



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:55 PM EDT

PDB ID : 4IN5 / pdb_00004in5
Title : (M)L214G mutant of the Rhodobacter sphaeroides Reaction Center
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.; Beatty, J.T.
Deposited on : 2013-01-04
Resolution : 2.20 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

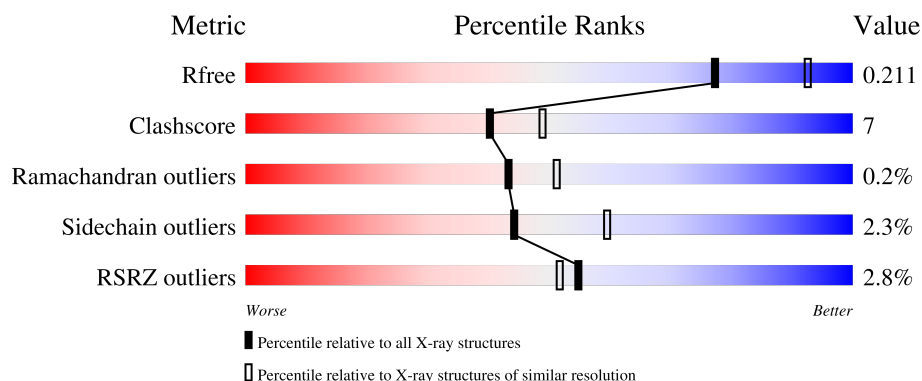
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

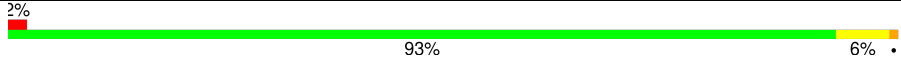
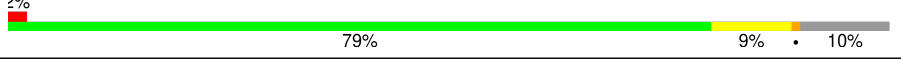
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	L	282	
2	M	307	
3	H	266	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	H	301	-	-	X	-
10	GOL	L	314	-	-	X	-
13	PC1	M	408	-	-	-	X
8	PO4	M	411	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7489 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	2	0
			2242	1515	356	363	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	1	0
			2407	1604	395	398	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	214	GLY	LEU	engineered mutation	UNP P0C0Y9

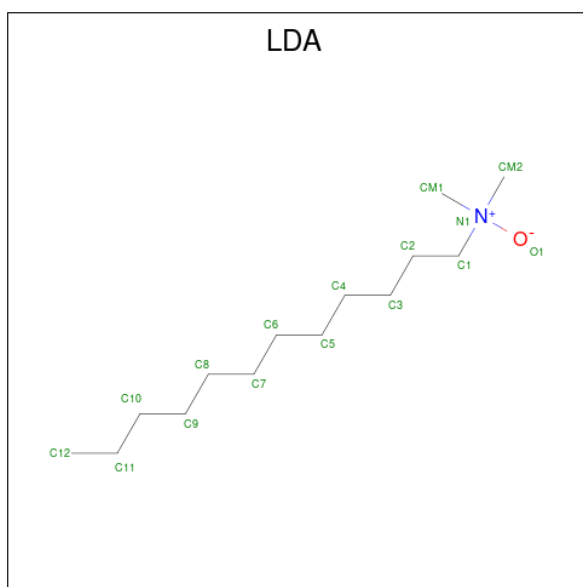
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	5	0
			1850	1184	320	337	9			

There are 6 discrepancies between the modelled and reference sequences:

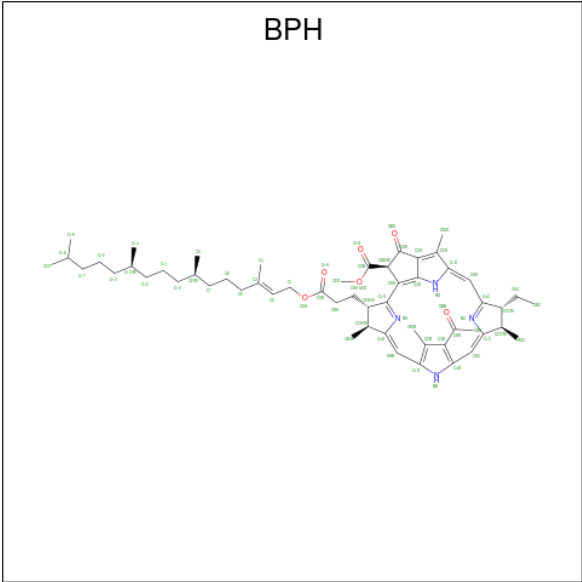
Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP P0C0Y7
H	-4	HIS	-	expression tag	UNP P0C0Y7
H	-3	HIS	-	expression tag	UNP P0C0Y7
H	-2	HIS	-	expression tag	UNP P0C0Y7
H	-1	HIS	-	expression tag	UNP P0C0Y7
H	0	HIS	-	expression tag	UNP P0C0Y7

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



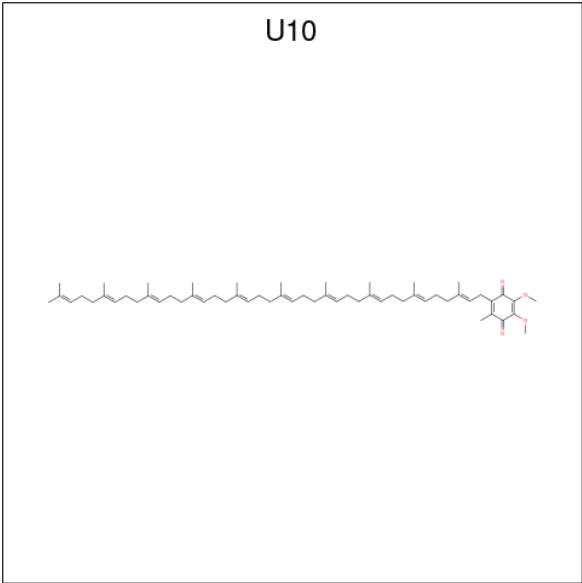
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			16	14	1	1		
4	L	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: 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	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



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

- # BCL

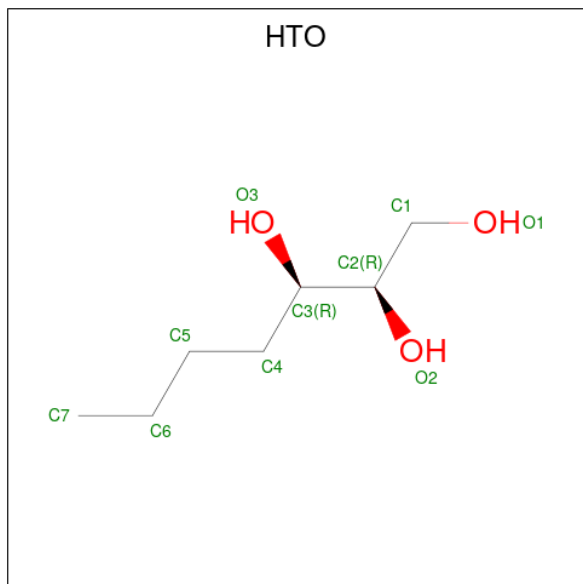
Diagram illustrating the Lewis structure of the phosphate ion (PO_4^{3-}). The central phosphorus atom (P) is bonded to four oxygen atoms (O). The bonds are as follows:

- Double bond to the right oxygen (O1).
- Single bond to the top oxygen (O3).
- Single bond to the bottom oxygen (O4).
- Single bond to the left oxygen (O2).

Each oxygen atom has a negative charge (O^-), and the phosphorus atom has a positive charge (P^+).

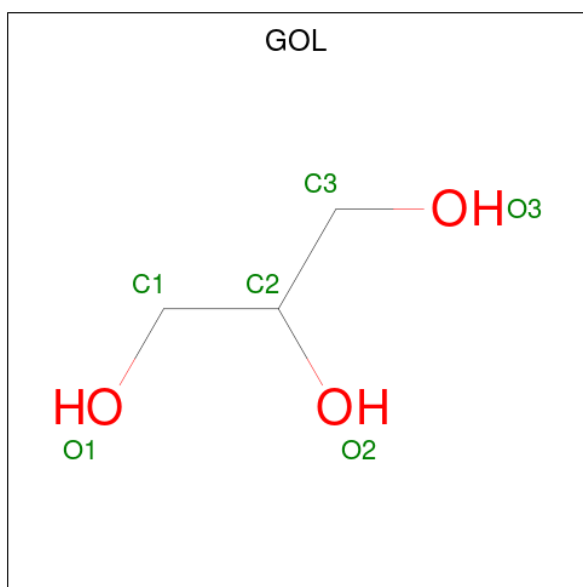
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

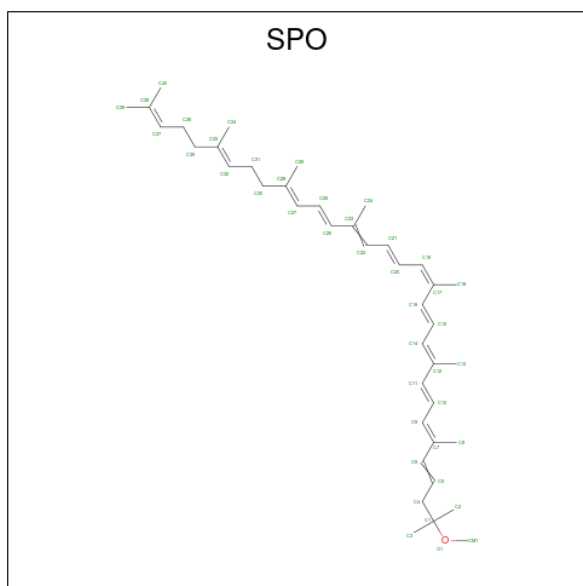


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10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

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

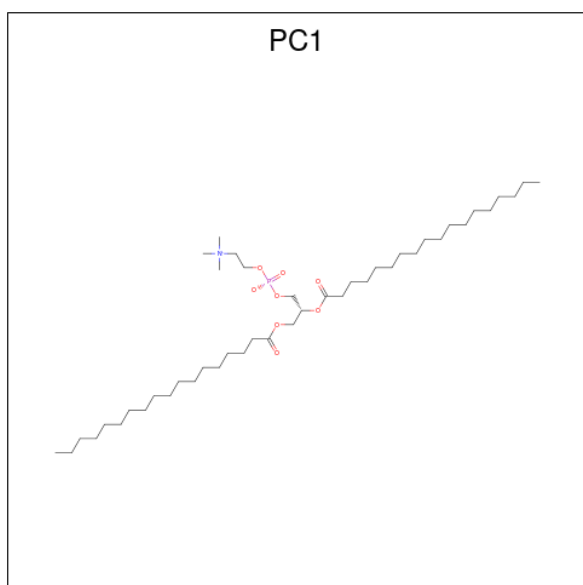
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 13 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



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

- Molecule 14 is POTASSIUM ION (CCD ID: K) (formula: K).

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

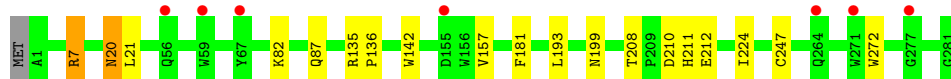
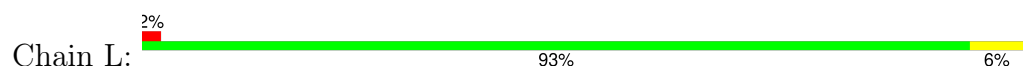
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	56	Total	O	0	0
			56	56		
15	M	53	Total	O	0	0
			53	53		
15	H	83	Total	O	0	0
			83	83		

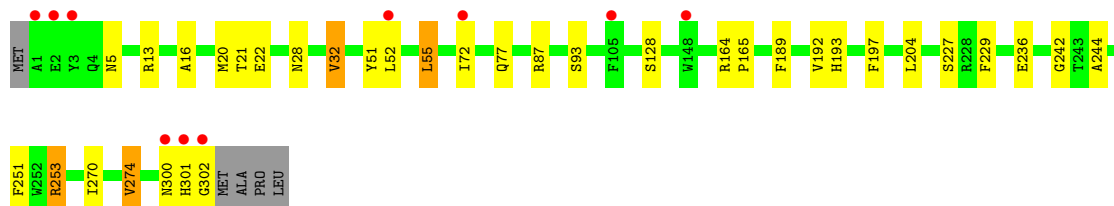
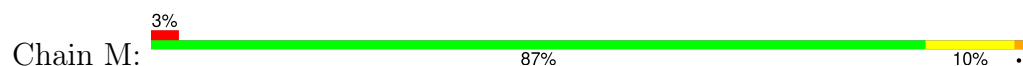
3 Residue-property plots [i](#)

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

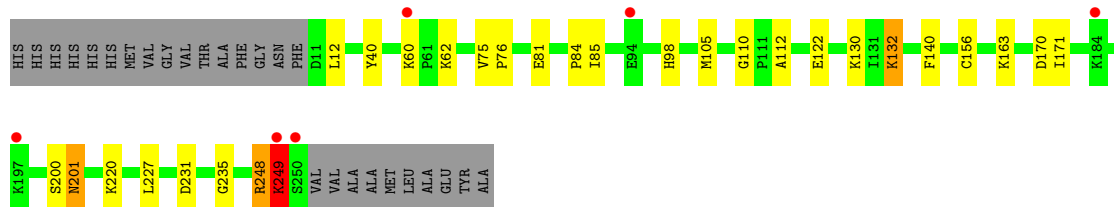
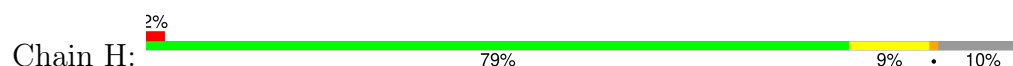
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.11Å 139.11Å 184.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.62 – 2.20 55.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.62-2.20) 99.9 (55.62-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.206 0.188 , 0.211	Depositor DCC
R_{free} test set	5239 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: FE, U10, K, SPO, PO4, PC1, BCL, BPH, HTO, GOL, LDA

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	1.18	0/2342	1.02	3/3206 (0.1%)
2	M	1.10	3/2504 (0.1%)	1.02	2/3418 (0.1%)
3	H	1.16	2/1923 (0.1%)	1.05	3/2611 (0.1%)
All	All	1.14	5/6769 (0.1%)	1.03	8/9235 (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
3	H	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	132	LYS	CA-C	-6.72	1.44	1.52
2	M	242	GLY	N-CA	5.76	1.49	1.44
2	M	32	VAL	N-CA	-5.60	1.39	1.46
2	M	227	SER	C-O	-5.50	1.17	1.24
3	H	105	MET	N-CA	5.19	1.52	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	5	ASN	N-CA-C	5.78	119.64	112.24
1	L	208	THR	CA-C-N	-5.53	113.97	119.56
1	L	208	THR	C-N-CA	-5.53	113.97	119.56
1	L	7	ARG	N-CA-C	5.47	117.24	111.28
3	H	62	LYS	N-CA-C	-5.28	101.34	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	253	ARG	NE-CZ-NH2	5.11	123.80	119.20
3	H	110	GLY	CA-C-N	-5.03	114.53	120.12
3	H	110	GLY	C-N-CA	-5.03	114.53	120.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	248	ARG	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	L	2242	0	2194	17	0
2	M	2407	0	2315	22	0
3	H	1850	0	1875	21	0
4	H	32	0	62	3	0
4	L	32	0	62	1	0
4	M	32	0	62	3	0
5	L	130	0	152	10	0
6	L	46	0	46	9	0
6	M	48	0	63	2	0
7	L	66	0	74	0	0
7	M	218	0	226	19	0
8	L	5	0	0	1	0
8	M	10	0	0	3	0
9	H	10	0	16	1	0
9	L	10	0	16	0	0
10	H	30	0	40	5	0
10	L	36	0	48	7	0
10	M	6	0	8	0	0
11	M	1	0	0	0	0
12	M	42	0	60	1	0
13	M	43	0	60	0	0
14	H	1	0	0	0	0
15	H	83	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	56	0	0	3	0
15	M	53	0	0	2	0
All	All	7489	0	7379	94	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 (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304[B]:U10:H1M3	6:L:304[B]:U10:C8	1.83	1.07
6:L:304[B]:U10:H1M3	6:L:304[B]:U10:H8	1.45	0.98
6:L:304[B]:U10:C8	6:L:304[B]:U10:C1M	2.54	0.84
5:L:313:BPH:HBB3	5:L:313:BPH:HHC	1.60	0.84
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.60	0.83
10:L:314:GOL:O1	15:L:454:HOH:O	2.00	0.80
10:L:314:GOL:C1	15:L:454:HOH:O	2.34	0.75
6:L:304[B]:U10:H3M2	6:L:304[B]:U10:H4M2	1.69	0.75
2:M:253:ARG:HD2	15:M:546:HOH:O	1.87	0.73
6:L:304[B]:U10:H4M2	6:L:304[B]:U10:C3M	2.19	0.72
2:M:197:PHE:CZ	7:M:403:BCL:HBB2	2.26	0.71
1:L:181:PHE:CD2	5:L:313:BPH:HBB1	2.28	0.69
10:L:314:GOL:H12	15:L:454:HOH:O	1.90	0.68
1:L:224:ILE:HB	6:L:304[A]:U10:H103	1.77	0.67
7:M:403:BCL:HBB3	7:M:403:BCL:HHC	1.78	0.65
7:M:403:BCL:HHC	7:M:403:BCL:CBB	2.26	0.65
2:M:197:PHE:HZ	7:M:403:BCL:HBB2	1.61	0.64
3:H:201:ASN:H	3:H:201:ASN:HD22	1.44	0.64
10:H:301:GOL:C3	15:H:451:HOH:O	2.48	0.61
5:L:313:BPH:HHD	5:L:313:BPH:HBC3	1.83	0.61
2:M:55:LEU:HD22	2:M:128:SER:HB2	1.82	0.61
10:H:301:GOL:H31	15:H:451:HOH:O	2.00	0.61
3:H:200:SER:H	9:H:308:HTO:H73	1.65	0.60
5:L:313:BPH:HMB2	7:M:402:BCL:H61	1.83	0.60
3:H:248:ARG:HA	3:H:249[A]:LYS:HB2	1.83	0.60
2:M:189:PHE:O	2:M:193:HIS:HD2	1.86	0.58
1:L:181:PHE:HB3	5:L:313:BPH:HBB2	1.85	0.58
2:M:270:ILE:O	2:M:274:VAL:HG13	2.05	0.56
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.24	0.56
2:M:300:ASN:O	2:M:302:GLY:N	2.40	0.55
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:304:LDA:H123	10:H:307:GOL:H11	1.89	0.54
1:L:20:ASN:C	1:L:20:ASN:HD22	2.16	0.54
1:L:20:ASN:HD22	1:L:21:LEU:N	2.06	0.54
1:L:224:ILE:H	6:L:304[A]:U10:H8	1.72	0.54
1:L:7:ARG:HH21	3:H:98:HIS:HD2	1.57	0.52
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.90	0.52
1:L:181:PHE:HB3	5:L:313:BPH:CBB	2.39	0.52
3:H:40:TYR:OH	4:H:304:LDA:HM12	2.10	0.52
7:M:402:BCL:HBB3	7:M:403:BCL:H41	1.90	0.52
7:M:403:BCL:HAA2	7:M:403:BCL:HBD	1.91	0.51
5:L:313:BPH:HBB3	5:L:313:BPH:CHC	2.38	0.50
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.94	0.49
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.94	0.49
10:L:314:GOL:H31	3:H:85[B]:ILE:CD1	2.43	0.49
1:L:272:TRP:CD1	2:M:87:ARG:HG3	2.48	0.49
2:M:13:ARG:O	3:H:140:PHE:HA	2.13	0.48
3:H:248:ARG:HA	3:H:249[B]:LYS:HB2	1.95	0.47
2:M:77:GLN:HE22	2:M:93:SER:H	1.60	0.47
7:M:402:BCL:HHC	7:M:402:BCL:CBB	2.45	0.47
3:H:40:TYR:OH	4:H:304:LDA:CM1	2.62	0.47
7:M:401[B]:BCL:H61	7:M:401[B]:BCL:H92	1.60	0.47
3:H:81:GLU:HG3	3:H:85[B]:ILE:HD11	1.97	0.47
3:H:84:PRO:O	3:H:85[A]:ILE:HD13	2.15	0.47
8:M:411:PO4:O3	10:H:301:GOL:O1	2.21	0.46
10:L:314:GOL:H31	3:H:85[B]:ILE:HD13	1.98	0.46
7:M:403:BCL:CBB	7:M:403:BCL:CHC	2.94	0.45
3:H:75:VAL:HA	3:H:76:PRO:C	2.41	0.45
2:M:204:LEU:HG	7:M:401[B]:BCL:H192	1.99	0.45
7:M:402:BCL:HBB2	12:M:407:SPO:H243	1.99	0.45
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.17	0.44
10:L:312:GOL:H12	2:M:236:GLU:OE1	2.18	0.44
7:M:401[A]:BCL:H62	7:M:401[A]:BCL:H2	1.30	0.44
5:L:303:BPH:HHC	5:L:303:BPH:CBB	2.41	0.44
8:M:411:PO4:P	4:M:412:LDA:HM22	2.58	0.44
7:M:401[B]:BCL:H111	7:M:401[B]:BCL:H142	1.52	0.44
6:M:406:U10:H322	6:M:406:U10:H301	1.76	0.44
2:M:197:PHE:CE1	7:M:403:BCL:HBB2	2.53	0.43
8:M:411:PO4:O2	4:M:412:LDA:HM22	2.18	0.43
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.36	0.43
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.43
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:301:GOL:H32	15:H:451:HOH:O	2.17	0.42
1:L:211:HIS:CE1	2:M:20:MET:HE2	2.54	0.42
2:M:197:PHE:HZ	7:M:403:BCL:CBB	2.31	0.42
4:L:302:LDA:H123	6:L:304[B]:U10:H102	2.01	0.42
4:M:412:LDA:HM23	4:M:412:LDA:H21	1.83	0.42
1:L:82:LYS:HE3	8:L:306:PO4:O2	2.19	0.42
2:M:21:THR:O	2:M:22:GLU:C	2.63	0.42
2:M:251:PHE:CD1	2:M:251:PHE:C	2.98	0.41
7:M:402:BCL:H71	7:M:403:BCL:H192	2.01	0.41
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.01	0.41
6:L:304[A]:U10:H1M1	6:L:304[A]:U10:H71	1.83	0.41
1:L:157:VAL:HG11	7:M:403:BCL:HBB1	2.02	0.41
1:L:199:ASN:HA	10:L:308:GOL:H31	2.03	0.41
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.56	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.21	0.41
3:H:201:ASN:H	3:H:201:ASN:ND2	2.16	0.41
3:H:132:LYS:HB2	3:H:171:ILE:HD11	2.04	0.40
1:L:193:LEU:HD21	1:L:212:GLU:HB3	2.03	0.40
6:M:406:U10:H303	6:M:406:U10:H261	2.03	0.40
2:M:253:ARG:NH1	15:M:509:HOH:O	2.39	0.40
3:H:248:ARG:CA	3:H:249[A]:LYS:HB2	2.50	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	L	281/282 (100%)	276 (98%)	5 (2%)	0	100	100
2	M	301/307 (98%)	290 (96%)	10 (3%)	1 (0%)	36	42
3	H	243/266 (91%)	240 (99%)	1 (0%)	2 (1%)	16	16
All	All	825/855 (96%)	806 (98%)	16 (2%)	3 (0%)	43	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	249[A]	LYS
3	H	249[B]	LYS
2	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	L	222/221 (100%)	219 (99%)	3 (1%)	59	75
2	M	236/239 (99%)	231 (98%)	5 (2%)	47	63
3	H	200/214 (94%)	190 (95%)	10 (5%)	22	28
All	All	658/674 (98%)	640 (97%)	18 (3%)	44	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	210	ASP
1	L	247	CYS
2	M	52	LEU
2	M	55	LEU
2	M	72	ILE
2	M	192	VAL
2	M	274	VAL
3	H	12	LEU
3	H	60	LYS
3	H	163[A]	LYS
3	H	163[B]	LYS
3	H	201	ASN
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	231	ASP
3	H	249[A]	LYS
3	H	249[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	159	ASN
2	M	4	GLN
2	M	77	GLN
2	M	187	ASN
2	M	193	HIS
3	H	98	HIS
3	H	201	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 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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[B]	-	69,74,74	1.77	18 (26%)	79,115,115	2.06	25 (31%)
4	LDA	M	412	-	13,15,15	1.97	2 (15%)	14,17,17	0.80	0
4	LDA	L	302	-	13,15,15	2.03	1 (7%)	14,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BPH	L	303	-	59,70,70	2.32	17 (28%)	59,101,101	2.13	16 (27%)
7	BCL	M	403	2	69,74,74	1.77	14 (20%)	79,115,115	2.05	22 (27%)
12	SPO	M	407	-	41,41,41	0.91	1 (2%)	47,50,50	1.65	7 (14%)
9	HTO	H	308	-	9,9,9	0.65	0	10,10,10	0.64	0
4	LDA	M	404	-	13,15,15	1.91	1 (7%)	14,17,17	0.68	0
13	PC1	M	408	-	42,42,53	1.18	2 (4%)	48,50,61	1.50	7 (14%)
10	GOL	H	303	-	5,5,5	0.50	0	5,5,5	0.50	0
6	U10	L	304[B]	-	23,23,63	2.04	2 (8%)	30,31,79	1.17	3 (10%)
8	PO4	M	409	-	4,4,4	0.62	0	6,6,6	0.81	0
8	PO4	L	306	-	4,4,4	0.73	0	6,6,6	1.02	0
7	BCL	M	401[A]	-	69,74,74	1.77	18 (26%)	79,115,115	2.19	27 (34%)
5	BPH	L	313	-	59,70,70	2.28	18 (30%)	59,101,101	2.03	14 (23%)
8	PO4	M	411	-	4,4,4	2.02	2 (50%)	6,6,6	1.42	1 (16%)
10	GOL	H	301	-	5,5,5	1.09	0	5,5,5	1.83	3 (60%)
10	GOL	L	314	-	5,5,5	0.77	0	5,5,5	0.61	0
9	HTO	L	307	-	9,9,9	0.98	0	10,10,10	0.71	0
10	GOL	L	308	-	5,5,5	1.22	0	5,5,5	1.35	0
10	GOL	H	302	-	5,5,5	0.58	0	5,5,5	0.80	0
10	GOL	L	312	-	5,5,5	0.43	0	5,5,5	0.75	0
4	LDA	L	301	-	13,15,15	1.94	1 (7%)	14,17,17	0.36	0
6	U10	L	304[A]	-	23,23,63	2.06	2 (8%)	30,31,79	2.09	11 (36%)
10	GOL	H	307	-	5,5,5	0.26	0	5,5,5	0.61	0
10	GOL	L	310	-	5,5,5	1.29	0	5,5,5	1.51	1 (20%)
4	LDA	H	309	-	13,15,15	1.97	1 (7%)	14,17,17	0.27	0
10	GOL	M	410	-	5,5,5	0.79	0	5,5,5	0.80	0
7	BCL	M	402	2	69,74,74	1.67	17 (24%)	79,115,115	2.15	25 (31%)
10	GOL	L	311	-	5,5,5	0.50	0	5,5,5	0.87	0
10	GOL	L	309	-	5,5,5	0.42	0	5,5,5	0.32	0
10	GOL	H	305	-	5,5,5	0.54	0	5,5,5	0.80	0
4	LDA	H	304	-	13,15,15	2.26	2 (15%)	14,17,17	1.15	1 (7%)
6	U10	M	406	-	48,48,63	1.36	3 (6%)	60,61,79	1.55	14 (23%)
7	BCL	L	305	1	69,74,74	1.50	12 (17%)	79,115,115	1.91	20 (25%)

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[B]	-	-	13/41/137/137	-
4	LDA	M	412	-	-	6/13/13/13	-
4	LDA	L	302	-	-	7/13/13/13	-
5	BPH	L	303	-	-	7/37/105/105	0/5/6/6
7	BCL	M	403	2	-	2/41/137/137	-
12	SPO	M	407	-	-	4/47/47/47	-
9	HTO	H	308	-	-	2/10/10/10	-
4	LDA	M	404	-	-	6/13/13/13	-
13	PC1	M	408	-	-	19/46/46/57	-
10	GOL	H	303	-	-	3/4/4/4	-
6	U10	L	304[B]	-	-	6/15/39/87	0/1/1/1
7	BCL	M	401[A]	-	-	7/41/137/137	-
5	BPH	L	313	-	-	5/37/105/105	0/5/6/6
10	GOL	H	301	-	-	0/4/4/4	-
10	GOL	L	314	-	-	2/4/4/4	-
9	HTO	L	307	-	-	7/10/10/10	-
10	GOL	L	308	-	-	2/4/4/4	-
10	GOL	H	302	-	-	2/4/4/4	-
10	GOL	L	312	-	-	1/4/4/4	-
4	LDA	L	301	-	-	7/13/13/13	-
6	U10	L	304[A]	-	-	1/15/39/87	0/1/1/1
10	GOL	H	307	-	-	3/4/4/4	-
10	GOL	L	310	-	-	0/4/4/4	-
4	LDA	H	309	-	-	6/13/13/13	-
10	GOL	M	410	-	-	2/4/4/4	-
7	BCL	M	402	2	-	9/41/137/137	-
10	GOL	L	311	-	-	0/4/4/4	-
10	GOL	L	309	-	-	0/4/4/4	-
10	GOL	H	305	-	-	2/4/4/4	-
4	LDA	H	304	-	-	4/13/13/13	-
6	U10	M	406	-	-	8/45/69/87	0/1/1/1
7	BCL	L	305	1	-	3/41/137/137	-

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	303	BPH	C1B-C2B	8.60	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	304[B]	U10	C6-C1	8.41	1.50	1.35
6	L	304[A]	U10	C6-C1	8.27	1.50	1.35
5	L	313	BPH	C1D-C2D	7.82	1.48	1.39
5	L	313	BPH	C1B-C2B	7.20	1.47	1.39
4	L	302	LDA	O1-N1	-6.99	1.25	1.42
4	H	309	LDA	O1-N1	-6.76	1.25	1.42
4	H	304	LDA	O1-N1	-6.70	1.25	1.42
6	M	406	U10	C6-C1	6.69	1.47	1.35
4	M	404	LDA	O1-N1	-6.54	1.26	1.42
4	L	301	LDA	O1-N1	-6.51	1.26	1.42
4	M	412	LDA	O1-N1	-6.45	1.26	1.42
5	L	303	BPH	C1D-C2D	6.21	1.46	1.39
7	M	403	BCL	O2D-CGD	5.54	1.46	1.33
5	L	303	BPH	C3B-C4B	5.33	1.50	1.41
7	M	403	BCL	OBD-CAD	5.24	1.31	1.22
5	L	313	BPH	C3A-C2A	-5.22	1.50	1.54
7	M	401[A]	BCL	O2A-CGA	5.18	1.48	1.33
7	M	401[B]	BCL	O2A-CGA	5.18	1.48	1.33
5	L	303	BPH	C3D-C2D	5.10	1.48	1.39
13	M	408	PC1	O21-C21	4.86	1.48	1.34
7	M	401[A]	BCL	O2D-CGD	4.68	1.44	1.33
7	M	401[B]	BCL	O2D-CGD	4.68	1.44	1.33
5	L	303	BPH	OBD-CAD	4.68	1.28	1.22
5	L	313	BPH	C4D-CHA	4.58	1.46	1.39
4	H	304	LDA	C1-N1	-4.57	1.46	1.51
13	M	408	PC1	O31-C31	4.55	1.46	1.33
5	L	303	BPH	C4B-NB	-4.35	1.30	1.38
7	M	403	BCL	CHC-C4B	4.24	1.48	1.39
7	M	403	BCL	CHD-C1D	4.12	1.46	1.38
7	M	401[A]	BCL	MG-NC	-4.03	1.96	2.06
7	M	401[B]	BCL	MG-NC	-4.03	1.96	2.06
7	L	305	BCL	O2A-CGA	4.01	1.45	1.33
7	L	305	BCL	CHC-C4B	3.98	1.48	1.39
7	M	402	BCL	O2A-CGA	3.94	1.44	1.33
5	L	303	BPH	C4D-CHA	3.92	1.45	1.39
5	L	303	BPH	O2D-CGD	3.85	1.42	1.33
7	M	402	BCL	C3D-C2D	3.82	1.49	1.39
5	L	313	BPH	C2C-C3C	-3.81	1.51	1.54
6	L	304[B]	U10	C4-C3	3.80	1.50	1.36
6	M	406	U10	C4-C3	3.59	1.49	1.36
7	L	305	BCL	CHB-C1B	3.53	1.47	1.39
7	L	305	BCL	OBD-CAD	3.52	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	402	BCL	C3B-C4B	3.52	1.48	1.41
7	M	401[A]	BCL	C4B-NB	-3.52	1.33	1.37
7	M	401[B]	BCL	C4B-NB	-3.52	1.33	1.37
7	M	402	BCL	C3D-C4D	-3.52	1.36	1.44
7	L	305	BCL	C3B-C4B	3.49	1.48	1.41
5	L	313	BPH	C3D-C4D	-3.49	1.36	1.41
5	L	313	BPH	O2A-CGA	3.48	1.43	1.33
7	M	402	BCL	O2D-CGD	3.48	1.41	1.33
7	M	402	BCL	CHC-C4B	3.45	1.47	1.39
5	L	303	BPH	C2C-C3C	-3.43	1.51	1.54
7	M	401[A]	BCL	MG-NA	-3.42	1.98	2.06
7	M	401[B]	BCL	MG-NA	-3.42	1.98	2.06
7	M	403	BCL	C3D-C2D	3.40	1.48	1.39
7	M	403	BCL	O2A-CGA	3.40	1.43	1.33
5	L	313	BPH	C3D-C2D	3.39	1.45	1.39
7	M	402	BCL	CBB-CAB	-3.36	1.43	1.50
5	L	313	BPH	O2D-CGD	3.31	1.41	1.33
7	M	403	BCL	CBB-CAB	-3.27	1.43	1.50
7	M	401[A]	BCL	OBD-CAD	3.17	1.28	1.22
7	M	401[B]	BCL	OBD-CAD	3.17	1.28	1.22
5	L	303	BPH	O2A-CGA	3.10	1.42	1.33
7	M	402	BCL	OBD-CAD	3.09	1.27	1.22
7	L	305	BCL	C3D-C4D	-3.05	1.37	1.44
7	M	402	BCL	MG-ND	-3.04	1.99	2.05
7	M	401[A]	BCL	CHC-C1C	-3.04	1.30	1.37
7	M	401[B]	BCL	CHC-C1C	-3.04	1.30	1.37
7	M	401[A]	BCL	C3D-C2D	3.01	1.47	1.39
7	M	401[B]	BCL	C3D-C2D	3.01	1.47	1.39
7	M	403	BCL	CHB-C1B	3.00	1.46	1.39
6	L	304[A]	U10	C4-C3	2.95	1.47	1.36
7	M	403	BCL	C3B-C4B	2.94	1.46	1.41
7	M	403	BCL	C3D-C4D	-2.93	1.37	1.44
7	L	305	BCL	CHD-C1D	2.92	1.44	1.38
7	L	305	BCL	C3D-C2D	2.92	1.47	1.39
5	L	313	BPH	CBD-CGD	-2.88	1.48	1.52
7	M	401[A]	BCL	MG-ND	-2.87	2.00	2.05
7	M	401[B]	BCL	MG-ND	-2.87	2.00	2.05
5	L	313	BPH	C3B-C4B	2.87	1.46	1.41
5	L	303	BPH	C1B-NB	-2.82	1.33	1.38
5	L	313	BPH	C3B-C2B	2.82	1.44	1.39
5	L	313	BPH	C4D-ND	-2.81	1.34	1.38
7	M	402	BCL	C1D-ND	-2.81	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401[A]	BCL	C3D-C4D	-2.71	1.38	1.44
7	M	401[B]	BCL	C3D-C4D	-2.71	1.38	1.44
6	M	406	U10	O3-C3M	-2.69	1.39	1.45
7	M	401[A]	BCL	CHB-C1B	2.67	1.45	1.39
7	M	401[B]	BCL	CHB-C1B	2.67	1.45	1.39
5	L	313	BPH	OBD-CAD	2.66	1.25	1.22
8	M	411	PO4	P-O4	-2.63	1.47	1.54
7	L	305	BCL	C4D-CHA	2.62	1.47	1.38
4	M	412	LDA	C1-N1	-2.61	1.48	1.51
7	M	401[A]	BCL	C1D-ND	-2.59	1.34	1.37
7	M	401[B]	BCL	C1D-ND	-2.59	1.34	1.37
7	M	402	BCL	MG-NA	-2.56	2.00	2.06
7	L	305	BCL	C1B-C2B	2.50	1.49	1.43
7	M	401[A]	BCL	C3B-C4B	2.46	1.46	1.41
7	M	401[B]	BCL	C3B-C4B	2.46	1.46	1.41
5	L	303	BPH	C3B-C2B	2.43	1.43	1.39
7	M	403	BCL	C4D-CHA	2.42	1.46	1.38
7	L	305	BCL	O2D-CGD	2.41	1.39	1.33
7	M	402	BCL	C4B-NB	-2.41	1.34	1.37
5	L	313	BPH	C1B-NB	-2.35	1.34	1.38
5	L	313	BPH	O2D-CED	-2.35	1.40	1.45
7	M	401[A]	BCL	CAA-C2A	2.35	1.58	1.54
7	M	401[B]	BCL	CAA-C2A	2.35	1.58	1.54
7	M	402	BCL	CHD-C1D	2.33	1.42	1.38
7	M	402	BCL	CHB-C1B	2.32	1.44	1.39
8	M	411	PO4	P-O3	-2.30	1.47	1.54
5	L	303	BPH	CBD-CGD	-2.29	1.49	1.52
5	L	303	BPH	O2D-CED	-2.29	1.40	1.45
7	M	403	BCL	O1D-CGD	2.27	1.27	1.21
7	L	305	BCL	CHB-C4A	-2.22	1.32	1.37
5	L	313	BPH	C1D-ND	-2.22	1.34	1.38
7	M	402	BCL	C4D-CHA	2.22	1.46	1.38
7	M	403	BCL	C1B-NB	-2.21	1.35	1.37
7	M	401[A]	BCL	C1B-NB	-2.21	1.35	1.37
7	M	401[B]	BCL	C1B-NB	-2.21	1.35	1.37
7	M	401[A]	BCL	MG-NB	-2.20	2.01	2.05
7	M	401[B]	BCL	MG-NB	-2.20	2.01	2.05
5	L	303	BPH	OBB-CAB	2.18	1.29	1.22
7	M	401[A]	BCL	CHC-C4B	2.16	1.44	1.39
7	M	401[B]	BCL	CHC-C4B	2.16	1.44	1.39
7	M	401[A]	BCL	C3C-C4C	-2.12	1.48	1.51
7	M	401[B]	BCL	C3C-C4C	-2.12	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	403	BCL	MG-NA	2.09	2.11	2.06
7	M	402	BCL	CBD-CGD	-2.09	1.46	1.52
12	M	407	SPO	C4-C5	2.08	1.53	1.50
5	L	313	BPH	CBB-CAB	-2.07	1.43	1.49
7	M	402	BCL	CHC-C1C	-2.01	1.32	1.37
5	L	303	BPH	C3A-C2A	-2.01	1.53	1.54
5	L	303	BPH	C4D-ND	-2.00	1.35	1.38

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401[A]	BCL	C1C-NC-C4C	-7.86	103.09	106.68
7	M	401[B]	BCL	C1C-NC-C4C	-7.86	103.09	106.68
7	M	403	BCL	CMD-C2D-C1D	7.83	138.51	124.73
5	L	303	BPH	O2D-CGD-CBD	7.38	119.06	110.95
7	L	305	BCL	CMD-C2D-C1D	7.12	137.26	124.73
7	M	402	BCL	C1C-NC-C4C	-7.01	103.48	106.68
12	M	407	SPO	C4-C5-C6	-7.00	115.08	124.91
13	M	408	PC1	O21-C21-C22	6.55	125.65	111.48
7	M	402	BCL	CMD-C2D-C1D	6.17	135.59	124.73
7	M	402	BCL	C1-O2A-CGA	6.15	131.55	116.65
5	L	313	BPH	O2D-CGD-CBD	6.09	117.63	110.95
7	M	401[A]	BCL	C3C-C4C-CHD	-5.33	112.15	123.39
7	M	401[B]	BCL	C3C-C4C-CHD	-5.33	112.15	123.39
5	L	313	BPH	C2B-C1B-NB	5.32	113.27	109.43
5	L	303	BPH	C2B-C1B-NB	5.13	113.14	109.43
5	L	313	BPH	OBD-CAD-C3D	-5.08	119.96	127.89
5	L	303	BPH	OBB-CAB-C3B	4.82	128.05	119.99
7	L	305	BCL	C4A-NA-C1A	-4.75	104.51	106.68
7	M	401[A]	BCL	C4-C3-C5	4.73	123.44	115.23
5	L	313	BPH	C3D-C4D-ND	4.69	113.72	107.71
7	M	401[A]	BCL	CMD-C2D-C1D	4.62	132.86	124.73
7	M	401[B]	BCL	CMD-C2D-C1D	4.62	132.86	124.73
6	L	304[A]	U10	C8-C7-C6	4.46	123.07	112.08
7	L	305	BCL	O1D-CGD-CBD	4.39	133.19	124.52
6	L	304[A]	U10	C1M-C1-C6	-4.37	117.26	124.45
5	L	303	BPH	CBB-CAB-C3B	-4.37	107.27	120.34
7	M	403	BCL	C3C-C4C-CHD	-4.34	114.24	123.39
7	M	403	BCL	C2B-C1B-NB	4.21	114.69	110.33
7	L	305	BCL	O2D-CGD-O1D	-4.20	115.68	123.85
7	M	402	BCL	C3D-C2D-C1D	-4.16	100.15	105.83
7	L	305	BCL	C3C-C4C-CHD	-4.13	114.67	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	303	BPH	C2D-C1D-ND	4.05	112.35	109.43
7	M	402	BCL	C3C-C4C-CHD	-4.04	114.88	123.39
7	M	401[A]	BCL	C5-C3-C2	-4.03	112.12	121.17
7	M	403	BCL	O2D-CGD-O1D	-4.02	116.02	123.85
7	M	403	BCL	CHD-C1D-ND	-4.02	119.15	124.80
7	M	402	BCL	C2B-C1B-NB	3.93	114.40	110.33
5	L	303	BPH	C4C-C3C-C2C	-3.90	99.13	102.84
6	M	406	U10	C32-C33-C34	-3.87	118.78	127.62
7	M	403	BCL	CBB-CAB-C3B	-3.81	112.37	120.40
7	M	403	BCL	C3D-C2D-C1D	-3.79	100.65	105.83
5	L	303	BPH	C3D-C4D-ND	3.76	112.53	107.71
5	L	303	BPH	O2D-CGD-O1D	-3.75	116.55	123.85
7	M	401[A]	BCL	C1D-CHD-C4C	-3.75	117.58	126.62
7	M	401[B]	BCL	C1D-CHD-C4C	-3.75	117.58	126.62
7	L	305	BCL	C3D-C2D-C1D	-3.63	100.88	105.83
7	M	402	BCL	CMB-C2B-C1B	3.60	130.90	125.42
5	L	313	BPH	C3D-CAD-CBD	3.58	112.33	107.61
7	M	401[A]	BCL	C2B-C1B-NB	3.56	114.01	110.33
7	M	401[B]	BCL	C2B-C1B-NB	3.56	114.01	110.33
7	L	305	BCL	C1C-NC-C4C	-3.50	105.08	106.68
7	M	403	BCL	C2D-C1D-ND	3.48	113.57	110.13
7	M	401[A]	BCL	C1-O2A-CGA	3.44	124.97	116.65
5	L	313	BPH	C1-O2A-CGA	3.40	124.89	116.65
7	M	402	BCL	CHD-C1D-ND	-3.39	120.03	124.80
7	L	305	BCL	C2A-C1A-CHA	-3.39	117.98	123.87
7	M	401[A]	BCL	C16-C15-C13	-3.35	104.85	115.97
6	M	406	U10	C1M-C1-C6	-3.34	118.96	124.45
13	M	408	PC1	O31-C31-C32	3.32	121.97	111.83
7	M	403	BCL	O2A-CGA-O1A	-3.31	115.36	123.63
13	M	408	PC1	O21-C21-O22	-3.27	116.06	123.70
7	M	403	BCL	CMB-C2B-C1B	3.26	130.39	125.42
7	M	402	BCL	O2D-CGD-CBD	3.26	116.93	111.23
7	M	401[A]	BCL	O2D-CGD-CBD	3.25	116.92	111.23
7	M	401[B]	BCL	O2D-CGD-CBD	3.25	116.92	111.23
7	M	401[A]	BCL	C2D-C1D-ND	3.25	113.34	110.13
7	M	401[B]	BCL	C2D-C1D-ND	3.25	113.34	110.13
6	L	304[A]	U10	C3M-O3-C3	3.22	127.80	116.47
7	L	305	BCL	C2B-C1B-NB	3.22	113.67	110.33
7	M	401[A]	BCL	C3B-C4B-NB	3.22	114.00	109.76
7	M	401[B]	BCL	C3B-C4B-NB	3.22	114.00	109.76
5	L	313	BPH	O2D-CGD-O1D	-3.21	117.60	123.85
13	M	408	PC1	C2-O21-C21	3.17	125.38	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401[A]	BCL	O2A-CGA-CBA	3.16	121.48	111.83
7	M	401[B]	BCL	O2A-CGA-CBA	3.16	121.48	111.83
7	M	401[A]	BCL	C3D-C2D-C1D	-3.16	101.51	105.83
7	M	401[B]	BCL	C3D-C2D-C1D	-3.16	101.51	105.83
7	M	401[A]	BCL	C3A-C2A-C1A	-3.16	96.61	101.34
7	M	401[B]	BCL	C3A-C2A-C1A	-3.16	96.61	101.34
7	M	403	BCL	C1-C2-C3	-3.13	121.07	126.20
7	M	402	BCL	C2D-C1D-ND	3.13	113.22	110.13
7	L	305	BCL	C3B-C4B-NB	3.08	113.83	109.76
6	M	406	U10	C30-C29-C31	3.07	120.56	115.23
6	L	304[A]	U10	O2-C2-C3	-3.07	114.52	121.03
5	L	313	BPH	C2D-C1D-ND	3.07	111.65	109.43
5	L	313	BPH	CBB-CAB-C3B	-3.06	111.16	120.34
6	L	304[A]	U10	C1-C6-C5	-3.06	116.65	119.62
7	M	403	BCL	C2A-C1A-CHA	-3.03	118.61	123.87
6	M	406	U10	C27-C28-C29	-3.01	120.73	127.62
6	M	406	U10	C6-C1-C2	3.01	121.55	119.17
7	M	403	BCL	CMD-C2D-C3D	-3.00	120.81	127.69
6	L	304[A]	U10	C7-C6-C5	2.99	121.99	118.52
7	M	403	BCL	OBb-CAB-C3B	2.99	125.72	120.43
7	M	401[A]	BCL	C2A-C1A-CHA	-2.97	118.71	123.87
7	M	401[B]	BCL	C2A-C1A-CHA	-2.97	118.71	123.87
7	M	402	BCL	CED-O2D-CGD	-2.97	109.17	115.92
7	M	402	BCL	C4-C3-C2	-2.96	116.03	123.63
13	M	408	PC1	O31-C31-O32	-2.96	116.23	123.63
7	M	403	BCL	O2A-CGA-CBA	2.90	120.69	111.83
7	M	401[A]	BCL	C3D-C4D-ND	2.90	114.70	109.99
7	M	401[B]	BCL	C3D-C4D-ND	2.90	114.70	109.99
7	M	402	BCL	CAB-C3B-C2B	-2.90	121.72	127.74
7	M	401[A]	BCL	OBb-CAB-C3B	2.88	125.53	120.43
7	M	401[B]	BCL	OBb-CAB-C3B	2.88	125.53	120.43
7	M	401[A]	BCL	CHD-C1D-ND	-2.88	120.75	124.80
7	M	401[B]	BCL	CHD-C1D-ND	-2.88	120.75	124.80
5	L	303	BPH	O2A-CGA-O1A	-2.87	116.44	123.63
5	L	303	BPH	C1-C2-C3	-2.82	121.57	126.20
7	M	403	BCL	C3D-C4D-ND	2.82	114.56	109.99
7	L	305	BCL	C2D-C1D-ND	2.80	112.90	110.13
7	L	305	BCL	CHD-C1D-ND	-2.80	120.86	124.80
6	M	406	U10	C17-C18-C19	-2.77	121.29	127.62
12	M	407	SPO	C40-C38-C39	2.76	120.94	114.59
7	M	402	BCL	O2A-CGA-CBA	2.73	120.15	111.83
7	M	402	BCL	C3D-C4D-ND	2.70	114.38	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	407	SPO	C20-C19-C17	-2.70	123.49	127.28
7	M	402	BCL	O2D-CGD-O1D	-2.70	118.60	123.85
5	L	303	BPH	CED-O2D-CGD	2.70	122.03	115.92
7	M	403	BCL	C1C-NC-C4C	-2.68	105.45	106.68
7	M	401[A]	BCL	CHC-C1C-NC	2.62	128.19	124.40
7	M	401[B]	BCL	CHC-C1C-NC	2.62	128.19	124.40
5	L	303	BPH	CBC-CAC-C3C	2.62	118.94	113.78
5	L	313	BPH	OB B-CAB-C3B	2.61	124.36	119.99
5	L	303	BPH	CMB-C2B-C3B	2.59	129.86	124.68
7	L	305	BCL	C1-O2A-CGA	2.59	122.91	116.65
5	L	303	BPH	OBD-CAD-C3D	-2.57	123.89	127.89
7	L	305	BCL	CMD-C2D-C3D	-2.57	121.80	127.69
7	M	402	BCL	C3A-C2A-C1A	-2.56	97.50	101.34
7	L	305	BCL	C3A-C2A-C1A	-2.56	97.50	101.34
12	M	407	SPO	C24-C23-C22	2.54	126.94	122.82
6	M	406	U10	C4M-O4-C4	2.54	125.40	116.47
10	H	301	GOL	C3-C2-C1	2.54	121.09	111.80
13	M	408	PC1	O21-C2-C3	2.52	117.38	108.34
6	L	304[B]	U10	C1M-C1-C6	-2.50	120.34	124.45
6	L	304[A]	U10	C4-C3-C2	-2.44	116.21	120.69
6	M	406	U10	C22-C21-C19	-2.43	105.12	113.19
7	L	305	BCL	C3D-C4D-ND	2.43	113.94	109.99
7	M	402	BCL	CHB-C4A-NA	2.41	127.88	124.40
7	M	401[A]	BCL	C16-C17-C18	-2.41	105.18	115.94
10	L	310	GOL	O3-C3-C2	2.39	121.13	110.38
6	M	406	U10	C3M-O3-C3	2.39	124.86	116.47
7	M	401[B]	BCL	C1-C2-C3	-2.36	122.33	126.20
6	M	406	U10	C41-C39-C40	2.36	120.02	114.59
7	M	402	BCL	O2A-CGA-O1A	-2.34	117.79	123.63
4	H	304	LDA	CM1-N1-C1	-2.33	105.33	110.23
7	M	401[B]	BCL	C4-C3-C2	-2.32	117.67	123.63
6	M	406	U10	C31-C29-C28	-2.31	115.97	121.17
7	L	305	BCL	O2A-CGA-O1A	-2.31	117.86	123.63
5	L	313	BPH	CMA-C3A-C4A	-2.31	109.64	114.61
10	H	301	GOL	O3-C3-C2	2.30	120.74	110.38
5	L	313	BPH	CBA-CAA-C2A	-2.29	107.02	113.78
6	L	304[A]	U10	O4-C4-C3	-2.28	115.00	123.64
7	M	402	BCL	O2A-C1-C2	2.28	116.89	108.11
6	M	406	U10	C25-C24-C26	2.27	119.16	115.23
7	M	401[A]	BCL	OBD-CAD-C3D	-2.26	123.13	128.42
7	M	401[B]	BCL	OBD-CAD-C3D	-2.26	123.13	128.42
7	M	401[A]	BCL	CBB-CAB-C3B	-2.26	115.64	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401[B]	BCL	CBB-CAB-C3B	-2.26	115.64	120.40
7	M	401[A]	BCL	CMB-C2B-C1B	2.26	128.86	125.42
7	M	401[B]	BCL	CMB-C2B-C1B	2.26	128.86	125.42
7	M	403	BCL	C1D-ND-C4D	-2.26	104.73	106.31
5	L	313	BPH	C4-C3-C2	-2.24	117.86	123.63
7	M	402	BCL	CHC-C1C-NC	2.24	127.63	124.40
7	M	401[A]	BCL	C1D-ND-C4D	-2.23	104.75	106.31
7	M	401[B]	BCL	C1D-ND-C4D	-2.23	104.75	106.31
5	L	313	BPH	C4D-ND-C1D	-2.23	106.21	108.87
7	M	401[B]	BCL	C4-C3-C5	2.22	119.09	115.23
7	M	402	BCL	CHB-C1B-C2B	-2.21	121.02	127.43
6	M	406	U10	C35-C34-C36	2.20	119.05	115.23
7	M	403	BCL	O1D-CGD-CBD	2.19	128.84	124.52
7	M	403	BCL	O2D-CGD-CBD	2.19	115.06	111.23
7	M	402	BCL	C4D-C3D-CAD	-2.18	105.74	108.11
12	M	407	SPO	C21-C20-C19	2.17	127.96	123.52
7	L	305	BCL	C1D-CHD-C4C	-2.15	121.43	126.62
6	L	304[A]	U10	C7-C6-C1	-2.14	121.22	124.89
13	M	408	PC1	C3-C2-C1	-2.13	106.81	111.78
6	L	304[A]	U10	C3-C2-C1	2.13	122.30	118.10
7	M	401[A]	BCL	CHC-C4B-C3B	-2.11	123.33	131.72
7	M	401[B]	BCL	CHC-C4B-C3B	-2.11	123.33	131.72
7	M	402	BCL	C5-C3-C2	2.10	125.89	121.17
8	M	411	PO4	O4-P-O2	2.10	114.45	107.91
5	L	303	BPH	OBB-CAB-CBB	2.10	124.66	120.19
6	M	406	U10	C15-C14-C16	2.09	118.86	115.23
7	M	402	BCL	CBB-CAB-C3B	-2.09	116.00	120.40
7	M	401[A]	BCL	CHB-C4A-NA	2.09	127.41	124.40
7	M	401[B]	BCL	CHB-C4A-NA	2.09	127.41	124.40
12	M	407	SPO	C27-C26-C25	-2.08	117.18	123.20
6	L	304[B]	U10	C12-C13-C14	-2.07	120.75	127.64
7	L	305	BCL	C4-C3-C5	2.06	118.81	115.23
6	L	304[A]	U10	O3-C3-C2	2.06	123.59	116.64
7	M	403	BCL	CHB-C4A-NA	2.06	127.37	124.40
6	L	304[B]	U10	C7-C8-C9	-2.04	123.31	126.83
12	M	407	SPO	C15-C14-C12	-2.03	124.42	127.28
5	L	303	BPH	C3D-CAD-CBD	2.03	110.27	107.61
10	H	301	GOL	O1-C1-C2	2.02	119.46	110.38
7	L	305	BCL	CMB-C2B-C1B	2.01	128.49	125.42
7	M	403	BCL	CAB-C3B-C2B	-2.01	123.57	127.74

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	404	LDA	C2-C1-N1-O1
4	M	404	LDA	C2-C1-N1-CM2
6	L	304[B]	U10	C1-C6-C7-C8
6	L	304[B]	U10	C5-C6-C7-C8
7	M	402	BCL	C2-C1-O2A-CGA
9	L	307	HTO	C1-C2-C3-O3
9	L	307	HTO	C1-C2-C3-C4
9	L	307	HTO	O2-C2-C3-O3
9	L	307	HTO	O2-C2-C3-C4
10	L	308	GOL	C1-C2-C3-O3
10	L	314	GOL	O1-C1-C2-C3
10	M	410	GOL	O1-C1-C2-C3
10	H	302	GOL	C1-C2-C3-O3
10	H	303	GOL	C1-C2-C3-O3
10	H	307	GOL	O1-C1-C2-C3
12	M	407	SPO	O1-C1-C4-C5
12	M	407	SPO	C2-C1-C4-C5
12	M	407	SPO	C3-C1-C4-C5
13	M	408	PC1	C11-O13-P-O14
13	M	408	PC1	C11-O13-P-O11
13	M	408	PC1	O22-C21-O21-C2
13	M	408	PC1	C2-C3-O31-C31
13	M	408	PC1	O32-C31-O31-C3
13	M	408	PC1	C32-C31-O31-C3
13	M	408	PC1	C22-C21-O21-C2
7	M	401[B]	BCL	C4-C3-C5-C6
6	L	304[B]	U10	C12-C11-C9-C10
6	L	304[B]	U10	C12-C11-C9-C8
6	L	304[B]	U10	C9-C11-C12-C13
6	M	406	U10	C30-C29-C31-C32
6	M	406	U10	C28-C29-C31-C32
7	M	401[B]	BCL	C2-C3-C5-C6
7	M	401[B]	BCL	C11-C12-C13-C14
7	M	401[B]	BCL	C12-C13-C15-C16
7	M	402	BCL	C6-C7-C8-C10
5	L	313	BPH	C5-C6-C7-C8
7	M	401[A]	BCL	C3-C5-C6-C7
7	L	305	BCL	C15-C16-C17-C18
7	M	401[B]	BCL	C10-C11-C12-C13
7	M	402	BCL	C8-C10-C11-C12
7	M	401[A]	BCL	C13-C15-C16-C17
7	M	401[B]	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	M	401[B]	BCL	C5-C6-C7-C8
6	L	304[A]	U10	C9-C11-C12-C13
6	M	406	U10	C29-C31-C32-C33
10	L	312	GOL	C1-C2-C3-O3
10	H	305	GOL	O1-C1-C2-C3
13	M	408	PC1	C3-C2-O21-C21
4	L	302	LDA	C2-C3-C4-C5
7	M	401[A]	BCL	C16-C17-C18-C19
4	L	301	LDA	C7-C8-C9-C10
7	M	402	BCL	CBA-CGA-O2A-C1
10	L	314	GOL	O1-C1-C2-O2
10	M	410	GOL	O1-C1-C2-O2
10	H	305	GOL	O1-C1-C2-O2
7	M	402	BCL	O1A-CGA-O2A-C1
4	H	304	LDA	C11-C10-C9-C8
4	L	302	LDA	C7-C8-C9-C10
13	M	408	PC1	C29-C2A-C2B-C2C
4	L	302	LDA	C3-C4-C5-C6
4	H	304	LDA	C7-C8-C9-C10
4	M	412	LDA	C1-C2-C3-C4
7	M	401[A]	BCL	C16-C17-C18-C20
12	M	407	SPO	C1-C4-C5-C6
13	M	408	PC1	C25-C26-C27-C28
4	H	309	LDA	C3-C4-C5-C6
7	M	401[B]	BCL	C8-C10-C11-C12
5	L	313	BPH	C15-C16-C17-C18
13	M	408	PC1	C26-C27-C28-C29
5	L	313	BPH	C16-C17-C18-C19
10	H	302	GOL	O2-C2-C3-O3
10	H	303	GOL	O2-C2-C3-O3
5	L	313	BPH	C8-C10-C11-C12
4	H	309	LDA	C1-C2-C3-C4
4	H	309	LDA	C11-C10-C9-C8
7	M	401[B]	BCL	C14-C13-C15-C16
4	L	301	LDA	C3-C4-C5-C6
4	L	301	LDA	C2-C3-C4-C5
4	L	302	LDA	C5-C6-C7-C8
4	H	309	LDA	C7-C8-C9-C10
4	L	301	LDA	C6-C7-C8-C9
4	H	309	LDA	C9-C10-C11-C12
5	L	313	BPH	C16-C17-C18-C20
10	L	308	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	M	402	BCL	C6-C7-C8-C9
4	M	412	LDA	C7-C8-C9-C10
7	M	402	BCL	C11-C10-C8-C7
13	M	408	PC1	C22-C23-C24-C25
4	H	309	LDA	C5-C6-C7-C8
5	L	303	BPH	C2-C3-C5-C6
4	M	412	LDA	C3-C4-C5-C6
7	M	401[A]	BCL	C6-C7-C8-C9
10	H	307	GOL	O1-C1-C2-O2
7	M	401[B]	BCL	C3-C5-C6-C7
13	M	408	PC1	C23-C24-C25-C26
4	L	301	LDA	C11-C10-C9-C8
4	M	404	LDA	C1-C2-C3-C4
5	L	303	BPH	C4-C3-C5-C6
4	M	412	LDA	C6-C7-C8-C9
4	H	304	LDA	C1-C2-C3-C4
4	M	404	LDA	C2-C1-N1-CM1
13	M	408	PC1	O13-C11-C12-N
4	M	404	LDA	C3-C4-C5-C6
5	L	303	BPH	C8-C10-C11-C12
4	L	302	LDA	C1-C2-C3-C4
4	L	301	LDA	C1-C2-C3-C4
7	M	401[A]	BCL	CHA-CBD-CGD-O1D
7	M	401[A]	BCL	CHA-CBD-CGD-O2D
7	M	401[B]	BCL	CHA-CBD-CGD-O1D
7	M	401[B]	BCL	CHA-CBD-CGD-O2D
4	M	404	LDA	C5-C6-C7-C8
7	L	305	BCL	C16-C17-C18-C20
4	L	301	LDA	C4-C5-C6-C7
4	M	412	LDA	N1-C1-C2-C3
9	H	308	HTO	O3-C3-C4-C5
9	L	307	HTO	C3-C4-C5-C6
6	M	406	U10	C35-C34-C36-C37
4	L	302	LDA	C11-C10-C9-C8
6	M	406	U10	C33-C34-C36-C37
7	M	403	BCL	C15-C16-C17-C18
6	M	406	U10	C5-C4-O4-C4M
9	L	307	HTO	C4-C5-C6-C7
5	L	303	BPH	C14-C13-C15-C16
7	M	402	BCL	C11-C10-C8-C9
6	M	406	U10	C25-C24-C26-C27
6	M	406	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
7	M	401[B]	BCL	C6-C7-C8-C9
13	M	408	PC1	C2-C1-O11-P
9	H	308	HTO	C4-C5-C6-C7
13	M	408	PC1	C31-C32-C33-C34
7	M	403	BCL	CAA-CBA-CGA-O2A
7	M	402	BCL	C4C-C3C-CAC-CBC
13	M	408	PC1	C27-C28-C29-C2A
4	L	302	LDA	C9-C10-C11-C12
5	L	303	BPH	O2A-C1-C2-C3
10	H	303	GOL	O1-C1-C2-O2
4	H	304	LDA	C6-C7-C8-C9
5	L	303	BPH	C16-C17-C18-C20
9	L	307	HTO	O3-C3-C4-C5
10	H	307	GOL	O2-C2-C3-O3
6	L	304[B]	U10	C2-C3-O3-C3M
13	M	408	PC1	O31-C31-C32-C33
7	L	305	BCL	C2-C1-O2A-CGA
4	M	412	LDA	C5-C6-C7-C8
13	M	408	PC1	O32-C31-C32-C33
5	L	303	BPH	C13-C15-C16-C17

There are no ring outliers.

21 monomers are involved in 58 short contacts:

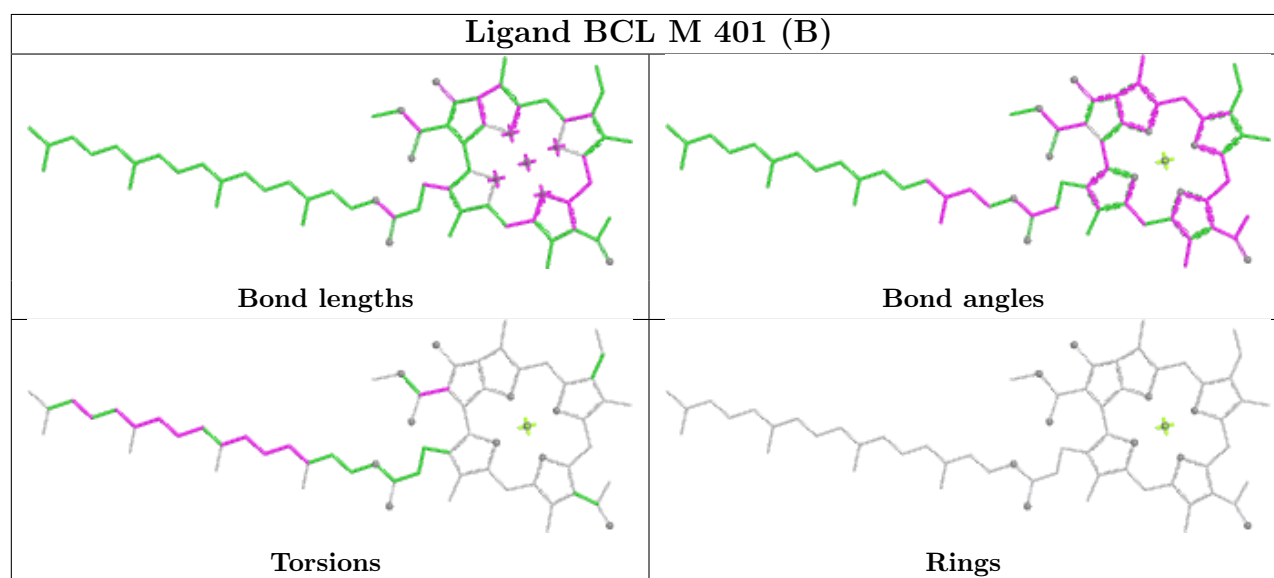
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	401[B]	BCL	3	0
4	M	412	LDA	3	0
4	L	302	LDA	1	0
5	L	303	BPH	3	0
7	M	403	BCL	11	0
12	M	407	SPO	1	0
9	H	308	HTO	1	0
6	L	304[B]	U10	6	0
8	L	306	PO4	1	0
7	M	401[A]	BCL	1	0
5	L	313	BPH	7	0
8	M	411	PO4	3	0
10	H	301	GOL	4	0
10	L	314	GOL	5	0
10	L	308	GOL	1	0
10	L	312	GOL	1	0
6	L	304[A]	U10	3	0

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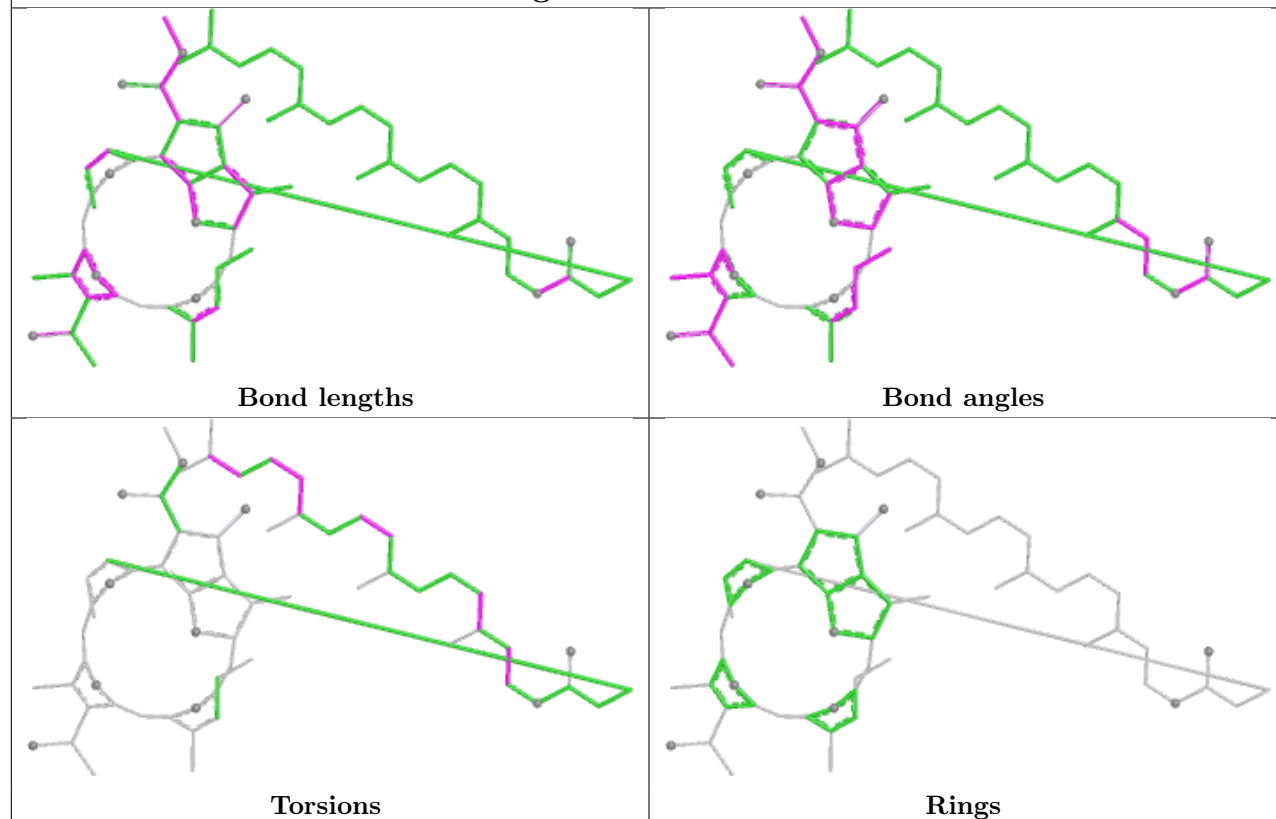
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	307	GOL	1	0
7	M	402	BCL	6	0
4	H	304	LDA	3	0
6	M	406	U10	2	0

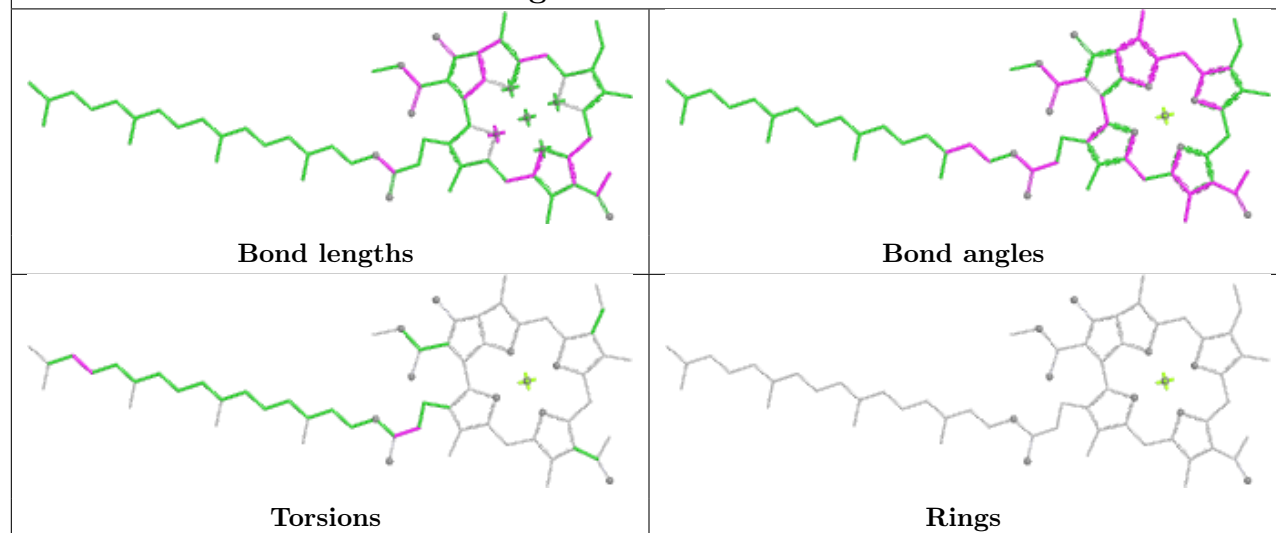
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

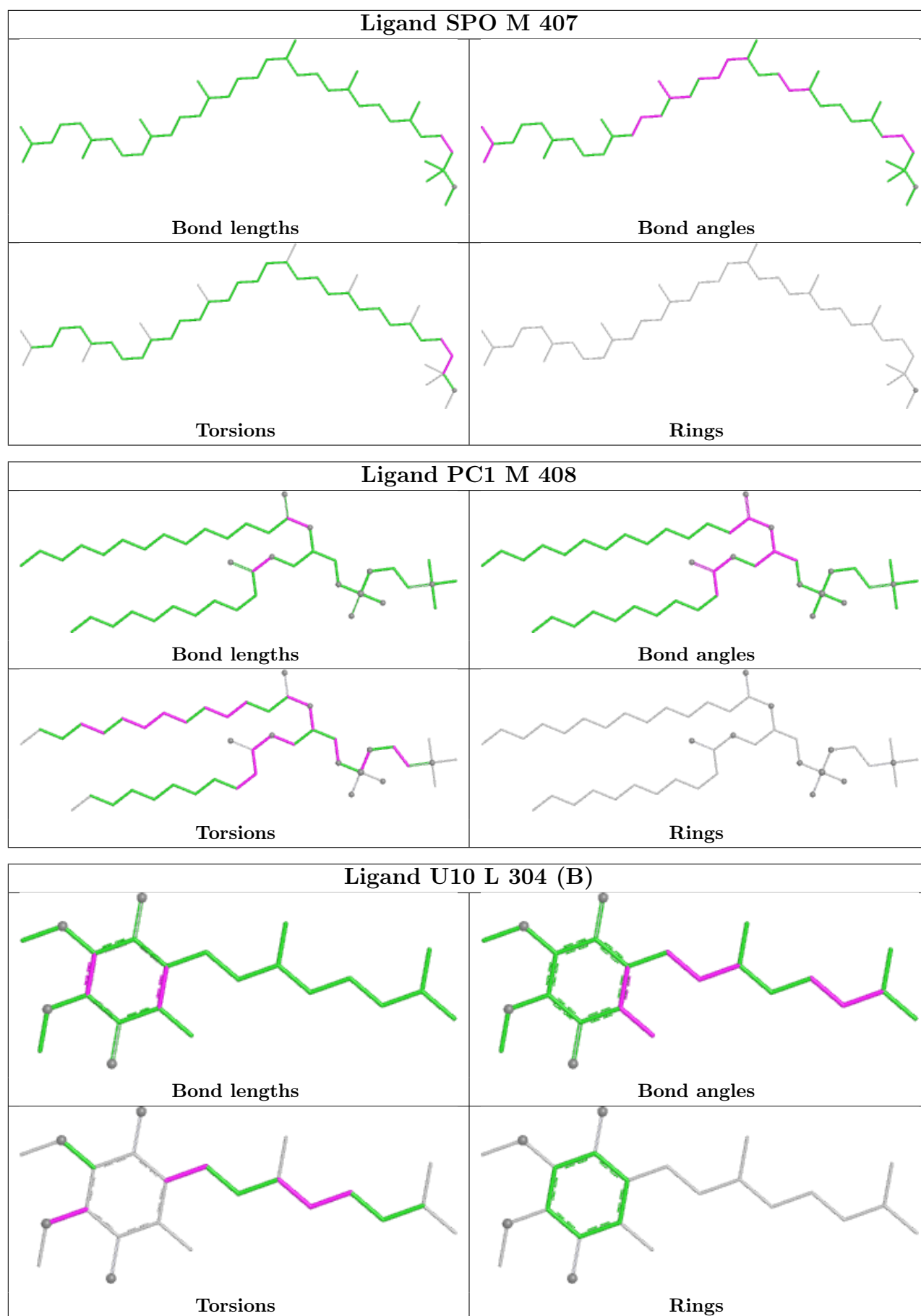


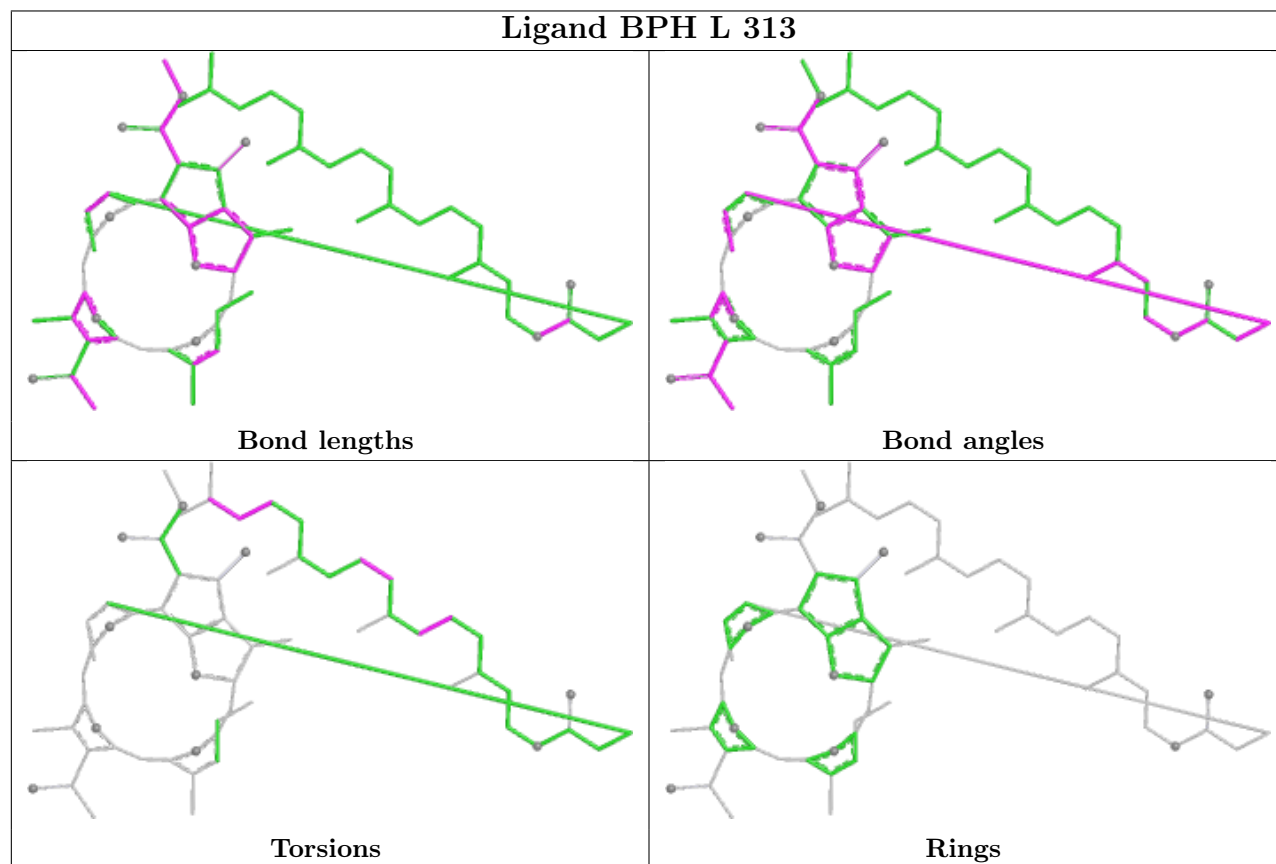
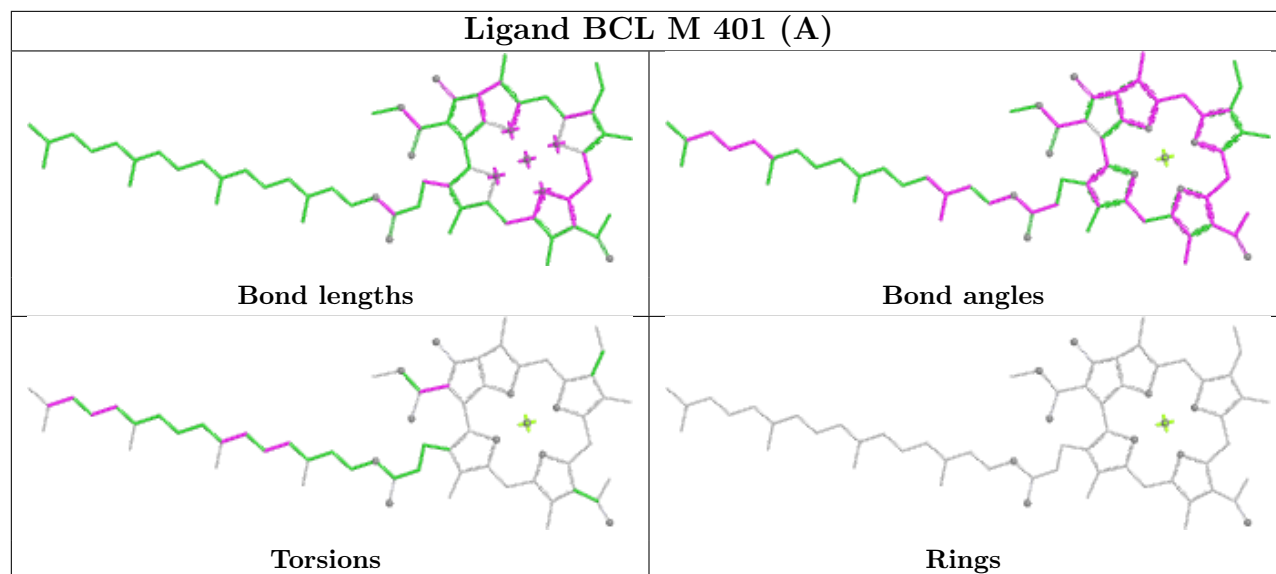
Ligand BPH L 303

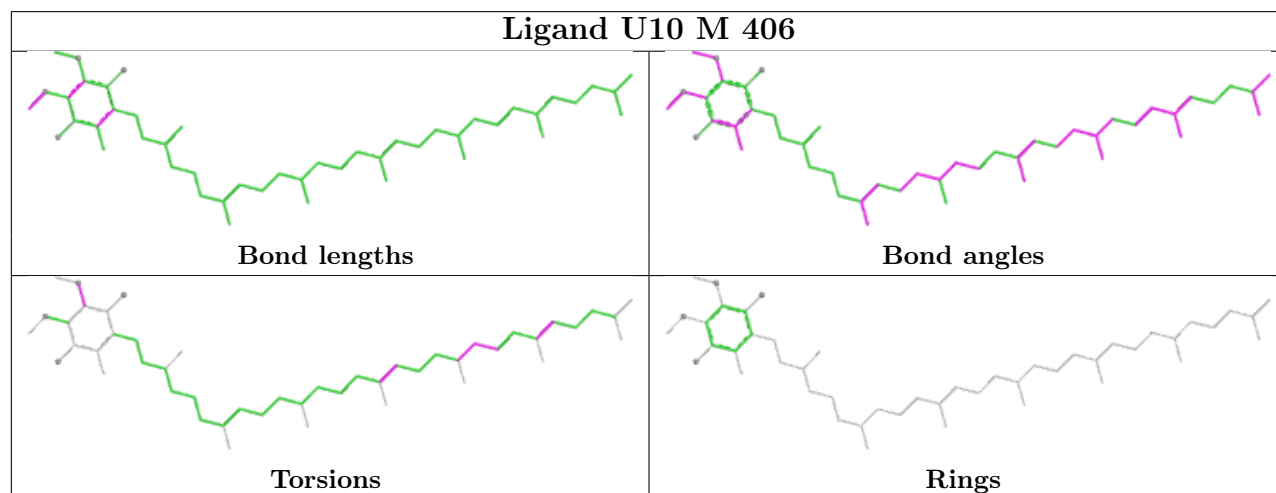
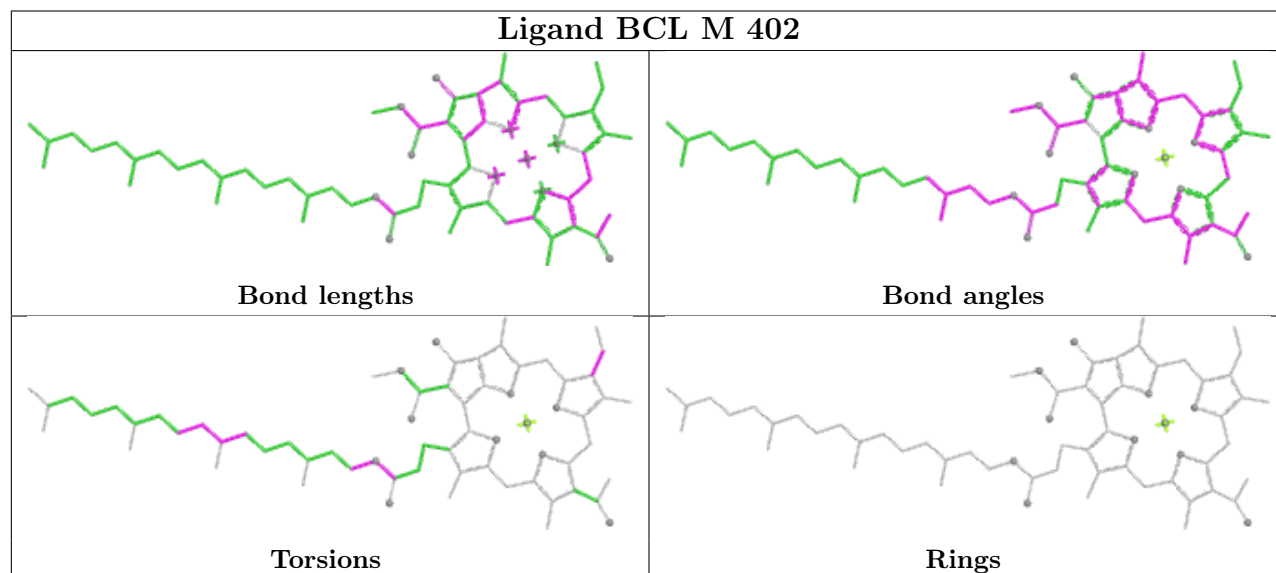
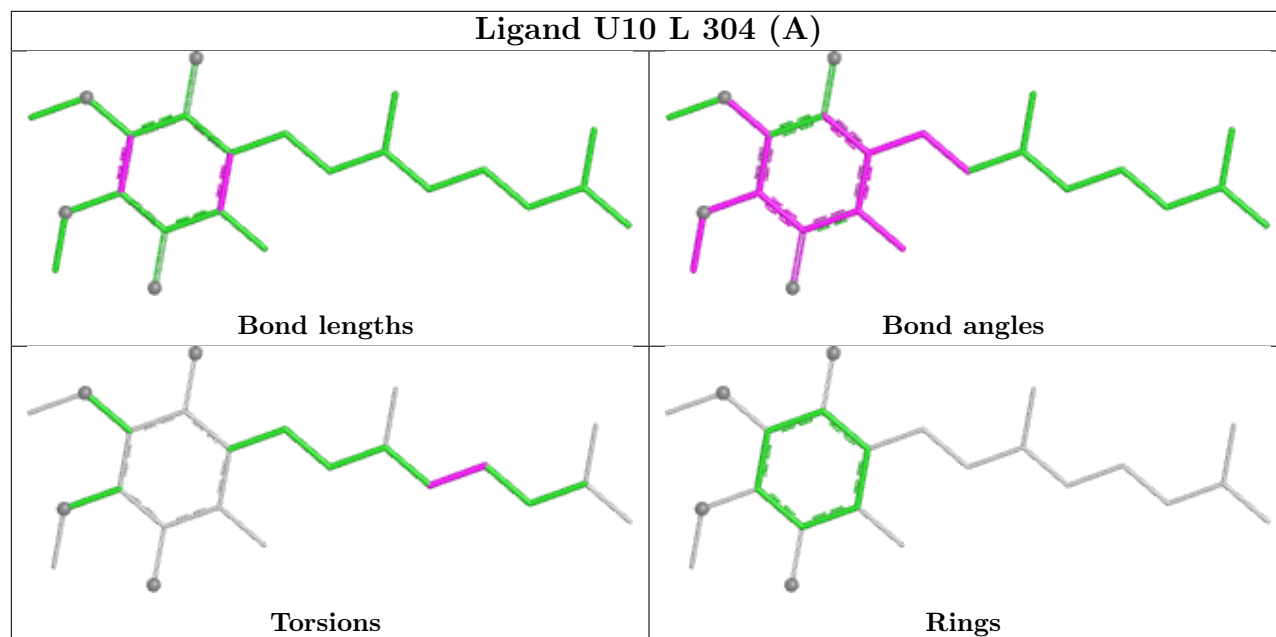


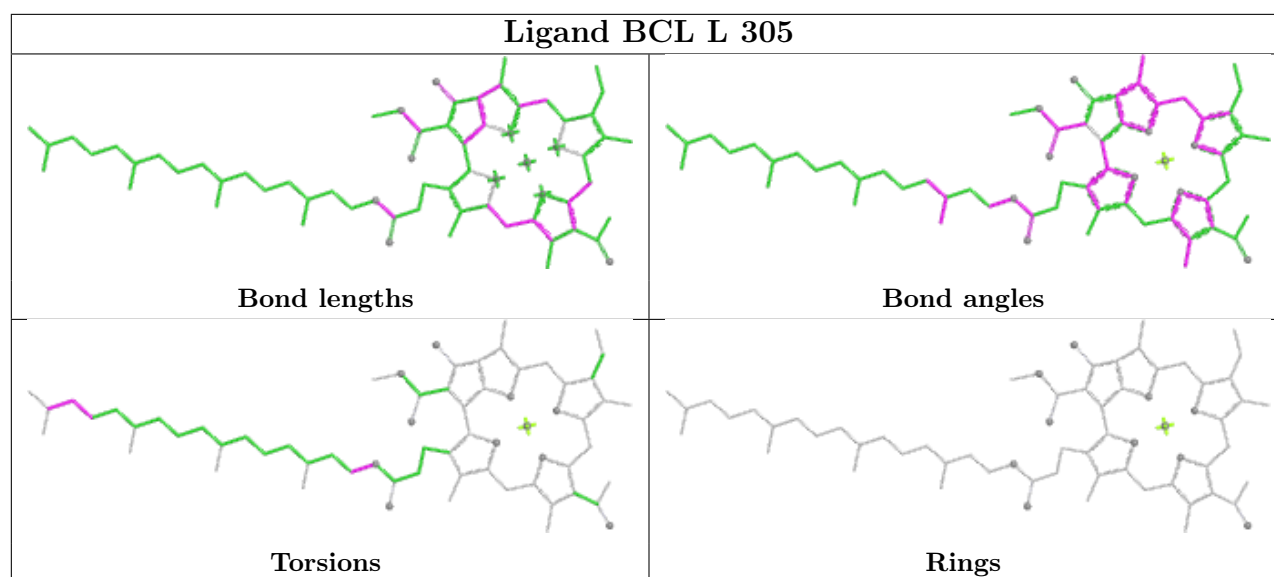
Ligand BCL M 403











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/282 (99%)	0.21	7 (2%) 58 55	28, 38, 63, 83	2 (0%)
2	M	302/307 (98%)	0.27	10 (3%) 49 46	29, 42, 63, 104	7 (2%)
3	H	240/266 (90%)	0.09	6 (2%) 58 55	30, 40, 56, 106	8 (3%)
All	All	823/855 (96%)	0.20	23 (2%) 55 52	28, 40, 62, 106	17 (2%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	17.6
2	M	2	GLU	9.8
2	M	301	HIS	7.0
3	H	250	SER	6.3
3	H	249[A]	LYS	5.9
2	M	52	LEU	4.8
3	H	184	LYS	4.4
2	M	302	GLY	4.2
1	L	277	GLY	4.0
1	L	271[A]	TRP	3.5
2	M	148	TRP	3.2
1	L	59	TRP	3.1
1	L	67	TYR	3.1
3	H	94	GLU	3.0
3	H	197	LYS	2.6
2	M	105	PHE	2.5
2	M	3	TYR	2.5
1	L	155	ASP	2.5
3	H	60	LYS	2.4
1	L	56	GLN	2.4
1	L	264	GLN	2.1
2	M	72	ILE	2.1
2	M	300	ASN	2.1

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 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.

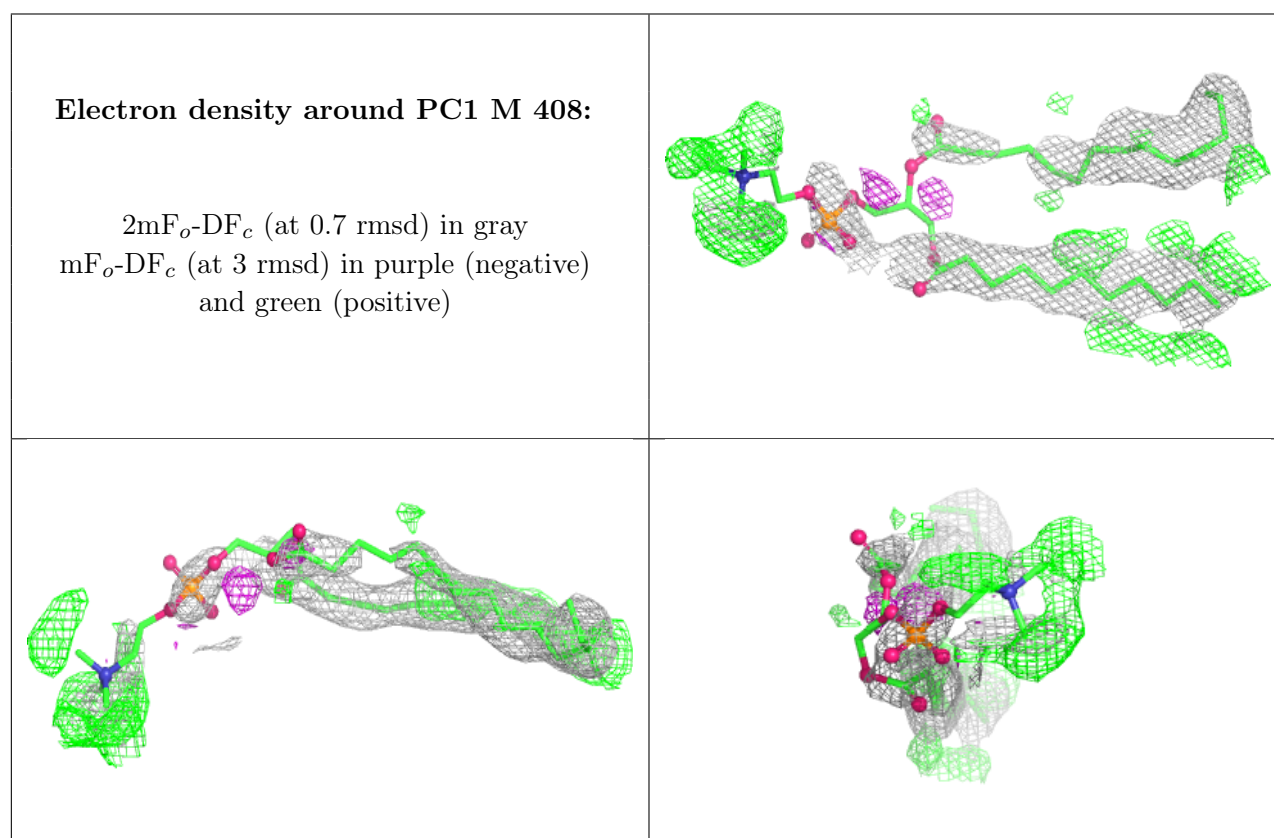
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	PC1	M	408	43/54	0.63	0.45	78,108,166,179	0
9	HTO	H	308	10/10	0.67	0.34	71,98,111,112	0
9	HTO	L	307	10/10	0.75	0.38	75,90,100,103	0
4	LDA	H	309	16/16	0.78	0.38	78,89,134,144	0
4	LDA	L	302	16/16	0.78	0.40	91,97,115,118	0
8	PO4	M	409	5/5	0.80	0.12	63,69,76,81	0
4	LDA	M	412	16/16	0.81	0.30	66,76,87,101	0
4	LDA	L	301	16/16	0.81	0.36	84,96,122,123	0
10	GOL	H	301	6/6	0.83	0.20	42,59,64,66	0
10	GOL	L	310	6/6	0.84	0.23	49,64,77,81	0
10	GOL	M	410	6/6	0.85	0.16	61,61,69,69	0
10	GOL	L	309	6/6	0.85	0.20	82,82,88,89	0
10	GOL	H	303	6/6	0.85	0.15	73,80,83,83	0
4	LDA	M	404	16/16	0.85	0.27	66,78,98,98	0
10	GOL	H	302	6/6	0.87	0.21	68,76,78,88	0
6	U10	L	304[A]	23/63	0.90	0.22	32,59,75,78	23
6	U10	L	304[B]	23/63	0.90	0.22	47,64,69,74	23
10	GOL	L	314	6/6	0.91	0.19	58,69,75,77	0
7	BCL	M	401[B]	66/66	0.91	0.17	24,35,62,70	20
10	GOL	L	308	6/6	0.91	0.18	42,58,66,72	0
4	LDA	H	304	16/16	0.91	0.18	49,66,81,82	0
7	BCL	M	401[A]	66/66	0.91	0.17	24,35,53,65	20
10	GOL	H	305	6/6	0.91	0.15	41,49,58,68	0
10	GOL	L	311	6/6	0.91	0.17	54,67,77,82	0
10	GOL	H	307	6/6	0.93	0.16	56,73,81,85	0
10	GOL	L	312	6/6	0.93	0.13	53,55,60,61	0
6	U10	M	406	48/63	0.94	0.14	30,53,78,90	0

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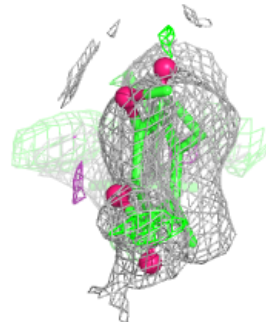
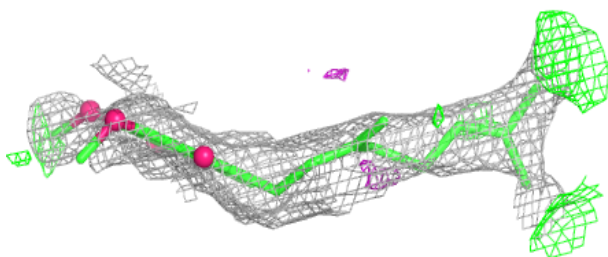
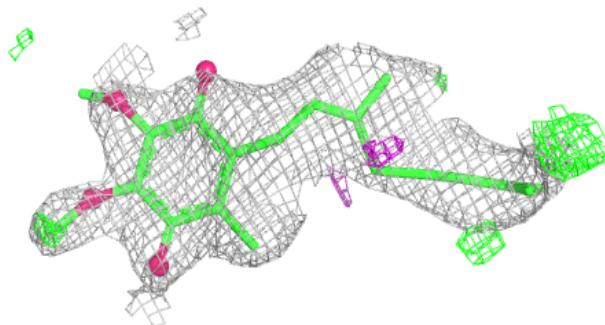
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	SPO	M	407	42/42	0.95	0.12	34,43,80,96	0
5	BPH	L	313	65/65	0.95	0.13	31,41,118,122	0
8	PO4	L	306	5/5	0.96	0.11	56,56,61,64	0
5	BPH	L	303	65/65	0.96	0.09	27,34,44,49	0
7	BCL	L	305	66/66	0.97	0.08	28,35,50,71	0
7	BCL	M	402	66/66	0.97	0.10	29,36,81,84	0
7	BCL	M	403	66/66	0.97	0.08	28,33,55,81	0
8	PO4	M	411	5/5	0.98	0.07	47,48,60,64	0
14	K	H	306	1/1	0.98	0.05	46,46,46,46	0
11	FE	M	405	1/1	1.00	0.01	30,30,30,30	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.

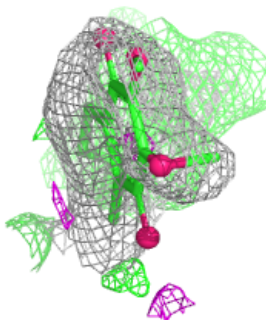
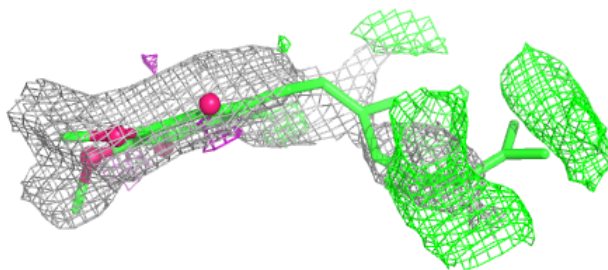
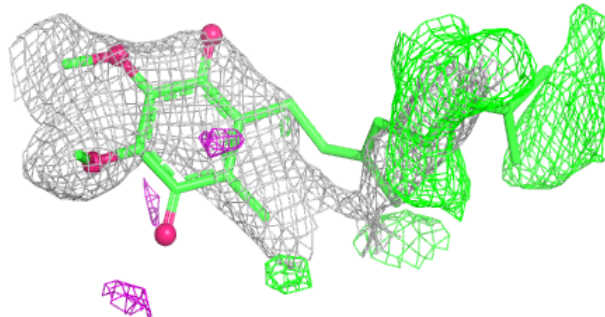


Electron density around U10 L 304 (A):

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

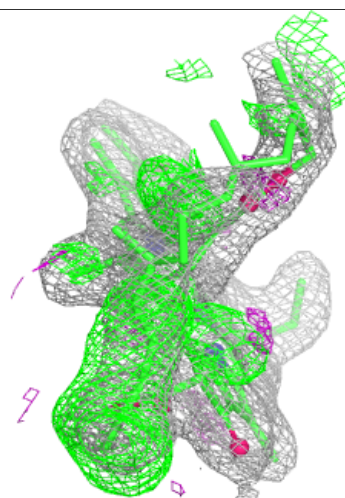
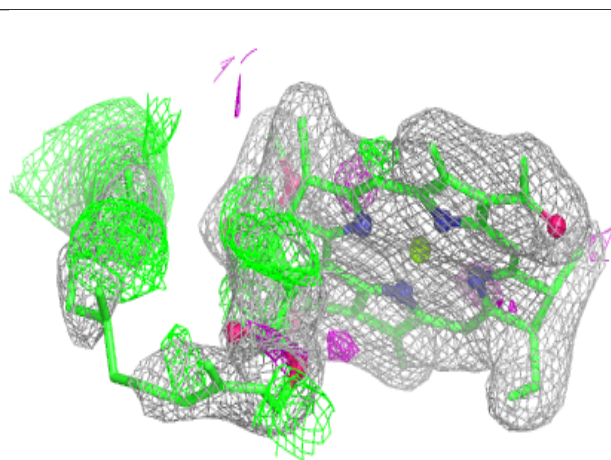
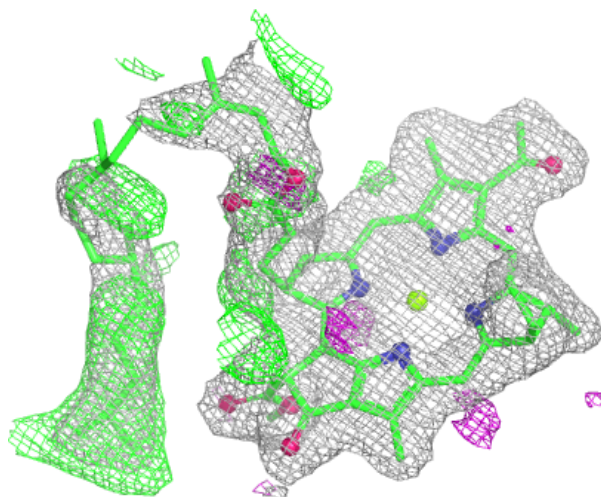
**Electron density around U10 L 304 (B):**

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



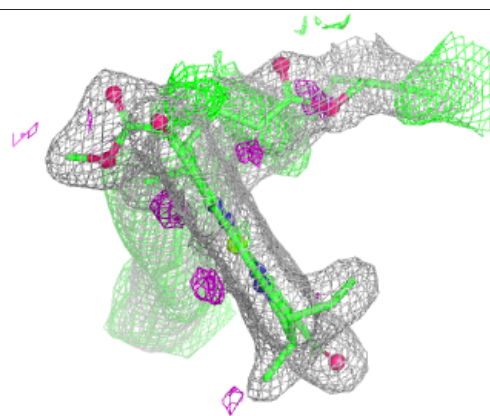
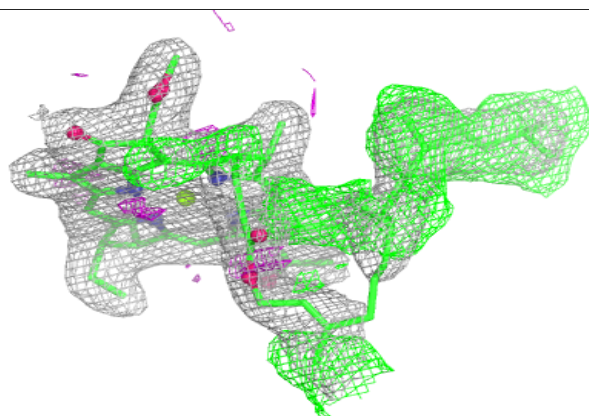
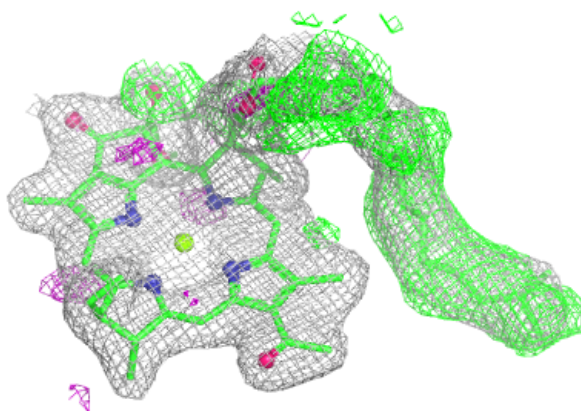
Electron density around BCL M 401 (B):

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

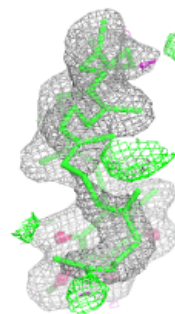
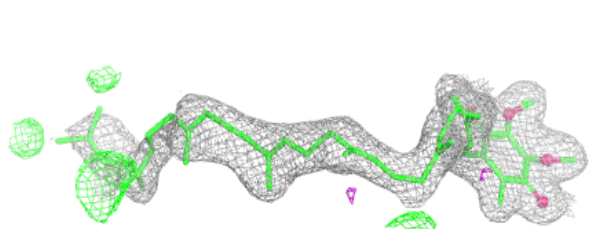
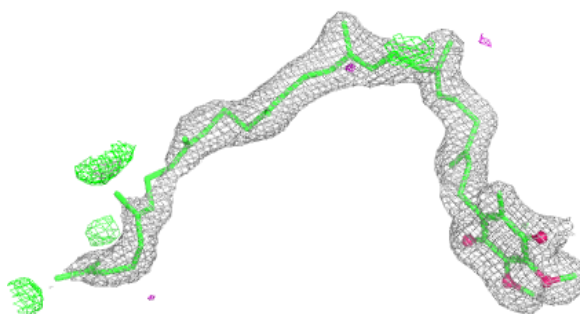


Electron density around BCL M 401 (A):

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

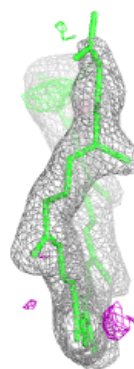
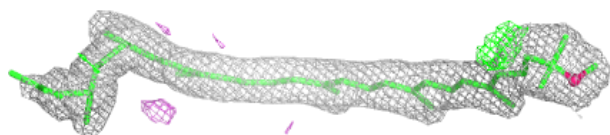
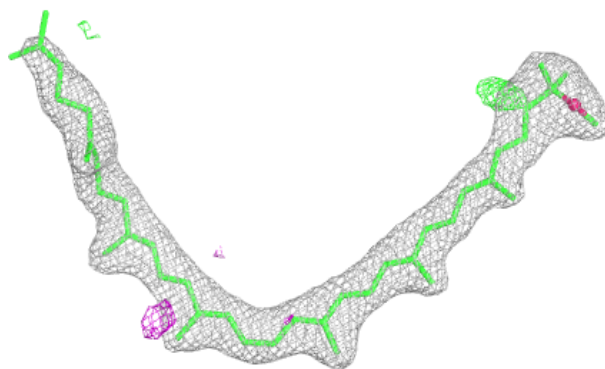
**Electron density around U10 M 406:**

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

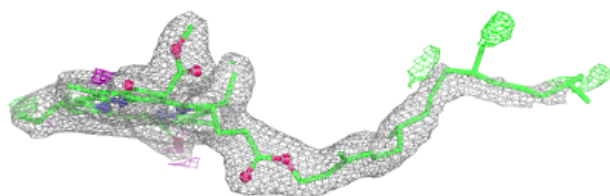
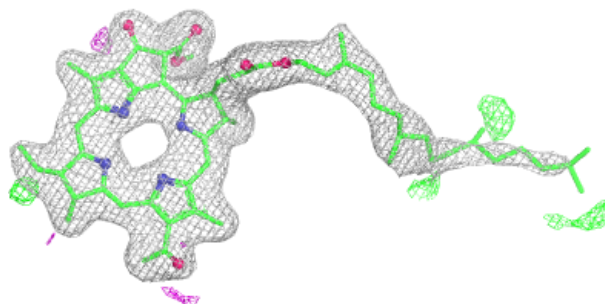


Electron density around SPO M 407:

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

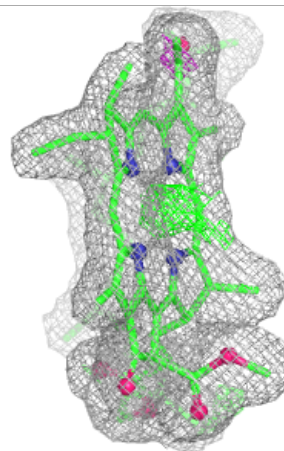
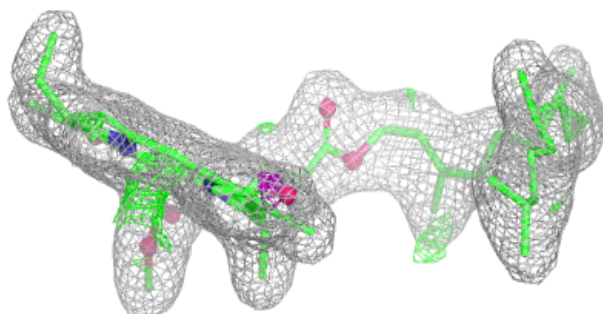
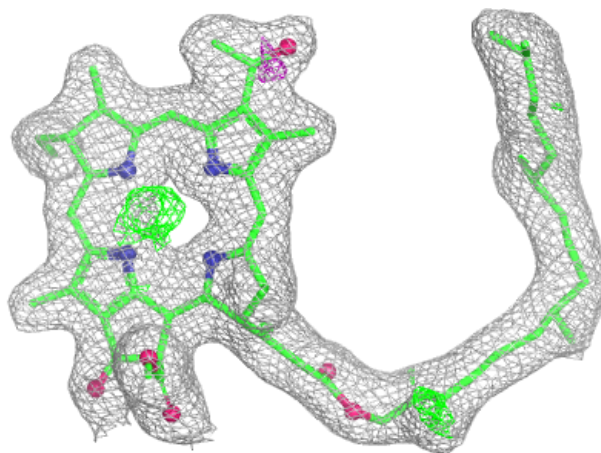
**Electron density around BPH L 313:**

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



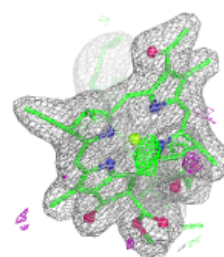
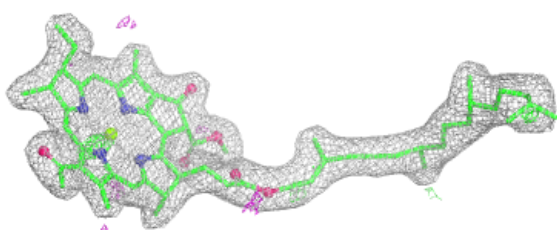
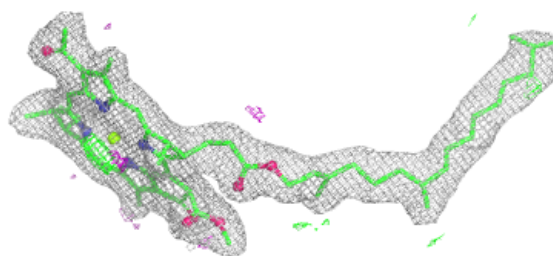
Electron density around BPH L 303:

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

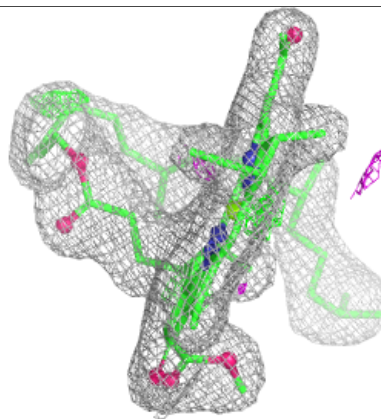
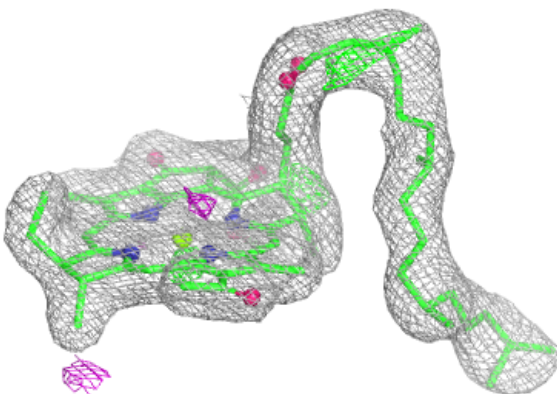
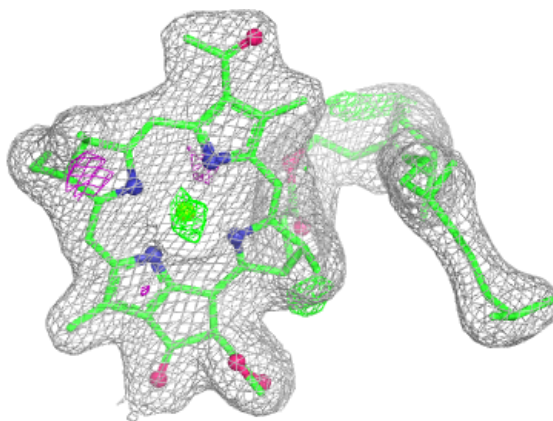


Electron density around BCL L 305:

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

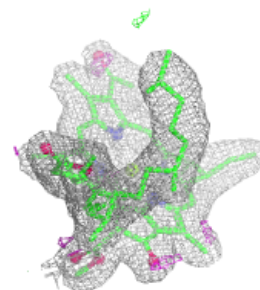
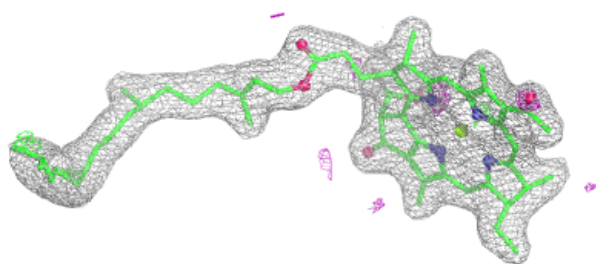
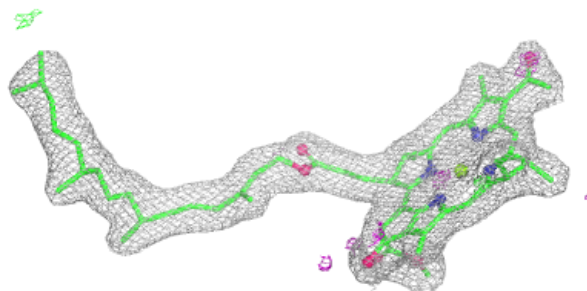
**Electron density around BCL M 402:**

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



Electron density around BCL M 403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.