



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 02:38 AM UTC

PDB ID : 7MH9 / pdb_00007mh9
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant;
Y(M210)3-nitrotyrosine
Authors : Mathews, I.; Weaver, J.; Boxer, S.G.
Deposited on : 2021-04-14
Resolution : 3.10 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

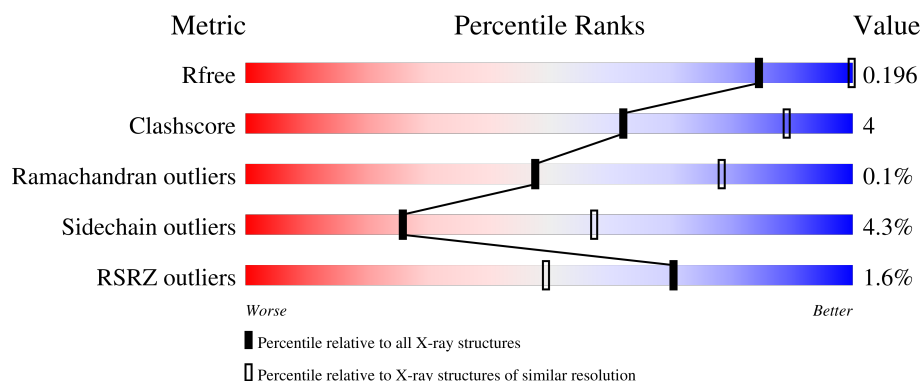
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	% 80% 10% 10%
2	L	282	2% 90% 9% .
3	M	308	% 86% 11% ..

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
6	BPH	L	406	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7240 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	0	0
			1829	1169	314	337	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	260	VAL	-	expression tag	UNP P0C0Y7
H	261	HIS	-	expression tag	UNP P0C0Y7
H	262	HIS	-	expression tag	UNP P0C0Y7
H	263	HIS	-	expression tag	UNP P0C0Y7
H	264	HIS	-	expression tag	UNP P0C0Y7
H	265	HIS	-	expression tag	UNP P0C0Y7
H	266	HIS	-	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	1	0
			2240	1513	356	363	8			

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

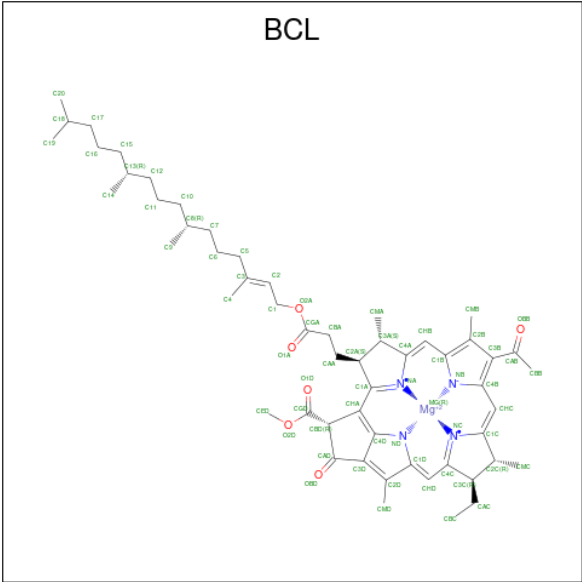
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2406	1604	394	398	10			

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



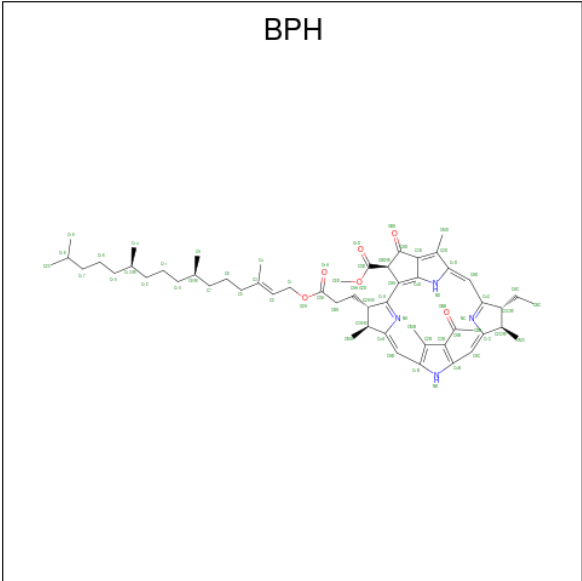
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



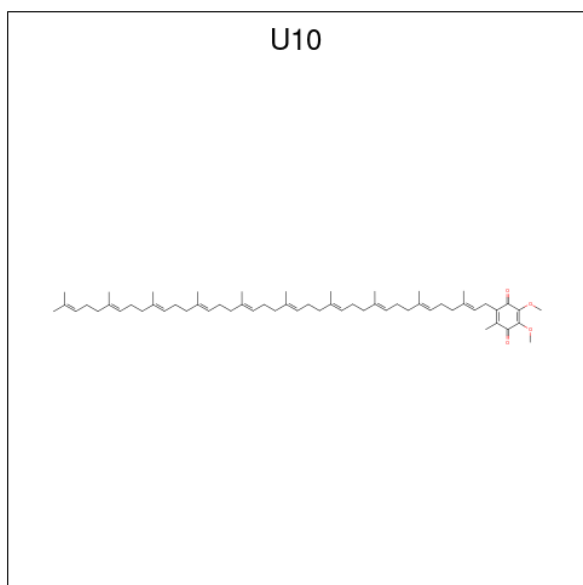
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			18	14	4		
7	M	1	Total	C	O	0	0
			48	44	4		

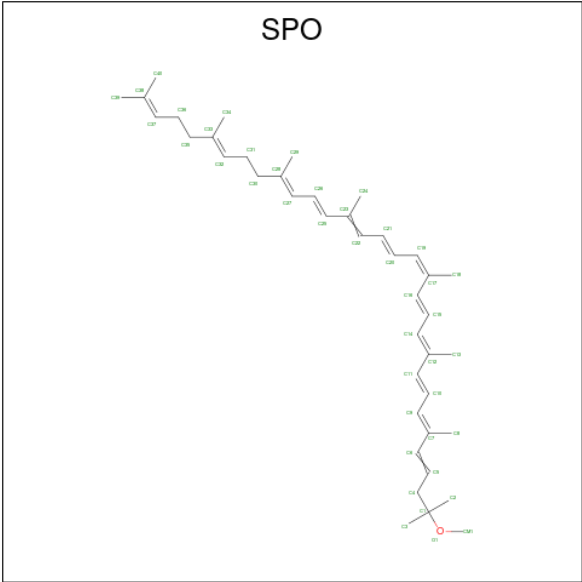
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Cl	0	0
			1	1		

- Molecule 9 is FE (III) ION (CCD ID: FE) (formula: Fe).

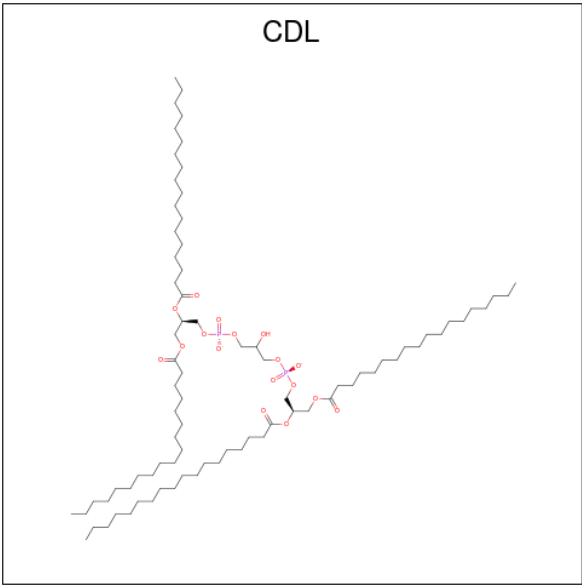
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			69	50	17	2		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	58	Total 58	O 58	0	0
12	L	31	Total 31	O 31	0	0
12	M	46	Total 48	O 48	0	2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.21Å 141.21Å 187.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.07 – 3.10 39.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.07-3.10) 99.9 (39.07-3.10)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.169 , 0.205 (Not available) , 0.196	Depositor DCC
R_{free} test set	1990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7240	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: U10, FE, LDA, CDL, CL, NIY, BCL, BPH, SPO

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	0.99	0/1877	1.40	1/2553 (0.0%)
2	L	0.96	0/2328	1.43	1/3186 (0.0%)
3	M	0.97	0/2481	1.48	0/3385
All	All	0.97	0/6686	1.44	2/9124 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	145	GLY	CA-C-O	-5.21	117.17	122.59
2	L	155	ASP	CB-CA-C	5.19	119.11	110.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	209	LEU	Mainchain

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	1829	0	1836	13	0
2	L	2240	0	2197	18	0
3	M	2406	0	2310	23	0
4	H	16	0	31	0	0
4	M	64	0	124	0	0
5	L	183	0	189	10	0
5	M	66	0	74	9	0
6	L	120	0	129	7	0
7	L	18	0	15	2	0
7	M	48	0	63	0	0
8	L	1	0	0	0	0
9	M	1	0	0	0	0
10	M	42	0	60	0	0
11	M	69	0	82	0	0
12	H	58	0	0	0	0
12	L	31	0	0	1	0
12	M	48	0	0	0	0
All	All	7240	0	7110	58	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 4.

All (58) 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)
1:H:201:ASN:H	1:H:201:ASN:HD22	1.31	0.77
5:L:401:BCL:HBB2	5:L:401:BCL:HHC	1.74	0.69
6:L:402:BPH:HBB2	3:M:210:NIY:HB2	1.75	0.68
6:L:402:BPH:HHC	6:L:402:BPH:HBB3	1.77	0.67
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.80	0.63
1:H:201:ASN:HD22	1:H:201:ASN:N	1.98	0.60
3:M:197:PHE:CZ	5:M:401:BCL:HBB2	2.37	0.60
5:M:401:BCL:HHC	5:M:401:BCL:HBB3	1.85	0.59
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.21	0.57
1:H:81:GLU:OE1	2:L:8:LYS:NZ	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:157:VAL:HG11	5:M:401:BCL:HBB1	1.86	0.56
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.41	0.55
2:L:181:PHE:CD2	6:L:406:BPH:HBB1	2.42	0.54
12:L:509:HOH:O	3:M:44:ASN:HB3	2.07	0.54
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.40	0.54
1:H:156:CYS:HB3	1:H:206:ASN:O	2.09	0.53
2:L:181:PHE:HB3	6:L:406:BPH:CBB	2.39	0.52
2:L:219:LEU:O	3:M:132:ARG:NH1	2.31	0.52
3:M:270:ILE:O	3:M:274:VAL:HG13	2.10	0.51
6:L:402:BPH:HBB1	3:M:210:NIY:CD2	2.40	0.51
1:H:140:PHE:HA	3:M:13:ARG:O	2.11	0.51
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.94	0.50
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.93	0.50
1:H:75:VAL:HA	1:H:76:PRO:C	2.37	0.49
2:L:181:PHE:HB3	6:L:406:BPH:HBB2	1.93	0.48
3:M:197:PHE:HZ	5:M:401:BCL:HBB2	1.78	0.48
5:L:405:BCL:HHC	5:L:405:BCL:CBB	2.44	0.48
5:L:405:BCL:HHC	5:L:405:BCL:HBB2	1.96	0.48
3:M:189:PHE:O	3:M:193:HIS:HD2	1.97	0.47
5:L:401:BCL:HBB3	5:L:404:BCL:H52	1.95	0.47
5:L:405:BCL:HBB3	5:M:401:BCL:H41	1.97	0.46
2:L:244:SER:OG	5:L:404:BCL:HMA2	2.15	0.46
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.52	0.45
5:M:401:BCL:HAA2	5:M:401:BCL:HBD	1.97	0.45
2:L:177:ILE:HD13	5:L:405:BCL:HMD2	1.99	0.45
3:M:197:PHE:HZ	5:M:401:BCL:CBB	2.30	0.45
1:H:201:ASN:H	1:H:201:ASN:ND2	2.09	0.44
2:L:216:PHE:CE1	7:L:403:U10:H72	2.53	0.44
5:L:404:BCL:HHC	5:L:404:BCL:OBB	2.18	0.44
3:M:187:ASN:HD22	5:M:401:BCL:HBC1	1.83	0.43
1:H:40:TYR:HA	1:H:41:PRO:C	2.44	0.43
5:L:404:BCL:HAA2	5:L:404:BCL:HBD	2.00	0.42
3:M:93:SER:OG	3:M:95:GLU:OE2	2.33	0.42
1:H:245:ALA:HA	1:H:248:ARG:NH2	2.35	0.42
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.82	0.42
3:M:194:GLY:O	3:M:195:ASN:HB3	2.20	0.41
3:M:136:ARG:CZ	3:M:136:ARG:HA	2.50	0.41
5:L:401:BCL:HMD2	3:M:206:ILE:HD13	2.02	0.41
2:L:182:THR:HG22	2:L:236:LEU:HD13	2.02	0.41
2:L:249:ILE:HD12	2:L:249:ILE:HA	1.89	0.41
2:L:210:ASP:OD1	2:L:210:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:GLY:O	2:L:21:LEU:HB2	2.21	0.40
2:L:216:PHE:CZ	7:L:403:U10:H72	2.56	0.40
1:H:245:ALA:N	1:H:246:PRO:CD	2.84	0.40
3:M:197:PHE:CE1	5:M:401:BCL:HBB2	2.55	0.40
1:H:63:THR:HA	1:H:73:LEU:O	2.22	0.40
2:L:48:LEU:CD1	2:L:88:ILE:HG22	2.52	0.40
6:L:406:BPH:H5C1	3:M:63:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/266 (90%)	232 (98%)	6 (2%)	0	100	100
2	L	280/282 (99%)	267 (95%)	13 (5%)	0	100	100
3	M	298/308 (97%)	284 (95%)	13 (4%)	1 (0%)	36	67
All	All	816/856 (95%)	783 (96%)	32 (4%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/215 (91%)	185 (95%)	10 (5%)	21	52
2	L	221/221 (100%)	212 (96%)	9 (4%)	27	59
3	M	235/240 (98%)	226 (96%)	9 (4%)	29	60
All	All	651/676 (96%)	623 (96%)	28 (4%)	26	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	92	VAL
1	H	118	ARG
1	H	173	GLU
1	H	197	LYS
1	H	200	SER
1	H	201	ASN
1	H	223	THR
1	H	231	ASP
2	L	17	VAL
2	L	21	LEU
2	L	82	LYS
2	L	158	SER
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	235	LEU
2	L	247	CYS
3	M	37	THR
3	M	39	LEU
3	M	47	LEU
3	M	60	LEU
3	M	72	ILE
3	M	170	SER
3	M	196	LEU
3	M	278	LEU
3	M	292	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS

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Mol	Chain	Res	Type
1	H	201	ASN
1	H	206	ASN
2	L	159	ASN
2	L	183	ASN
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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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$
3	NIY	M	210	3	14,15,16	1.19	2 (14%)	11,20,22	1.18	1 (9%)

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
3	NIY	M	210	3	-	2/7/10/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	NIY	CE1-NN	-3.02	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	NIY	O1-NN	-2.21	1.20	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	210	NIY	O2-NN-CE1	2.93	124.04	119.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	NIY	CA-CB-CG-CD1
3	M	210	NIY	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	210	NIY	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
5	BCL	L	405	-	54,59,74	1.98	15 (27%)	61,97,115	2.35	20 (32%)
5	BCL	M	401	-	69,74,74	1.71	16 (23%)	79,115,115	2.16	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	U10	L	403	-	18,18,63	1.00	1 (5%)	24,25,79	1.13	3 (12%)
7	U10	M	407	-	48,48,63	0.67	3 (6%)	60,61,79	0.56	0
10	SPO	M	408	-	41,41,41	1.26	6 (14%)	47,50,50	1.20	7 (14%)
4	LDA	M	403	-	13,15,15	0.16	0	14,17,17	0.29	0
4	LDA	M	402	-	13,15,15	0.26	0	14,17,17	0.34	0
5	BCL	L	404	-	69,74,74	1.69	15 (21%)	79,115,115	2.11	21 (26%)
4	LDA	M	404	-	13,15,15	0.16	0	14,17,17	0.22	0
11	CDL	M	409	-	68,68,99	0.39	0	74,80,111	0.44	0
5	BCL	L	401	-	69,74,74	1.71	16 (23%)	79,115,115	2.18	21 (26%)
4	LDA	M	405	-	13,15,15	0.17	0	14,17,17	0.21	0
4	LDA	H	401	-	13,15,15	0.15	0	14,17,17	0.40	0
6	BPH	L	406	-	49,60,70	0.91	2 (4%)	47,89,101	1.20	4 (8%)
6	BPH	L	402	-	59,70,70	0.81	2 (3%)	59,101,101	1.01	3 (5%)

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
5	BCL	L	405	-	-	2/23/119/137	-
5	BCL	M	401	-	-	8/41/137/137	-
7	U10	L	403	-	-	5/9/33/87	0/1/1/1
7	U10	M	407	-	-	8/45/69/87	0/1/1/1
10	SPO	M	408	-	-	3/47/47/47	-
4	LDA	M	403	-	-	5/13/13/13	-
4	LDA	M	402	-	-	6/13/13/13	-
5	BCL	L	404	-	-	2/41/137/137	-
4	LDA	M	404	-	-	3/13/13/13	-
11	CDL	M	409	-	-	29/79/79/110	-
5	BCL	L	401	-	-	9/41/137/137	-
4	LDA	M	405	-	-	4/13/13/13	-
4	LDA	H	401	-	-	7/13/13/13	-
6	BPH	L	406	-	1/1/16/22	7/25/93/105	0/5/6/6
6	BPH	L	402	-	-	7/37/105/105	0/5/6/6

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	404	BCL	O2D-CGD	5.35	1.46	1.33
5	L	401	BCL	O2D-CGD	5.14	1.45	1.33
5	L	405	BCL	O2D-CGD	5.05	1.45	1.33
5	L	405	BCL	O2A-CGA	4.87	1.47	1.33
5	M	401	BCL	O2D-CGD	4.74	1.44	1.33
5	L	405	BCL	C3D-C4D	-4.59	1.33	1.44
5	L	401	BCL	C3D-C4D	-4.49	1.34	1.44
5	M	401	BCL	C3D-C4D	-4.48	1.34	1.44
5	L	404	BCL	C3D-C4D	-4.41	1.34	1.44
5	L	401	BCL	O2A-CGA	4.17	1.45	1.33
5	L	405	BCL	CHB-C1B	4.09	1.48	1.39
5	L	405	BCL	C3B-C4B	3.99	1.49	1.41
6	L	406	BPH	C4D-CHA	3.96	1.45	1.39
5	L	404	BCL	O2A-CGA	3.95	1.44	1.33
5	M	401	BCL	OBD-CAD	3.86	1.29	1.22
5	L	404	BCL	CHC-C4B	3.80	1.47	1.39
5	M	401	BCL	O2A-CGA	3.79	1.44	1.33
5	M	401	BCL	C3B-C4B	3.74	1.48	1.41
5	L	401	BCL	CHB-C1B	3.67	1.47	1.39
5	L	404	BCL	C3B-C4B	3.65	1.48	1.41
5	L	405	BCL	CHD-C1D	3.59	1.45	1.38
5	M	401	BCL	CHD-C1D	3.55	1.45	1.38
5	M	401	BCL	CHB-C1B	3.35	1.46	1.39
5	L	401	BCL	C3B-C4B	3.35	1.47	1.41
5	L	401	BCL	OBD-CAD	3.34	1.28	1.22
5	L	405	BCL	OBD-CAD	3.29	1.28	1.22
5	L	404	BCL	OBD-CAD	3.28	1.28	1.22
5	L	405	BCL	CHC-C4B	3.24	1.46	1.39
5	L	401	BCL	CHC-C4B	3.23	1.46	1.39
6	L	402	BPH	C4D-CHA	3.17	1.44	1.39
6	L	402	BPH	C1B-C2B	3.16	1.43	1.39
5	L	404	BCL	CHB-C1B	3.16	1.46	1.39
5	L	401	BCL	C3D-C2D	3.09	1.47	1.39
5	L	404	BCL	CHD-C1D	3.06	1.44	1.38
5	L	405	BCL	C3D-C2D	3.04	1.47	1.39
5	L	405	BCL	CHD-C4C	3.01	1.47	1.39
5	M	401	BCL	CHC-C4B	3.00	1.46	1.39
5	L	404	BCL	CHD-C4C	2.91	1.47	1.39
5	L	401	BCL	CHD-C1D	2.87	1.44	1.38
5	M	401	BCL	CHD-C4C	2.86	1.47	1.39
7	L	403	U10	C3-C2	-2.86	1.40	1.48
5	L	401	BCL	MG-NA	-2.81	1.99	2.06
5	L	401	BCL	C1D-ND	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	401	BCL	C3D-C2D	2.72	1.46	1.39
5	L	404	BCL	C3D-C2D	2.67	1.46	1.39
10	M	408	SPO	C25-C23	-2.64	1.40	1.46
5	L	404	BCL	C1B-C2B	2.55	1.49	1.43
10	M	408	SPO	C9-C7	2.54	1.41	1.35
6	L	406	BPH	C1B-C2B	2.52	1.42	1.39
5	L	404	BCL	C1D-ND	-2.50	1.34	1.37
5	L	401	BCL	CHD-C4C	2.46	1.46	1.39
10	M	408	SPO	C11-C12	-2.41	1.40	1.46
5	L	405	BCL	C1D-C2D	2.36	1.50	1.45
5	L	401	BCL	C1B-C2B	2.35	1.48	1.43
10	M	408	SPO	C14-C12	2.35	1.41	1.35
10	M	408	SPO	C22-C23	2.34	1.41	1.35
5	M	401	BCL	C1B-NB	-2.32	1.34	1.37
5	M	401	BCL	C1D-C2D	2.32	1.49	1.45
5	M	401	BCL	C1D-ND	-2.31	1.34	1.37
5	L	405	BCL	C1B-C2B	2.26	1.48	1.43
5	L	405	BCL	C1D-ND	-2.25	1.34	1.37
10	M	408	SPO	C19-C17	2.25	1.41	1.35
5	L	401	BCL	C4B-NB	-2.22	1.34	1.37
7	M	407	U10	C6-C1	2.21	1.39	1.35
7	M	407	U10	C4-C5	-2.17	1.42	1.48
5	M	401	BCL	MG-NA	-2.16	2.01	2.06
5	L	405	BCL	C4B-NB	-2.15	1.35	1.37
5	L	404	BCL	C4D-CHA	2.14	1.45	1.38
5	M	401	BCL	C1B-C2B	2.14	1.48	1.43
5	L	404	BCL	MG-NC	-2.13	2.01	2.06
5	L	405	BCL	MG-NA	-2.13	2.01	2.06
5	M	401	BCL	C4B-NB	-2.11	1.35	1.37
5	L	401	BCL	C1D-C2D	2.04	1.49	1.45
5	L	404	BCL	C1D-C2D	2.03	1.49	1.45
7	M	407	U10	C3-C2	-2.03	1.43	1.48
5	L	401	BCL	C4D-CHA	2.02	1.45	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BCL	CMD-C2D-C1D	8.04	138.89	124.73
5	L	404	BCL	CMD-C2D-C1D	7.77	138.42	124.73
5	L	405	BCL	CMD-C2D-C1D	7.22	137.44	124.73
5	L	401	BCL	CMD-C2D-C1D	6.91	136.89	124.73
5	M	401	BCL	C2B-C1B-NB	5.57	116.10	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	404	BCL	C2B-C1B-NB	5.34	115.86	110.33
5	L	405	BCL	O2D-CGD-CBD	5.25	120.41	111.23
5	L	401	BCL	CHD-C1D-ND	-5.23	117.44	124.80
5	M	401	BCL	CHD-C1D-ND	-5.23	117.44	124.80
5	L	401	BCL	C2B-C1B-NB	5.23	115.75	110.33
5	L	405	BCL	CHD-C1D-ND	-5.12	117.60	124.80
5	L	404	BCL	CHD-C1D-ND	-4.92	117.88	124.80
5	L	404	BCL	C3D-C2D-C1D	-4.92	99.12	105.83
5	L	401	BCL	C3D-C2D-C1D	-4.88	99.17	105.83
5	L	405	BCL	C3D-C2D-C1D	-4.88	99.17	105.83
5	L	404	BCL	C1D-ND-C4D	-4.85	102.91	106.31
5	L	401	BCL	C1C-NC-C4C	-4.80	104.49	106.68
6	L	406	BPH	C4D-CHA-CBD	-4.73	106.19	108.45
5	M	401	BCL	C3D-C2D-C1D	-4.55	99.63	105.83
5	L	405	BCL	C2B-C1B-NB	4.44	114.93	110.33
6	L	402	BPH	C4D-CHA-CBD	-4.42	106.34	108.45
5	L	401	BCL	O2D-CGD-CBD	4.33	118.80	111.23
5	L	404	BCL	C2D-C1D-ND	4.32	114.40	110.13
5	L	405	BCL	C1D-ND-C4D	-4.29	103.30	106.31
5	L	404	BCL	C3C-C4C-CHD	-4.28	114.36	123.39
5	L	401	BCL	C3C-C4C-CHD	-4.27	114.39	123.39
5	M	401	BCL	C1D-ND-C4D	-4.23	103.34	106.31
5	L	401	BCL	C2D-C1D-ND	4.19	114.28	110.13
5	L	401	BCL	C1D-ND-C4D	-4.19	103.37	106.31
5	L	405	BCL	C3C-C4C-CHD	-4.18	114.58	123.39
5	M	401	BCL	O2D-CGD-CBD	4.10	118.39	111.23
5	M	401	BCL	C3C-C4C-CHD	-4.06	114.84	123.39
5	L	405	BCL	C2D-C1D-ND	3.80	113.89	110.13
5	L	401	BCL	C4A-NA-C1A	3.80	108.41	106.68
6	L	402	BPH	C2B-C1B-NB	-3.75	106.72	109.43
5	M	401	BCL	C1C-NC-C4C	-3.63	105.02	106.68
5	L	405	BCL	C1-O2A-CGA	3.57	125.30	116.65
5	M	401	BCL	C2D-C1D-ND	3.53	113.62	110.13
5	L	405	BCL	C3D-C4D-ND	3.53	115.72	109.99
5	L	401	BCL	C3B-C4B-NB	3.52	114.40	109.76
5	M	401	BCL	C3D-C4D-ND	3.47	115.63	109.99
5	L	404	BCL	C3D-C4D-ND	3.41	115.53	109.99
5	L	404	BCL	CHB-C4A-NA	3.39	129.29	124.40
5	L	404	BCL	C3B-C4B-NB	3.38	114.22	109.76
5	L	401	BCL	C3D-C4D-ND	3.36	115.45	109.99
6	L	406	BPH	C2B-C1B-NB	-3.27	107.07	109.43
5	L	404	BCL	C1C-NC-C4C	-3.26	105.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	401	BCL	CHC-C1C-NC	3.22	129.05	124.40
5	M	401	BCL	CHC-C1C-NC	3.21	129.04	124.40
5	L	404	BCL	O2A-CGA-CBA	3.20	121.58	111.83
5	L	401	BCL	C4-C3-C5	3.16	120.70	115.23
7	L	403	U10	C7-C6-C1	-3.15	119.49	124.89
5	L	401	BCL	CHB-C4A-NA	3.05	128.81	124.40
5	M	401	BCL	C3B-C4B-NB	3.02	113.74	109.76
5	L	405	BCL	O1D-CGD-CBD	-3.02	118.57	124.52
5	L	404	BCL	C4-C3-C5	2.98	120.40	115.23
5	L	405	BCL	C3B-C4B-NB	2.96	113.67	109.76
5	M	401	BCL	O2A-CGA-CBA	2.96	120.85	111.83
5	L	404	BCL	C1D-CHD-C4C	-2.93	119.55	126.62
5	L	405	BCL	CHC-C1C-NC	2.92	128.61	124.40
5	M	401	BCL	O2D-CGD-O1D	-2.88	118.24	123.85
5	M	401	BCL	CMD-C2D-C3D	-2.71	121.48	127.69
5	L	401	BCL	C1D-CHD-C4C	-2.70	120.11	126.62
5	L	401	BCL	CED-O2D-CGD	2.66	121.96	115.92
10	M	408	SPO	C21-C20-C19	2.66	128.97	123.52
5	L	404	BCL	O2A-CGA-O1A	-2.66	116.98	123.63
5	L	405	BCL	C1C-NC-C4C	-2.64	105.47	106.68
5	L	404	BCL	C2A-C1A-CHA	-2.62	119.32	123.87
5	M	401	BCL	CHB-C4A-NA	2.61	128.17	124.40
5	M	401	BCL	C1D-CHD-C4C	-2.61	120.33	126.62
5	L	404	BCL	CMB-C2B-C1B	2.57	129.33	125.42
5	L	405	BCL	CHB-C4A-NA	2.51	128.02	124.40
10	M	408	SPO	C21-C22-C23	2.50	130.78	127.28
5	L	405	BCL	O2A-CGA-CBA	2.46	119.33	111.83
5	L	405	BCL	C1D-CHD-C4C	-2.45	120.71	126.62
10	M	408	SPO	C10-C9-C7	2.43	130.69	127.28
6	L	406	BPH	C1A-C2A-C3A	-2.40	100.55	102.84
5	L	405	BCL	CHC-C4B-NB	-2.40	120.46	124.05
5	L	401	BCL	O1D-CGD-CBD	-2.38	119.82	124.52
5	M	401	BCL	CED-O2D-CGD	2.38	121.32	115.92
5	M	401	BCL	CHB-C1B-C2B	-2.37	120.54	127.43
5	L	404	BCL	CHC-C1C-NC	2.34	127.78	124.40
7	L	403	U10	C7-C6-C5	2.34	121.23	118.52
5	M	401	BCL	O2A-CGA-O1A	-2.32	117.84	123.63
5	L	404	BCL	CMD-C2D-C3D	-2.28	122.46	127.69
5	L	404	BCL	CED-O2D-CGD	2.23	120.97	115.92
5	L	401	BCL	C5-C3-C2	-2.21	116.20	121.17
5	L	405	BCL	C2A-C1A-CHA	-2.20	120.06	123.87
5	L	404	BCL	CHC-C4B-C3B	-2.18	123.06	131.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	403	U10	C1M-C1-C6	-2.17	120.88	124.45
10	M	408	SPO	C15-C14-C12	2.17	130.32	127.28
6	L	402	BPH	C1A-C2A-C3A	-2.14	100.80	102.84
10	M	408	SPO	C18-C17-C19	-2.14	119.35	122.82
5	M	401	BCL	C4A-NA-C1A	2.11	107.64	106.68
10	M	408	SPO	C20-C21-C22	2.11	127.83	123.52
5	L	401	BCL	O2A-CGA-CBA	2.09	118.22	111.83
10	M	408	SPO	C20-C19-C17	2.07	130.18	127.28
5	L	401	BCL	CMB-C2B-C1B	2.06	128.56	125.42
6	L	406	BPH	C2D-C1D-ND	-2.06	107.94	109.43
5	M	401	BCL	CMB-C2B-C1B	2.04	128.53	125.42
5	L	405	BCL	CHB-C1B-C2B	-2.03	121.53	127.43
5	M	401	BCL	C1-C2-C3	-2.01	122.90	126.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	406	BPH	C8

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	401	LDA	C2-C1-N1-O1
4	H	401	LDA	C2-C1-N1-CM1
4	M	402	LDA	C2-C1-N1-O1
4	M	402	LDA	C2-C1-N1-CM1
4	M	403	LDA	N1-C1-C2-C3
6	L	406	BPH	C4C-C3C-CAC-CBC
6	L	406	BPH	C2C-C3C-CAC-CBC
7	L	403	U10	C1-C6-C7-C8
7	L	403	U10	C5-C6-C7-C8
7	M	407	U10	C32-C33-C34-C35
7	M	407	U10	C32-C33-C34-C36
10	M	408	SPO	C4-C1-O1-CM1
11	M	409	CDL	CA3-OA5-PA1-OA2
11	M	409	CDL	CA3-OA5-PA1-OA3
11	M	409	CDL	CA3-OA5-PA1-OA4
11	M	409	CDL	CB2-OB2-PB2-OB3
11	M	409	CDL	CB2-OB2-PB2-OB5
7	M	407	U10	C24-C26-C27-C28
7	M	407	U10	C29-C31-C32-C33
7	M	407	U10	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
5	M	401	BCL	CBD-CGD-O2D-CED
6	L	402	BPH	CBD-CGD-O2D-CED
11	M	409	CDL	CB7-C71-C72-C73
5	L	401	BCL	C15-C16-C17-C18
7	M	407	U10	C27-C28-C29-C30
11	M	409	CDL	OA7-CA5-OA6-CA4
5	L	404	BCL	C2A-CAA-CBA-CGA
11	M	409	CDL	C11-CA5-OA6-CA4
11	M	409	CDL	C33-C34-C35-C36
11	M	409	CDL	CA5-C11-C12-C13
4	H	401	LDA	C6-C7-C8-C9
4	M	404	LDA	C1-C2-C3-C4
6	L	406	BPH	C5-C6-C7-C8
4	M	403	LDA	C1-C2-C3-C4
4	M	402	LDA	C4-C5-C6-C7
5	M	401	BCL	O1D-CGD-O2D-CED
11	M	409	CDL	CA7-C31-C32-C33
6	L	402	BPH	O2A-C1-C2-C3
4	H	401	LDA	C9-C10-C11-C12
11	M	409	CDL	C13-C14-C15-C16
10	M	408	SPO	C2-C1-O1-CM1
10	M	408	SPO	C3-C1-O1-CM1
6	L	402	BPH	O1D-CGD-O2D-CED
6	L	402	BPH	C4-C3-C5-C6
11	M	409	CDL	C72-C71-CB7-OB8
7	L	403	U10	C7-C8-C9-C10
4	M	402	LDA	C1-C2-C3-C4
11	M	409	CDL	C17-C18-C19-C20
11	M	409	CDL	OA5-CA3-CA4-CA6
4	M	402	LDA	C11-C10-C9-C8
11	M	409	CDL	C71-C72-C73-C74
5	L	401	BCL	C11-C12-C13-C15
4	M	404	LDA	C9-C10-C11-C12
6	L	402	BPH	C13-C15-C16-C17
7	M	407	U10	C14-C16-C17-C18
6	L	402	BPH	C2-C3-C5-C6
11	M	409	CDL	OA5-CA3-CA4-OA6
5	M	401	BCL	C16-C17-C18-C20
5	L	401	BCL	C4B-C3B-CAB-CBB
6	L	402	BPH	C14-C13-C15-C16
5	L	405	BCL	C4C-C3C-CAC-CBC
5	L	401	BCL	C2B-C3B-CAB-OB8

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Mol	Chain	Res	Type	Atoms
5	L	401	BCL	C2B-C3B-CAB-CBB
7	L	403	U10	C7-C8-C9-C11
11	M	409	CDL	C39-C40-C41-C42
4	H	401	LDA	C2-C1-N1-CM2
4	M	402	LDA	C2-C1-N1-CM2
4	M	404	LDA	C4-C5-C6-C7
11	M	409	CDL	C72-C73-C74-C75
4	M	405	LDA	C1-C2-C3-C4
11	M	409	CDL	C11-C12-C13-C14
11	M	409	CDL	C36-C37-C38-C39
5	M	401	BCL	C16-C17-C18-C19
5	L	401	BCL	C4B-C3B-CAB-OB
4	H	401	LDA	C11-C10-C9-C8
5	L	401	BCL	CHA-CBD-CGD-O2D
11	M	409	CDL	CB2-OB2-PB2-OB4
4	M	405	LDA	N1-C1-C2-C3
6	L	406	BPH	O1A-CGA-O2A-C1
5	L	401	BCL	C11-C12-C13-C14
5	L	404	BCL	C15-C16-C17-C18
6	L	406	BPH	C4-C3-C5-C6
11	M	409	CDL	C51-C52-C53-C54
7	M	407	U10	C5-C4-O4-C4M
4	M	405	LDA	C3-C4-C5-C6
5	M	401	BCL	C2B-C3B-CAB-OB
6	L	406	BPH	C2-C3-C5-C6
11	M	409	CDL	C37-C38-C39-C40
7	L	403	U10	C5-C4-O4-C4M
4	H	401	LDA	C5-C6-C7-C8
4	M	403	LDA	C7-C8-C9-C10
11	M	409	CDL	CA3-CA4-CA6-OA8
4	M	403	LDA	C6-C7-C8-C9
11	M	409	CDL	C72-C71-CB7-OB9
4	M	403	LDA	C9-C10-C11-C12
6	L	406	BPH	CBA-CGA-O2A-C1
4	M	405	LDA	C7-C8-C9-C10
5	M	401	BCL	C2B-C3B-CAB-CBB
5	M	401	BCL	C4B-C3B-CAB-OB
11	M	409	CDL	C31-C32-C33-C34
5	L	401	BCL	C13-C15-C16-C17
11	M	409	CDL	C52-C51-CB5-OB6
5	L	405	BCL	CAD-CBD-CGD-O2D
5	M	401	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	M	409	CDL	C34-C35-C36-C37

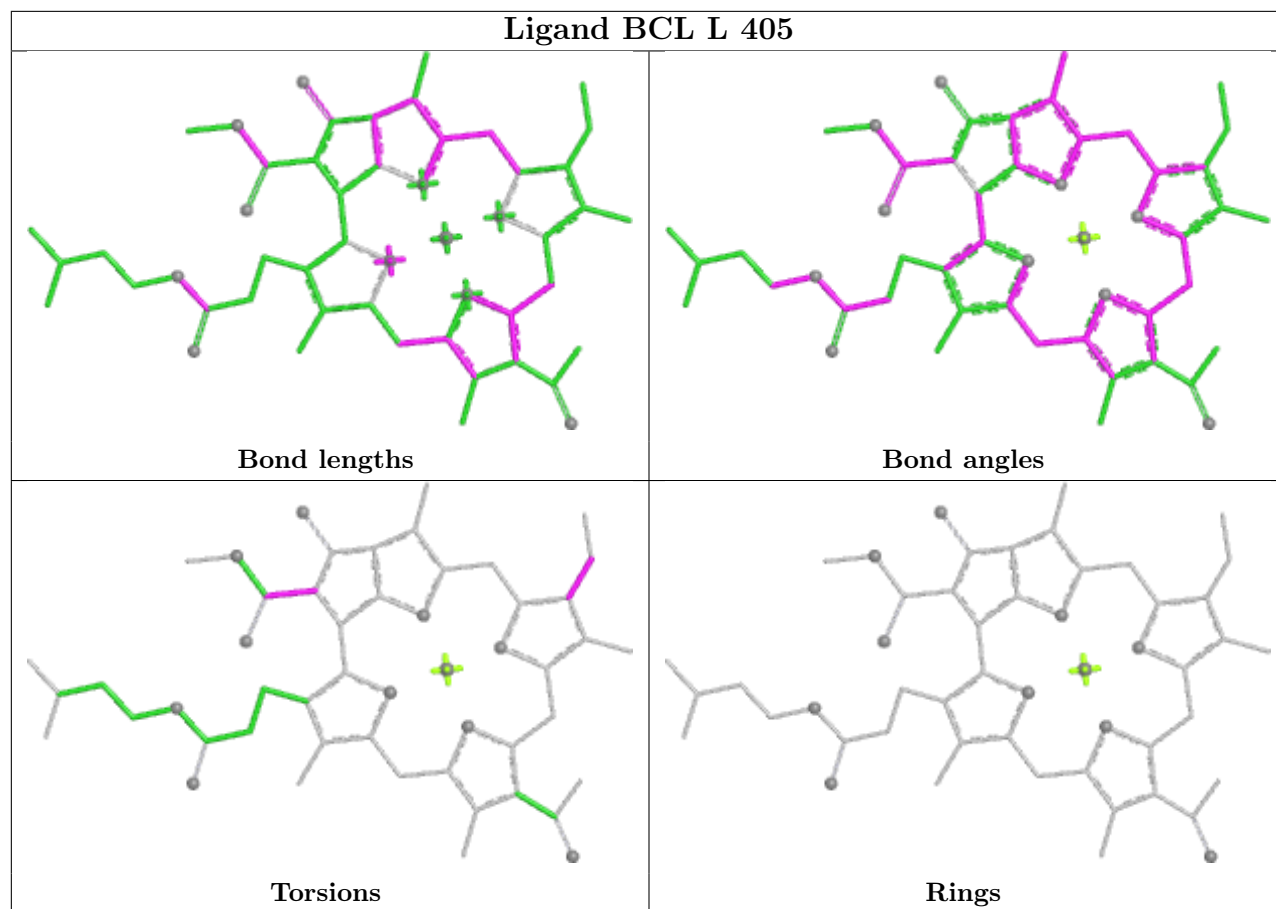
There are no ring outliers.

7 monomers are involved in 27 short contacts:

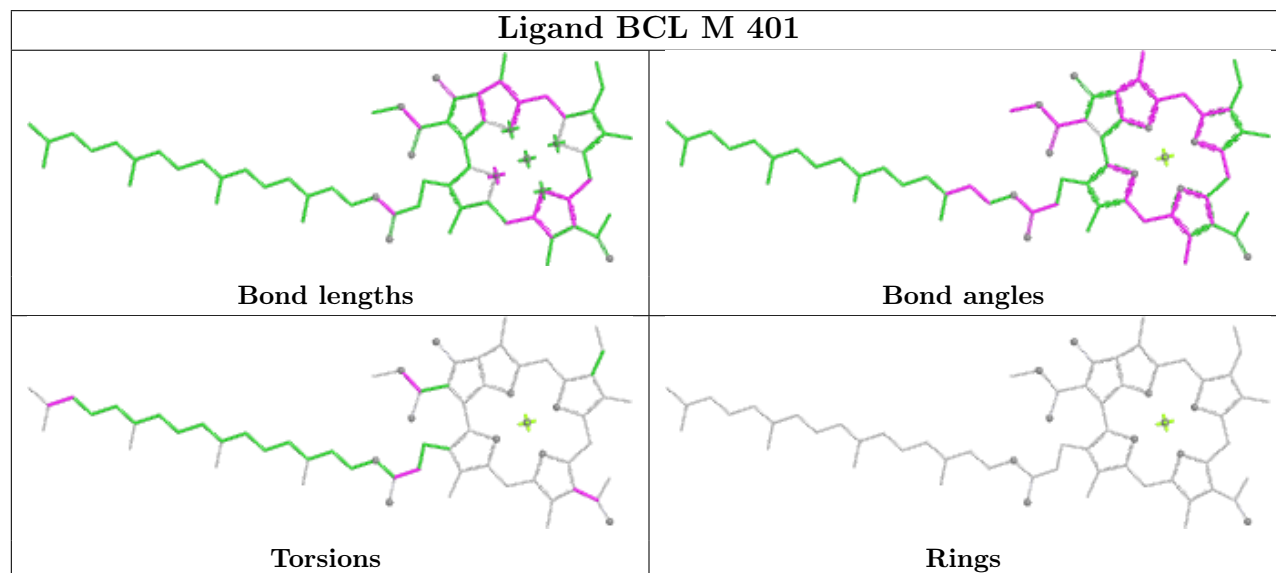
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	405	BCL	4	0
5	M	401	BCL	9	0
7	L	403	U10	2	0
5	L	404	BCL	4	0
5	L	401	BCL	3	0
6	L	406	BPH	4	0
6	L	402	BPH	3	0

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.

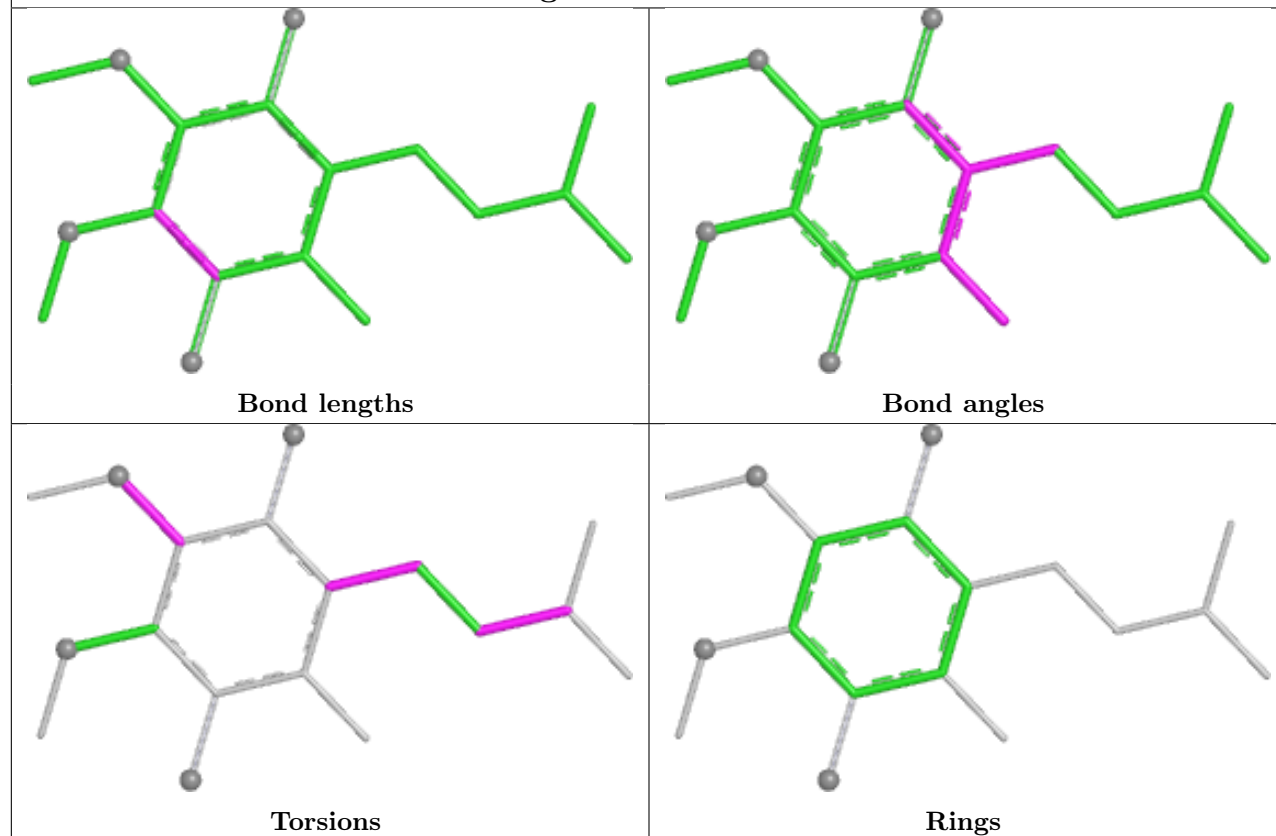
Ligand BCL L 405



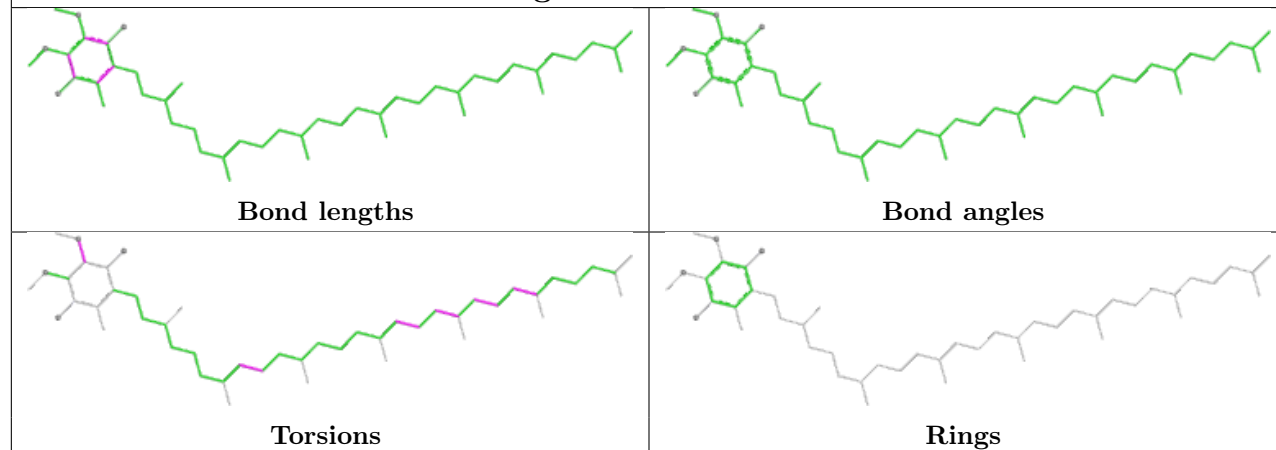
Ligand BCL M 401

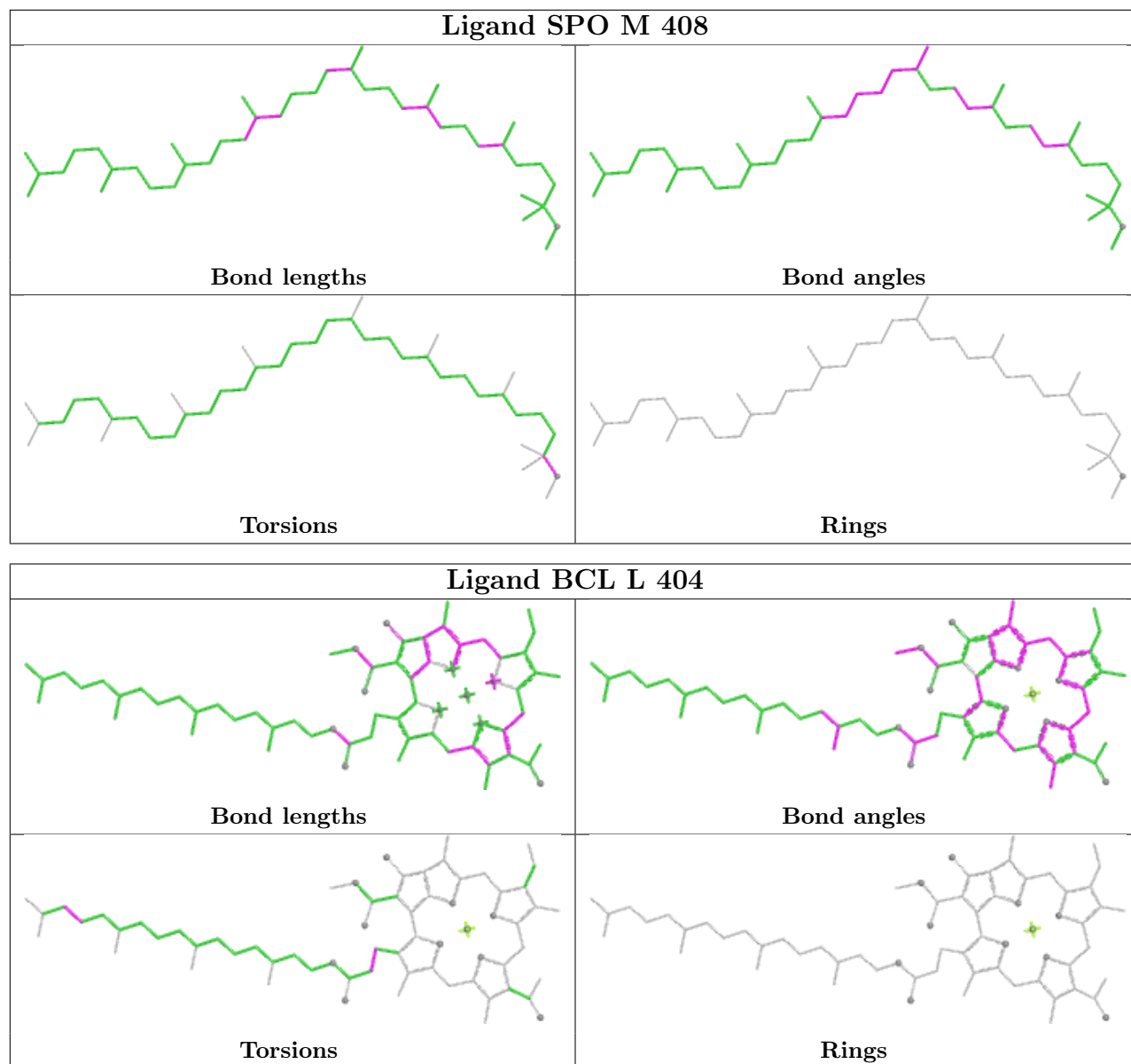


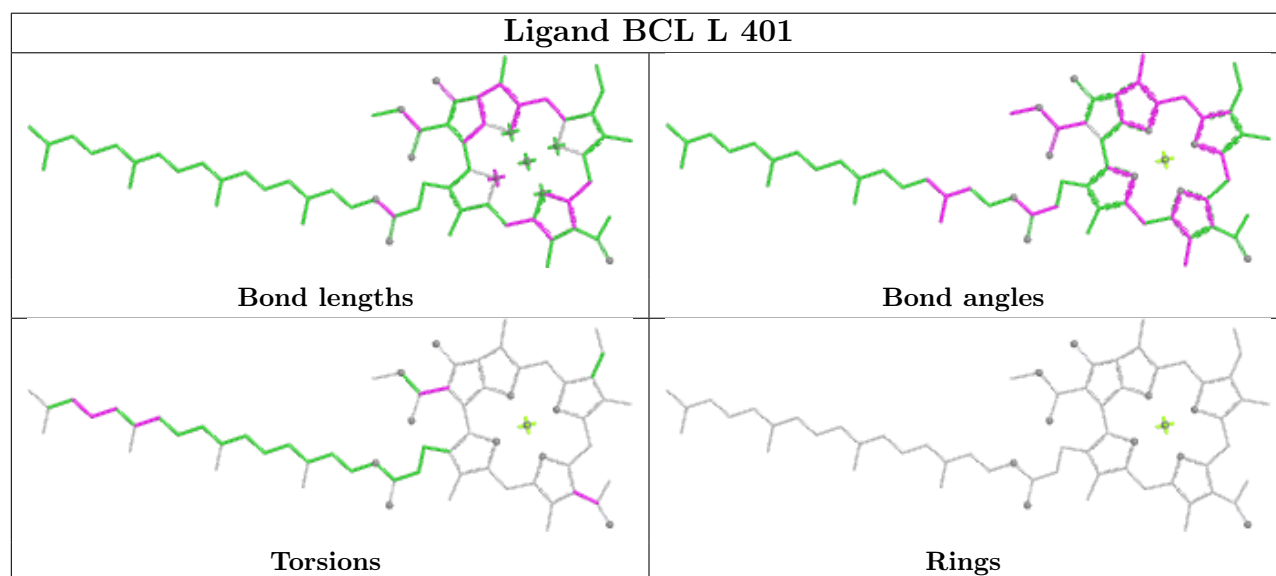
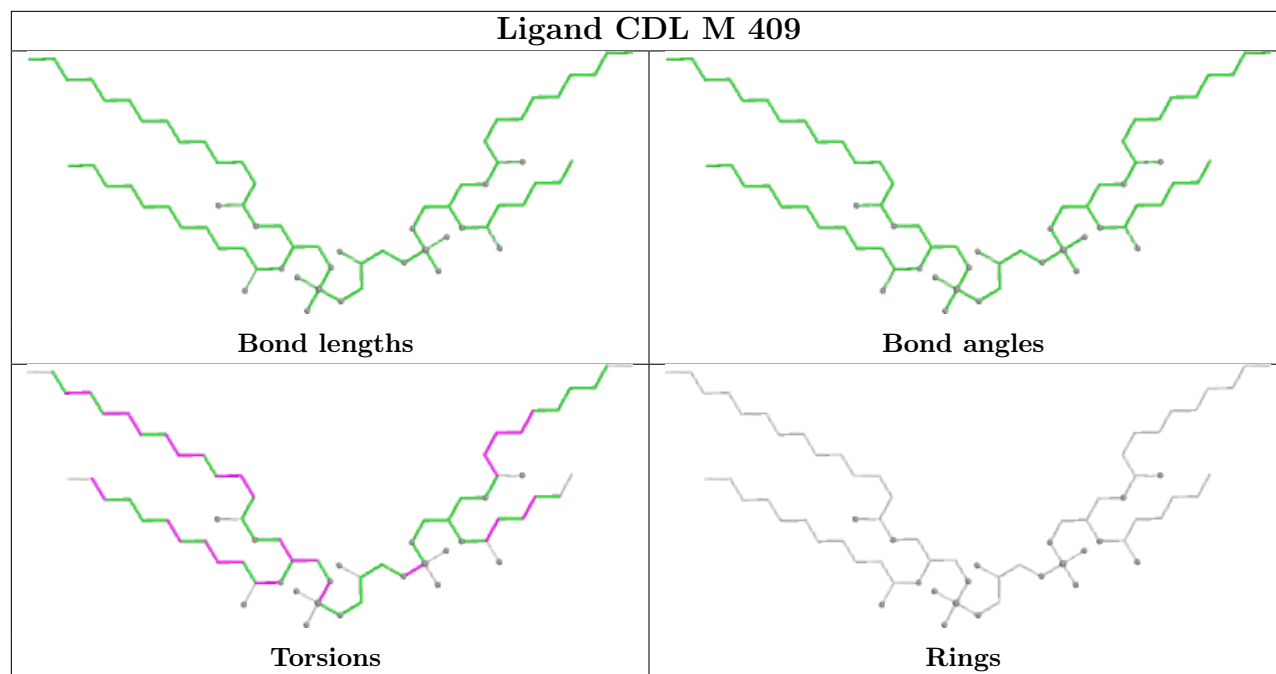
Ligand U10 L 403



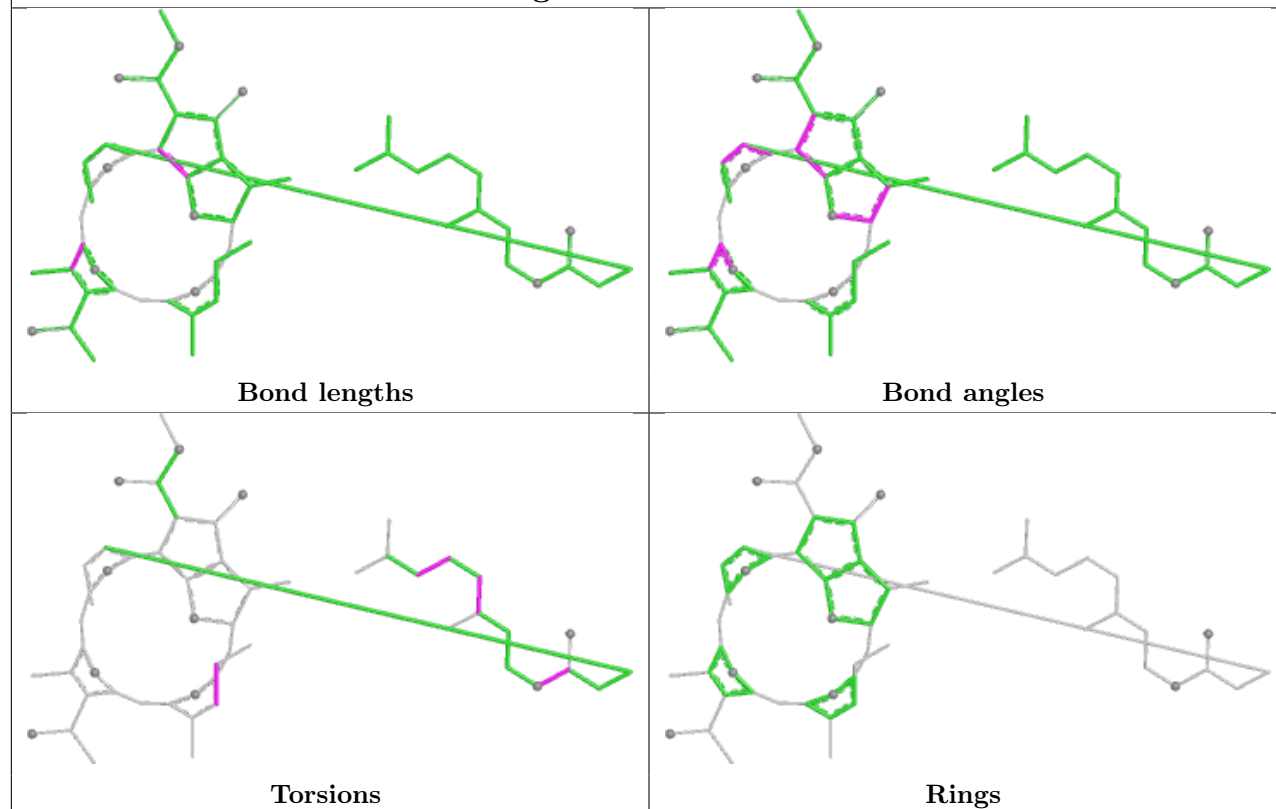
Ligand U10 M 407



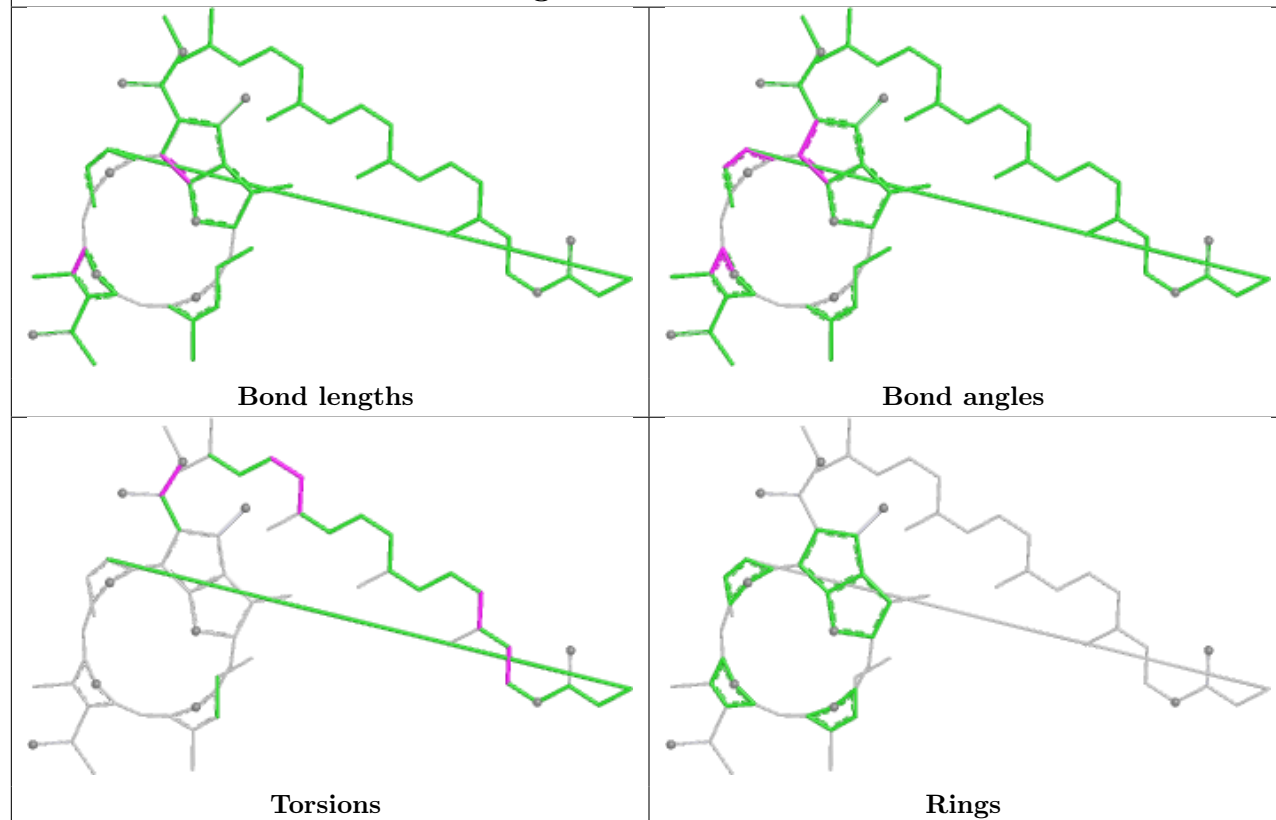




Ligand BPH L 406



Ligand BPH L 402



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	240/266 (90%)	-0.29	2 (0%) 82 65	46, 59, 83, 116	0
2	L	281/282 (99%)	-0.19	7 (2%) 58 37	28, 56, 89, 103	1 (0%)
3	M	300/308 (97%)	-0.26	4 (1%) 75 56	41, 60, 91, 112	0
All	All	821/856 (95%)	-0.24	13 (1%) 70 49	28, 58, 88, 116	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	4.7
1	H	250	SER	4.4
2	L	62	GLN	4.1
3	M	2	GLU	3.4
1	H	102	GLY	3.0
3	M	301	HIS	2.8
2	L	270	PRO	2.6
2	L	155	ASP	2.4
3	M	25	ASN	2.4
2	L	61	PRO	2.3
3	M	23	ASP	2.3
2	L	202	LYS	2.2
2	L	59	TRP	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NIY	M	210	15/16	0.98	0.05	48,50,55,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

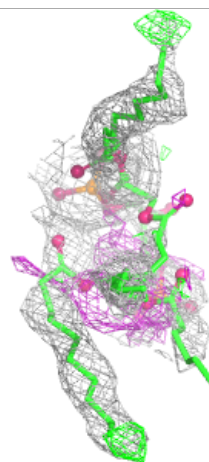
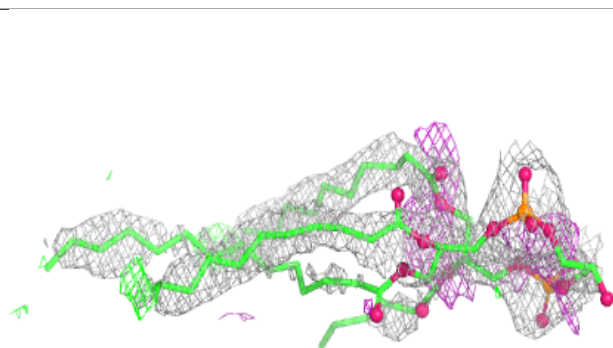
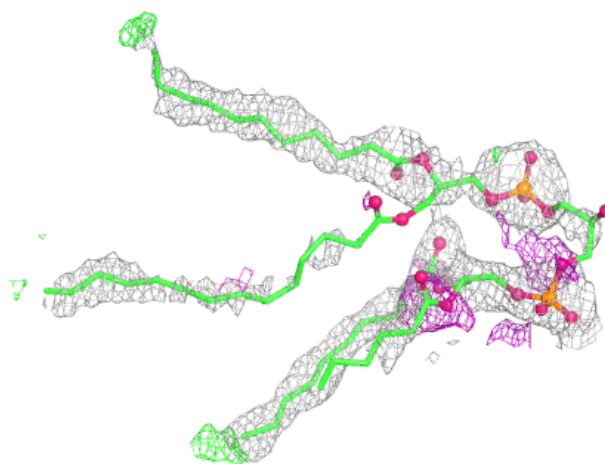
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CDL	M	409	69/100	0.82	0.26	78,124,156,178	0
7	U10	L	403	18/63	0.87	0.30	31,36,37,37	18
4	LDA	M	405	16/16	0.87	0.26	91,98,137,140	0
4	LDA	M	404	16/16	0.88	0.28	94,109,119,122	0
4	LDA	M	403	16/16	0.92	0.21	92,98,125,128	0
7	U10	M	407	48/63	0.93	0.19	47,62,114,118	0
8	CL	L	407	1/1	0.94	0.09	87,87,87,87	0
10	SPO	M	408	42/42	0.94	0.16	53,69,100,109	0
6	BPH	L	406	55/65	0.94	0.12	47,60,84,91	0
4	LDA	M	402	16/16	0.95	0.16	80,86,91,91	0
4	LDA	H	401	16/16	0.96	0.15	69,76,104,105	0
5	BCL	L	405	51/66	0.96	0.10	45,49,64,66	0
6	BPH	L	402	65/65	0.96	0.11	45,51,64,65	0
5	BCL	L	401	66/66	0.97	0.09	45,51,76,81	0
5	BCL	M	401	66/66	0.97	0.09	47,51,78,95	0
5	BCL	L	404	66/66	0.97	0.09	40,47,75,84	0
9	FE	M	406	1/1	1.00	0.05	46,46,46,46	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.

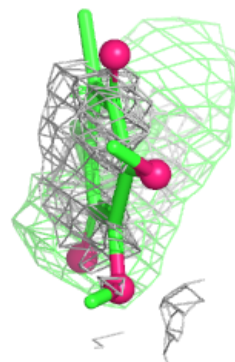
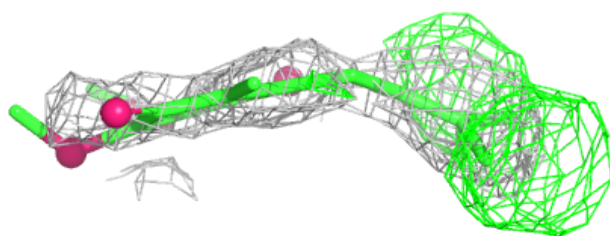
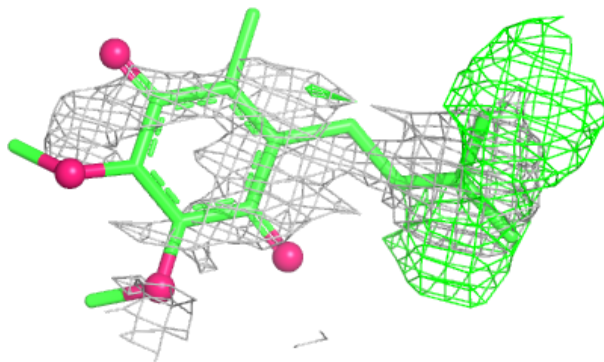
Electron density around CDL M 409:

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

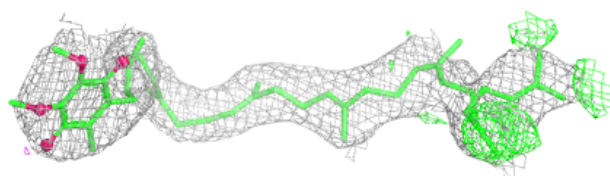
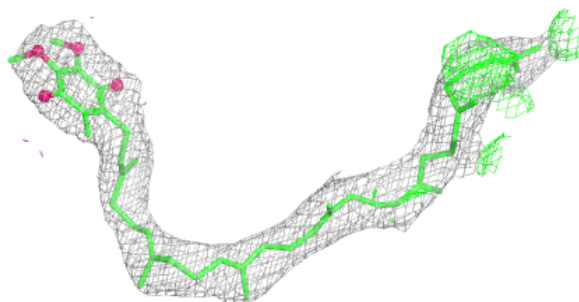


Electron density around U10 L 403:

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

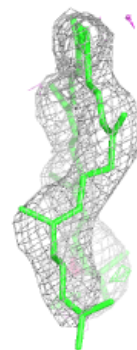
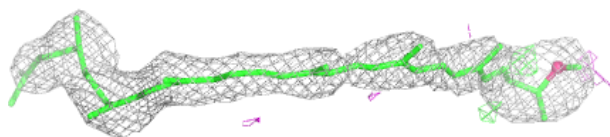
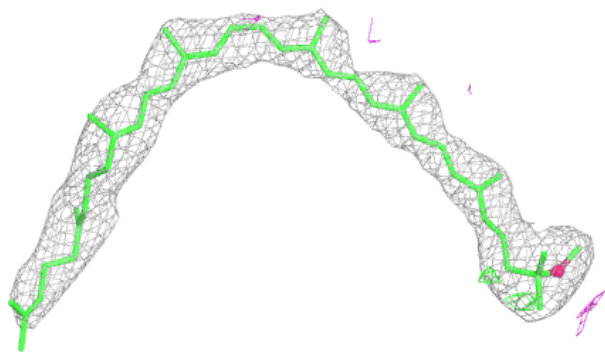
**Electron density around U10 M 407:**

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



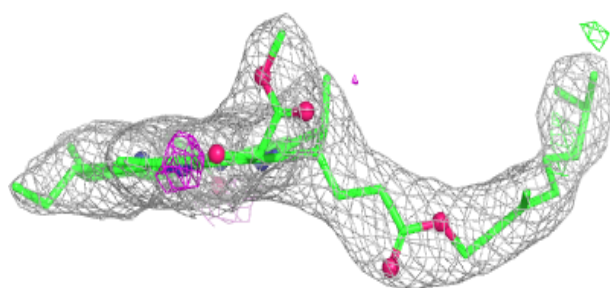
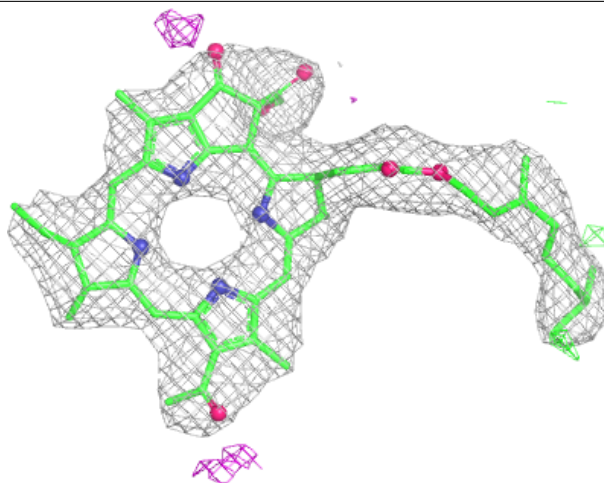
Electron density around SPO M 408:

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



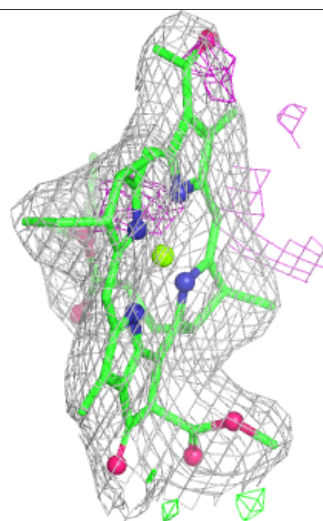
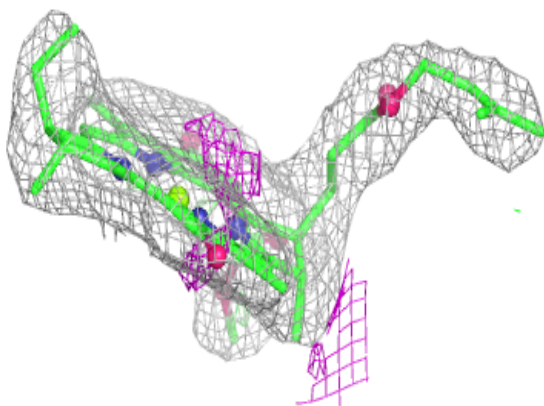
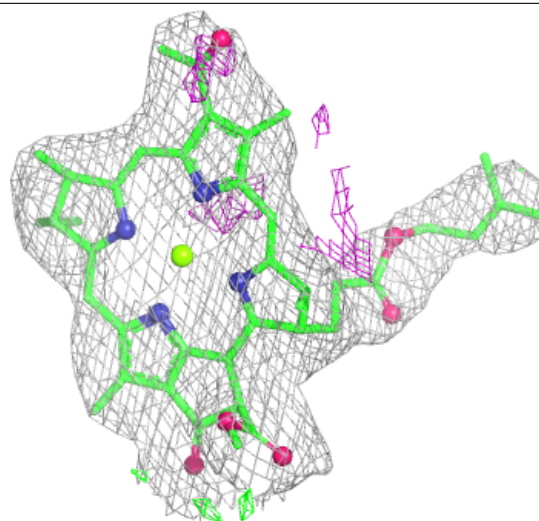
Electron density around BPH L 406:

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



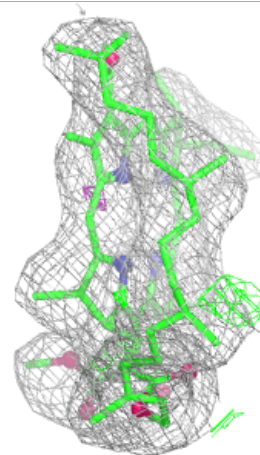
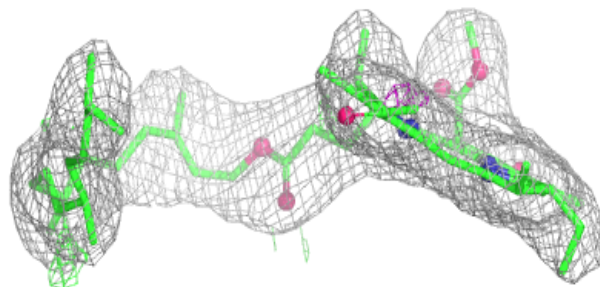
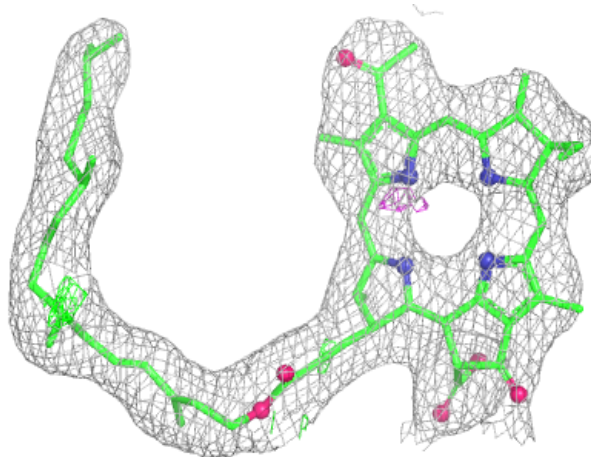
Electron density around BCL L 405:

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



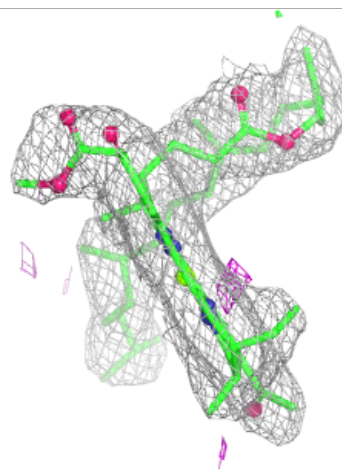
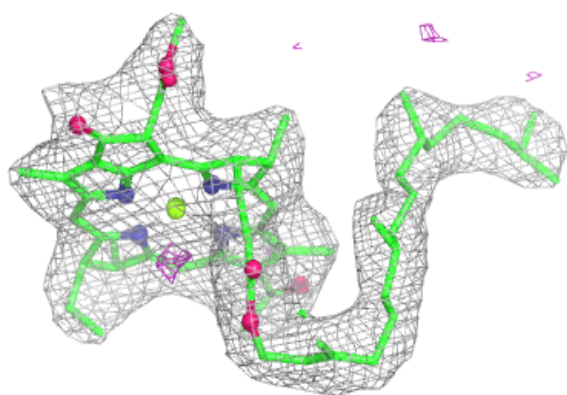
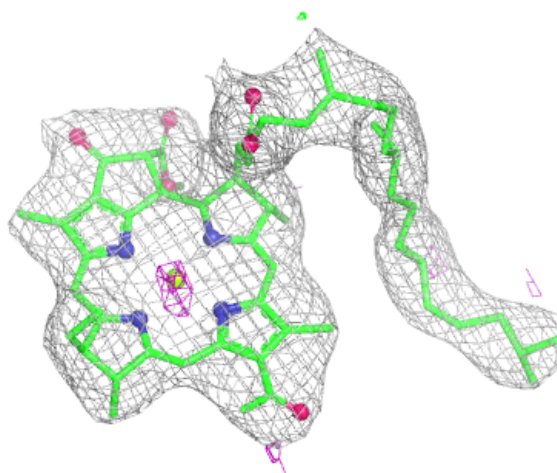
Electron density around BPH L 402:

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



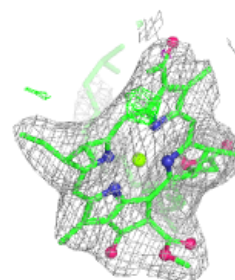
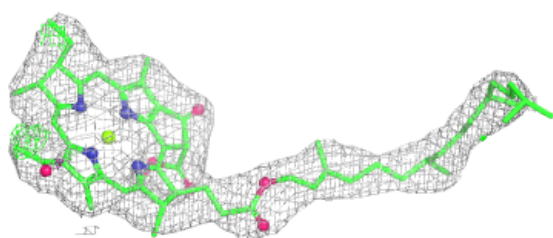
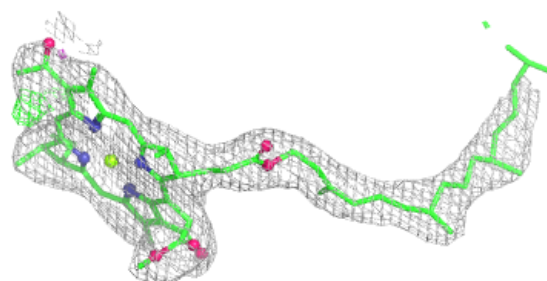
Electron density around BCL L 401:

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

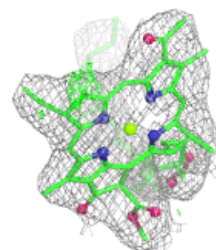
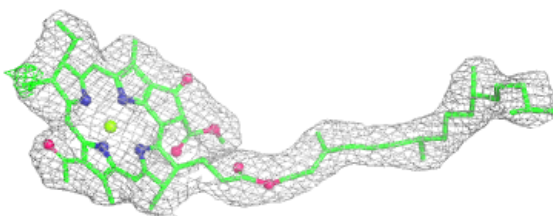
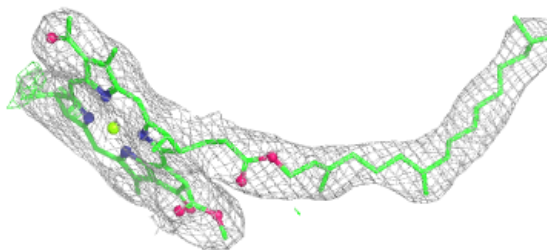


Electron density around BCL M 401:

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

**Electron density around BCL L 404:**

$2mF_o-DF_c$ (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.