wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 11:15 AM EDT

PDB ID	:	1KBY / pdb_00001kby
Title	:	Structure of Photosynthetic Reaction Center with bacteriochlorophyll-bacteri opheophytin heterodimer
Authors	:	Camara-Artigas, A.; Magee, C.; Goetsch, A.; Allen, J.P.
Deposited on	:	2001-11-07
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:

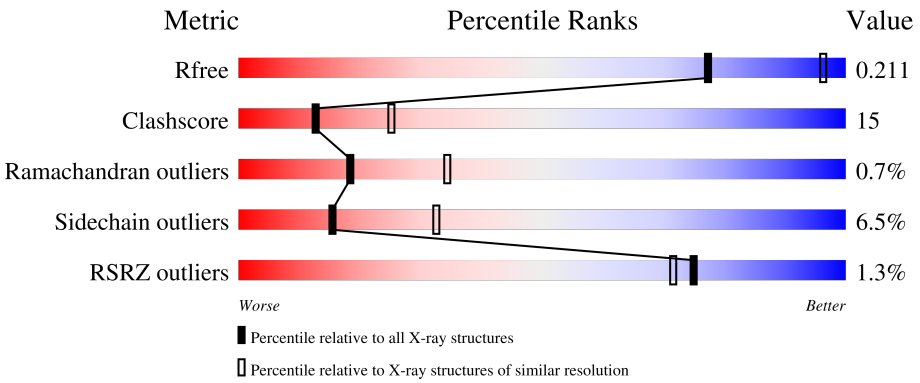
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	% 74% 23% •
2	M	307	2% 63% 32% • •
3	H	260	% 59% 25% 6% 9%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7220 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 PHOTOSYNTHETIC REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2232	1507	355	362	8	0	0	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2406	1607	392	397	10	0	0	0

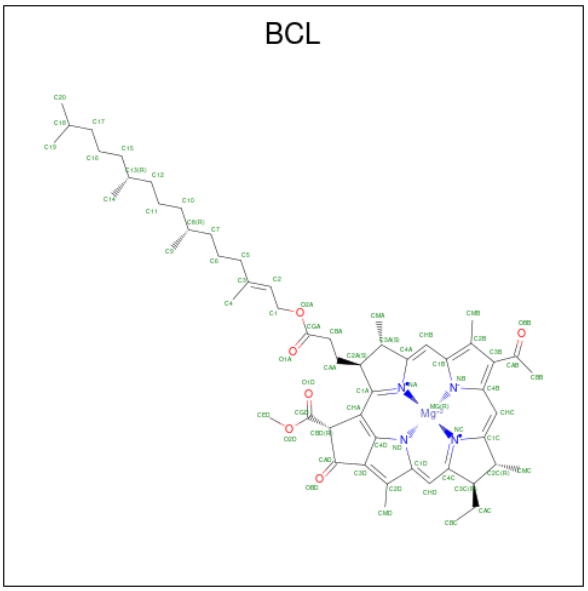
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	202	LEU	HIS	engineered mutation	UNP P02953

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER PROTEIN H CHAIN.

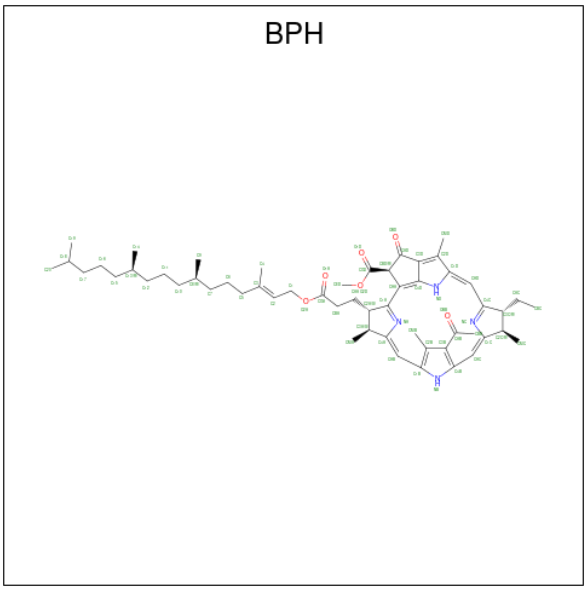
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	236	1794	1148	305	332	9	0	0	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: 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	L	1	66	55	1	4	6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: 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

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

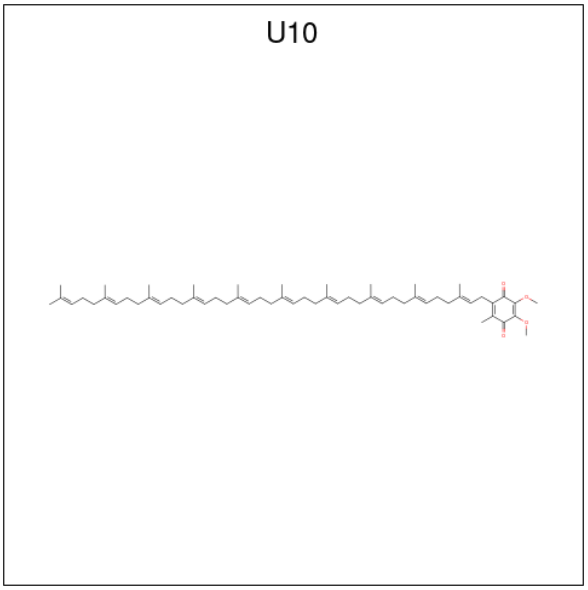
- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

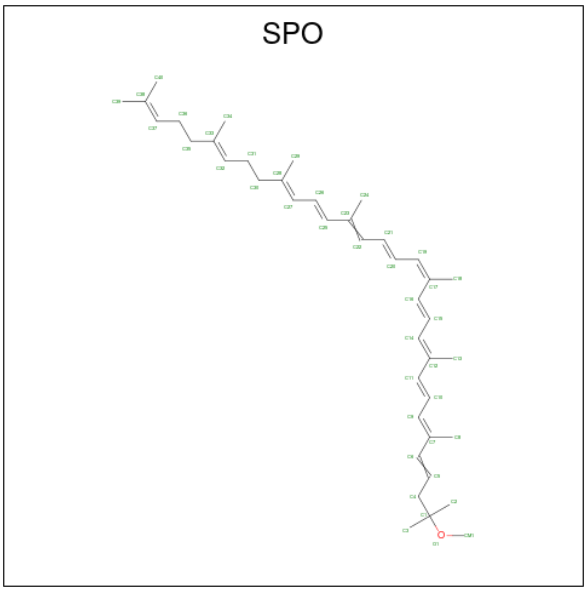
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	M	1	1	1	0	0

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



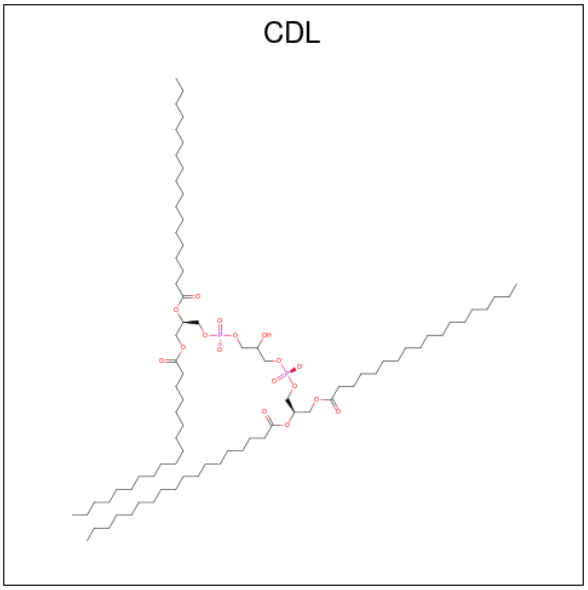
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	M	1	48	44	4	0	0

- Molecule 9 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 10 is CARDIOLIPIN (CCD ID: 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.

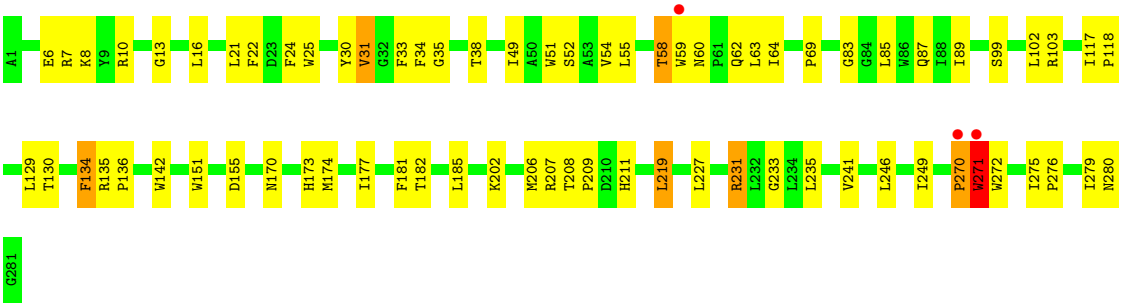
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	L	74	74	74	0	0
			Total	O		
11	M	71	71	71	0	0
			Total	O		
11	H	77	77	77	0	0

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.

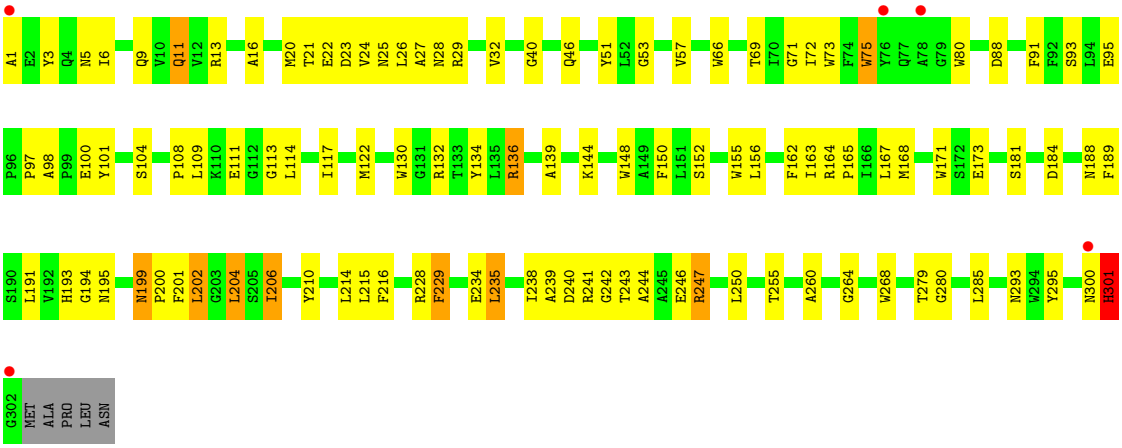
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER PROTEIN L CHAIN

Chain L:



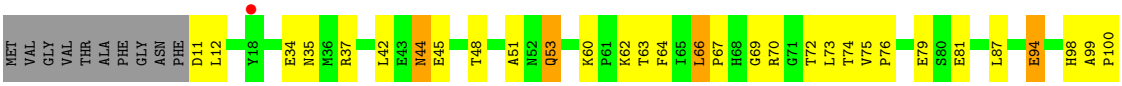
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER PROTEIN M CHAIN

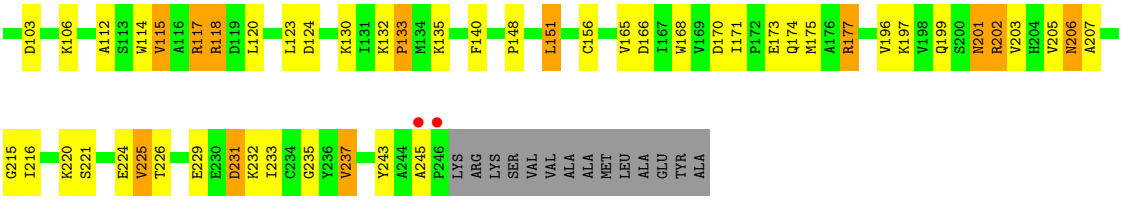
Chain M:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER PROTEIN H CHAIN

Chain H:




D103
K106
A112
S113
W114
V115
A116
R117
R118
D119
L120
L123
D124
K130
I131
K132
P133
M134
K135
F140
P148
L151
C156
V165
D166
I167
W168
V169
D170
I171
P172
E173
Q174
M175
A176
R177
V196
K197
V198
Q199
S200
N201
R202
V203
H204
V205
N206
A207
G215
I216
K220
S221
E224
V225
T226
E229
E230
D231
K232
I233
C234
G235
Y236
V237
Y243
A244
A245
P246
LYS
ARG
LYS
SER
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	142.31Å 142.31Å 187.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.07 – 2.50 27.07 – 2.56	Depositor EDS
% Data completeness (in resolution range)	81.4 (27.07-2.50) 83.6 (27.07-2.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.224 0.196 , 0.211	Depositor DCC
R_{free} test set	6034 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7220	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: FE, U10, CL, SPO, BPH, BCL, CDL

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	0.49	0/2320	0.96	11/3175 (0.3%)
2	M	0.46	0/2497	0.91	7/3409 (0.2%)
3	H	0.46	0/1842	0.99	8/2509 (0.3%)
All	All	0.47	0/6659	0.95	26/9093 (0.3%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	66	LEU	CA-C-N	9.16	131.29	119.84
3	H	66	LEU	C-N-CA	9.16	131.29	119.84
1	L	6	GLU	N-CA-C	8.94	122.69	111.69
1	L	35	GLY	N-CA-C	-7.36	103.35	112.77
1	L	31	VAL	CA-C-N	-7.25	115.09	122.27

There are no chirality outliers.

There are no planarity outliers.

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	2187	62	0
2	M	2406	0	2325	81	0
3	H	1794	0	1792	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	198	0	222	14	0
5	L	130	0	152	14	0
5	M	65	0	76	9	0
6	M	1	0	0	0	0
7	M	1	0	0	0	0
8	M	48	0	63	2	0
9	M	42	0	60	1	0
10	M	81	0	106	1	0
11	H	77	0	0	1	0
11	L	74	0	0	2	0
11	M	71	0	0	3	0
All	All	7220	0	6983	213	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 15.

The worst 5 of 213 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:L:271:TRP:H	1:L:271:TRP:CD1	1.68	1.00
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.42	1.00
5:M:852:BPH:HAA2	5:M:852:BPH:HBD	1.47	0.96
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.45	0.95
1:L:34:PHE:O	1:L:38:THR:HG23	1.74	0.88

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%)	15 (5%)	2 (1%)	18 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	300/307 (98%)	286 (95%)	13 (4%)	1 (0%)	36	55
3	H	234/260 (90%)	222 (95%)	9 (4%)	3 (1%)	9	18
All	All	813/848 (96%)	770 (95%)	37 (5%)	6 (1%)	18	34

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
3	H	220	LYS
3	H	51	ALA
1	L	270	PRO
1	L	271	TRP

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%)	210 (96%)	10 (4%)	24	49
2	M	236/240 (98%)	220 (93%)	16 (7%)	14	31
3	H	191/208 (92%)	175 (92%)	16 (8%)	10	22
All	All	647/668 (97%)	605 (94%)	42 (6%)	15	32

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	72	THR
3	H	177	ARG
3	H	79	GLU
3	H	117	ARG
3	H	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	32	GLN
3	H	44	ASN
3	H	206	ASN
3	H	98	HIS
2	M	77	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	BPH	L	855	-	59,70,70	1.88	11 (18%)	59,101,101	2.51	18 (30%)
10	CDL	M	5000	-	80,80,99	0.73	1 (1%)	86,92,111	0.95	6 (6%)
4	BCL	L	851	1	69,74,74	1.42	9 (13%)	79,115,115	1.63	16 (20%)
8	U10	M	857	-	48,48,63	2.49	14 (29%)	60,61,79	2.11	20 (33%)
9	SPO	M	859	-	41,41,41	3.32	24 (58%)	47,50,50	2.76	15 (31%)
5	BPH	L	854	-	59,70,70	1.89	13 (22%)	59,101,101	2.44	16 (27%)
5	BPH	M	852	-	59,70,70	1.96	14 (23%)	59,101,101	3.25	24 (40%)
4	BCL	L	850	2	69,74,74	2.27	16 (23%)	79,115,115	4.68	26 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	L	853	1	69,74,74	1.48	11 (15%)	79,115,115	1.94	23 (29%)

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	BPH	L	855	-	-	8/37/105/105	0/5/6/6
10	CDL	M	5000	-	-	33/91/91/110	-
4	BCL	L	851	1	-	5/41/137/137	-
8	U10	M	857	-	-	15/45/69/87	0/1/1/1
9	SPO	M	859	-	-	12/47/47/47	-
5	BPH	L	854	-	-	7/37/105/105	0/5/6/6
5	BPH	M	852	-	-	9/37/105/105	0/5/6/6
4	BCL	L	850	2	-	7/41/137/137	-
4	BCL	L	853	1	-	8/41/137/137	-

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	857	U10	C6-C1	10.46	1.54	1.35
4	L	850	BCL	C1B-NB	-10.32	1.24	1.37
9	M	859	SPO	C15-C16	9.17	1.58	1.34
4	L	850	BCL	C3B-C4B	8.54	1.58	1.41
5	L	855	BPH	C3A-C2A	-8.38	1.47	1.54

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	850	BCL	OBB-CAB-C3B	24.05	162.96	120.43
4	L	850	BCL	OBB-CAB-CBB	-18.59	78.14	119.77
4	L	850	BCL	CBB-CAB-C3B	-16.88	84.83	120.40
4	L	850	BCL	C3B-C4B-NB	12.63	126.43	109.76
5	M	852	BPH	C4D-CHA-CBD	-12.47	102.47	108.45

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	851	BCL	C2C-C3C-CAC-CBC
4	L	851	BCL	C4C-C3C-CAC-CBC
5	L	854	BPH	C4C-C3C-CAC-CBC
5	L	854	BPH	C2C-C3C-CAC-CBC
5	L	855	BPH	C4C-C3C-CAC-CBC

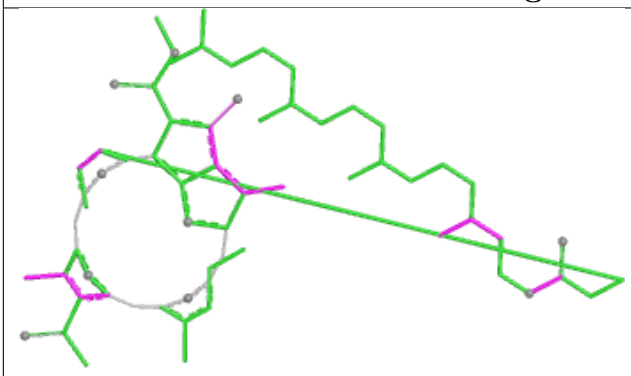
There are no ring outliers.

9 monomers are involved in 33 short contacts:

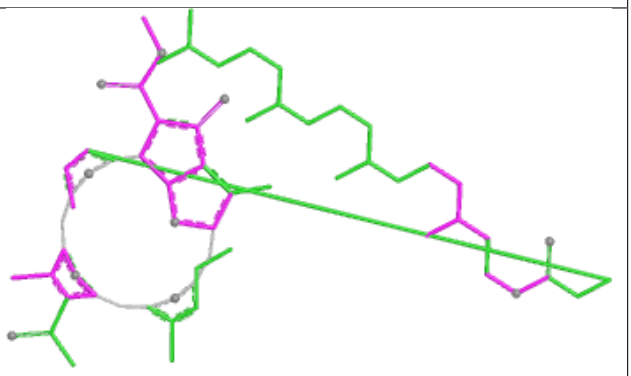
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	855	BPH	5	0
10	M	5000	CDL	1	0
4	L	851	BCL	4	0
8	M	857	U10	2	0
9	M	859	SPO	1	0
5	L	854	BPH	9	0
5	M	852	BPH	9	0
4	L	850	BCL	8	0
4	L	853	BCL	4	0

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.

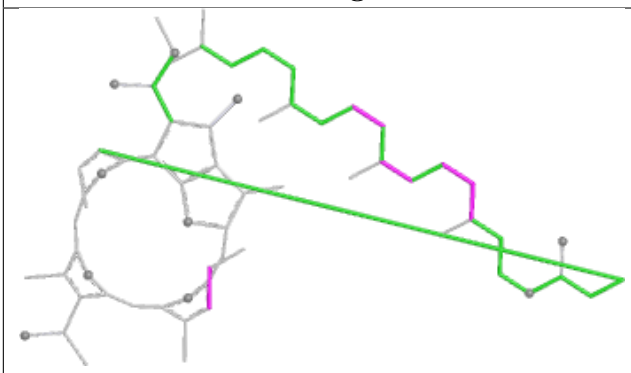
Ligand BPH L 855



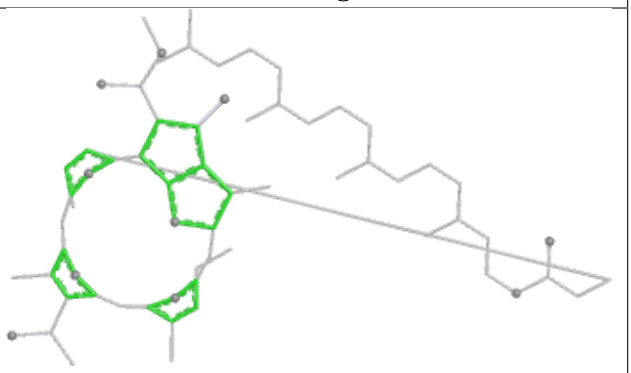
Bond lengths



Bond angles

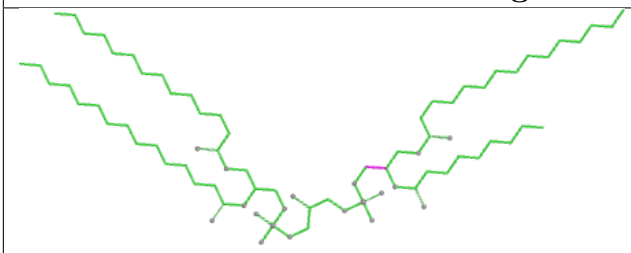


Torsions

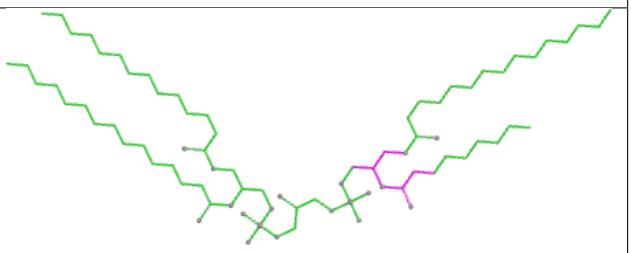


Rings

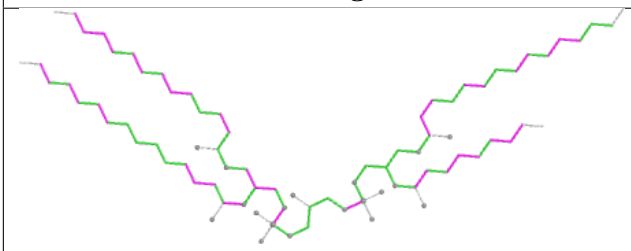
Ligand CDL M 5000



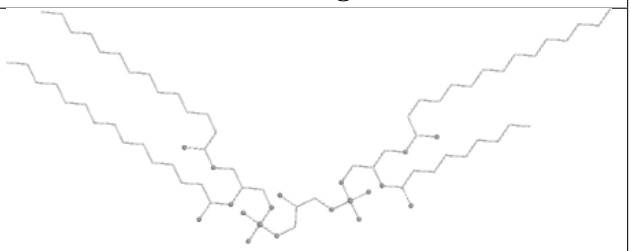
Bond lengths



Bond angles

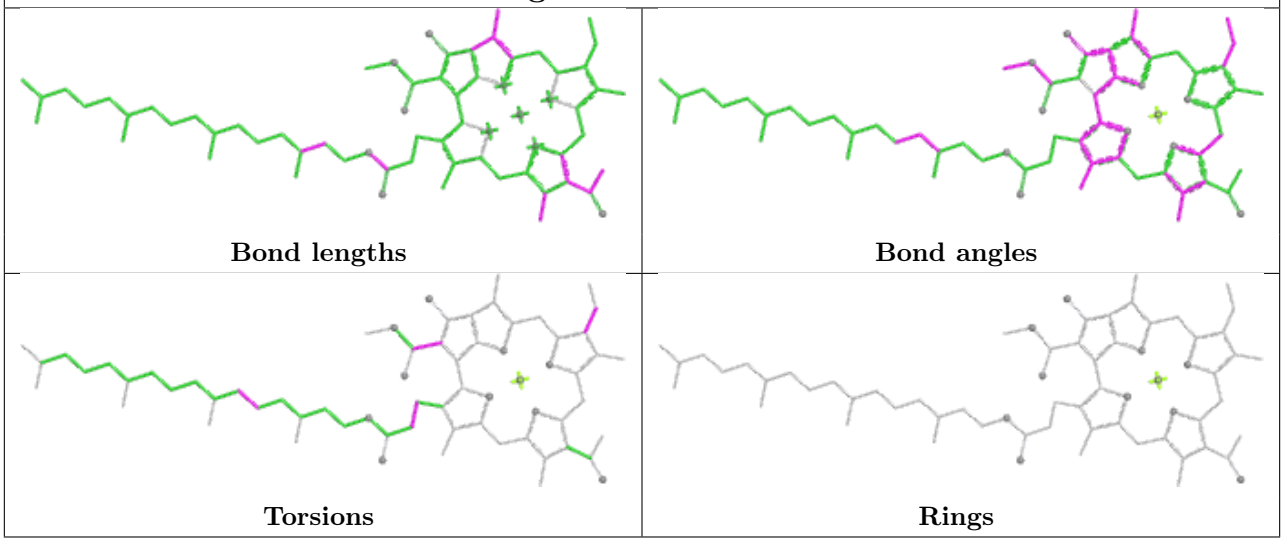


Torsions

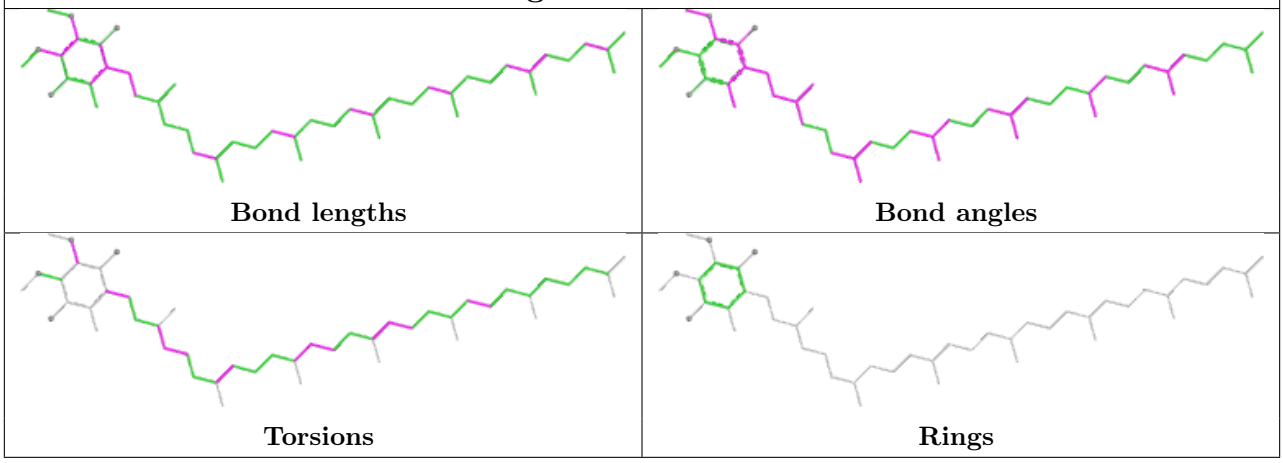


Rings

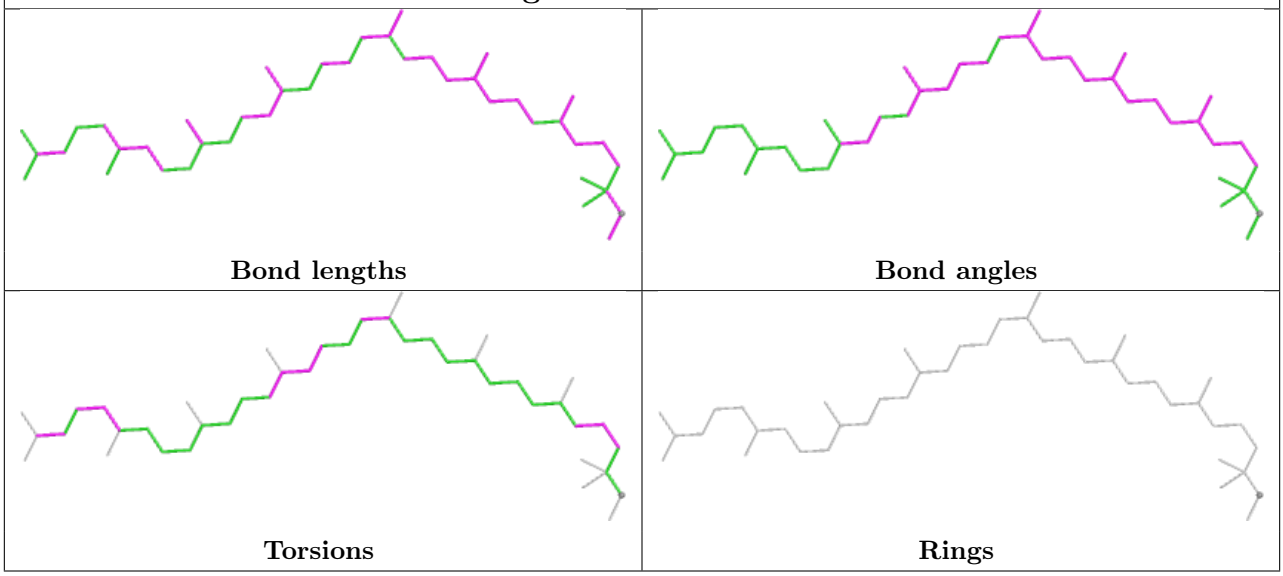
Ligand BCL L 851



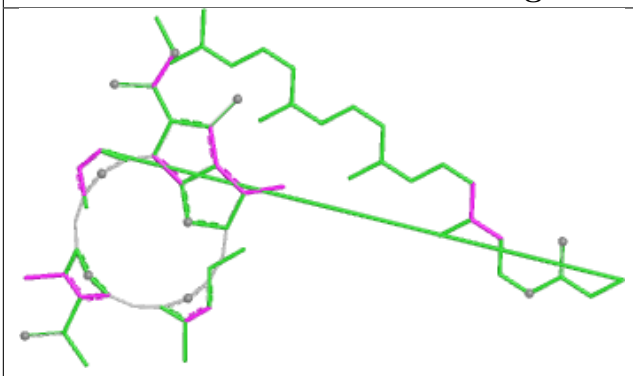
Ligand U10 M 857



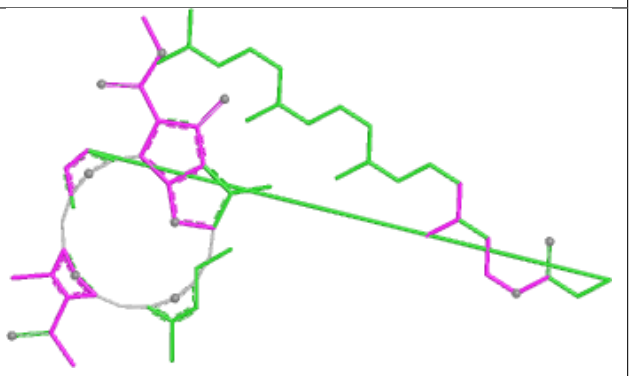
Ligand SPO M 859



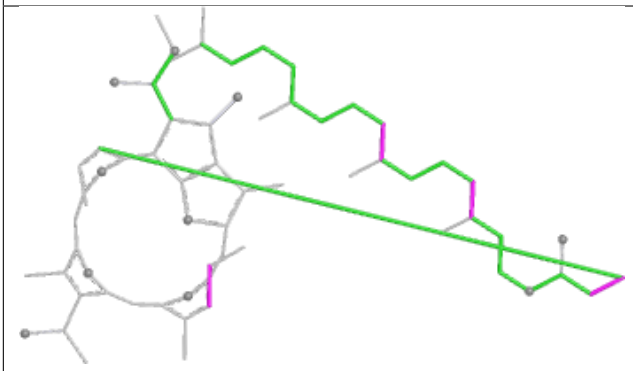
Ligand BPH L 854



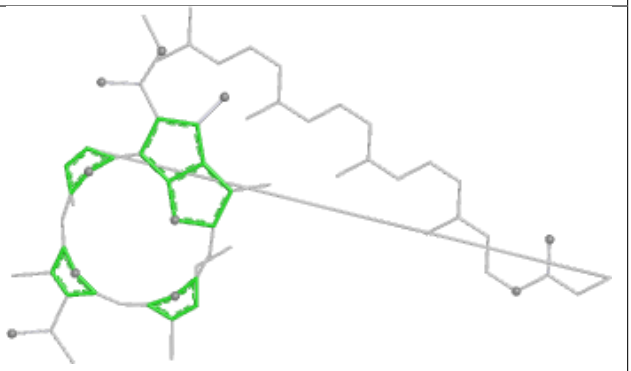
Bond lengths



Bond angles

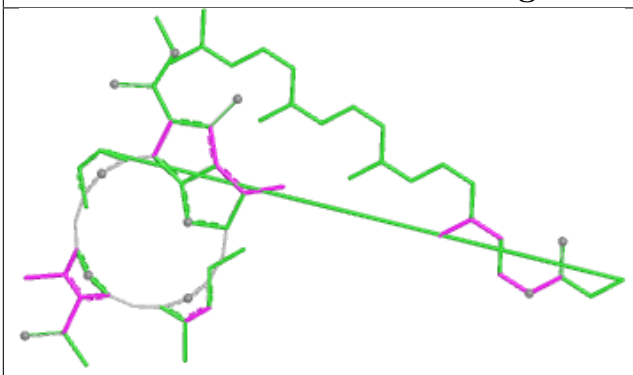


Torsions

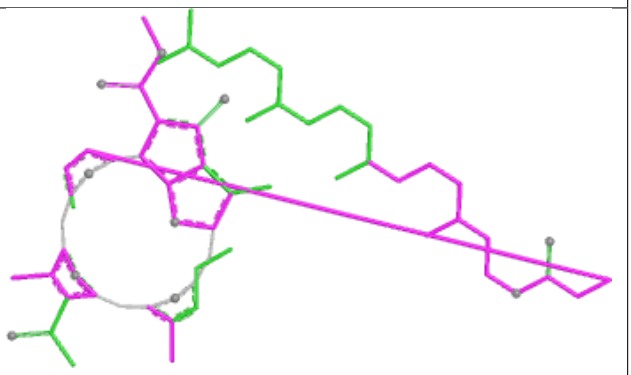


Rings

Ligand BPH M 852

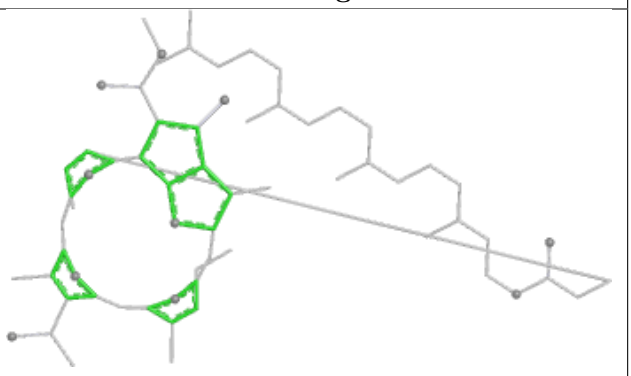


Bond lengths



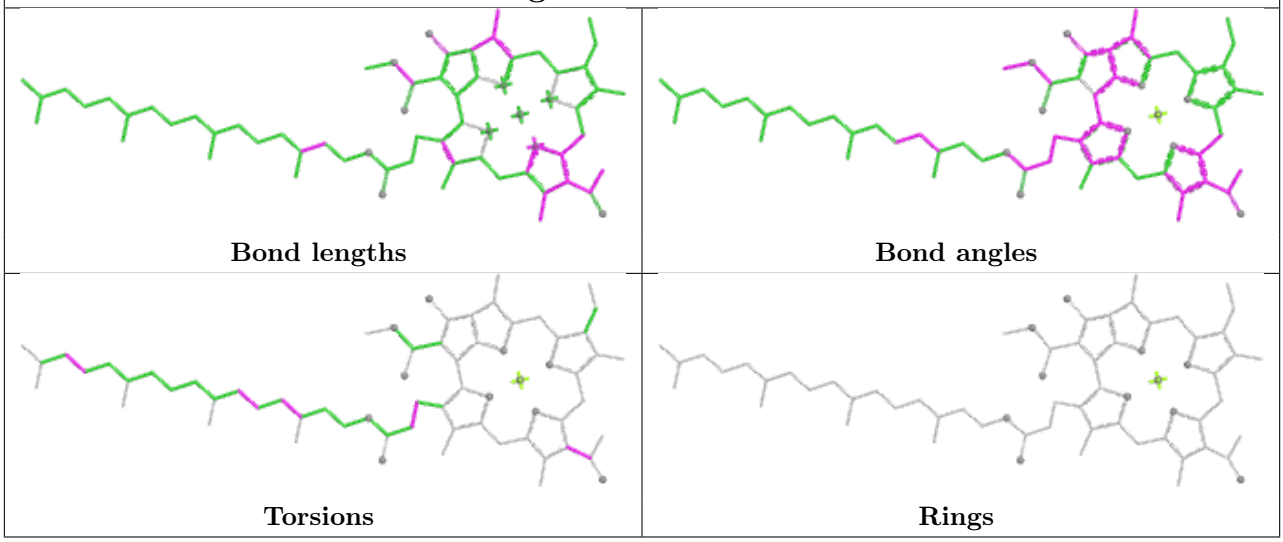
Bond angles

Torsions

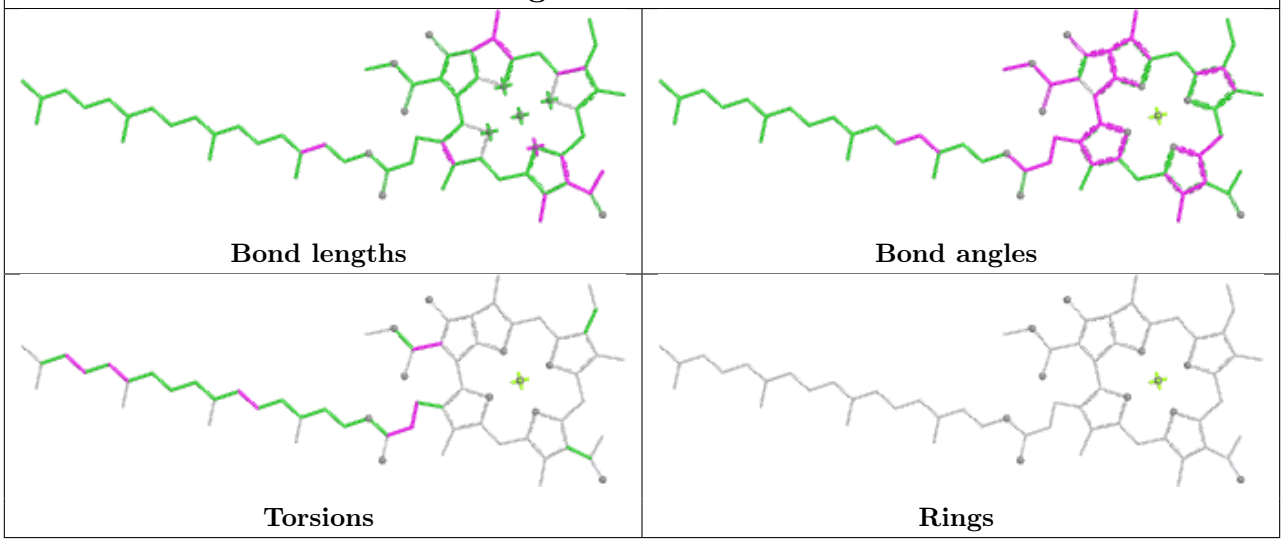


Rings

Ligand BCL L 850



Ligand BCL L 853



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%)	-0.16	3 (1%)	78	75	24, 39, 73, 82	0
2	M	302/307 (98%)	-0.06	5 (1%)	69	65	23, 45, 74, 89	0
3	H	236/260 (90%)	-0.12	3 (1%)	75	71	28, 45, 65, 85	0
All	All	819/848 (96%)	-0.11	11 (1%)	75	71	23, 44, 72, 89	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	302	GLY	5.9
2	M	1	ALA	3.1
3	H	245	ALA	3.1
3	H	246	PRO	3.0
3	H	18	TYR	2.8

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

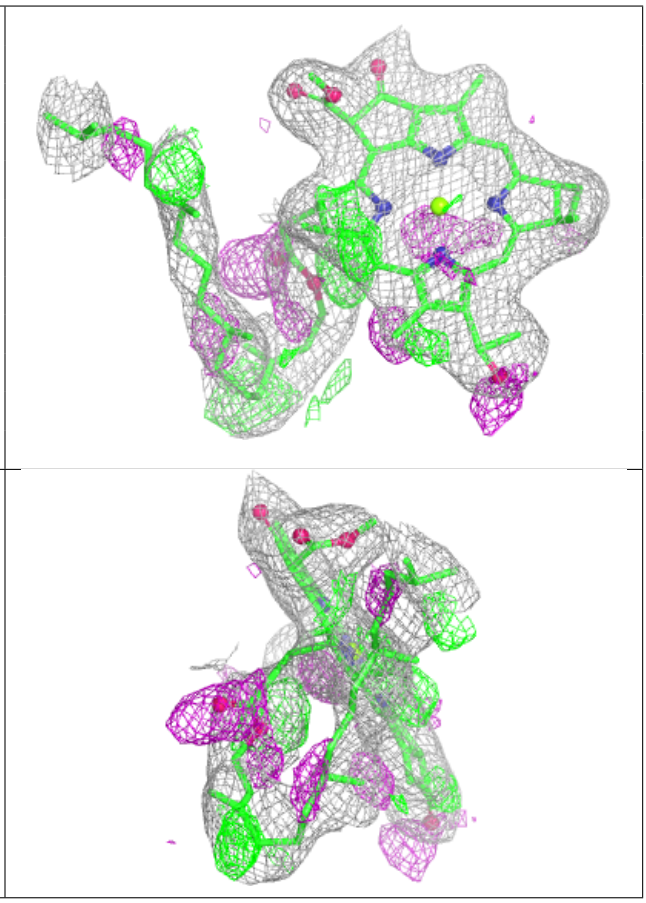
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CL	M	6000	1/1	0.77	0.16	100,100,100,100	0
4	BCL	L	850	66/66	0.89	0.16	35,46,96,98	0
10	CDL	M	5000	81/100	0.90	0.15	59,76,86,90	0
5	BPH	M	852	65/65	0.91	0.12	33,37,66,76	0
5	BPH	L	854	65/65	0.92	0.12	39,44,95,98	0
8	U10	M	857	48/63	0.92	0.13	41,51,69,70	0
4	BCL	L	853	66/66	0.92	0.11	24,30,60,66	0
9	SPO	M	859	42/42	0.93	0.14	47,62,74,75	0
5	BPH	L	855	65/65	0.93	0.10	26,35,46,53	0
4	BCL	L	851	66/66	0.95	0.09	30,37,47,60	0
6	FE	M	856	1/1	1.00	0.02	28,28,28,28	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.

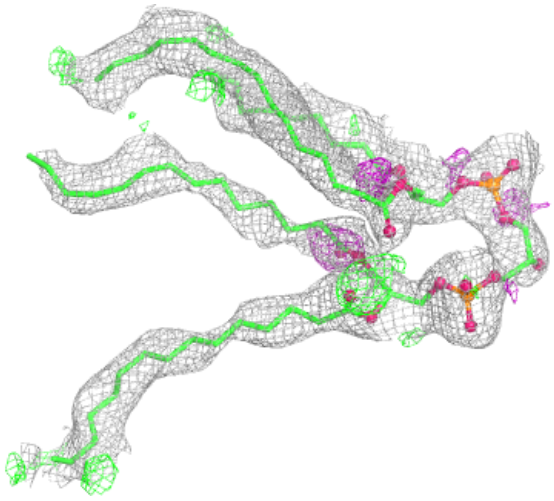
Electron density around BCL L 850:

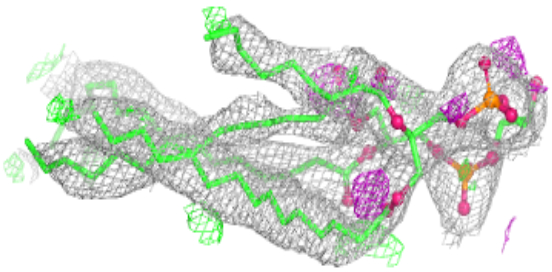
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

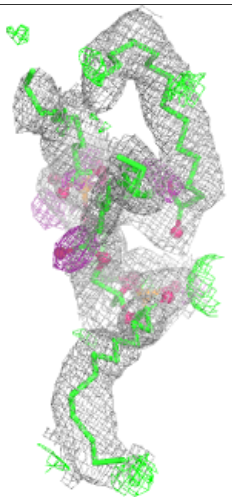


Electron density around CDL M 5000:

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

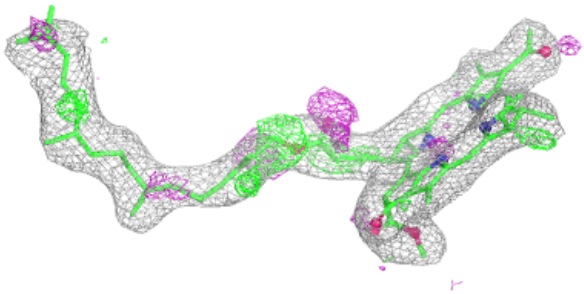


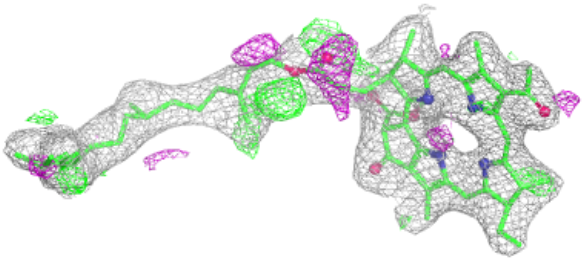


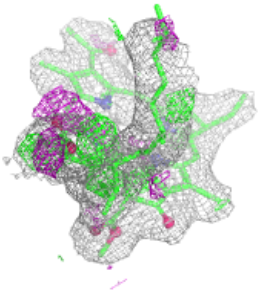


Electron density around BPH M 852:

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

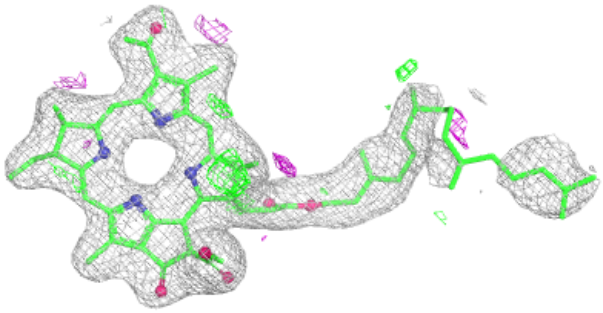


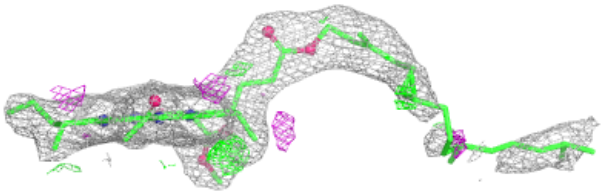


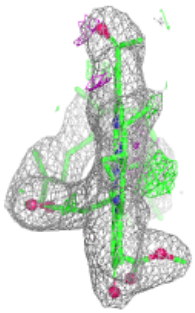


Electron density around BPH L 854:

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

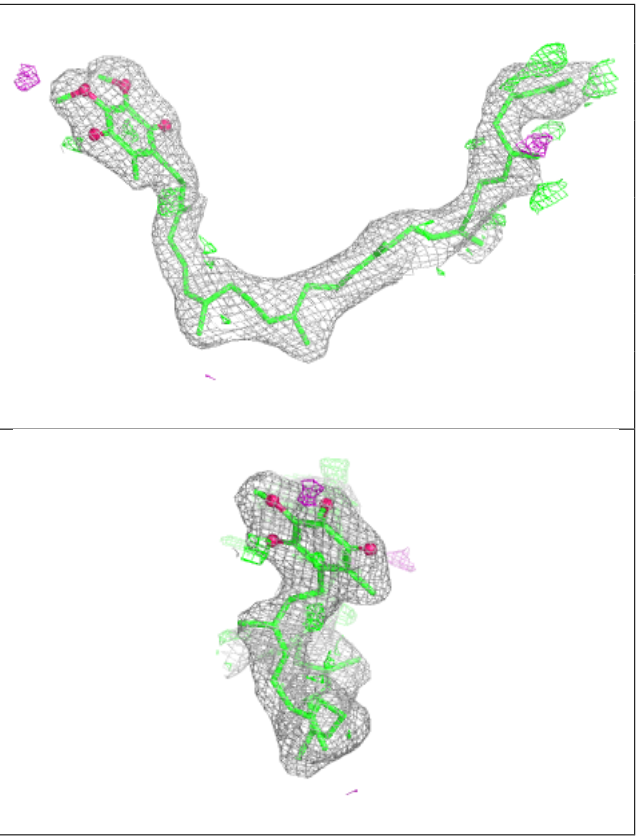






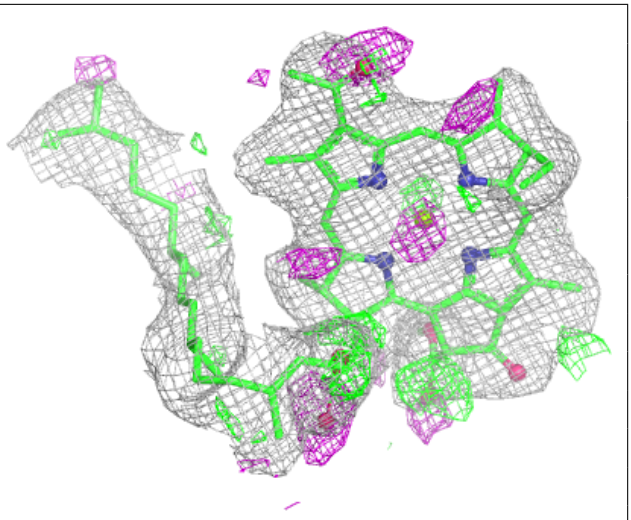
Electron density around U10 M 857:

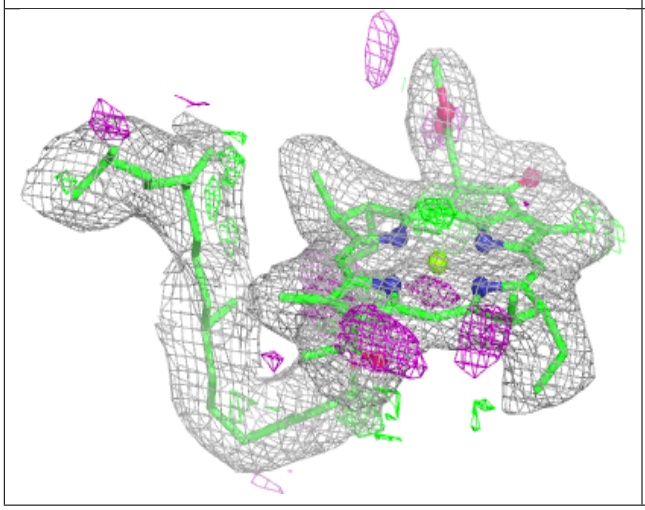
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

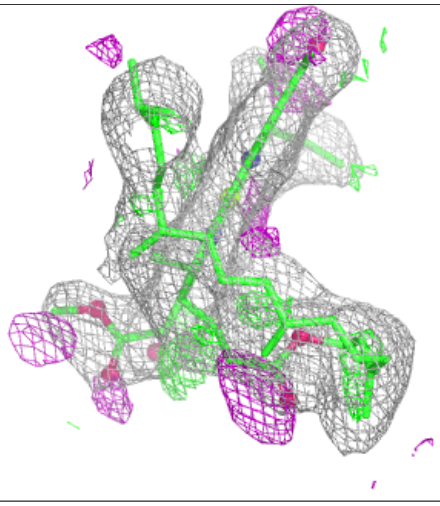


Electron density around BCL L 853:

$2mF_o$-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 859:

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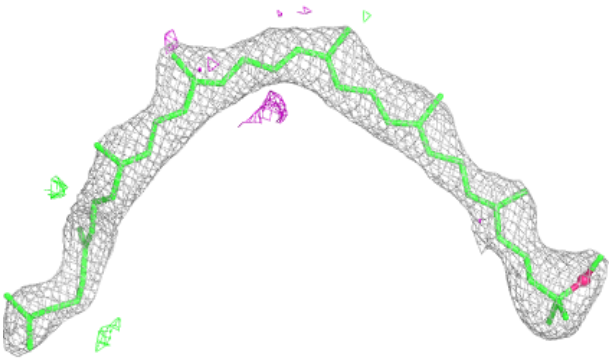
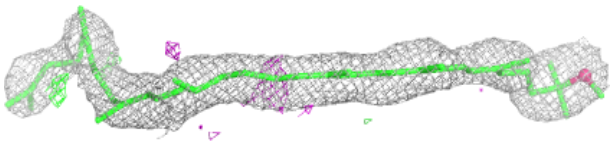
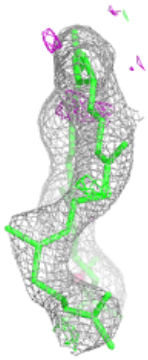
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BPH L 855:

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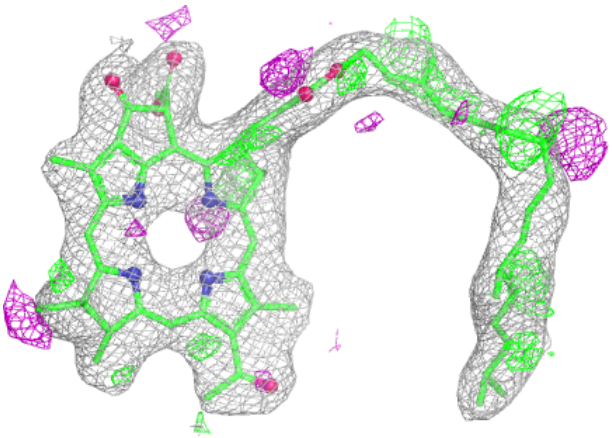
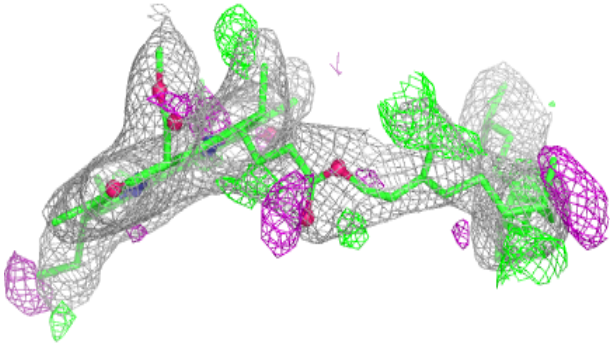
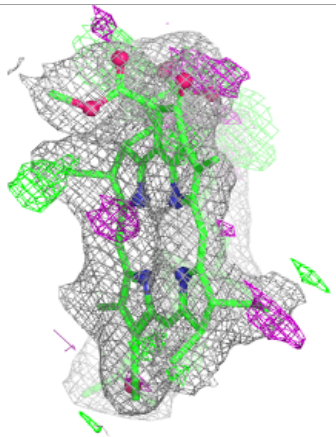
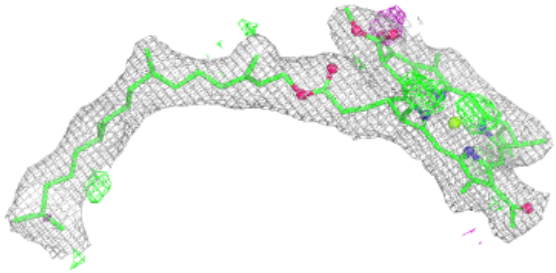
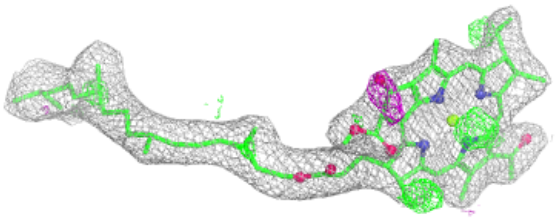
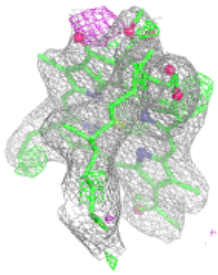
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCL L 851: $2mF_o$-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.