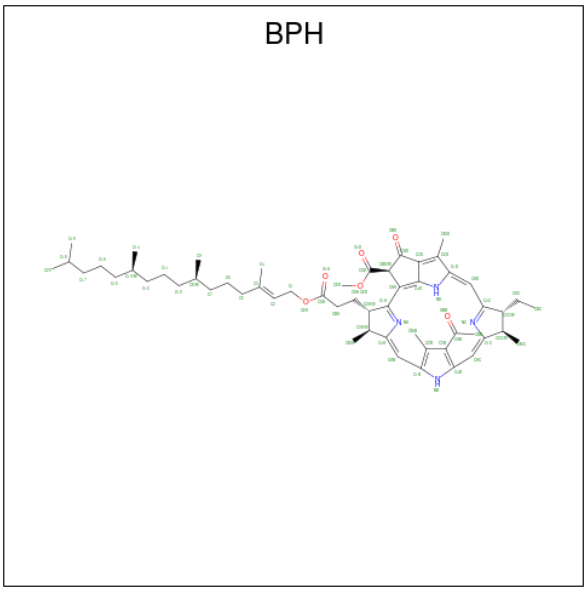
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
4	L	1	5	4	1		0	0
			Total	O	P			
4	M	1	5	4	1		0	0
			Total	O	P			
4	M	1	5	4	1		0	0
			Total	O	P			
4	M	1	5	4	1		0	0

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



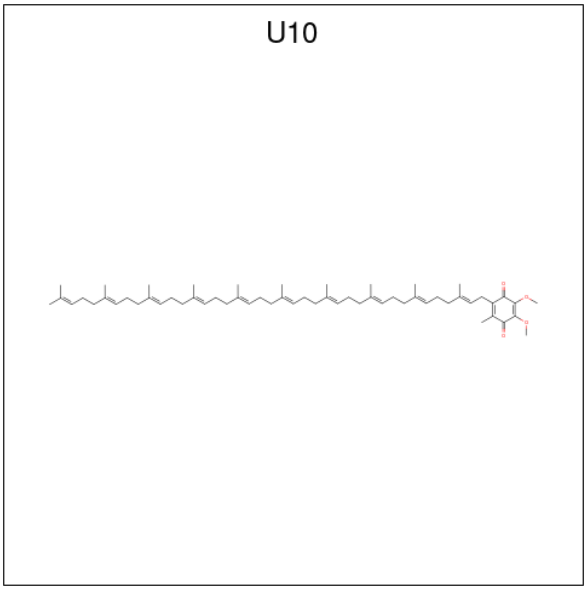
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

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



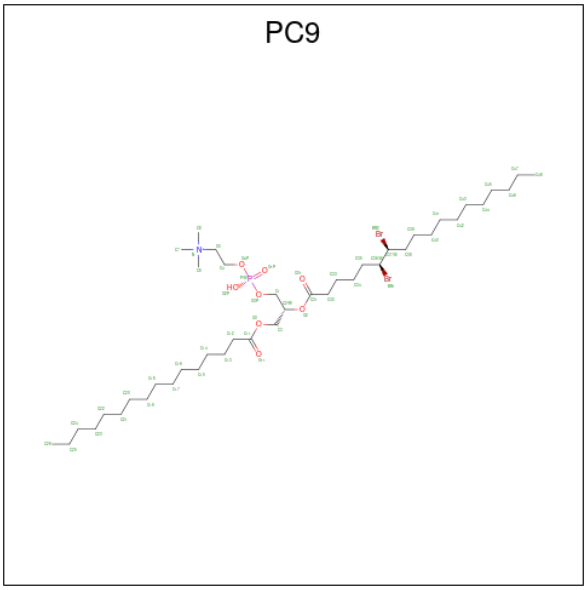
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	65	55	4	6	0	0
6	M	1	65	55	4	6	0	0

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



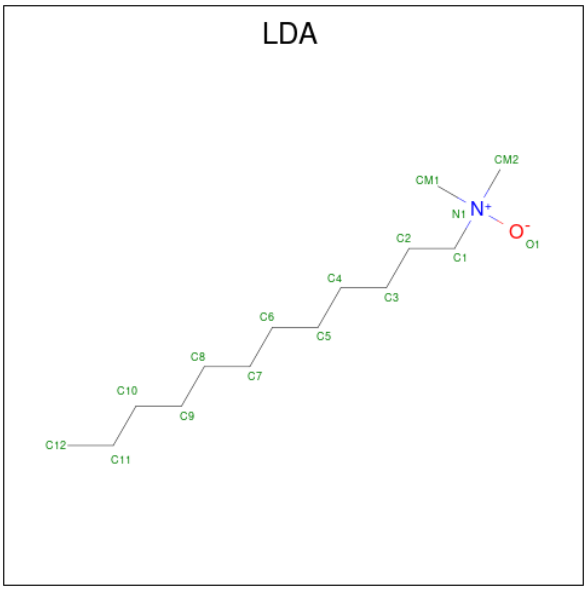
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	L	1	48	44	4	0	0
7	M	1	48	44	4	0	0

- Molecule 8 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
			Total	Br	C	N	O	P		
8	L	1	54	2	42	1	8	1	0	0

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

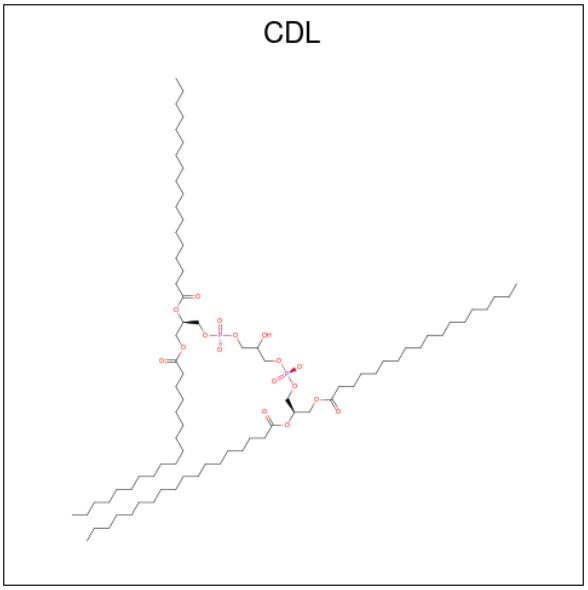


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	L	1	16	14	1	1	0	0
			Total	C	N	O		
9	L	1	16	14	1	1	0	0
			Total	C	N	O		
9	M	1	16	14	1	1	0	0
			Total	C	N	O		
9	M	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0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

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

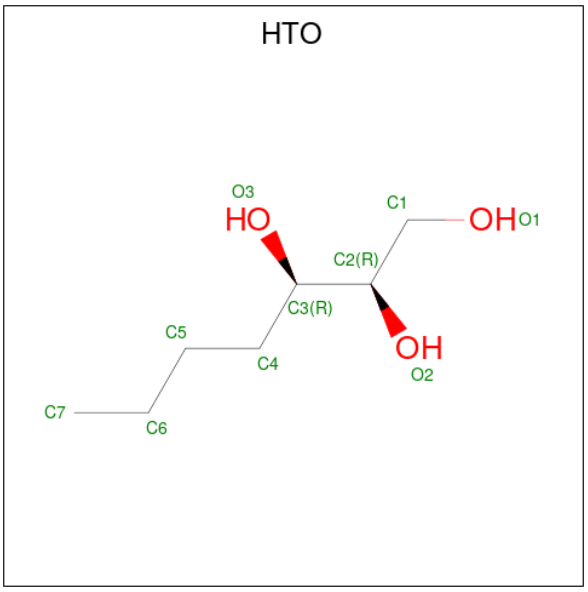


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
11	M	1	81	62	17	2	0	0

- Molecule 12 is POTASSIUM ION (three-letter code: K) (formula: K).

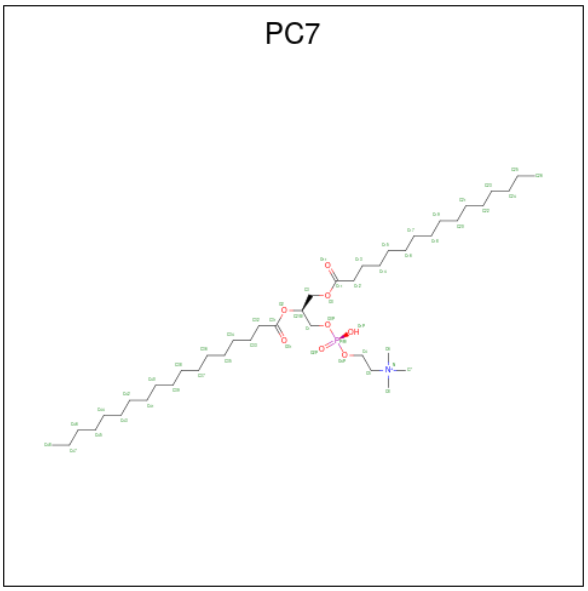
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total K 1 1	0	0

- Molecule 13 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



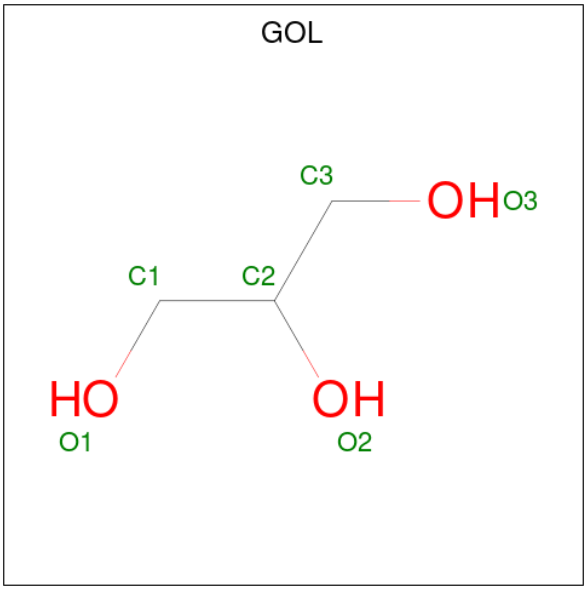
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total C O 10 7 3	0	0

- Molecule 14 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$).



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

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

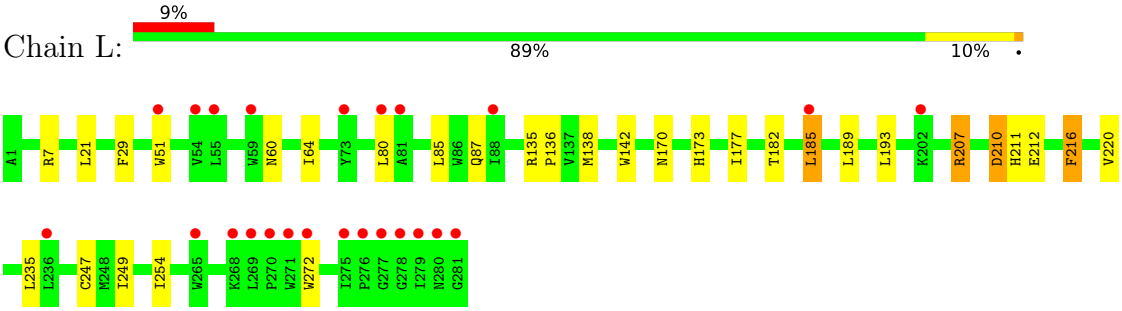
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	L	113	113	113	0	0
			Total	O		
16	M	139	139	139	0	0
			Total	O		
16	H	225	225	225	0	0

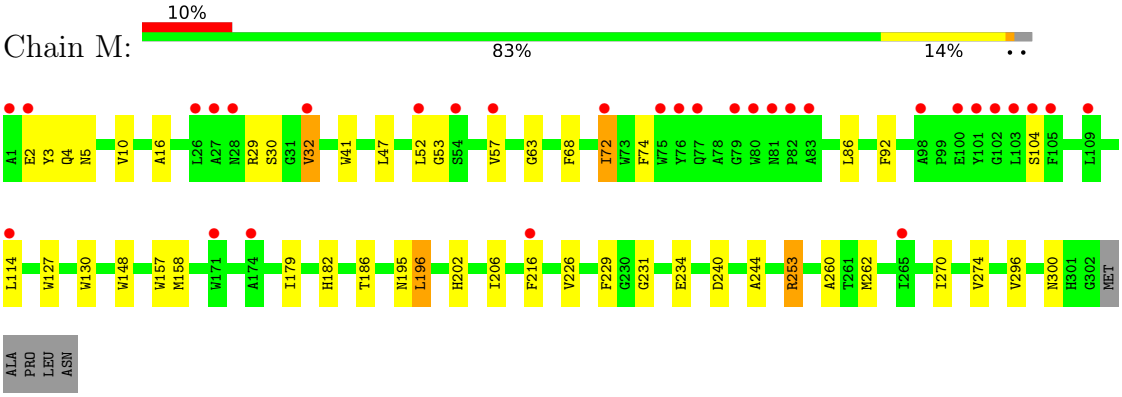
3 Residue-property plots (i)

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.

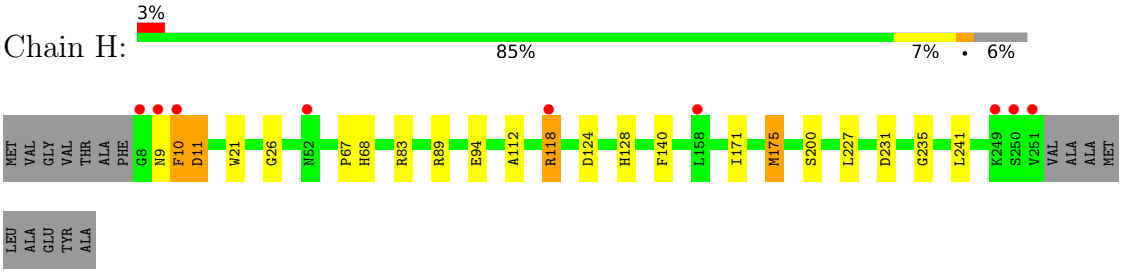
• Molecule 1: Reaction center protein L chain



• 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	139.54Å 139.54Å 183.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.03 – 2.55 45.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.03-2.55) 100.0 (45.68-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.210 0.182 , 0.211	Depositor DCC
R_{free} test set	3362 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: U10, LDA, HTO, K, PC9, BPH, FE, CDL, GOL, PO4, PC7, 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	0.89	0/2334	0.75	2/3194 (0.1%)
2	M	0.88	1/2590 (0.0%)	0.80	5/3532 (0.1%)
3	H	0.93	0/1986	0.86	3/2697 (0.1%)
All	All	0.90	1/6910 (0.0%)	0.80	10/9423 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	260	ALA	CA-CB	5.14	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	253[A]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	M	253[B]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
3	H	83	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	L	210	ASP	CB-CG-OD1	5.57	123.32	118.30
1	L	7	ARG	NE-CZ-NH2	5.51	123.05	120.30
3	H	124	ASP	CB-CG-OD1	5.42	123.18	118.30
2	M	240	ASP	CB-CG-OD1	5.33	123.09	118.30
3	H	83	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	M	29	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	M	29	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2234	0	2193	21	0
2	M	2466	0	2371	35	0
3	H	1891	0	1902	14	0
4	L	5	0	0	1	0
4	M	15	0	0	0	0
5	L	132	0	148	6	0
5	M	132	0	148	19	0
6	L	65	0	75	0	0
6	M	65	0	76	11	0
7	L	48	0	63	12	0
7	M	48	0	63	1	0
8	L	54	0	80	36	0
9	H	64	0	124	7	0
9	L	32	0	62	1	0
9	M	32	0	62	1	0
10	M	1	0	0	0	0
11	M	81	0	106	2	0
12	H	1	0	0	0	0
13	H	10	0	16	1	0
14	H	52	0	84	8	0
15	H	18	0	24	2	0
16	H	225	0	0	2	0
16	L	113	0	0	1	0
16	M	139	0	0	3	0
All	All	7923	0	7597	128	0

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

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:802:PC9:H442	8:L:802:PC9:C48	1.58	1.26
8:L:802:PC9:H482	8:L:802:PC9:C44	1.67	1.19
7:L:502:U10:H351	7:L:502:U10:H38	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:802:PC9:H483	6:M:401:BPH:HED1	1.40	1.03
7:L:502:U10:H153	8:L:802:PC9:H471	1.38	1.02
1:L:189:LEU:CD1	8:L:802:PC9:H472	1.96	0.95
8:L:802:PC9:C48	8:L:802:PC9:C44	2.29	0.94
14:H:801:PC7:H73	9:H:905:LDA:H112	1.50	0.92
14:H:801:PC7:H451	9:H:901:LDA:H122	1.53	0.89
7:L:502:U10:H351	7:L:502:U10:C38	2.04	0.87
7:L:502:U10:H153	8:L:802:PC9:C47	2.03	0.87
2:M:253[B]:ARG:NH1	16:M:1468:HOH:O	2.07	0.85
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.59	0.84
5:M:311:BCL:H41	5:M:311:BCL:H71	1.61	0.81
8:L:802:PC9:C26	6:M:401:BPH:HED2	2.12	0.79
14:H:801:PC7:H431	9:H:901:LDA:H121	1.69	0.75
8:L:802:PC9:H483	6:M:401:BPH:CED	2.17	0.73
14:H:801:PC7:O31	14:H:801:PC7:H32	1.87	0.72
7:L:502:U10:C15	8:L:802:PC9:H471	2.18	0.69
1:L:189:LEU:HD12	8:L:802:PC9:H472	1.72	0.69
8:L:802:PC9:H231	5:M:313:BCL:C20	2.23	0.69
2:M:2[B]:GLU:O	2:M:4:GLN:NE2	2.26	0.68
5:L:314:BCL:HMB1	5:L:314:BCL:HBB2	1.77	0.67
8:L:802:PC9:C23	5:M:313:BCL:C20	2.73	0.66
3:H:128[B]:HIS:HD1	15:H:708:GOL:C2	2.09	0.65
5:M:311:BCL:H41	5:M:311:BCL:C7	2.19	0.65
5:M:311:BCL:H102	5:M:313:BCL:H191	1.79	0.65
8:L:802:PC9:H52	2:M:30:SER:HA	1.79	0.64
8:L:802:PC9:H442	8:L:802:PC9:H482	0.75	0.64
8:L:802:PC9:C23	5:M:313:BCL:H201	2.28	0.64
2:M:63:GLY:HA3	6:M:401:BPH:H5C2	1.79	0.63
2:M:270:ILE:HD13	11:M:800:CDL:H711	1.81	0.62
5:M:311:BCL:HMB1	5:M:311:BCL:HBB2	1.81	0.62
14:H:801:PC7:C7	9:H:905:LDA:H112	2.28	0.62
7:L:502:U10:C12	8:L:802:PC9:H471	2.30	0.61
5:M:311:BCL:HMB1	5:M:311:BCL:CBB	2.31	0.61
2:M:179:ILE:HG23	5:M:311:BCL:HED1	1.83	0.60
2:M:72:ILE:N	2:M:72:ILE:HD13	2.17	0.59
2:M:262:MET:HE3	2:M:262:MET:CA	2.31	0.59
8:L:802:PC9:BR2	2:M:47:LEU:HD22	2.58	0.59
2:M:68[A]:PHE:CD1	2:M:72:ILE:HD11	2.38	0.58
2:M:253[A]:ARG:NH2	16:M:1461:HOH:O	2.36	0.58
8:L:802:PC9:H231	5:M:313:BCL:H203	1.86	0.58
8:L:802:PC9:H251	8:L:802:PC9:H202	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:LEU:HD13	8:L:802:PC9:H461	1.86	0.57
3:H:200:SER:H	13:H:709:HTO:H73	1.69	0.57
7:L:502:U10:H153	8:L:802:PC9:C46	2.35	0.57
5:M:311:BCL:H71	5:M:311:BCL:C4	2.34	0.56
7:L:502:U10:H122	8:L:802:PC9:C48	2.36	0.56
2:M:68[A]:PHE:CE1	2:M:72:ILE:HD11	2.41	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.56
5:L:314:BCL:HMB1	5:L:314:BCL:CBB	2.37	0.55
1:L:51:TRP:CZ3	1:L:80:LEU:HD13	2.42	0.54
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.43	0.53
2:M:179:ILE:CG2	5:M:311:BCL:HED1	2.39	0.53
1:L:189:LEU:HD11	8:L:802:PC9:H472	1.89	0.53
9:H:904:LDA:C3	9:H:904:LDA:HM13	2.39	0.53
3:H:9:ASN:C	3:H:11:ASP:H	2.13	0.52
8:L:802:PC9:O1P	8:L:802:PC9:H31	2.09	0.52
2:M:68[A]:PHE:O	2:M:72:ILE:HD13	2.10	0.52
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.45	0.51
2:M:41:TRP:CZ3	9:M:907:LDA:HM22	2.45	0.51
7:L:502:U10:H153	8:L:802:PC9:H461	1.92	0.51
8:L:802:PC9:C44	8:L:802:PC9:H483	2.32	0.51
2:M:72:ILE:N	2:M:72:ILE:CD1	2.74	0.51
2:M:68[B]:PHE:O	2:M:72:ILE:HD13	2.11	0.50
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.47	0.50
6:M:401:BPH:C15	6:M:401:BPH:H192	2.42	0.49
1:L:29:PHE:CE1	7:M:501:U10:H311	2.48	0.49
6:M:401:BPH:HHD	6:M:401:BPH:CBC	2.43	0.49
1:L:182:THR:OG1	5:M:311:BCL:H2	2.13	0.49
7:L:502:U10:H122	8:L:802:PC9:H471	1.95	0.49
4:L:703:PO4:O1	16:L:1467:HOH:O	2.20	0.49
3:H:21:TRP:CZ3	14:H:801:PC7:H72	2.48	0.48
8:L:802:PC9:BR1	5:M:311:BCL:H193	2.68	0.48
8:L:802:PC9:C48	6:M:401:BPH:HED1	2.27	0.47
2:M:10:VAL:HG22	16:H:1457:HOH:O	2.14	0.47
3:H:112:ALA:HA	3:H:235:GLY:O	2.14	0.47
2:M:234:GLU:CG	2:M:262:MET:HE1	2.45	0.47
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.50	0.47
8:L:802:PC9:H232	5:M:313:BCL:C20	2.44	0.47
16:M:1078:HOH:O	3:H:175:MET:HE1	2.14	0.47
3:H:128[B]:HIS:HD1	15:H:708:GOL:H2	1.80	0.47
8:L:802:PC9:H261	6:M:401:BPH:HED2	1.95	0.47
5:L:312:BCL:CBB	5:L:312:BCL:HMB1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:802:PC9:H232	5:M:313:BCL:H201	1.97	0.46
6:M:401:BPH:H192	6:M:401:BPH:H152	1.96	0.46
1:L:207:ARG:CG	1:L:211:HIS:CG	2.99	0.46
1:L:138:MET:SD	1:L:249:ILE:HD11	2.56	0.46
5:L:312:BCL:OBB	5:L:312:BCL:HHC	2.15	0.46
11:M:800:CDL:H172	3:H:26:GLY:HA3	1.97	0.46
3:H:118[A]:ARG:NH2	16:H:1237:HOH:O	2.48	0.46
2:M:53:GLY:O	2:M:57:VAL:HG23	2.16	0.45
5:M:311:BCL:H102	5:M:313:BCL:C19	2.45	0.45
5:L:314:BCL:HBA1	5:L:314:BCL:C4A	2.47	0.45
2:M:186:THR:HG23	5:M:313:BCL:HMD2	1.98	0.45
2:M:262:MET:HE3	2:M:262:MET:HA	1.99	0.45
14:H:801:PC7:C43	9:H:901:LDA:H121	2.43	0.45
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.52	0.44
1:L:51:TRP:HZ3	1:L:80:LEU:HD13	1.83	0.44
3:H:89:ARG:NH2	3:H:94[A]:GLU:HG2	2.31	0.44
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.43
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.52	0.43
2:M:226:VAL:HG23	2:M:231:GLY:HA3	2.00	0.43
1:L:216:PHE:CD2	7:L:502:U10:H102	2.54	0.43
8:L:802:PC9:H241	6:M:401:BPH:HMA1	2.00	0.43
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.01	0.43
5:L:312:BCL:NA	5:M:313:BCL:HBB2	2.34	0.43
9:H:904:LDA:HM13	9:H:904:LDA:H31	2.00	0.43
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.53	0.42
9:L:906:LDA:H32	9:L:906:LDA:HM13	2.01	0.42
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.54	0.42
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.82	0.42
2:M:296:VAL:O	2:M:300:ASN:ND2	2.49	0.42
1:L:51:TRP:CE3	1:L:85:LEU:HD21	2.55	0.42
1:L:60:ASN:O	1:L:64:ILE:HG13	2.20	0.42
1:L:220:VAL:HG11	8:L:802:PC9:H263	2.02	0.42
8:L:802:PC9:H263	6:M:401:BPH:HED2	1.98	0.42
7:L:502:U10:H322	7:L:502:U10:H301	1.81	0.42
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.88	0.41
14:H:801:PC7:H11	14:H:801:PC7:H41	2.02	0.41
1:L:80:LEU:O	1:L:85:LEU:HD12	2.21	0.41
2:M:2[B]:GLU:OE2	3:H:241:LEU:HD21	2.20	0.41
3:H:140:PHE:CE1	3:H:171:ILE:HG23	2.56	0.41
2:M:127:TRP:O	2:M:130:TRP:HB3	2.21	0.41
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:LEU:HD21	1:L:212:GLU:HB3	2.03	0.40
3:H:227:LEU:HD23	3:H:227:LEU:HA	1.89	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%)	275 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	299 (96%)	10 (3%)	1 (0%)	41	51
3	H	251/260 (96%)	245 (98%)	5 (2%)	1 (0%)	34	46
All	All	842/848 (99%)	819 (97%)	21 (2%)	2 (0%)	47	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	10	PHE
2	M	195	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	222/220 (101%)	213 (96%)	9 (4%)	30	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	246/240 (102%)	236 (96%)	10 (4%)	30	41
3	H	207/208 (100%)	201 (97%)	6 (3%)	42	57
All	All	675/668 (101%)	650 (96%)	25 (4%)	34	46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	254	ILE
1	L	272	TRP
2	M	32	VAL
2	M	52	LEU
2	M	72	ILE
2	M	86	LEU
2	M	104	SER
2	M	114	LEU
2	M	182	HIS
2	M	196	LEU
2	M	216	PHE
2	M	274	VAL
3	H	10	PHE
3	H	11	ASP
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	175	MET
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	HTO	H	709	-	9,9,9	0.45	0	10,10,10	0.46	0
9	LDA	H	904	-	12,15,15	1.94	1 (8%)	14,17,17	0.55	0
9	LDA	M	907	-	12,15,15	1.90	1 (8%)	14,17,17	0.50	0
9	LDA	M	920	-	12,15,15	1.80	1 (8%)	14,17,17	0.84	1 (7%)
9	LDA	L	902	-	12,15,15	1.87	1 (8%)	14,17,17	0.86	1 (7%)
6	BPH	M	401	-	51,70,70	0.79	2 (3%)	52,101,101	1.82	12 (23%)
5	BCL	L	314	1	64,74,74	1.13	4 (6%)	78,115,115	1.69	16 (20%)
8	PC9	L	802	-	53,53,53	0.82	2 (3%)	59,63,63	1.25	6 (10%)
5	BCL	M	311	2	64,74,74	1.16	4 (6%)	78,115,115	1.61	15 (19%)
7	U10	M	501	-	48,48,63	1.19	6 (12%)	58,61,79	1.71	12 (20%)
9	LDA	H	903	-	12,15,15	1.99	1 (8%)	14,17,17	0.59	0
9	LDA	L	906	-	12,15,15	2.02	1 (8%)	14,17,17	0.65	0
15	GOL	H	706	-	5,5,5	0.52	0	5,5,5	0.92	0
14	PC7	H	801	-	51,51,51	0.89	1 (1%)	57,59,59	1.01	3 (5%)
4	PO4	M	701	-	4,4,4	0.80	0	6,6,6	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BCL	L	312	1	64,74,74	1.16	5 (7%)	78,115,115	1.60	15 (19%)
9	LDA	H	905	-	12,15,15	2.01	1 (8%)	14,17,17	0.42	0
7	U10	L	502	-	48,48,63	1.00	3 (6%)	58,61,79	1.78	13 (22%)
15	GOL	H	708	-	5,5,5	0.37	0	5,5,5	0.58	0
5	BCL	M	313	2	64,74,74	1.35	5 (7%)	78,115,115	1.92	21 (26%)
15	GOL	H	705	-	5,5,5	0.48	0	5,5,5	0.48	0
11	CDL	M	800	-	80,80,99	1.19	5 (6%)	86,92,111	1.30	8 (9%)
9	LDA	H	901	-	12,15,15	1.75	1 (8%)	14,17,17	0.67	0
6	BPH	L	402	-	51,70,70	0.91	2 (3%)	52,101,101	1.58	9 (17%)
4	PO4	M	704	-	4,4,4	0.84	0	6,6,6	0.74	0
4	PO4	M	702	-	4,4,4	0.67	0	6,6,6	0.73	0
4	PO4	L	703	-	4,4,4	0.75	0	6,6,6	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HTO	H	709	-	-	2/10/10/10	-
9	LDA	H	904	-	-	5/13/13/13	-
9	LDA	M	907	-	-	10/13/13/13	-
9	LDA	M	920	-	-	7/13/13/13	-
9	LDA	L	902	-	-	4/13/13/13	-
6	BPH	M	401	-	-	12/37/105/105	0/5/6/6
5	BCL	L	314	1	-	3/37/137/137	-
8	PC9	L	802	-	-	24/60/60/60	-
5	BCL	M	311	2	-	11/37/137/137	-
7	U10	M	501	-	-	4/45/69/87	0/1/1/1
9	LDA	H	903	-	-	4/13/13/13	-
9	LDA	L	906	-	-	5/13/13/13	-
15	GOL	H	706	-	-	2/4/4/4	-
14	PC7	H	801	-	-	30/55/55/55	-
9	LDA	H	905	-	-	9/13/13/13	-
7	U10	L	502	-	-	12/45/69/87	0/1/1/1
15	GOL	H	708	-	-	2/4/4/4	-
5	BCL	M	313	2	-	3/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GOL	H	705	-	-	3/4/4/4	-
11	CDL	M	800	-	-	33/91/91/110	-
9	LDA	H	901	-	-	6/13/13/13	-
6	BPH	L	402	-	-	5/37/105/105	0/5/6/6
5	BCL	L	312	1	-	6/37/137/137	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	906	LDA	O1-N1	-6.86	1.26	1.42
9	H	905	LDA	O1-N1	-6.85	1.26	1.42
9	H	903	LDA	O1-N1	-6.83	1.26	1.42
9	H	904	LDA	O1-N1	-6.60	1.26	1.42
9	M	907	LDA	O1-N1	-6.46	1.27	1.42
9	L	902	LDA	O1-N1	-6.38	1.27	1.42
9	H	901	LDA	O1-N1	-6.01	1.28	1.42
9	M	920	LDA	O1-N1	-5.99	1.28	1.42
5	M	311	BCL	MG-NA	5.41	2.19	2.06
5	L	312	BCL	MG-NA	5.18	2.18	2.06
5	M	313	BCL	C4B-NB	5.04	1.39	1.35
11	M	800	CDL	OA8-CA7	4.87	1.47	1.33
11	M	800	CDL	OB6-CB5	4.85	1.48	1.34
11	M	800	CDL	OA6-CA5	4.69	1.47	1.34
5	M	313	BCL	MG-NA	4.62	2.17	2.06
5	L	314	BCL	MG-NA	4.39	2.16	2.06
7	M	501	U10	O3-C3	4.19	1.47	1.36
7	L	502	U10	O3-C3	4.15	1.47	1.36
11	M	800	CDL	OB8-CB7	4.01	1.45	1.33
5	M	313	BCL	C3C-C4C	-3.59	1.47	1.51
5	L	312	BCL	C1B-NB	3.43	1.38	1.35
5	M	311	BCL	C1B-NB	3.29	1.38	1.35
5	L	314	BCL	C4B-NB	3.13	1.38	1.35
5	M	313	BCL	MG-ND	3.09	2.11	2.05
8	L	802	PC9	P-O1P	2.98	1.61	1.50
5	M	313	BCL	C4D-ND	-2.89	1.33	1.37
7	M	501	U10	O2-C2	2.87	1.29	1.23
5	L	314	BCL	C1B-NB	2.59	1.37	1.35
5	L	312	BCL	C4-C3	2.48	1.57	1.50
7	M	501	U10	C13-C14	2.46	1.38	1.33
6	M	401	BPH	C3A-C2A	-2.46	1.52	1.54
7	L	502	U10	C13-C14	2.46	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	502	U10	O4-C4	2.40	1.42	1.36
7	M	501	U10	C33-C34	2.26	1.38	1.33
5	L	312	BCL	C5-C3	2.24	1.55	1.51
7	M	501	U10	O3-C3M	-2.22	1.40	1.45
5	M	311	BCL	MG-NC	2.20	2.11	2.06
14	H	801	PC7	C1-C2	2.19	1.57	1.50
5	L	314	BCL	C4D-ND	-2.18	1.34	1.37
8	L	802	PC9	O3-C3	2.15	1.50	1.45
6	L	402	BPH	C3A-C2A	-2.11	1.52	1.54
7	M	501	U10	O4-C4	2.11	1.42	1.36
5	L	312	BCL	MG-NC	2.07	2.11	2.06
11	M	800	CDL	PA1-OA3	-2.07	1.43	1.50
5	M	311	BCL	C3D-C4D	-2.06	1.39	1.44
6	L	402	BPH	CBD-CGD	2.04	1.55	1.52
6	M	401	BPH	CBA-CGA	-2.00	1.44	1.50

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	313	BCL	CMB-C2B-C1B	-6.45	118.55	128.46
11	M	800	CDL	OA6-CA5-C11	5.84	124.10	111.50
6	L	402	BPH	O2D-CGD-CBD	5.68	118.19	111.00
5	M	313	BCL	C1C-NC-C4C	5.57	109.21	106.71
6	M	401	BPH	O2D-CGD-CBD	5.54	118.02	111.00
6	M	401	BPH	OBD-CAD-CBD	-4.75	118.85	125.82
11	M	800	CDL	OB6-CB5-C51	4.64	121.50	111.50
7	M	501	U10	C30-C29-C31	4.59	122.99	115.27
7	L	502	U10	C30-C29-C31	4.45	122.76	115.27
5	M	313	BCL	C4D-CHA-C1A	4.41	126.61	121.25
5	M	313	BCL	CHD-C1D-ND	-4.32	120.48	124.45
5	M	311	BCL	CMB-C2B-C1B	-4.26	121.91	128.46
7	M	501	U10	C32-C33-C34	-4.19	117.57	127.66
14	H	801	PC7	O2-C31-C32	4.15	120.45	111.50
7	M	501	U10	C17-C18-C19	-4.12	117.74	127.66
7	L	502	U10	C25-C24-C26	4.09	122.14	115.27
6	M	401	BPH	CAC-C3C-C4C	4.08	122.87	113.73
5	L	312	BCL	CMB-C2B-C1B	-4.02	122.29	128.46
5	L	314	BCL	O2D-CGD-CBD	3.97	118.32	111.27
5	M	311	BCL	C4-C3-C2	-3.96	113.52	123.68
7	M	501	U10	C6-C1-C2	3.95	122.30	119.18
8	L	802	PC9	C2-O2-C31	-3.91	108.15	117.79
5	L	312	BCL	C1D-ND-C4D	3.89	109.10	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	802	PC9	O2-C31-C32	3.85	119.79	111.50
5	L	314	BCL	CAA-C2A-C3A	-3.81	102.34	112.78
5	M	313	BCL	CMB-C2B-C3B	3.78	131.76	124.68
5	L	314	BCL	CMB-C2B-C1B	-3.75	122.71	128.46
5	M	313	BCL	CAC-C3C-C2C	-3.74	104.91	114.26
7	L	502	U10	C31-C29-C28	-3.74	113.55	121.12
7	M	501	U10	C7-C6-C5	-3.72	114.00	118.48
6	M	401	BPH	C1-C2-C3	-3.71	119.62	126.04
5	L	314	BCL	CAC-C3C-C2C	-3.68	105.06	114.26
5	L	312	BCL	CMB-C2B-C3B	3.67	131.55	124.68
5	L	314	BCL	CAC-C3C-C4C	-3.59	104.61	112.58
5	L	312	BCL	CAA-C2A-C3A	-3.58	102.97	112.78
7	L	502	U10	C35-C34-C33	-3.58	114.51	123.68
7	M	501	U10	C26-C27-C28	-3.54	100.23	111.88
6	L	402	BPH	O2D-CGD-O1D	-3.54	116.92	123.84
6	L	402	BPH	C1-C2-C3	-3.53	119.94	126.04
5	L	312	BCL	CHD-C1D-ND	-3.53	121.21	124.45
5	L	314	BCL	CAA-CBA-CGA	3.46	123.36	113.25
7	L	502	U10	O2-C2-C3	-3.42	113.66	120.93
5	L	314	BCL	CHD-C1D-ND	-3.40	121.33	124.45
6	M	401	BPH	CMA-C3A-C4A	-3.34	107.06	114.38
5	M	311	BCL	CED-O2D-CGD	-3.30	108.47	115.94
7	L	502	U10	C35-C34-C36	3.29	120.81	115.27
5	L	312	BCL	C4B-C3B-CAB	-3.27	120.81	127.13
6	M	401	BPH	CMB-C2B-C3B	3.26	130.77	124.68
5	M	311	BCL	C4D-CHA-C1A	3.19	125.13	121.25
5	L	312	BCL	C2D-C1D-ND	-3.16	107.77	110.10
11	M	800	CDL	CB6-CB4-CB3	-3.13	104.38	111.79
7	M	501	U10	C31-C29-C28	-3.09	114.86	121.12
5	L	312	BCL	C4A-NA-C1A	-3.04	105.34	106.71
5	M	311	BCL	CMA-C3A-C4A	-3.03	103.63	111.77
5	L	314	BCL	C4D-CHA-C1A	3.03	124.94	121.25
5	L	314	BCL	OBB-CAB-C3B	2.99	125.30	119.99
5	L	314	BCL	C5-C3-C2	-2.99	115.07	121.12
5	L	314	BCL	O1D-CGD-CBD	-2.97	118.41	124.48
6	L	402	BPH	CAC-C3C-C4C	2.96	120.35	113.73
6	M	401	BPH	CAA-C2A-C3A	-2.96	104.68	112.78
5	L	312	BCL	C1C-NC-C4C	2.95	108.03	106.71
5	L	312	BCL	CHA-C1A-NA	-2.93	119.68	126.40
7	L	502	U10	C1M-C1-C6	-2.93	119.62	124.40
5	M	313	BCL	CHA-C1A-NA	-2.91	119.73	126.40
14	H	801	PC7	C3-C2-C1	2.88	118.59	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	800	CDL	OB8-CB7-OB9	-2.87	116.35	123.59
5	M	311	BCL	CMB-C2B-C3B	2.87	130.04	124.68
5	M	311	BCL	CHD-C1D-ND	-2.86	121.82	124.45
5	M	313	BCL	C1D-ND-C4D	2.85	108.36	106.33
11	M	800	CDL	OB8-CB7-C71	2.83	120.80	111.91
5	M	311	BCL	C5-C3-C2	2.83	126.85	121.12
5	M	311	BCL	CHA-C1A-NA	-2.81	119.95	126.40
5	M	313	BCL	O2A-C1-C2	2.78	115.95	108.64
5	M	313	BCL	O2D-CGD-O1D	-2.77	118.42	123.84
7	L	502	U10	C12-C13-C14	-2.71	121.14	127.66
5	M	311	BCL	OBB-CAB-C3B	2.70	124.79	119.99
5	M	313	BCL	CHD-C4C-NC	2.70	128.07	125.08
5	M	311	BCL	C1-O2A-CGA	2.69	123.51	116.44
6	L	402	BPH	CMB-C2B-C3B	2.66	129.66	124.68
7	M	501	U10	C22-C23-C24	-2.66	121.26	127.66
5	M	313	BCL	CHC-C1C-NC	2.66	128.18	124.51
5	L	312	BCL	CHD-C1D-C2D	2.64	131.01	125.48
5	M	313	BCL	CHD-C1D-C2D	2.62	130.97	125.48
5	M	313	BCL	C4B-CHC-C1C	-2.60	124.97	130.12
5	M	311	BCL	C4-C3-C5	2.59	119.63	115.27
6	L	402	BPH	CMD-C2D-C3D	2.53	129.42	124.68
7	L	502	U10	C3M-O3-C3	2.51	125.37	116.47
9	M	920	LDA	O1-N1-C1	2.50	115.41	109.27
5	L	314	BCL	CMA-C3A-C2A	-2.49	103.78	113.83
5	M	311	BCL	CAA-CBA-CGA	2.49	120.53	113.25
5	M	311	BCL	C1D-ND-C4D	2.48	108.10	106.33
11	M	800	CDL	OA8-CA7-C31	2.46	119.63	111.91
5	L	314	BCL	CMB-C2B-C3B	2.45	129.27	124.68
7	L	502	U10	C21-C22-C23	-2.45	103.84	111.88
7	M	501	U10	C4M-O4-C4	2.44	125.11	116.47
5	L	312	BCL	C5-C3-C2	-2.44	116.19	121.12
5	L	312	BCL	C1-O2A-CGA	2.42	122.81	116.44
5	M	313	BCL	C4-C3-C5	2.41	119.33	115.27
8	L	802	PC9	C35-C36-C37	-2.40	109.55	115.61
6	L	402	BPH	CAC-C3C-C2C	2.38	120.22	114.26
8	L	802	PC9	O3-C11-C12	2.36	119.32	111.91
6	M	401	BPH	CMA-C3A-C2A	-2.33	104.60	113.99
5	M	313	BCL	C2C-C3C-C4C	2.32	104.81	101.34
5	M	313	BCL	OBB-CAB-CBB	-2.30	115.00	120.17
6	L	402	BPH	CMA-C3A-C4A	-2.29	109.36	114.38
5	M	311	BCL	O2D-CGD-CBD	2.26	115.28	111.27
5	L	312	BCL	CED-O2D-CGD	2.23	120.98	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	401	BPH	C4C-C3C-C2C	2.22	104.95	102.84
7	M	501	U10	C22-C21-C19	-2.22	105.67	112.98
6	M	401	BPH	O2D-CGD-O1D	-2.22	119.50	123.84
9	L	902	LDA	CM1-N1-C1	2.21	114.87	110.23
5	M	313	BCL	C2D-C1D-ND	-2.20	108.48	110.10
14	H	801	PC7	O3-C11-C12	2.20	118.81	111.91
7	M	501	U10	C15-C14-C16	2.20	118.97	115.27
5	M	313	BCL	CAC-C3C-C4C	-2.19	107.72	112.58
5	L	312	BCL	C4-C3-C5	2.19	118.96	115.27
7	L	502	U10	C22-C23-C24	-2.18	122.42	127.66
5	L	314	BCL	C2C-C3C-C4C	2.17	104.59	101.34
7	L	502	U10	C16-C17-C18	-2.16	104.77	111.88
6	M	401	BPH	C1C-C2C-C3C	-2.15	100.80	102.84
5	M	313	BCL	C1-C2-C3	-2.14	122.34	126.04
7	L	502	U10	C7-C6-C5	-2.12	115.93	118.48
11	M	800	CDL	OA6-CA5-OA7	-2.12	118.59	123.70
6	L	402	BPH	CMA-C3A-C2A	-2.10	105.52	113.99
8	L	802	PC9	O3-C3-C2	2.09	114.52	108.43
5	L	314	BCL	CHD-C1D-C2D	2.07	129.83	125.48
5	L	314	BCL	C4-C3-C5	2.06	118.73	115.27
7	M	501	U10	C41-C39-C40	2.06	119.15	114.60
8	L	802	PC9	C24-C23-C22	-2.05	104.01	114.42
11	M	800	CDL	CA4-OA6-CA5	-2.05	112.75	117.79
5	M	313	BCL	C4D-C3D-CAD	-2.04	105.69	108.10
6	M	401	BPH	O2A-C1-C2	-2.04	103.28	108.64

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	311	BCL	C4-C3-C5-C6
6	M	401	BPH	C2C-C3C-CAC-CBC
6	M	401	BPH	C11-C12-C13-C14
8	L	802	PC9	C1-O3P-P-O4P
9	L	906	LDA	N1-C1-C2-C3
9	H	901	LDA	C2-C1-N1-O1
9	H	901	LDA	C2-C1-N1-CM1
9	H	905	LDA	C2-C1-N1-O1
9	H	905	LDA	C2-C1-N1-CM1
9	H	905	LDA	C2-C1-N1-CM2
11	M	800	CDL	CB2-OB2-PB2-OB3
11	M	800	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
14	H	801	PC7	C1-O3P-P-O1P
14	H	801	PC7	O4P-C4-C5-N
15	H	705	GOL	C1-C2-C3-O3
15	H	706	GOL	C1-C2-C3-O3
15	H	708	GOL	O1-C1-C2-C3
5	M	311	BCL	C2-C3-C5-C6
11	M	800	CDL	C38-C39-C40-C41
7	L	502	U10	C30-C29-C31-C32
7	L	502	U10	C28-C29-C31-C32
11	M	800	CDL	C36-C37-C38-C39
8	L	802	PC9	C22-C23-C24-C25
11	M	800	CDL	CB7-C71-C72-C73
5	M	311	BCL	C15-C16-C17-C18
15	H	708	GOL	O1-C1-C2-O2
8	L	802	PC9	C31-C32-C33-C34
14	H	801	PC7	C31-C32-C33-C34
7	L	502	U10	C29-C31-C32-C33
7	M	501	U10	C29-C31-C32-C33
11	M	800	CDL	CA2-OA2-PA1-OA5
14	H	801	PC7	C1-O3P-P-O4P
8	L	802	PC9	C44-C45-C46-C47
11	M	800	CDL	C51-CB5-OB6-CB4
8	L	802	PC9	C40-C41-C42-C43
9	L	902	LDA	C11-C10-C9-C8
11	M	800	CDL	C18-C19-C20-C21
9	L	906	LDA	C3-C4-C5-C6
9	M	920	LDA	C4-C5-C6-C7
9	H	905	LDA	C6-C7-C8-C9
11	M	800	CDL	OB7-CB5-OB6-CB4
9	H	905	LDA	C4-C5-C6-C7
11	M	800	CDL	C15-C16-C17-C18
9	H	905	LDA	C11-C10-C9-C8
8	L	802	PC9	C41-C42-C43-C44
5	L	312	BCL	C11-C10-C8-C9
5	M	311	BCL	C11-C12-C13-C14
8	L	802	PC9	C11-C12-C13-C14
9	L	906	LDA	C4-C5-C6-C7
11	M	800	CDL	C71-C72-C73-C74
13	H	709	HTO	C2-C3-C4-C5
9	L	906	LDA	C2-C3-C4-C5
11	M	800	CDL	C19-C20-C21-C22
14	H	801	PC7	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
9	M	920	LDA	C5-C6-C7-C8
7	L	502	U10	C18-C19-C21-C22
9	M	907	LDA	C4-C5-C6-C7
15	H	706	GOL	O2-C2-C3-O3
9	L	906	LDA	C9-C10-C11-C12
9	H	901	LDA	C1-C2-C3-C4
8	L	802	PC9	C13-C14-C15-C16
5	L	312	BCL	C11-C10-C8-C7
9	H	905	LDA	C1-C2-C3-C4
8	L	802	PC9	C32-C31-O2-C2
9	M	907	LDA	C11-C10-C9-C8
9	H	903	LDA	C6-C7-C8-C9
8	L	802	PC9	O31-C31-O2-C2
8	L	802	PC9	C39-C40-C41-C42
5	M	311	BCL	C16-C17-C18-C19
7	L	502	U10	C20-C19-C21-C22
9	M	920	LDA	C1-C2-C3-C4
6	M	401	BPH	C6-C7-C8-C9
14	H	801	PC7	C32-C31-O2-C2
6	M	401	BPH	C10-C11-C12-C13
9	L	902	LDA	C1-C2-C3-C4
9	H	905	LDA	C3-C4-C5-C6
11	M	800	CDL	OA5-CA3-CA4-CA6
7	L	502	U10	C15-C14-C16-C17
6	M	401	BPH	C15-C16-C17-C18
13	H	709	HTO	O3-C3-C4-C5
9	H	901	LDA	C11-C10-C9-C8
14	H	801	PC7	C44-C45-C46-C47
8	L	802	PC9	C21-C22-C23-C24
11	M	800	CDL	C52-C53-C54-C55
9	M	907	LDA	C9-C10-C11-C12
7	L	502	U10	C24-C26-C27-C28
8	L	802	PC9	C45-C46-C47-C48
15	H	705	GOL	O2-C2-C3-O3
6	L	402	BPH	C4-C3-C5-C6
5	M	311	BCL	C2-C1-O2A-CGA
11	M	800	CDL	C75-C76-C77-C78
14	H	801	PC7	C35-C36-C37-C38
14	H	801	PC7	C15-C16-C17-C18
9	M	907	LDA	C7-C8-C9-C10
9	M	920	LDA	C11-C10-C9-C8
14	H	801	PC7	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
9	M	920	LDA	C3-C4-C5-C6
6	M	401	BPH	C6-C7-C8-C10
7	L	502	U10	C13-C14-C16-C17
11	M	800	CDL	C81-C82-C83-C84
14	H	801	PC7	C17-C18-C19-C20
9	M	907	LDA	C1-C2-C3-C4
9	M	920	LDA	C2-C3-C4-C5
11	M	800	CDL	C74-C75-C76-C77
14	H	801	PC7	C39-C40-C41-C42
11	M	800	CDL	C11-C12-C13-C14
5	M	311	BCL	C16-C17-C18-C20
14	H	801	PC7	C1-C2-C3-O3
9	H	904	LDA	C6-C7-C8-C9
11	M	800	CDL	C53-C54-C55-C56
6	L	402	BPH	C8-C10-C11-C12
11	M	800	CDL	OA5-CA3-CA4-OA6
14	H	801	PC7	C42-C43-C44-C45
11	M	800	CDL	C1-CB2-OB2-PB2
9	L	902	LDA	C9-C10-C11-C12
9	L	902	LDA	C3-C4-C5-C6
6	L	402	BPH	C2-C3-C5-C6
11	M	800	CDL	C31-CA7-OA8-CA6
5	L	312	BCL	CAD-CBD-CGD-O2D
6	L	402	BPH	CAD-CBD-CGD-O2D
6	M	401	BPH	CAD-CBD-CGD-O2D
11	M	800	CDL	C34-C35-C36-C37
9	M	907	LDA	C2-C1-N1-CM1
9	M	907	LDA	C2-C1-N1-CM2
9	M	920	LDA	C2-C1-N1-CM2
9	H	904	LDA	C2-C1-N1-CM1
8	L	802	PC9	C16-C17-C18-C19
14	H	801	PC7	C13-C14-C15-C16
8	L	802	PC9	C19-C20-C21-C22
14	H	801	PC7	C2-C1-O3P-P
8	L	802	PC9	C1-O3P-P-O2P
11	M	800	CDL	CA2-OA2-PA1-OA3
14	H	801	PC7	C1-O3P-P-O2P
14	H	801	PC7	O3P-C1-C2-C3
5	M	313	BCL	C16-C17-C18-C19
9	M	907	LDA	C2-C1-N1-O1
5	L	314	BCL	C15-C16-C17-C18
11	M	800	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
5	L	314	BCL	C12-C13-C15-C16
5	M	311	BCL	C11-C10-C8-C7
6	M	401	BPH	C4C-C3C-CAC-CBC
9	M	907	LDA	C3-C4-C5-C6
11	M	800	CDL	OA9-CA7-OA8-CA6
5	M	311	BCL	C14-C13-C15-C16
7	M	501	U10	C30-C29-C31-C32
9	M	907	LDA	C2-C3-C4-C5
14	H	801	PC7	C3-C2-O2-C31
14	H	801	PC7	C11-C12-C13-C14
8	L	802	PC9	C2-C1-O3P-P
9	H	901	LDA	C6-C7-C8-C9
8	L	802	PC9	C4-O4P-P-O3P
5	L	314	BCL	C14-C13-C15-C16
5	M	313	BCL	C16-C17-C18-C20
8	L	802	PC9	C38-C39-C40-C41
14	H	801	PC7	C18-C19-C20-C21
6	M	401	BPH	C4-C3-C5-C6
5	L	312	BCL	C2-C1-O2A-CGA
9	H	903	LDA	C4-C5-C6-C7
11	M	800	CDL	C72-C73-C74-C75
14	H	801	PC7	C23-C24-C25-C26
7	L	502	U10	C5-C4-O4-C4M
14	H	801	PC7	O2-C2-C3-O3
15	H	705	GOL	O1-C1-C2-C3
7	M	501	U10	C28-C29-C31-C32
5	M	313	BCL	CAA-CBA-CGA-O2A
9	H	904	LDA	C1-C2-C3-C4
7	M	501	U10	C5-C4-O4-C4M
7	L	502	U10	C35-C34-C36-C37
14	H	801	PC7	C32-C33-C34-C35
8	L	802	PC9	C14-C15-C16-C17
14	H	801	PC7	C20-C21-C22-C23
9	H	904	LDA	C2-C3-C4-C5
9	H	903	LDA	C7-C8-C9-C10
7	L	502	U10	C25-C24-C26-C27
9	H	901	LDA	C5-C6-C7-C8
5	M	311	BCL	CAD-CBD-CGD-O2D
14	H	801	PC7	O3-C11-C12-C13
6	L	402	BPH	O2A-C1-C2-C3
9	H	904	LDA	C2-C1-N1-CM2
8	L	802	PC9	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	M	401	BPH	C16-C17-C18-C20
5	M	311	BCL	C11-C10-C8-C9
7	L	502	U10	C3-C4-O4-C4M
6	M	401	BPH	C2-C3-C5-C6
11	M	800	CDL	C52-C51-CB5-OB6
9	H	903	LDA	C2-C3-C4-C5
9	H	905	LDA	C2-C3-C4-C5
8	L	802	PC9	C15-C16-C17-C18
5	L	312	BCL	C16-C17-C18-C19
11	M	800	CDL	CB3-OB5-PB2-OB3
14	H	801	PC7	O11-C11-C12-C13
11	M	800	CDL	C12-C13-C14-C15
8	L	802	PC9	O3-C11-C12-C13
11	M	800	CDL	CB4-CB3-OB5-PB2
6	M	401	BPH	C11-C12-C13-C15
14	H	801	PC7	O3P-C1-C2-O2
11	M	800	CDL	C32-C31-CA7-OA8
8	L	802	PC9	O11-C11-C12-C13
11	M	800	CDL	C52-C51-CB5-OB7
14	H	801	PC7	C38-C39-C40-C41
5	L	312	BCL	C15-C16-C17-C18
14	H	801	PC7	O2-C31-C32-C33

There are no ring outliers.

18 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	709	HTO	1	0
9	H	904	LDA	2	0
9	M	907	LDA	1	0
6	M	401	BPH	11	0
5	L	314	BCL	3	0
8	L	802	PC9	36	0
5	M	311	BCL	11	0
7	M	501	U10	1	0
9	L	906	LDA	1	0
14	H	801	PC7	8	0
5	L	312	BCL	3	0
9	H	905	LDA	2	0
7	L	502	U10	12	0
15	H	708	GOL	2	0
5	M	313	BCL	10	0

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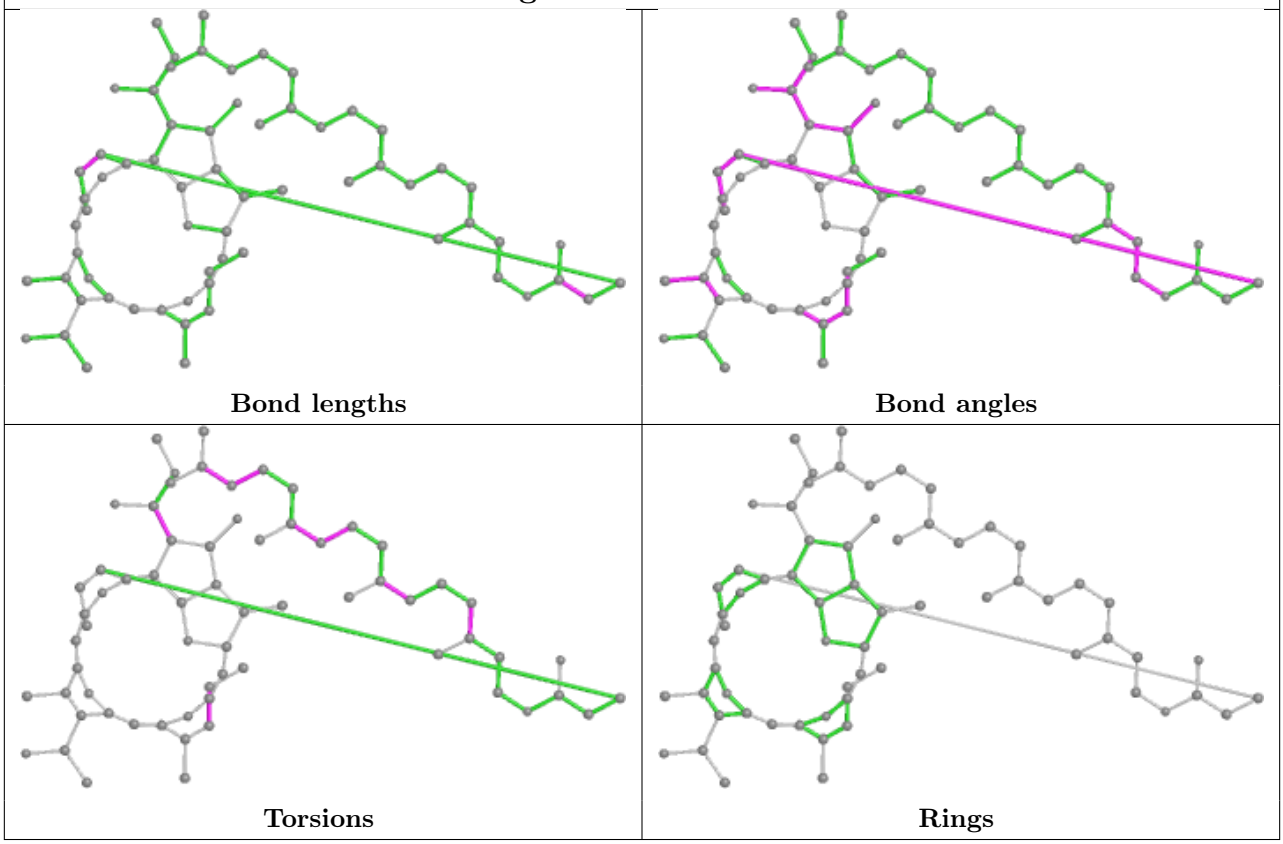
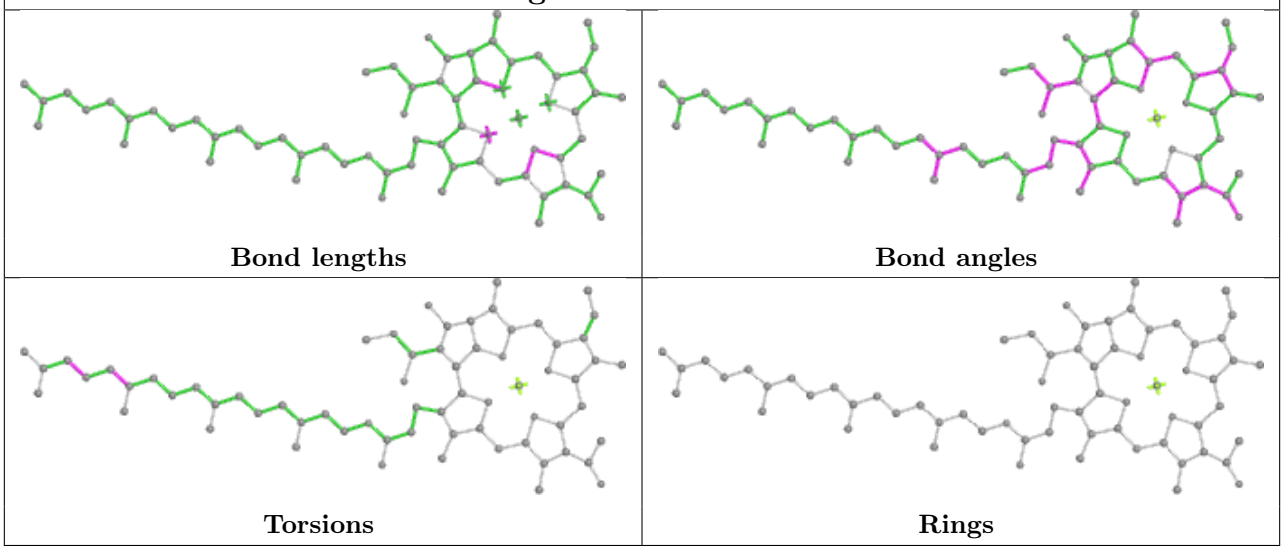
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	800	CDL	2	0
9	H	901	LDA	3	0
4	L	703	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

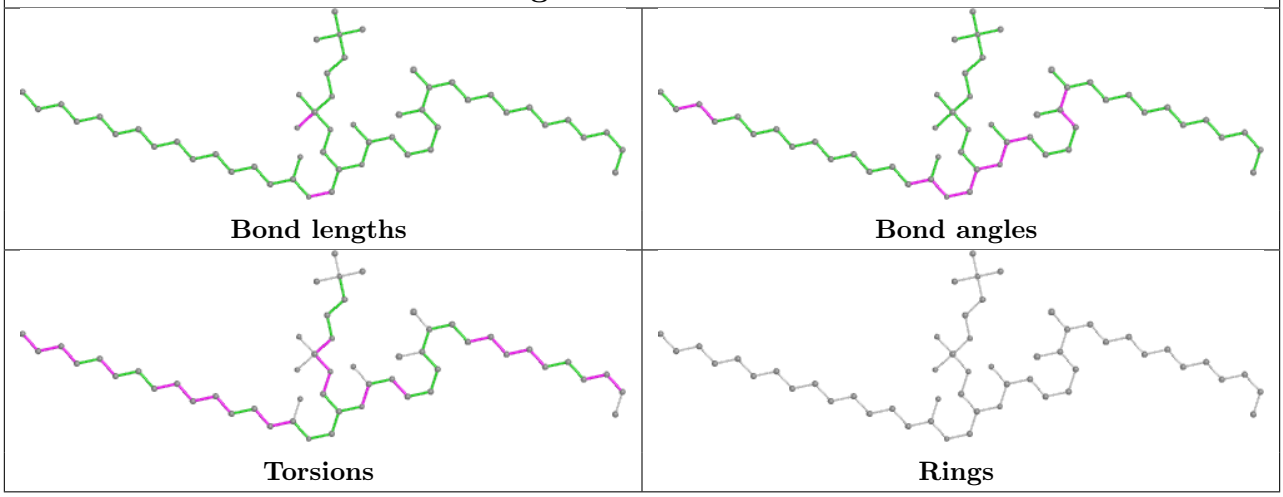
Ligand BPH M 401



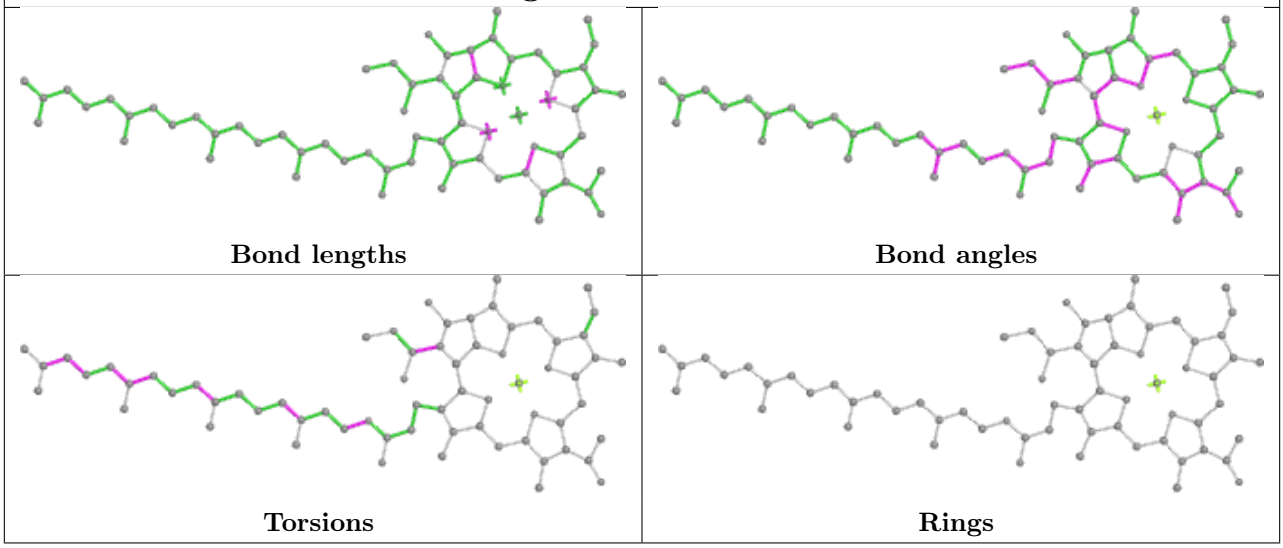
Ligand BCL L 314



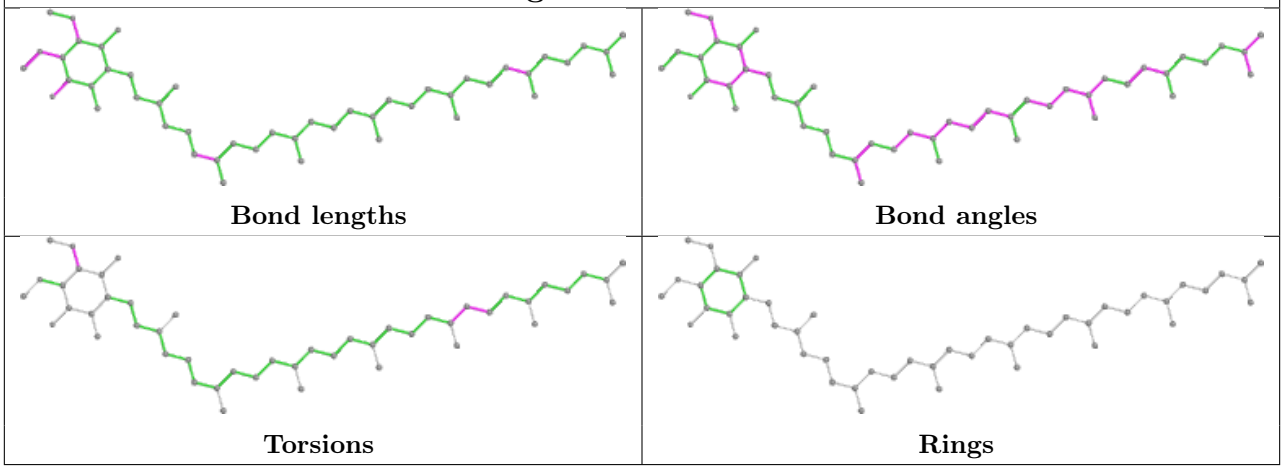
Ligand PC9 L 802



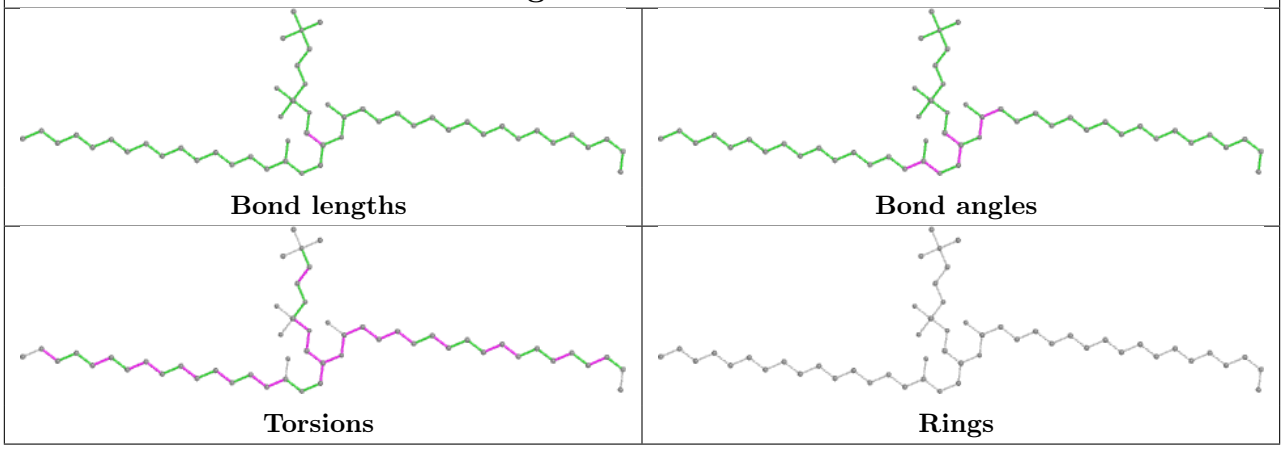
Ligand BCL M 311



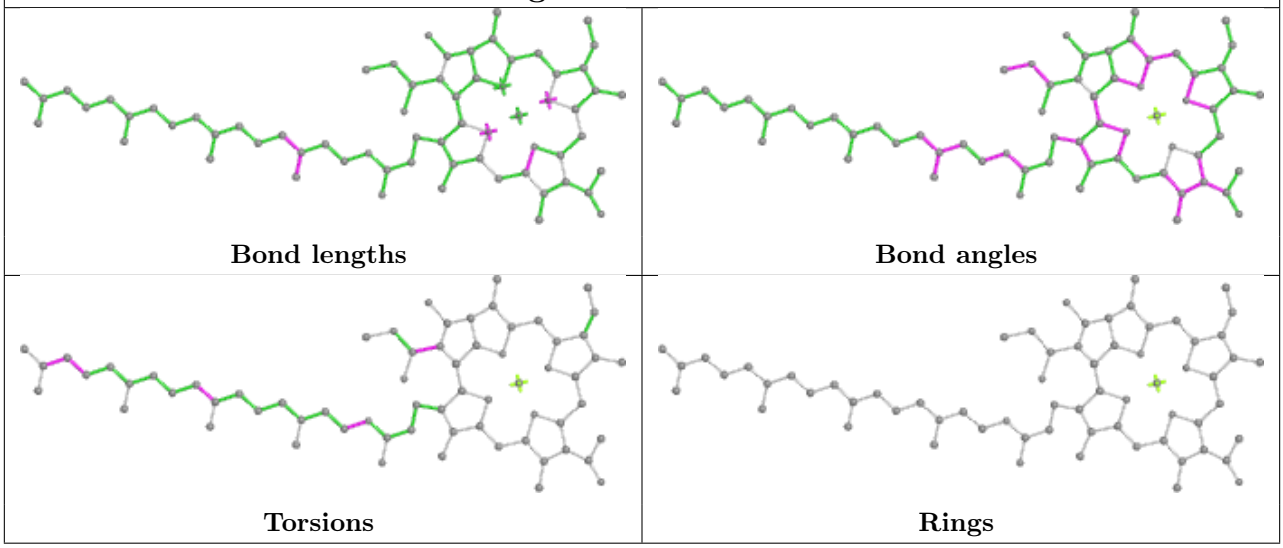
Ligand U10 M 501



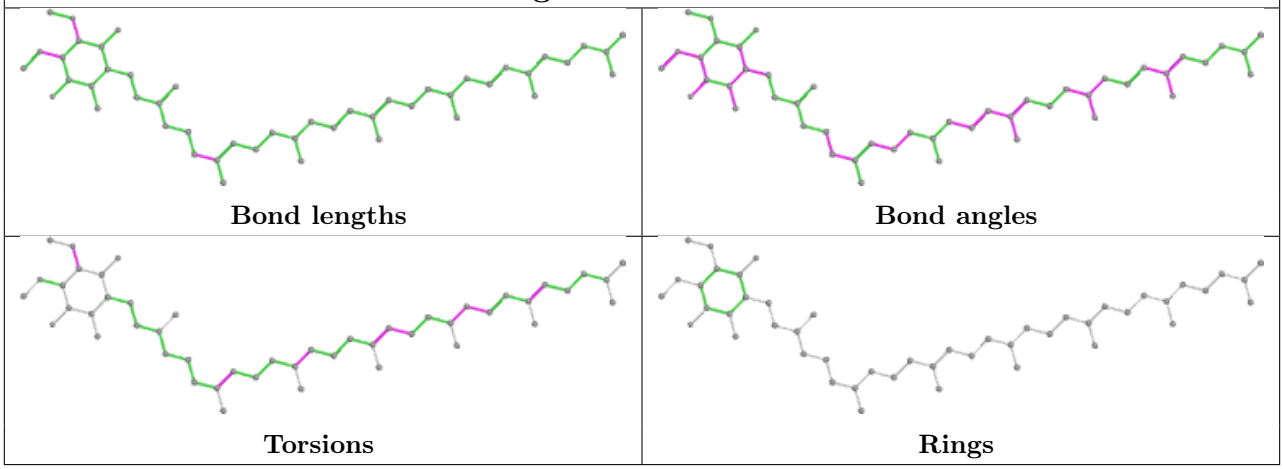
Ligand PC7 H 801



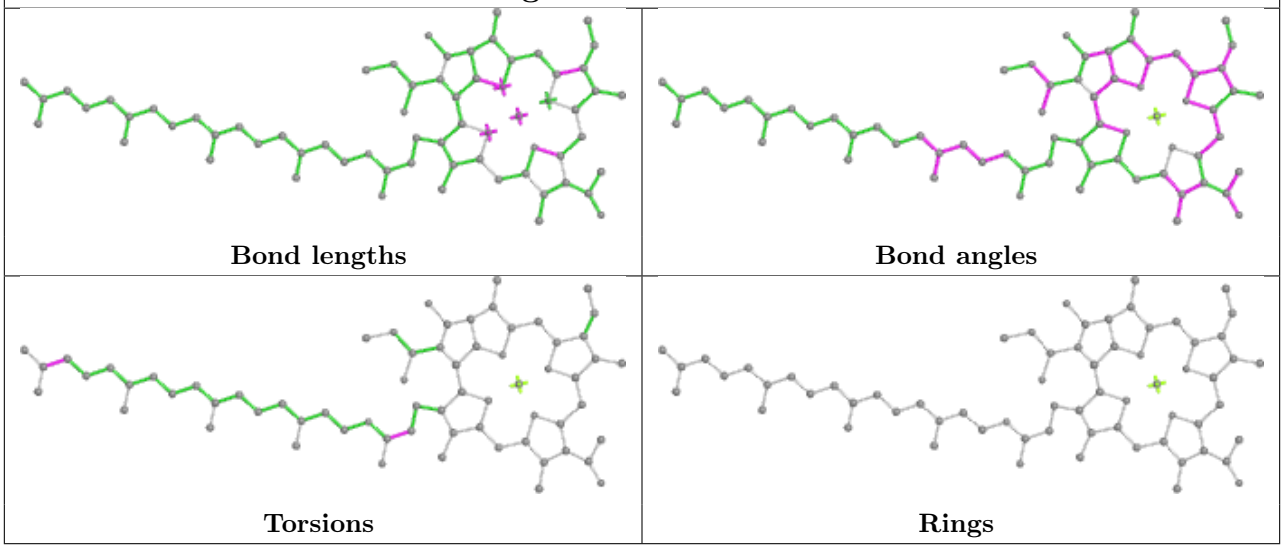
Ligand BCL L 312



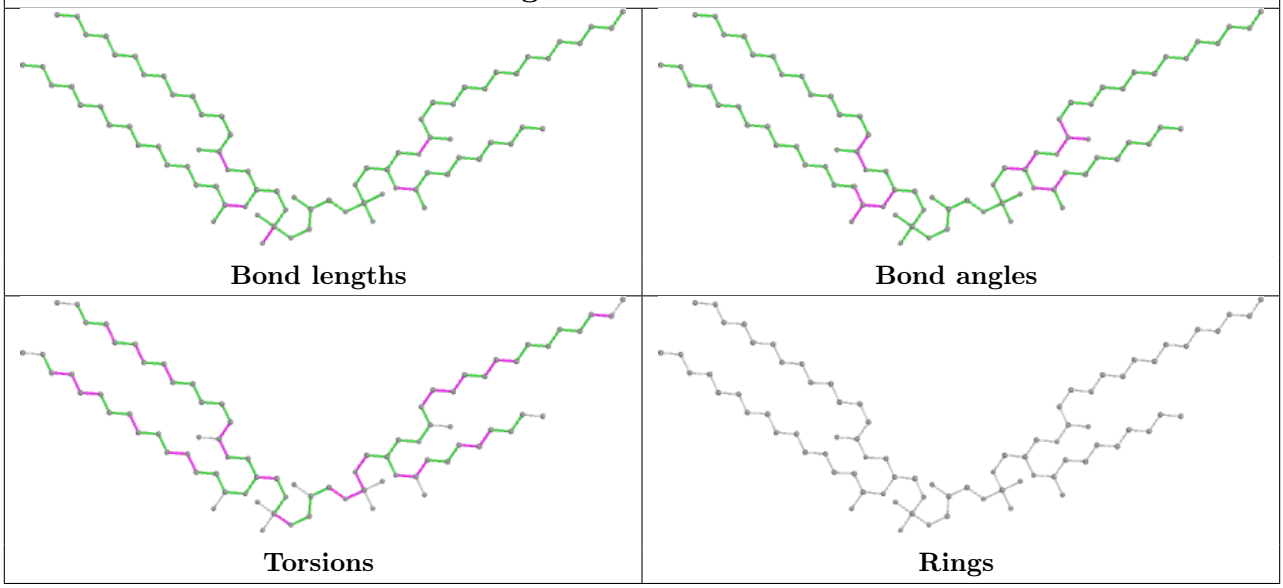
Ligand U10 L 502



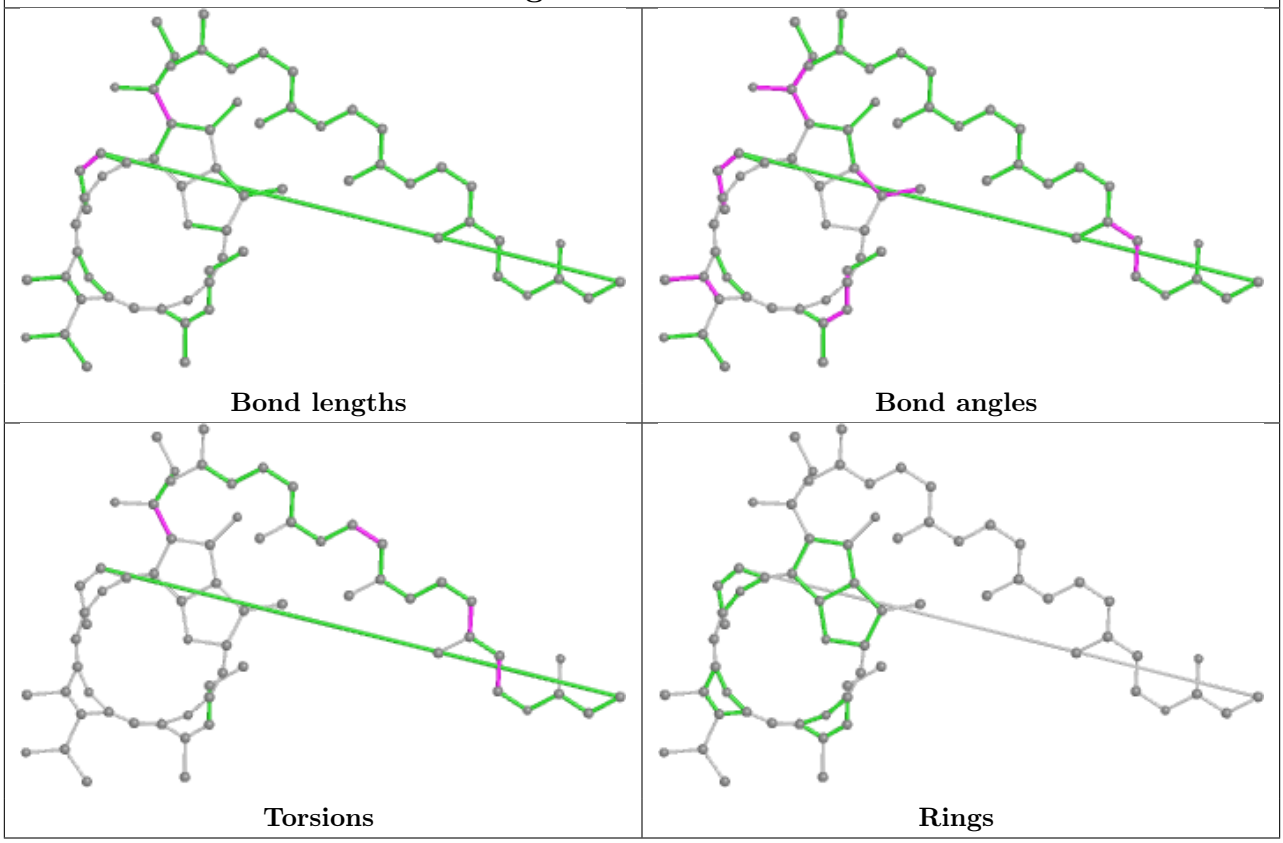
Ligand BCL M 313



Ligand CDL M 800



Ligand BPH L 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	0.16	24 (8%) 10 12	38, 51, 61, 72	0
2	M	302/307 (98%)	0.36	31 (10%) 6 8	40, 50, 60, 76	0
3	H	244/260 (93%)	0.03	9 (3%) 41 48	42, 49, 60, 87	1 (0%)
All	All	827/848 (97%)	0.19	64 (7%) 13 17	38, 50, 61, 87	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	9	ASN	8.8
3	H	8	GLY	8.5
3	H	251	VAL	7.7
3	H	10	PHE	7.2
3	H	250	SER	6.4
1	L	279	ILE	6.2
2	M	80	TRP	5.3
1	L	281	GLY	5.2
2	M	83	ALA	4.5
1	L	55	LEU	4.4
1	L	81	ALA	4.3
1	L	277	GLY	4.2
1	L	51	TRP	4.1
2	M	82	PRO	4.1
1	L	280	ASN	4.1
3	H	249	LYS	4.0
3	H	118[A]	ARG	3.9
2	M	75	TRP	3.8
2	M	1	ALA	3.7
2	M	171	TRP	3.7
1	L	59	TRP	3.5
2	M	114	LEU	3.4
2	M	26	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	M	76	TYR	3.3
2	M	98	ALA	3.3
2	M	2[A]	GLU	3.2
2	M	109	LEU	3.2
1	L	276[A]	PRO	3.0
2	M	79	GLY	3.0
3	H	52	ASN	2.9
1	L	278	GLY	2.9
2	M	101	TYR	2.9
2	M	32	VAL	2.7
2	M	174	ALA	2.7
1	L	270	PRO	2.7
2	M	216	PHE	2.7
1	L	73	TYR	2.7
1	L	236	LEU	2.7
2	M	81	ASN	2.7
2	M	102	GLY	2.6
1	L	80	LEU	2.6
2	M	103	LEU	2.5
2	M	104	SER	2.5
1	L	275	ILE	2.4
1	L	269	LEU	2.4
2	M	72	ILE	2.4
2	M	105	PHE	2.4
1	L	185	LEU	2.4
2	M	265	ILE	2.4
1	L	54	VAL	2.4
1	L	271	TRP	2.3
2	M	100	GLU	2.3
1	L	202	LYS	2.3
3	H	158	LEU	2.3
2	M	57	VAL	2.2
2	M	52	LEU	2.2
1	L	265	TRP	2.2
1	L	88	ILE	2.2
2	M	54	SER	2.2
2	M	28	ASN	2.1
2	M	27	ALA	2.1
1	L	268	LYS	2.1
1	L	272	TRP	2.0
2	M	77	GLN	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, 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
9	LDA	H	905	16/16	0.20	0.75	61,69,78,78	16
9	LDA	H	904	16/16	0.30	0.61	65,68,72,72	16
9	LDA	H	903	16/16	0.44	0.48	63,65,74,75	16
8	PC9	L	802	54/54	0.55	0.62	57,66,75,79	54
9	LDA	M	920	16/16	0.56	0.48	59,74,88,88	16
14	PC7	H	801	52/52	0.60	0.81	26,68,76,78	52
9	LDA	L	902	16/16	0.66	0.50	68,73,77,80	16
13	HTO	H	709	10/10	0.67	0.26	50,56,56,58	10
9	LDA	L	906	16/16	0.68	0.35	54,56,59,60	16
11	CDL	M	800	81/100	0.68	0.40	43,71,83,85	81
9	LDA	M	907	16/16	0.71	0.42	56,61,66,67	16
15	GOL	H	708	6/6	0.77	0.89	46,46,47,49	6
7	U10	L	502	48/63	0.78	0.65	34,48,60,62	48
15	GOL	H	705	6/6	0.84	0.30	58,69,70,72	0
4	PO4	M	702	5/5	0.84	0.22	66,67,68,68	5
4	PO4	M	704	5/5	0.85	0.34	76,76,77,78	5
15	GOL	H	706	6/6	0.87	0.29	74,76,77,77	0
9	LDA	H	901	16/16	0.89	0.28	60,65,69,71	0
7	U10	M	501	48/63	0.89	0.22	43,54,77,80	0
4	PO4	L	703	5/5	0.90	0.39	70,72,73,75	5
6	BPH	M	401	65/65	0.91	0.18	45,51,92,93	0
5	BCL	L	314	66/66	0.94	0.17	38,47,62,66	0
5	BCL	L	312	66/66	0.95	0.15	41,46,58,61	0
5	BCL	M	311	66/66	0.95	0.17	42,51,96,97	0
6	BPH	L	402	65/65	0.95	0.15	35,47,52,53	0
5	BCL	M	313	66/66	0.97	0.15	38,46,70,79	0
4	PO4	M	701	5/5	0.97	0.31	57,59,62,63	0

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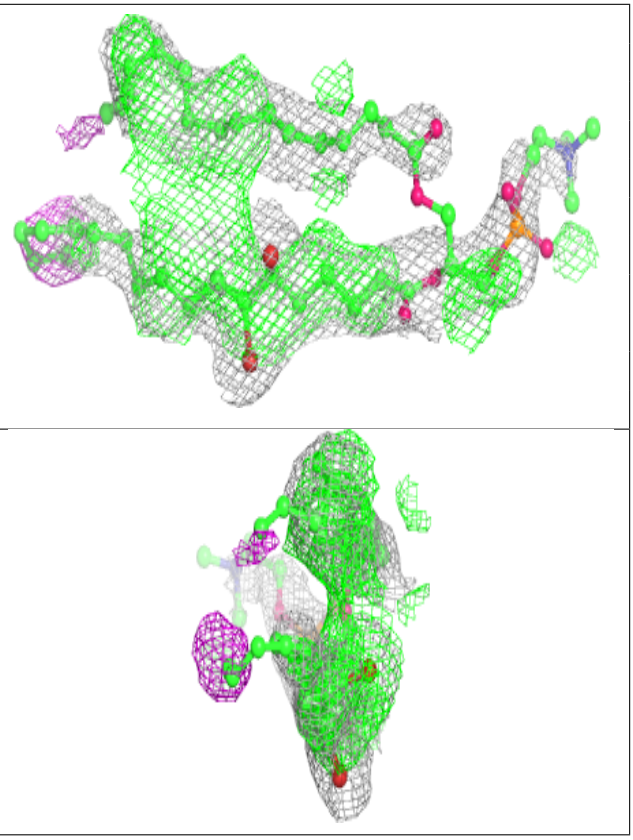
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	K	H	700	1/1	0.98	0.07	54,54,54,54	0
10	FE	M	500	1/1	1.00	0.16	49,49,49,49	0

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.

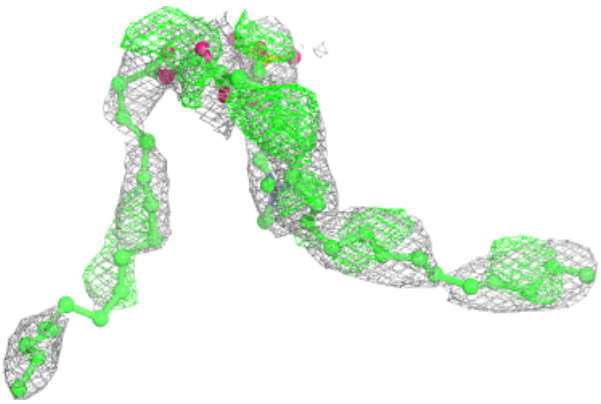
Electron density around PC9 L 802:

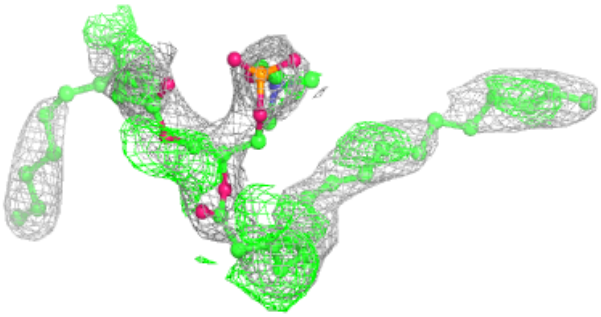
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

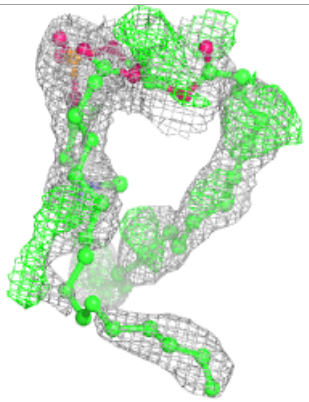


Electron density around PC7 H 801:

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

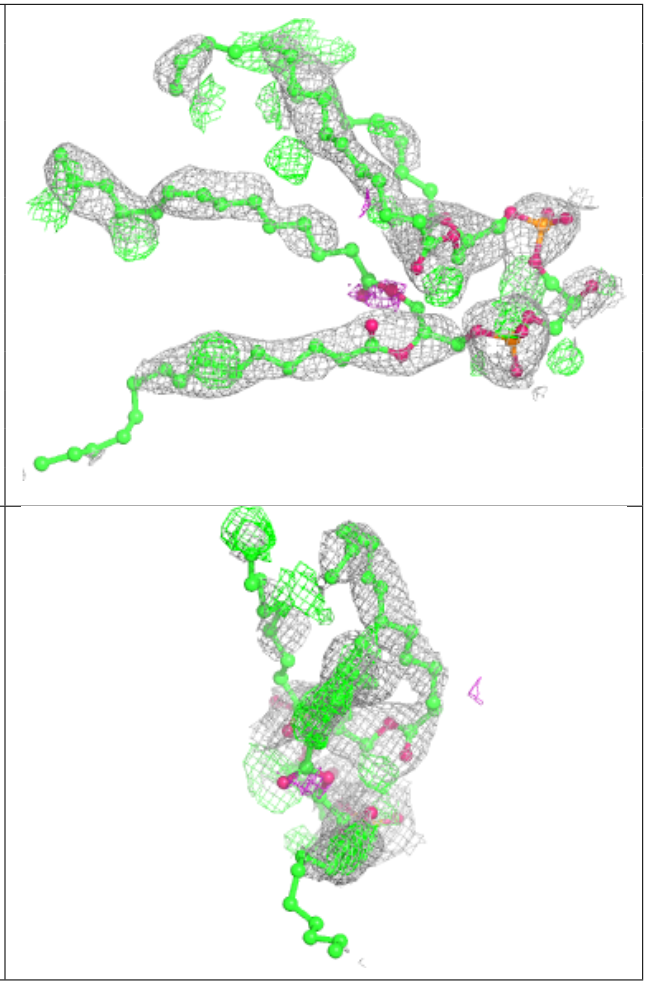






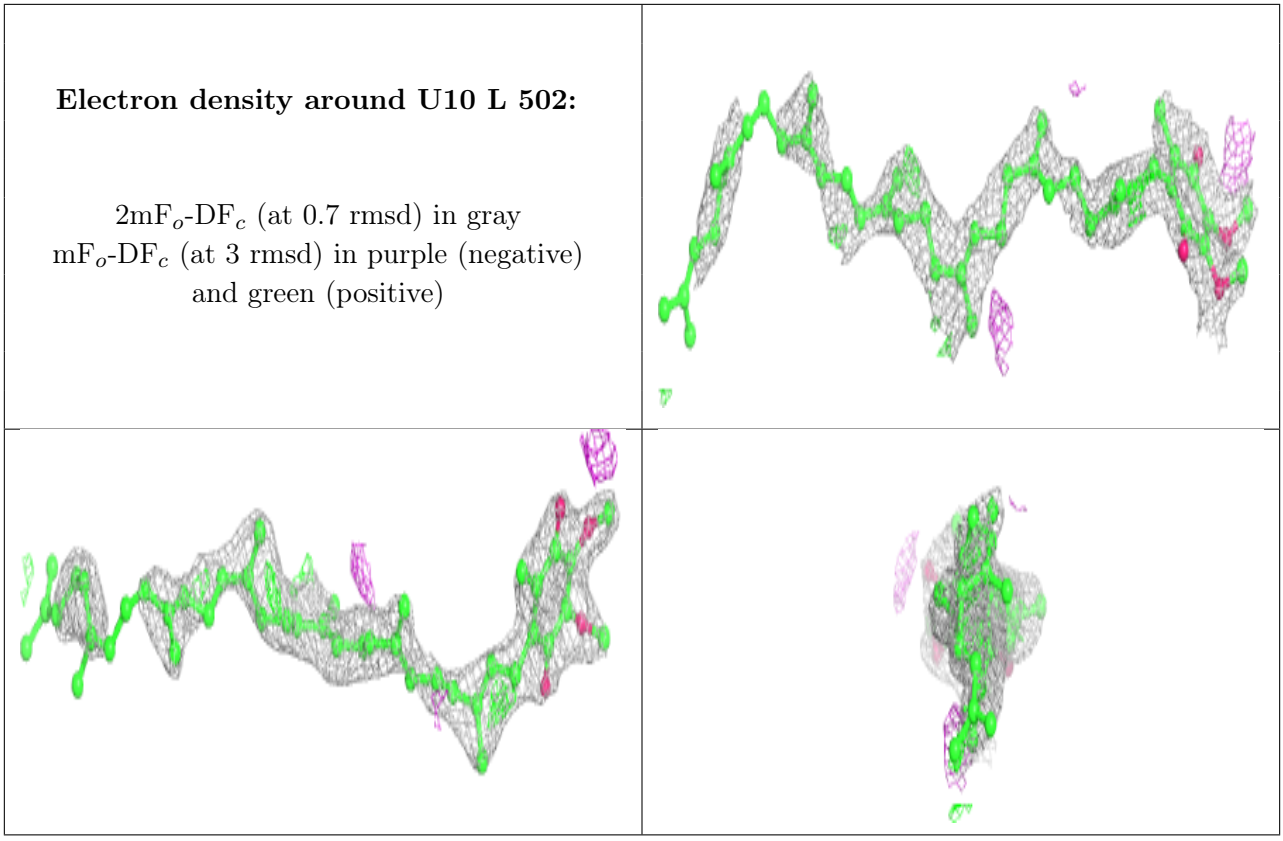
Electron density around CDL M 800:

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



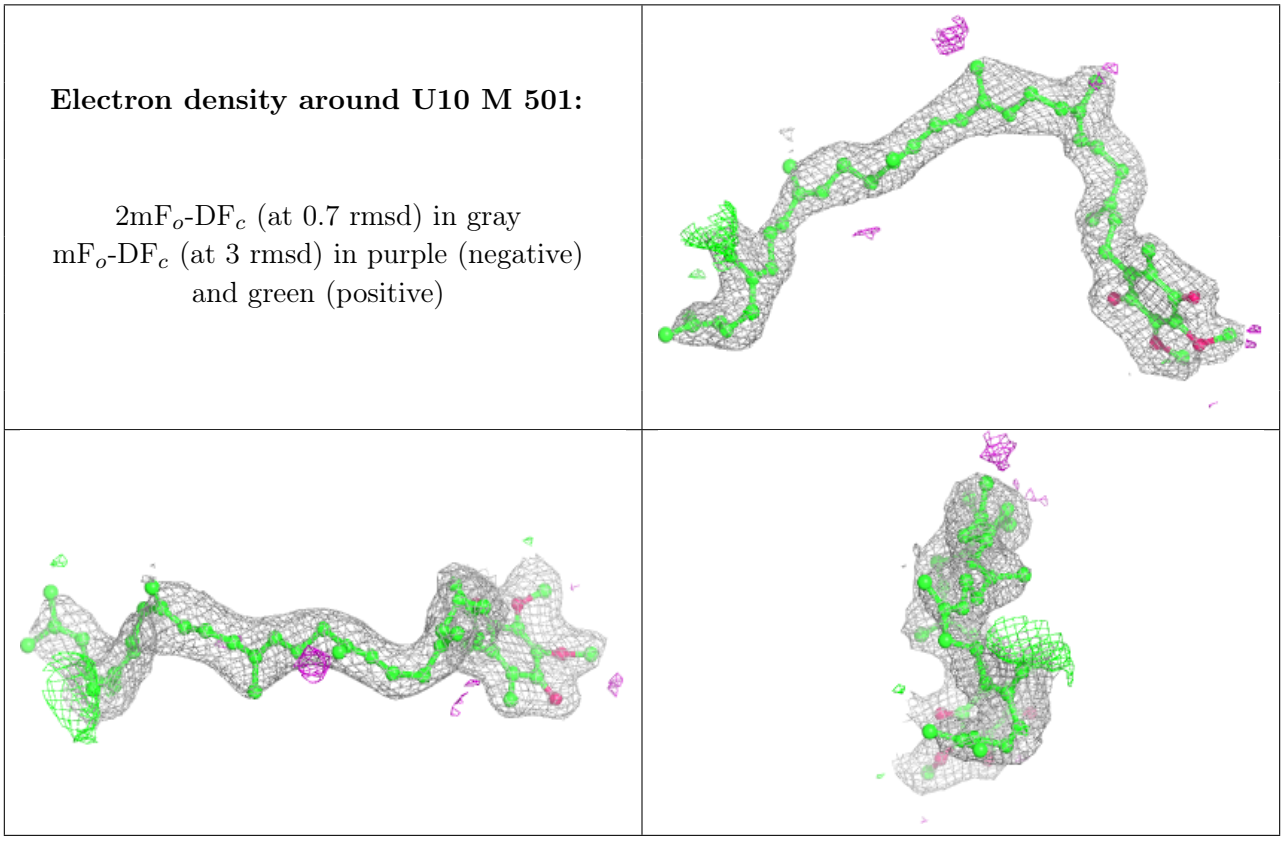
Electron density around U10 L 502:

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



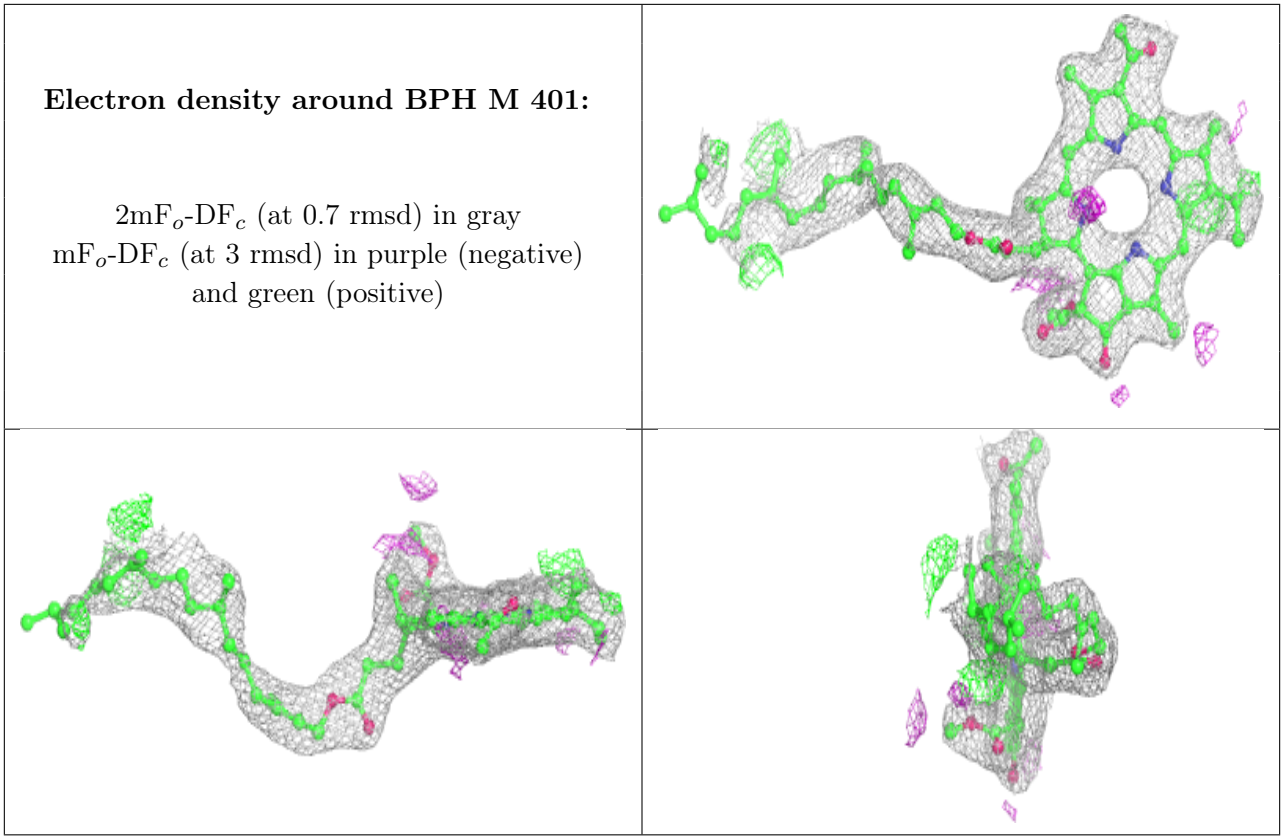
Electron density around U10 M 501:

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



Electron density around 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 314:

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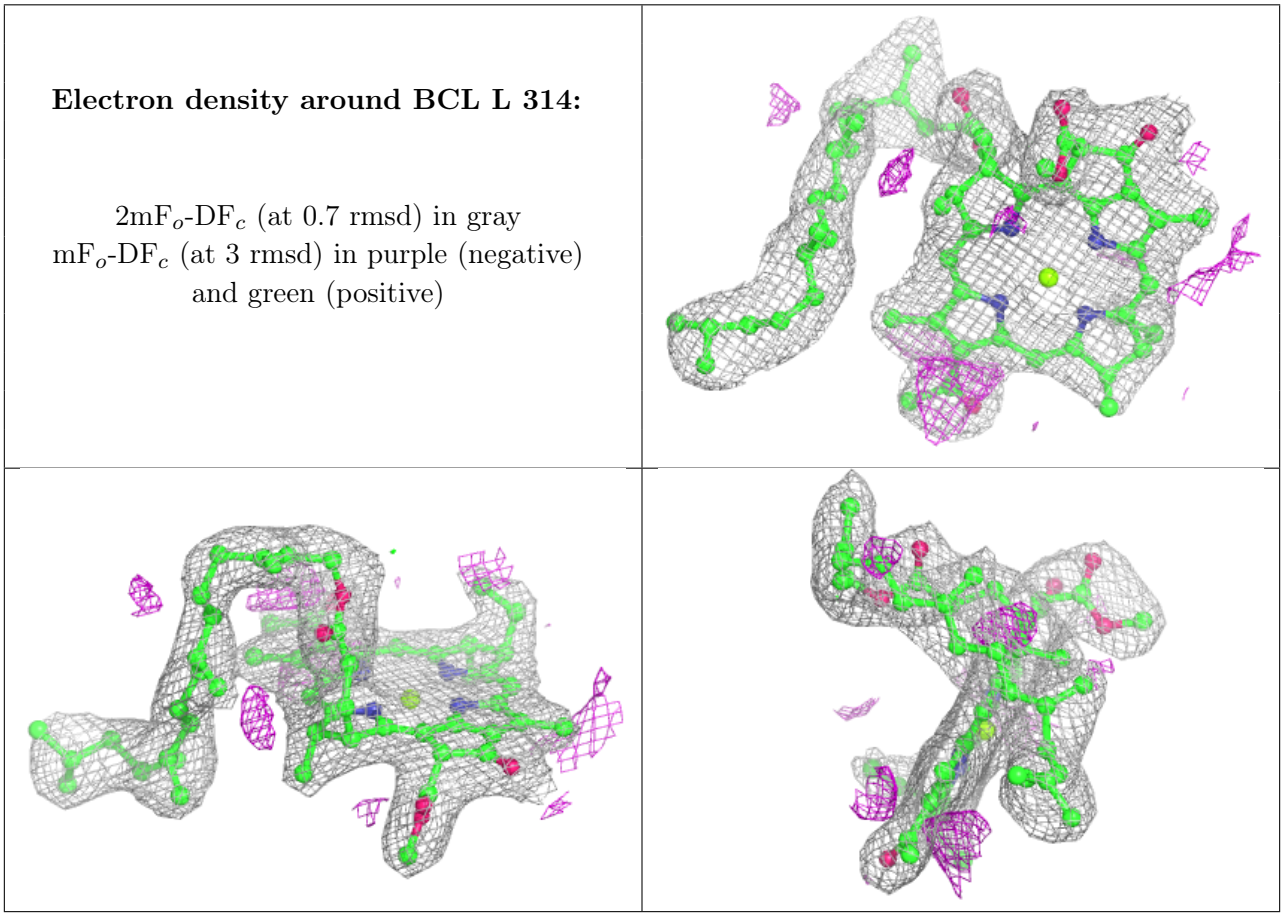
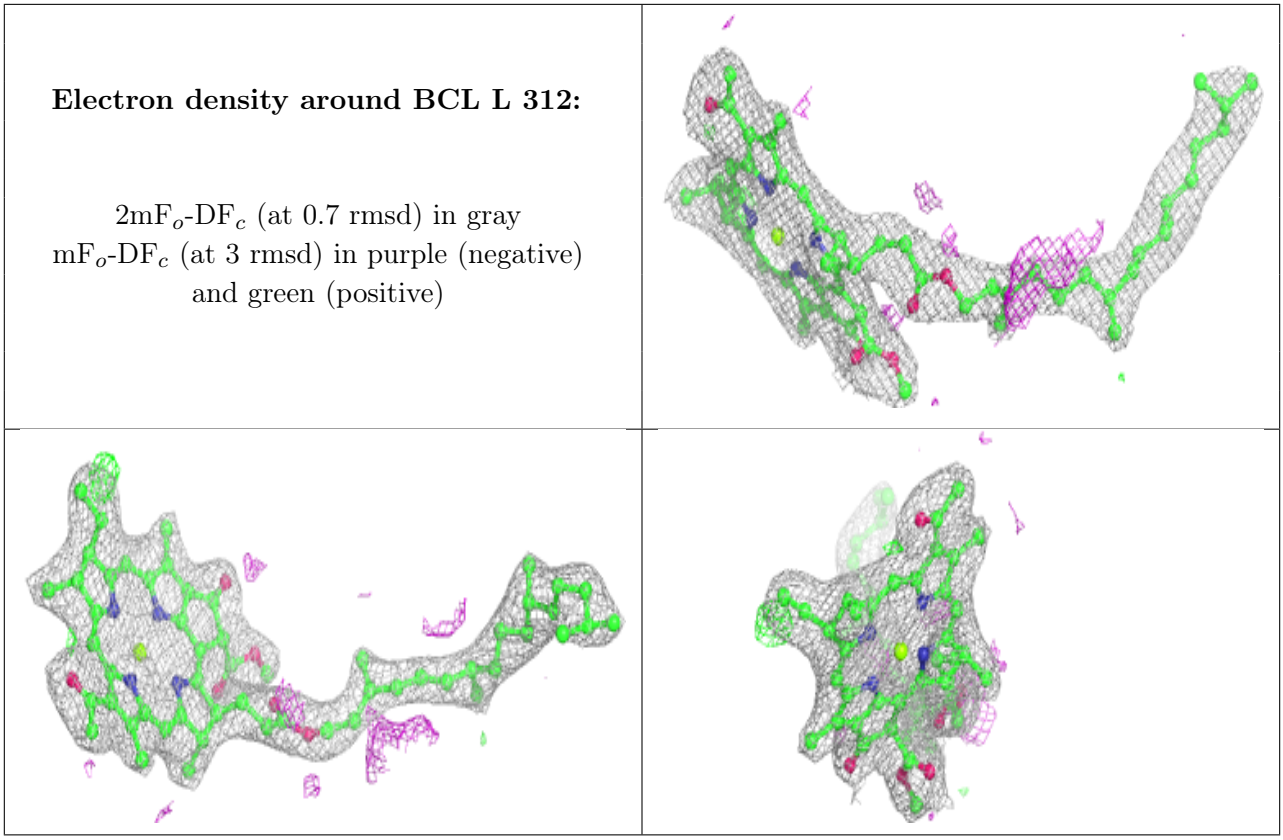
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



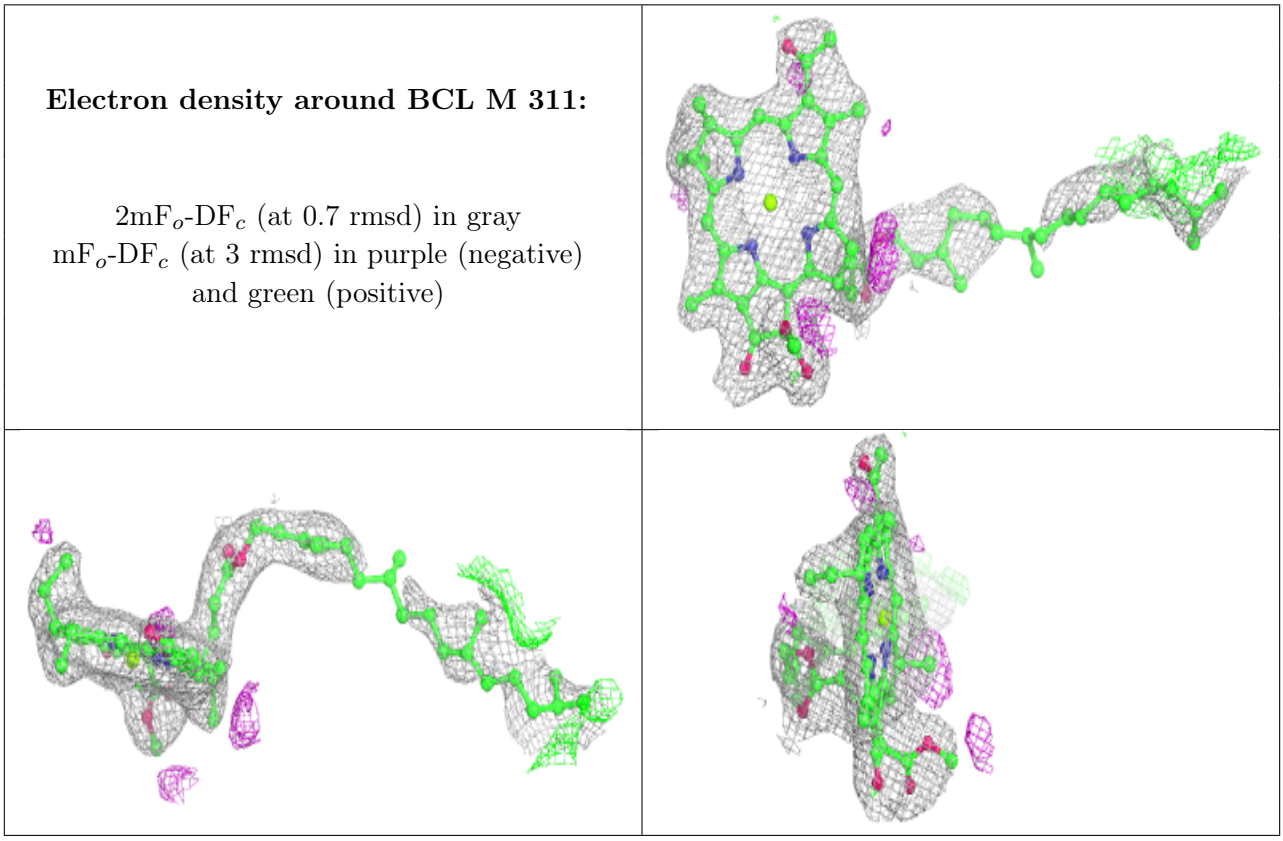
Electron density around BCL L 312:

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



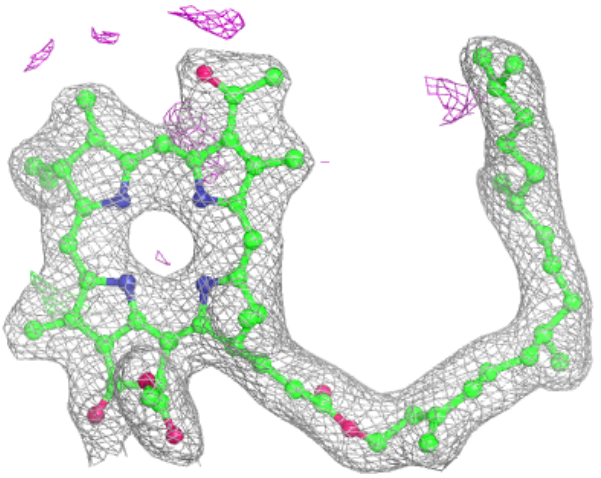
Electron density around BCL M 311:

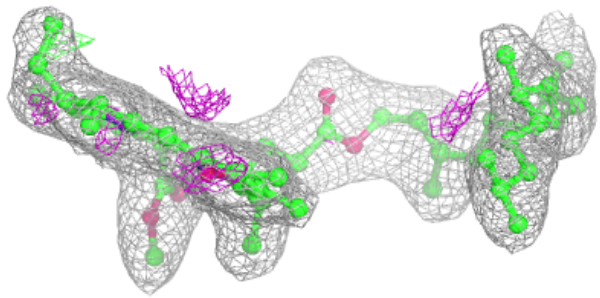
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

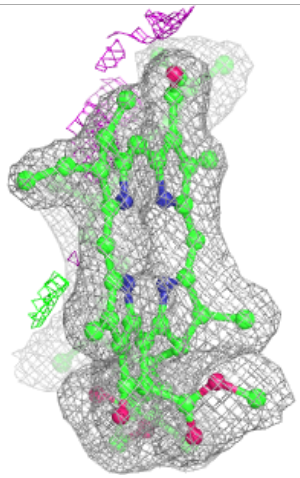


Electron density around BPH L 402:

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

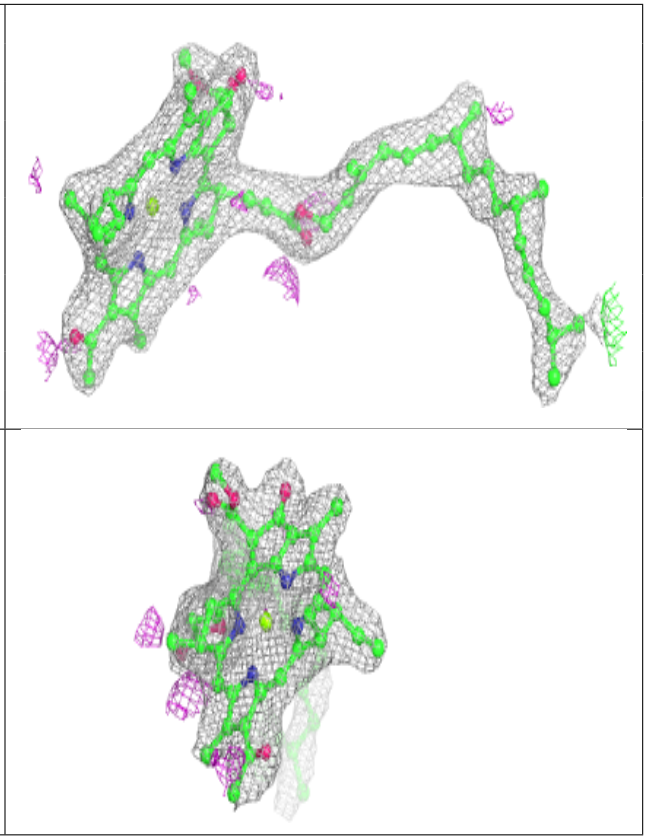






Electron density around BCL M 313:

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



6.5 Other polymers (i)

There are no such residues in this entry.