wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 03:29 AM EDT

PDB ID	:	3DTA
Title	:	E(L212)Q, N(M44)D double mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides
Authors	:	Pokkuluri, P.R.; Schiffer, M.
Deposited on	:	2008-07-14
Resolution	:	3.20 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:

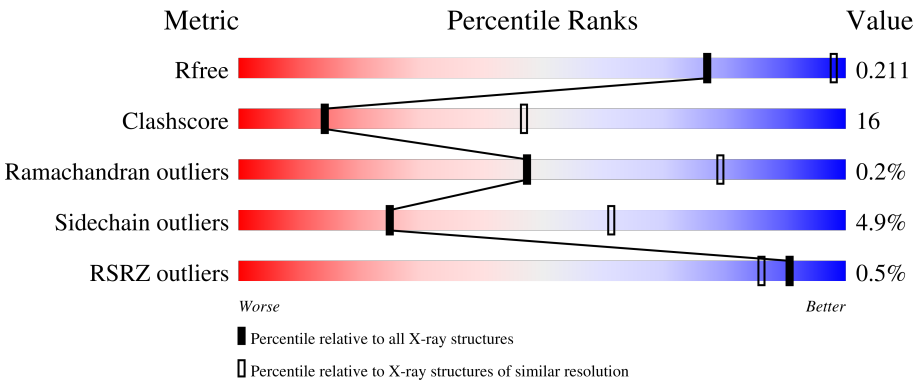
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	68% 27% ·
2	M	314	64% 27% · ·
3	H	260	% 61% 28% · 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
10	CDL	M	800	-	-	-	X
4	BCL	L	501	X	-	-	-
4	BCL	M	501	X	-	-	-
5	BPH	M	503	X	-	-	-
6	U10	L	504	-	-	-	X
7	LDA	M	704	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7296 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
			Total	C	N	O	S			
1	L	281	2232	1507	356	361	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	GLN	GLU	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2408	1607	393	398	10	0	0	0

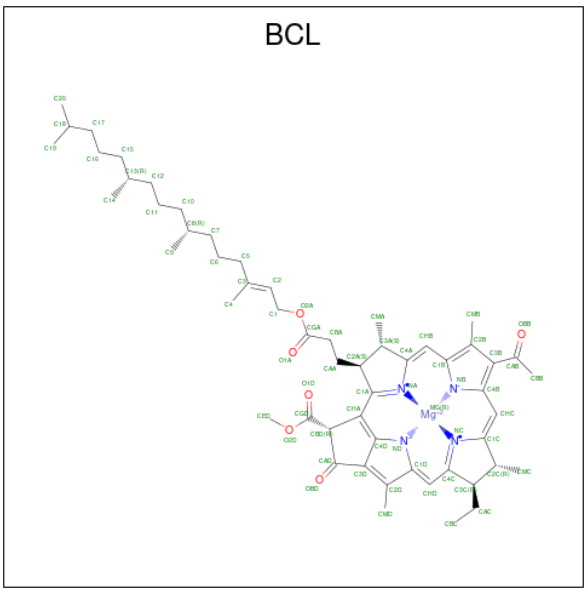
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	44	ASP	ASN	engineered mutation	UNP P0C0Y9
M	308	HIS	-	expression tag	UNP P0C0Y9
M	309	HIS	-	expression tag	UNP P0C0Y9
M	310	HIS	-	expression tag	UNP P0C0Y9
M	311	HIS	-	expression tag	UNP P0C0Y9
M	312	HIS	-	expression tag	UNP P0C0Y9
M	313	HIS	-	expression tag	UNP P0C0Y9
M	314	HIS	-	expression tag	UNP P0C0Y9

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

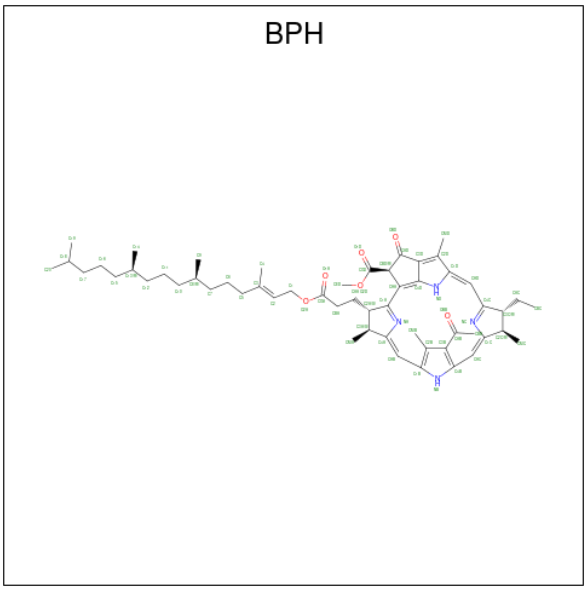
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	240	1829	1169	314	337	9	0	0	0

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



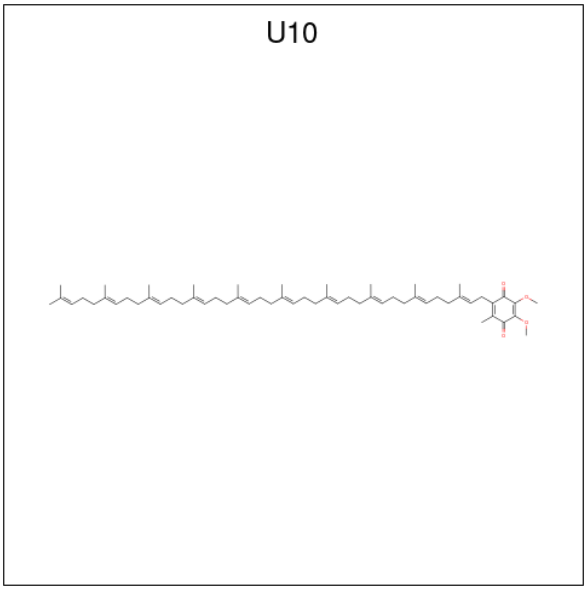
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0

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



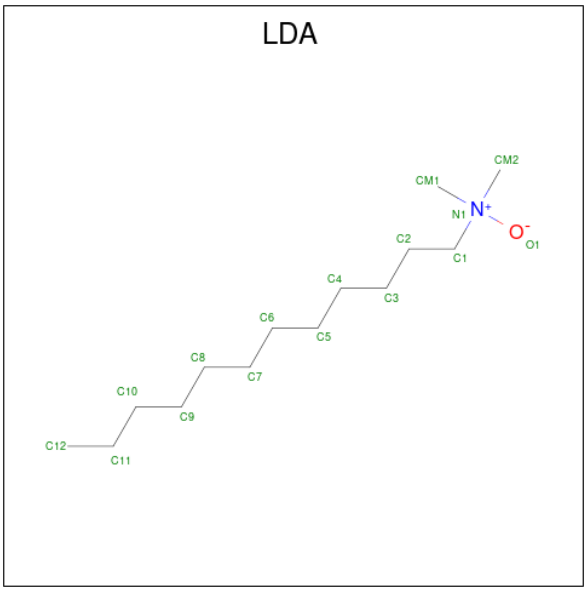
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	0	0
			Total	C	N	O		
5	M	1	65	55	4	6	10	0

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



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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

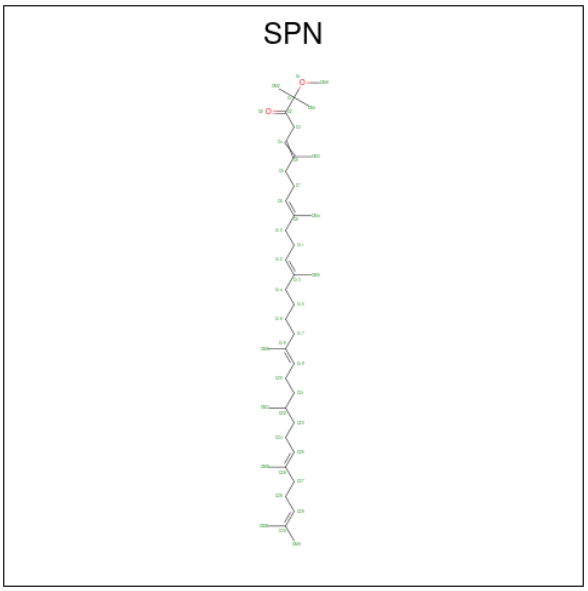


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	16	14	1	1	0	0
			Total	C	N	O		
7	M	1	16	14	1	1	0	0
			Total	C	N	O		
7	M	1	16	14	1	1	0	0
			Total	C	N	O		
7	H	1	16	14	1	1	0	0

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

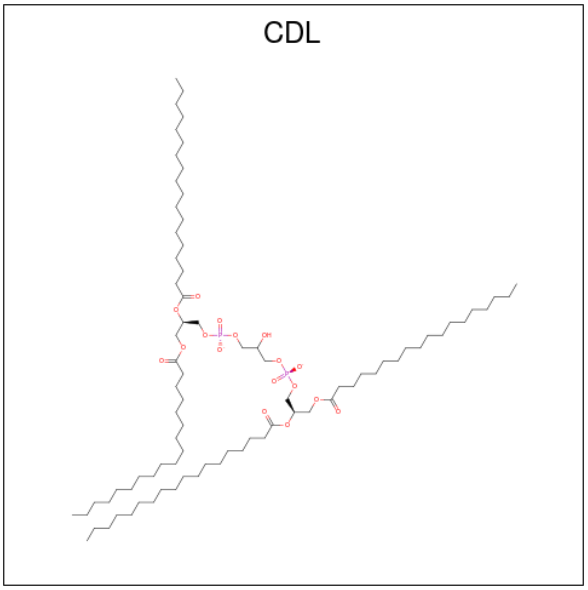
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
8	M	1	1	1	0	0

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



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

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 11 is water.

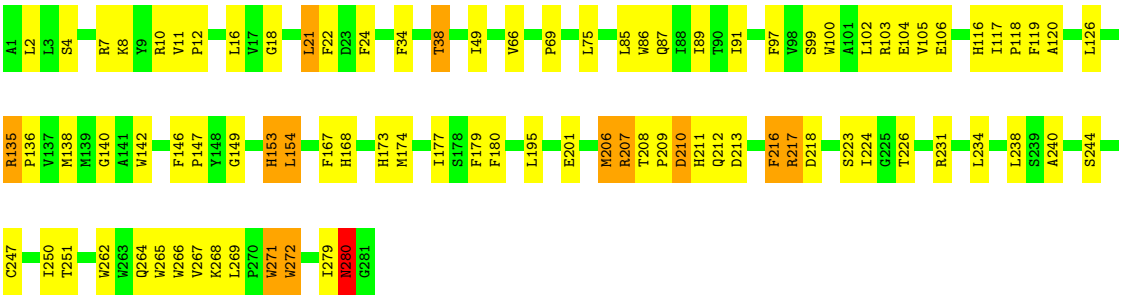
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	L	40	40	40	0	0
			Total	O		
11	M	44	44	44	0	0
			Total	O		
11	H	64	64	64	0	0

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.

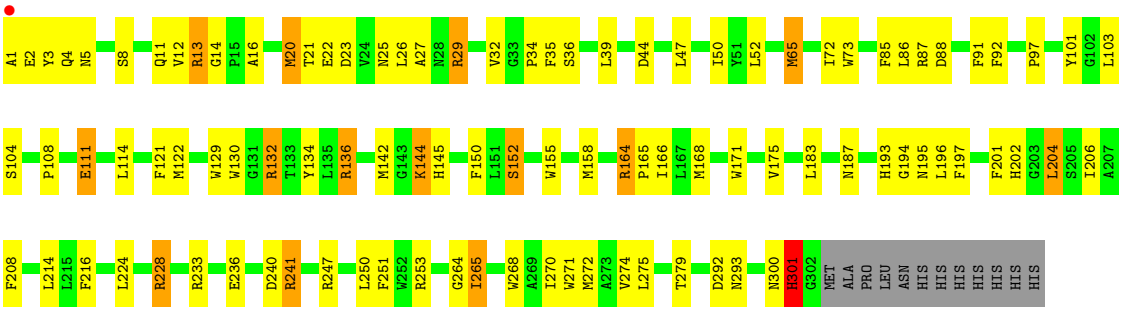
- Molecule 1: Reaction center protein L chain

Chain L:



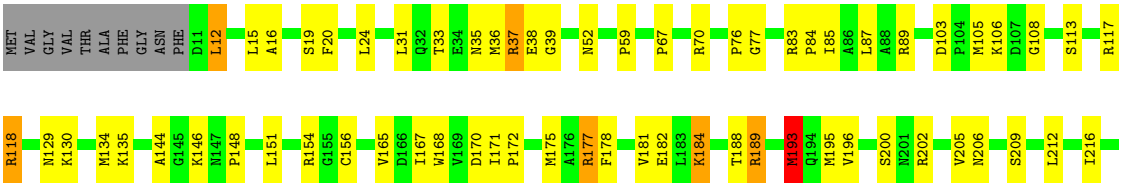
- Molecule 2: Reaction center protein M chain

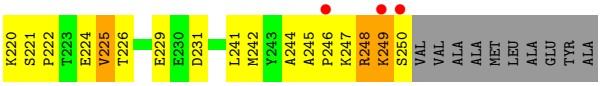
Chain M:



- Molecule 3: Reaction center protein H chain

Chain H:




K220
S221
P222
T223
E224
V225
T226
E229
E230
D231
L241
M242
Y243
A244
A245
P246
K247
R248
K249
S250
VAL
VAL
ALA
ALA
MET
LEU
ALA
GLU
TYR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.50Å 141.50Å 187.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.20 28.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.9 (28.52-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.17Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.203 0.205 , 0.211	Depositor DCC
R_{free} test set	2410 reflections (6.99%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 80.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, U10, SPN, CDL, BPH, FE, 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	0.95	0/2320	1.08	13/3175 (0.4%)
2	M	1.08	3/2500 (0.1%)	1.17	21/3413 (0.6%)
3	H	0.95	2/1877 (0.1%)	1.25	21/2553 (0.8%)
All	All	1.00	5/6697 (0.1%)	1.17	55/9141 (0.6%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	76	PRO	C-N	-6.35	1.21	1.33
2	M	14	GLY	N-CA	5.91	1.54	1.46
3	H	77	GLY	N-CA	5.73	1.54	1.46
2	M	247	ARG	CG-CD	-5.41	1.38	1.51
2	M	301	HIS	CA-C	-5.14	1.39	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	248	ARG	CD-NE-CZ	13.08	141.92	123.60
2	M	247	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	L	103	ARG	NE-CZ-NH1	11.02	125.81	120.30
3	H	250	SER	CA-C-O	-8.25	102.78	120.10
1	L	207	ARG	NE-CZ-NH2	7.67	124.13	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	280	ASN	Mainchain

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	2232	0	2189	79	0
2	M	2408	0	2319	86	0
3	H	1829	0	1836	46	0
4	L	132	0	148	16	0
4	M	132	0	148	19	0
5	L	65	0	76	2	0
5	M	65	0	76	1	0
6	L	48	0	63	7	0
6	M	48	0	63	6	0
7	H	16	0	31	4	0
7	L	16	0	31	3	0
7	M	32	0	62	4	0
8	M	1	0	0	0	0
9	M	43	0	69	1	0
10	M	81	0	106	1	0
11	H	64	0	0	3	0
11	L	40	0	0	1	0
11	M	44	0	0	3	0
All	All	7296	0	7217	223	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 16.

The worst 5 of 223 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:13:ARG:HD3	2:M:35:PHE:CD2	1.72	1.23
2:M:13:ARG:CD	2:M:35:PHE:CD2	2.43	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:13:ARG:HD3	2:M:35:PHE:CE2	1.94	1.00
3:H:33:THR:O	3:H:59:PRO:HG3	1.69	0.91
1:L:34:PHE:O	1:L:38:THR:HG23	1.71	0.89

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%)	262 (94%)	16 (6%)	1 (0%)	34	69
2	M	300/314 (96%)	285 (95%)	14 (5%)	1 (0%)	41	74
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/855 (96%)	776 (95%)	39 (5%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
1	L	210	ASP

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	220/220 (100%)	208 (94%)	12 (6%)	21	57
2	M	236/247 (96%)	227 (96%)	9 (4%)	33	67
3	H	195/208 (94%)	184 (94%)	11 (6%)	21	57
All	All	651/675 (96%)	619 (95%)	32 (5%)	25	61

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	222	PRO
3	H	225	VAL
2	M	111	GLU
1	L	272	TRP
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
2	M	188	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\#\|Z\| > 2$
4	BCL	M	501	2	58,74,74	1.57	10 (17%)	69,115,115	2.55	27 (39%)
6	U10	L	504	-	48,48,63	2.15	21 (43%)	58,61,79	1.01	3 (5%)
5	BPH	L	503	-	51,70,70	1.76	11 (21%)	52,101,101	2.49	14 (26%)
5	BPH	M	503	-	51,70,70	1.77	9 (17%)	52,101,101	2.83	24 (46%)
4	BCL	M	502	2	58,74,74	1.31	8 (13%)	69,115,115	1.94	13 (18%)
7	LDA	M	704	-	12,15,15	2.06	1 (8%)	14,17,17	0.52	0
4	BCL	L	502	1	58,74,74	1.61	10 (17%)	69,115,115	2.61	14 (20%)
9	SPN	M	600	-	40,42,42	3.75	18 (45%)	50,52,52	2.58	16 (32%)
10	CDL	M	800	-	80,80,99	0.48	0	86,92,111	0.93	6 (6%)
4	BCL	L	501	1	58,74,74	1.39	9 (15%)	69,115,115	2.24	14 (20%)
7	LDA	M	701	-	12,15,15	2.57	1 (8%)	14,17,17	0.40	0
6	U10	M	504	-	48,48,63	2.46	21 (43%)	58,61,79	1.30	7 (12%)
7	LDA	H	703	-	12,15,15	2.40	1 (8%)	14,17,17	0.65	0
7	LDA	L	709	-	12,15,15	2.42	1 (8%)	14,17,17	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	501	2	2/2/21/25	15/37/137/137	-
6	U10	L	504	-	-	9/45/69/87	0/1/1/1
5	BPH	L	503	-	-	5/37/105/105	0/5/6/6
5	BPH	M	503	-	1/1/18/22	12/37/105/105	0/5/6/6
4	BCL	M	502	2	-	8/37/137/137	-
7	LDA	M	704	-	-	2/13/13/13	-
4	BCL	L	502	1	-	6/37/137/137	-
9	SPN	M	600	-	-	19/50/51/51	-
10	CDL	M	800	-	-	30/91/91/110	-
4	BCL	L	501	1	1/1/21/25	10/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	M	701	-	-	8/13/13/13	-
6	U10	M	504	-	-	10/45/69/87	0/1/1/1
7	LDA	H	703	-	-	5/13/13/13	-
7	LDA	L	709	-	-	4/13/13/13	-

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C4-C5	8.92	1.54	1.33
9	M	600	SPN	C19-C18	8.79	1.54	1.33
7	M	701	LDA	O1-N1	-8.77	1.21	1.42
9	M	600	SPN	C8-C9	8.43	1.53	1.33
7	H	703	LDA	O1-N1	-8.30	1.22	1.42

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	503	BPH	O2D-CGD-CBD	11.86	126.03	111.00
5	L	503	BPH	O2D-CGD-CBD	11.28	125.28	111.00
4	L	502	BCL	C4B-C3B-CAB	-11.05	105.79	127.13
4	L	502	BCL	OBB-CAB-C3B	9.30	136.49	119.99
4	L	501	BCL	C4A-NA-C1A	8.47	110.51	106.71

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	501	BCL	C13
4	M	501	BCL	C13
4	M	501	BCL	C8
5	M	503	BPH	C8

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	501	BCL	C2C-C3C-CAC-CBC
4	L	501	BCL	C4C-C3C-CAC-CBC
4	M	501	BCL	C1-C2-C3-C4
5	M	503	BPH	O2A-C1-C2-C3
5	M	503	BPH	C1-C2-C3-C4

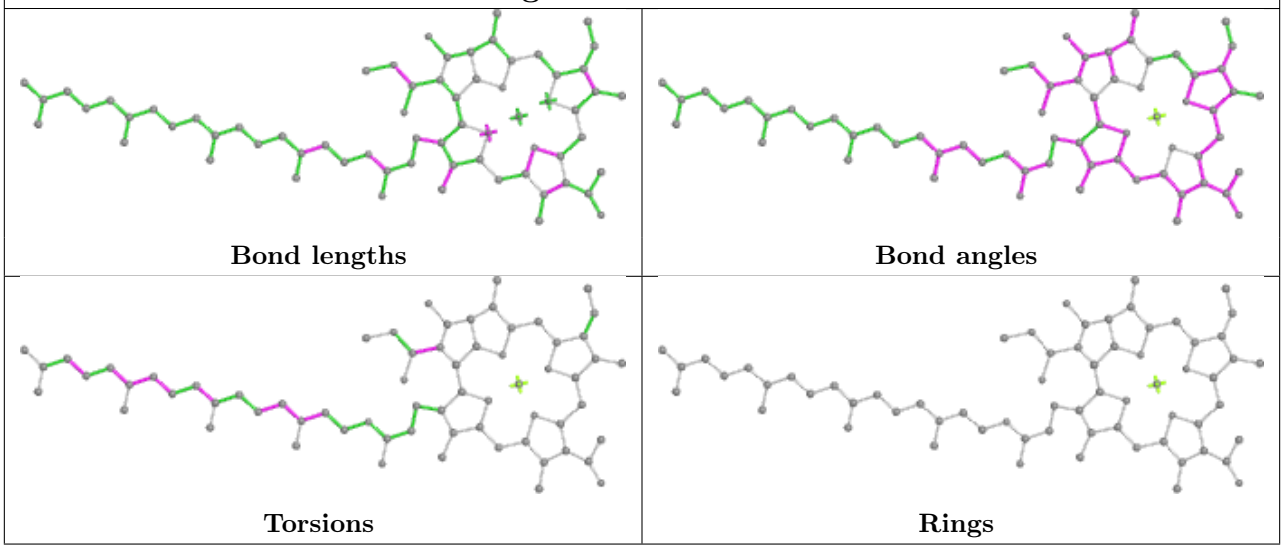
There are no ring outliers.

13 monomers are involved in 58 short contacts:

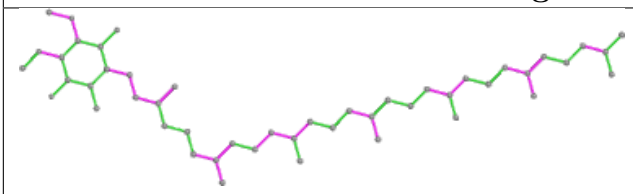
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	501	BCL	9	0
6	L	504	U10	7	0
5	L	503	BPH	2	0
5	M	503	BPH	1	0
4	M	502	BCL	12	0
4	L	502	BCL	11	0
9	M	600	SPN	1	0
10	M	800	CDL	1	0
4	L	501	BCL	7	0
7	M	701	LDA	4	0
6	M	504	U10	6	0
7	H	703	LDA	4	0
7	L	709	LDA	3	0

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 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.

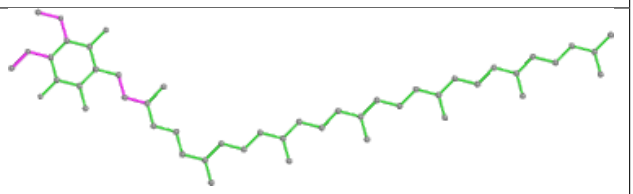
Ligand BCL M 501



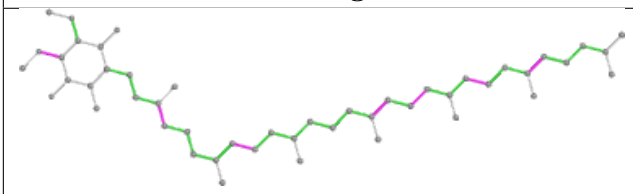
Ligand U10 L 504



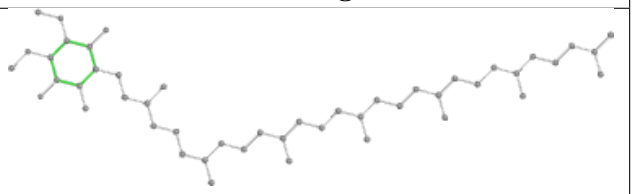
Bond lengths



Bond angles

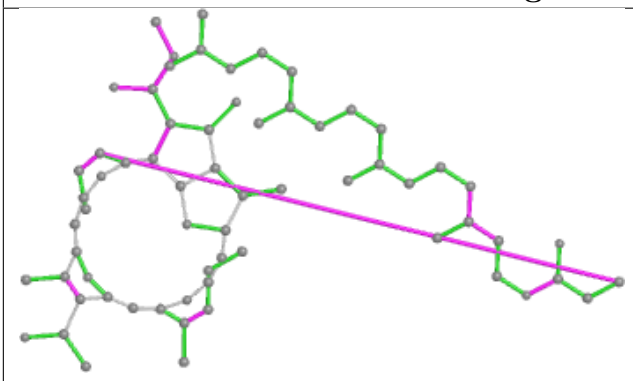


Torsions

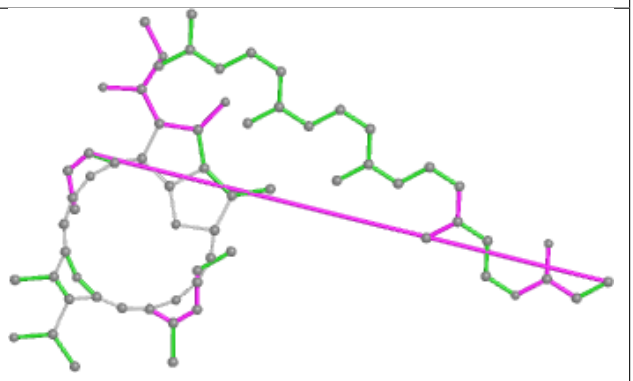


Rings

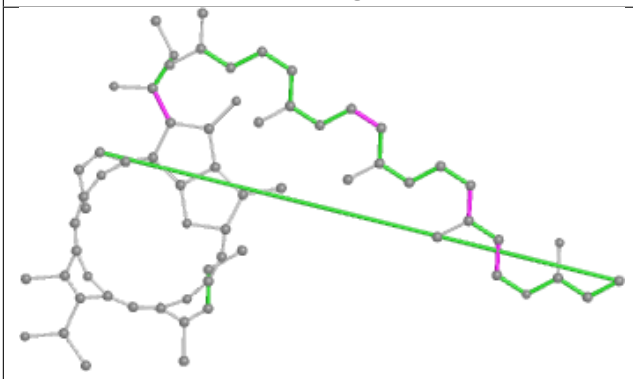
Ligand BPH L 503



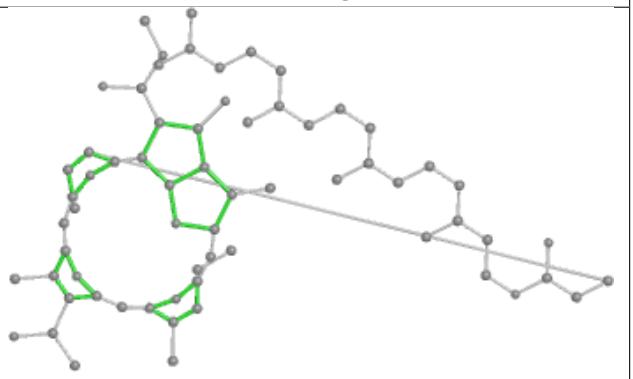
Bond lengths



Bond angles

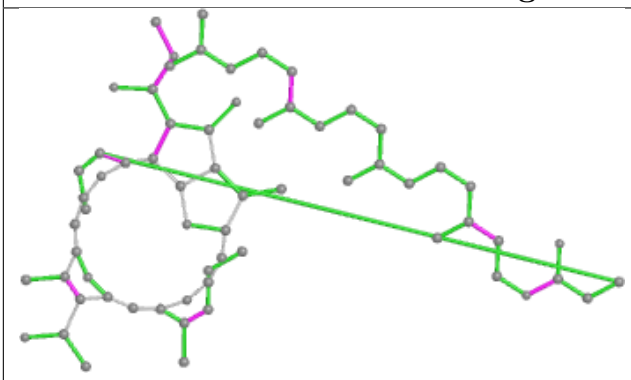


Torsions

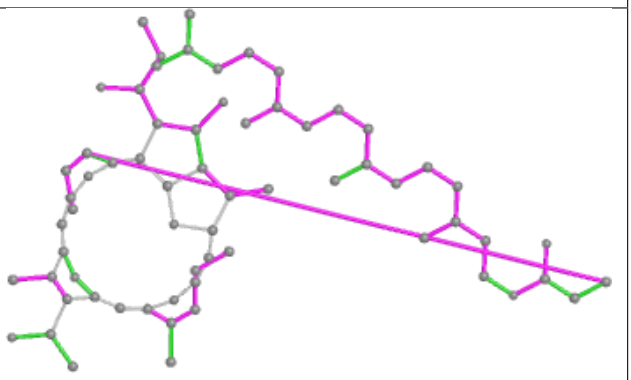


Rings

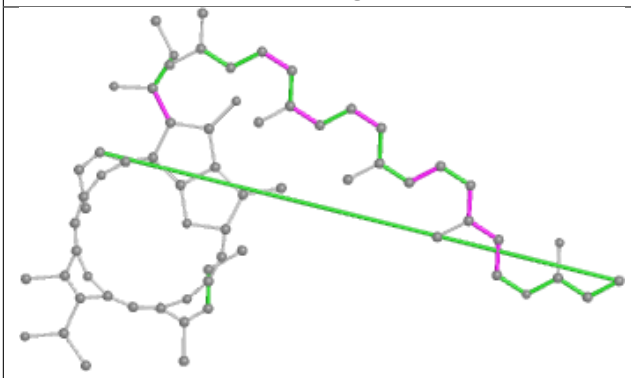
Ligand BPH M 503



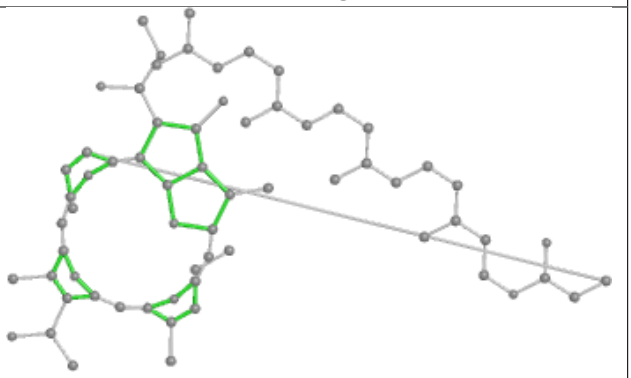
Bond lengths



Bond angles

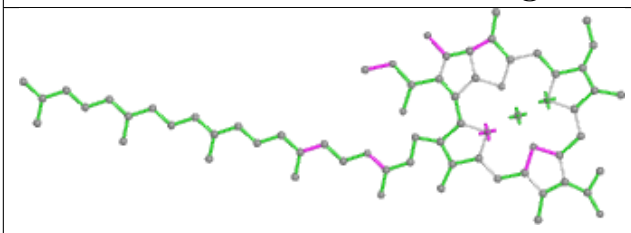


Torsions

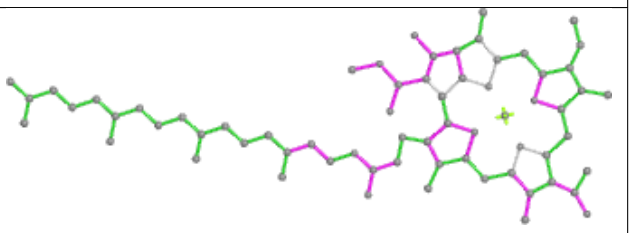


Rings

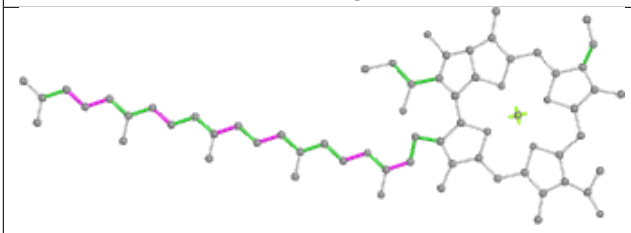
Ligand BCL M 502



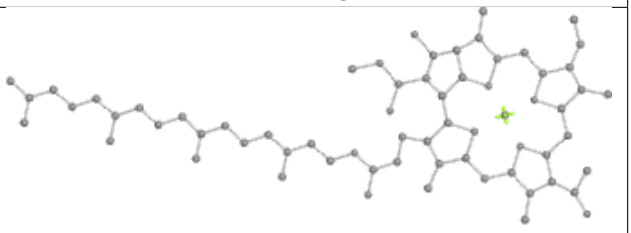
Bond lengths



Bond angles

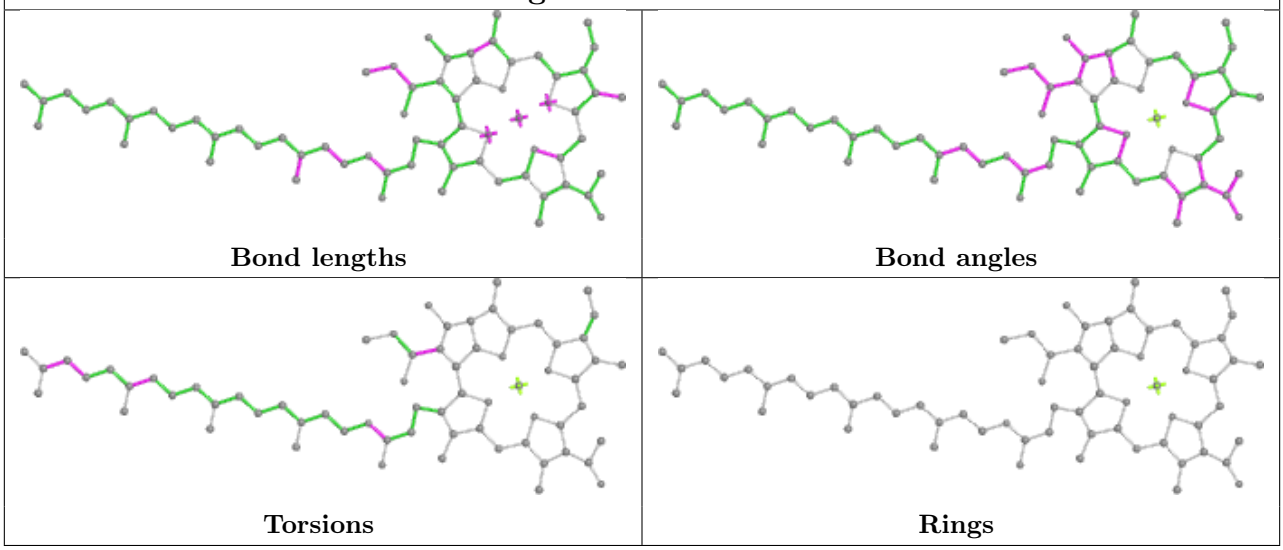


Torsions

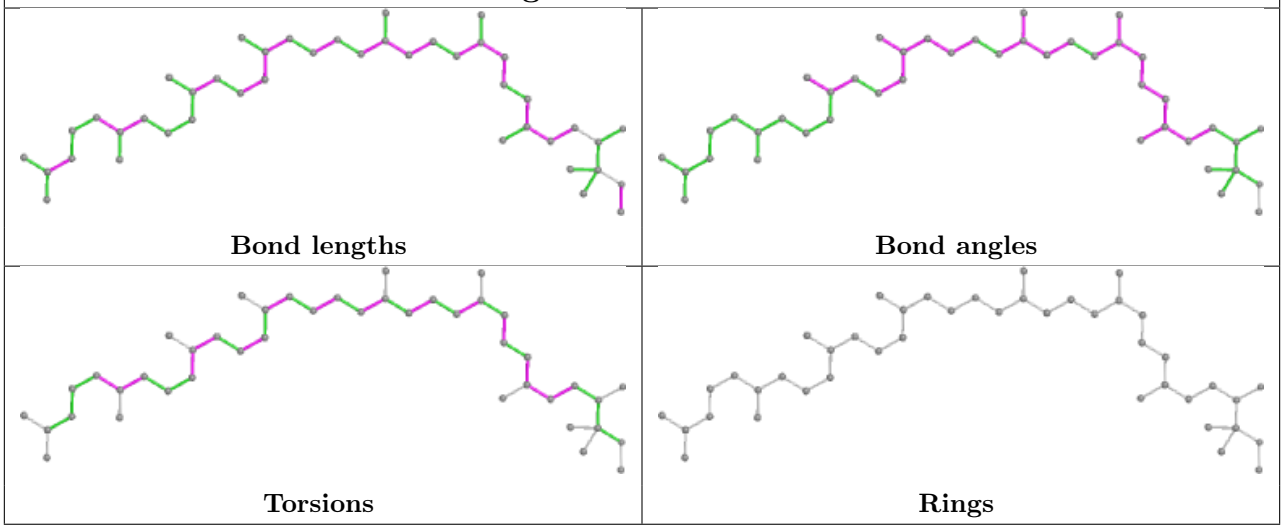


Rings

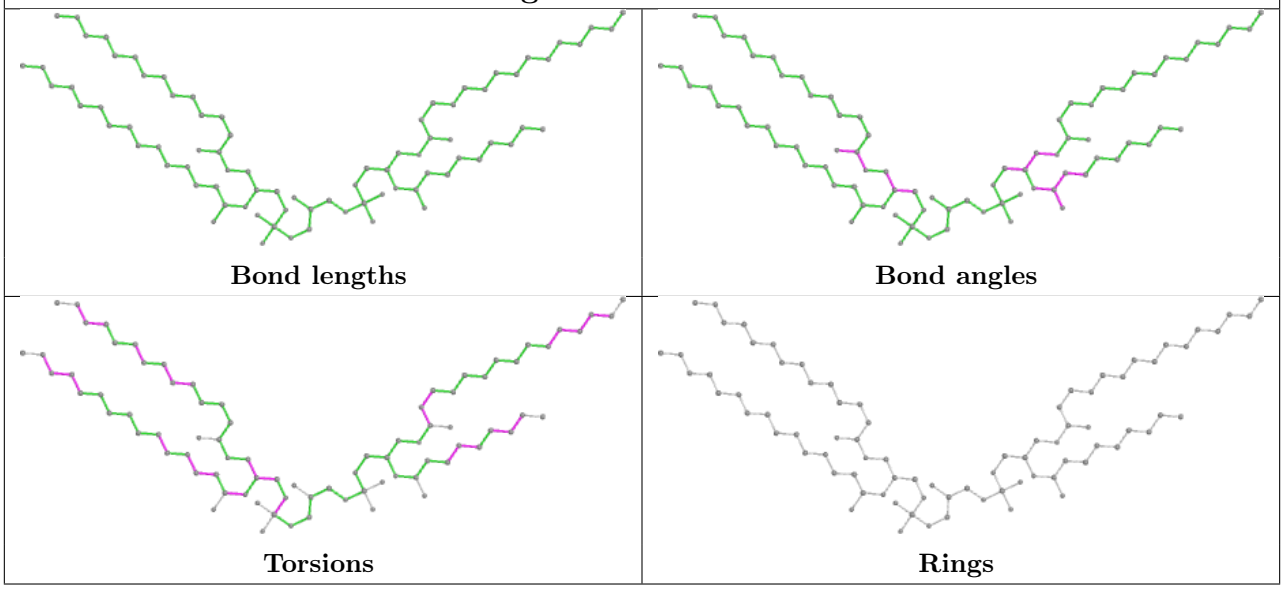
Ligand BCL L 502



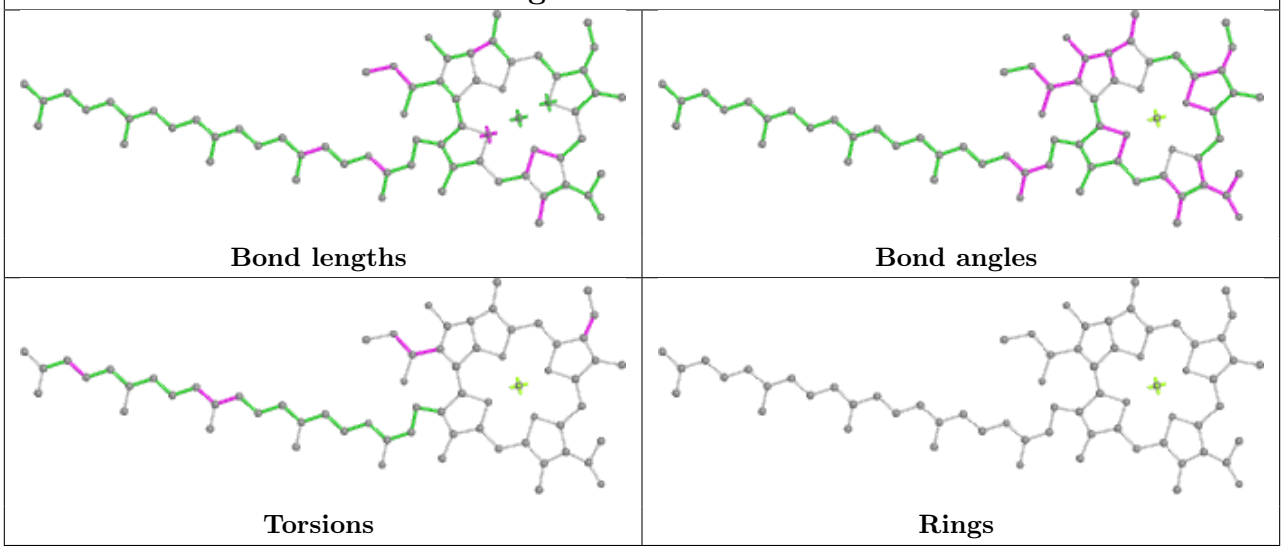
Ligand SPN M 600



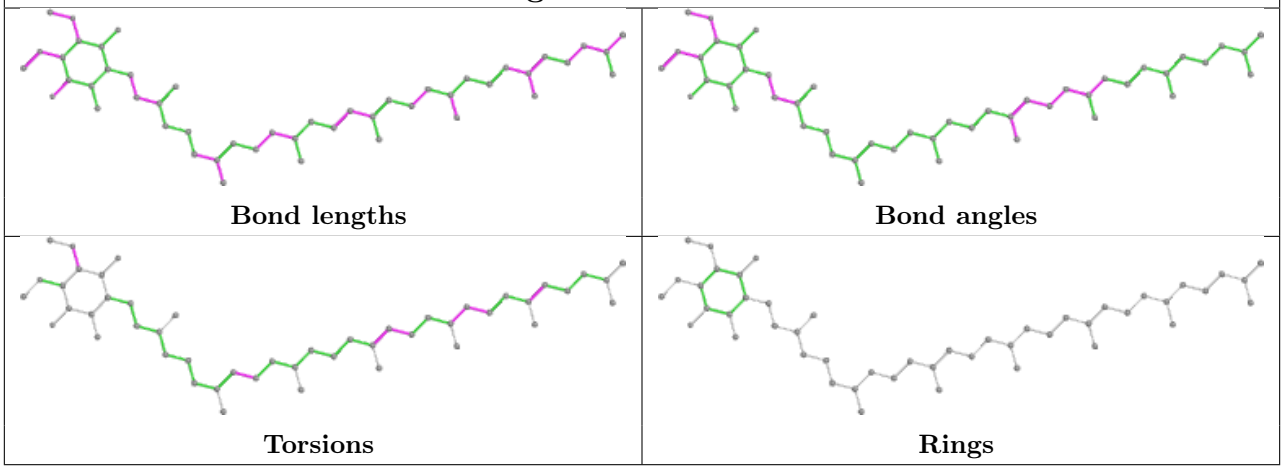
Ligand CDL M 800



Ligand BCL L 501



Ligand U10 M 504



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	L	281/281 (100%)	-0.64	0	100	100	26, 44, 79, 100	0
2	M	302/314 (96%)	-0.56	1 (0%)	94	92	25, 52, 87, 106	0
3	H	240/260 (92%)	-0.47	3 (1%)	77	65	29, 49, 70, 110	0
All	All	823/855 (96%)	-0.56	4 (0%)	91	86	25, 48, 83, 110	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	5.0
2	M	1	ALA	4.8
3	H	249	LYS	3.7
3	H	246	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

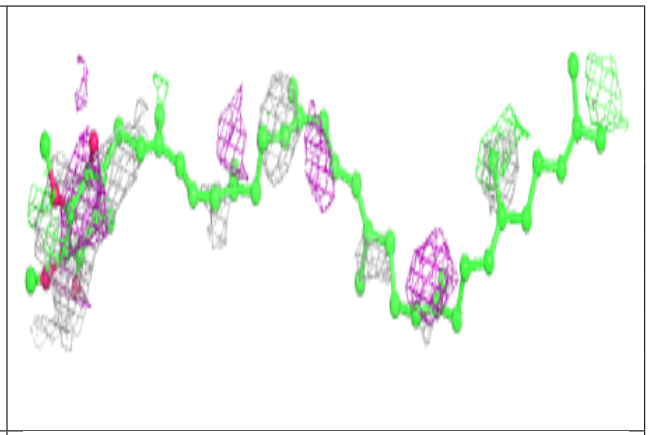
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

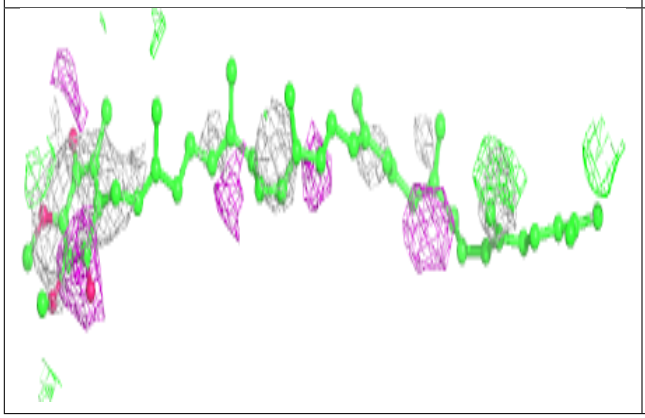
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	LDA	M	704	16/16	0.62	0.43	78,97,117,117	0
6	U10	L	504	48/63	0.65	0.74	97,99,105,105	0
10	CDL	M	800	81/100	0.78	0.44	56,75,87,90	81
9	SPN	M	600	43/43	0.80	0.35	52,67,84,85	0
7	LDA	L	709	16/16	0.80	0.63	105,107,110,110	0
7	LDA	M	701	16/16	0.90	0.23	53,61,72,73	0
7	LDA	H	703	16/16	0.90	0.27	64,66,72,73	0
5	BPH	M	503	65/65	0.94	0.18	42,55,69,73	10
6	U10	M	504	48/63	0.94	0.20	36,40,77,78	0
4	BCL	M	501	66/66	0.95	0.21	32,40,106,107	0
5	BPH	L	503	65/65	0.96	0.17	31,40,48,49	0
4	BCL	L	501	66/66	0.96	0.15	17,25,56,59	0
4	BCL	L	502	66/66	0.97	0.15	22,27,51,52	0
4	BCL	M	502	66/66	0.97	0.16	26,31,64,69	0
8	FE	M	500	1/1	0.99	0.07	35,35,35,35	0

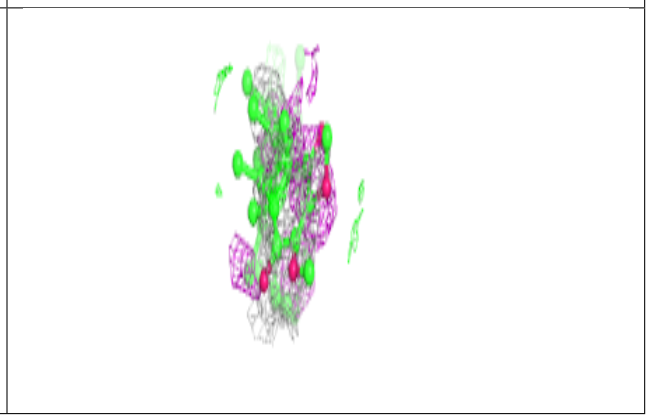
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 L 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

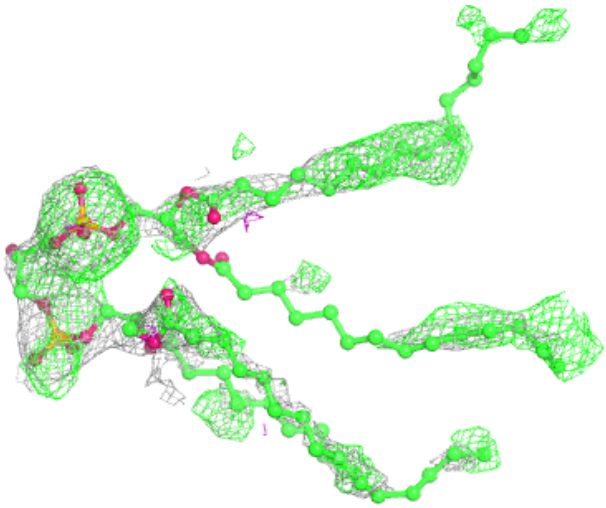


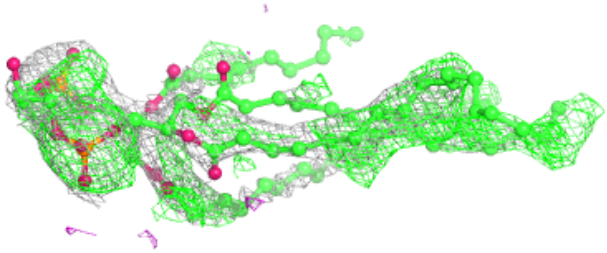


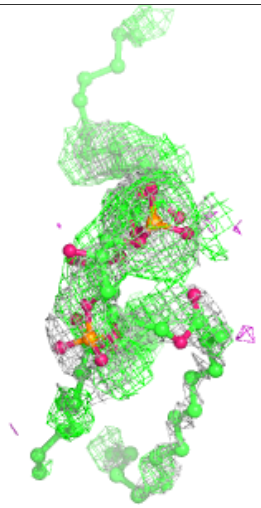


Electron density around CDL M 800:

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







Electron density around SPN M 600:

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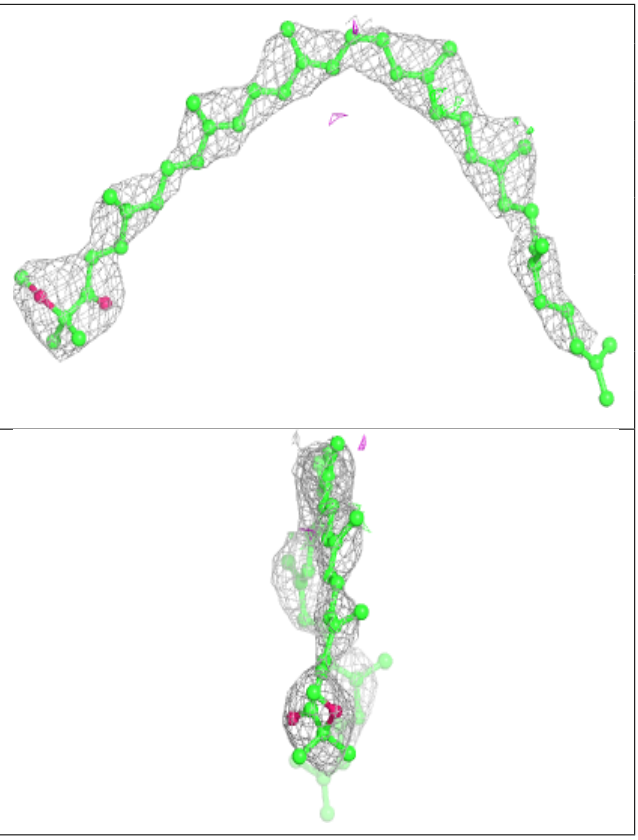
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BPH M 503:

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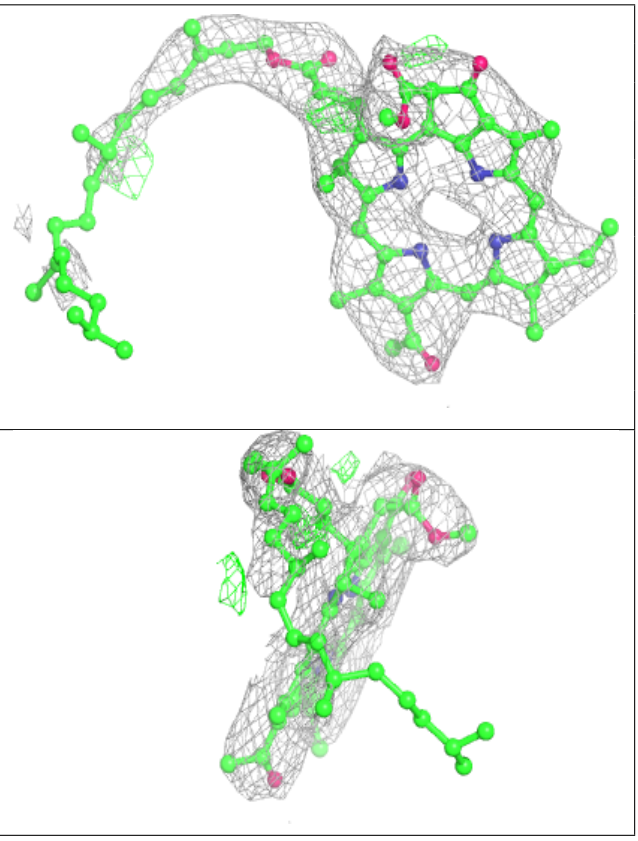
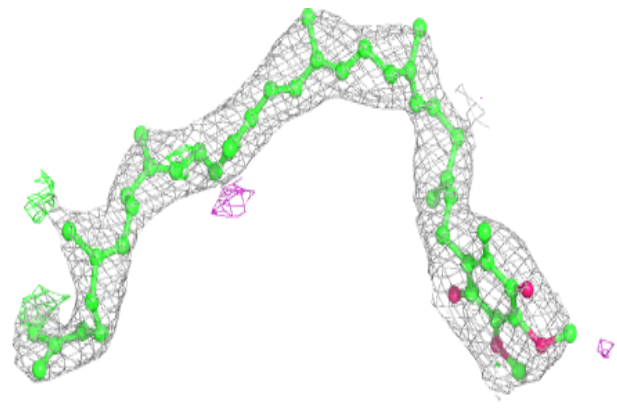
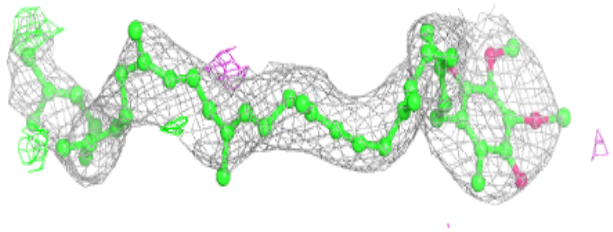
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

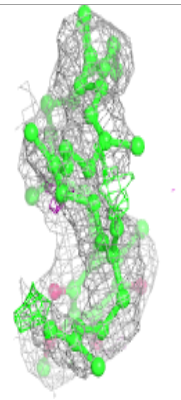


Electron density around U10 M 504:

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

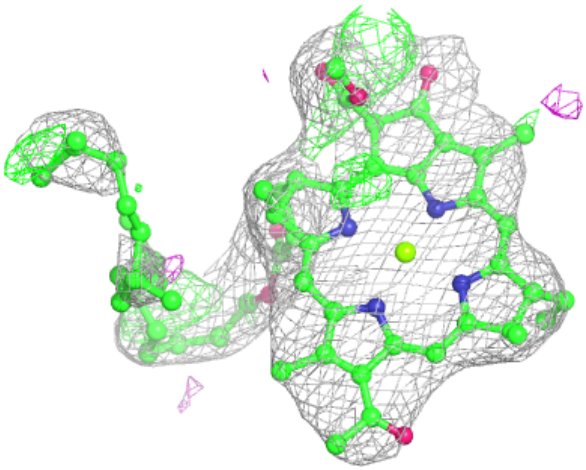


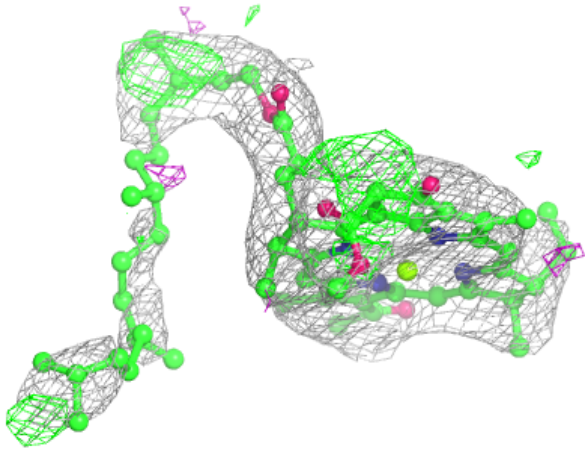


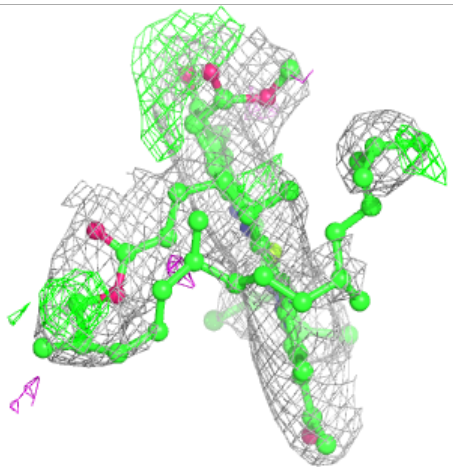


Electron density around BCL M 501:

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

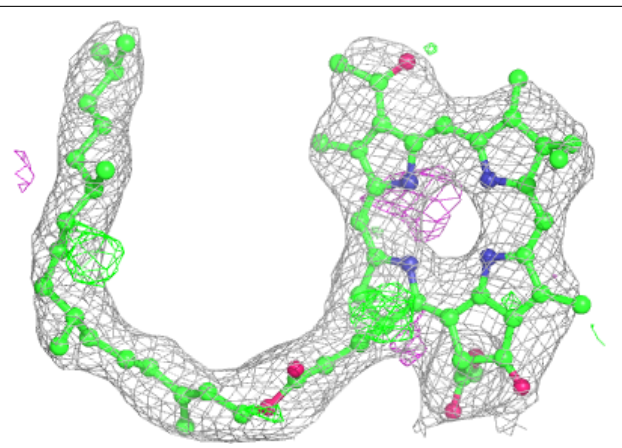


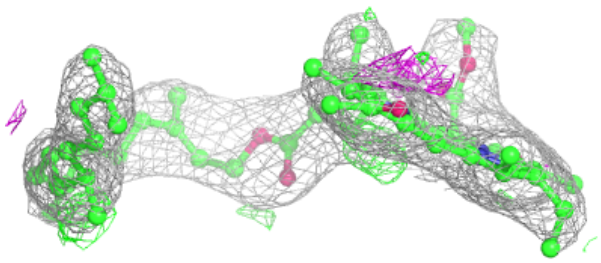


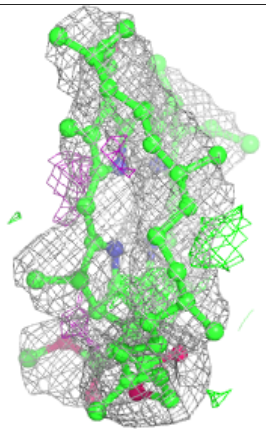


Electron density around BPH L 503:

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

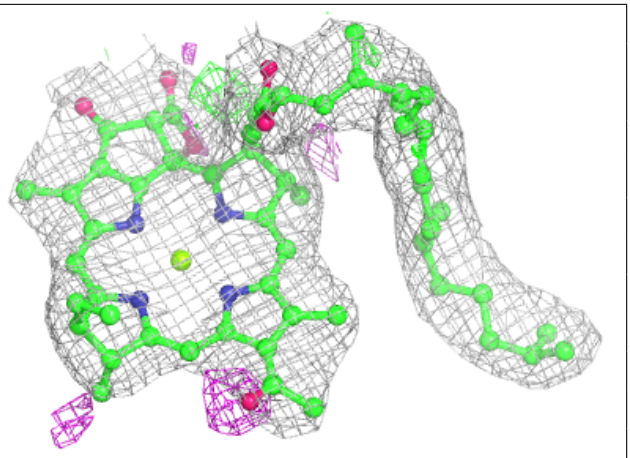


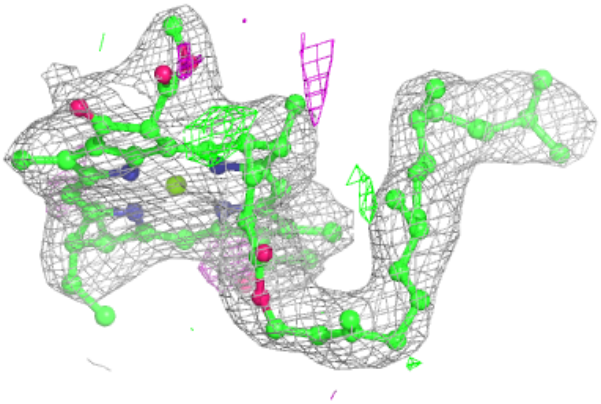


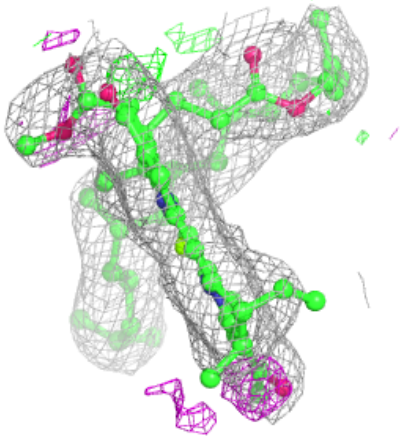


Electron density around BCL L 501:

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

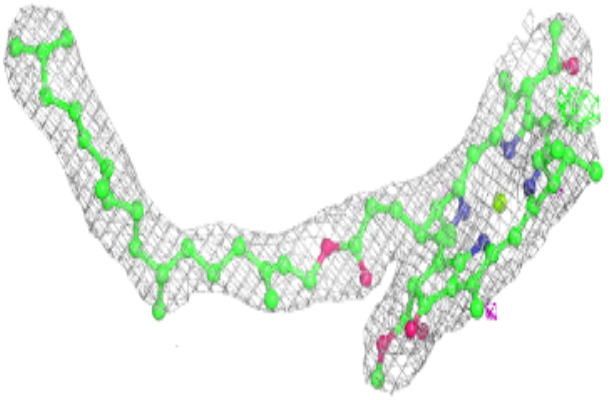


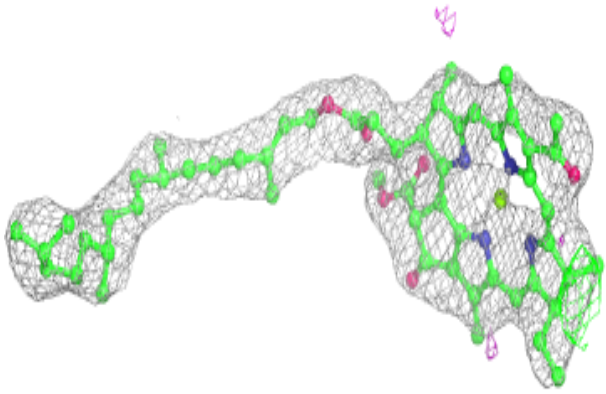


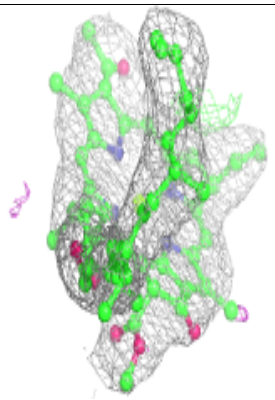


Electron density around BCL L 502:

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

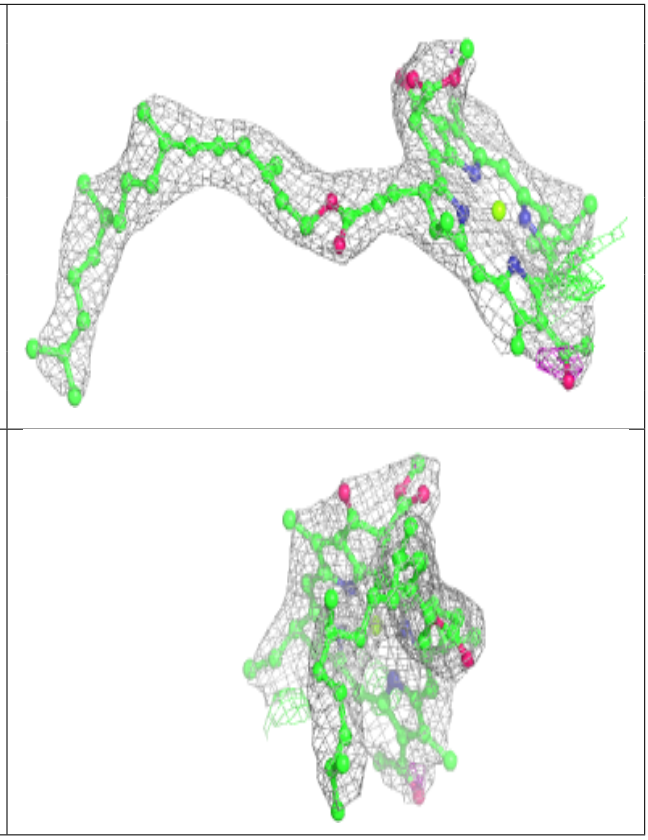






Electron density around BCL M 502:

$2mF_o$-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.