wwPDB X-ray Structure Validation Summary Report (i)

Apr 20, 2024 – 01:03 pm BST

PDB ID	:	5LSE
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT WITH Glu L212 replaced with Ala (CHAIN L, EL212W), Asp L213 replaced with ALA (Chain L, DL213A) AND LEU M215 REPLACED WITH ALA (CHAIN M, LM215A)
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Deposited on	:	2016-08-25
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

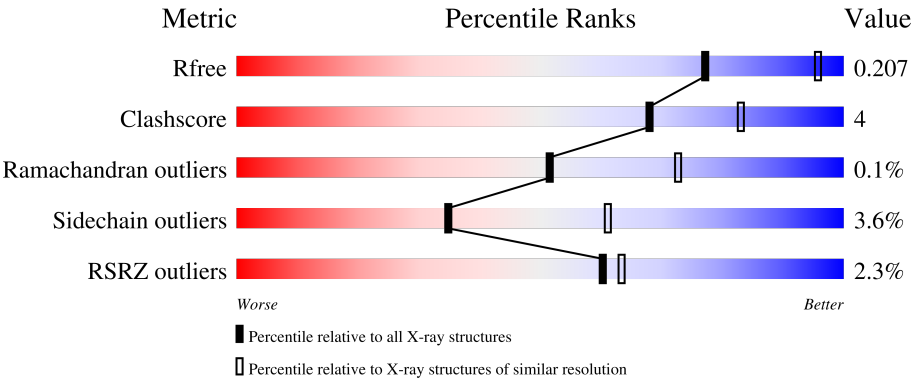
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	L	281	2% 93% 6%
2	M	307	% 87% 9%
3	H	260	3% 83% 8% 8%

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
7	D12	H	305	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7439 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	0	0
			2225	1504	355	358	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	engineered mutation	UNP P0C0Y8
L	213	ALA	ASP	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	300	Total	C	N	O	S	0	1	0
			2397	1599	395	393	10			

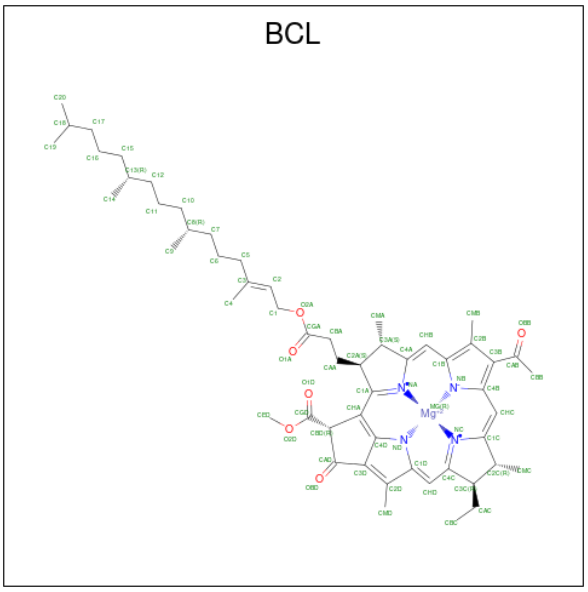
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	215	ALA	LEU	engineered mutation	UNP P0C0Y9

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

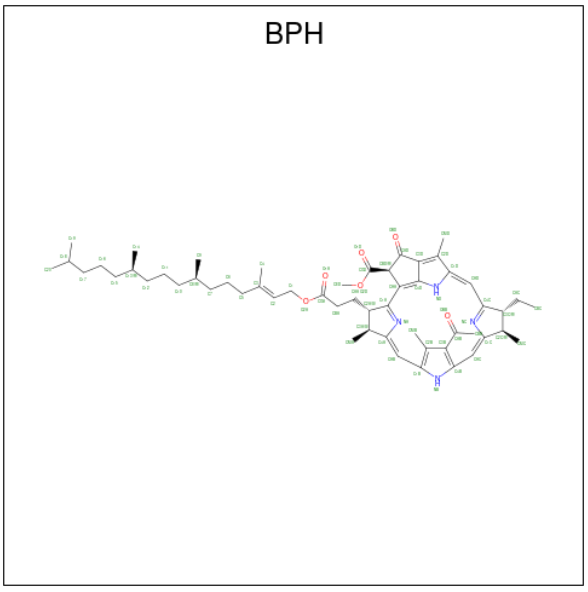
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	1	0
			1837	1173	316	339	9			

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



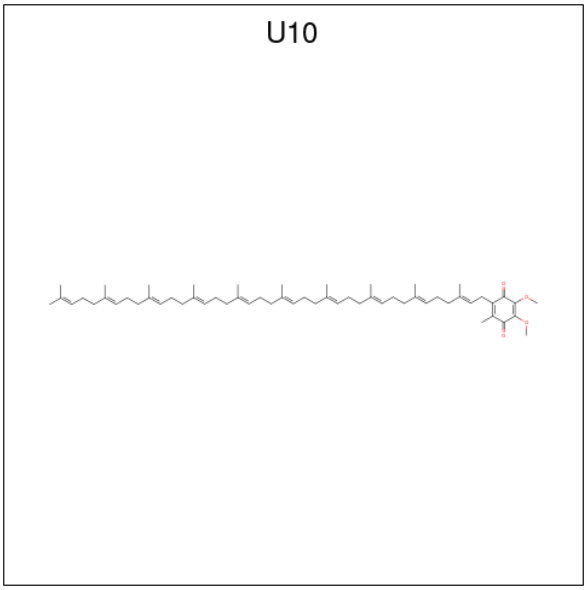
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



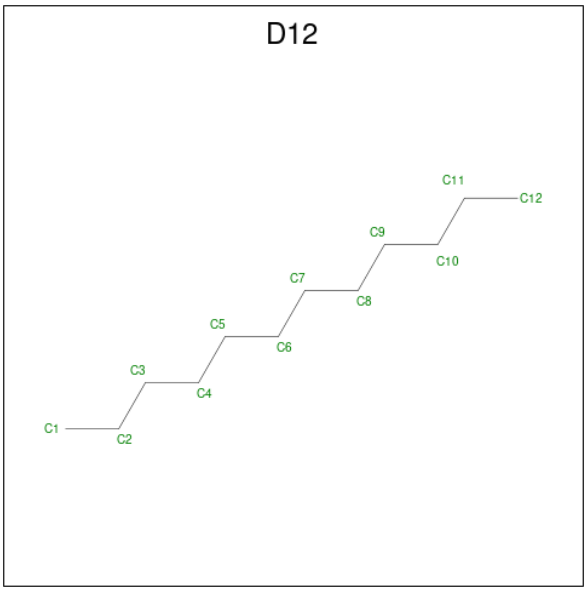
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 7 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).

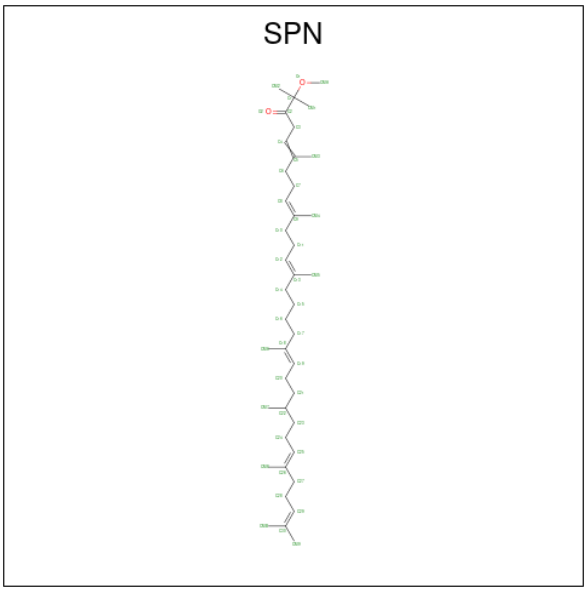


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C 8 8	0	0
7	H	1	Total C 12 12	0	0
7	H	1	Total C 9 9	0	0
7	H	1	Total C 8 8	0	0
7	H	1	Total C 8 8	0	0

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

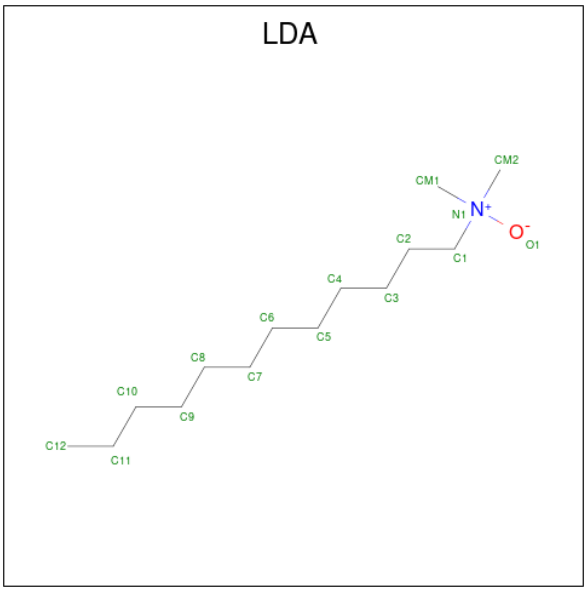
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total Fe 1 1	0	0

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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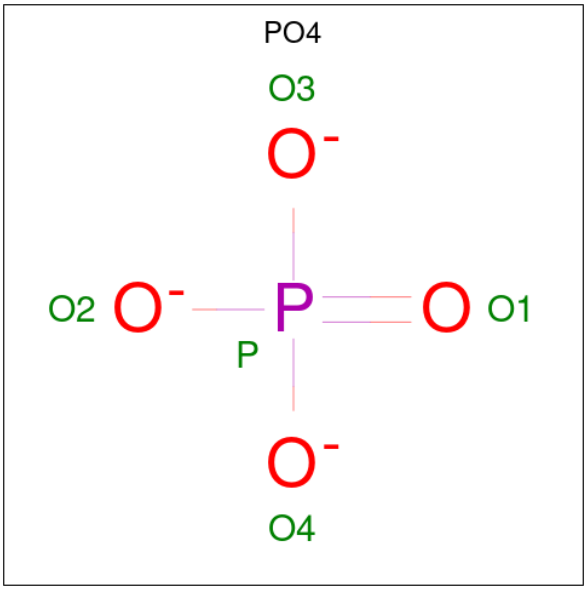
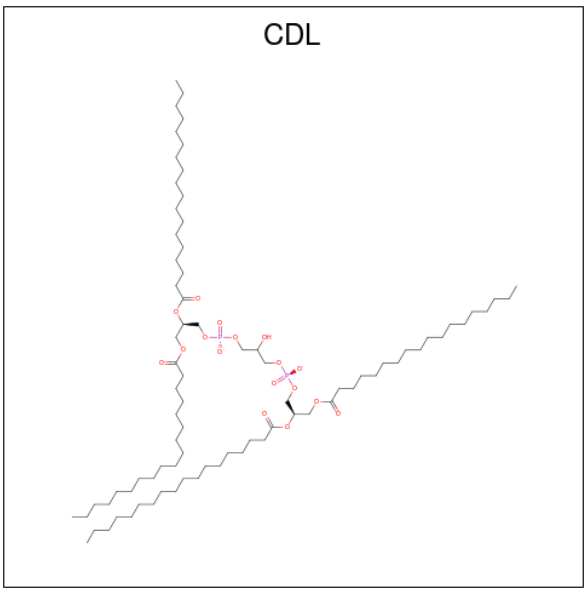
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total C N O 16 14 1 1	0	0

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total	C	O	P	0	0
			78	59	17	2		

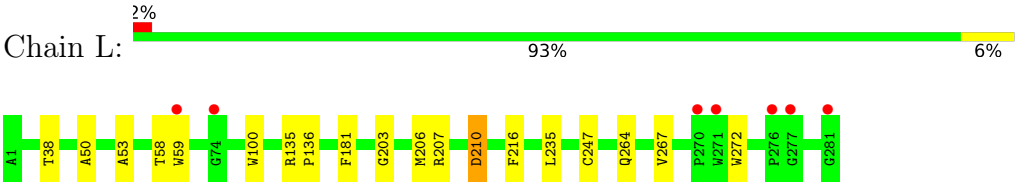
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	72	Total	O	0	0
			72	72		
13	M	83	Total	O	0	0
			83	83		
13	H	115	Total	O	0	0
			115	115		

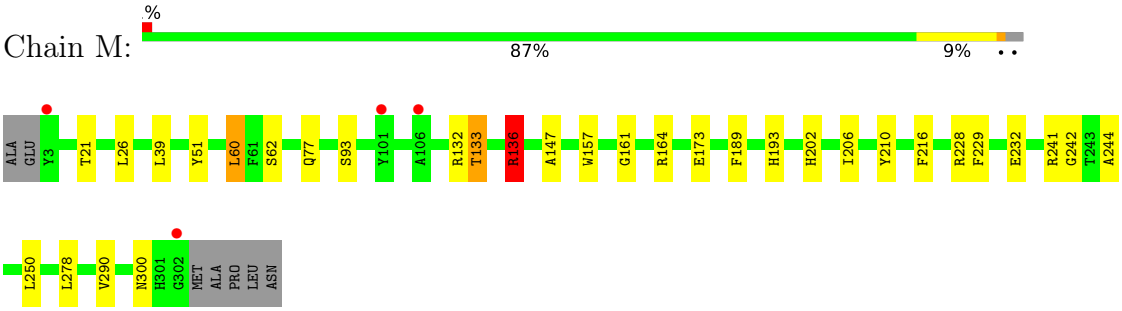
3 Residue-property plots (i)

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

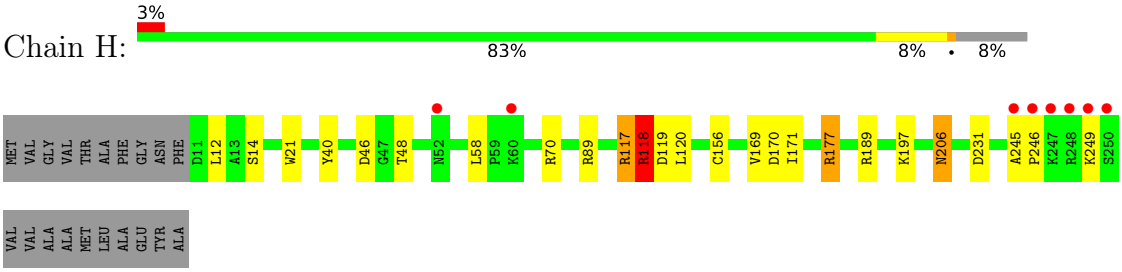
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.99Å 138.99Å 184.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.90 – 2.50 27.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (23.90-2.50) 98.9 (27.05-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.168 , 0.201 0.175 , 0.207	Depositor DCC
R_{free} test set	3515 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7439	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, U10, FE, D12, SPN, CDL, LDA, BPH, BCL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	L	0.77	0/2313	0.77	3/3166 (0.1%)
2	M	0.76	0/2494	0.82	5/3404 (0.1%)
3	H	0.79	0/1885	0.94	9/2564 (0.4%)
All	All	0.77	0/6692	0.84	17/9134 (0.2%)

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
1	L	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	241	ARG	NE-CZ-NH1	9.11	124.86	120.30
2	M	241	ARG	NE-CZ-NH2	-8.28	116.16	120.30
3	H	117	ARG	NE-CZ-NH2	-8.12	116.24	120.30
3	H	117	ARG	NE-CZ-NH1	7.65	124.13	120.30
3	H	177	ARG	NE-CZ-NH1	7.06	123.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	203	GLY	Peptide
2	M	300	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2225	0	2187	6	0
2	M	2397	0	2310	20	0
3	H	1837	0	1841	12	0
4	L	132	0	148	6	0
4	M	132	0	148	7	0
5	L	65	0	75	4	0
5	M	65	0	76	9	0
6	L	48	0	63	1	0
6	M	48	0	63	0	0
7	H	37	0	73	0	0
7	L	8	0	15	0	0
8	L	1	0	0	0	0
9	M	43	0	69	5	0
10	H	16	0	31	1	0
10	M	32	0	62	3	0
11	M	5	0	0	0	0
12	M	78	0	100	0	0
13	H	115	0	0	0	0
13	L	72	0	0	0	0
13	M	83	0	0	0	0
All	All	7439	0	7261	55	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.

The worst 5 of 55 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)
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.60	0.84
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:46:ASP:OD1	3:H:48:THR:HB	1.94	0.67
4:M:401:BCL:HMB1	4:M:401:BCL:HBB2	1.78	0.65
4:L:302:BCL:HMB1	4:L:302:BCL:HBB2	1.80	0.63

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	34 54
2	M	299/307 (97%)	285 (95%)	14 (5%)	0	100 100
3	H	239/260 (92%)	236 (99%)	3 (1%)	0	100 100
All	All	817/848 (96%)	792 (97%)	24 (3%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	58	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	218/218 (100%)	209 (96%)	9 (4%)	30 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	235/239 (98%)	227 (97%)	8 (3%)	37 63
3	H	196/208 (94%)	190 (97%)	6 (3%)	40 67
All	All	649/665 (98%)	626 (96%)	23 (4%)	35 62

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	216	PHE
3	H	14	SER
2	M	278	LEU
3	H	118	ARG
1	L	264	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	44	ASN
2	M	77	GLN
2	M	193	HIS
3	H	44	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	D12	H	302	-	11,11,11	0.38	0	10,10,10	0.27	0
10	LDA	H	301	-	12,15,15	2.23	1 (8%)	14,17,17	2.73	3 (21%)
4	BCL	L	302	-	64,74,74	1.06	4 (6%)	78,115,115	1.52	15 (19%)
5	BPH	L	303	-	51,70,70	0.71	1 (1%)	52,101,101	1.48	9 (17%)
4	BCL	L	301	-	64,74,74	1.01	4 (6%)	78,115,115	1.42	14 (17%)
9	SPN	M	405	-	40,42,42	3.63	17 (42%)	50,52,52	2.35	19 (38%)
10	LDA	M	407	-	12,15,15	2.44	1 (8%)	14,17,17	2.15	3 (21%)
6	U10	L	304	-	48,48,63	1.83	5 (10%)	58,61,79	1.66	12 (20%)
6	U10	M	404	-	48,48,63	1.71	3 (6%)	58,61,79	1.41	6 (10%)
10	LDA	M	406	-	12,15,15	2.47	1 (8%)	14,17,17	1.69	3 (21%)
12	CDL	M	409	-	77,77,99	1.20	4 (5%)	83,89,111	1.09	7 (8%)
7	D12	H	305	-	7,7,11	0.51	0	6,6,10	0.17	0
7	D12	H	304	-	7,7,11	0.45	0	6,6,10	0.43	0
11	PO4	M	408	-	4,4,4	0.92	0	6,6,6	0.55	0
7	D12	L	305	-	7,7,11	0.48	0	6,6,10	0.30	0
4	BCL	M	401	-	64,74,74	1.10	4 (6%)	78,115,115	1.64	15 (19%)
7	D12	H	303	-	8,8,11	0.44	0	7,7,10	0.25	0
4	BCL	M	402	-	64,74,74	1.36	4 (6%)	78,115,115	1.48	17 (21%)
5	BPH	M	403	-	51,70,70	0.72	0	52,101,101	1.68	12 (23%)

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
10	LDA	M	406	-	-	2/13/13/13	-
12	CDL	M	409	-	-	36/88/88/110	-
7	D12	H	305	-	-	1/5/5/9	-
6	U10	L	304	-	-	17/45/69/87	0/1/1/1
7	D12	H	302	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	D12	H	303	-	-	1/6/6/9	-
7	D12	H	304	-	-	1/5/5/9	-
4	BCL	L	302	-	-	4/37/137/137	-
5	BPH	L	303	-	-	3/37/105/105	0/5/6/6
6	U10	M	404	-	-	14/45/69/87	0/1/1/1
4	BCL	M	402	-	-	3/37/137/137	-
9	SPN	M	405	-	-	21/50/51/51	-
4	BCL	L	301	-	-	2/37/137/137	-
10	LDA	H	301	-	-	7/13/13/13	-
7	D12	L	305	-	-	2/5/5/9	-
5	BPH	M	403	-	-	14/37/105/105	0/5/6/6
10	LDA	M	407	-	-	5/13/13/13	-
4	BCL	M	401	-	-	9/37/137/137	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	405	SPN	C3-C4	-9.33	1.37	1.50
10	M	407	LDA	O1-N1	-8.26	1.22	1.42
10	M	406	LDA	O1-N1	-8.24	1.22	1.42
6	L	304	U10	C6-C1	7.96	1.49	1.35
10	H	301	LDA	O1-N1	-7.63	1.24	1.42

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	301	LDA	O1-N1-C1	-6.58	93.13	109.27
10	M	407	LDA	O1-N1-C1	-5.70	95.29	109.27
9	M	405	SPN	CM5-C13-C14	5.54	124.59	115.27
9	M	405	SPN	CM3-C5-C6	5.48	124.50	115.27
10	H	301	LDA	CM1-N1-C1	-5.35	98.99	110.23

There are no chirality outliers.

5 of 145 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	401	BCL	C11-C10-C8-C9
5	M	403	BPH	C2-C3-C5-C6
5	M	403	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	L	304	U10	C28-C29-C31-C32
6	L	304	U10	C30-C29-C31-C32

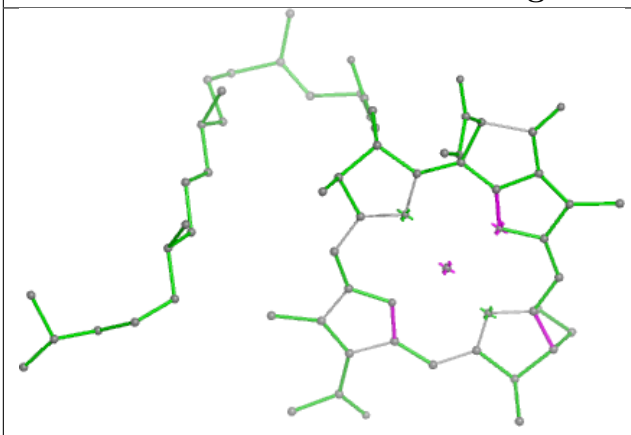
There are no ring outliers.

10 monomers are involved in 31 short contacts:

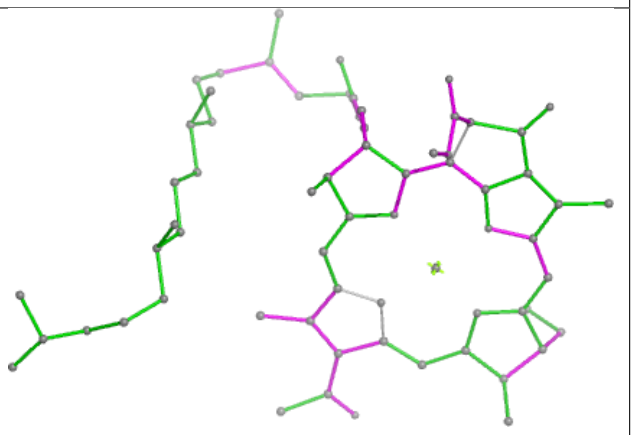
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	301	LDA	1	0
4	L	302	BCL	4	0
5	L	303	BPH	4	0
4	L	301	BCL	3	0
9	M	405	SPN	5	0
6	L	304	U10	1	0
10	M	406	LDA	3	0
4	M	401	BCL	6	0
4	M	402	BCL	2	0
5	M	403	BPH	9	0

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

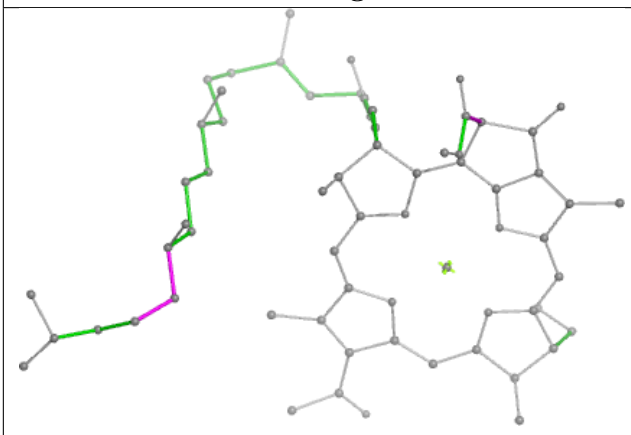
Ligand BCL L 302



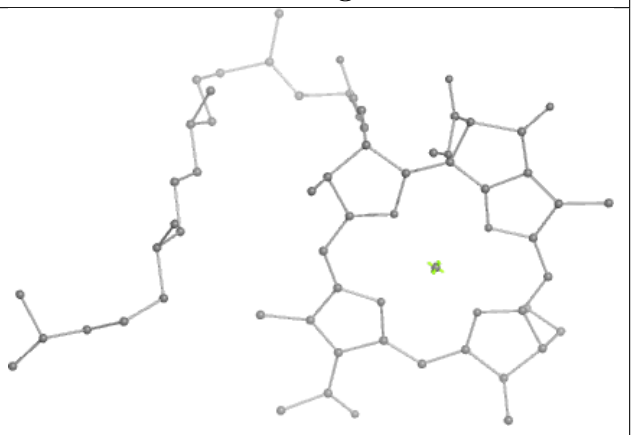
Bond lengths



Bond angles

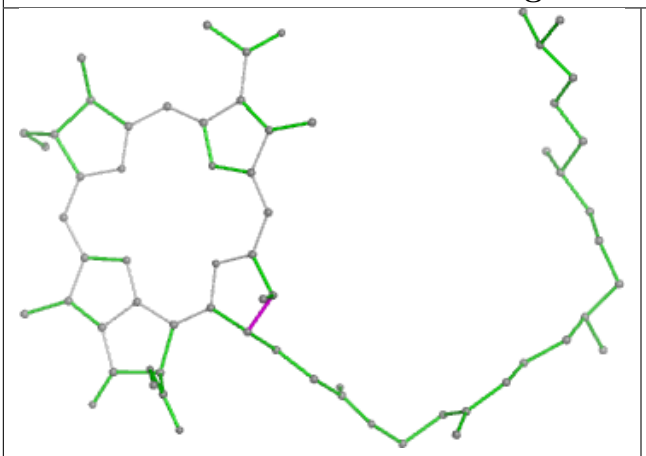


Torsions

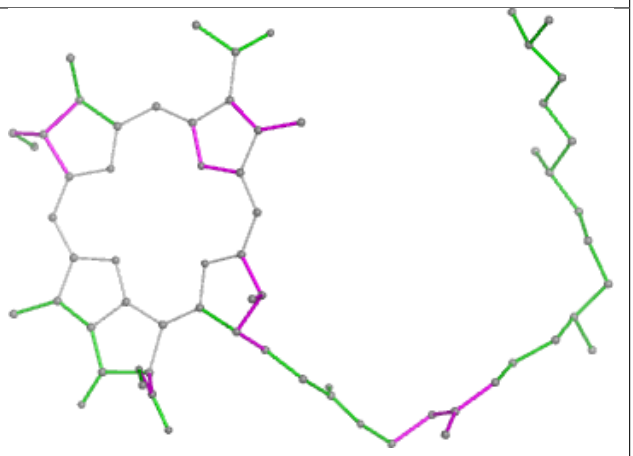


Rings

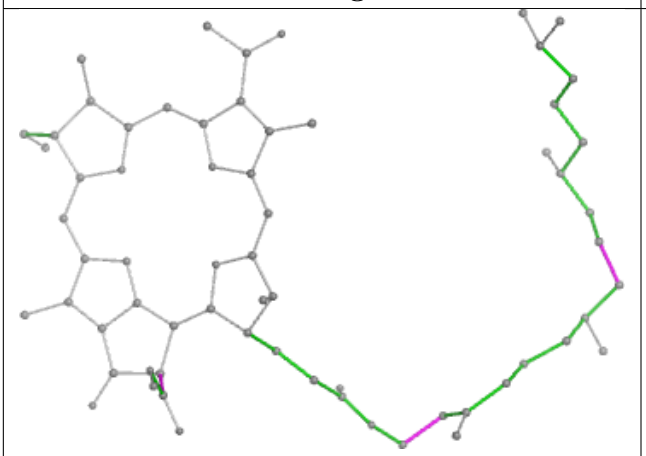
Ligand BPH L 303



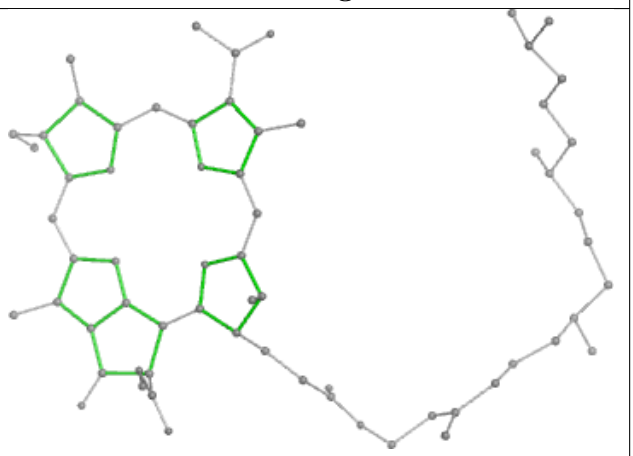
Bond lengths



Bond angles

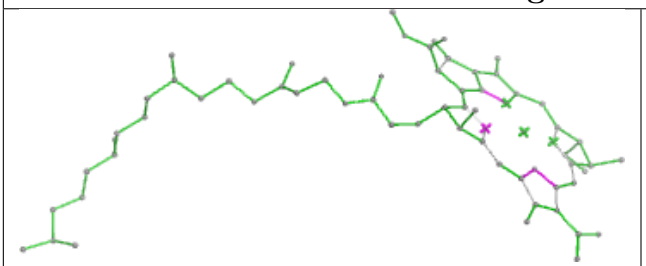


Torsions

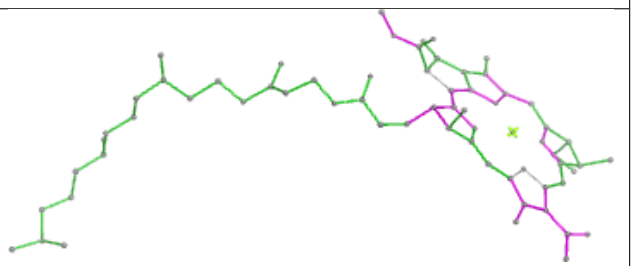


Rings

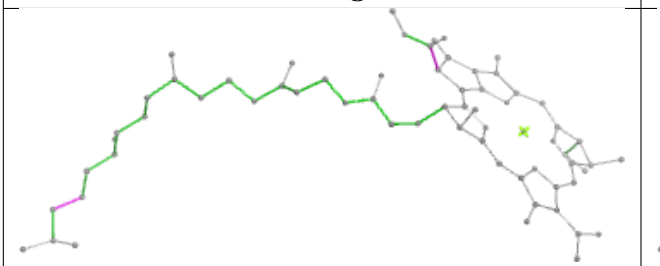
Ligand BCL L 301



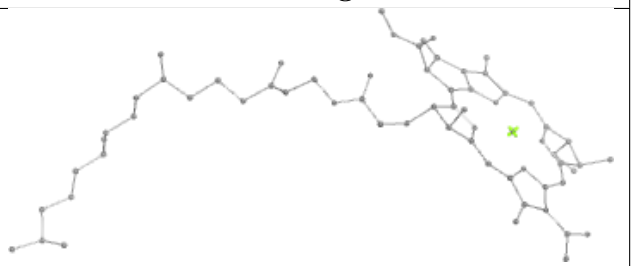
Bond lengths



Bond angles

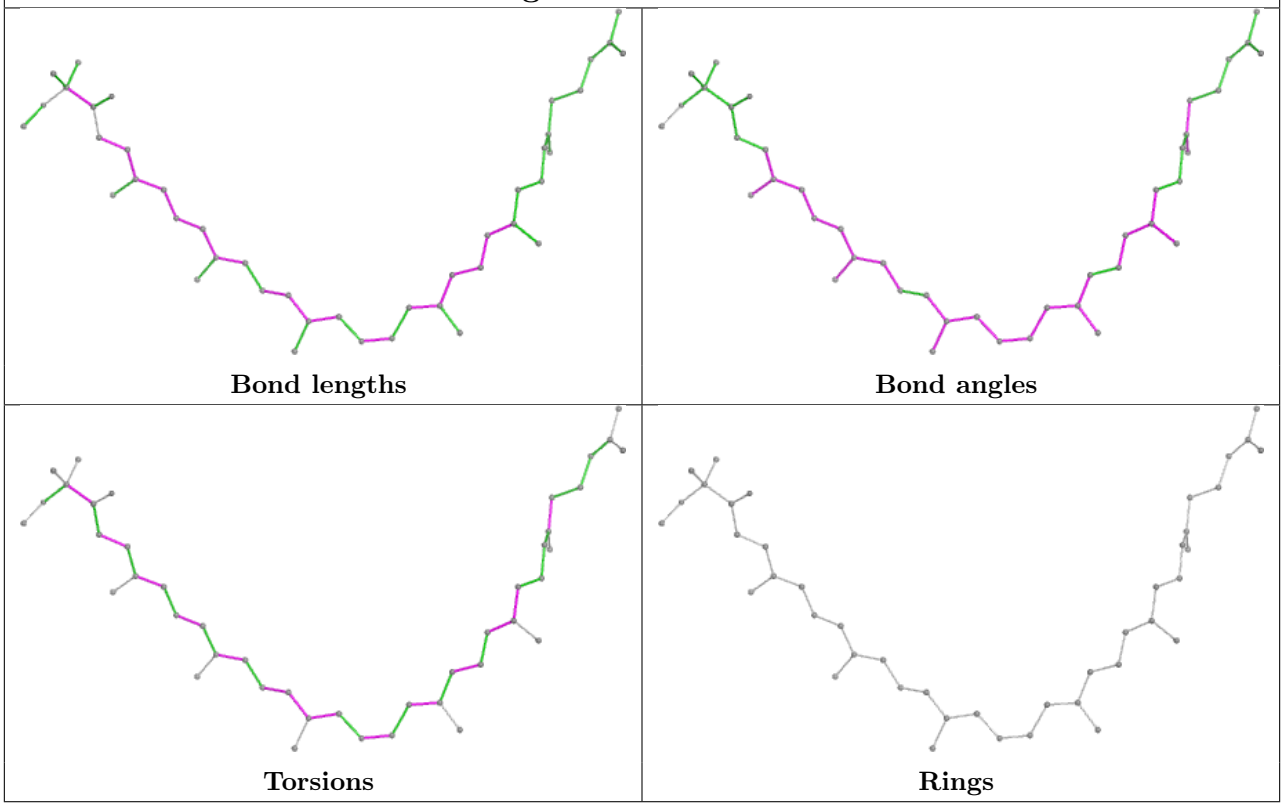


Torsions

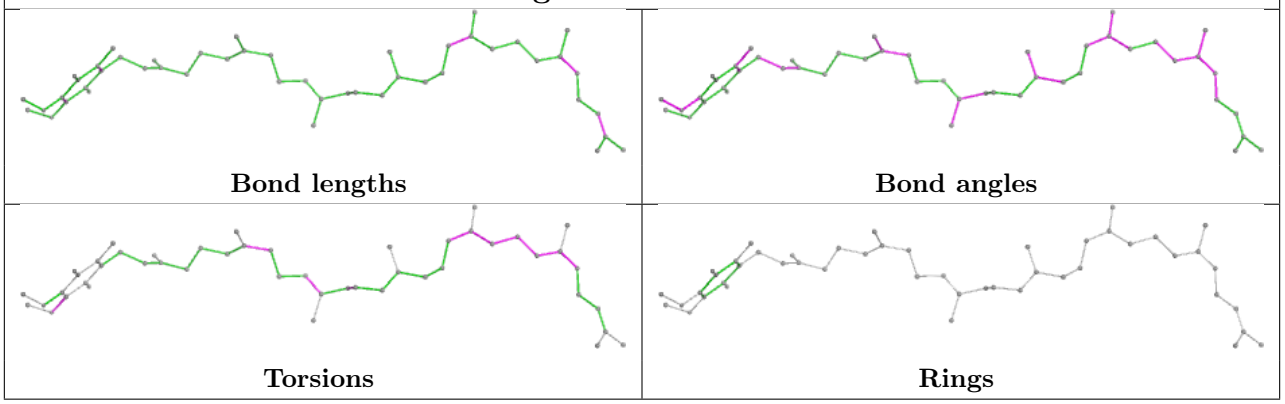


Rings

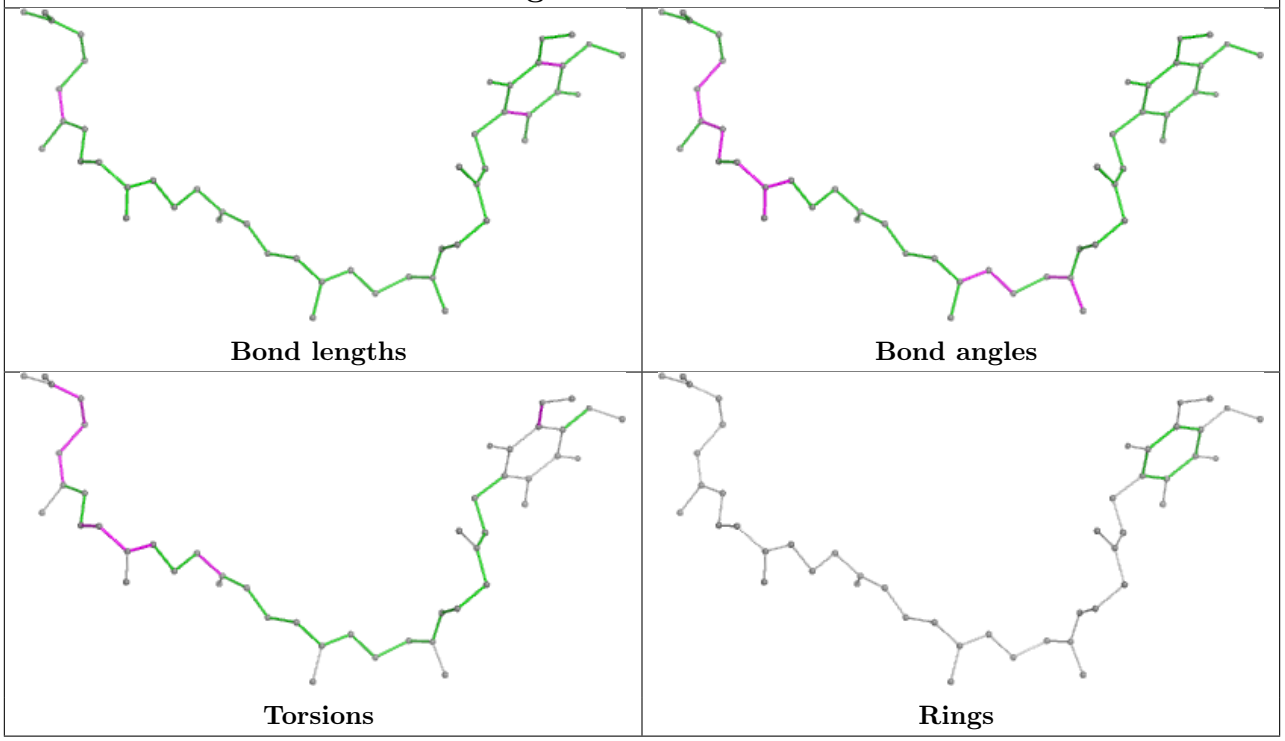
Ligand SPN M 405



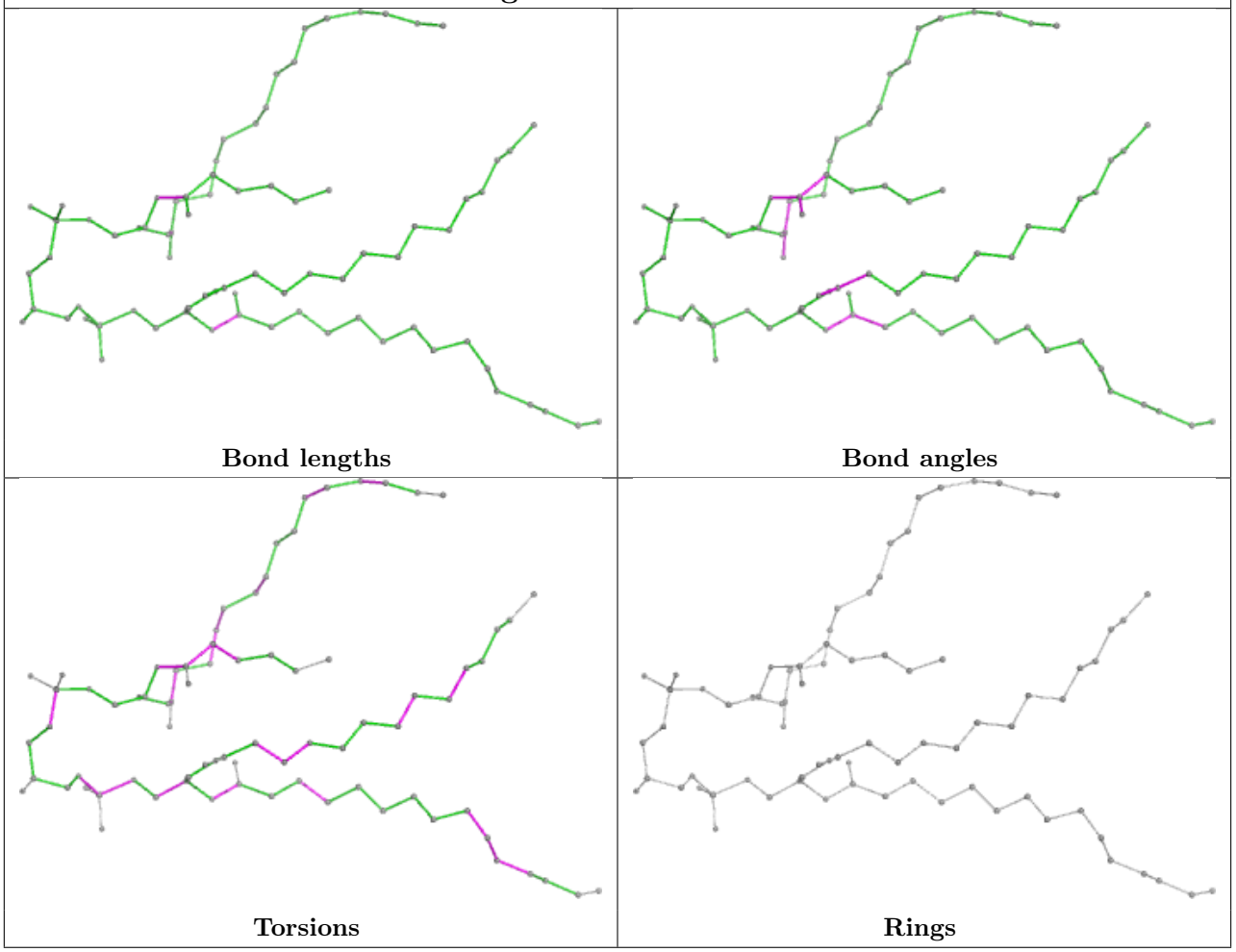
Ligand U10 L 304



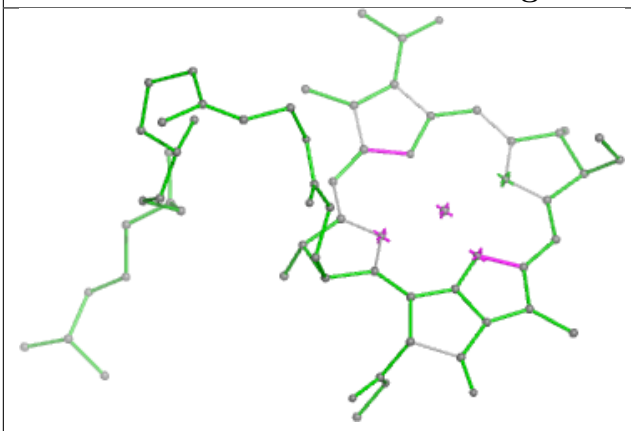
Ligand U10 M 404



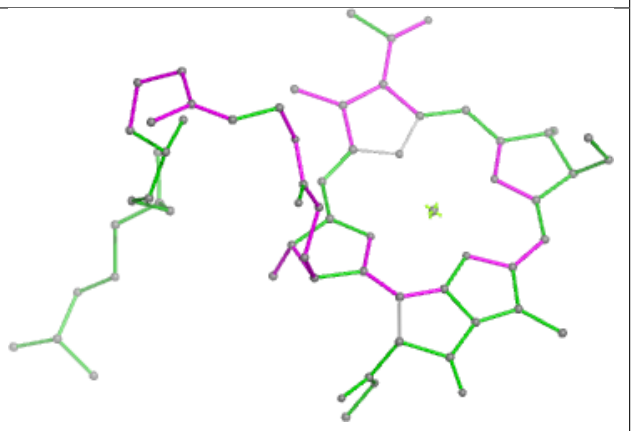
Ligand CDL M 409



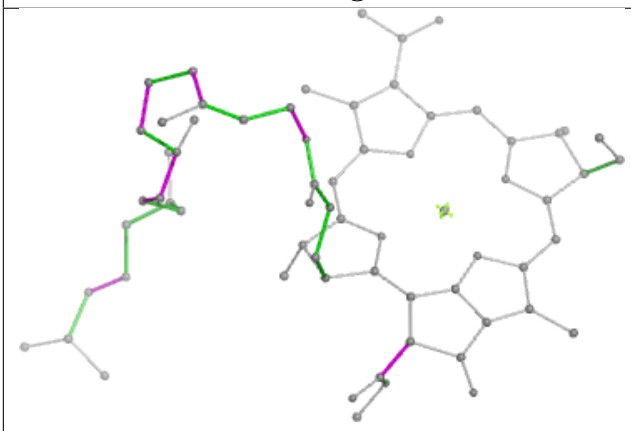
Ligand BCL M 401



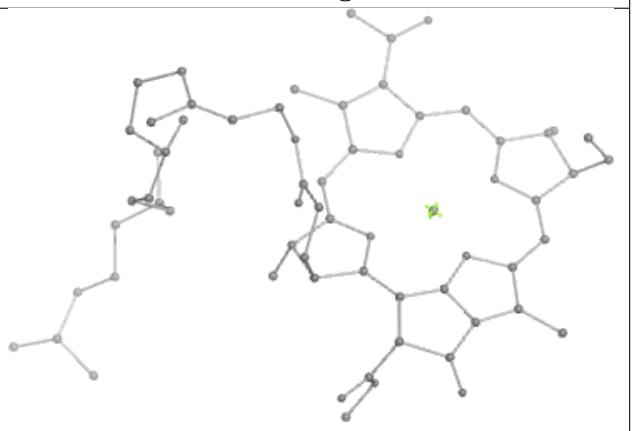
Bond lengths



Bond angles

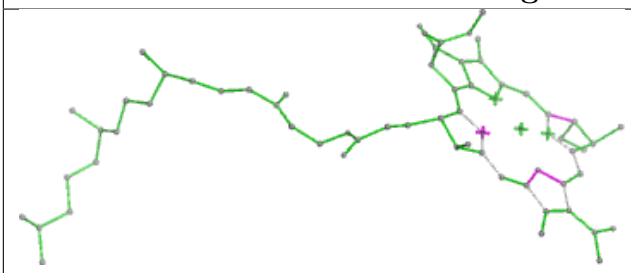


Torsions

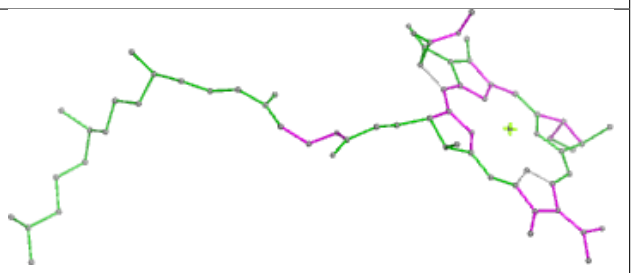


Rings

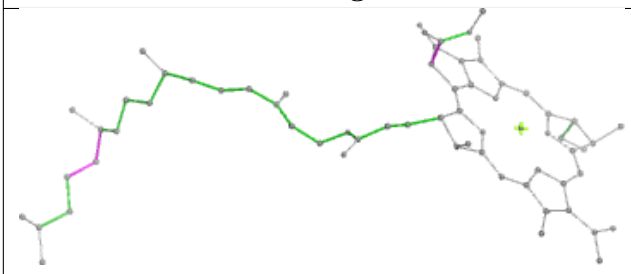
Ligand BCL M 402



Bond lengths



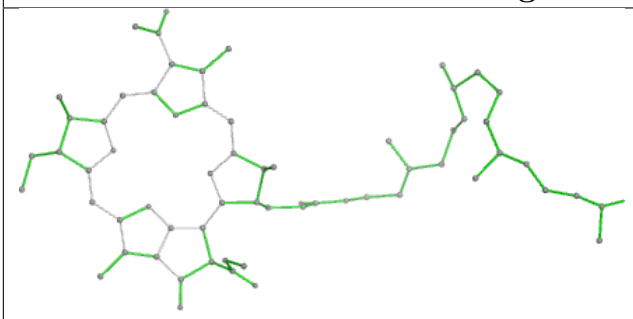
Bond angles



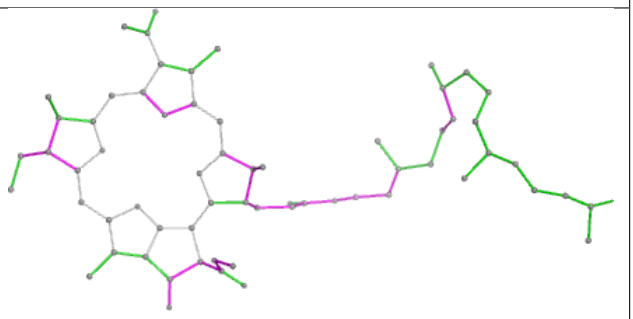
Torsions

Rings

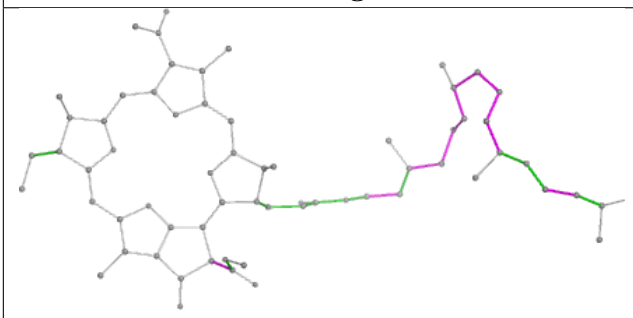
Ligand BPH M 403



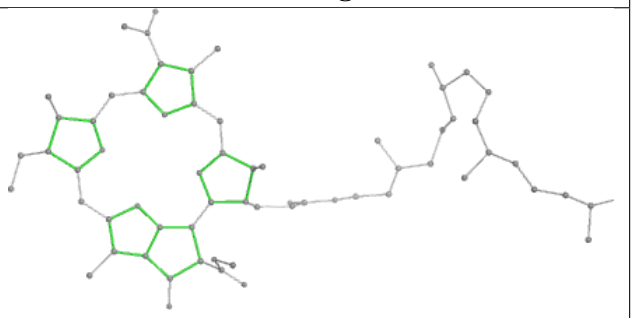
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	-0.50	7 (2%)	57	61	33, 43, 76, 118	0
2	M	300/307 (97%)	-0.45	4 (1%)	77	79	32, 47, 74, 108	0
3	H	240/260 (92%)	-0.39	8 (3%)	46	50	37, 46, 66, 146	0
All	All	821/848 (96%)	-0.45	19 (2%)	60	63	32, 46, 74, 146	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	7.7
1	L	59	TRP	6.3
3	H	246	PRO	6.2
3	H	249	LYS	6.1
3	H	247	LYS	5.2

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 monosaccharides in this entry.

6.4 Ligands

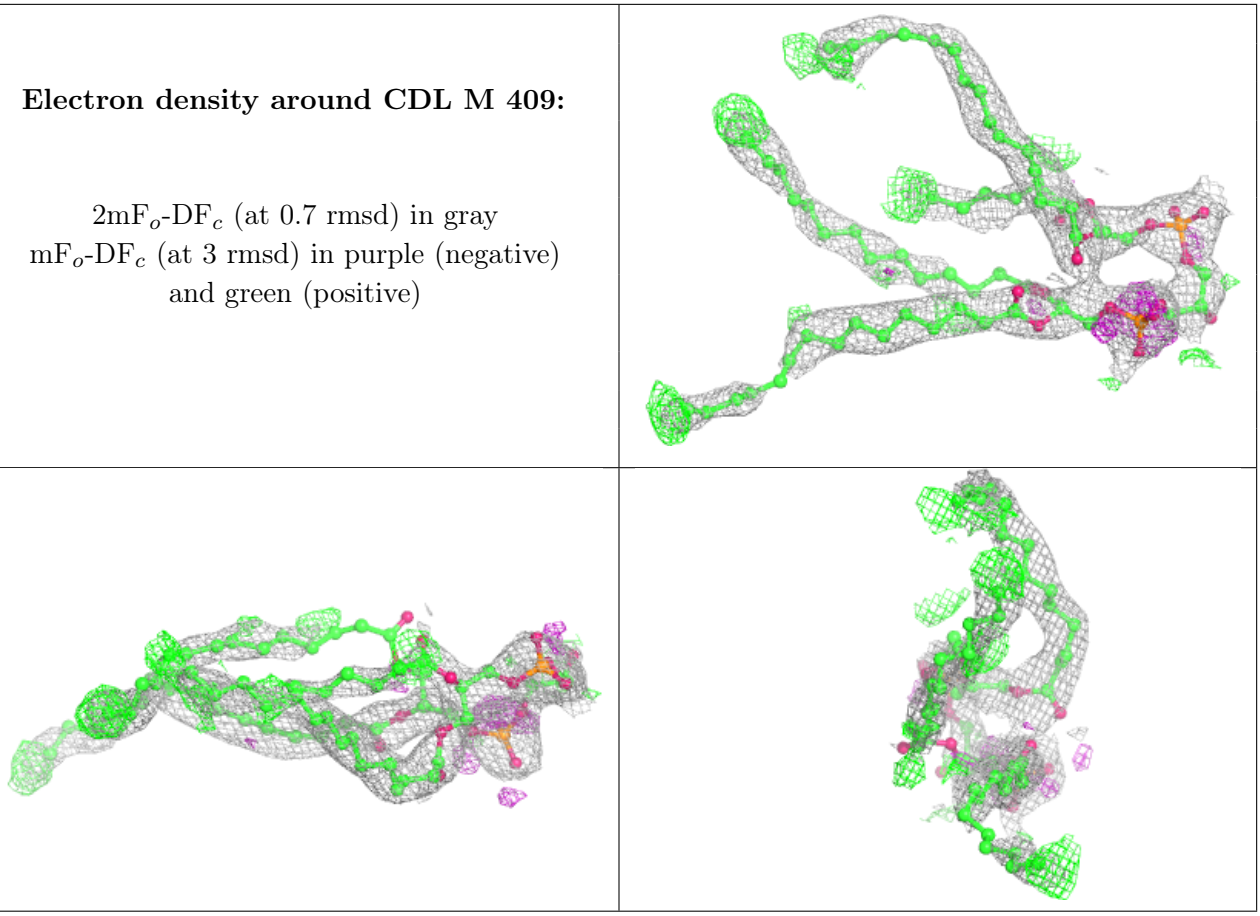
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	D12	H	305	8/12	0.57	0.50	81,85,87,88	0
7	D12	L	305	8/12	0.67	0.23	83,90,93,94	0
10	LDA	M	407	16/16	0.73	0.29	79,92,108,111	0
12	CDL	M	409	78/100	0.78	0.30	50,93,130,139	0
6	U10	L	304	48/63	0.79	0.26	47,68,94,100	0
7	D12	H	304	8/12	0.84	0.20	74,76,86,87	0
10	LDA	M	406	16/16	0.86	0.22	43,62,79,80	0
7	D12	H	303	9/12	0.87	0.23	75,76,81,83	0
7	D12	H	302	12/12	0.88	0.28	75,78,80,81	0
5	BPH	M	403	65/65	0.91	0.16	38,45,97,103	0
6	U10	M	404	48/63	0.91	0.23	34,49,91,103	0
9	SPN	M	405	43/43	0.92	0.18	38,51,90,98	0
10	LDA	H	301	16/16	0.95	0.12	57,65,75,78	0
4	BCL	M	401	66/66	0.96	0.16	32,37,90,93	0
4	BCL	L	301	66/66	0.97	0.16	33,40,50,64	0
4	BCL	M	402	66/66	0.97	0.16	34,40,60,71	0
5	BPH	L	303	65/65	0.97	0.14	30,37,46,48	0
11	PO4	M	408	5/5	0.97	0.20	70,71,78,79	0
4	BCL	L	302	66/66	0.97	0.15	28,34,60,72	0
8	FE	L	306	1/1	0.99	0.12	35,35,35,35	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.

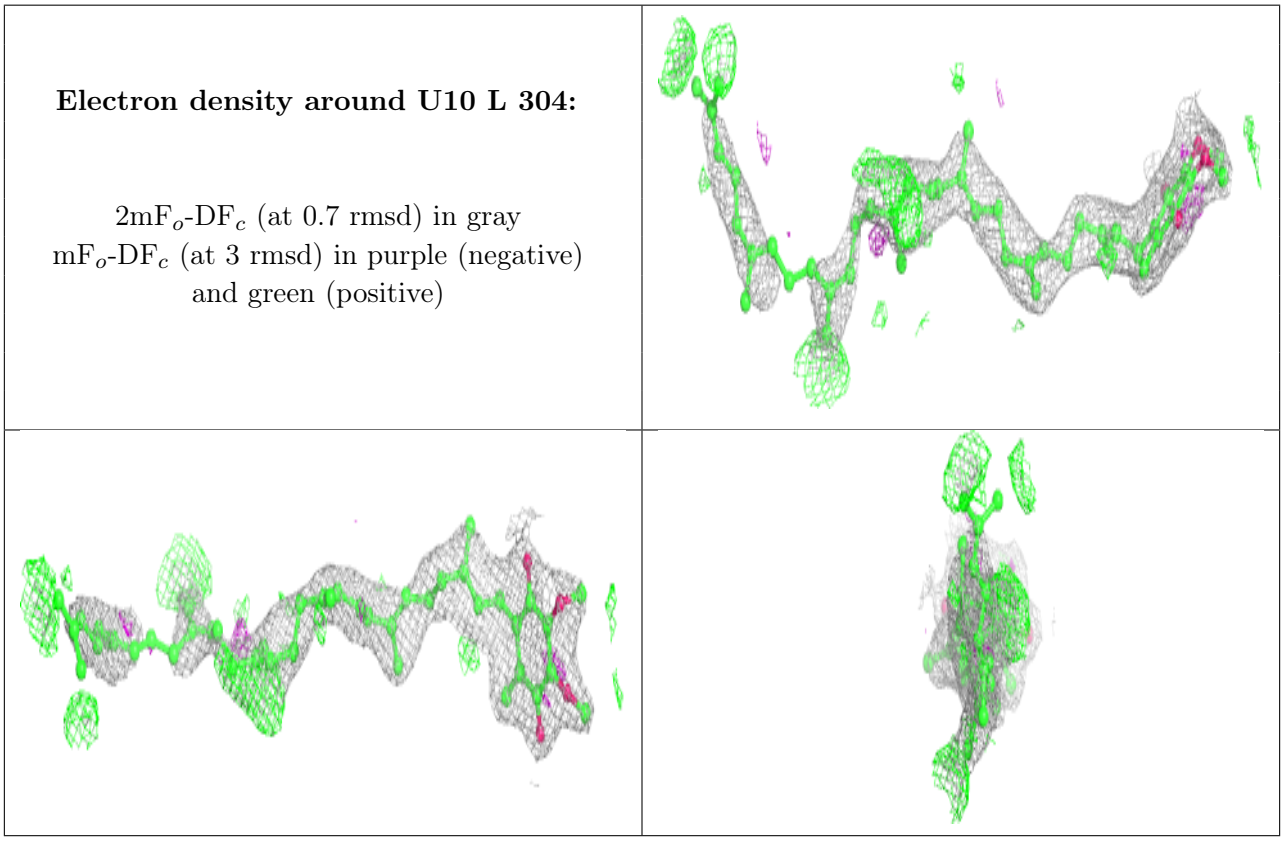
Electron density around CDL M 409:

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



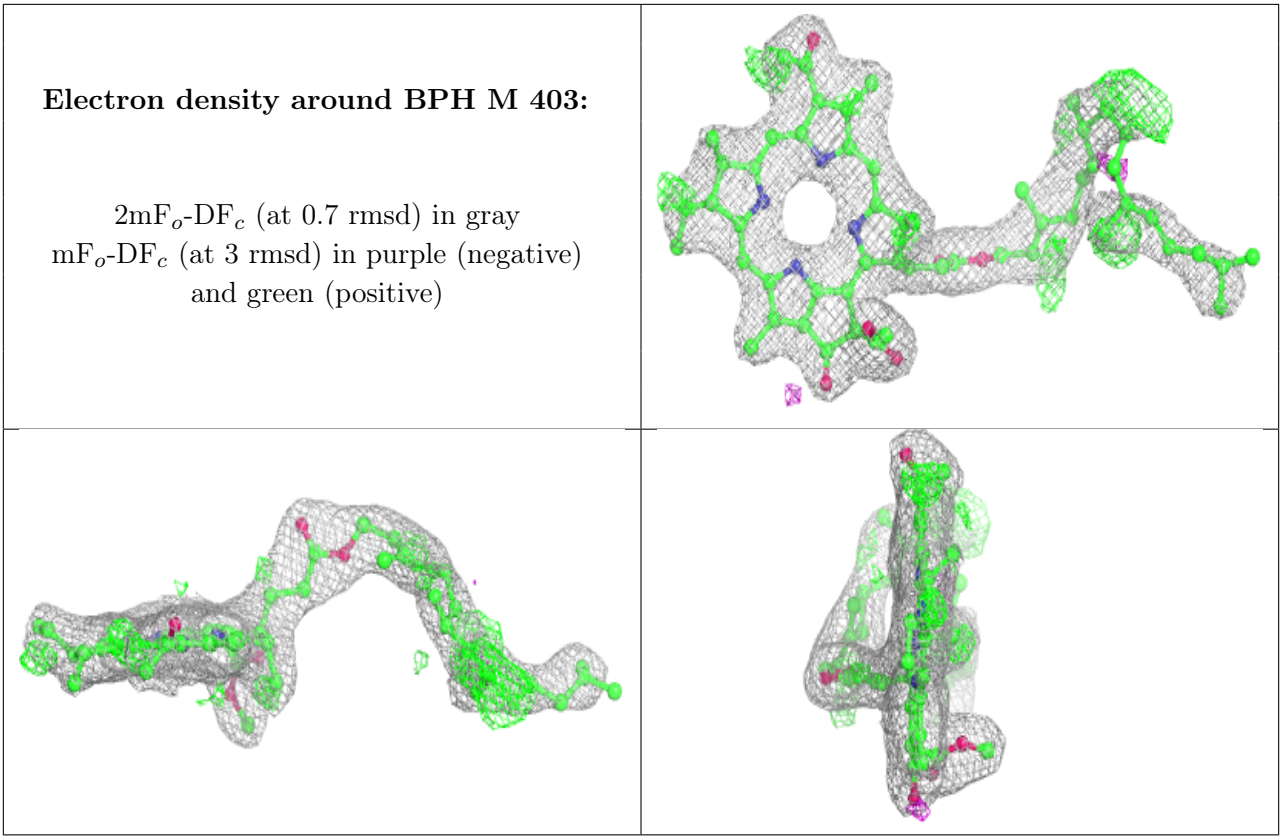
Electron density around U10 L 304:

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



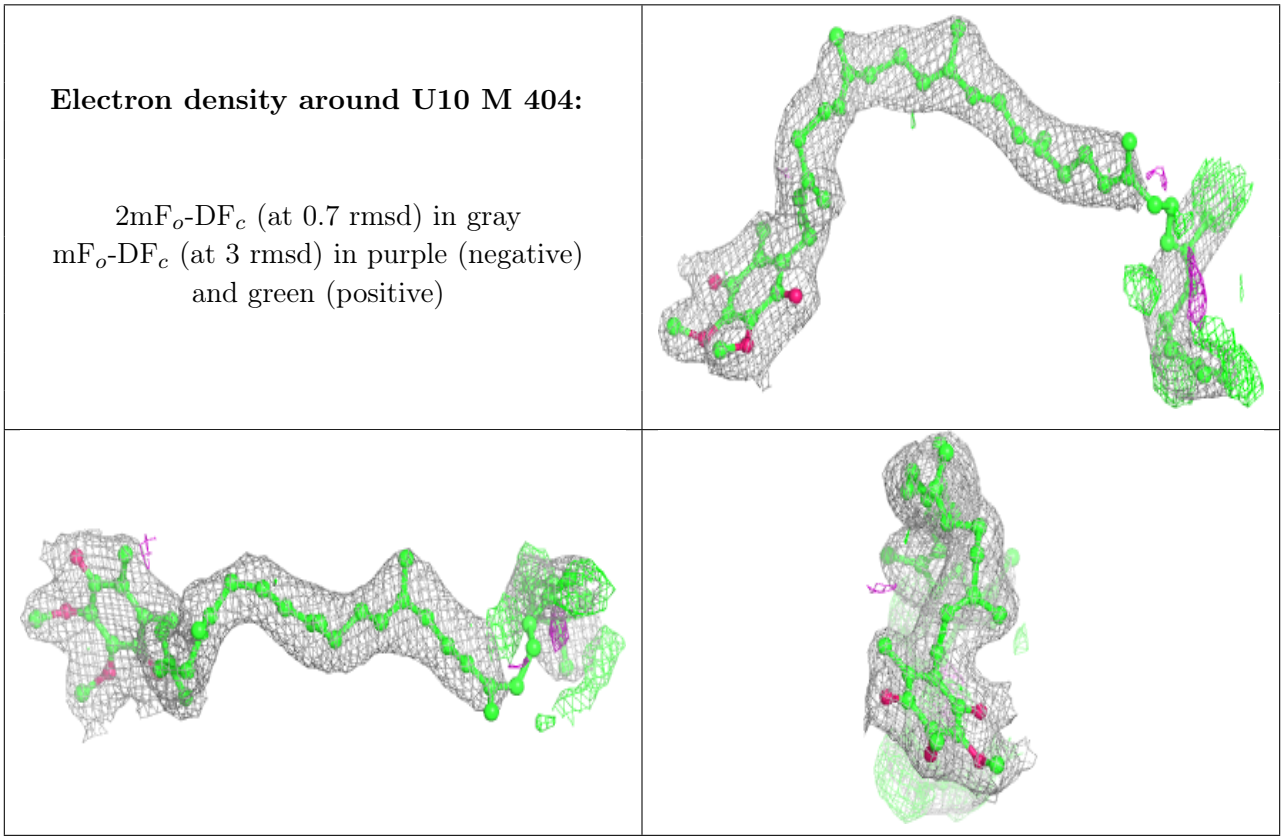
Electron density around BPH M 403:

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



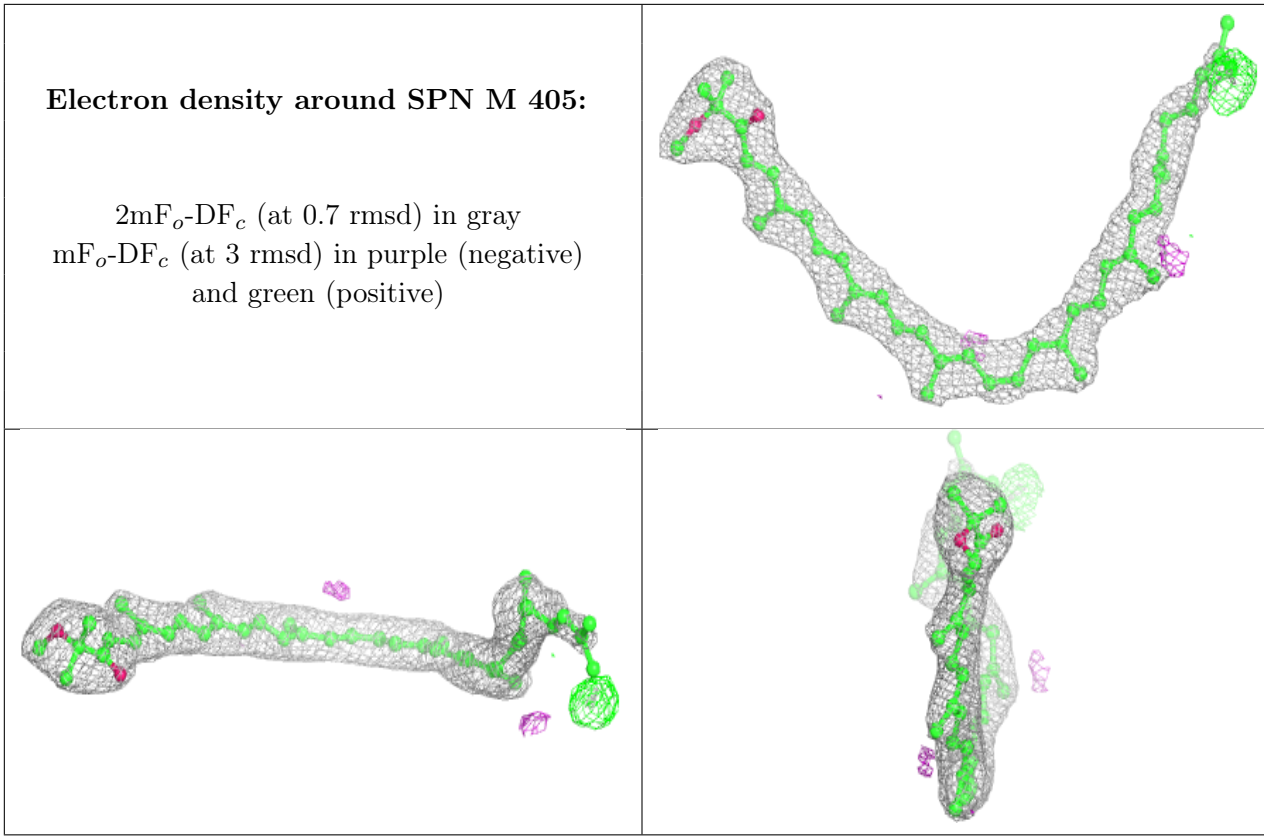
Electron density around U10 M 404:

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



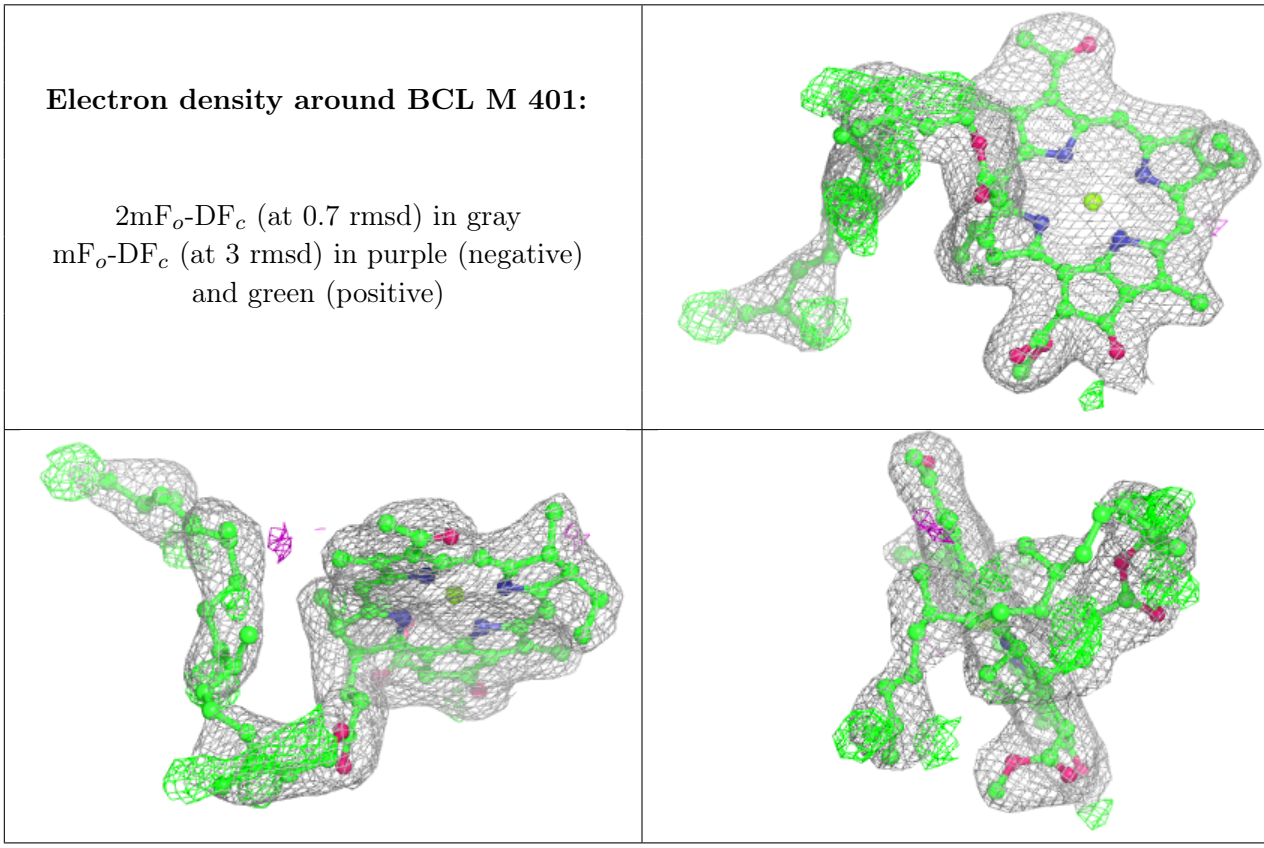
Electron density around SPN M 405:

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



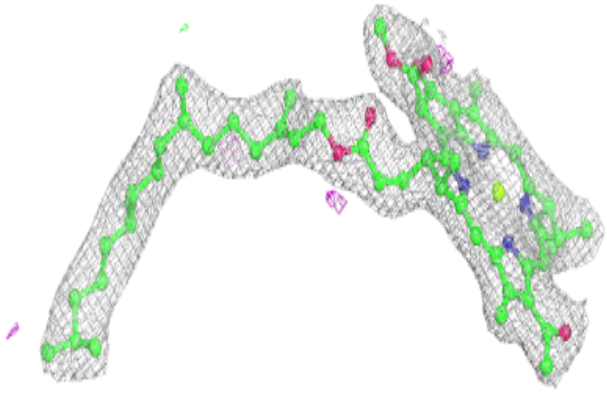
Electron density around BCL M 401:

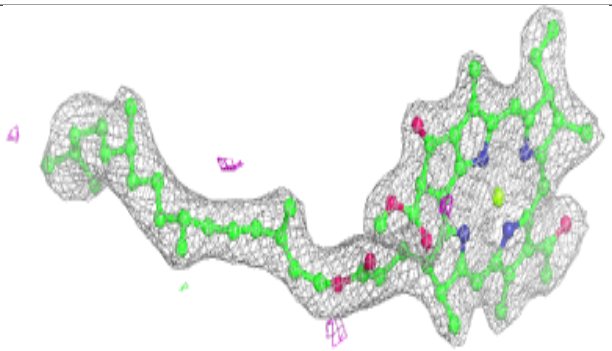
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

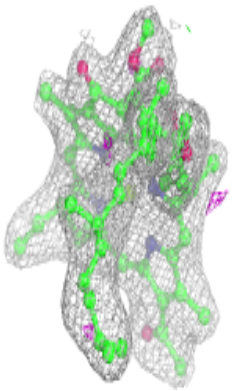


Electron density around BCL L 301:

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

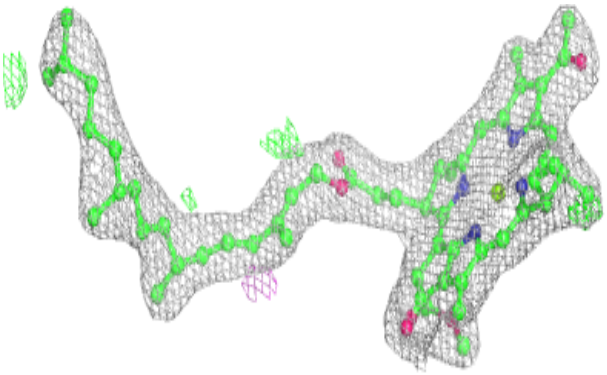


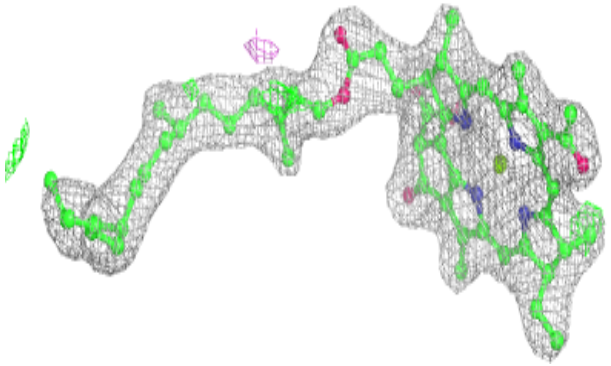


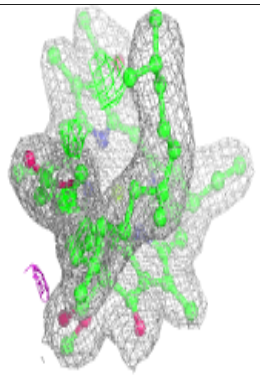


Electron density around BCL M 402:

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

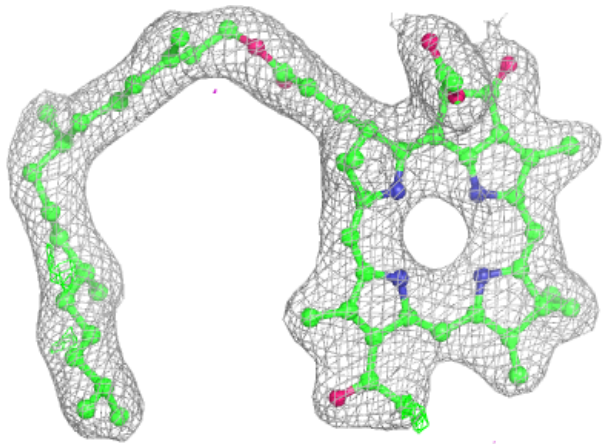


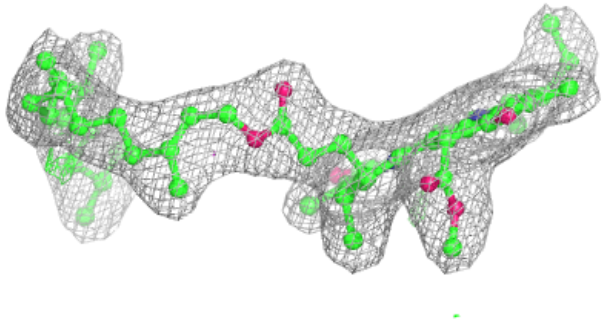




Electron density around BPH L 303:

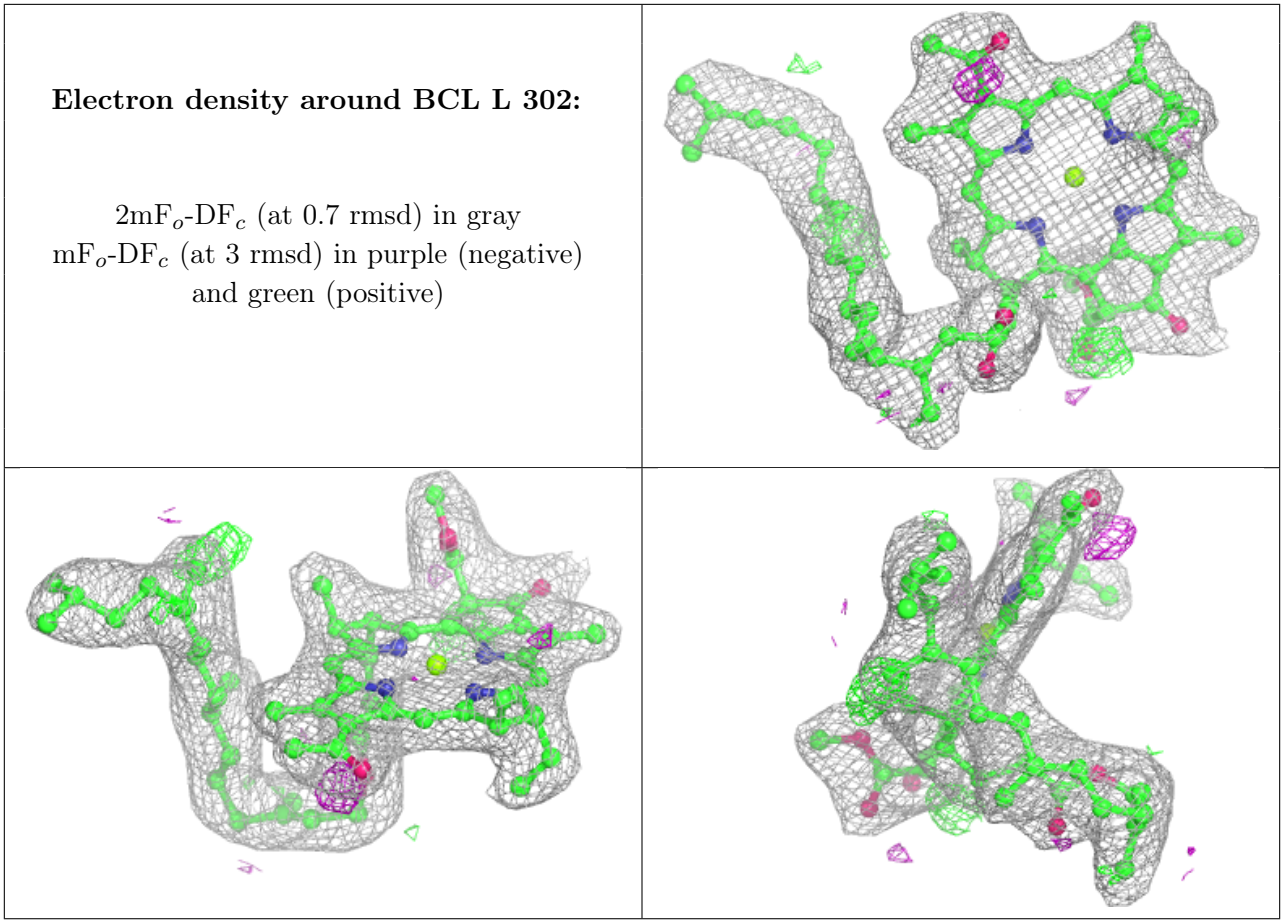
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around BCL L 302:

$2mF_o$-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.