



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:25 PM EDT

PDB ID : 4IN7 / pdb_00004in7
Title : (M)L214N mutant of the Rhodobacter sphaeroides Reaction Center
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.P.; Beatty, J.T.
Deposited on : 2013-01-04
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

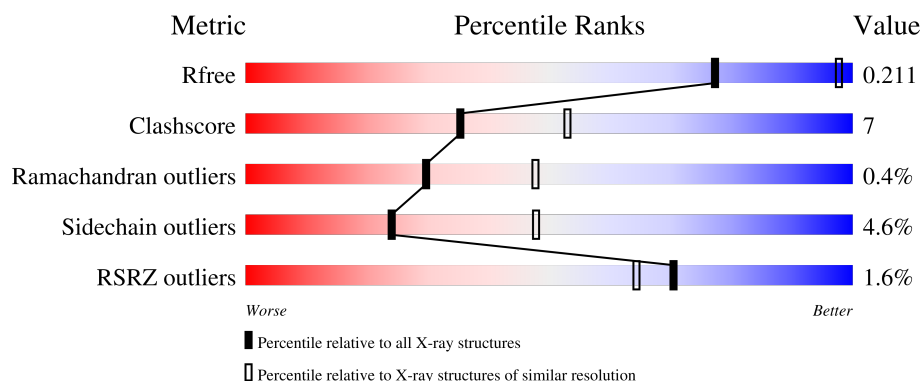
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	H	266	
2	L	282	
3	M	307	

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	HTO	L	309	-	X	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7359 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	5	0
			1849	1183	320	337	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP P0C0Y7
H	-4	HIS	-	expression tag	UNP P0C0Y7
H	-3	HIS	-	expression tag	UNP P0C0Y7
H	-2	HIS	-	expression tag	UNP P0C0Y7
H	-1	HIS	-	expression tag	UNP P0C0Y7
H	0	HIS	-	expression tag	UNP P0C0Y7
H	251	VAL	-	expression tag	UNP P0C0Y7
H	252	VAL	-	expression tag	UNP P0C0Y7
H	253	ALA	-	expression tag	UNP P0C0Y7
H	254	ALA	-	expression tag	UNP P0C0Y7
H	255	MET	-	expression tag	UNP P0C0Y7
H	256	LEU	-	expression tag	UNP P0C0Y7
H	257	ALA	-	expression tag	UNP P0C0Y7
H	258	GLU	-	expression tag	UNP P0C0Y7
H	259	TYR	-	expression tag	UNP P0C0Y7
H	260	ALA	-	expression tag	UNP P0C0Y7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2239	1513	355	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	expression tag	UNP P0C0Y8

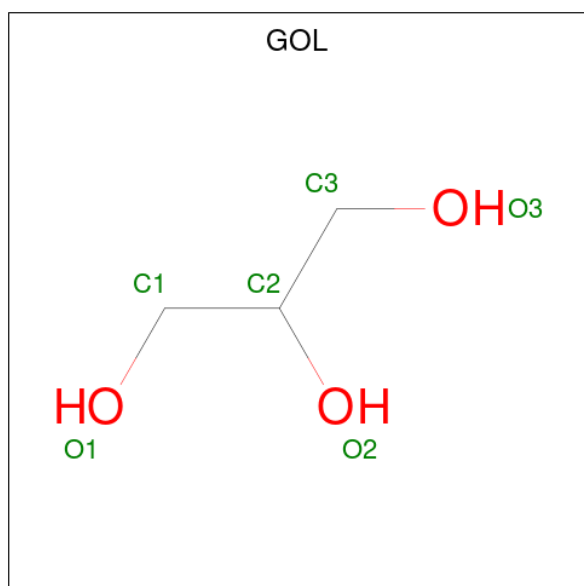
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	1	0
			2410	1605	396	399	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	expression tag	UNP P0C0Y9
M	214	ASN	LEU	engineered mutation	UNP P0C0Y9
M	303	MET	-	expression tag	UNP P0C0Y9
M	304	ALA	-	expression tag	UNP P0C0Y9
M	305	PRO	-	expression tag	UNP P0C0Y9
M	306	LEU	-	expression tag	UNP P0C0Y9

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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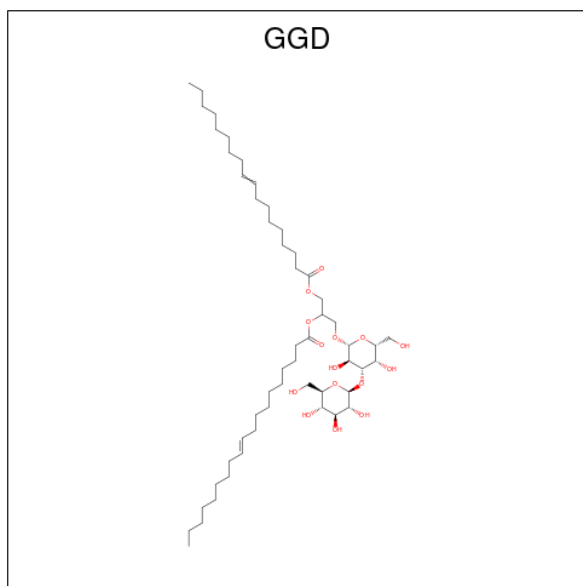
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

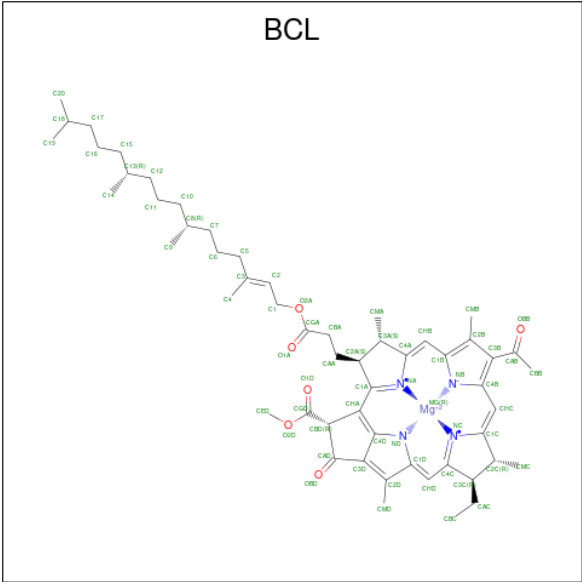
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY] -1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (CCD ID: GGD) (formula: C₅₂H₉₄O₁₅).



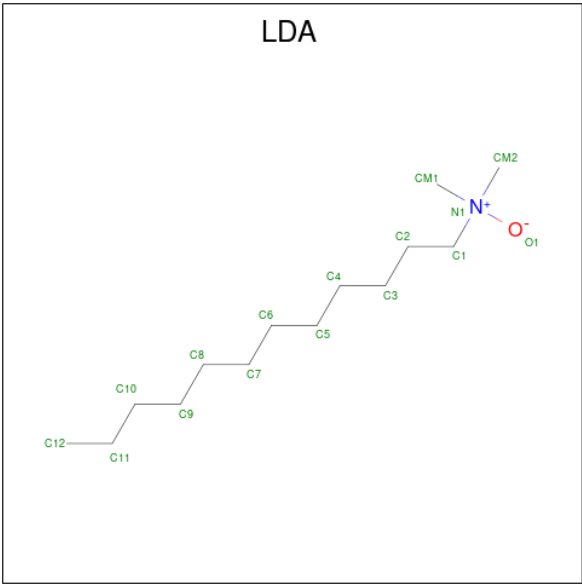
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



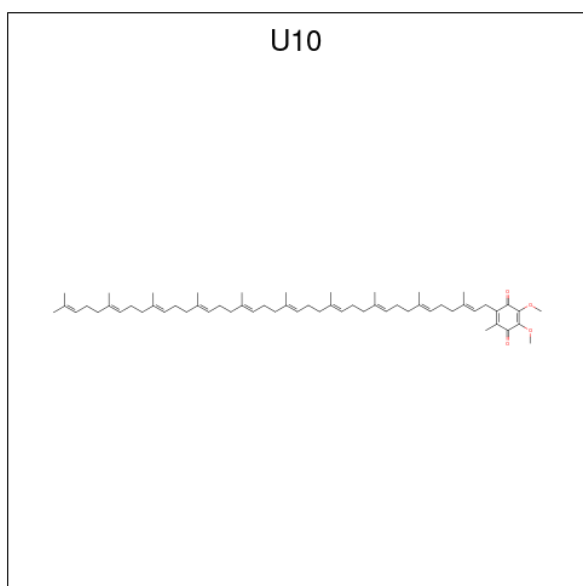
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



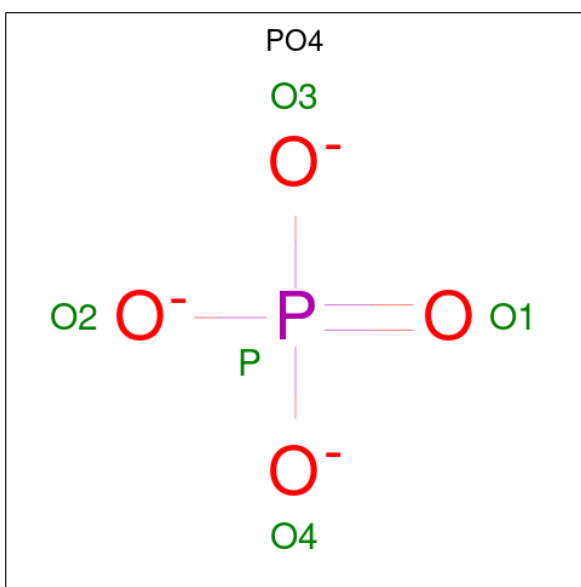
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



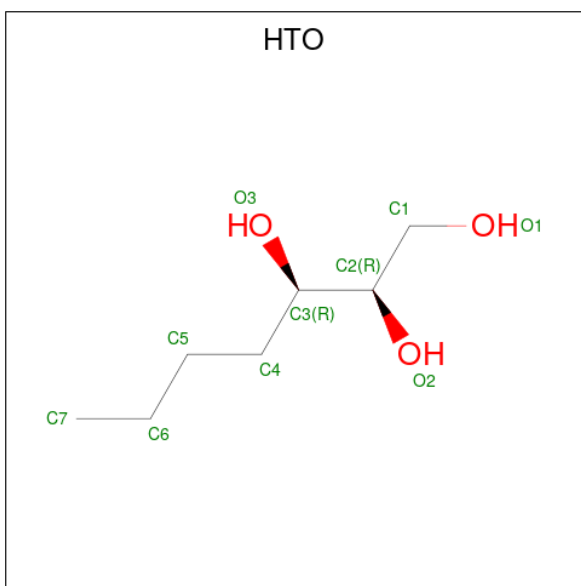
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	1
			46	38	8		
9	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 11 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).

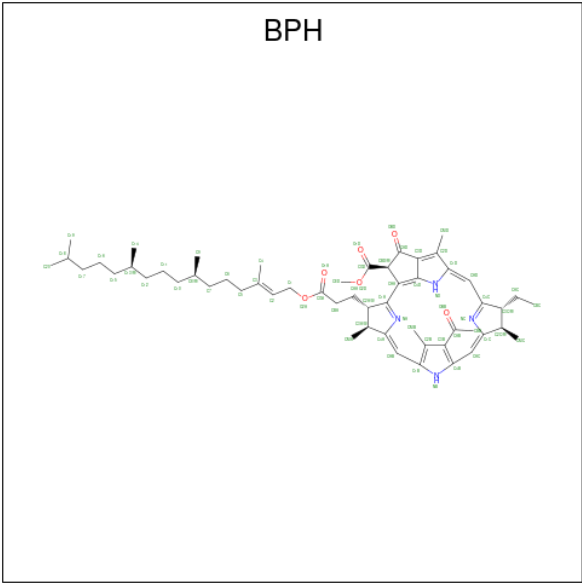


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			10	7	3		
11	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

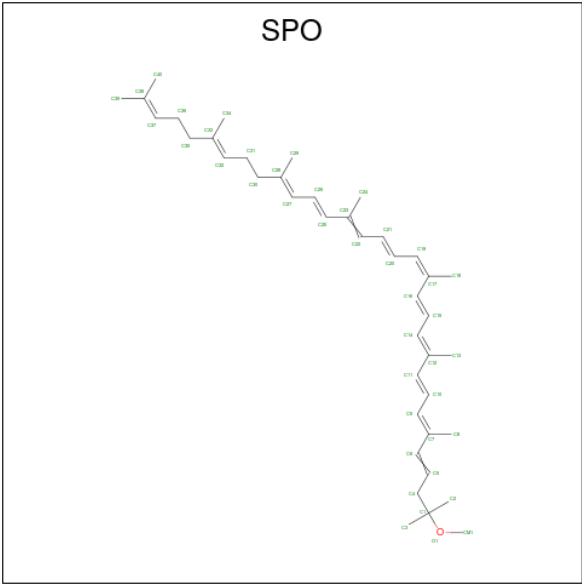
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	Fe		0	0
			1	1			

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



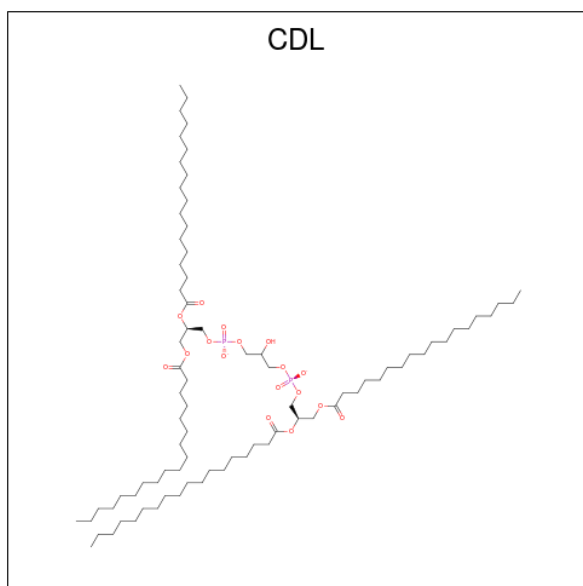
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			65	55	4	6		
13	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 14 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



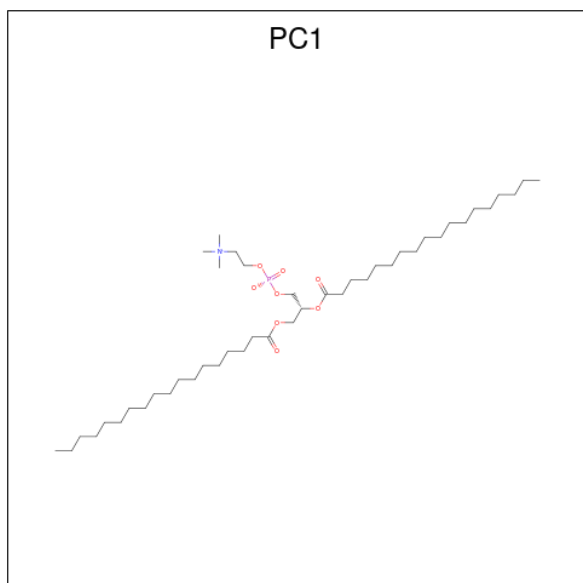
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

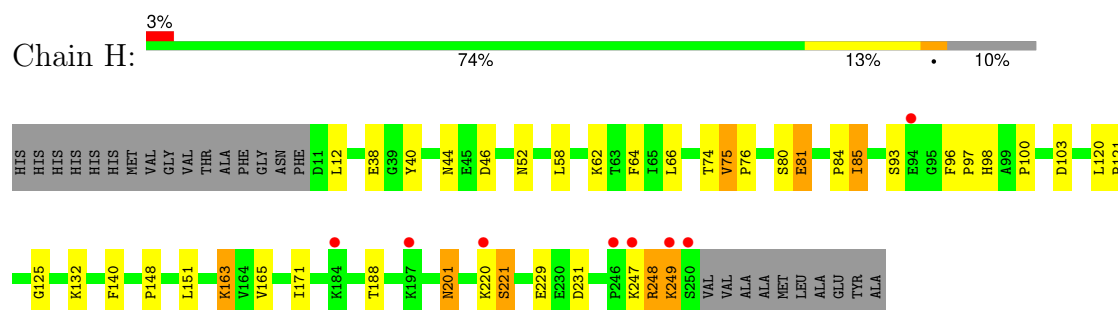
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

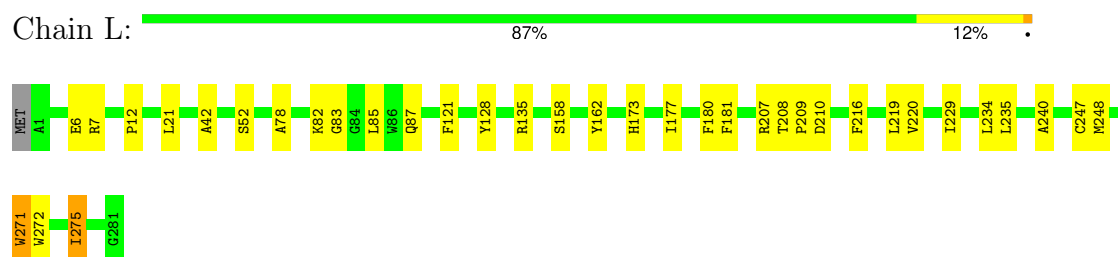
3 Residue-property plots [i](#)

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.

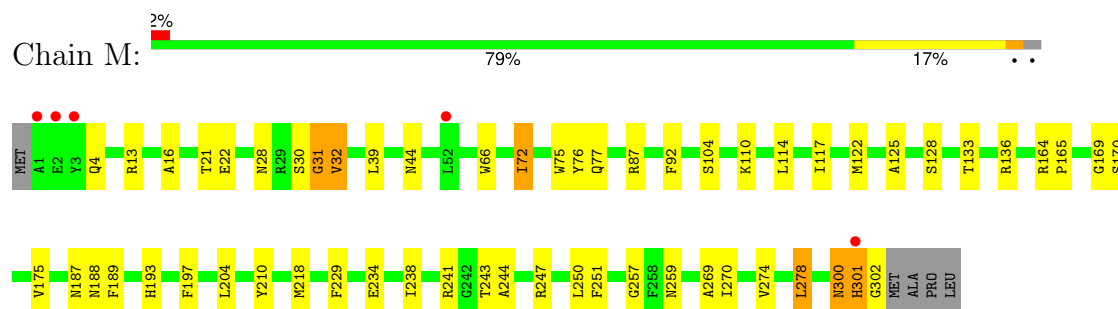
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.14Å 139.14Å 185.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.57 – 2.85 38.57 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.57-2.85) 99.8 (38.57-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.213 0.179 , 0.211	Depositor DCC
R_{free} test set	2474 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDL, FE, BCL, PO4, U10, GOL, K, SPO, PC1, HTO, GGD, LDA, BPH

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	H	1.20	4/1929 (0.2%)	1.24	6/2619 (0.2%)
2	L	1.10	1/2339 (0.0%)	1.14	10/3203 (0.3%)
3	M	1.12	3/2507 (0.1%)	1.14	12/3422 (0.4%)
All	All	1.14	8/6775 (0.1%)	1.17	28/9244 (0.3%)

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
3	M	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	85[A]	ILE	C-O	-7.12	1.15	1.24
1	H	85[B]	ILE	C-O	-7.12	1.15	1.24
1	H	100	PRO	C-O	-6.79	1.15	1.23
3	M	301	HIS	N-CA	6.79	1.54	1.46
3	M	259	ASN	C-O	-6.34	1.17	1.23
1	H	132	LYS	CA-C	-5.66	1.46	1.52
2	L	234	LEU	C-O	-5.29	1.18	1.24
3	M	72	ILE	CA-CB	5.24	1.60	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	28	ASN	N-CA-C	7.43	122.38	113.16
3	M	175	VAL	CA-C-N	7.31	127.89	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	175	VAL	C-N-CA	7.31	127.89	120.14
2	L	220	VAL	CB-CA-C	-7.26	103.51	110.70
3	M	44[A]	ASN	N-CA-C	6.86	120.17	110.23
3	M	44[B]	ASN	N-CA-C	6.86	120.17	110.23
3	M	72	ILE	N-CA-C	-6.65	104.28	110.53
2	L	275	ILE	CA-C-N	-6.41	114.13	120.98
2	L	275	ILE	C-N-CA	-6.41	114.13	120.98
1	H	80	SER	N-CA-C	6.39	119.60	109.50
2	L	234	LEU	N-CA-C	-6.22	104.42	111.07
2	L	6	GLU	N-CA-C	6.13	118.04	111.36
3	M	31	GLY	N-CA-C	-6.11	101.92	112.06
2	L	271[A]	TRP	N-CA-CB	5.85	120.37	110.49
2	L	271[B]	TRP	N-CA-CB	5.85	120.37	110.49
1	H	248	ARG	CA-C-N	5.79	132.12	121.70
1	H	248	ARG	C-N-CA	5.79	132.12	121.70
3	M	259	ASN	N-CA-C	5.66	116.74	108.14
2	L	12	PRO	CB-CA-C	-5.61	104.23	111.46
3	M	117	ILE	N-CA-C	-5.51	105.24	110.42
3	M	75	TRP	N-CA-C	-5.42	105.45	111.36
1	H	125	GLY	N-CA-C	-5.30	108.38	115.32
3	M	125	ALA	N-CA-C	5.26	117.02	111.28
1	H	81	GLU	N-CA-C	5.19	117.67	111.71
1	H	188	THR	N-CA-C	5.14	117.97	109.85
3	M	169	GLY	N-CA-C	5.07	122.71	114.90
2	L	78	ALA	CA-C-N	-5.01	114.62	119.78
2	L	78	ALA	C-N-CA	-5.01	114.62	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1849	0	1873	29	0
2	L	2239	0	2185	24	0
3	M	2410	0	2314	31	0
4	H	30	0	40	0	0
4	L	12	0	16	1	0
5	H	1	0	0	0	0
6	H	57	0	68	3	0
7	L	132	0	148	12	0
7	M	132	0	148	13	0
8	L	48	0	93	0	0
8	M	32	0	62	4	0
9	L	46	0	46	4	0
9	M	48	0	63	2	0
10	L	5	0	0	1	0
11	L	20	0	32	0	0
12	M	1	0	0	0	0
13	M	130	0	150	17	0
14	M	42	0	60	3	0
15	M	81	0	102	1	0
16	M	43	0	60	1	0
17	M	1	0	0	0	0
All	All	7359	0	7460	109	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 7.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:412:BPH:HBB3	13:M:412:BPH:HHC	1.50	0.91
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.63	0.78
13:M:406:BPH:HHC	13:M:406:BPH:HBB3	1.66	0.78
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.68	0.75
1:H:220[B]:LYS:HE2	1:H:221:SER:OG	1.91	0.71
2:L:229:ILE:HD13	9:L:305[B]:U10:H3M2	1.73	0.71
1:H:248:ARG:HA	1:H:249[B]:LYS:HB2	1.73	0.70
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.75	0.67
3:M:210:TYR:HB3	13:M:412:BPH:HBB2	1.77	0.67
1:H:84:PRO:O	1:H:85[A]:ILE:HD13	1.95	0.67
1:H:120:LEU:HB3	1:H:121:PRO:HD2	1.76	0.67
7:M:402:BCL:CBB	7:M:402:BCL:HHC	2.24	0.67
7:L:301:BCL:HBB2	7:L:301:BCL:HHC	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:ASN:H	1:H:201:ASN:HD22	1.45	0.63
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.80	0.63
7:M:401:BCL:HBB2	14:M:408:SPO:H243	1.82	0.61
1:H:120:LEU:HB3	1:H:121:PRO:CD	2.30	0.60
3:M:189:PHE:O	3:M:193:HIS:HD2	1.84	0.60
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.84	0.59
1:H:163[A]:LYS:HE2	1:H:165:VAL:HG12	1.83	0.59
13:M:412:BPH:C2	13:M:412:BPH:O1A	2.50	0.59
3:M:31:GLY:N	16:M:410:PC1:O12	2.31	0.57
1:H:220[B]:LYS:HD3	1:H:229:GLU:OE2	2.05	0.57
3:M:270:ILE:O	3:M:274:VAL:HG13	2.03	0.57
2:L:128:TYR:HD1	7:L:301:BCL:HBB1	1.69	0.57
7:M:401:BCL:CBB	7:M:401:BCL:HHC	2.34	0.57
13:M:412:BPH:HHC	13:M:412:BPH:CBB	2.29	0.57
7:M:401:BCL:HBB2	7:M:401:BCL:HHC	1.88	0.55
7:M:401:BCL:H72	7:M:402:BCL:H192	1.89	0.55
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.42	0.55
7:L:306:BCL:C1C	7:M:402:BCL:HBB3	2.38	0.54
2:L:181:PHE:CD2	13:M:406:BPH:HBB1	2.43	0.53
7:L:306:BCL:CBB	7:L:306:BCL:HMB3	2.37	0.53
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.91	0.53
2:L:181:PHE:HB3	13:M:406:BPH:HBB2	1.90	0.53
2:L:82:LYS:NZ	10:L:307:PO4:O4	2.40	0.53
13:M:412:BPH:HBB3	13:M:412:BPH:CHC	2.31	0.52
3:M:234:GLU:O	3:M:238:ILE:HG13	2.09	0.52
7:M:401:BCL:C7	7:M:402:BCL:H192	2.40	0.52
7:M:401:BCL:CBB	14:M:408:SPO:H243	2.40	0.52
3:M:300:ASN:O	3:M:302:GLY:N	2.44	0.51
3:M:300:ASN:C	3:M:302:GLY:N	2.69	0.51
9:L:305[B]:U10:H103	8:M:404:LDA:H121	1.93	0.50
2:L:121:PHE:CZ	13:M:412:BPH:HBA2	2.46	0.50
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.45	0.49
1:H:38:GLU:OE1	3:M:241:ARG:NH2	2.46	0.49
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.60	0.49
1:H:52:ASN:ND2	6:H:307:GGD:HA41	2.27	0.49
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.95	0.49
3:M:269:ALA:O	3:M:270:ILE:C	2.55	0.49
1:H:62:LYS:HE3	1:H:64:PHE:CZ	2.47	0.49
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.47	0.49
3:M:251:PHE:CD1	3:M:251:PHE:C	2.90	0.49
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:PHE:HA	3:M:13:ARG:O	2.14	0.48
7:L:301:BCL:HHC	7:L:301:BCL:CBB	2.43	0.48
2:L:181:PHE:HB3	13:M:406:BPH:CBB	2.44	0.48
2:L:42:ALA:HA	13:M:412:BPH:H9C3	1.95	0.47
3:M:197:PHE:CZ	7:M:402:BCL:HBB2	2.49	0.47
2:L:128:TYR:CD1	7:L:301:BCL:HBB1	2.48	0.47
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.50	0.47
4:L:311:GOL:H12	8:M:403:LDA:O1	2.15	0.47
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.32	0.46
3:M:77:GLN:NE2	3:M:92:PHE:HB3	2.31	0.46
13:M:412:BPH:CBB	13:M:412:BPH:CHC	2.91	0.46
1:H:62:LYS:O	1:H:74:THR:HA	2.16	0.45
13:M:406:BPH:HBC2	13:M:406:BPH:HHD	1.99	0.45
3:M:197:PHE:HZ	7:M:402:BCL:HBB2	1.82	0.45
1:H:52:ASN:HD21	6:H:307:GGD:HA41	1.83	0.44
7:L:306:BCL:H193	9:M:407:U10:H252	2.00	0.44
3:M:204:LEU:HG	8:M:403:LDA:HM13	1.99	0.44
9:L:305[B]:U10:C10	8:M:404:LDA:H121	2.47	0.44
3:M:21:THR:O	3:M:22:GLU:C	2.60	0.44
7:L:301:BCL:H193	13:M:412:BPH:H7C1	2.00	0.44
1:H:40:TYR:HB3	1:H:58:LEU:HD21	1.98	0.44
2:L:229:ILE:HD13	9:L:305[B]:U10:C3M	2.43	0.44
3:M:243:THR:O	3:M:247:ARG:HG3	2.19	0.43
7:M:402:BCL:HAA2	7:M:402:BCL:HBD	1.98	0.43
1:H:44:ASN:C	1:H:46:ASP:H	2.26	0.43
3:M:16:ALA:CB	3:M:32:VAL:HG11	2.40	0.43
2:L:83:GLY:O	2:L:87:GLN:HG3	2.19	0.43
7:L:306:BCL:H203	7:L:306:BCL:H161	1.91	0.43
1:H:44:ASN:C	1:H:46:ASP:N	2.77	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.43	0.43
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.54	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.37	0.43
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.02	0.42
2:L:135:ARG:HD2	2:L:248:MET:O	2.19	0.42
2:L:208:THR:HB	2:L:209:PRO:HD2	2.00	0.42
3:M:274:VAL:O	3:M:278:LEU:HB2	2.19	0.42
13:M:412:BPH:H4C1	13:M:412:BPH:H6C2	1.81	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.00	0.42
13:M:412:BPH:H5C2	13:M:412:BPH:H1C1	1.82	0.42
15:M:409:CDL:C36	15:M:409:CDL:C34	2.97	0.42
3:M:76:TYR:CD2	3:M:76:TYR:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.55	0.41
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.03	0.41
1:H:103:ASP:OD1	1:H:103:ASP:C	2.64	0.41
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.96	0.41
7:L:301:BCL:HBC1	7:L:306:BCL:CGA	2.51	0.41
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.90	0.41
7:L:301:BCL:C2B	13:M:412:BPH:H202	2.51	0.41
3:M:218:MET:HE1	9:M:407:U10:H162	2.03	0.41
3:M:300:ASN:C	3:M:302:GLY:H	2.28	0.41
7:L:306:BCL:NC	7:M:402:BCL:HBB3	2.35	0.41
14:M:408:SPO:H181	14:M:408:SPO:H20	1.86	0.40
6:H:307:GGD:HC62	3:M:257:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	H	244/266 (92%)	231 (95%)	11 (4%)	2 (1%)	16	31
2	L	281/282 (100%)	265 (94%)	16 (6%)	0	100	100
3	M	301/307 (98%)	288 (96%)	11 (4%)	2 (1%)	18	35
All	All	826/855 (97%)	784 (95%)	38 (5%)	4 (0%)	30	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	30	SER
3	M	301	HIS

5.3.2 Protein sidechains ⓘ

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	H	200/214 (94%)	189 (94%)	11 (6%)	19	41
2	L	221/221 (100%)	212 (96%)	9 (4%)	27	52
3	M	237/240 (99%)	225 (95%)	12 (5%)	21	43
All	All	658/675 (98%)	626 (95%)	32 (5%)	24	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	66	LEU
1	H	75	VAL
1	H	93	SER
1	H	163[A]	LYS
1	H	163[B]	LYS
1	H	171	ILE
1	H	201	ASN
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
2	L	21	LEU
2	L	158	SER
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	271[A]	TRP
2	L	271[B]	TRP
3	M	4	GLN
3	M	32	VAL
3	M	39	LEU
3	M	72	ILE
3	M	104	SER
3	M	110	LYS

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Mol	Chain	Res	Type
3	M	114	LEU
3	M	128	SER
3	M	136	ARG
3	M	170	SER
3	M	188	ASN
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	H	98	HIS
1	H	201	ASN
2	L	159	ASN
2	L	258	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	202	HIS
3	M	300	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	M	401	3	69,74,74	1.76	14 (20%)	79,115,115	2.02	23 (29%)
11	HTO	L	309	-	9,9,9	1.61	3 (33%)	10,10,10	2.00	4 (40%)
4	GOL	L	311	-	5,5,5	0.37	0	5,5,5	0.37	0
7	BCL	L	301	2	69,74,74	1.66	17 (24%)	79,115,115	2.31	30 (37%)
16	PC1	M	410	-	42,42,53	1.52	3 (7%)	48,50,61	1.51	6 (12%)
7	BCL	M	402	3	69,74,74	1.72	17 (24%)	79,115,115	2.03	20 (25%)
9	U10	M	407	-	48,48,63	1.38	5 (10%)	60,61,79	2.15	15 (25%)
4	GOL	H	304	-	5,5,5	0.82	0	5,5,5	0.79	0
15	CDL	M	409	-	79,79,99	1.54	5 (6%)	84,90,111	1.45	9 (10%)
8	LDA	M	404	-	13,15,15	1.98	1 (7%)	14,17,17	0.56	0
7	BCL	L	306	2	69,74,74	1.78	14 (20%)	79,115,115	1.93	22 (27%)
8	LDA	L	302	-	13,15,15	2.08	2 (15%)	14,17,17	0.86	0
13	BPH	M	406	-	59,70,70	2.35	15 (25%)	59,101,101	2.14	13 (22%)
8	LDA	M	403	-	13,15,15	2.16	1 (7%)	14,17,17	0.92	1 (7%)
4	GOL	H	301	-	5,5,5	0.80	0	5,5,5	1.15	0
13	BPH	M	412	17	59,70,70	2.45	16 (27%)	59,101,101	2.70	24 (40%)
8	LDA	L	304	-	13,15,15	2.02	1 (7%)	14,17,17	0.78	0
11	HTO	L	308	-	9,9,9	1.39	2 (22%)	10,10,10	1.24	1 (10%)
4	GOL	L	310	-	5,5,5	0.48	0	5,5,5	0.52	0
8	LDA	L	303	-	13,15,15	2.12	1 (7%)	14,17,17	0.79	1 (7%)
6	GGD	H	307	-	58,58,68	1.15	3 (5%)	72,72,82	1.71	14 (19%)
4	GOL	H	306	-	5,5,5	1.18	0	5,5,5	1.06	1 (20%)
9	U10	L	305[A]	-	23,23,63	1.85	2 (8%)	30,31,79	1.56	6 (20%)
14	SPO	M	408	-	41,41,41	0.81	1 (2%)	47,50,50	1.87	11 (23%)
4	GOL	H	303	-	5,5,5	0.58	0	5,5,5	0.68	0
4	GOL	H	302	-	5,5,5	0.51	0	5,5,5	0.69	0
9	U10	L	305[B]	-	23,23,63	2.12	2 (8%)	30,31,79	1.46	5 (16%)
10	PO4	L	307	-	4,4,4	1.22	1 (25%)	6,6,6	0.85	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
7	BCL	M	401	3	-	11/41/137/137	-
11	HTO	L	309	-	-	5/10/10/10	-
4	GOL	L	311	-	-	4/4/4/4	-
7	BCL	L	301	2	-	5/41/137/137	-
16	PC1	M	410	-	-	23/46/46/57	-
7	BCL	M	402	3	-	2/41/137/137	-
9	U10	M	407	-	-	9/45/69/87	0/1/1/1
4	GOL	H	304	-	-	2/4/4/4	-
15	CDL	M	409	-	-	48/88/88/110	-
8	LDA	M	404	-	-	7/13/13/13	-
7	BCL	L	306	2	-	3/41/137/137	-
8	LDA	L	302	-	-	5/13/13/13	-
13	BPH	M	406	-	-	12/37/105/105	0/5/6/6
8	LDA	M	403	-	-	7/13/13/13	-
4	GOL	H	301	-	-	2/4/4/4	-
13	BPH	M	412	17	-	9/37/105/105	0/5/6/6
8	LDA	L	304	-	-	8/13/13/13	-
11	HTO	L	308	-	-	6/10/10/10	-
4	GOL	L	310	-	-	4/4/4/4	-
8	LDA	L	303	-	-	7/13/13/13	-
6	GGD	H	307	-	-	20/47/87/97	0/2/2/2
4	GOL	H	306	-	-	2/4/4/4	-
9	U10	L	305[A]	-	-	1/15/39/87	0/1/1/1
14	SPO	M	408	-	-	4/47/47/47	-
4	GOL	H	303	-	-	2/4/4/4	-
4	GOL	H	302	-	-	2/4/4/4	-
9	U10	L	305[B]	-	-	4/15/39/87	0/1/1/1

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	305[B]	U10	C6-C1	8.63	1.50	1.35
13	M	412	BPH	C1D-C2D	7.83	1.48	1.39
9	L	305[A]	U10	C6-C1	7.81	1.49	1.35
13	M	412	BPH	C1B-C2B	7.30	1.47	1.39
8	L	303	LDA	O1-N1	-7.10	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	304	LDA	O1-N1	-6.99	1.25	1.42
13	M	406	BPH	C1D-C2D	6.98	1.47	1.39
8	M	403	LDA	O1-N1	-6.79	1.25	1.42
8	M	404	LDA	O1-N1	-6.73	1.25	1.42
8	L	302	LDA	O1-N1	-6.66	1.25	1.42
13	M	412	BPH	C3A-C2A	-6.59	1.49	1.54
13	M	412	BPH	OBD-CAD	6.40	1.30	1.22
13	M	406	BPH	C1B-C2B	6.10	1.46	1.39
13	M	406	BPH	C2C-C3C	-5.96	1.49	1.54
16	M	410	PC1	O31-C31	5.95	1.50	1.33
15	M	409	CDL	OB6-CB5	5.60	1.50	1.34
15	M	409	CDL	OA6-CA5	5.52	1.49	1.34
7	L	306	BCL	C1D-ND	-5.51	1.30	1.37
9	M	407	U10	C6-C1	5.44	1.44	1.35
13	M	406	BPH	C3D-C4D	-5.43	1.33	1.41
15	M	409	CDL	OA8-CA7	5.33	1.48	1.33
16	M	410	PC1	O21-C21	5.24	1.49	1.34
7	M	401	BCL	O2A-CGA	5.09	1.48	1.33
13	M	406	BPH	C3D-C2D	4.95	1.48	1.39
13	M	406	BPH	C4D-CHA	4.88	1.46	1.39
7	M	401	BCL	OBD-CAD	4.87	1.30	1.22
7	L	301	BCL	O2A-CGA	4.70	1.47	1.33
15	M	409	CDL	OB8-CB7	4.67	1.47	1.33
7	L	301	BCL	O2D-CGD	4.61	1.44	1.33
7	M	402	BCL	C1D-ND	-4.51	1.31	1.37
13	M	406	BPH	O2A-CGA	4.43	1.46	1.33
7	L	306	BCL	C3D-C4D	-4.43	1.34	1.44
7	M	402	BCL	C3D-C4D	-4.37	1.34	1.44
13	M	412	BPH	CHA-CBD	-4.28	1.46	1.51
7	L	306	BCL	O2D-CGD	4.26	1.43	1.33
13	M	412	BPH	C3D-C2D	4.22	1.46	1.39
7	M	401	BCL	CHB-C1B	4.17	1.48	1.39
6	H	307	GGD	OC6-CC5	4.17	1.46	1.34
13	M	412	BPH	C3D-C4D	-4.04	1.35	1.41
7	M	401	BCL	C3D-C4D	-4.03	1.35	1.44
7	M	402	BCL	O2D-CGD	3.99	1.43	1.33
6	H	307	GGD	OC8-CC7	3.97	1.44	1.33
7	L	306	BCL	C3C-C4C	-3.96	1.46	1.51
13	M	412	BPH	C4D-CHA	3.87	1.45	1.39
9	L	305[B]	U10	C4-C3	3.69	1.49	1.36
7	L	301	BCL	CHB-C1B	3.66	1.47	1.39
7	M	402	BCL	O2A-CGA	3.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	406	BPH	C3B-C2B	3.66	1.45	1.39
7	L	306	BCL	C3B-C4B	3.65	1.48	1.41
7	M	402	BCL	OBD-CAD	3.59	1.28	1.22
7	L	301	BCL	C1D-ND	-3.48	1.33	1.37
7	L	306	BCL	O2A-CGA	3.48	1.43	1.33
7	M	401	BCL	O2D-CGD	3.47	1.41	1.33
7	M	401	BCL	C3D-C2D	3.40	1.48	1.39
7	L	306	BCL	OBD-CAD	3.37	1.28	1.22
13	M	412	BPH	O2A-CGA	3.36	1.43	1.33
7	M	402	BCL	C3B-C4B	3.31	1.47	1.41
7	M	401	BCL	C3B-C4B	3.30	1.47	1.41
9	M	407	U10	C4-C3	3.26	1.48	1.36
13	M	406	BPH	CHA-CBD	-3.22	1.47	1.51
7	M	402	BCL	CHD-C1D	3.18	1.44	1.38
7	L	301	BCL	C3B-C4B	3.17	1.47	1.41
13	M	406	BPH	O2D-CGD	3.08	1.40	1.33
9	M	407	U10	C31-C29	3.07	1.57	1.51
7	L	306	BCL	MG-ND	-3.04	1.99	2.05
11	L	309	HTO	C4-C3	3.02	1.57	1.52
13	M	406	BPH	C3B-C4B	3.00	1.46	1.41
13	M	412	BPH	C3B-C2B	3.00	1.44	1.39
7	M	401	BCL	CHD-C1D	2.99	1.44	1.38
9	L	305[A]	U10	C4-C3	2.99	1.47	1.36
7	M	402	BCL	CHC-C4B	2.97	1.46	1.39
7	L	306	BCL	CHC-C4B	2.95	1.46	1.39
7	L	301	BCL	C3D-C2D	2.94	1.47	1.39
7	L	306	BCL	CHB-C1B	2.93	1.46	1.39
6	H	307	GGD	OA1-CA1	2.85	1.44	1.40
13	M	412	BPH	C3B-C4B	2.84	1.46	1.41
7	M	402	BCL	C4B-NB	-2.82	1.34	1.37
13	M	412	BPH	C1B-NB	-2.80	1.33	1.38
11	L	308	HTO	C4-C3	2.76	1.57	1.52
13	M	406	BPH	OBD-CAD	2.76	1.25	1.22
7	L	301	BCL	C3D-C4D	-2.76	1.38	1.44
7	L	306	BCL	MG-NA	-2.74	1.99	2.06
7	L	301	BCL	CHD-C4C	2.69	1.46	1.39
7	M	401	BCL	C1D-ND	-2.68	1.34	1.37
7	L	301	BCL	CHC-C4B	2.64	1.45	1.39
7	M	401	BCL	CHC-C4B	2.62	1.45	1.39
16	M	410	PC1	C3-C2	2.58	1.58	1.50
7	L	301	BCL	CHC-C1C	-2.54	1.31	1.37
7	L	306	BCL	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	BCL	MG-NA	-2.49	2.00	2.06
13	M	406	BPH	C3A-C2A	-2.48	1.52	1.54
7	M	402	BCL	CHB-C4A	-2.47	1.31	1.37
7	L	301	BCL	OBD-CAD	2.47	1.26	1.22
7	M	402	BCL	CHB-C1B	2.47	1.45	1.39
7	M	402	BCL	C2C-C3C	-2.47	1.47	1.54
14	M	408	SPO	C25-C23	2.43	1.51	1.46
7	L	301	BCL	CHD-C1D	2.41	1.43	1.38
9	M	407	U10	C18-C19	2.39	1.38	1.33
13	M	412	BPH	C1D-ND	-2.37	1.34	1.38
7	M	401	BCL	CHC-C1C	-2.37	1.31	1.37
13	M	412	BPH	O2D-CGD	2.36	1.39	1.33
10	L	307	PO4	P-O4	-2.34	1.47	1.54
7	M	402	BCL	C4D-CHA	2.33	1.46	1.38
7	L	301	BCL	MG-NA	-2.31	2.00	2.06
15	M	409	CDL	CA3-CA4	2.29	1.58	1.50
11	L	309	HTO	C1-C2	2.28	1.57	1.52
7	L	301	BCL	C2C-C3C	-2.28	1.48	1.54
7	M	401	BCL	CHD-C4C	2.28	1.45	1.39
7	M	402	BCL	C1B-NB	-2.26	1.34	1.37
7	M	402	BCL	CHC-C1C	-2.23	1.32	1.37
7	L	306	BCL	C4B-NB	-2.23	1.34	1.37
13	M	412	BPH	O1D-CGD	2.22	1.26	1.21
13	M	412	BPH	CBD-CGD	-2.21	1.49	1.52
11	L	309	HTO	C3-C2	2.21	1.58	1.53
13	M	406	BPH	C1-C2	2.20	1.55	1.49
7	L	301	BCL	C1B-C2B	2.17	1.48	1.43
11	L	308	HTO	C3-C2	2.13	1.58	1.53
7	M	402	BCL	MG-NC	-2.11	2.01	2.06
7	L	301	BCL	C4D-CHA	2.08	1.45	1.38
9	M	407	U10	C33-C34	2.08	1.37	1.33
7	L	306	BCL	C3D-C2D	2.06	1.44	1.39
7	M	401	BCL	MG-NC	-2.05	2.01	2.06
13	M	406	BPH	C4B-NB	-2.05	1.34	1.38
7	M	402	BCL	CHD-C4C	2.03	1.44	1.39
8	L	302	LDA	C1-N1	-2.02	1.49	1.51
7	L	301	BCL	MG-NC	-2.01	2.01	2.06

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	407	U10	C30-C29-C31	9.78	132.20	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	412	BPH	O1D-CGD-CBD	8.90	138.23	124.72
7	L	301	BCL	O2D-CGD-CBD	7.80	124.87	111.23
14	M	408	SPO	C4-C5-C6	-7.35	114.60	124.91
15	M	409	CDL	OB6-CB5-C51	6.36	125.23	111.48
7	M	402	BCL	C1C-NC-C4C	-6.35	103.78	106.68
13	M	412	BPH	CED-O2D-CGD	-6.31	101.60	115.92
13	M	412	BPH	C4D-CHA-CBD	-6.09	105.53	108.45
7	L	306	BCL	CMD-C2D-C1D	5.96	135.23	124.73
7	M	402	BCL	CMD-C2D-C1D	5.78	134.91	124.73
13	M	406	BPH	O2D-CGD-CBD	5.71	117.22	110.95
9	M	407	U10	C31-C29-C28	-5.58	108.64	121.17
13	M	412	BPH	C3D-C4D-ND	5.47	114.72	107.71
16	M	410	PC1	O21-C21-C22	5.32	122.99	111.48
15	M	409	CDL	OA6-CA5-C11	5.22	122.78	111.48
7	L	306	BCL	C2B-C1B-NB	5.22	115.74	110.33
13	M	406	BPH	C2B-C1B-NB	5.17	113.17	109.43
6	H	307	GGD	OB1-CA3-CA2	5.14	120.30	107.23
7	M	401	BCL	O2D-CGD-CBD	5.01	119.99	111.23
6	H	307	GGD	OC6-CC5-C14	5.00	122.30	111.48
6	H	307	GGD	CA1-OA5-CA5	4.92	123.32	113.72
7	L	301	BCL	C2D-C1D-ND	4.88	114.96	110.13
7	M	401	BCL	CMD-C2D-C1D	4.75	133.09	124.73
7	L	301	BCL	C1C-NC-C4C	-4.67	104.55	106.68
7	L	306	BCL	C3C-C4C-CHD	-4.63	113.62	123.39
7	M	402	BCL	C3C-C4C-CHD	-4.58	113.73	123.39
6	H	307	GGD	CC4-OC6-CC5	-4.58	106.84	117.80
13	M	406	BPH	C3D-CAD-CBD	4.57	113.62	107.61
13	M	412	BPH	CAA-CBA-CGA	-4.48	100.48	113.21
7	M	401	BCL	C3C-C4C-CHD	-4.47	113.97	123.39
13	M	412	BPH	C2B-C1B-NB	4.45	112.64	109.43
6	H	307	GGD	CA4-CA3-CA2	-4.40	104.76	110.86
7	L	301	BCL	CMD-C2D-C1D	4.38	132.45	124.73
7	L	301	BCL	O2D-CGD-O1D	-4.38	115.32	123.85
7	L	301	BCL	OBD-CAD-C3D	-4.37	118.19	128.42
7	L	301	BCL	C3C-C4C-CHD	-4.37	114.17	123.39
7	L	301	BCL	C3D-C2D-C1D	-4.36	99.88	105.83
13	M	406	BPH	CMA-C3A-C4A	-4.35	105.23	114.61
13	M	412	BPH	O2D-CGD-O1D	-4.31	115.45	123.85
13	M	406	BPH	OBD-CAD-CBD	-4.29	119.53	125.82
13	M	406	BPH	C3D-C4D-ND	4.24	113.15	107.71
13	M	412	BPH	O2D-CGD-CBD	-4.24	106.28	110.95
7	M	402	BCL	C4A-NA-C1A	4.24	108.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	407	U10	C32-C31-C29	4.21	127.13	113.19
7	M	401	BCL	C1C-NC-C4C	-4.18	104.77	106.68
7	L	301	BCL	C3B-C4B-NB	4.17	115.26	109.76
7	M	402	BCL	C2B-C1B-NB	4.15	114.63	110.33
16	M	410	PC1	C3-O31-C31	4.13	132.21	117.12
7	M	401	BCL	C3D-C4D-ND	4.11	116.67	109.99
7	L	301	BCL	C4A-NA-C1A	4.02	108.52	106.68
7	M	402	BCL	C3D-C2D-C1D	-4.01	100.36	105.83
13	M	406	BPH	C1-O2A-CGA	4.01	126.35	116.65
14	M	408	SPO	C15-C14-C12	-4.00	121.67	127.28
7	L	306	BCL	C1D-ND-C4D	-3.92	103.56	106.31
7	M	401	BCL	C1-O2A-CGA	3.91	126.12	116.65
7	L	306	BCL	CMB-C2B-C1B	3.86	131.30	125.42
13	M	412	BPH	C1-C2-C3	-3.84	119.91	126.20
7	M	402	BCL	C1D-ND-C4D	-3.82	103.63	106.31
11	L	309	HTO	O1-C1-C2	3.80	119.14	111.16
13	M	406	BPH	O2D-CGD-O1D	-3.79	116.47	123.85
13	M	412	BPH	C4-C3-C5	3.78	121.78	115.23
13	M	406	BPH	C1A-C2A-C3A	-3.76	99.26	102.84
7	M	402	BCL	C2D-C1D-ND	3.72	113.81	110.13
7	M	401	BCL	O2D-CGD-O1D	-3.70	116.65	123.85
7	L	306	BCL	C2D-C1D-ND	3.65	113.73	110.13
9	M	407	U10	C7-C8-C9	-3.63	120.58	126.83
7	M	401	BCL	O2A-C1-C2	3.57	121.85	108.11
9	L	305[A]	U10	C8-C7-C6	3.54	120.79	112.08
7	M	401	BCL	CHD-C1D-ND	-3.53	119.83	124.80
7	L	306	BCL	C3D-C4D-ND	3.52	115.71	109.99
7	M	402	BCL	O2D-CGD-O1D	-3.50	117.03	123.85
13	M	412	BPH	C2D-C1D-ND	3.49	111.95	109.43
16	M	410	PC1	O31-C3-C2	3.42	118.25	108.40
9	M	407	U10	C4M-O4-C4	3.39	128.39	116.47
7	L	301	BCL	C1D-ND-C4D	-3.36	103.95	106.31
7	M	401	BCL	C1D-ND-C4D	-3.31	103.99	106.31
7	L	306	BCL	CHD-C1D-ND	-3.30	120.16	124.80
16	M	410	PC1	O31-C31-C32	3.28	121.85	111.83
7	M	402	BCL	CHD-C1D-ND	-3.25	120.23	124.80
7	L	301	BCL	CHB-C4A-NA	3.25	129.09	124.40
7	L	306	BCL	C1C-NC-C4C	-3.24	105.20	106.68
7	M	401	BCL	O2A-CGA-CBA	3.24	121.72	111.83
7	M	402	BCL	C3D-C4D-ND	3.23	115.24	109.99
15	M	409	CDL	OA8-CA7-C31	3.22	121.64	111.83
13	M	406	BPH	C4C-C3C-C2C	-3.20	99.79	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	402	BCL	CHB-C4A-NA	3.20	129.01	124.40
13	M	406	BPH	C4-C3-C2	-3.19	115.44	123.63
7	M	401	BCL	CMB-C2B-C1B	3.17	130.24	125.42
7	L	306	BCL	C1-O2A-CGA	3.16	124.31	116.65
13	M	412	BPH	C4C-C3C-C2C	-3.15	99.84	102.84
13	M	406	BPH	C6-C5-C3	3.14	121.12	113.47
7	L	301	BCL	CHC-C1C-NC	3.11	128.89	124.40
7	M	402	BCL	OBD-CAD-C3D	-3.10	121.18	128.42
13	M	412	BPH	OBB-CAB-C3B	3.09	125.16	119.99
7	L	306	BCL	C3B-C4B-NB	3.09	113.84	109.76
15	M	409	CDL	OA6-CA5-OA7	-3.08	116.50	123.70
9	L	305[A]	U10	C16-C14-C15	3.07	121.66	114.59
7	L	301	BCL	C2A-C1A-CHA	-3.06	118.56	123.87
13	M	412	BPH	C4D-ND-C1D	-3.06	105.21	108.87
9	L	305[B]	U10	C10-C9-C11	3.04	120.51	115.23
7	L	301	BCL	O2A-CGA-CBA	3.04	121.11	111.83
7	L	301	BCL	C1D-CHD-C4C	-3.03	119.32	126.62
7	L	306	BCL	O2A-CGA-O1A	-3.01	116.11	123.63
7	L	306	BCL	O2A-CGA-CBA	3.00	120.97	111.83
7	M	401	BCL	C1-C2-C3	3.00	131.10	126.20
7	L	306	BCL	C3D-C2D-C1D	-2.98	101.76	105.83
7	L	301	BCL	C5-C3-C2	-2.98	114.48	121.17
7	L	301	BCL	C3D-C4D-ND	2.97	114.81	109.99
7	L	306	BCL	CHB-C4A-NA	2.96	128.67	124.40
13	M	412	BPH	C4-C3-C2	-2.96	116.03	123.63
14	M	408	SPO	C27-C26-C25	-2.94	114.67	123.20
15	M	409	CDL	OA8-CA7-OA9	-2.92	116.31	123.63
6	H	307	GGD	OC8-CC7-OC9	-2.92	116.33	123.63
13	M	412	BPH	CBB-CAB-C3B	-2.91	111.63	120.34
11	L	309	HTO	C4-C3-C2	2.90	120.71	113.73
7	M	401	BCL	C2B-C1B-NB	2.90	113.33	110.33
7	L	301	BCL	C4-C3-C5	2.90	120.26	115.23
9	M	407	U10	C26-C27-C28	-2.89	97.71	112.02
7	M	402	BCL	C1D-CHD-C4C	-2.89	119.65	126.62
14	M	408	SPO	C20-C19-C17	-2.89	123.22	127.28
9	L	305[B]	U10	O5-C5-C4	-2.85	115.00	121.03
9	L	305[A]	U10	C16-C14-C13	-2.84	114.12	122.66
11	L	309	HTO	C1-C2-C3	2.84	118.79	113.00
7	M	401	BCL	C1D-CHD-C4C	-2.82	119.81	126.62
7	L	301	BCL	OBB-CAB-C3B	2.80	125.39	120.43
9	L	305[B]	U10	C16-C14-C15	2.79	121.01	114.59
7	L	306	BCL	CHC-C1C-NC	2.78	128.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401	BCL	CHC-C1C-NC	2.76	128.39	124.40
7	M	402	BCL	C3B-C4B-NB	2.71	113.33	109.76
15	M	409	CDL	OB8-CB7-OB9	-2.71	116.86	123.63
13	M	412	BPH	O2A-CGA-CBA	2.69	120.04	111.83
6	H	307	GGD	OC8-CC7-C31	2.68	120.01	111.83
13	M	412	BPH	O2A-CGA-O1A	-2.67	116.95	123.63
15	M	409	CDL	OB6-CB5-OB7	-2.65	117.50	123.70
13	M	412	BPH	O2A-C1-C2	2.65	118.30	108.11
7	L	301	BCL	C2B-C1B-NB	2.63	113.06	110.33
9	M	407	U10	C32-C33-C34	-2.63	121.60	127.62
7	L	301	BCL	CHD-C1D-ND	-2.62	121.11	124.80
14	M	408	SPO	C6-C7-C9	-2.62	114.89	119.01
11	L	309	HTO	C5-C4-C3	2.62	118.41	114.11
7	L	306	BCL	C2A-C1A-CHA	-2.61	119.33	123.87
9	L	305[A]	U10	O2-C2-C3	-2.59	115.55	121.03
7	L	306	BCL	C1D-CHD-C4C	-2.58	120.40	126.62
6	H	307	GGD	OA5-CA1-CA2	2.58	115.67	110.37
9	M	407	U10	C17-C18-C19	-2.57	121.73	127.62
7	M	401	BCL	CED-O2D-CGD	-2.55	110.13	115.92
15	M	409	CDL	CA6-OA8-CA7	2.53	126.38	117.12
6	H	307	GGD	OB5-CB5-CB6	2.52	112.70	106.44
14	M	408	SPO	C21-C22-C23	-2.52	123.74	127.28
16	M	410	PC1	O21-C2-C3	2.52	117.38	108.34
9	M	407	U10	C6-C1-C2	2.51	121.15	119.17
13	M	412	BPH	CBA-CAA-C2A	2.50	121.14	113.78
7	L	301	BCL	C1-O2A-CGA	2.50	122.69	116.65
7	M	401	BCL	C3D-C2D-C1D	-2.49	102.44	105.83
7	L	301	BCL	C4D-CHA-C1A	-2.48	118.28	121.24
9	L	305[A]	U10	C7-C6-C5	-2.47	115.65	118.52
9	M	407	U10	C35-C34-C36	2.46	119.50	115.23
9	L	305[B]	U10	C1-C6-C5	-2.45	117.24	119.62
7	M	401	BCL	CHB-C4A-NA	2.43	127.91	124.40
14	M	408	SPO	C40-C38-C37	-2.43	115.38	122.66
6	H	307	GGD	OA2-CA2-CA3	2.42	116.15	109.94
13	M	412	BPH	C7-C6-C5	2.41	119.69	113.26
7	L	301	BCL	O1D-CGD-CBD	-2.40	119.78	124.52
6	H	307	GGD	OC8-CC6-CC4	2.39	115.28	108.40
7	M	401	BCL	C3A-C2A-C1A	-2.38	97.77	101.34
13	M	406	BPH	C5-C3-C2	2.37	126.50	121.17
6	H	307	GGD	OB1-CA3-CA4	2.37	113.25	107.23
9	M	407	U10	C25-C24-C26	2.36	119.33	115.23
7	M	402	BCL	O2D-CGD-CBD	2.35	115.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	402	BCL	O2A-C1-C2	2.35	117.14	108.11
7	M	401	BCL	C2D-C1D-ND	2.34	112.44	110.13
9	L	305[A]	U10	C7-C8-C9	-2.34	122.80	126.83
9	M	407	U10	C41-C39-C40	2.34	119.97	114.59
7	L	301	BCL	C6-C5-C3	-2.33	107.79	113.47
6	H	307	GGD	OC6-CC5-OC7	-2.31	118.29	123.70
16	M	410	PC1	O21-C21-O22	-2.30	118.33	123.70
6	H	307	GGD	CB1-OB1-CA3	2.27	123.36	117.98
9	L	305[B]	U10	C15-C14-C13	-2.26	115.87	122.66
9	M	407	U10	C15-C14-C16	2.26	119.15	115.23
7	L	301	BCL	C16-C15-C13	-2.26	108.47	115.97
7	L	301	BCL	O2A-CGA-O1A	-2.25	117.99	123.63
13	M	412	BPH	CBC-CAC-C3C	-2.21	109.42	113.78
14	M	408	SPO	C13-C12-C11	2.21	121.46	118.09
9	M	407	U10	C10-C9-C11	2.21	119.06	115.23
7	L	301	BCL	CHC-C4B-NB	-2.20	120.75	124.05
7	L	306	BCL	CHC-C4B-C3B	-2.20	123.00	131.72
8	L	303	LDA	CM1-N1-C1	2.20	114.85	110.23
13	M	412	BPH	C1A-C2A-C3A	2.16	104.90	102.84
7	M	401	BCL	CMC-C2C-C3C	-2.16	105.64	113.98
7	L	301	BCL	CED-O2D-CGD	2.15	120.80	115.92
11	L	308	HTO	C1-C2-C3	2.12	117.33	113.00
7	M	402	BCL	CMC-C2C-C3C	-2.12	105.79	113.98
7	M	402	BCL	CHB-C1B-C2B	-2.10	121.33	127.43
13	M	412	BPH	C1-O2A-CGA	2.10	121.73	116.65
7	M	402	BCL	OBb-CAB-C3B	2.09	124.13	120.43
7	L	306	BCL	C3A-C2A-C1A	-2.07	98.23	101.34
4	H	306	GOL	O1-C1-C2	2.07	119.71	110.38
14	M	408	SPO	C26-C27-C28	-2.05	124.80	127.69
7	L	306	BCL	CMD-C2D-C3D	-2.05	122.99	127.69
9	M	407	U10	C1M-C1-C6	-2.05	121.09	124.45
14	M	408	SPO	C14-C15-C16	-2.04	117.28	123.20
8	M	403	LDA	O1-N1-C1	2.04	114.28	109.27
7	L	306	BCL	OBd-CAD-C3D	-2.03	123.67	128.42
7	M	401	BCL	CMA-C3A-C4A	-2.03	106.32	111.77
14	M	408	SPO	C13-C12-C14	-2.02	119.55	122.82
15	M	409	CDL	OB8-CB7-C71	2.00	117.95	111.83

There are no chirality outliers.

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	306	GOL	O1-C1-C2-O2
4	H	306	GOL	O1-C1-C2-C3
4	H	302	GOL	O1-C1-C2-O2
4	H	302	GOL	O1-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3
4	H	304	GOL	C1-C2-C3-O3
4	L	311	GOL	O1-C1-C2-C3
6	H	307	GGD	OC7-CC5-OC6-CC4
8	L	303	LDA	C2-C1-N1-O1
8	L	303	LDA	C2-C1-N1-CM1
8	L	303	LDA	C2-C1-N1-CM2
8	M	403	LDA	C2-C1-N1-O1
8	M	403	LDA	C2-C1-N1-CM1
8	M	403	LDA	C2-C1-N1-CM2
9	M	407	U10	C29-C31-C32-C33
11	L	308	HTO	C1-C2-C3-O3
11	L	308	HTO	O3-C3-C4-C5
11	L	309	HTO	C1-C2-C3-O3
11	L	309	HTO	C1-C2-C3-C4
11	L	309	HTO	O2-C2-C3-O3
11	L	309	HTO	O2-C2-C3-C4
13	M	406	BPH	C4C-C3C-CAC-CBC
13	M	406	BPH	C2C-C3C-CAC-CBC
13	M	412	BPH	C4C-C3C-CAC-CBC
13	M	412	BPH	C2C-C3C-CAC-CBC
13	M	412	BPH	C2-C1-O2A-CGA
13	M	412	BPH	C4-C3-C5-C6
13	M	412	BPH	C6-C7-C8-C9
14	M	408	SPO	O1-C1-C4-C5
14	M	408	SPO	C2-C1-C4-C5
14	M	408	SPO	C3-C1-C4-C5
15	M	409	CDL	CB2-OB2-PB2-OB3
15	M	409	CDL	CB2-OB2-PB2-OB5
15	M	409	CDL	CB3-OB5-PB2-OB2
15	M	409	CDL	CB3-OB5-PB2-OB3
15	M	409	CDL	CB3-OB5-PB2-OB4
16	M	410	PC1	C1-O11-P-O13
16	M	410	PC1	O13-C11-C12-N
6	H	307	GGD	CA2-CA3-OB1-CB1
15	M	409	CDL	OB9-CB7-OB8-CB6
6	H	307	GGD	C14-CC5-OC6-CC4
9	M	407	U10	C30-C29-C31-C32
13	M	412	BPH	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	M	401	BCL	C3-C5-C6-C7
6	H	307	GGD	C31-CC7-OC8-CC6
15	M	409	CDL	C71-CB7-OB8-CB6
6	H	307	GGD	OC9-CC7-OC8-CC6
15	M	409	CDL	OA9-CA7-OA8-CA6
15	M	409	CDL	O1-C1-CB2-OB2
15	M	409	CDL	C31-CA7-OA8-CA6
6	H	307	GGD	OA5-CA5-CA6-OA6
15	M	409	CDL	C11-CA5-OA6-CA4
9	M	407	U10	C28-C29-C31-C32
9	L	305[B]	U10	C9-C11-C12-C13
9	M	407	U10	C24-C26-C27-C28
9	M	407	U10	C34-C36-C37-C38
7	M	401	BCL	C11-C12-C13-C14
16	M	410	PC1	O22-C21-O21-C2
16	M	410	PC1	C22-C21-O21-C2
15	M	409	CDL	OA7-CA5-OA6-CA4
9	L	305[A]	U10	C9-C11-C12-C13
7	L	306	BCL	C15-C16-C17-C18
13	M	406	BPH	C5-C6-C7-C8
7	M	401	BCL	C13-C15-C16-C17
13	M	406	BPH	C10-C11-C12-C13
6	H	307	GGD	CC5-C14-C15-C16
7	M	401	BCL	C8-C10-C11-C12
16	M	410	PC1	C31-C32-C33-C34
7	L	301	BCL	C13-C15-C16-C17
6	H	307	GGD	CA4-CA5-CA6-OA6
8	L	302	LDA	C7-C8-C9-C10
4	L	310	GOL	O1-C1-C2-C3
4	L	311	GOL	C1-C2-C3-O3
16	M	410	PC1	C3-C2-O21-C21
7	M	401	BCL	C16-C17-C18-C20
15	M	409	CDL	C80-C81-C82-C83
15	M	409	CDL	C71-C72-C73-C74
4	H	303	GOL	O2-C2-C3-O3
15	M	409	CDL	C53-C54-C55-C56
8	L	304	LDA	C5-C6-C7-C8
16	M	410	PC1	C2A-C2B-C2C-C2D
15	M	409	CDL	C11-C12-C13-C14
15	M	409	CDL	CA2-C1-CB2-OB2
15	M	409	CDL	C38-C39-C40-C41
15	M	409	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
15	M	409	CDL	C20-C21-C22-C23
8	L	303	LDA	C1-C2-C3-C4
16	M	410	PC1	C22-C23-C24-C25
8	M	404	LDA	C1-C2-C3-C4
6	H	307	GGD	C34-C35-C36-C37
13	M	412	BPH	C3-C5-C6-C7
8	M	404	LDA	C4-C5-C6-C7
15	M	409	CDL	C16-C17-C18-C19
8	M	403	LDA	C2-C3-C4-C5
13	M	412	BPH	C13-C15-C16-C17
8	L	302	LDA	C6-C7-C8-C9
15	M	409	CDL	C14-C15-C16-C17
6	H	307	GGD	CC7-C31-C32-C33
8	L	302	LDA	C3-C4-C5-C6
6	H	307	GGD	C40-C41-C42-C43
13	M	412	BPH	C5-C6-C7-C8
16	M	410	PC1	C28-C29-C2A-C2B
15	M	409	CDL	C52-C53-C54-C55
8	L	302	LDA	C1-C2-C3-C4
8	L	303	LDA	C4-C5-C6-C7
8	L	304	LDA	C4-C5-C6-C7
4	L	311	GOL	O1-C1-C2-O2
4	L	311	GOL	O2-C2-C3-O3
6	H	307	GGD	C31-C32-C33-C34
15	M	409	CDL	C15-C16-C17-C18
7	M	401	BCL	C10-C11-C12-C13
8	L	302	LDA	C4-C5-C6-C7
11	L	308	HTO	O2-C2-C3-O3
15	M	409	CDL	CB7-C71-C72-C73
7	M	401	BCL	O2A-C1-C2-C3
15	M	409	CDL	C12-C13-C14-C15
15	M	409	CDL	C78-C79-C80-C81
8	L	304	LDA	C9-C10-C11-C12
15	M	409	CDL	C13-C14-C15-C16
8	L	304	LDA	C1-C2-C3-C4
15	M	409	CDL	C31-C32-C33-C34
16	M	410	PC1	C27-C28-C29-C2A
13	M	406	BPH	C13-C15-C16-C17
16	M	410	PC1	C2-C1-O11-P
7	M	402	BCL	C15-C16-C17-C18
8	M	404	LDA	C9-C10-C11-C12
16	M	410	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
15	M	409	CDL	CA5-C11-C12-C13
15	M	409	CDL	CB3-CB4-CB6-OB8
15	M	409	CDL	OB5-CB3-CB4-OB6
6	H	307	GGD	C38-C39-C40-C41
15	M	409	CDL	C39-C40-C41-C42
6	H	307	GGD	C17-C18-C19-C20
16	M	410	PC1	C2B-C2C-C2D-C2E
8	M	404	LDA	C6-C7-C8-C9
7	M	401	BCL	C4C-C3C-CAC-CBC
8	L	303	LDA	C2-C3-C4-C5
4	H	301	GOL	O2-C2-C3-O3
7	M	401	BCL	C16-C17-C18-C19
16	M	410	PC1	O11-C1-C2-C3
8	M	403	LDA	C11-C10-C9-C8
14	M	408	SPO	C1-C4-C5-C6
15	M	409	CDL	CA3-CA4-CA6-OA8
6	H	307	GGD	OC6-CC4-CC6-OC8
7	L	306	BCL	C16-C17-C18-C20
8	L	304	LDA	C2-C1-N1-CM1
6	H	307	GGD	C41-C42-C43-C44
15	M	409	CDL	O1-C1-CA2-OA2
13	M	406	BPH	CBA-CGA-O2A-C1
8	M	404	LDA	C7-C8-C9-C10
15	M	409	CDL	OA6-CA4-CA6-OA8
6	H	307	GGD	CC3-CC4-CC6-OC8
9	M	407	U10	C31-C32-C33-C34
13	M	406	BPH	O1A-CGA-O2A-C1
7	L	301	BCL	CHA-CBD-CGD-O1D
7	L	301	BCL	CHA-CBD-CGD-O2D
15	M	409	CDL	CB2-OB2-PB2-OB4
16	M	410	PC1	C11-O13-P-O14
16	M	410	PC1	C1-O11-P-O14
15	M	409	CDL	OB5-CB3-CB4-CB6
13	M	406	BPH	C11-C12-C13-C14
9	M	407	U10	C25-C24-C26-C27
8	L	304	LDA	N1-C1-C2-C3
8	M	403	LDA	N1-C1-C2-C3
11	L	309	HTO	C3-C4-C5-C6
11	L	308	HTO	C4-C5-C6-C7
4	L	310	GOL	O2-C2-C3-O3
16	M	410	PC1	C32-C33-C34-C35
7	M	401	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	M	409	CDL	C40-C41-C42-C43
6	H	307	GGD	CB2-CB1-OB1-CA3
7	L	301	BCL	C3-C5-C6-C7
4	H	304	GOL	O2-C2-C3-O3
7	M	401	BCL	C12-C13-C15-C16
13	M	406	BPH	C11-C12-C13-C15
15	M	409	CDL	OB6-CB4-CB6-OB8
11	L	308	HTO	C2-C3-C4-C5
9	M	407	U10	C23-C24-C26-C27
15	M	409	CDL	C17-C18-C19-C20
8	L	303	LDA	C5-C6-C7-C8
6	H	307	GGD	OB5-CB1-OB1-CA3
9	M	407	U10	C5-C4-O4-C4M
9	L	305[B]	U10	C3-C4-O4-C4M
7	M	402	BCL	CAA-CBA-CGA-O2A
4	H	301	GOL	C1-C2-C3-O3
4	L	310	GOL	C1-C2-C3-O3
4	L	310	GOL	O1-C1-C2-O2
8	L	304	LDA	C2-C3-C4-C5
8	M	403	LDA	C7-C8-C9-C10
16	M	410	PC1	C36-C37-C38-C39
16	M	410	PC1	C11-C12-N-C14
13	M	406	BPH	C16-C17-C18-C20
15	M	409	CDL	C79-C80-C81-C82
8	M	404	LDA	C2-C1-N1-CM1
8	M	404	LDA	C2-C1-N1-CM2
7	L	306	BCL	C16-C17-C18-C19
15	M	409	CDL	C12-C11-CA5-OA6
16	M	410	PC1	C11-C12-N-C13
15	M	409	CDL	C41-C42-C43-C44
15	M	409	CDL	C81-C82-C83-C84
8	L	304	LDA	C11-C10-C9-C8
15	M	409	CDL	C72-C71-CB7-OB8
7	L	301	BCL	C12-C13-C15-C16
13	M	406	BPH	C12-C13-C15-C16
16	M	410	PC1	C11-C12-N-C15
9	L	305[B]	U10	C6-C7-C8-C9
15	M	409	CDL	C12-C11-CA5-OA7
11	L	308	HTO	C1-C2-C3-C4
16	M	410	PC1	O31-C31-C32-C33
6	H	307	GGD	C20-C21-C22-C23
15	M	409	CDL	C72-C71-CB7-OB9

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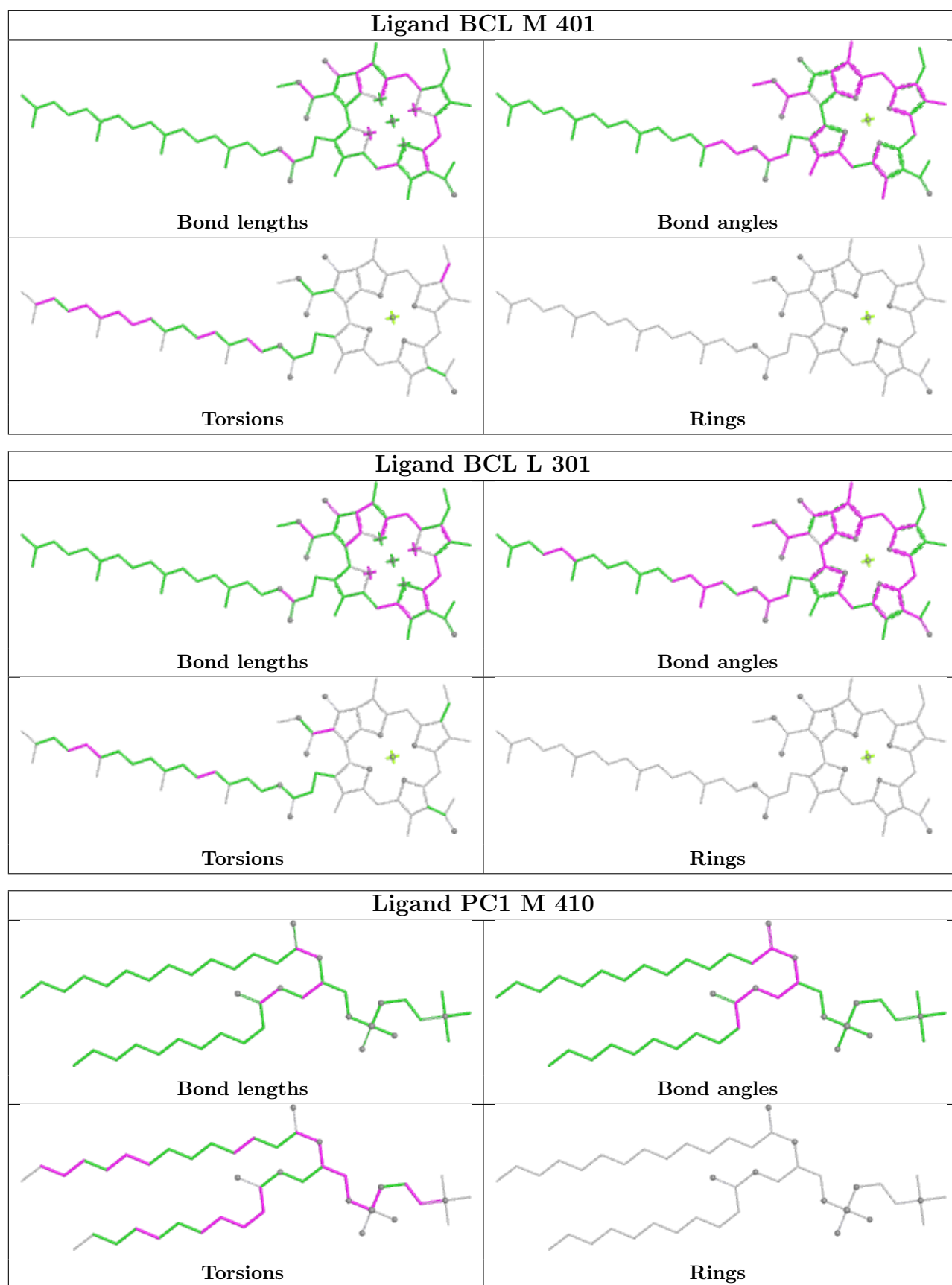
Mol	Chain	Res	Type	Atoms
13	M	406	BPH	C2-C1-O2A-CGA
16	M	410	PC1	O32-C31-C32-C33
9	L	305[B]	U10	C5-C4-O4-C4M

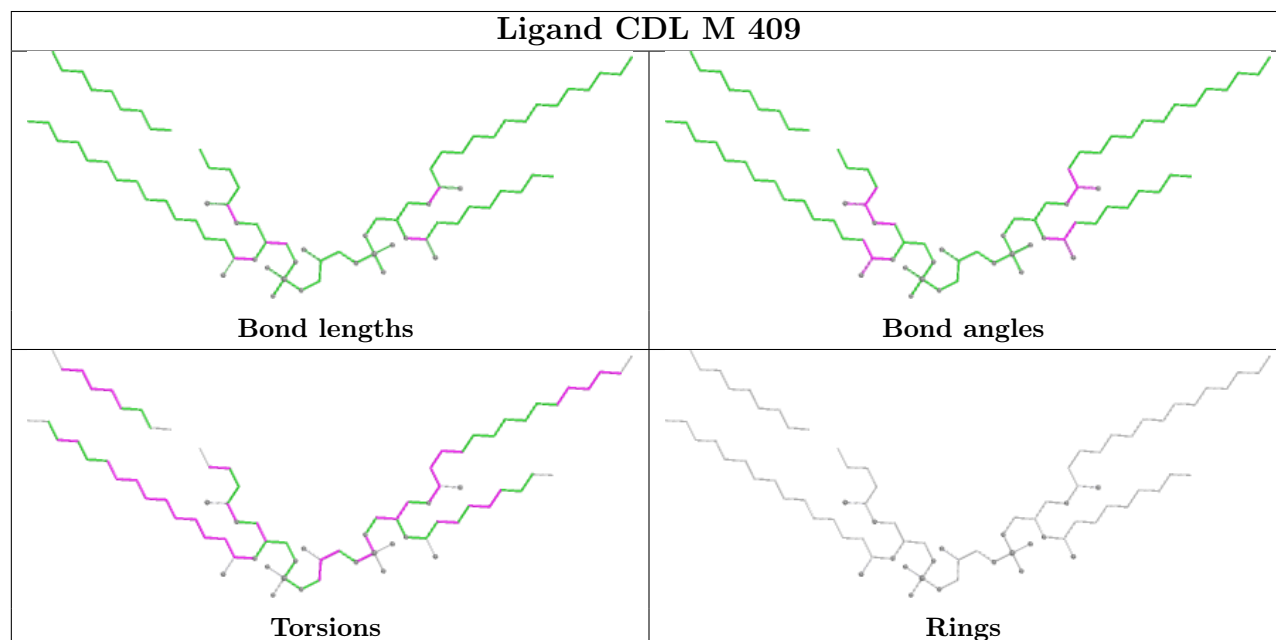
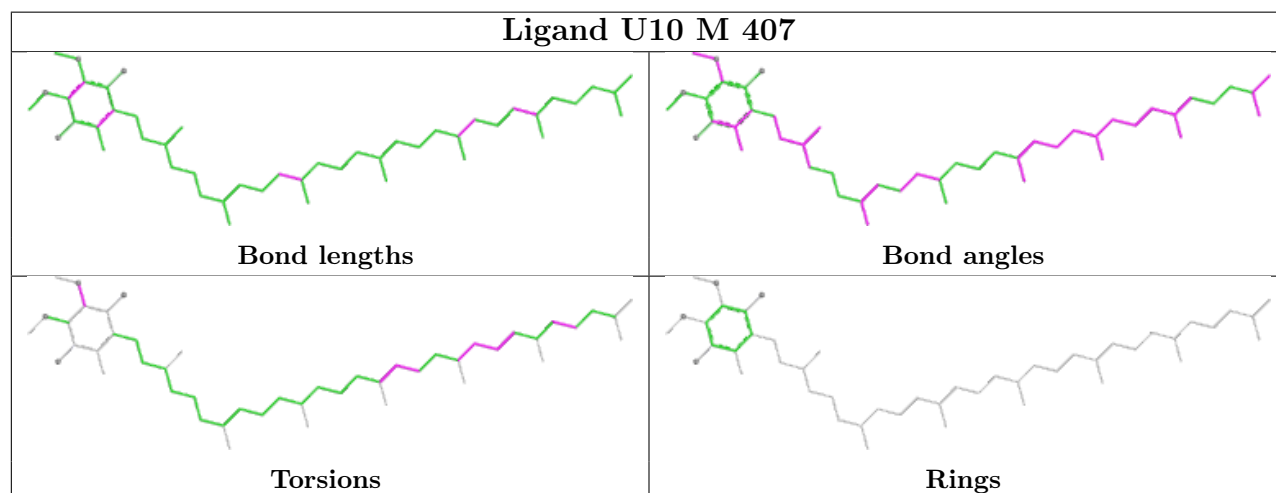
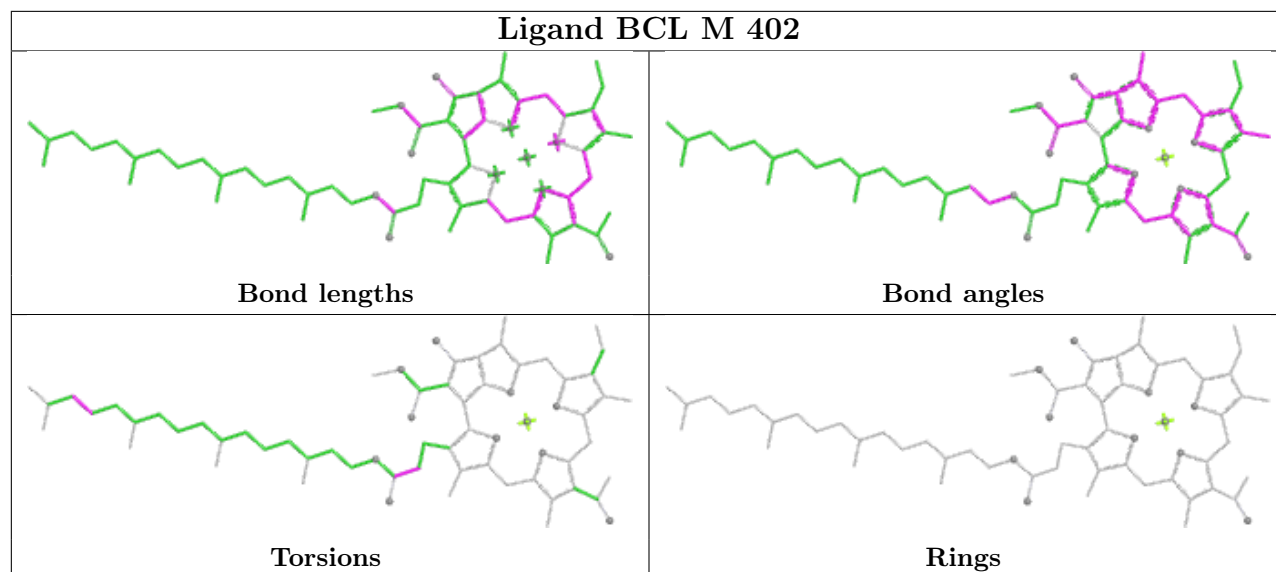
There are no ring outliers.

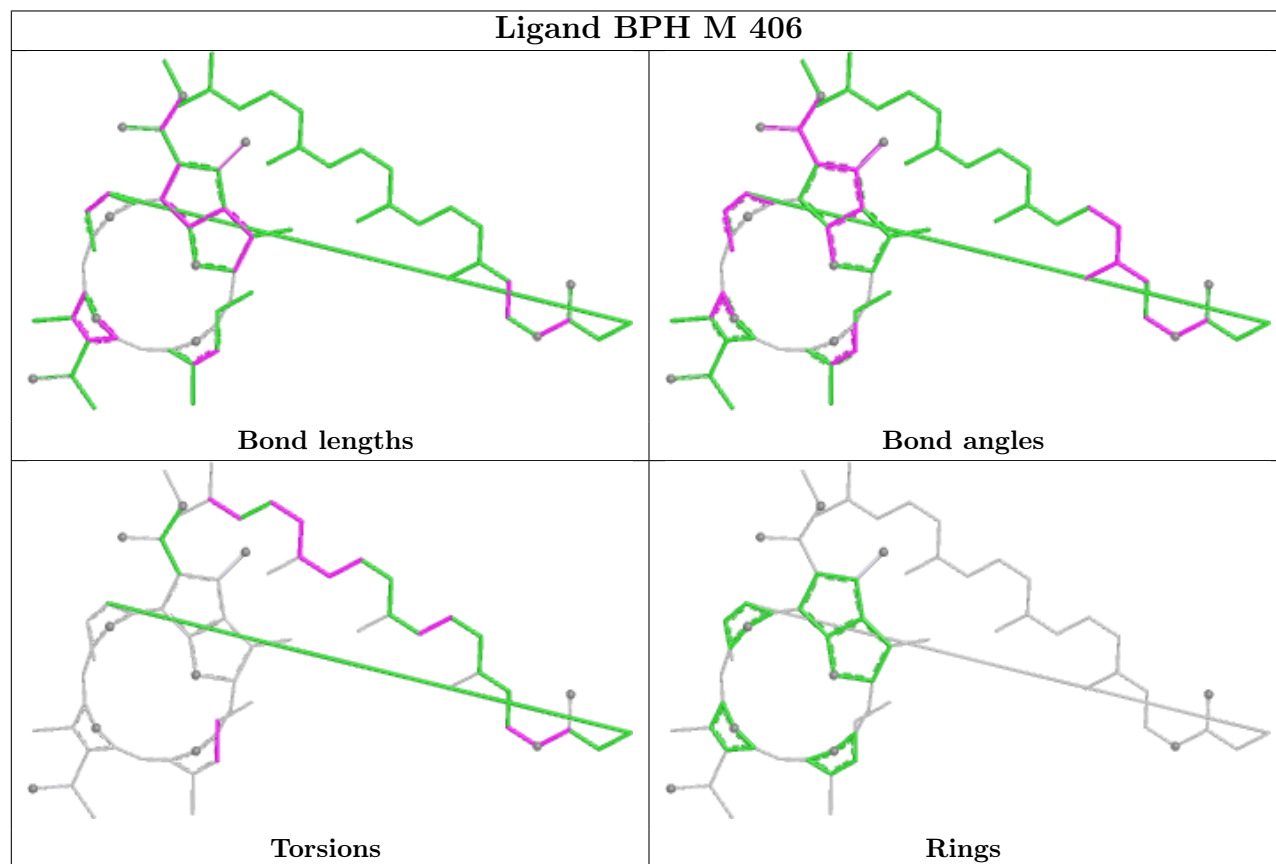
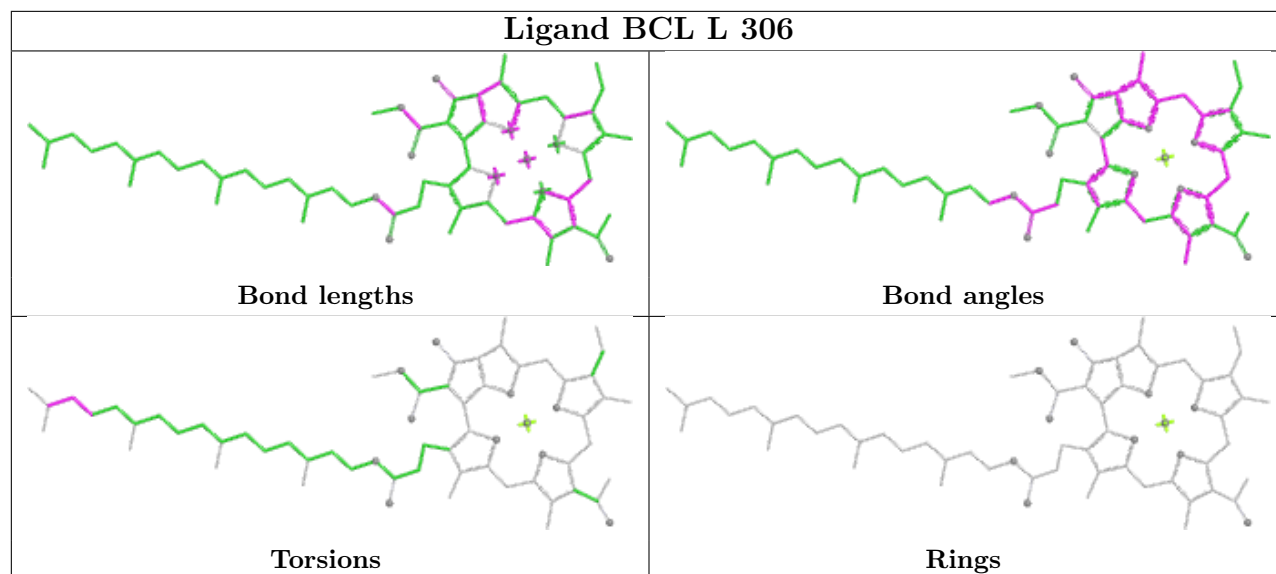
16 monomers are involved in 52 short contacts:

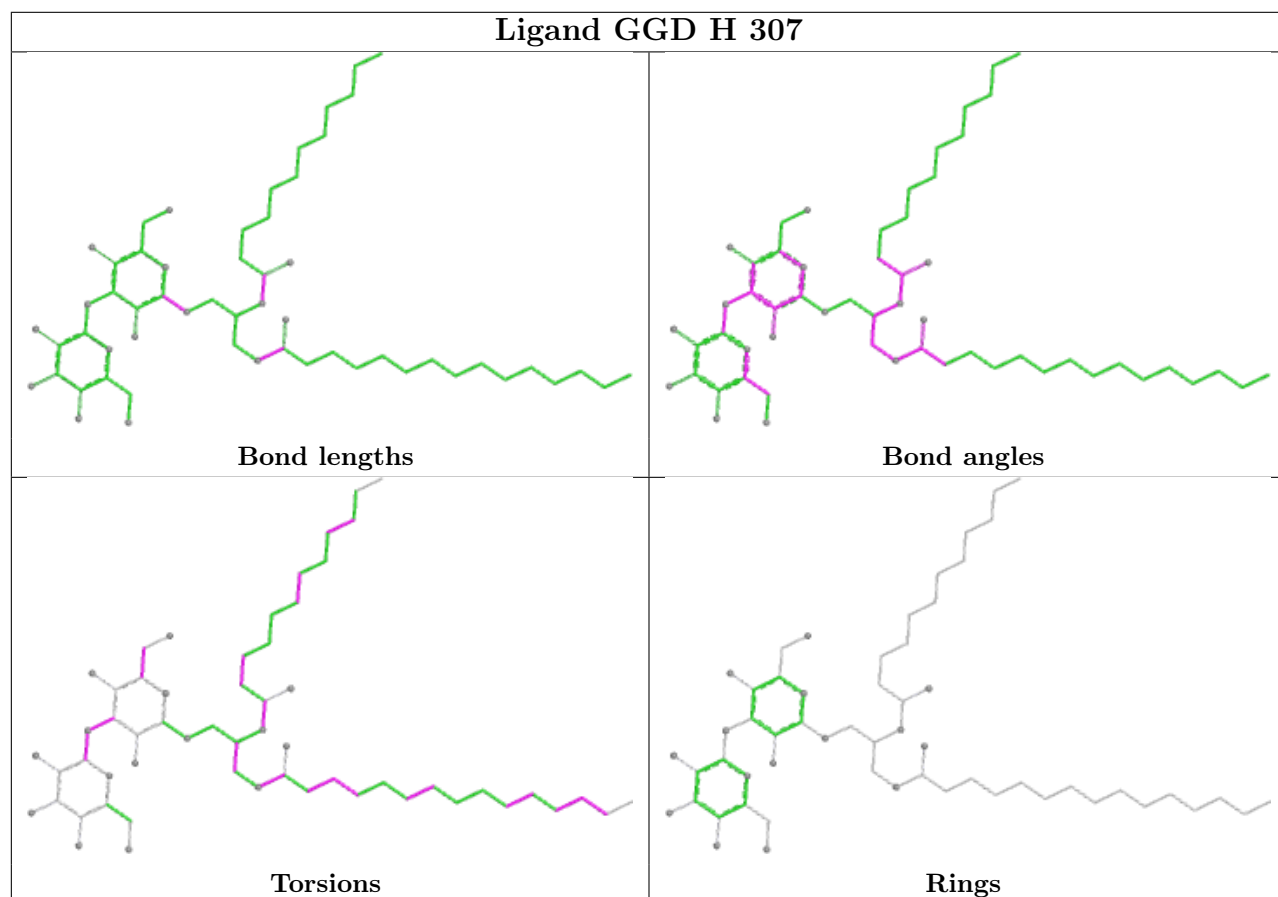
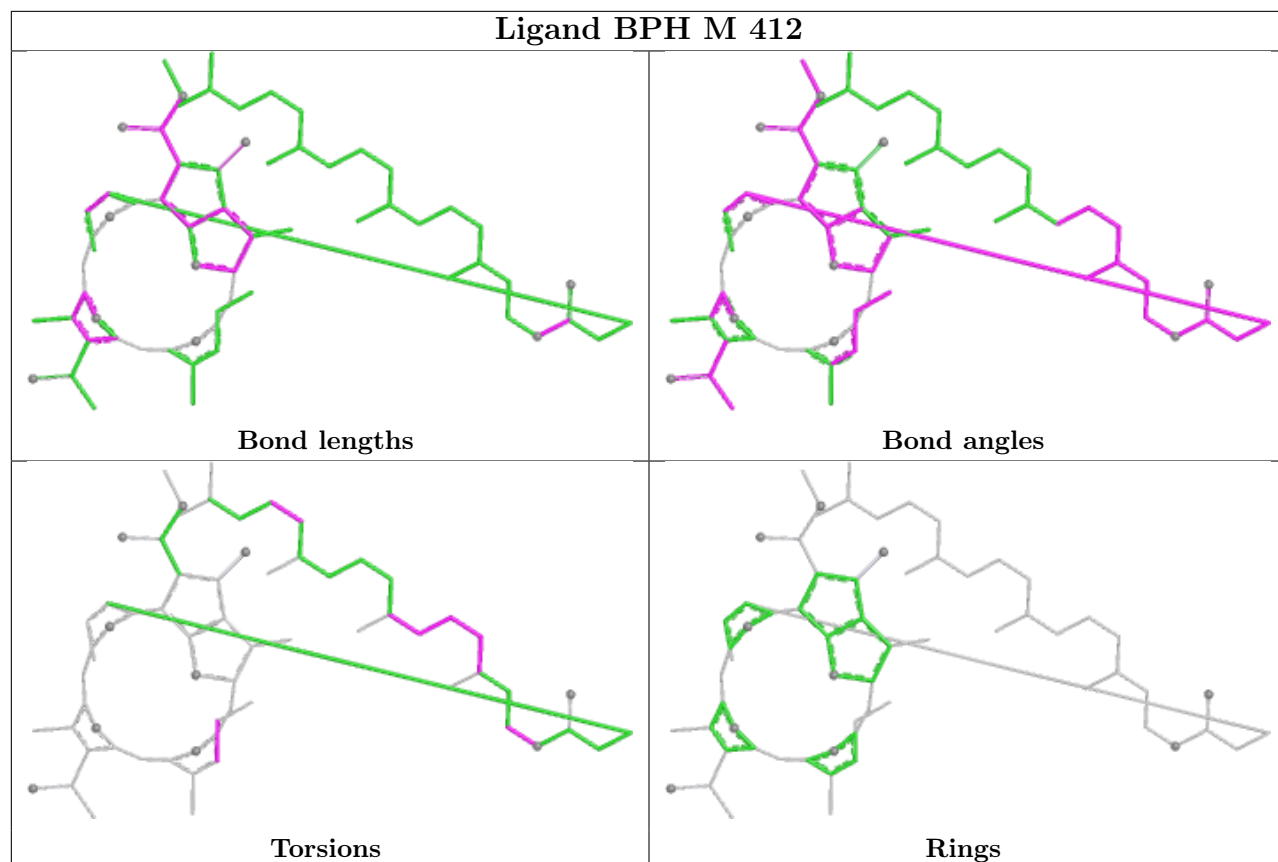
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	401	BCL	6	0
4	L	311	GOL	1	0
7	L	301	BCL	7	0
16	M	410	PC1	1	0
7	M	402	BCL	9	0
9	M	407	U10	2	0
15	M	409	CDL	1	0
8	M	404	LDA	2	0
7	L	306	BCL	6	0
13	M	406	BPH	5	0
8	M	403	LDA	2	0
13	M	412	BPH	12	0
6	H	307	GGD	3	0
14	M	408	SPO	3	0
9	L	305[B]	U10	4	0
10	L	307	PO4	1	0

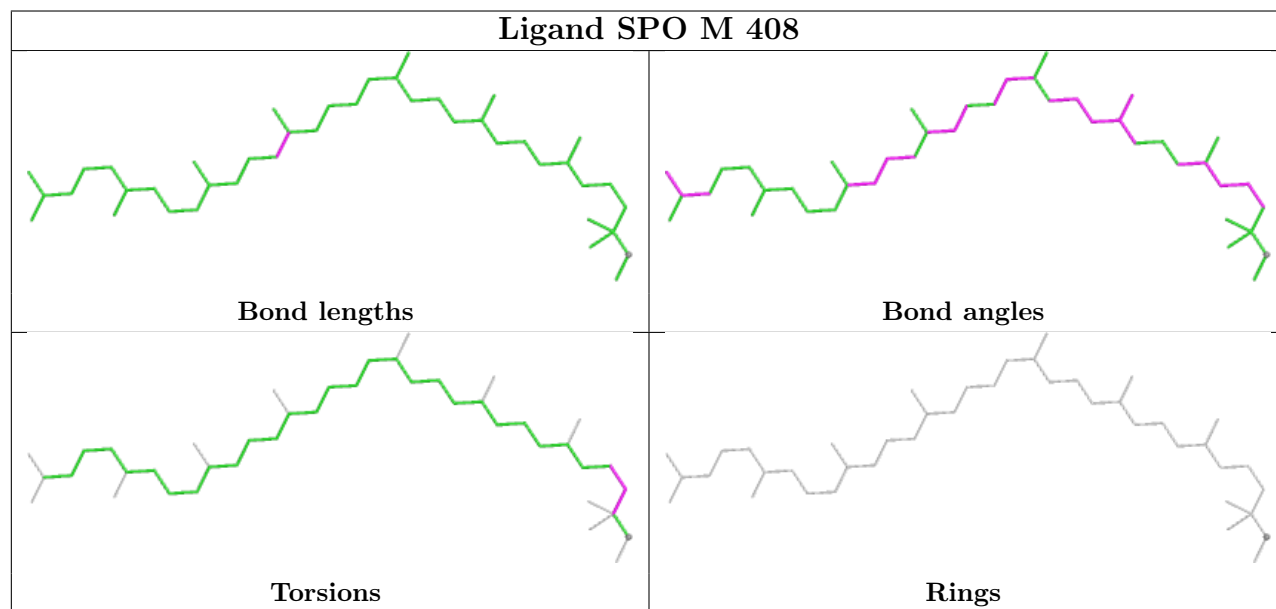
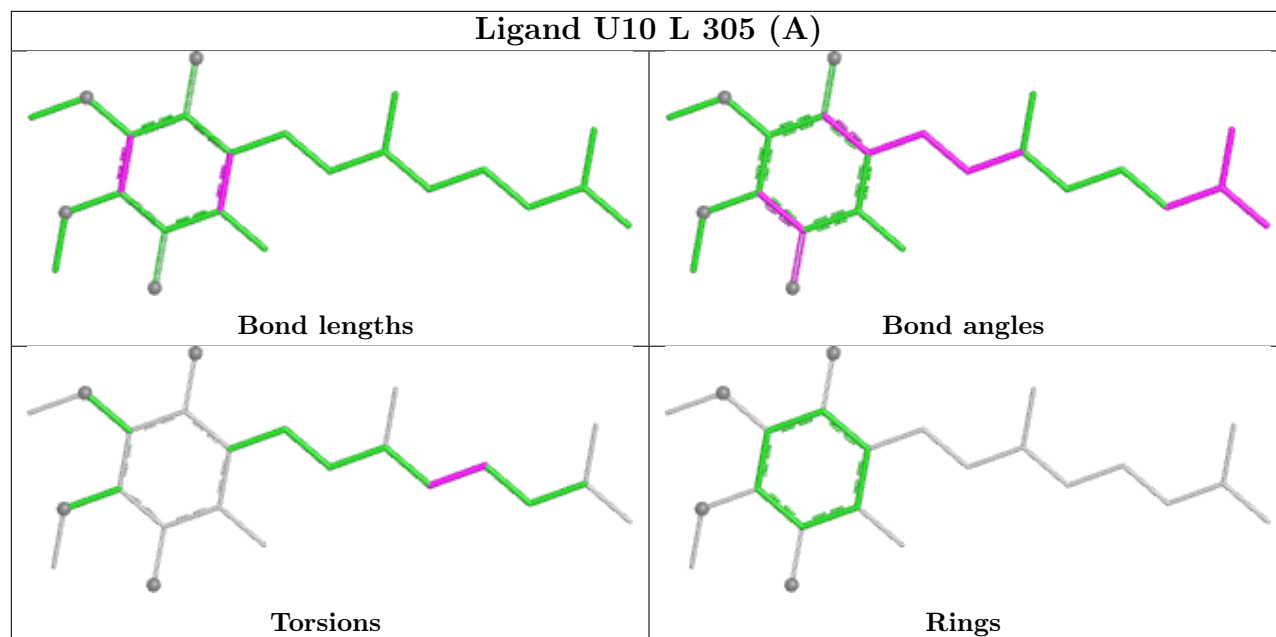
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

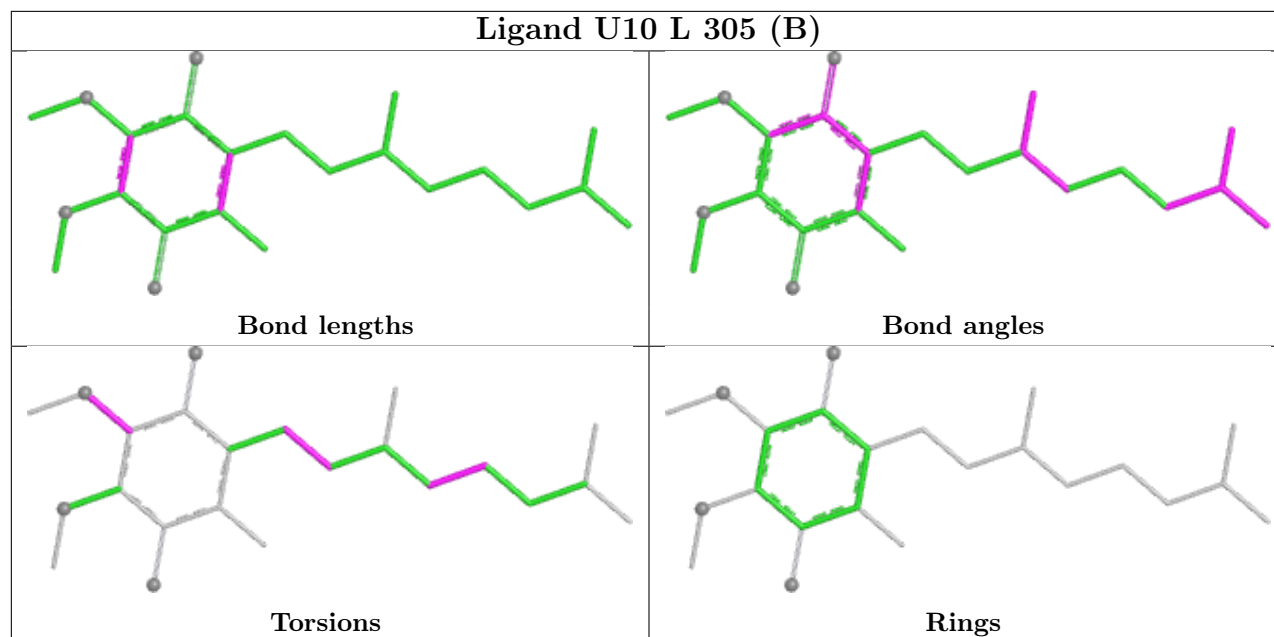












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	H	240/266 (90%)	-0.36	8 (3%)	49	40	22, 43, 61, 133	8 (3%)
2	L	281/282 (99%)	-0.41	0	100	100	30, 41, 64, 89	2 (0%)
3	M	302/307 (98%)	-0.36	5 (1%)	69	63	28, 44, 65, 99	7 (2%)
All	All	823/855 (96%)	-0.38	13 (1%)	70	64	22, 43, 64, 133	17 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	18.0
3	M	2	GLU	6.0
3	M	301	HIS	5.5
1	H	247	LYS	3.9
1	H	249[A]	LYS	3.1
1	H	250	SER	3.1
1	H	184	LYS	2.7
3	M	52	LEU	2.6
1	H	246	PRO	2.6
3	M	3	TYR	2.5
1	H	220[A]	LYS	2.1
1	H	197	LYS	2.1
1	H	94	GLU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

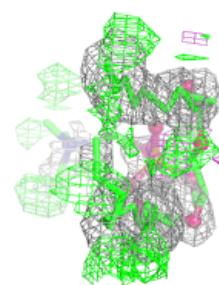
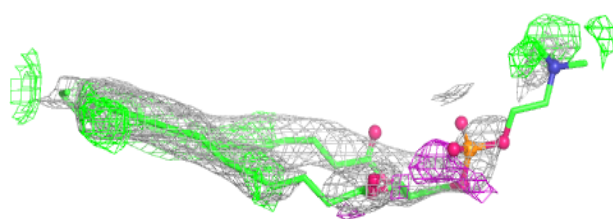
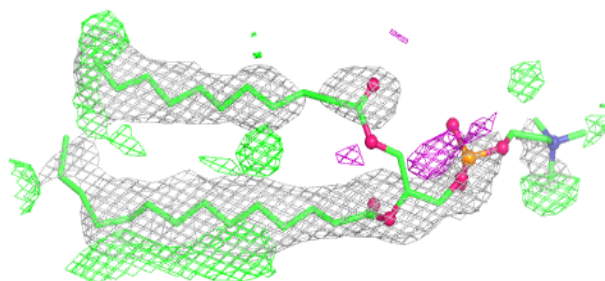
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	HTO	L	309	10/10	0.65	0.31	72,96,120,121	0
8	LDA	L	302	16/16	0.73	0.38	47,125,153,155	0
16	PC1	M	410	43/54	0.73	0.38	61,99,145,170	0
4	GOL	H	306	6/6	0.77	0.21	69,76,89,90	0
8	LDA	L	303	16/16	0.83	0.33	80,90,108,114	0
6	GGD	H	307	57/67	0.85	0.23	51,108,185,203	0
15	CDL	M	409	81/100	0.87	0.26	53,96,139,153	0
8	LDA	L	304	16/16	0.88	0.24	71,98,123,128	0
11	HTO	L	308	10/10	0.90	0.22	66,87,102,105	0
4	GOL	H	303	6/6	0.90	0.13	85,89,92,95	0
4	GOL	L	310	6/6	0.91	0.15	73,81,85,86	0
8	LDA	M	404	16/16	0.91	0.18	59,69,92,96	0
4	GOL	L	311	6/6	0.92	0.12	83,88,91,94	0
4	GOL	H	302	6/6	0.93	0.15	81,82,85,90	0
9	U10	L	305[A]	23/63	0.93	0.13	33,37,65,71	23
9	U10	L	305[B]	23/63	0.93	0.13	35,50,60,62	23
9	U10	M	407	48/63	0.93	0.15	33,46,91,110	0
4	GOL	H	301	6/6	0.94	0.13	59,65,69,80	0
4	GOL	H	304	6/6	0.94	0.13	40,52,63,71	0
7	BCL	M	401	66/66	0.95	0.11	28,38,95,105	0
13	BPH	M	406	65/65	0.95	0.13	35,47,119,134	0
13	BPH	M	412	65/65	0.96	0.09	30,39,48,57	0
14	SPO	M	408	42/42	0.96	0.12	33,47,80,92	0
8	LDA	M	403	16/16	0.96	0.12	52,68,77,78	0
7	BCL	L	301	66/66	0.96	0.10	26,34,56,61	0
10	PO4	L	307	5/5	0.97	0.10	60,62,66,67	0
7	BCL	L	306	66/66	0.97	0.07	28,39,49,65	0
5	K	H	305	1/1	0.98	0.04	50,50,50,50	0
7	BCL	M	402	66/66	0.98	0.08	33,40,51,75	0
17	MG	M	411	1/1	0.99	0.03	39,39,39,39	0
12	FE	M	405	1/1	1.00	0.02	36,36,36,36	0

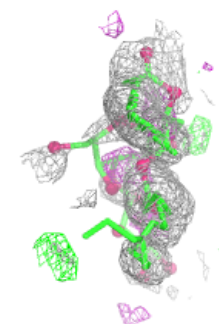
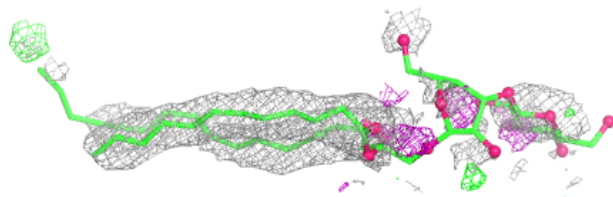
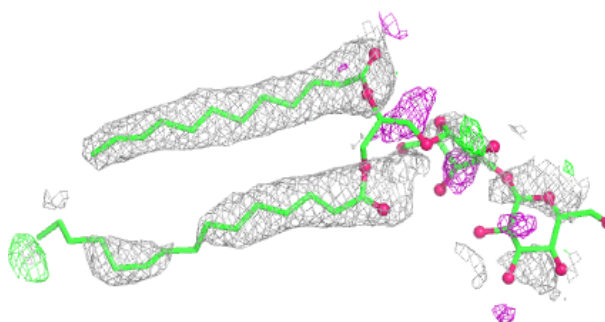
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 M 410:

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

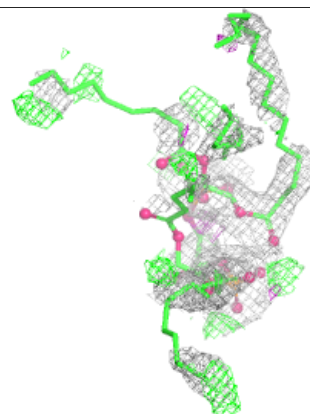
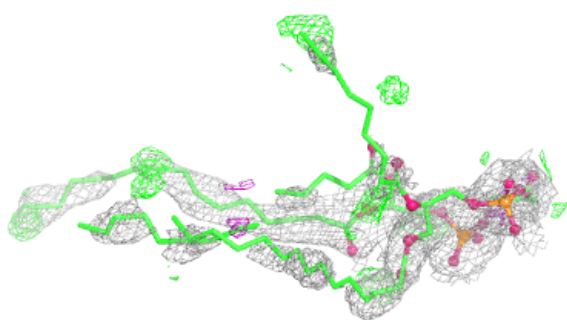
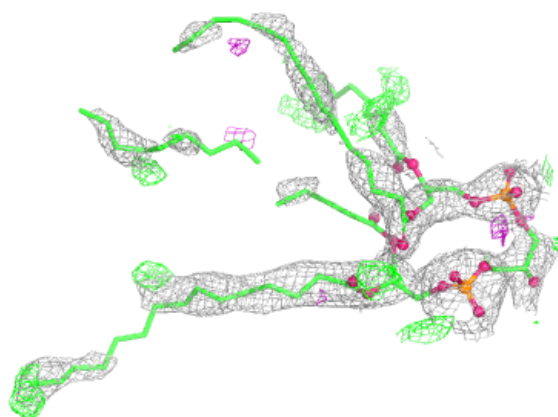
**Electron density around GGD H 307:**

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

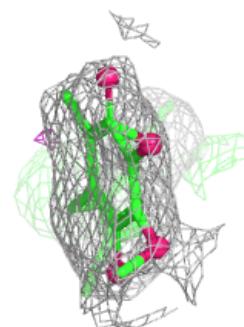
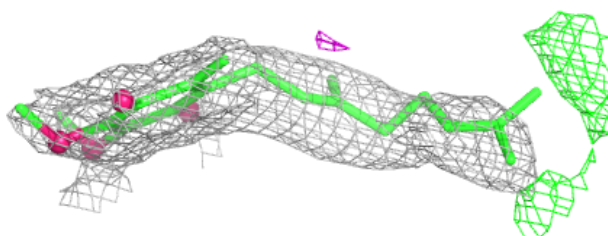


Electron density around CDL M 409:

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

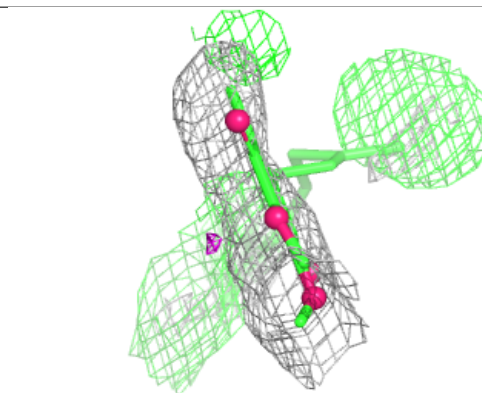
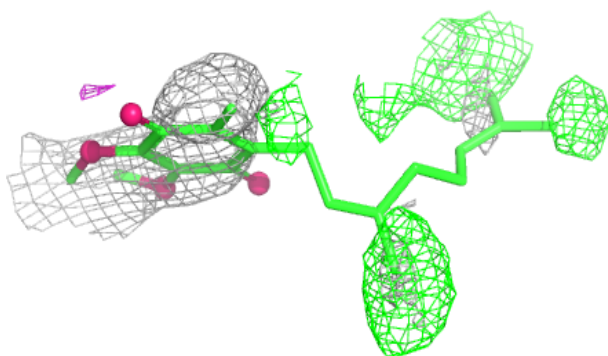
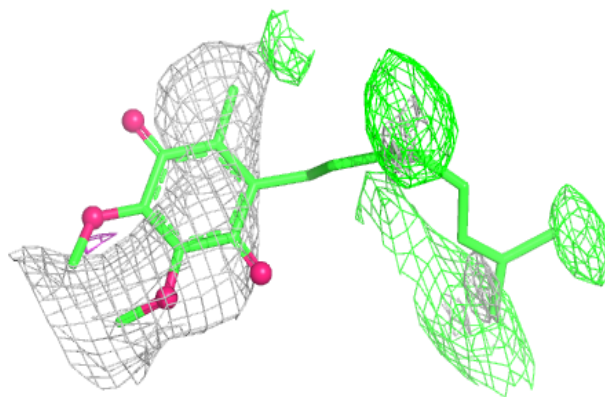
**Electron density around U10 L 305 (A):**

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

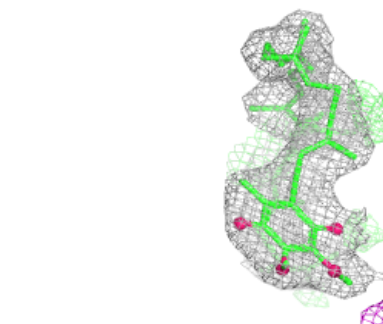
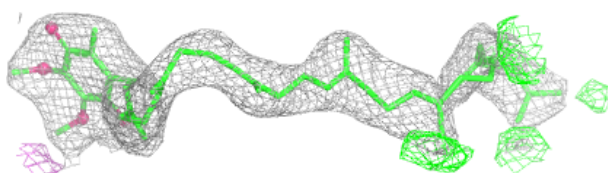
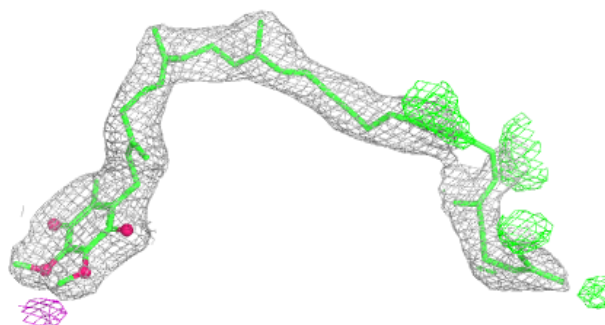


Electron density around U10 L 305 (B):

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

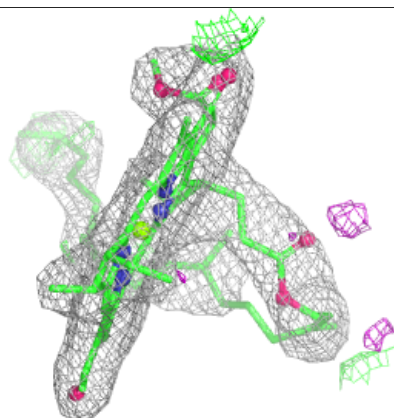
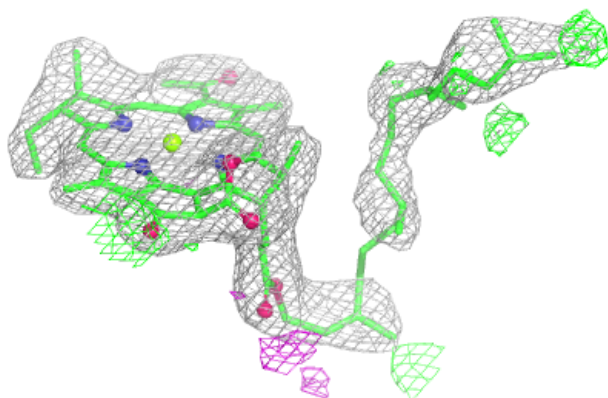
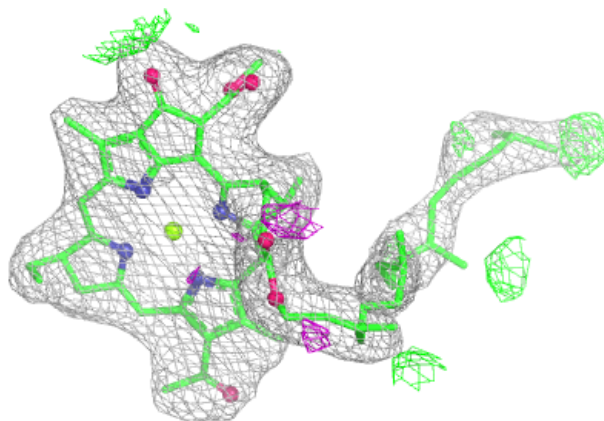
**Electron density around U10 M 407:**

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

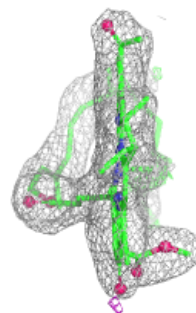
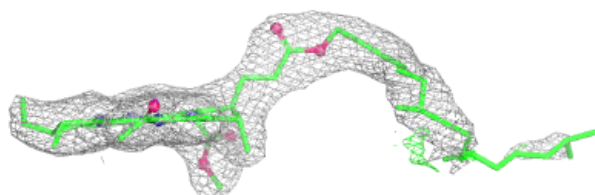
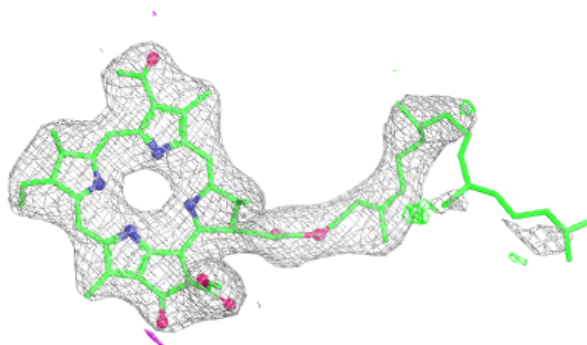


Electron density around BCL M 401:

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

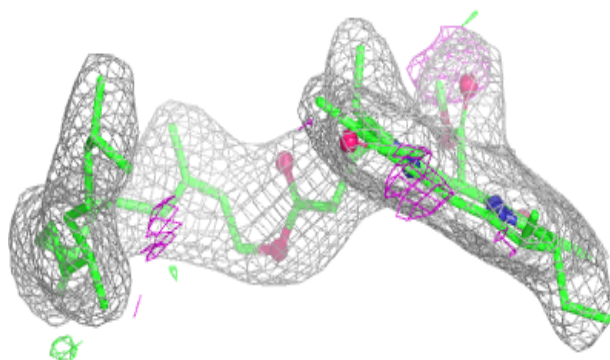
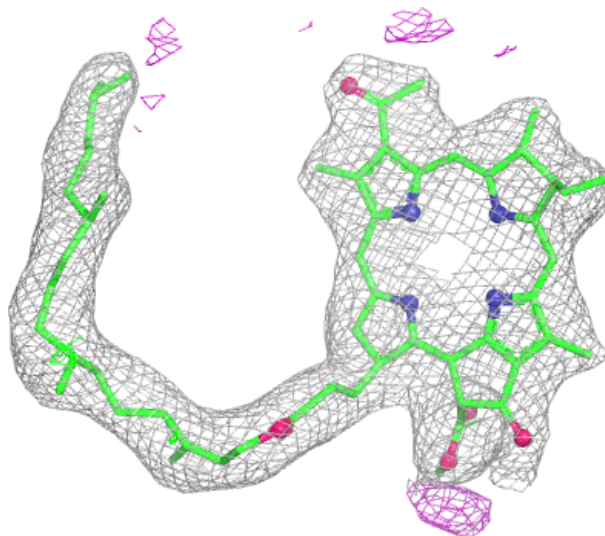
**Electron density around BPH M 406:**

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



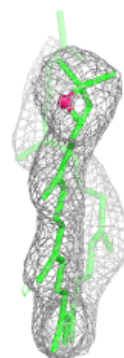
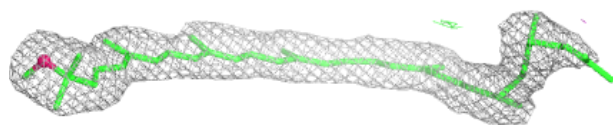
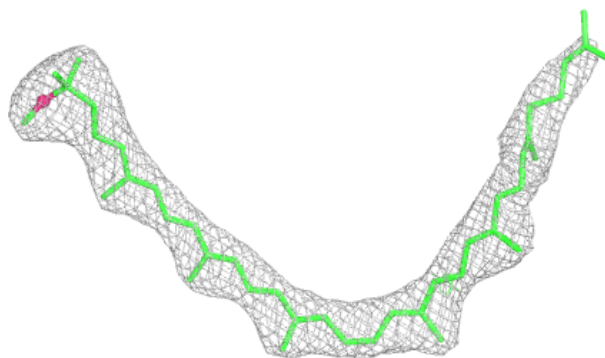
Electron density around BPH M 412:

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

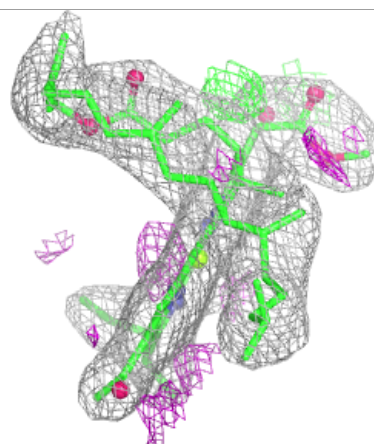
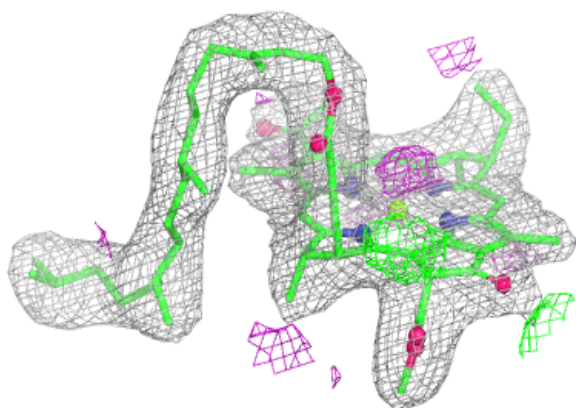
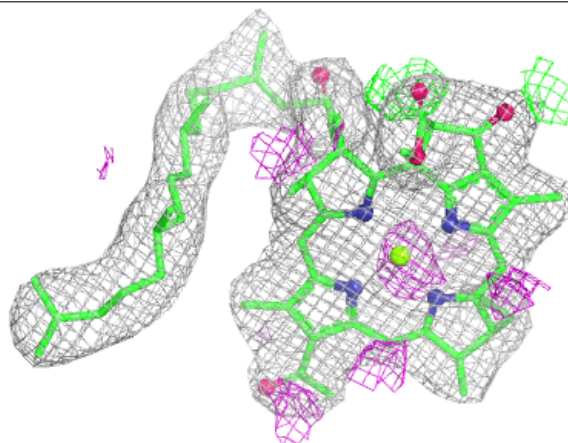


Electron density around SPO M 408:

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

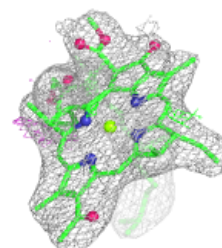
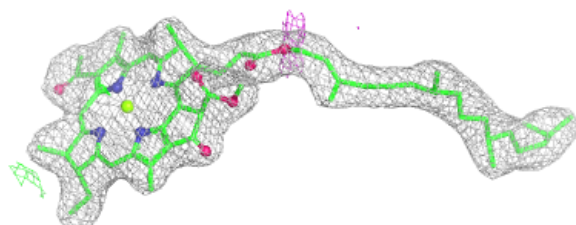
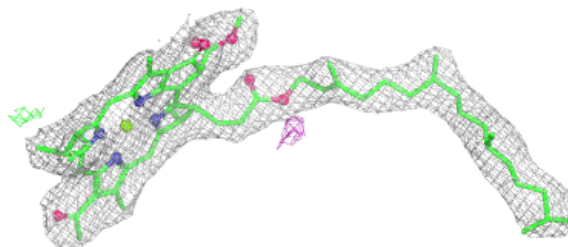
**Electron density around BCL L 301:**

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

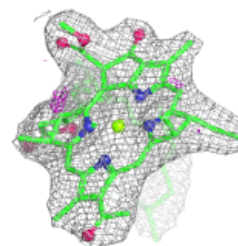
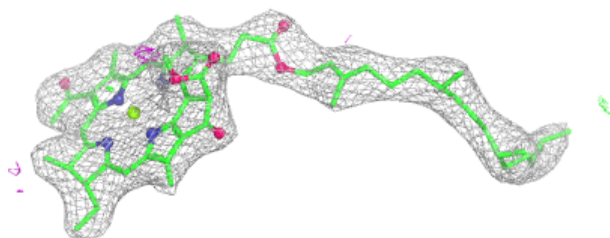
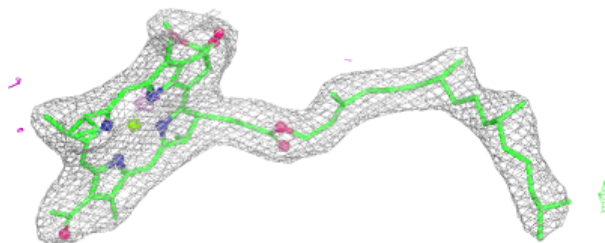


Electron density around BCL L 306:

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

**Electron density around BCL M 402:**

$2mF_o-DF_c$ (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.