



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:09 am BST

PDB ID : 2HHK
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylglycerol
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-28
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

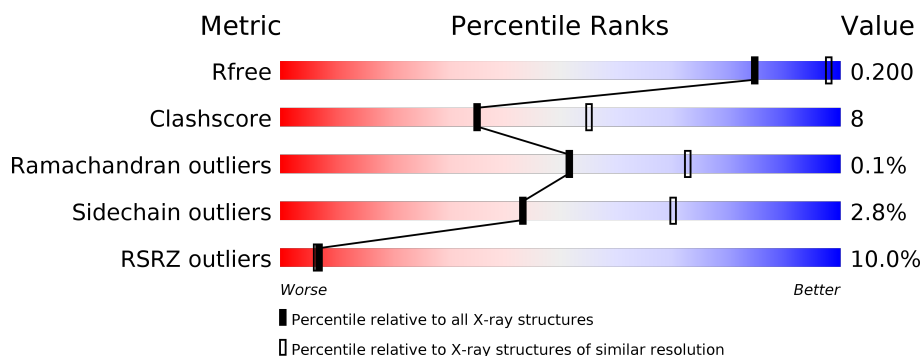
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>12%</div> <div>94%</div> <div>• •</div> </div>
2	M	307	<div> <div>12%</div> <div>89%</div> <div>9% • •</div> </div>
3	H	260	<div> <div>4%</div> <div>78%</div> <div>13% • 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CDL	M	800	-	-	-	X
12	PGK	M	802	-	-	-	X
13	LDA	H	901	-	-	X	-
13	LDA	H	903	-	-	X	X
13	LDA	H	904	-	-	-	X
13	LDA	M	902	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	920	-	-	-	X
15	PGT	H	801[A]	-	-	-	X
15	PGT	H	801[B]	-	-	-	X
6	U10	L	502	-	-	-	X
7	GOL	L	709	-	-	X	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2235	1510	356	361	8			

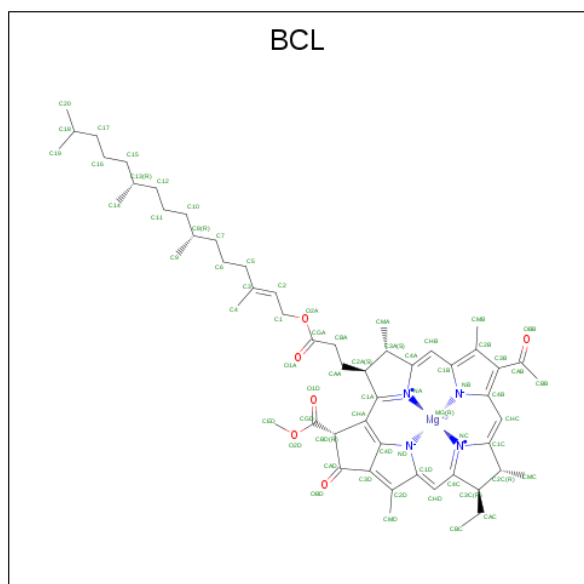
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	10	0
			2448	1633	402	402	11			

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

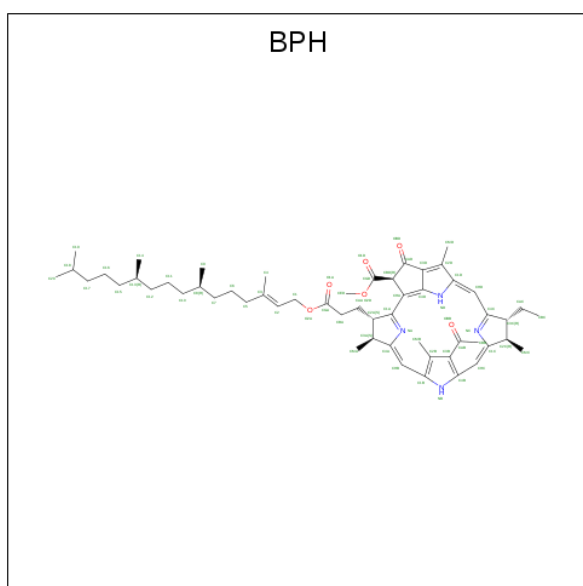
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1862	1189	323	339	11			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



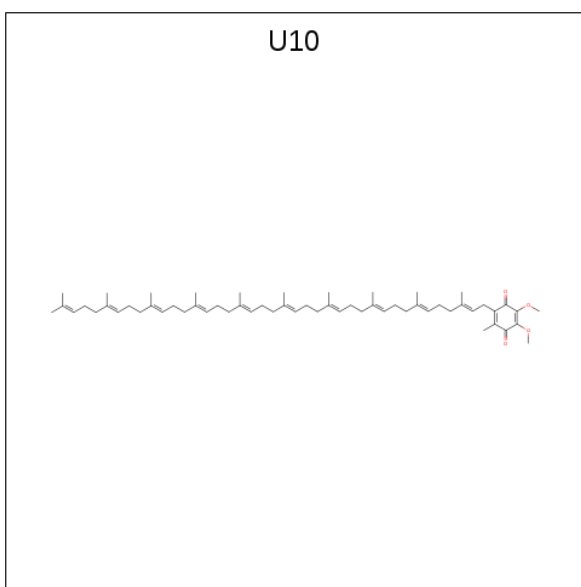
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



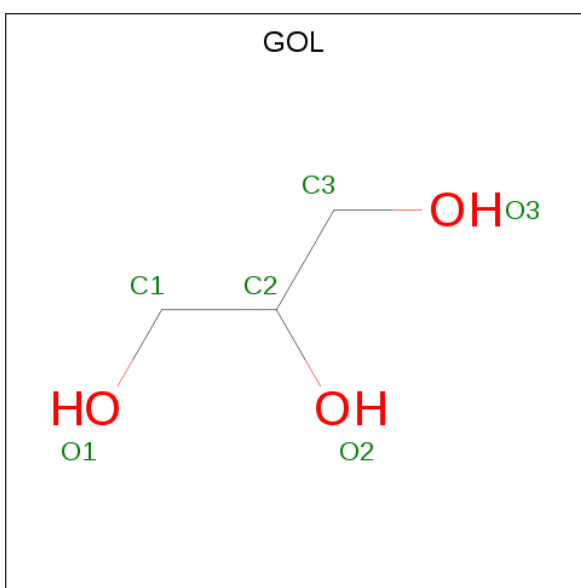
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

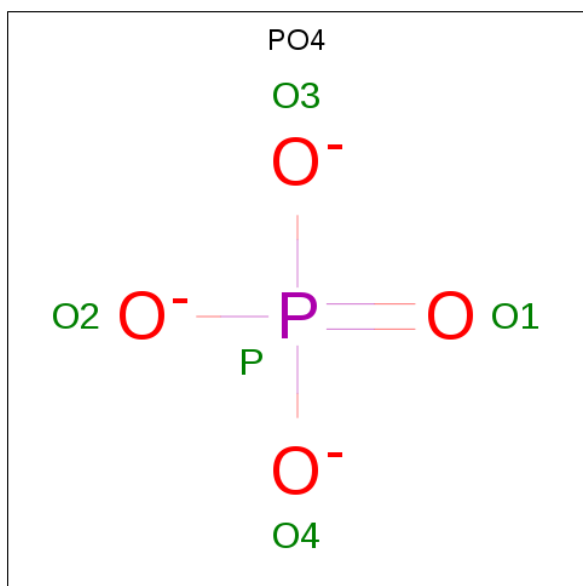
- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



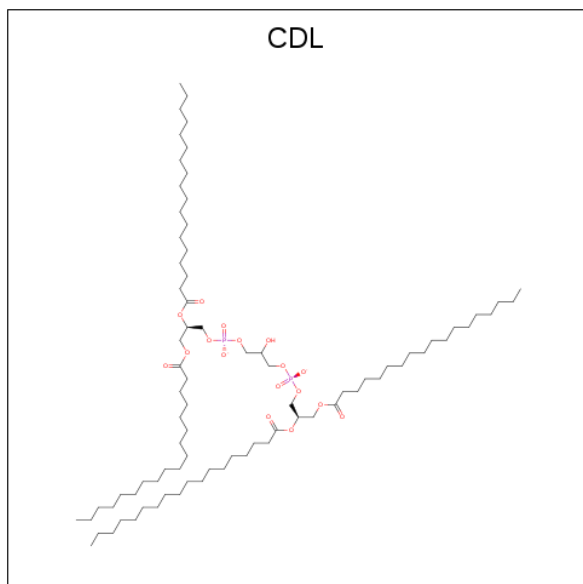
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		

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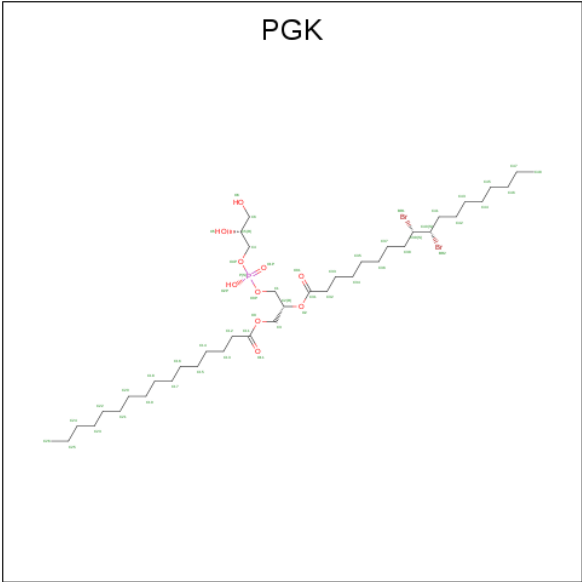
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	O	P	0	0
			5	4	1		

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



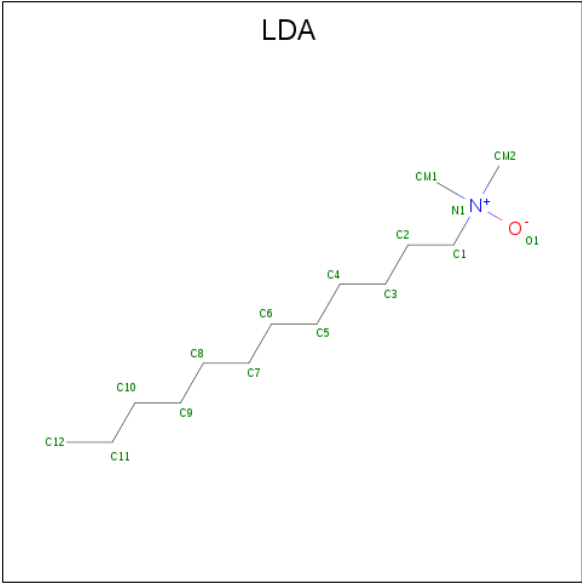
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 12 is (1R)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PGK) (formula: $C_{40}H_{77}Br_2O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	M	1	Total	Br	C	O	P	0	0
			53	2	40	10	1		

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



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

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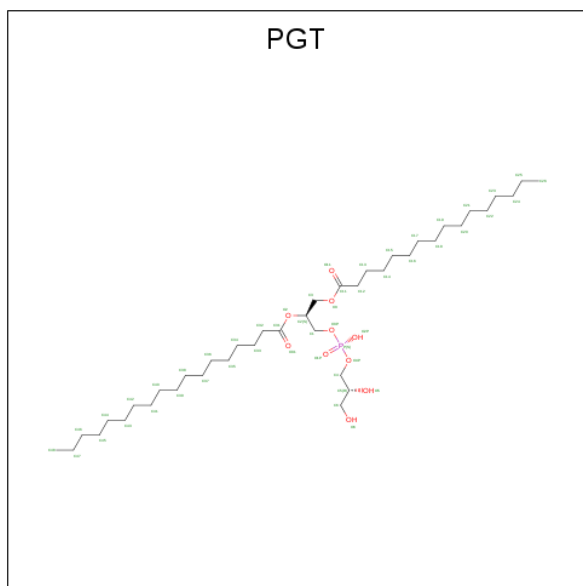
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		

- 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 (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	O	P	0	1
			102	80	20	2		

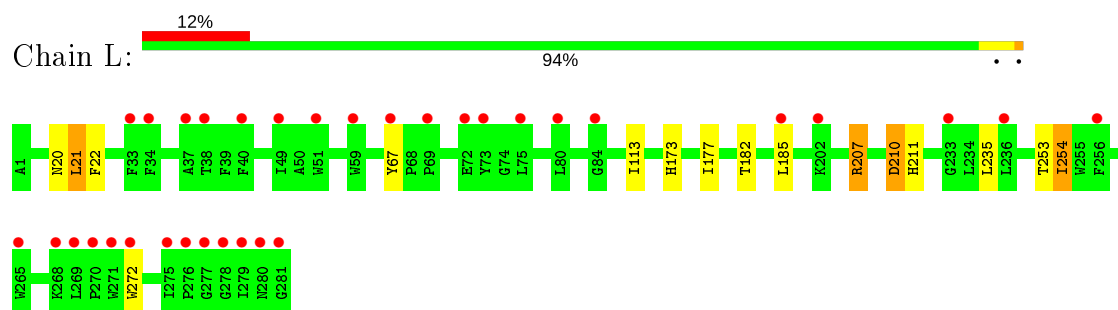
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	92	Total 92	O 92	0	0
16	M	119	Total 119	O 119	0	0
16	H	199	Total 199	O 199	0	0

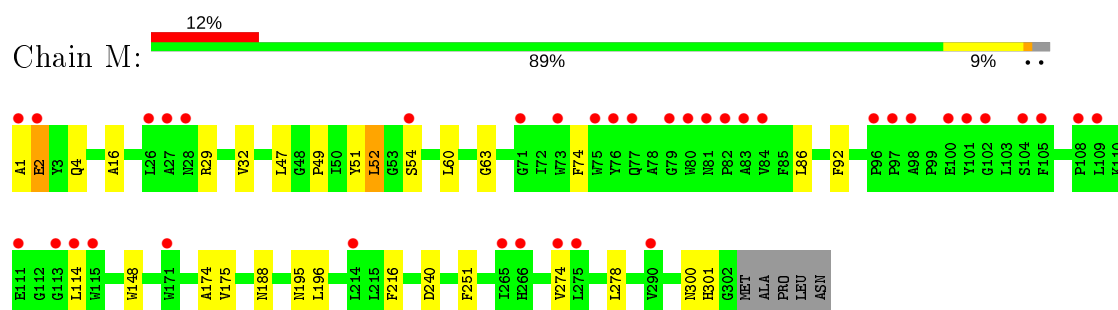
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

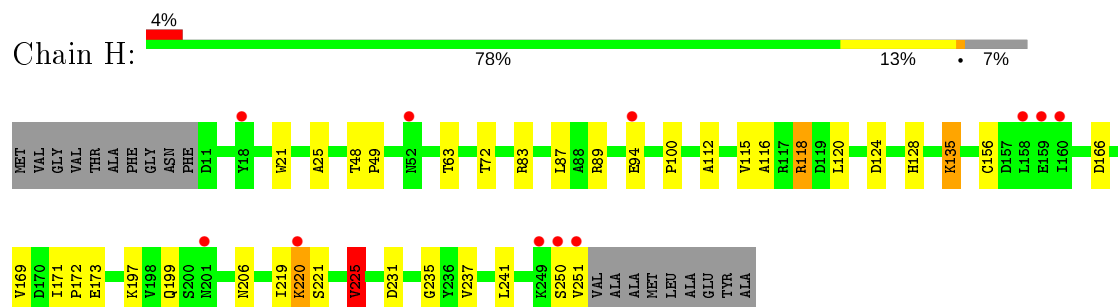
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.42Å 139.42Å 183.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.50 45.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.00-2.50) 99.5 (45.63-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.197 0.177 , 0.200	Depositor DCC
R_{free} test set	3548 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 97.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CL, CDL, BPH, K, PGK, PGT, FE, U10, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.88	0/2328	0.73	1/3186 (0.0%)
2	M	0.87	0/2592	0.78	1/3536 (0.0%)
3	H	0.93	5/1953 (0.3%)	0.82	4/2652 (0.2%)
All	All	0.89	5/6873 (0.1%)	0.78	6/9374 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	173	GLU	CD-OE2	5.32	1.31	1.25
3	H	237	VAL	CB-CG2	5.12	1.63	1.52
3	H	221[A]	SER	CB-OG	5.07	1.48	1.42
3	H	221[B]	SER	CB-OG	5.07	1.48	1.42
3	H	94	GLU	CG-CD	5.05	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.50	124.15	118.30
3	H	124	ASP	CB-CG-OD1	6.31	123.98	118.30
3	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
3	H	89	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	M	240	ASP	CB-CG-OD1	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	83	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	ALA	Peptide

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	2235	0	2196	10	0
2	M	2448	0	2367	26	0
3	H	1862	0	1883	25	0
4	L	132	0	148	6	0
4	M	132	0	148	20	0
5	L	65	0	75	0	0
5	M	65	0	76	4	0
6	L	48	0	63	4	0
6	M	48	0	63	1	0
7	H	6	0	8	0	0
7	L	18	0	24	5	0
8	M	1	0	0	0	0
9	M	1	0	0	0	0
10	H	5	0	0	0	0
10	M	15	0	0	1	0
11	M	81	0	106	3	0
12	M	53	0	74	11	0
13	H	48	0	93	25	0
13	M	48	0	93	12	0
14	H	1	0	0	0	0
15	H	102	0	156	20	0
16	H	199	0	0	4	0
16	L	92	0	0	2	0
16	M	119	0	0	2	0
All	All	7824	0	7573	123	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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:301[A]:HIS:HE1	16:M:1031:HOH:O	1.41	1.03
4:M:311:BCL:C9	4:M:311:BCL:H41	1.91	0.99
4:M:311:BCL:C7	4:M:311:BCL:H41	1.92	0.98
13:M:902:LDA:C12	13:H:903:LDA:C12	2.43	0.96
13:M:902:LDA:C12	13:H:903:LDA:H123	1.96	0.95
4:M:311:BCL:C4	4:M:311:BCL:H92	1.98	0.94
13:M:902:LDA:H122	13:H:903:LDA:C12	1.98	0.93
13:M:902:LDA:H122	13:H:903:LDA:H123	1.49	0.93
4:M:311:BCL:H92	4:M:311:BCL:H41	1.48	0.92
7:L:709:GOL:H2	3:H:241:LEU:HD13	1.54	0.89
15:H:801[A]:PGT:C44	13:H:901:LDA:H121	2.05	0.86
15:H:801[A]:PGT:C43	13:H:901:LDA:H121	2.05	0.85
4:M:313:BCL:H201	12:M:802:PGK:H252	1.59	0.84
4:M:311:BCL:HBB2	4:M:311:BCL:HMB1	1.63	0.81
4:M:311:BCL:CBB	4:M:311:BCL:HMB1	2.13	0.79
4:M:311:BCL:H41	4:M:311:BCL:H71	1.64	0.77
13:M:902:LDA:H123	13:H:903:LDA:C12	2.15	0.77
3:H:250:SER:O	3:H:251:VAL:HG23	1.85	0.76
6:L:502:U10:H153	12:M:802:PGK:H482	1.69	0.74
15:H:801[A]:PGT:H442	13:H:901:LDA:C12	2.20	0.71
4:M:311:BCL:C8	4:M:311:BCL:H41	2.20	0.71
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.73	0.69
1:L:254:ILE:C	1:L:254:ILE:HD12	2.13	0.69
4:L:314:BCL:HBB2	4:L:314:BCL:HMB1	1.74	0.68
15:H:801[B]:PGT:C32	15:H:801[B]:PGT:H12	2.22	0.68
15:H:801[A]:PGT:H362	15:H:801[A]:PGT:H321	1.75	0.68
1:L:182:THR:OG1	4:M:311:BCL:H2	1.94	0.68
15:H:801[A]:PGT:H442	13:H:901:LDA:H121	1.72	0.68
3:H:220[B]:LYS:NZ	16:H:1209:HOH:O	2.25	0.67
6:L:502:U10:H153	12:M:802:PGK:C48	2.25	0.66
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.78	0.66
15:H:801[B]:PGT:C43	13:H:901:LDA:H121	2.24	0.66
15:H:801[B]:PGT:C44	13:H:901:LDA:H121	2.26	0.65
4:M:313:BCL:C20	12:M:802:PGK:H252	2.26	0.64
4:M:311:BCL:C4	4:M:311:BCL:C9	2.63	0.64
15:H:801[A]:PGT:H412	13:H:903:LDA:H111	1.82	0.62
15:H:801[A]:PGT:H432	13:H:901:LDA:H121	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:902:LDA:H122	13:H:903:LDA:H122	1.80	0.62
11:M:800:CDL:H231	13:H:904:LDA:HM12	1.82	0.60
2:M:174:ALA:HB1	13:M:920:LDA:H121	1.83	0.60
2:M:175:VAL:H	13:M:920:LDA:H123	1.66	0.60
4:M:311:BCL:H191	12:M:802:PGK:BR2	2.57	0.60
4:M:311:BCL:H42	4:M:311:BCL:H92	1.84	0.60
3:H:118[B]:ARG:HE	3:H:120:LEU:HD12	1.68	0.57
13:M:902:LDA:C12	13:H:903:LDA:H122	2.33	0.57
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.40	0.57
4:M:311:BCL:C4	4:M:311:BCL:H71	2.33	0.57
3:H:21:TRP:CD1	15:H:801[B]:PGT:H5	2.41	0.56
4:L:314:BCL:CBB	4:L:314:BCL:HMB1	2.37	0.55
11:M:800:CDL:C23	13:H:904:LDA:HM12	2.37	0.54
4:M:311:BCL:H8	12:M:802:PGK:H471	1.91	0.52
2:M:60[A]:LEU:HD23	5:M:401:BPH:H4C1	1.92	0.52
15:H:801[B]:PGT:H322	15:H:801[B]:PGT:H12	1.92	0.52
7:L:709:GOL:H2	3:H:241:LEU:CD1	2.35	0.51
2:M:278[B]:LEU:HD11	11:M:800:CDL:H811	1.91	0.51
3:H:197[A]:LYS:NZ	3:H:199:GLN:HE21	2.09	0.51
15:H:801[B]:PGT:H431	13:H:901:LDA:H121	1.90	0.50
6:L:502:U10:C15	12:M:802:PGK:H482	2.41	0.50
2:M:175:VAL:N	13:M:920:LDA:H123	2.26	0.50
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.93	0.50
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.93	0.50
2:M:51:TYR:O	2:M:52:LEU:HD23	2.11	0.50
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.47	0.50
4:L:312:BCL:CBB	4:L:312:BCL:HMB1	2.43	0.48
2:M:188[B]:ASN:ND2	16:M:1077:HOH:O	2.43	0.48
3:H:220[B]:LYS:NZ	16:H:1100:HOH:O	2.41	0.48
2:M:175:VAL:H	13:M:920:LDA:C12	2.27	0.47
2:M:54:SER:OG	10:M:703:PO4:O2	2.32	0.47
15:H:801[A]:PGT:H442	13:H:901:LDA:H123	1.96	0.47
6:L:502:U10:H4M3	6:L:502:U10:H3M2	1.96	0.47
15:H:801[A]:PGT:C41	13:H:903:LDA:H111	2.44	0.47
1:L:113:ILE:O	7:L:709:GOL:H11	2.15	0.47
2:M:175:VAL:HB	13:M:920:LDA:H123	1.97	0.47
2:M:29:ARG:O	12:M:802:PGK:H42	2.15	0.47
4:L:312:BCL:HHC	4:L:312:BCL:OBB	2.15	0.46
1:L:113:ILE:O	7:L:709:GOL:C1	2.63	0.46
4:M:313:BCL:HMB1	4:M:313:BCL:CBB	2.45	0.46
3:H:63:THR:CG2	3:H:72:THR:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.51	0.46
7:L:709:GOL:C2	3:H:241:LEU:HD13	2.36	0.46
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
4:M:313:BCL:HAA2	4:M:313:BCL:HBD	1.99	0.45
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.81	0.45
3:H:128[B]:HIS:HE1	16:H:1109:HOH:O	1.99	0.45
5:M:401:BPH:CBC	5:M:401:BPH:HHD	2.47	0.45
12:M:802:PGK:H121	12:M:802:PGK:H31	1.53	0.45
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.52	0.44
3:H:135:LYS:HB3	3:H:135:LYS:HE3	1.57	0.44
15:H:801[A]:PGT:H362	15:H:801[A]:PGT:C32	2.46	0.44
2:M:63:GLY:HA3	5:M:401:BPH:H5C2	1.99	0.44
4:L:312:BCL:HMB1	4:L:312:BCL:HBB3	1.99	0.44
2:M:47:LEU:HD22	12:M:802:PGK:BR2	2.73	0.43
15:H:801[B]:PGT:H322	15:H:801[B]:PGT:H351	1.58	0.43
15:H:801[A]:PGT:H432	13:H:903:LDA:H112	2.00	0.43
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.91	0.43
3:H:128[B]:HIS:HD2	16:H:1280:HOH:O	2.01	0.42
1:L:67:TYR:HB3	16:L:1167:HOH:O	2.19	0.42
3:H:135:LYS:HB3	3:H:166:ASP:OD2	2.20	0.42
1:L:253:THR:OG1	1:L:254:ILE:N	2.51	0.42
4:M:313:BCL:H201	12:M:802:PGK:C25	2.40	0.42
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.54	0.42
3:H:48:THR:HB	3:H:49:PRO:HD2	2.02	0.42
3:H:25:ALA:HB2	13:H:903:LDA:H52	2.01	0.42
15:H:801[A]:PGT:C44	13:H:901:LDA:C12	2.81	0.42
2:M:2:GLU:HG3	2:M:2:GLU:H	1.53	0.42
2:M:2:GLU:O	2:M:4:GLN:NE2	2.52	0.42
3:H:115:VAL:HG12	3:H:116:ALA:N	2.35	0.42
13:H:901:LDA:H22	13:H:901:LDA:HM11	1.80	0.42
2:M:32:VAL:HG12	2:M:49:PRO:HD3	2.02	0.42
6:M:501:U10:H322	6:M:501:U10:H28	1.80	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.41
15:H:801[B]:PGT:C41	13:H:903:LDA:H111	2.50	0.41
1:L:20:ASN:ND2	16:L:1300:HOH:O	2.52	0.41
4:L:312:BCL:CGA	4:L:314:BCL:HBC1	2.51	0.41
3:H:118[B]:ARG:NE	3:H:120:LEU:HD12	2.35	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.01	0.41
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.41
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:401:BPH:HBC3	5:M:401:BPH:HHD	2.02	0.40
4:M:311:BCL:HMB1	4:M:311:BCL:HBB3	2.00	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	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	298 (96%)	11 (4%)	1 (0%)	41	61
3	H	247/260 (95%)	242 (98%)	5 (2%)	0	100	100
All	All	837/848 (99%)	814 (97%)	22 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	221/220 (100%)	214 (97%)	7 (3%)	39	65
2	M	246/240 (102%)	240 (98%)	6 (2%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	204/208 (98%)	197 (97%)	7 (3%)	37	63
All	All	671/668 (100%)	651 (97%)	20 (3%)	43	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	254	ILE
1	L	272	TRP
2	M	2	GLU
2	M	52	LEU
2	M	86	LEU
2	M	114	LEU
2	M	216	PHE
2	M	274	VAL
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	135	LYS
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
3	H	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LDA	H	901	-	12,15,15	1.77	1 (8%)	14,17,17	0.86	0
10	PO4	M	702	-	4,4,4	0.63	0	6,6,6	0.66	0
4	BCL	L	314	1	58,74,74	1.17	3 (5%)	69,115,115	1.60	15 (21%)
4	BCL	M	313	2	58,74,74	1.20	3 (5%)	69,115,115	1.86	17 (24%)
13	LDA	H	903	-	12,15,15	1.91	1 (8%)	14,17,17	0.54	0
10	PO4	M	703	-	4,4,4	0.90	0	6,6,6	1.43	1 (16%)
13	LDA	H	904	-	12,15,15	2.02	1 (8%)	14,17,17	0.53	0
7	GOL	L	707	-	5,5,5	0.38	0	5,5,5	0.48	0
11	CDL	M	800	-	80,80,99	1.25	4 (5%)	86,92,111	1.44	12 (13%)
10	PO4	M	705	-	4,4,4	0.85	0	6,6,6	0.78	0
7	GOL	H	706	-	5,5,5	0.27	0	5,5,5	0.85	0
4	BCL	L	312	1	58,74,74	1.23	4 (6%)	69,115,115	1.56	15 (21%)
13	LDA	M	902	-	12,15,15	1.93	1 (8%)	14,17,17	0.54	0
12	PGK	M	802	-	52,52,52	0.88	3 (5%)	55,60,60	1.48	5 (9%)
4	BCL	M	311	2	58,74,74	1.14	3 (5%)	69,115,115	1.83	20 (28%)
5	BPH	L	402	-	64,70,70	0.83	1 (1%)	76,101,101	1.20	11 (14%)
10	PO4	H	704	-	4,4,4	0.90	0	6,6,6	0.68	0
13	LDA	M	920	-	12,15,15	1.87	1 (8%)	14,17,17	0.83	0
13	LDA	M	907	-	12,15,15	2.06	1 (8%)	14,17,17	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U10	M	501	-	48,48,63	1.15	2 (4%)	58,61,79	1.49	8 (13%)
7	GOL	L	708	-	5,5,5	0.49	0	5,5,5	0.56	0
6	U10	L	502	-	48,48,63	1.10	4 (8%)	58,61,79	1.65	11 (18%)
5	BPH	M	401	-	64,70,70	0.89	1 (1%)	76,101,101	1.56	14 (18%)
15	PGT	H	801[A]	-	50,50,50	0.71	0	53,56,56	0.97	3 (5%)
15	PGT	H	801[B]	-	50,50,50	0.83	1 (2%)	53,56,56	1.10	5 (9%)
7	GOL	L	709	-	5,5,5	0.64	0	5,5,5	0.66	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	LDA	H	901	-	-	4/13/13/13	-
4	BCL	L	314	1	-	3/37/137/137	-
4	BCL	M	313	2	-	2/37/137/137	-
13	LDA	H	903	-	-	5/13/13/13	-
13	LDA	H	904	-	-	7/13/13/13	-
7	GOL	L	707	-	-	4/4/4/4	-
11	CDL	M	800	-	-	37/91/91/110	-
7	GOL	H	706	-	-	2/4/4/4	-
4	BCL	L	312	1	-	3/37/137/137	-
13	LDA	M	902	-	-	1/13/13/13	-
12	PGK	M	802	-	-	24/60/60/60	-
4	BCL	M	311	2	-	10/37/137/137	-
5	BPH	L	402	-	-	6/54/105/105	0/5/6/6
13	LDA	M	920	-	-	7/13/13/13	-
13	LDA	M	907	-	-	7/13/13/13	-
6	U10	M	501	-	-	5/45/69/87	0/1/1/1
7	GOL	L	708	-	-	4/4/4/4	-
6	U10	L	502	-	-	11/45/69/87	0/1/1/1
5	BPH	M	401	-	-	13/54/105/105	0/5/6/6
15	PGT	H	801[A]	-	-	30/55/55/55	-
15	PGT	H	801[B]	-	-	24/55/55/55	-
7	GOL	L	709	-	-	2/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	907	LDA	O1-N1	-6.96	1.25	1.42
13	H	904	LDA	O1-N1	-6.90	1.26	1.42
13	M	902	LDA	O1-N1	-6.59	1.26	1.42
13	H	903	LDA	O1-N1	-6.53	1.26	1.42
13	M	920	LDA	O1-N1	-6.35	1.27	1.42
13	H	901	LDA	O1-N1	-6.10	1.27	1.42
4	M	313	BCL	MG-NA	5.74	2.19	2.06
4	L	312	BCL	MG-NA	5.47	2.19	2.06
11	M	800	CDL	OA8-CA7	5.42	1.49	1.33
4	M	311	BCL	MG-NA	4.98	2.18	2.06
11	M	800	CDL	OB6-CB5	4.62	1.47	1.34
4	L	314	BCL	MG-NA	4.45	2.16	2.06
11	M	800	CDL	OA6-CA5	4.35	1.46	1.34
4	M	311	BCL	C1B-NB	4.35	1.39	1.35
11	M	800	CDL	OB8-CB7	4.33	1.46	1.33
6	M	501	U10	O3-C3	4.21	1.47	1.36
6	L	502	U10	O3-C3	4.15	1.47	1.36
4	L	312	BCL	C1B-NB	3.65	1.38	1.35
4	M	313	BCL	C4B-NB	3.59	1.38	1.35
12	M	802	PGK	P-O1P	3.35	1.62	1.50
6	M	501	U10	O4-C4	3.06	1.44	1.36
4	L	312	BCL	C4-C3	2.89	1.58	1.50
6	L	502	U10	C13-C14	2.85	1.39	1.33
15	H	801[B]	PGT	C1-C2	2.82	1.59	1.50
4	L	314	BCL	MG-NC	-2.78	1.99	2.06
4	L	312	BCL	C4B-NB	2.75	1.37	1.35
6	L	502	U10	O4-C4	2.58	1.43	1.36
4	L	314	BCL	C1B-NB	2.49	1.37	1.35
4	M	311	BCL	MG-NC	2.47	2.12	2.06
5	M	401	BPH	CHC-C1C	2.36	1.41	1.36
6	L	502	U10	C33-C34	2.21	1.38	1.33
5	L	402	BPH	CHC-C1C	2.16	1.41	1.36
12	M	802	PGK	O2-C2	-2.15	1.41	1.46
4	M	313	BCL	C5-C3	2.13	1.55	1.51
12	M	802	PGK	BR1-C39	-2.07	1.92	1.97

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	313	BCL	CMB-C2B-C1B	-5.91	119.38	128.46
11	M	800	CDL	OB6-CB5-C51	5.38	123.09	111.50
12	M	802	PGK	BR1-C39-C40	-5.10	100.39	110.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	313	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
5	M	401	BPH	O2D-CGD-CBD	4.68	119.59	111.27
6	L	502	U10	C25-C24-C26	4.63	123.07	115.27
12	M	802	PGK	C3-C2-C1	-4.60	100.90	111.79
4	L	312	BCL	CMB-C2B-C1B	-4.59	121.41	128.46
5	M	401	BPH	C1-C2-C3	-4.39	118.45	126.04
4	M	311	BCL	OB B-CAB-C3B	4.36	127.73	119.99
4	M	313	BCL	C1C-NC-C4C	4.25	108.61	106.71
6	L	502	U10	O2-C2-C3	-4.17	112.07	120.93
4	M	313	BCL	CMB-C2B-C3B	4.17	132.48	124.68
15	H	801[A]	PGT	O2-C31-C32	4.16	120.47	111.50
11	M	800	CDL	CA4-OA6-CA5	-4.16	107.55	117.79
12	M	802	PGK	O2-C31-C32	4.15	120.45	111.50
4	M	311	BCL	O2D-CGD-CBD	4.10	118.56	111.27
4	M	311	BCL	C4-C3-C2	-4.04	113.32	123.68
4	M	311	BCL	C1-O2A-CGA	4.01	126.97	116.44
4	M	313	BCL	CMD-C2D-C3D	4.00	132.16	124.68
4	L	312	BCL	CMB-C2B-C3B	4.00	132.16	124.68
15	H	801[B]	PGT	O2-C31-C32	3.98	120.08	111.50
11	M	800	CDL	OB8-CB6-CB4	3.94	119.91	108.43
11	M	800	CDL	OA6-CA5-C11	3.93	119.98	111.50
4	L	314	BCL	CAA-C2A-C3A	-3.86	102.21	112.78
4	M	311	BCL	CMB-C2B-C1B	-3.80	122.63	128.46
4	L	314	BCL	CAC-C3C-C2C	-3.78	104.81	114.26
6	M	501	U10	C17-C18-C19	-3.69	118.77	127.66
4	M	313	BCL	C4D-C3D-CAD	-3.68	106.42	108.47
5	M	401	BPH	CAC-C3C-C4C	3.64	122.03	112.67
4	M	311	BCL	CED-O2D-CGD	-3.63	107.73	115.94
4	L	314	BCL	O2D-CGD-CBD	3.52	117.53	111.27
15	H	801[B]	PGT	C2-O2-C31	-3.45	109.30	117.79
6	M	501	U10	C22-C23-C24	-3.43	119.41	127.66
5	M	401	BPH	OB D-CAD-CBD	-3.41	121.02	125.89
6	L	502	U10	C12-C13-C14	-3.41	119.44	127.66
4	L	312	BCL	C4D-C3D-CAD	-3.32	106.62	108.47
4	L	312	BCL	C4B-C3B-CAB	-3.31	120.73	127.13
5	M	401	BPH	CAA-C2A-C3A	-3.28	103.80	112.78
4	M	311	BCL	C5-C3-C2	3.26	127.70	121.12
6	L	502	U10	C3M-O3-C3	3.23	127.91	116.47
6	L	502	U10	C30-C29-C31	3.22	120.68	115.27
6	M	501	U10	C15-C14-C16	3.17	120.61	115.27
11	M	800	CDL	OA8-CA7-C31	3.13	121.72	111.91
6	M	501	U10	C30-C29-C31	3.11	120.50	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	312	BCL	CAA-C2A-C3A	-3.11	104.27	112.78
6	M	501	U10	C26-C27-C28	-3.09	101.73	111.88
4	L	314	BCL	C5-C3-C2	-3.06	114.92	121.12
4	L	314	BCL	CAA-CBA-CGA	3.04	122.13	113.25
5	L	402	BPH	C1-C2-C3	-3.01	120.84	126.04
6	M	501	U10	C41-C39-C40	2.99	121.20	114.60
6	M	501	U10	C32-C33-C34	-2.97	120.50	127.66
6	M	501	U10	C7-C6-C5	-2.97	114.90	118.48
5	M	401	BPH	C4D-C3D-CAD	-2.94	106.00	107.87
4	M	313	BCL	O2A-C1-C2	2.94	116.36	108.64
11	M	800	CDL	OB8-CB7-C71	2.94	121.12	111.91
6	L	502	U10	C25-C24-C23	-2.93	116.15	123.68
5	L	402	BPH	O2D-CGD-CBD	2.93	116.48	111.27
4	L	312	BCL	CHA-C1A-NA	-2.89	119.78	126.40
6	L	502	U10	C22-C23-C24	-2.87	120.75	127.66
4	M	313	BCL	C4-C3-C5	2.85	120.06	115.27
12	M	802	PGK	C2-O2-C31	-2.82	110.85	117.79
4	M	313	BCL	O2D-CGD-O1D	-2.81	118.34	123.84
6	L	502	U10	C7-C6-C5	-2.77	115.15	118.48
6	L	502	U10	C1M-C1-C6	-2.77	119.88	124.40
5	M	401	BPH	O2D-CGD-O1D	-2.76	118.44	123.84
4	L	314	BCL	C1C-NC-C4C	2.75	107.94	106.71
4	L	312	BCL	C2C-C3C-C4C	2.65	105.31	101.34
4	M	311	BCL	CHA-C1A-NA	-2.65	120.33	126.40
5	L	402	BPH	C1B-NB-C4B	2.62	111.45	106.51
15	H	801[B]	PGT	O3-C11-C12	2.61	120.11	111.91
4	M	311	BCL	CAA-CBA-CGA	2.59	120.82	113.25
4	L	312	BCL	OBD-CAD-CBD	-2.58	122.21	125.89
4	L	314	BCL	CMB-C2B-C1B	-2.53	124.58	128.46
4	L	314	BCL	C4-C3-C5	2.53	119.52	115.27
4	M	313	BCL	CHA-C1A-NA	-2.53	120.61	126.40
11	M	800	CDL	OB8-CB7-OB9	-2.52	117.23	123.59
4	M	313	BCL	C4B-CHC-C1C	-2.51	125.15	130.12
11	M	800	CDL	C72-C71-CB7	-2.50	104.53	113.62
4	L	314	BCL	O1D-CGD-CBD	-2.50	119.38	124.48
4	L	314	BCL	C2C-C3C-C4C	2.49	105.08	101.34
4	L	312	BCL	CAC-C3C-C2C	-2.49	108.05	114.26
4	M	313	BCL	CMA-C3A-C4A	2.47	118.41	111.77
5	L	402	BPH	CAC-C3C-C4C	2.45	118.96	112.67
12	M	802	PGK	BR2-C40-C39	-2.44	105.55	110.27
5	M	401	BPH	C4-C3-C2	-2.43	117.43	123.68
5	L	402	BPH	CMA-C3A-C2A	-2.43	104.01	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	800	CDL	C74-C73-C72	-2.43	102.08	114.42
15	H	801[A]	PGT	O3-C3-C2	2.43	115.50	108.43
4	M	311	BCL	CMB-C2B-C3B	2.42	129.21	124.68
4	M	311	BCL	C1D-CHD-C4C	2.41	129.44	125.88
5	L	402	BPH	CAC-C3C-C2C	2.40	120.26	114.26
4	L	312	BCL	C4-C3-C5	2.40	119.30	115.27
5	L	402	BPH	O2D-CGD-O1D	-2.39	119.17	123.84
15	H	801[B]	PGT	O2-C31-O31	-2.39	117.94	123.70
4	L	314	BCL	CMC-C2C-C3C	-2.36	104.31	113.83
11	M	800	CDL	OA6-CA5-OA7	-2.36	118.01	123.70
5	M	401	BPH	C1B-NB-C4B	2.35	110.94	106.51
4	M	311	BCL	OBD-CAD-C3D	2.35	131.88	127.98
4	M	311	BCL	CAA-C2A-C3A	-2.34	106.38	112.78
4	L	314	BCL	CAC-C3C-C4C	-2.32	107.43	112.58
4	M	313	BCL	C1-C2-C3	-2.31	122.04	126.04
10	M	703	PO4	O4-P-O3	2.30	115.36	107.97
4	L	312	BCL	C1-O2A-CGA	2.29	122.46	116.44
5	M	401	BPH	C1-O2A-CGA	2.28	122.41	116.44
15	H	801[A]	PGT	O3-C11-C12	2.27	119.05	111.91
4	M	313	BCL	C2C-C3C-C4C	2.25	104.70	101.34
4	L	312	BCL	C4A-NA-C1A	-2.24	105.70	106.71
5	M	401	BPH	C3A-C2A-C1A	2.24	104.32	101.64
4	M	313	BCL	C16-C15-C13	-2.23	108.70	115.92
5	M	401	BPH	CMA-C3A-C2A	-2.22	104.88	113.83
4	M	311	BCL	C6-C5-C3	-2.21	107.65	113.45
4	M	311	BCL	C4-C3-C5	2.20	118.97	115.27
5	M	401	BPH	C2B-C1B-NB	-2.19	106.49	109.79
4	M	311	BCL	OBD-CAD-CBD	-2.18	122.78	125.89
4	M	311	BCL	C4A-NA-C1A	2.17	107.68	106.71
4	L	312	BCL	CMA-C3A-C2A	-2.17	105.08	113.83
4	M	311	BCL	CMA-C3A-C4A	-2.13	106.04	111.77
4	L	314	BCL	C4A-NA-C1A	2.12	107.66	106.71
15	H	801[B]	PGT	O3-C3-C2	2.11	114.58	108.43
4	L	314	BCL	CMA-C3A-C2A	-2.11	105.33	113.83
5	L	402	BPH	CAA-C2A-C3A	-2.10	107.02	112.78
4	L	314	BCL	OBB-CAB-C3B	2.10	123.71	119.99
5	L	402	BPH	CMD-C2D-C3D	2.09	128.59	124.68
5	L	402	BPH	C7-C6-C5	-2.08	107.72	113.36
5	M	401	BPH	CAA-C2A-C1A	-2.07	106.98	112.33
6	L	502	U10	O2-C2-C1	2.07	126.82	120.73
4	M	311	BCL	C4D-C3D-CAD	-2.06	107.32	108.47
4	L	312	BCL	CMA-C3A-C4A	-2.05	106.25	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502	U10	C41-C39-C40	2.04	119.12	114.60
4	M	313	BCL	O2D-CGD-CBD	2.04	114.89	111.27
4	M	311	BCL	C2A-C1A-CHA	2.04	127.43	123.86
4	M	313	BCL	CHC-C1C-NC	2.03	127.32	124.51
4	L	312	BCL	C1C-NC-C4C	2.02	107.61	106.71
11	M	800	CDL	OB6-CB5-OB7	-2.02	118.82	123.70
11	M	800	CDL	CA6-OA8-CA7	2.01	124.57	117.12
5	L	402	BPH	CBC-CAC-C3C	2.00	117.93	113.47

There are no chirality outliers.

All (211) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	H	904	LDA	N1-C1-C2-C3
7	L	707	GOL	O1-C1-C2-C3
11	M	800	CDL	CA2-OA2-PA1-OA3
11	M	800	CDL	CA2-OA2-PA1-OA4
11	M	800	CDL	CA2-OA2-PA1-OA5
11	M	800	CDL	CA3-OA5-PA1-OA4
11	M	800	CDL	CB2-OB2-PB2-OB5
11	M	800	CDL	CB3-OB5-PB2-OB3
11	M	800	CDL	CB3-OB5-PB2-OB4
13	M	902	LDA	C2-C1-N1-CM1
12	M	802	PGK	C1-O3P-P-O1P
12	M	802	PGK	C1-O3P-P-O2P
12	M	802	PGK	C4-O4P-P-O1P
12	M	802	PGK	C4-O4P-P-O2P
12	M	802	PGK	C5-C4-O4P-P
4	M	311	BCL	C2-C3-C5-C6
4	M	311	BCL	C4-C3-C5-C6
13	M	920	LDA	N1-C1-C2-C3
13	M	907	LDA	C2-C1-N1-CM2
7	L	708	GOL	O1-C1-C2-C3
7	L	708	GOL	C1-C2-C3-O3
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C4B-C3B-CAB-CBB
5	M	401	BPH	C4B-C3B-CAB-OB
5	M	401	BPH	C2B-C3B-CAB-CBB
15	H	801[A]	PGT	C32-C31-O2-C2
15	H	801[A]	PGT	C4-O4P-P-O3P
15	H	801[A]	PGT	C4-O4P-P-O1P
15	H	801[A]	PGT	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
15	H	801[A]	PGT	C4-C5-C6-O6
15	H	801[B]	PGT	C32-C31-O2-C2
15	H	801[B]	PGT	C1-O3P-P-O1P
12	M	802	PGK	O11-C11-O3-C3
12	M	802	PGK	C12-C11-O3-C3
15	H	801[A]	PGT	O31-C31-O2-C2
15	H	801[B]	PGT	O31-C31-O2-C2
15	H	801[B]	PGT	C12-C11-O3-C3
15	H	801[B]	PGT	O11-C11-O3-C3
6	L	502	U10	C25-C24-C26-C27
6	L	502	U10	C23-C24-C26-C27
6	M	501	U10	C29-C31-C32-C33
15	H	801[B]	PGT	C32-C33-C34-C35
4	M	311	BCL	C10-C11-C12-C13
7	L	708	GOL	O2-C2-C3-O3
15	H	801[A]	PGT	C31-C32-C33-C34
15	H	801[A]	PGT	C11-C12-C13-C14
6	L	502	U10	C19-C21-C22-C23
6	L	502	U10	C34-C36-C37-C38
15	H	801[A]	PGT	O4P-C4-C5-O5
15	H	801[A]	PGT	C12-C11-O3-C3
11	M	800	CDL	CB3-OB5-PB2-OB2
12	M	802	PGK	C1-O3P-P-O4P
12	M	802	PGK	C4-O4P-P-O3P
15	H	801[A]	PGT	O4P-C4-C5-C6
13	H	903	LDA	C2-C3-C4-C5
5	M	401	BPH	C2B-C3B-CAB-OB2
13	H	904	LDA	C7-C8-C9-C10
15	H	801[B]	PGT	C14-C15-C16-C17
13	H	904	LDA	C2-C3-C4-C5
11	M	800	CDL	C38-C39-C40-C41
11	M	800	CDL	CB7-C71-C72-C73
15	H	801[A]	PGT	O11-C11-O3-C3
5	L	402	BPH	C4-C3-C5-C6
6	M	501	U10	C30-C29-C31-C32
13	M	920	LDA	C3-C4-C5-C6
15	H	801[B]	PGT	C42-C43-C44-C45
15	H	801[B]	PGT	C33-C34-C35-C36
15	H	801[B]	PGT	C17-C18-C19-C20
7	L	707	GOL	C1-C2-C3-O3
12	M	802	PGK	C4-C5-C6-O6
11	M	800	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
11	M	800	CDL	C11-C12-C13-C14
12	M	802	PGK	C16-C17-C18-C19
13	M	920	LDA	C11-C10-C9-C8
13	M	907	LDA	C4-C5-C6-C7
13	H	901	LDA	C5-C6-C7-C8
13	H	901	LDA	C11-C10-C9-C8
15	H	801[A]	PGT	C17-C18-C19-C20
15	H	801[A]	PGT	C14-C15-C16-C17
12	M	802	PGK	C34-C35-C36-C37
12	M	802	PGK	C32-C33-C34-C35
15	H	801[B]	PGT	C11-C12-C13-C14
5	M	401	BPH	C13-C15-C16-C17
12	M	802	PGK	C21-C22-C23-C24
15	H	801[A]	PGT	C20-C21-C22-C23
11	M	800	CDL	CA3-CA4-CA6-OA8
11	M	800	CDL	OA7-CA5-OA6-CA4
6	L	502	U10	C15-C14-C16-C17
5	L	402	BPH	C2-C3-C5-C6
6	M	501	U10	C28-C29-C31-C32
15	H	801[B]	PGT	C39-C40-C41-C42
15	H	801[B]	PGT	C37-C38-C39-C40
7	L	707	GOL	O2-C2-C3-O3
12	M	802	PGK	O5-C5-C6-O6
15	H	801[A]	PGT	O5-C5-C6-O6
15	H	801[B]	PGT	C20-C21-C22-C23
4	M	311	BCL	C5-C6-C7-C8
11	M	800	CDL	C51-CB5-OB6-CB4
11	M	800	CDL	C13-C14-C15-C16
6	L	502	U10	C13-C14-C16-C17
13	H	904	LDA	C1-C2-C3-C4
5	M	401	BPH	C16-C17-C18-C19
12	M	802	PGK	C23-C24-C25-C26
11	M	800	CDL	CA5-C11-C12-C13
12	M	802	PGK	C32-C31-O2-C2
15	H	801[A]	PGT	C34-C35-C36-C37
13	M	907	LDA	C11-C10-C9-C8
11	M	800	CDL	OB7-CB5-OB6-CB4
11	M	800	CDL	C17-C18-C19-C20
11	M	800	CDL	OA5-CA3-CA4-CA6
11	M	800	CDL	C19-C20-C21-C22
13	M	920	LDA	C9-C10-C11-C12
13	M	907	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	L	709	GOL	O2-C2-C3-O3
15	H	801[B]	PGT	C1-C2-O2-C31
4	M	311	BCL	C2-C1-O2A-CGA
15	H	801[A]	PGT	C2-C3-O3-C11
13	H	904	LDA	C9-C10-C11-C12
13	M	920	LDA	C5-C6-C7-C8
13	H	903	LDA	C6-C7-C8-C9
13	H	903	LDA	N1-C1-C2-C3
12	M	802	PGK	O31-C31-O2-C2
11	M	800	CDL	C20-C21-C22-C23
4	M	311	BCL	C15-C16-C17-C18
11	M	800	CDL	C75-C76-C77-C78
12	M	802	PGK	C44-C45-C46-C47
13	H	904	LDA	C6-C7-C8-C9
12	M	802	PGK	C18-C19-C20-C21
15	H	801[A]	PGT	C1-C2-C3-O3
7	H	706	GOL	O2-C2-C3-O3
11	M	800	CDL	OA5-CA3-CA4-OA6
5	M	401	BPH	C16-C17-C18-C20
13	H	901	LDA	C3-C4-C5-C6
5	L	402	BPH	C8-C10-C11-C12
11	M	800	CDL	C18-C19-C20-C21
11	M	800	CDL	C1-CB2-OB2-PB2
13	H	903	LDA	C11-C10-C9-C8
15	H	801[B]	PGT	C44-C45-C46-C47
13	M	920	LDA	C4-C5-C6-C7
5	L	402	BPH	CAD-CBD-CGD-O2D
5	M	401	BPH	CAD-CBD-CGD-O2D
15	H	801[A]	PGT	C2-C1-O3P-P
15	H	801[B]	PGT	C5-C4-O4P-P
15	H	801[A]	PGT	C42-C43-C44-C45
13	H	901	LDA	C4-C5-C6-C7
11	M	800	CDL	OA6-CA4-CA6-OA8
15	H	801[B]	PGT	O5-C5-C6-O6
13	M	907	LDA	C7-C8-C9-C10
15	H	801[B]	PGT	C4-C5-C6-O6
7	L	709	GOL	C1-C2-C3-O3
11	M	800	CDL	O1-C1-CA2-OA2
11	M	800	CDL	CA3-OA5-PA1-OA3
11	M	800	CDL	CB2-OB2-PB2-OB4
11	M	800	CDL	C39-C40-C41-C42
5	M	401	BPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	L	314	BCL	C12-C13-C15-C16
4	M	311	BCL	C6-C7-C8-C10
15	H	801[B]	PGT	O3P-C1-C2-O2
15	H	801[A]	PGT	O2-C2-C3-O3
15	H	801[A]	PGT	C37-C38-C39-C40
7	L	707	GOL	O1-C1-C2-O2
7	L	708	GOL	O1-C1-C2-O2
5	L	402	BPH	C2B-C3B-CAB-OB6
15	H	801[B]	PGT	C12-C13-C14-C15
11	M	800	CDL	CB3-CB4-OB6-CB5
15	H	801[A]	PGT	C1-C2-O2-C31
11	M	800	CDL	OB6-CB4-CB6-OB8
15	H	801[B]	PGT	C1-O3P-P-O4P
4	L	314	BCL	C14-C13-C15-C16
4	L	312	BCL	C11-C10-C8-C9
15	H	801[A]	PGT	C12-C13-C14-C15
11	M	800	CDL	CB6-CB4-OB6-CB5
12	M	802	PGK	C1-C2-O2-C31
15	H	801[A]	PGT	C22-C23-C24-C25
15	H	801[B]	PGT	C22-C23-C24-C25
5	M	401	BPH	C15-C16-C17-C18
13	M	907	LDA	C2-C3-C4-C5
6	M	501	U10	C5-C4-O4-C4M
4	M	313	BCL	C16-C17-C18-C19
12	M	802	PGK	O4P-C4-C5-C6
15	H	801[A]	PGT	O2-C31-C32-C33
4	M	311	BCL	C11-C10-C8-C9
15	H	801[A]	PGT	C33-C34-C35-C36
4	M	313	BCL	CAA-CBA-CGA-O2A
12	M	802	PGK	C1-C2-C3-O3
6	L	502	U10	C18-C19-C21-C22
12	M	802	PGK	C41-C42-C43-C44
4	L	312	BCL	CAD-CBD-CGD-O2D
4	M	311	BCL	CAD-CBD-CGD-O2D
5	L	402	BPH	O2A-C1-C2-C3
13	H	903	LDA	C5-C6-C7-C8
4	L	312	BCL	C16-C17-C18-C19
13	M	907	LDA	C2-C1-N1-CM1
15	H	801[A]	PGT	C35-C36-C37-C38
11	M	800	CDL	C72-C71-CB7-OB8
4	M	311	BCL	C6-C7-C8-C9
6	L	502	U10	C3-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
6	L	502	U10	C5-C4-O4-C4M
13	M	920	LDA	C7-C8-C9-C10
7	H	706	GOL	C1-C2-C3-O3
11	M	800	CDL	C36-C37-C38-C39
5	M	401	BPH	C2-C1-O2A-CGA
11	M	800	CDL	C72-C71-CB7-OB9
6	L	502	U10	C20-C19-C21-C22
15	H	801[B]	PGT	C2-C1-O3P-P
15	H	801[A]	PGT	C1-O3P-P-O1P
6	M	501	U10	C24-C26-C27-C28
13	H	904	LDA	C2-C1-N1-O1
6	L	502	U10	C30-C29-C31-C32
5	M	401	BPH	C6-C7-C8-C10
4	L	314	BCL	C15-C16-C17-C18

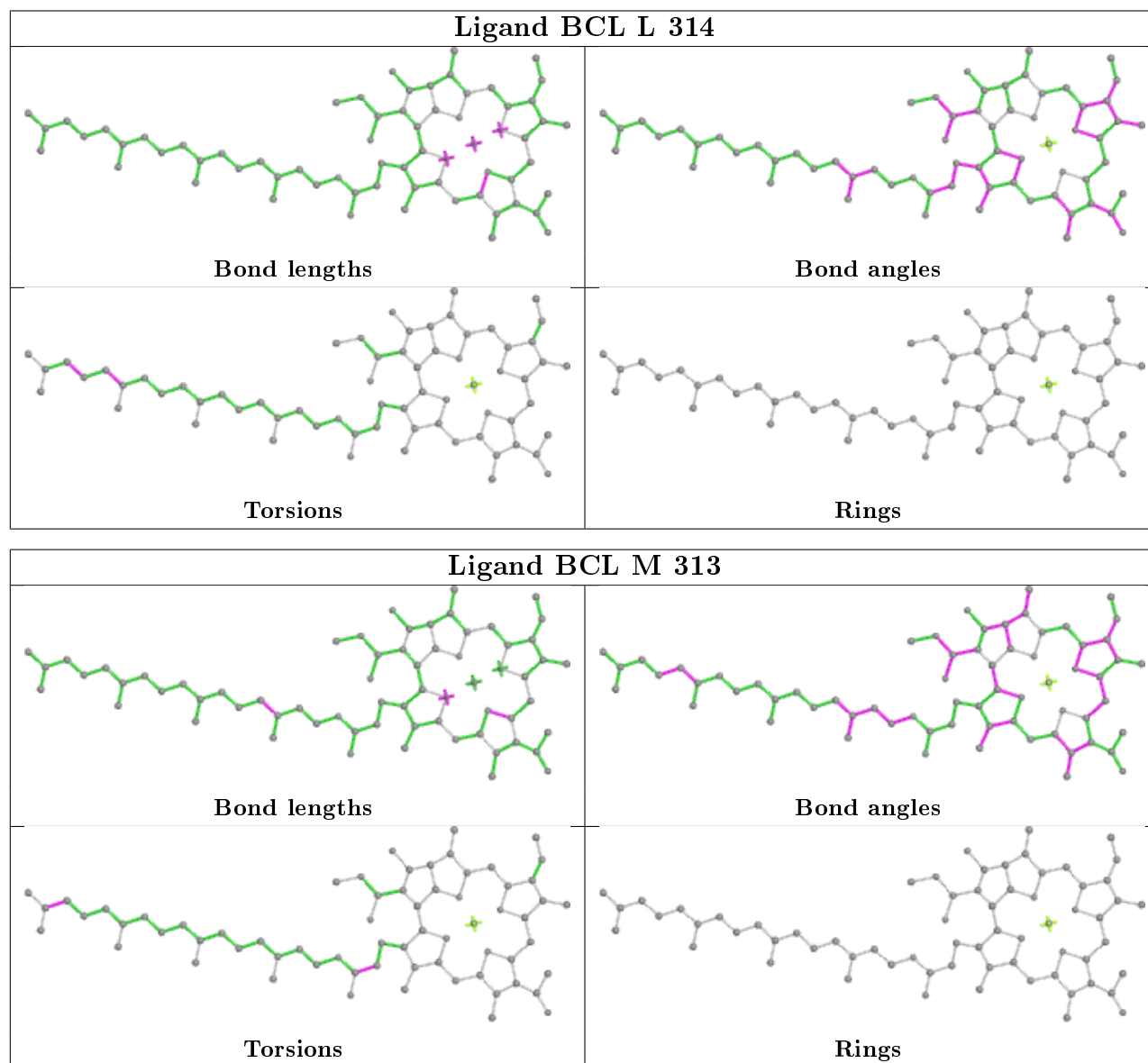
There are no ring outliers.

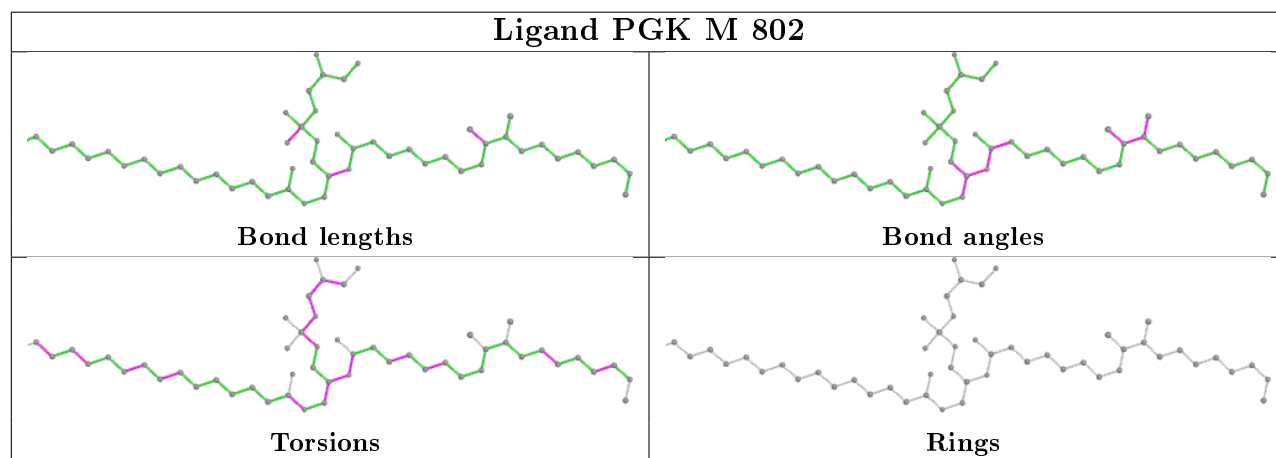
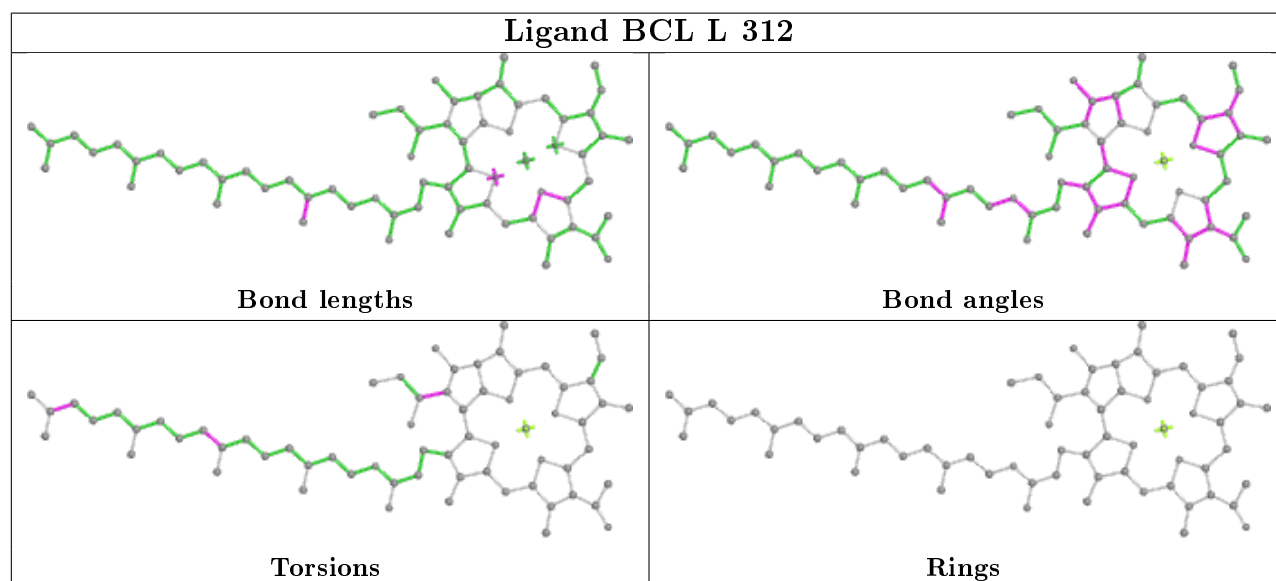
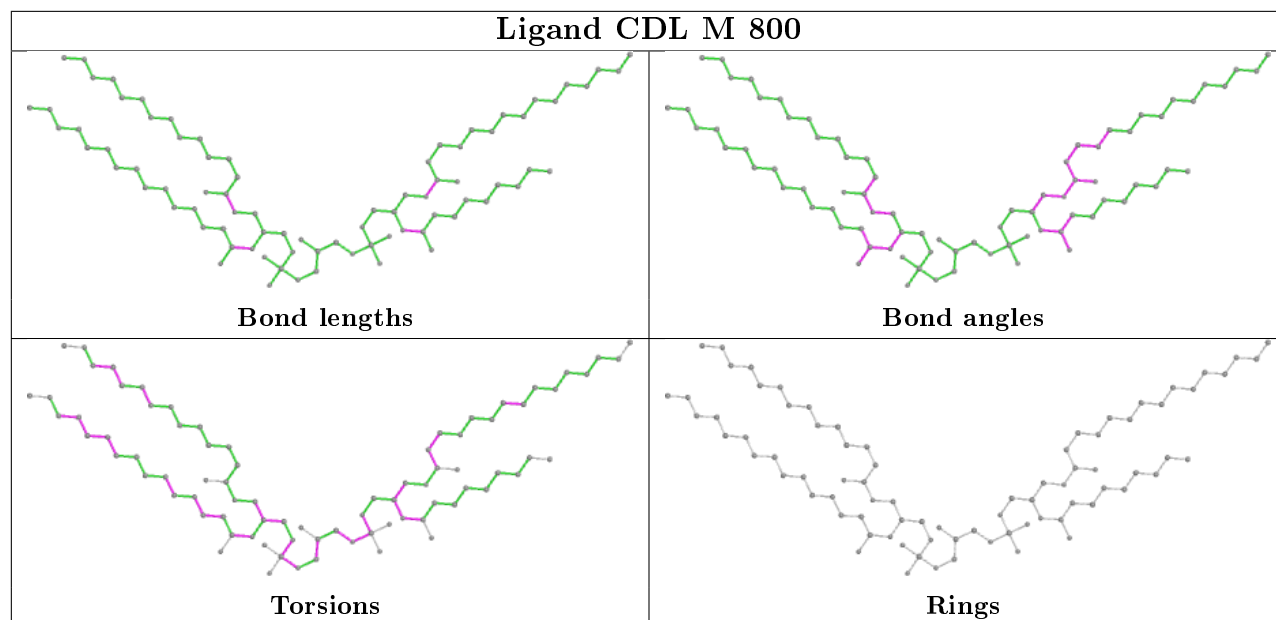
18 monomers are involved in 81 short contacts:

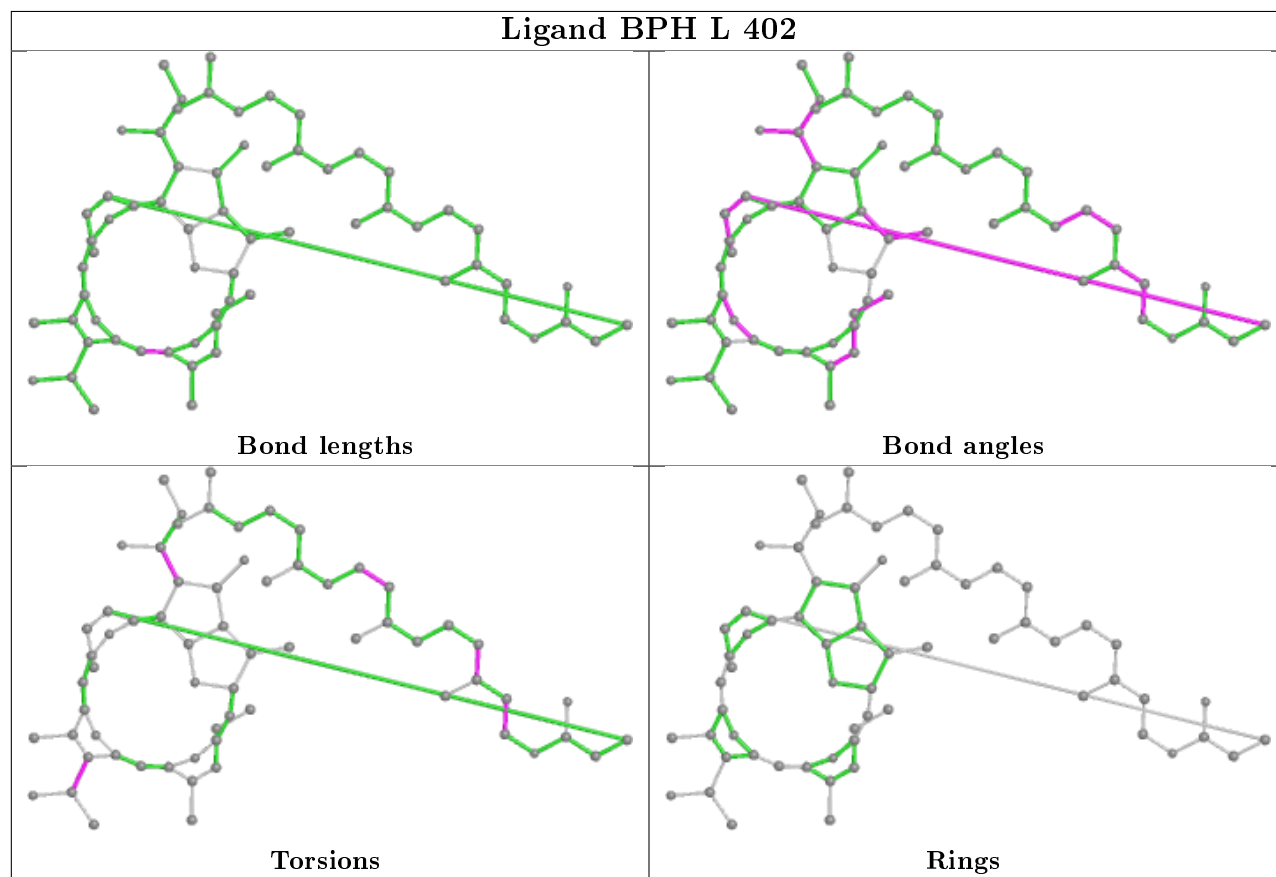
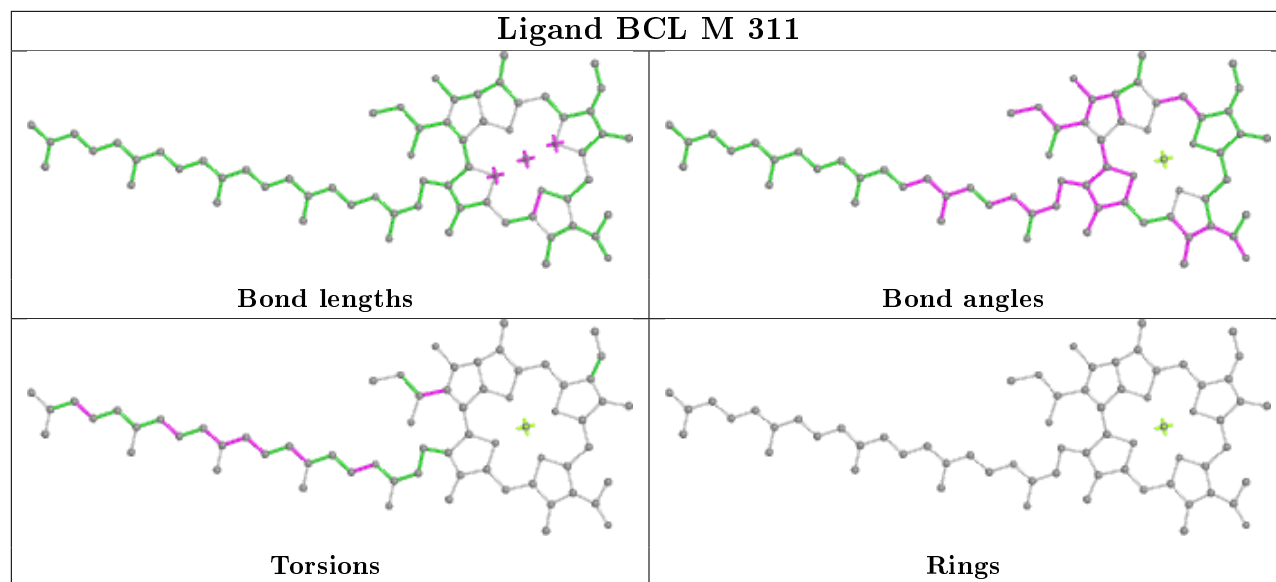
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	901	LDA	11	0
4	L	314	BCL	3	0
4	M	313	BCL	5	0
13	H	903	LDA	12	0
10	M	703	PO4	1	0
13	H	904	LDA	2	0
11	M	800	CDL	3	0
4	L	312	BCL	4	0
13	M	902	LDA	7	0
12	M	802	PGK	11	0
4	M	311	BCL	15	0
13	M	920	LDA	5	0
6	M	501	U10	1	0
6	L	502	U10	4	0
5	M	401	BPH	4	0
15	H	801[A]	PGT	12	0
15	H	801[B]	PGT	8	0
7	L	709	GOL	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

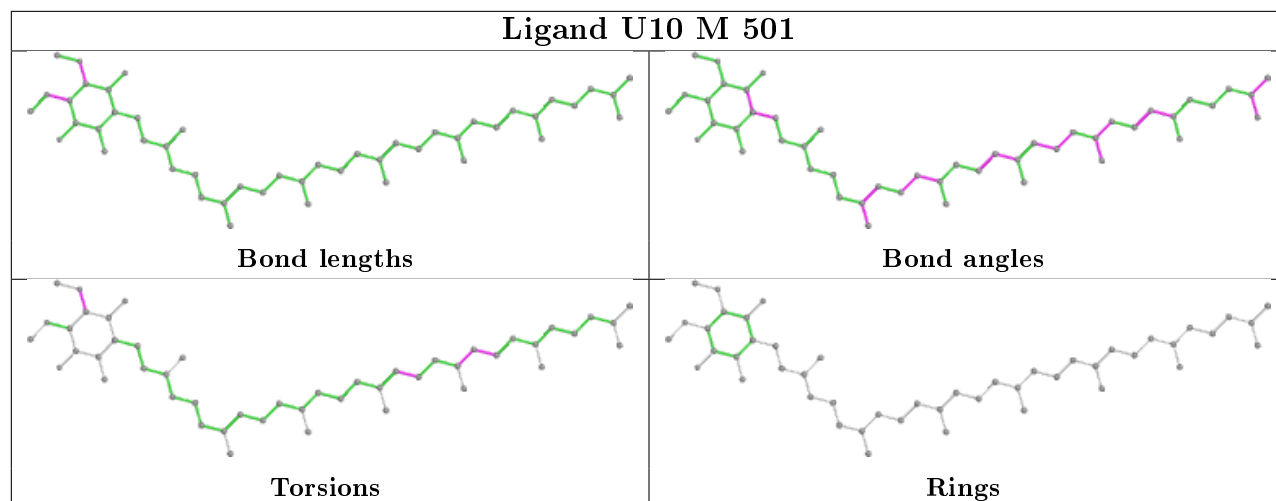
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



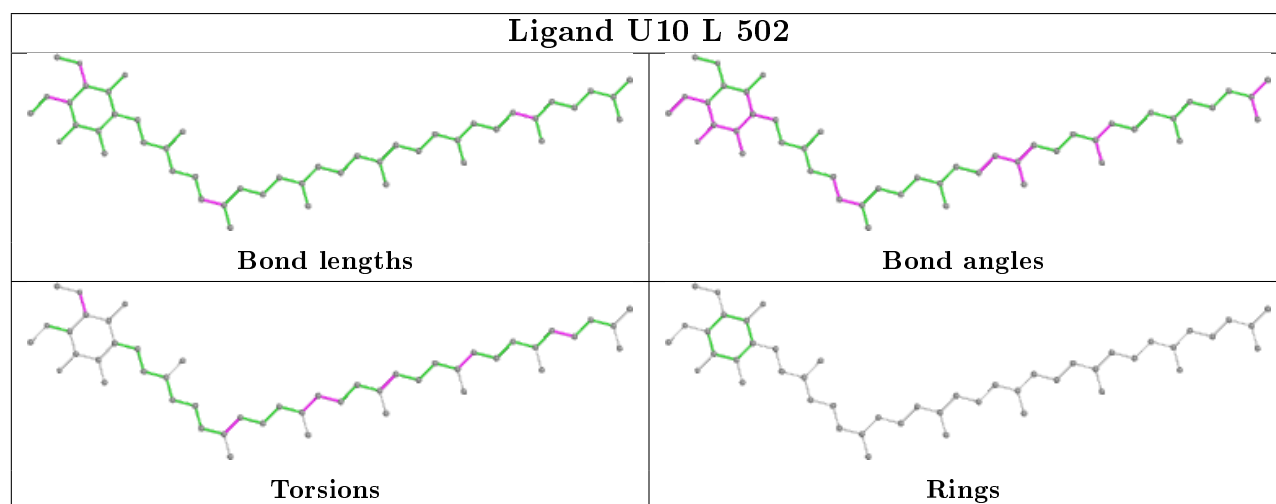


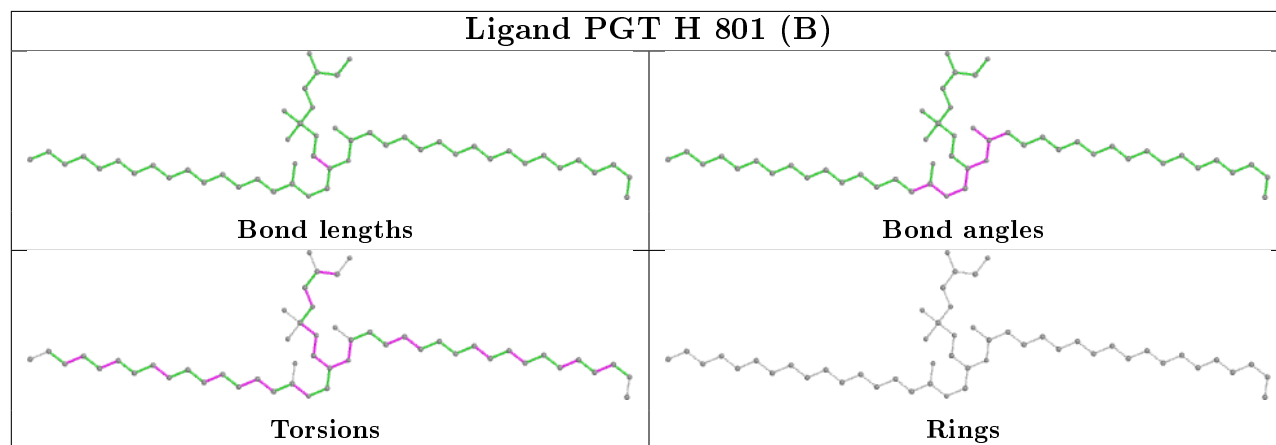
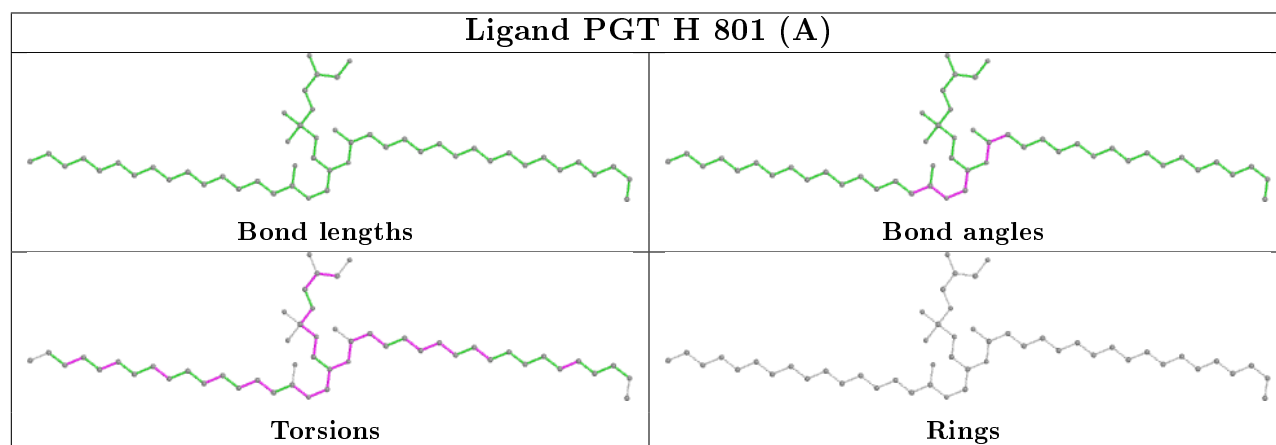
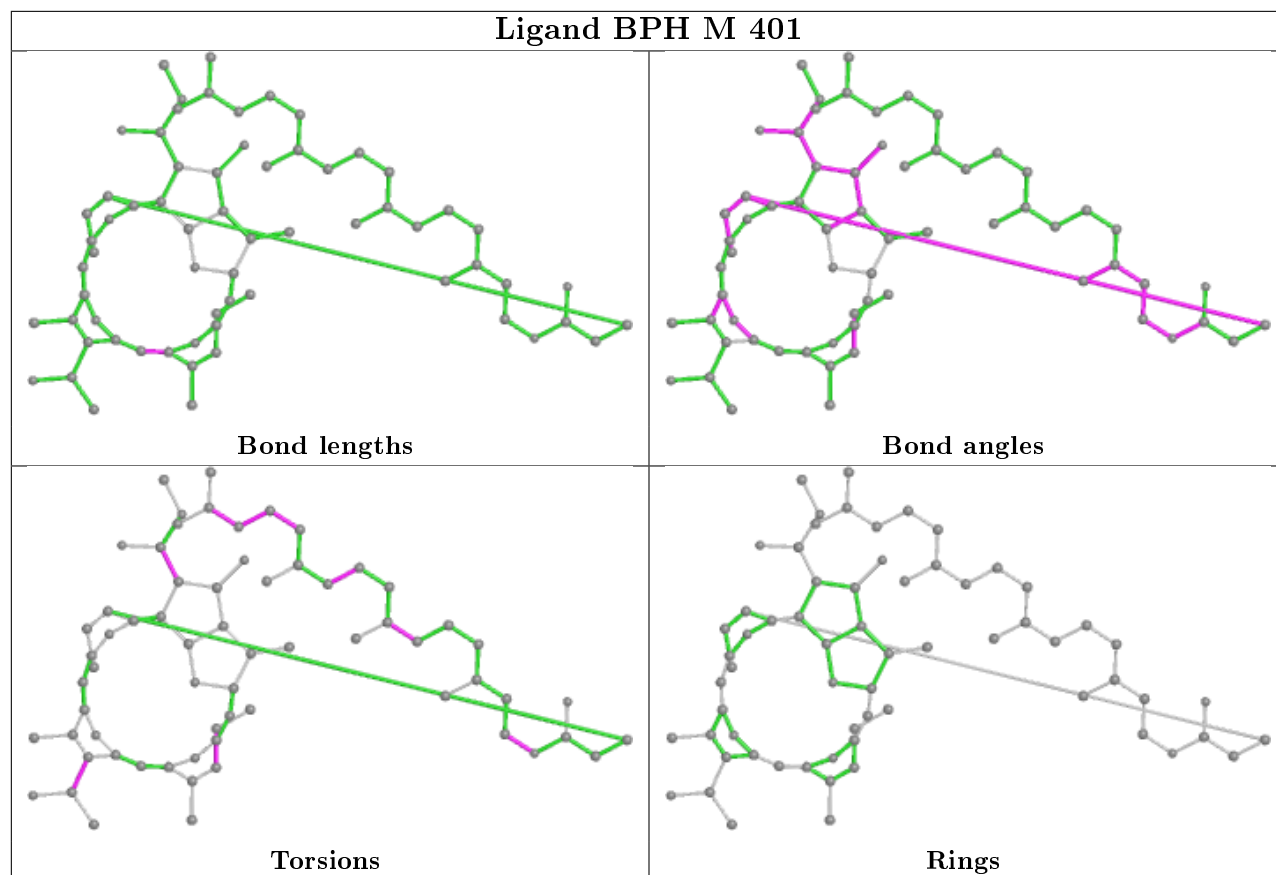


Ligand U10 M 501



Ligand U10 L 502





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	0.48	33 (11%) 4 4	54, 62, 73, 80	0
2	M	302/307 (98%)	0.59	38 (12%) 3 3	54, 62, 73, 94	0
3	H	241/260 (92%)	0.16	11 (4%) 32 34	54, 62, 73, 100	0
All	All	824/848 (97%)	0.42	82 (9%) 7 6	54, 62, 73, 100	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.7
2	M	80	TRP	6.5
3	H	250	SER	6.2
3	H	251	VAL	5.7
1	L	277	GLY	5.0
3	H	249	LYS	4.8
1	L	270	PRO	4.7
1	L	202	LYS	4.5
2	M	79	GLY	4.4
1	L	281	GLY	4.2
2	M	28	ASN	4.2
1	L	269	LEU	4.2
1	L	271	TRP	4.1
2	M	75	TRP	3.9
1	L	278	GLY	3.7
2	M	265	ILE	3.7
1	L	275	ILE	3.6
3	H	52	ASN	3.5
2	M	101	TYR	3.4
1	L	51	TRP	3.4
1	L	279	ILE	3.4
2	M	100[A]	GLU	3.3
1	L	73	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	M	104	SER	3.3
2	M	114	LEU	3.2
3	H	158	LEU	3.2
2	M	102	GLY	3.1
3	H	159	GLU	3.1
1	L	80	LEU	3.1
2	M	97	PRO	3.0
2	M	82	PRO	3.0
1	L	33	PHE	3.0
1	L	268	LYS	3.0
1	L	185	LEU	2.9
2	M	81	ASN	2.9
1	L	75	LEU	2.9
2	M	71	GLY	2.9
2	M	84	VAL	2.8
1	L	84	GLY	2.8
2	M	108	PRO	2.8
1	L	276	PRO	2.8
2	M	2	GLU	2.7
1	L	38	THR	2.7
2	M	98	ALA	2.7
1	L	40	PHE	2.7
2	M	73	TRP	2.7
2	M	77	GLN	2.6
1	L	280	ASN	2.6
2	M	111	GLU	2.6
1	L	236	LEU	2.6
2	M	171	TRP	2.5
1	L	72	GLU	2.5
1	L	272	TRP	2.5
1	L	59	TRP	2.5
1	L	256	PHE	2.5
2	M	26	LEU	2.4
3	H	160	ILE	2.4
2	M	96	PRO	2.4
3	H	94	GLU	2.4
2	M	76	TYR	2.4
2	M	83	ALA	2.4
2	M	275	LEU	2.4
3	H	18	TYR	2.4
2	M	27	ALA	2.3
1	L	69	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	113	GLY	2.2
2	M	54	SER	2.2
1	L	49	ILE	2.2
3	H	201	ASN	2.2
1	L	265	TRP	2.2
2	M	290	VAL	2.2
2	M	105	PHE	2.2
2	M	274	VAL	2.1
1	L	37	ALA	2.1
1	L	34	PHE	2.1
3	H	220[A]	LYS	2.1
1	L	233	GLY	2.1
1	L	67	TYR	2.0
2	M	115	TRP	2.0
2	M	266	HIS	2.0
2	M	109	LEU	2.0
2	M	214	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	LDA	H	903	16/16	-0.13	1.34	73,75,78,78	16
12	PGK	M	802	53/53	0.19	0.75	61,67,76,77	53
13	LDA	M	902	16/16	0.22	0.93	66,71,75,79	16
15	PGT	H	801[A]	51/51	0.41	1.25	45,73,81,82	51
15	PGT	H	801[B]	51/51	0.41	1.25	47,76,84,85	51
13	LDA	H	904	16/16	0.44	0.74	76,79,86,86	16

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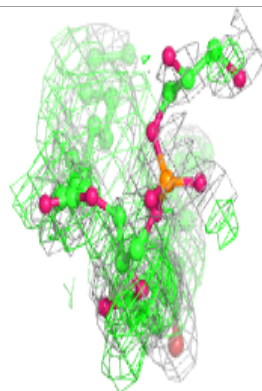
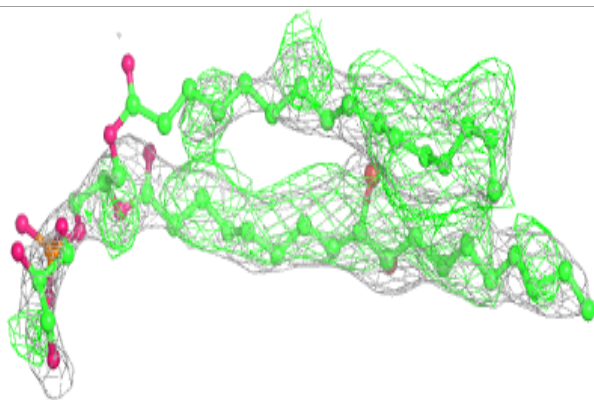
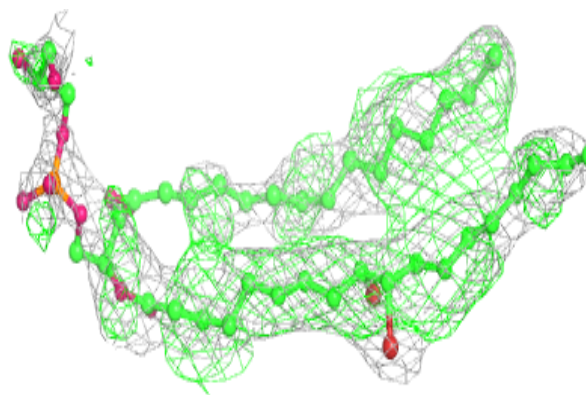
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	LDA	M	920	16/16	0.61	0.62	41,60,78,80	16
11	CDL	M	800	81/100	0.64	0.49	49,74,88,90	81
7	GOL	L	707	6/6	0.65	0.35	65,67,68,68	6
10	PO4	H	704	5/5	0.68	0.26	61,61,63,63	5
13	LDA	M	907	16/16	0.75	0.47	69,72,77,77	16
7	GOL	L	709	6/6	0.75	0.46	65,66,68,70	6
6	U10	L	502	48/63	0.76	0.59	53,68,86,90	48
10	PO4	M	705	5/5	0.78	0.25	63,64,65,65	5
7	GOL	L	708	6/6	0.81	0.32	60,66,68,68	6
13	LDA	H	901	16/16	0.83	0.41	72,77,86,88	16
6	U10	M	501	48/63	0.84	0.31	56,69,90,93	0
5	BPH	M	401	65/65	0.90	0.20	56,62,116,118	0
7	GOL	H	706	6/6	0.91	0.39	72,72,73,74	6
4	BCL	L	312	66/66	0.93	0.17	49,59,70,78	0
5	BPH	L	402	65/65	0.93	0.17	50,62,66,68	0
4	BCL	L	314	66/66	0.93	0.19	50,59,75,80	0
9	CL	M	701	1/1	0.93	0.32	73,73,73,73	1
4	BCL	M	313	66/66	0.94	0.20	51,59,84,95	0
10	PO4	M	702	5/5	0.95	0.21	69,71,74,77	5
10	PO4	M	703	5/5	0.95	0.21	59,59,63,64	5
4	BCL	M	311	66/66	0.95	0.20	55,62,119,120	0
14	K	H	700	1/1	0.96	0.10	58,58,58,58	0
8	FE	M	500	1/1	1.00	0.18	59,59,59,59	0

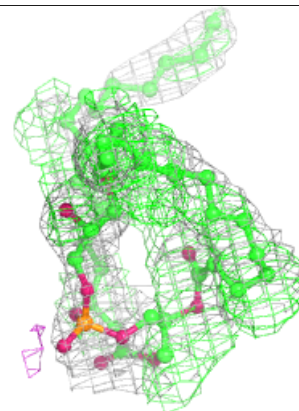
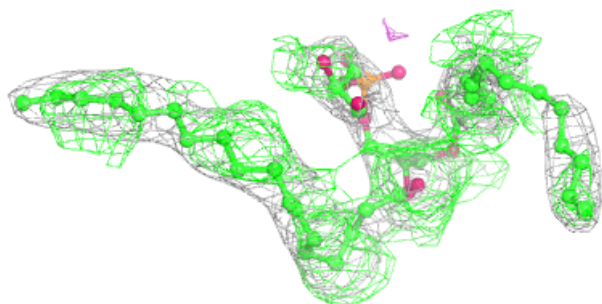
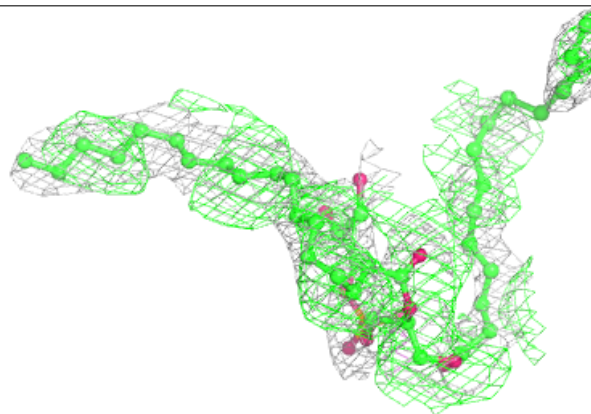
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGK 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)

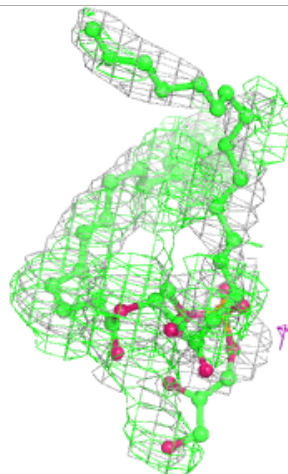
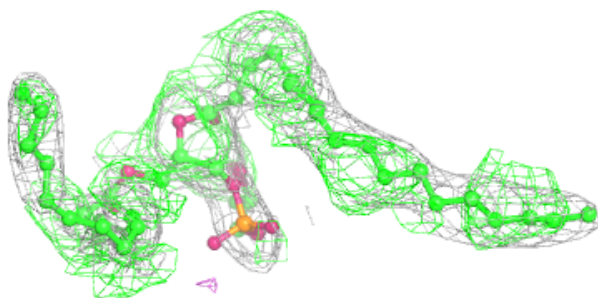
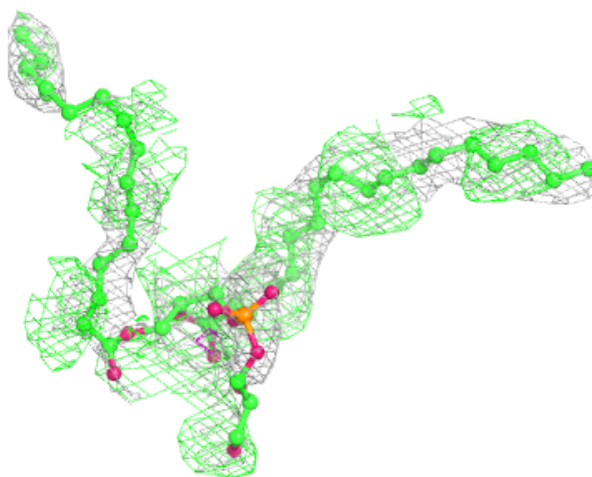
**Electron density around PGT H 801 (A):**

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



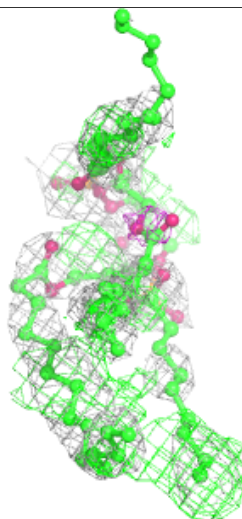
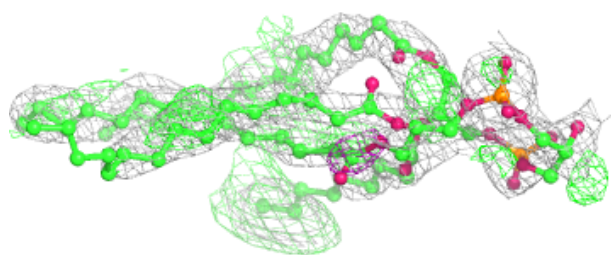
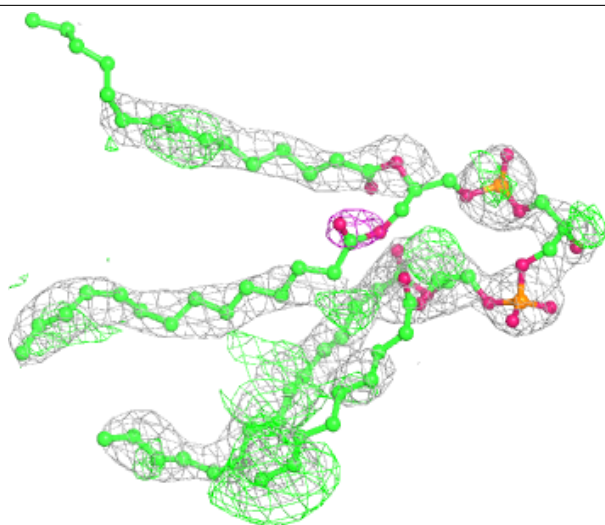
Electron density around PGT H 801 (B):

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



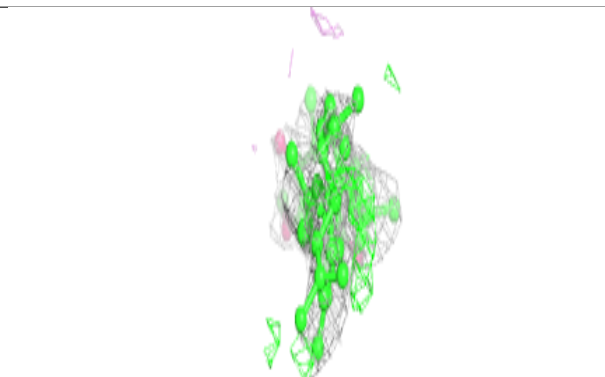
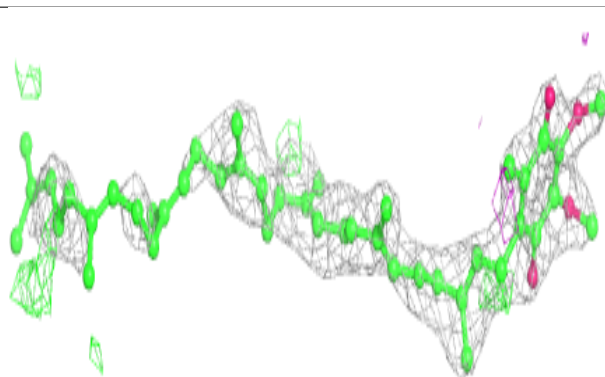
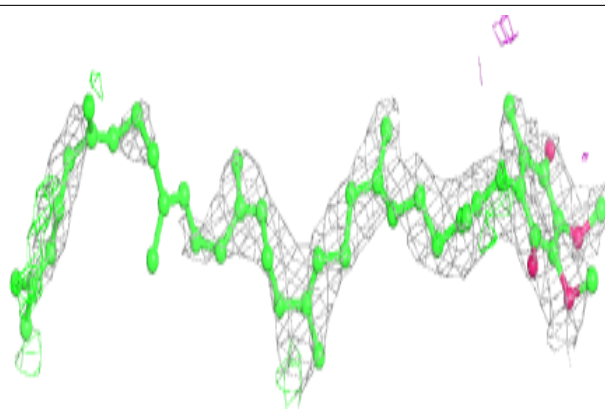
Electron density around CDL M 800:

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

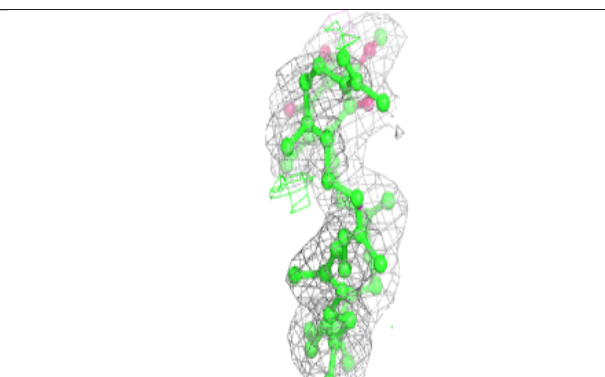
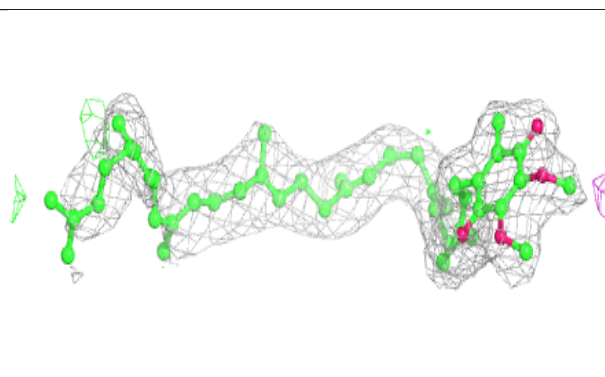
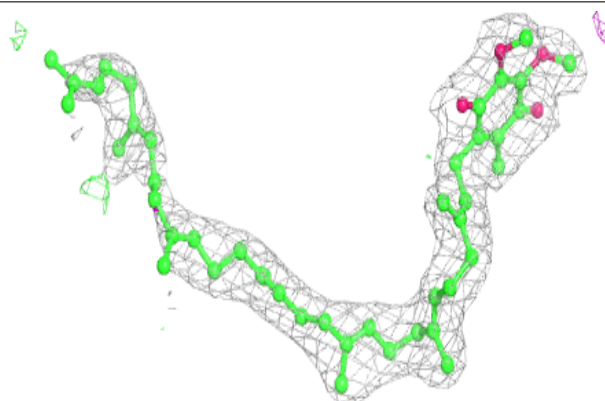


Electron density around U10 L 502:

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

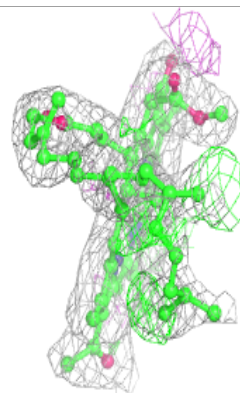
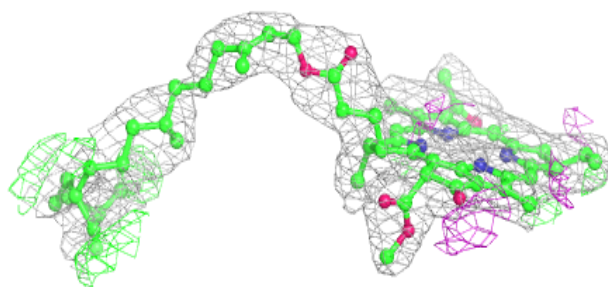
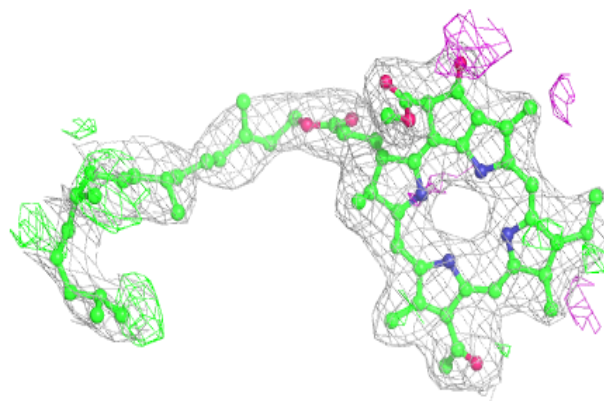
**Electron density around U10 M 501:**

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

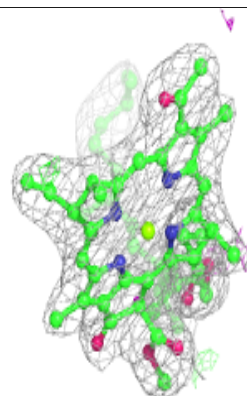
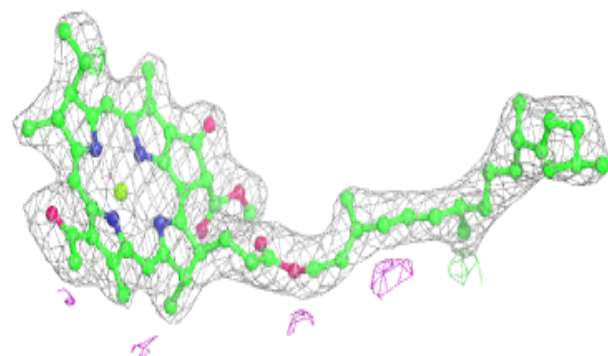
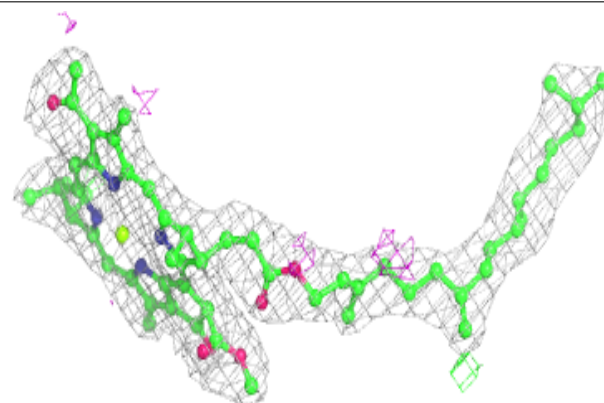


Electron density around BPH M 401:

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

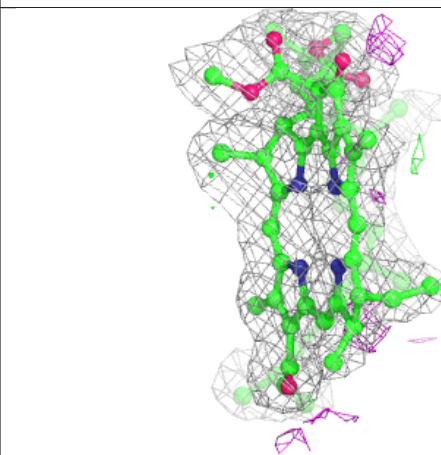
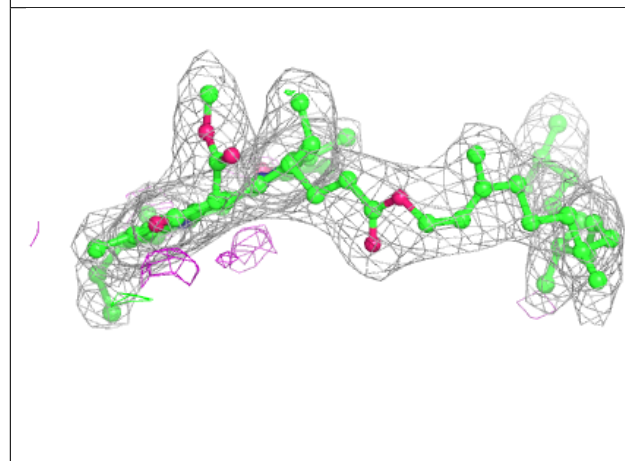
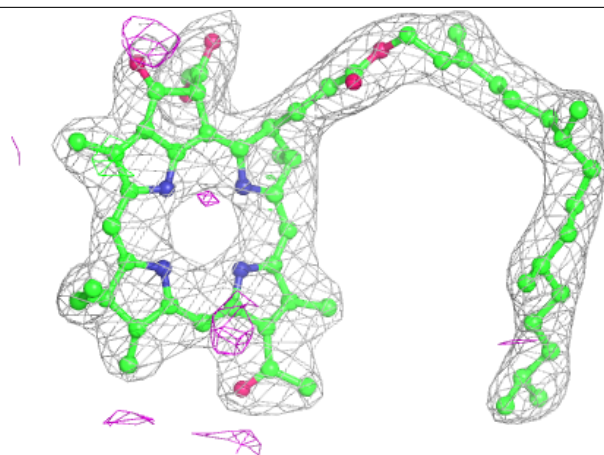
**Electron density around BCL L 312:**

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



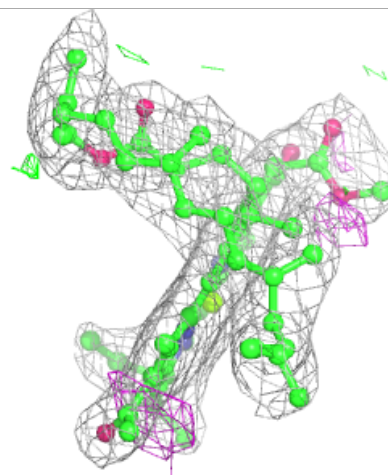
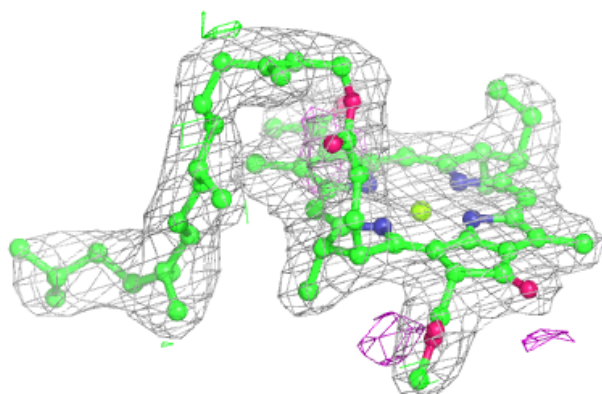
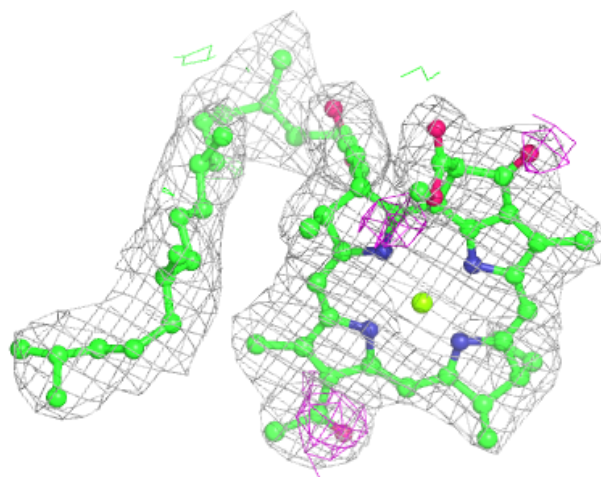
Electron density around BPH L 402:

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



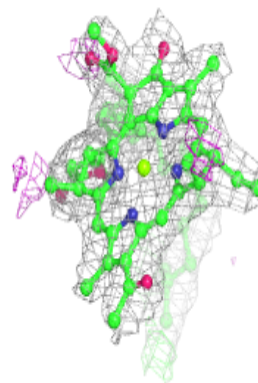
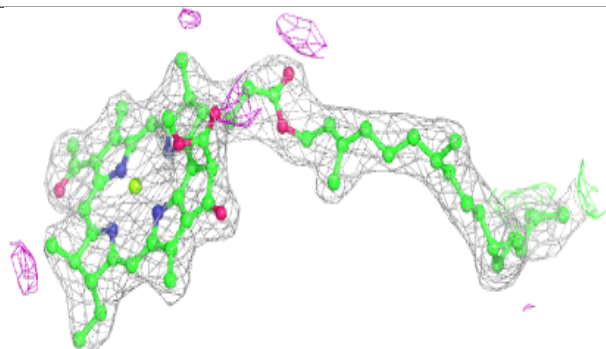
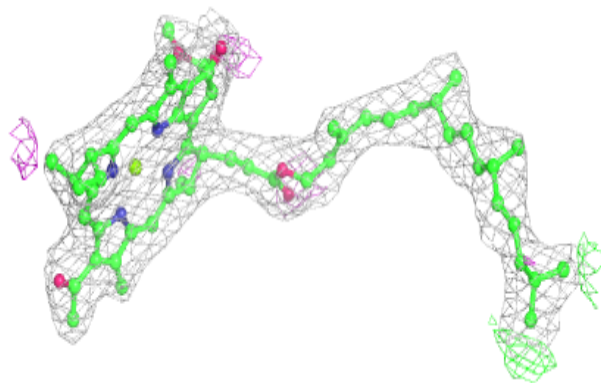
Electron density around BCL L 314:

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

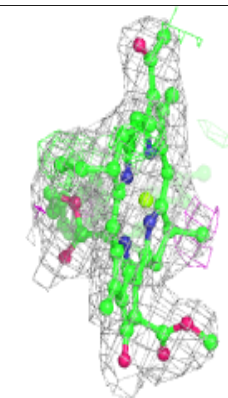
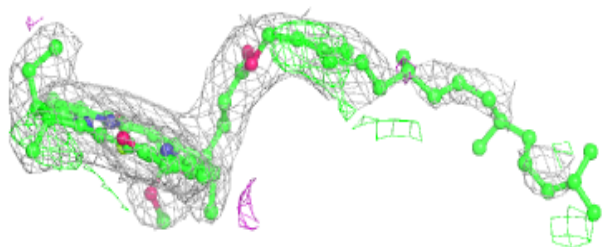
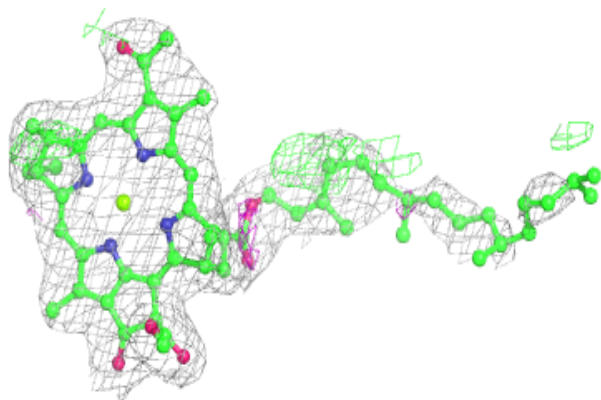


Electron density around BCL M 313:

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

**Electron density around BCL 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)



6.5 Other polymers

There are no such residues in this entry.