wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 01:45 PM EDT

PDB ID	:	1RZZ
Title	:	PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TETRAGONAL FORM)
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on	:	2003-12-29
Resolution	:	2.40 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:

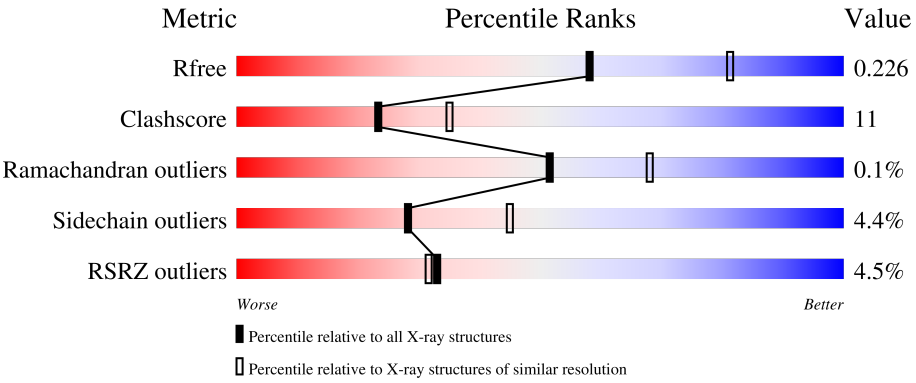
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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% 77% 21%
1	R	281	6% 75% 22%
2	M	307	4% 78% 18%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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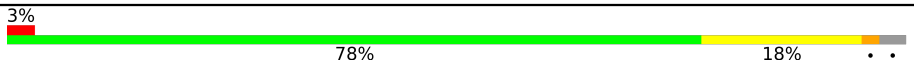
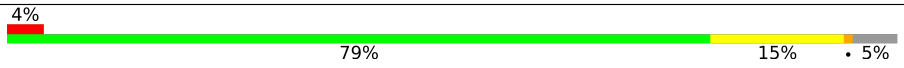
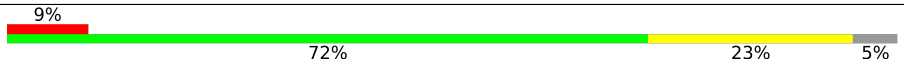
Mol	Chain	Length	Quality of chain
2	S	307	
3	H	260	
3	T	260	

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
5	U10	R	2009	-	-	-	X
7	BPH	M	1005	X	-	-	-
7	BPH	M	1006	X	-	-	-
7	BPH	R	2006	X	-	-	-
7	BPH	S	2005	X	-	-	-
9	LDA	S	2011	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14481 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
			2232	1507	356	361	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	engineered mutation	UNP P02954
R	213	ASN	ASP	engineered mutation	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			
2	S	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			

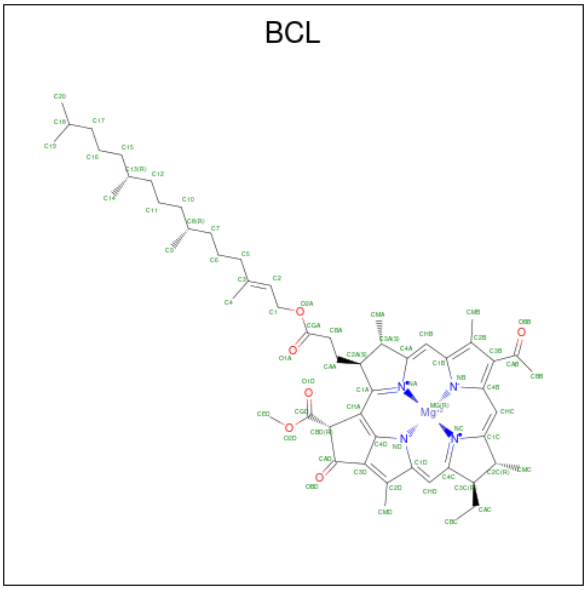
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	engineered mutation	UNP P02953
S	233	CYS	ARG	engineered mutation	UNP P02953

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

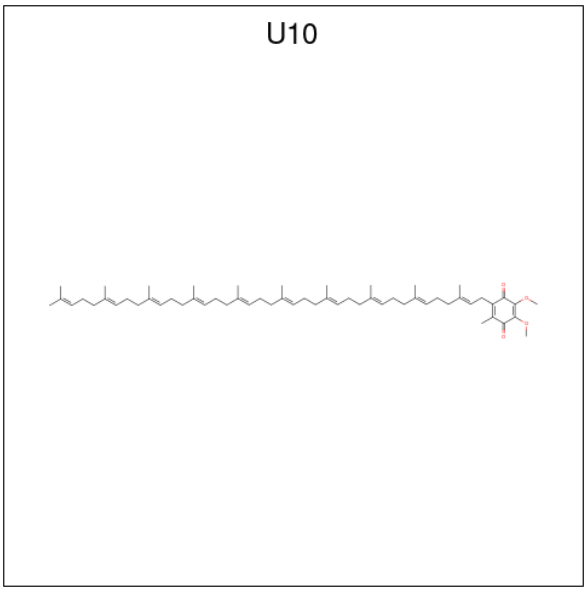
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

- 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
			51	40	1	4	6		
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	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

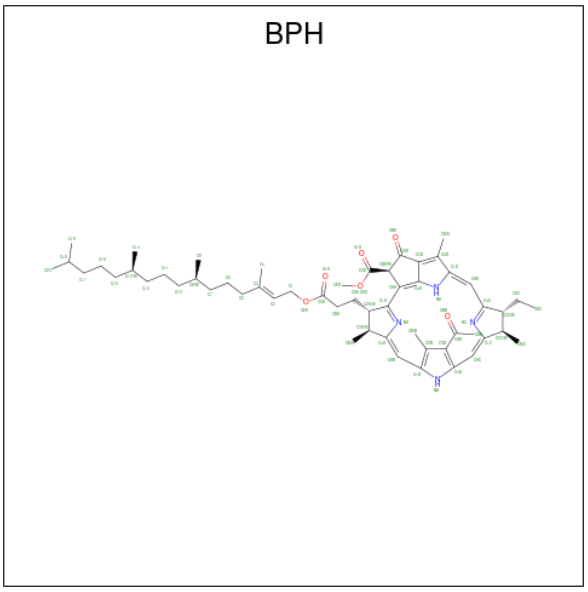


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 44 40 4	0	0
5	M	1	Total C O 38 34 4	0	0
5	R	1	Total C O 18 14 4	0	0
5	S	1	Total C O 32 28 4	0	0

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

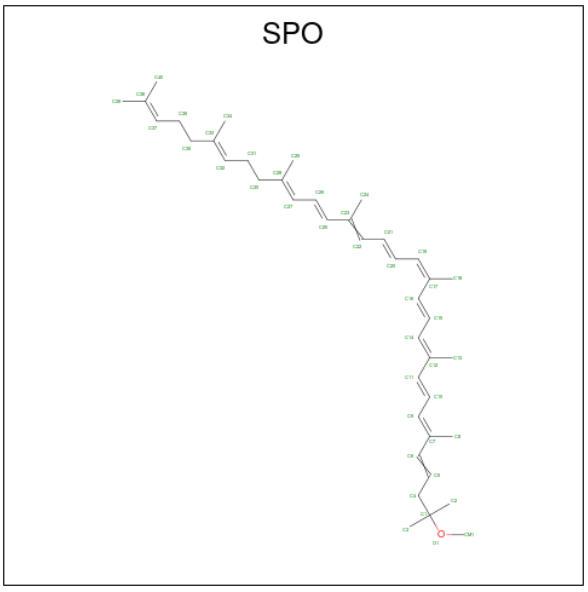
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Fe 1 1	0	0
6	S	1	Total Fe 1 1	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



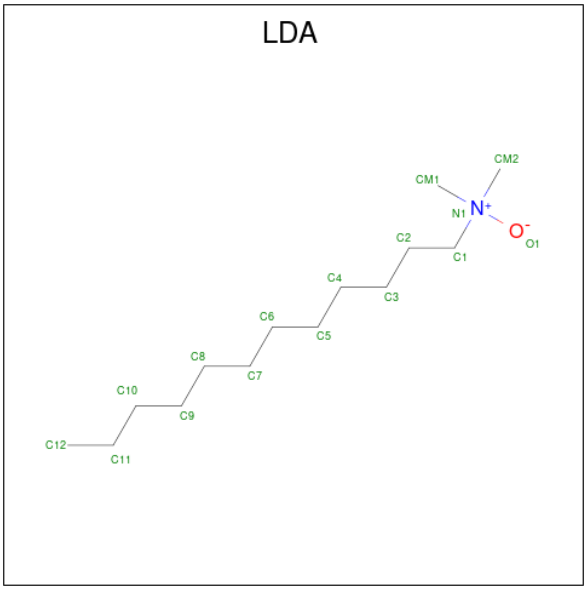
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			55	45	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	R	1	Total	C	N	O	0	0
			65	55	4	6		
7	S	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	72	Total O 72 72	0	0
10	M	107	Total O 107 107	0	0

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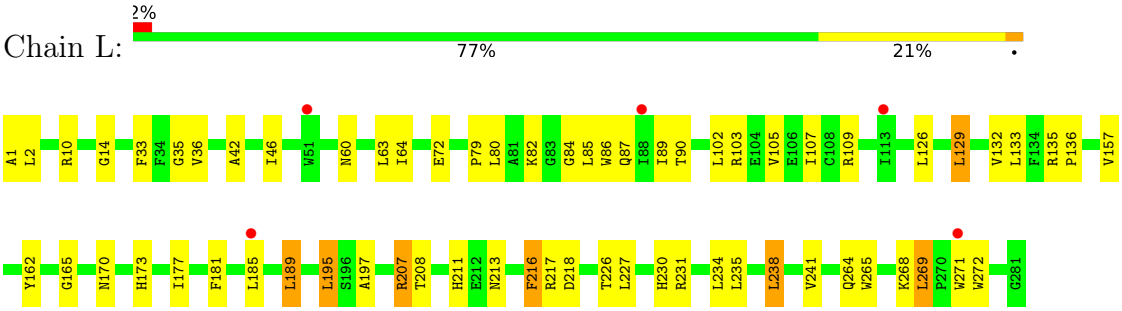
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	109	Total O 109 109	0	0
10	R	47	Total O 47 47	0	0
10	S	75	Total O 75 75	0	0
10	T	63	Total O 63 63	0	0

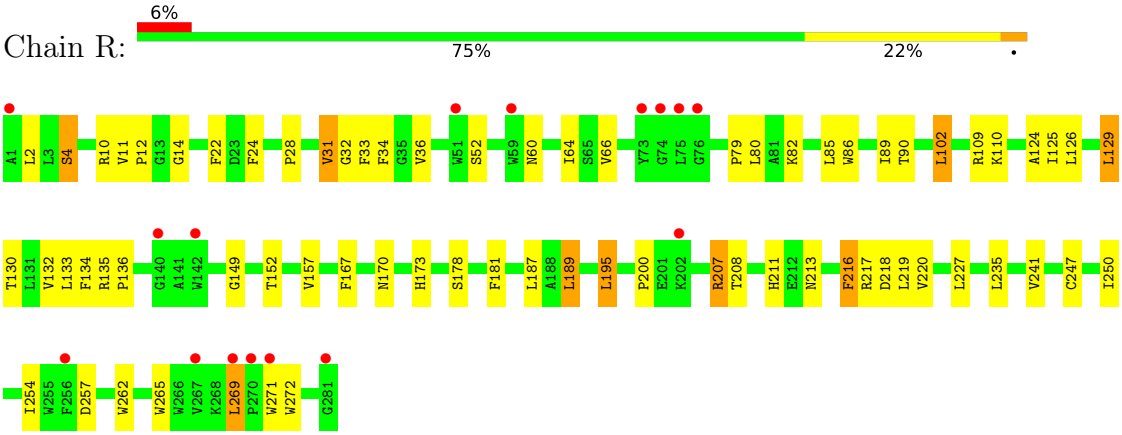
3 Residue-property plots (i)

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.

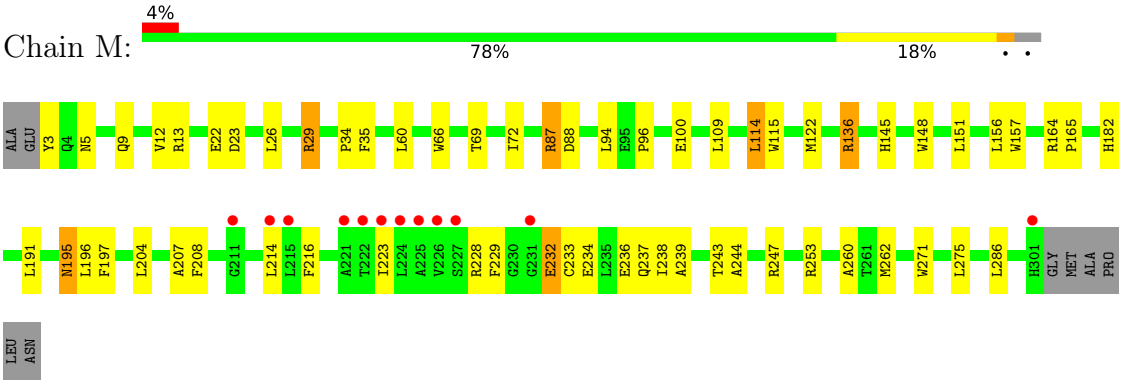
• Molecule 1: Reaction center protein L chain



• Molecule 1: Reaction center protein L chain

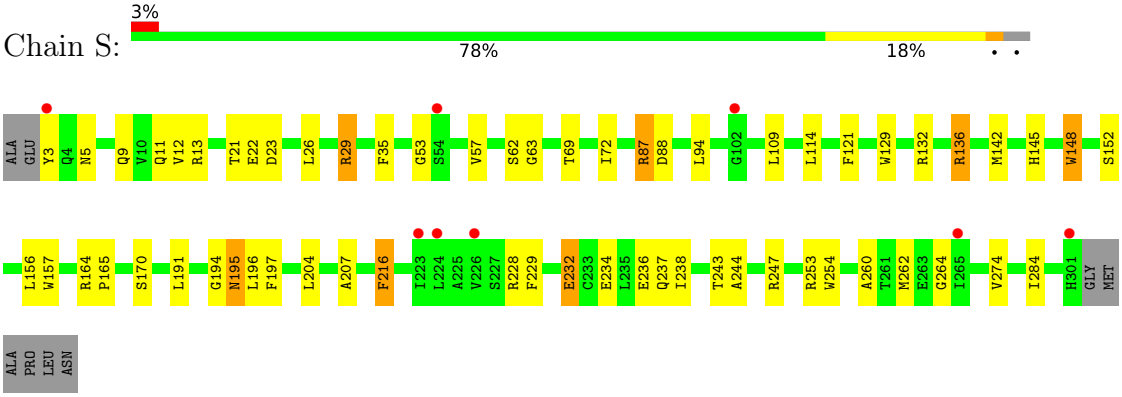


• Molecule 2: Reaction center protein M chain



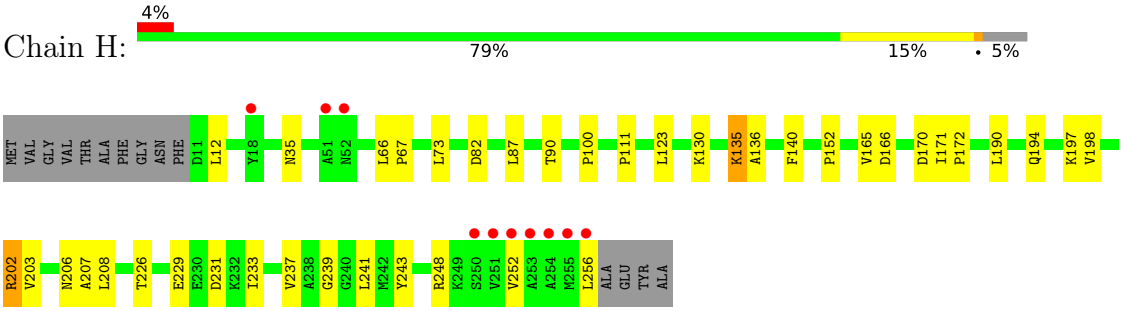
• Molecule 2: Reaction center protein M chain

Chain S:



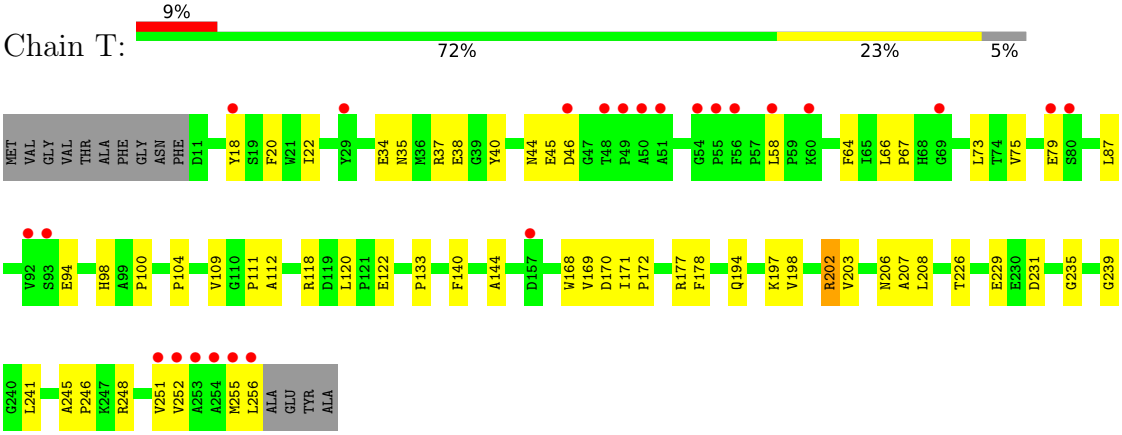
• Molecule 3: Reaction center protein H chain

Chain H:



• Molecule 3: Reaction center protein H chain

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.58Å 139.58Å 274.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 2.40 39.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.76-2.40) 98.3 (39.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.238 0.200 , 0.226	Depositor DCC
R_{free} test set	5283 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14481	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: LDA, SPO, U10, BPH, FE2, 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	0.42	0/2320	0.57	0/3175
1	R	0.37	0/2320	0.55	0/3175
2	M	0.41	0/2477	0.56	0/3383
2	S	0.39	0/2477	0.53	0/3383
3	H	0.35	0/1917	0.60	0/2608
3	T	0.31	0/1917	0.56	0/2608
All	All	0.38	0/13428	0.56	0/18332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2189	57	0
1	R	2232	0	2189	60	0
2	M	2385	0	2296	51	0
2	S	2385	0	2296	63	0
3	H	1869	0	1884	36	0
3	T	1869	0	1884	52	0
4	L	183	0	189	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	66	0	74	13	0
4	R	66	0	74	5	0
4	S	183	0	189	21	0
5	L	44	0	56	3	0
5	M	38	0	47	4	0
5	R	18	0	15	0	0
5	S	32	0	39	1	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	M	120	0	127	6	0
7	R	65	0	74	5	0
7	S	55	0	53	2	0
8	M	42	0	60	4	0
8	S	42	0	60	3	0
9	M	64	0	124	3	0
9	S	16	0	31	0	0
10	H	109	0	0	1	0
10	L	72	0	0	1	0
10	M	107	0	0	2	0
10	R	47	0	0	2	0
10	S	75	0	0	3	0
10	T	63	0	0	1	0
All	All	14481	0	13950	317	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 11.

The worst 5 of 317 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:R:241:VAL:HG21	7:R:2006:BPH:HAC1	1.40	1.03
1:L:241:VAL:HG21	7:M:1006:BPH:HAC2	1.38	1.01
2:M:109:LEU:HD12	2:M:114:LEU:HD13	1.56	0.86
2:S:157:TRP:HB2	4:S:2003:BCL:H62	1.58	0.84
4:S:2001:BCL:HBC1	4:S:2003:BCL:CAD	2.09	0.82

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%)	269 (96%)	10 (4%)	0	100 100
1	R	279/281 (99%)	263 (94%)	14 (5%)	2 (1%)	22 32
2	M	297/307 (97%)	285 (96%)	12 (4%)	0	100 100
2	S	297/307 (97%)	287 (97%)	10 (3%)	0	100 100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100 100
3	T	244/260 (94%)	235 (96%)	9 (4%)	0	100 100
All	All	1640/1696 (97%)	1575 (96%)	63 (4%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	4	SER
1	R	31	VAL

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%)	207 (94%)	13 (6%)	19 32
1	R	220/220 (100%)	208 (94%)	12 (6%)	21 35
2	M	235/240 (98%)	220 (94%)	15 (6%)	17 28
2	S	235/240 (98%)	225 (96%)	10 (4%)	29 46
3	H	199/208 (96%)	194 (98%)	5 (2%)	47 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	199/208 (96%)	196 (98%)	3 (2%)	65 80
All	All	1308/1336 (98%)	1250 (96%)	58 (4%)	28 45

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	73	LEU
3	T	202	ARG
1	R	129	LEU
2	S	232	GLU
2	S	148	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	T	128	HIS
3	T	206	ASN
1	R	87	GLN
1	R	159	ASN
1	R	183	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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
9	LDA	M	1014	-	12,15,15	2.11	1 (8%)	14,17,17	1.74	5 (35%)
5	U10	S	2008	-	32,32,63	1.98	10 (31%)	38,41,79	1.96	10 (26%)
4	BCL	R	2002	-	58,74,74	1.20	4 (6%)	69,115,115	2.06	22 (31%)
9	LDA	S	2011	-	12,15,15	2.06	1 (8%)	14,17,17	1.71	4 (28%)
4	BCL	S	2001	-	43,59,74	1.45	6 (13%)	51,97,115	2.18	14 (27%)
8	SPO	M	1010	-	40,41,41	3.47	24 (60%)	47,50,50	4.02	14 (29%)
7	BPH	S	2005	-	41,60,70	1.94	9 (21%)	40,89,101	3.14	20 (50%)
7	BPH	M	1006	-	51,70,70	1.76	9 (17%)	52,101,101	2.68	18 (34%)
9	LDA	M	1012	-	12,15,15	2.10	1 (8%)	14,17,17	1.71	4 (28%)
8	SPO	S	2010	-	40,41,41	3.39	24 (60%)	47,50,50	4.13	14 (29%)
4	BCL	L	1002	-	58,74,74	1.10	4 (6%)	69,115,115	2.05	20 (28%)
4	BCL	S	2004	-	58,74,74	1.32	9 (15%)	69,115,115	1.99	22 (31%)
5	U10	L	1009	-	44,44,63	2.09	17 (38%)	53,56,79	2.96	16 (30%)
5	U10	R	2009	-	18,18,63	2.26	7 (38%)	22,25,79	2.29	7 (31%)
9	LDA	M	1013	-	12,15,15	2.08	1 (8%)	14,17,17	1.70	4 (28%)
4	BCL	L	1004	-	58,74,74	1.32	7 (12%)	69,115,115	2.10	21 (30%)
4	BCL	L	1001	-	43,59,74	1.61	7 (16%)	51,97,115	2.20	14 (27%)
4	BCL	M	1003	-	58,74,74	1.25	7 (12%)	69,115,115	2.03	23 (33%)
5	U10	M	1008	-	38,38,63	1.98	11 (28%)	46,49,79	1.92	11 (23%)
7	BPH	R	2006	-	51,70,70	1.86	11 (21%)	52,101,101	2.75	18 (34%)
9	LDA	M	1011	-	12,15,15	1.99	1 (8%)	14,17,17	1.66	4 (28%)
4	BCL	S	2003	-	58,74,74	1.23	4 (6%)	69,115,115	2.15	27 (39%)
7	BPH	M	1005	-	41,60,70	1.87	10 (24%)	40,89,101	2.90	18 (45%)

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
9	LDA	M	1014	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	U10	S	2008	-	-	2/26/50/87	0/1/1/1
4	BCL	R	2002	-	-	5/37/137/137	-
9	LDA	S	2011	-	-	7/13/13/13	-
4	BCL	S	2001	-	-	3/19/119/137	-
8	SPO	M	1010	-	-	13/47/47/47	-
7	BPH	S	2005	-	1/1/16/22	10/25/93/105	0/5/6/6
7	BPH	M	1006	-	2/2/18/22	14/37/105/105	0/5/6/6
9	LDA	M	1012	-	-	6/13/13/13	-
8	SPO	S	2010	-	-	12/47/47/47	-
4	BCL	L	1002	-	-	6/37/137/137	-
4	BCL	S	2004	-	-	7/37/137/137	-
5	U10	L	1009	-	-	7/41/65/87	0/1/1/1
5	U10	R	2009	-	-	1/9/33/87	0/1/1/1
9	LDA	M	1013	-	-	4/13/13/13	-
4	BCL	L	1004	-	-	10/37/137/137	-
4	BCL	L	1001	-	-	2/19/119/137	-
4	BCL	M	1003	-	-	10/37/137/137	-
7	BPH	R	2006	-	2/2/18/22	12/37/105/105	0/5/6/6
5	U10	M	1008	-	-	2/33/57/87	0/1/1/1
9	LDA	M	1011	-	-	6/13/13/13	-
4	BCL	S	2003	-	-	8/37/137/137	-
7	BPH	M	1005	-	1/1/16/22	7/25/93/105	0/5/6/6

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1010	SPO	C6-C5	9.15	1.55	1.32
8	S	2010	SPO	C6-C5	8.71	1.54	1.32
8	M	1010	SPO	C15-C16	8.59	1.56	1.34
8	M	1010	SPO	C10-C11	7.86	1.54	1.34
8	S	2010	SPO	C10-C11	7.82	1.54	1.34

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	2010	SPO	C3-C1-C4	-17.48	84.02	110.86
8	M	1010	SPO	C3-C1-C4	-17.14	84.55	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	2010	SPO	C2-C1-C4	-16.17	86.04	110.86
8	M	1010	SPO	C2-C1-C4	-15.62	86.88	110.86
5	L	1009	U10	C32-C33-C34	14.51	162.60	127.66

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	1005	BPH	C8
7	M	1006	BPH	C13
7	M	1006	BPH	C8
7	R	2006	BPH	C13
7	R	2006	BPH	C8

5 of 160 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1004	BCL	C1A-C2A-CAA-CBA
4	L	1004	BCL	C3A-C2A-CAA-CBA
4	M	1003	BCL	C4-C3-C5-C6
4	S	2003	BCL	C2-C3-C5-C6
4	S	2003	BCL	C4-C3-C5-C6

There are no ring outliers.

19 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	1014	LDA	2	0
5	S	2008	U10	1	0
4	R	2002	BCL	5	0
4	S	2001	BCL	8	0
8	M	1010	SPO	4	0
7	S	2005	BPH	2	0
7	M	1006	BPH	4	0
9	M	1012	LDA	1	0
8	S	2010	SPO	3	0
4	L	1002	BCL	6	0
4	S	2004	BCL	5	0
5	L	1009	U10	3	0
4	L	1004	BCL	9	0
4	L	1001	BCL	11	0
4	M	1003	BCL	13	0
5	M	1008	U10	4	0

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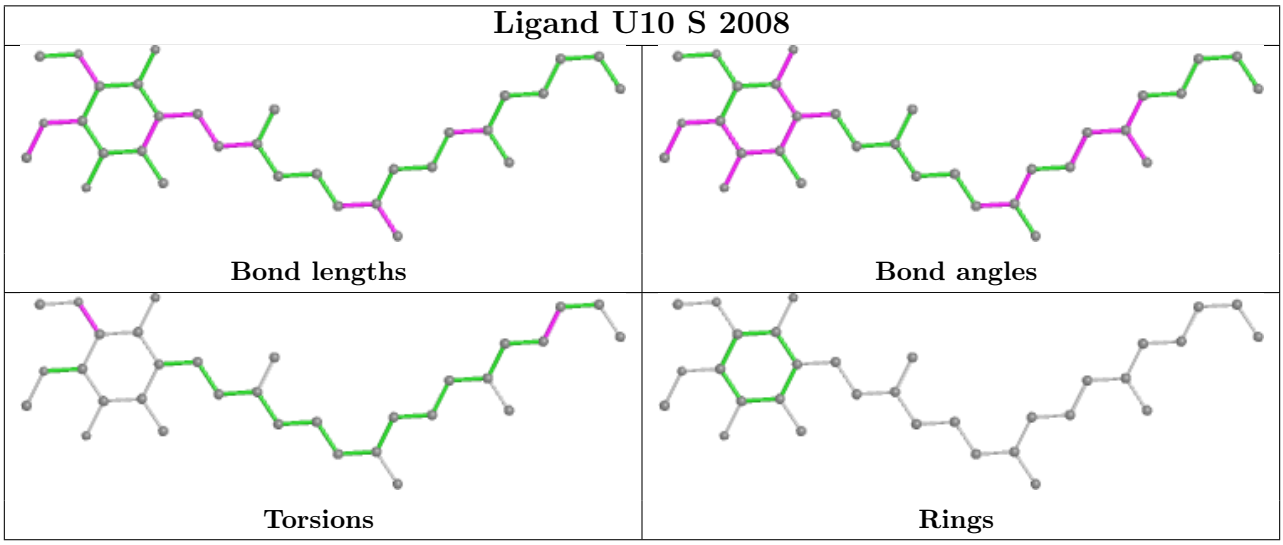
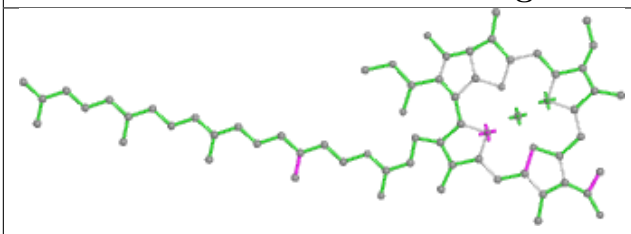
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	2006	BPH	5	0
4	S	2003	BCL	11	0
7	M	1005	BPH	2	0

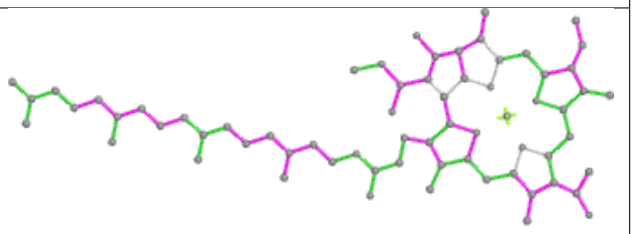
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



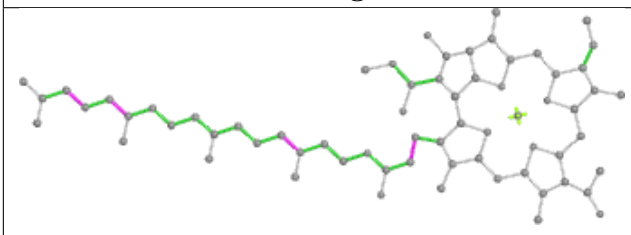
Ligand BCL R 2002



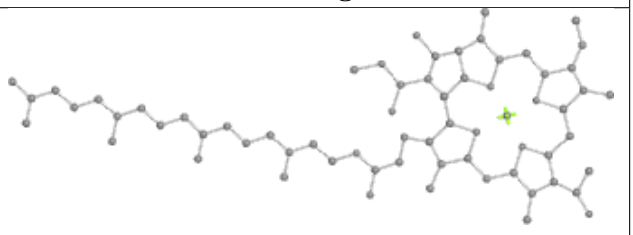
Bond lengths



Bond angles

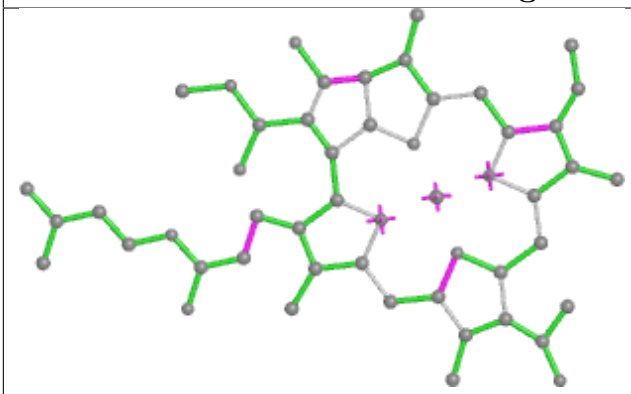


Torsions



Rings

Ligand BCL S 2001



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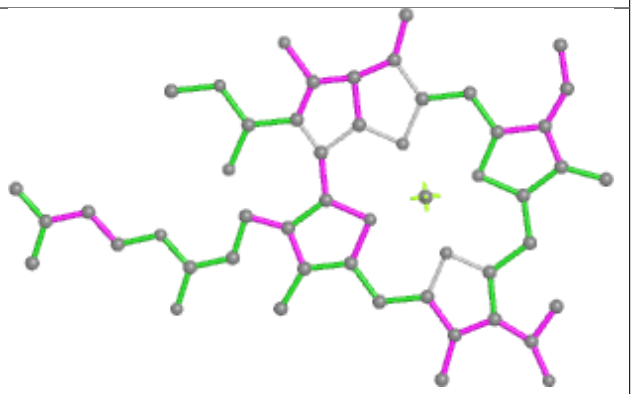
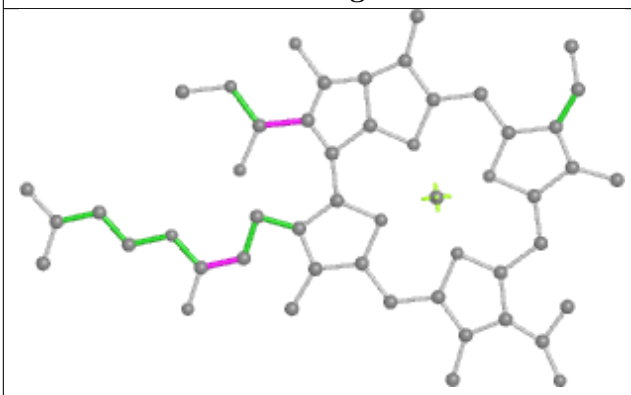
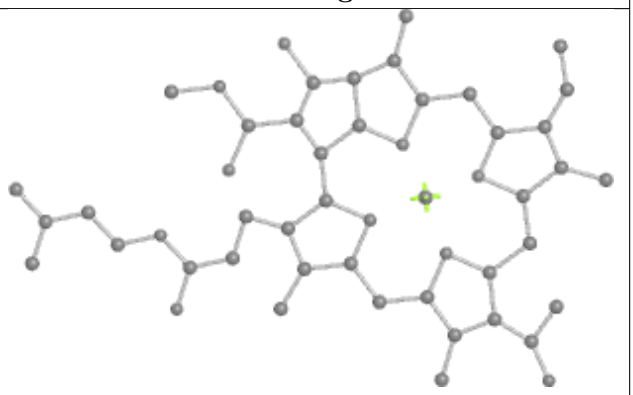


Bond angles

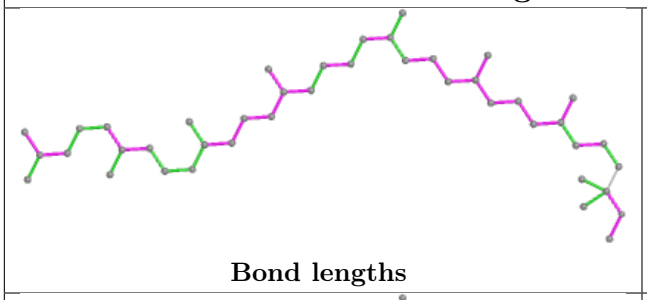


Torsions

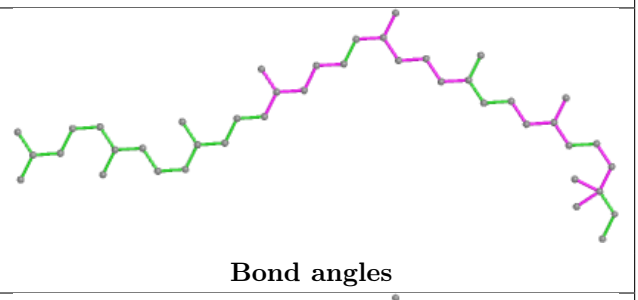


Rings

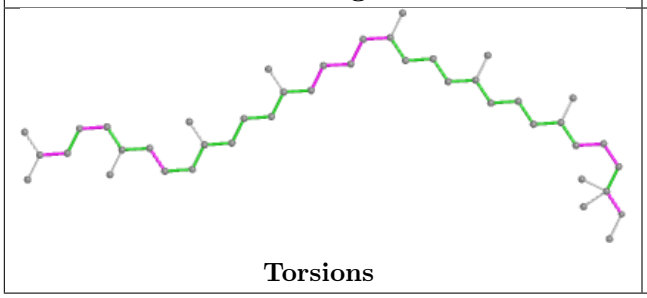
Ligand SPO M 1010



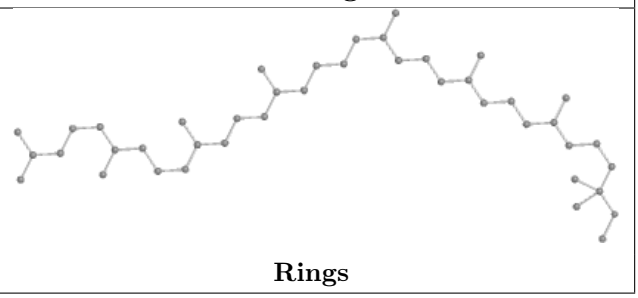
Bond lengths



Bond angles

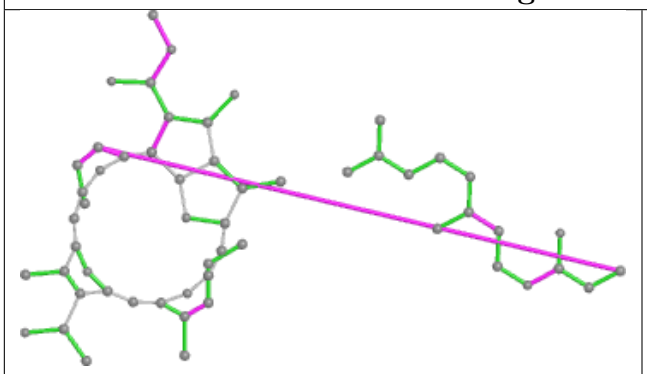


Torsions

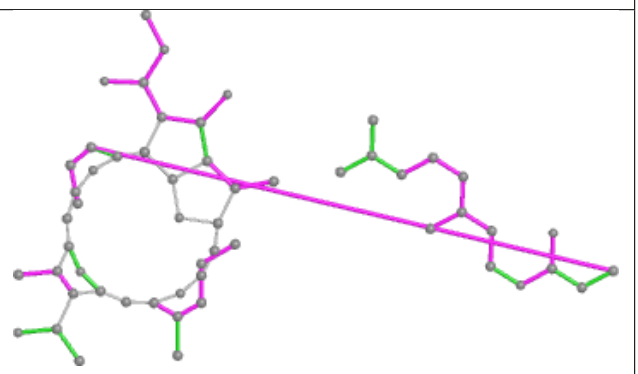


Rings

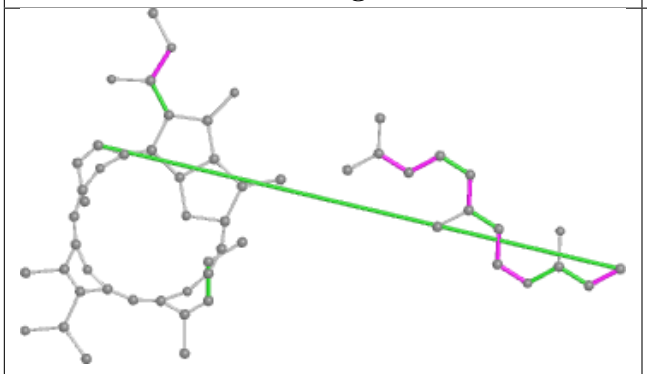
Ligand BPH S 2005



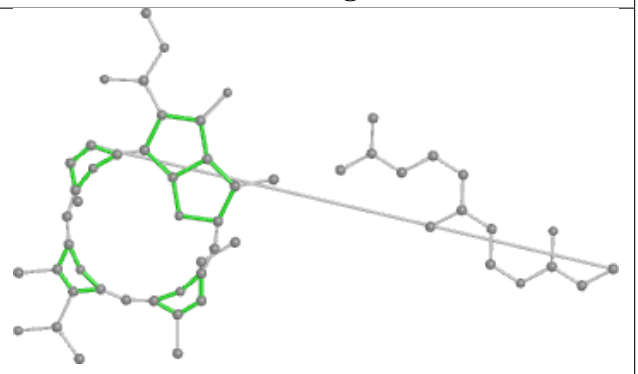
Bond lengths



Bond angles

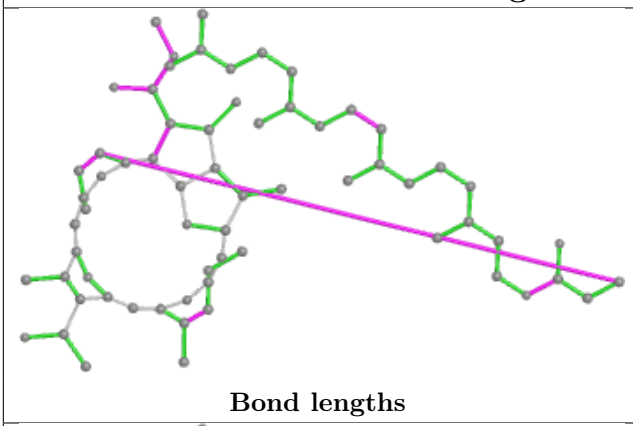


Torsions

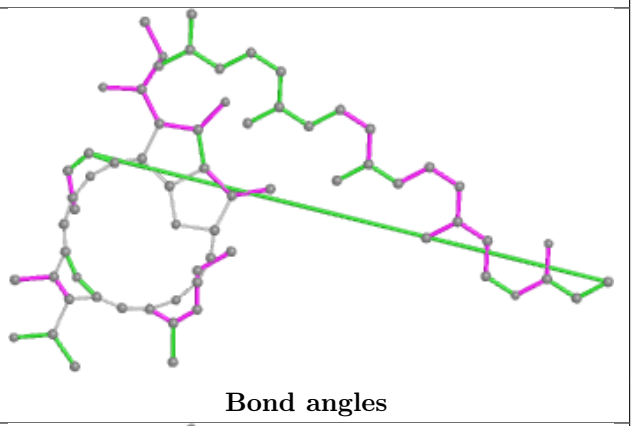


Rings

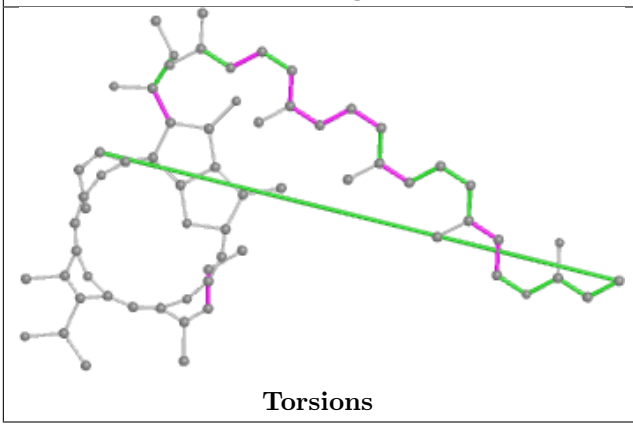
Ligand BPH M 1006



Bond lengths



Bond angles



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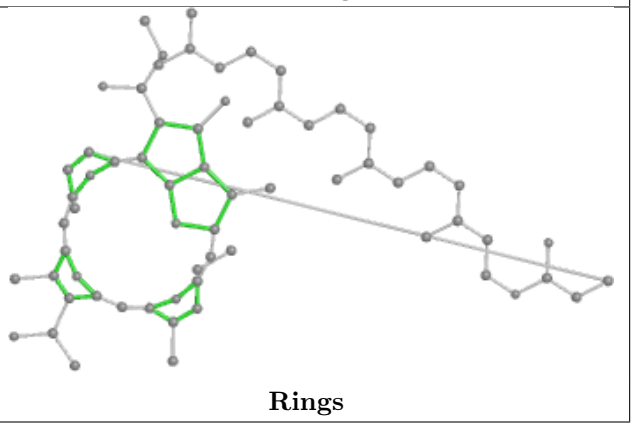
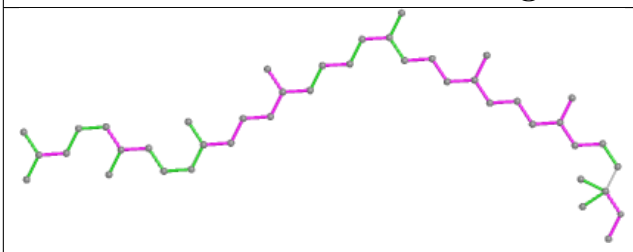
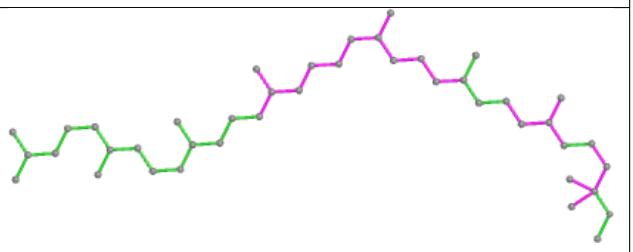


Rings

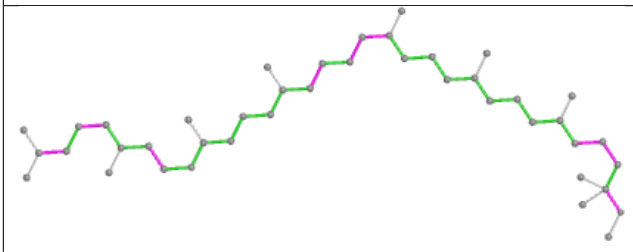
Ligand SPO S 2010



Bond lengths



Bond angles



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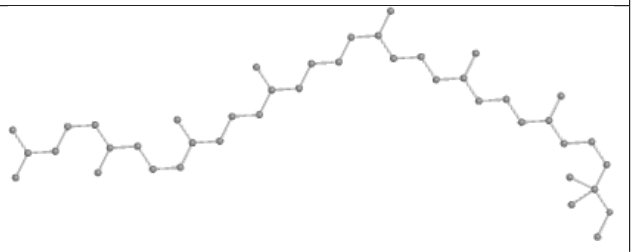
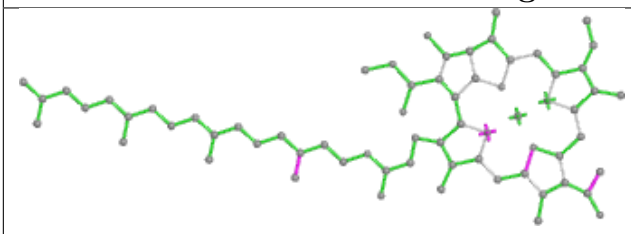
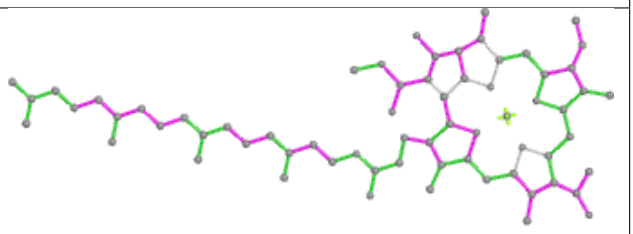


Rings

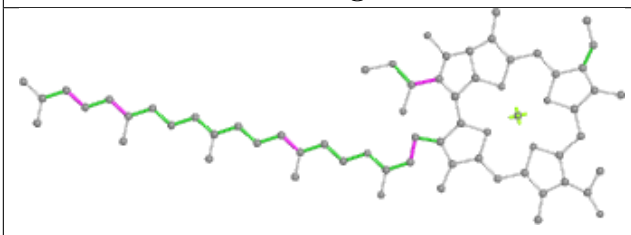
Ligand BCL L 1002



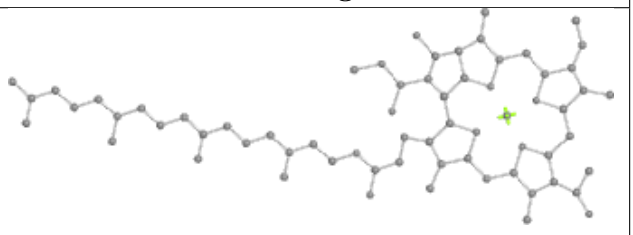
Bond lengths



Bond angles

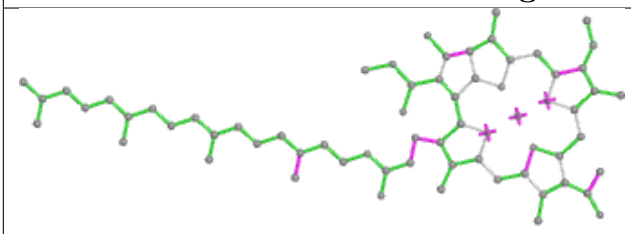


Torsions

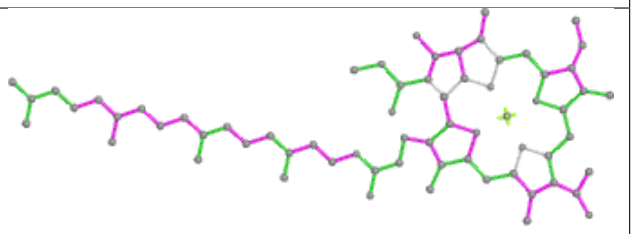


Rings

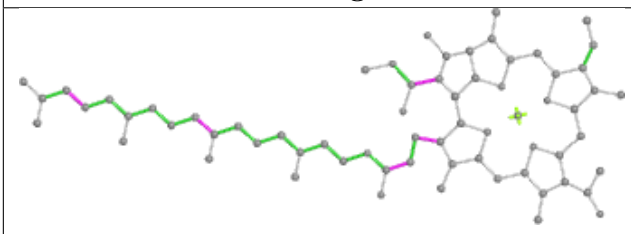
Ligand BCL S 2004



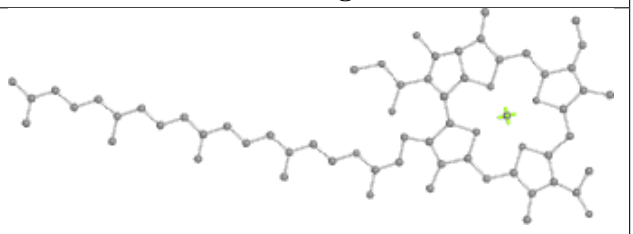
Bond lengths



Bond angles

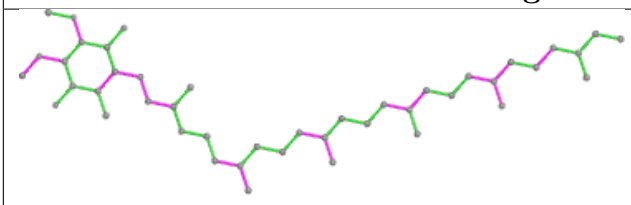


Torsions

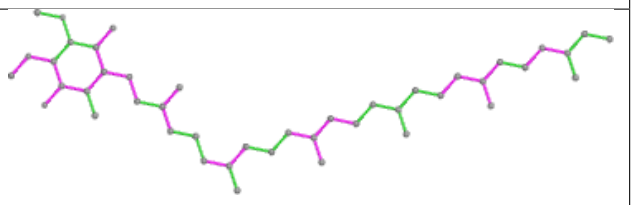


Rings

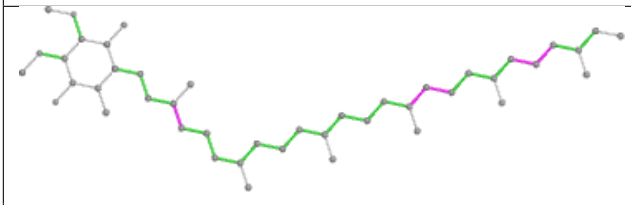
Ligand U10 L 1009



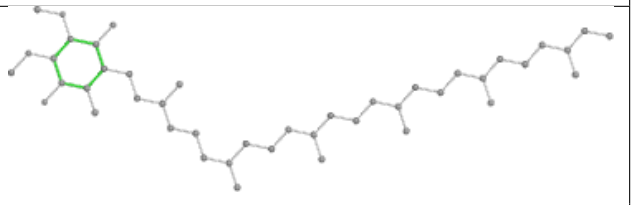
Bond lengths



Bond angles

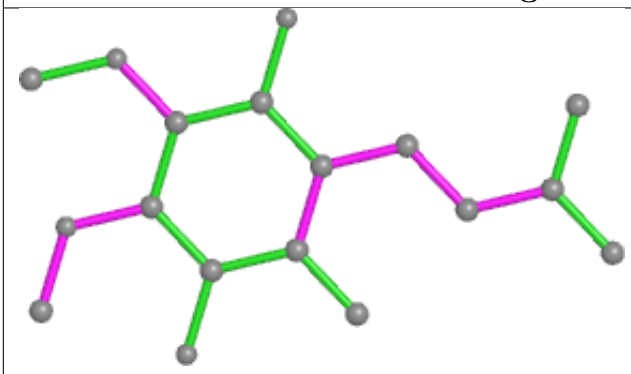


Torsions

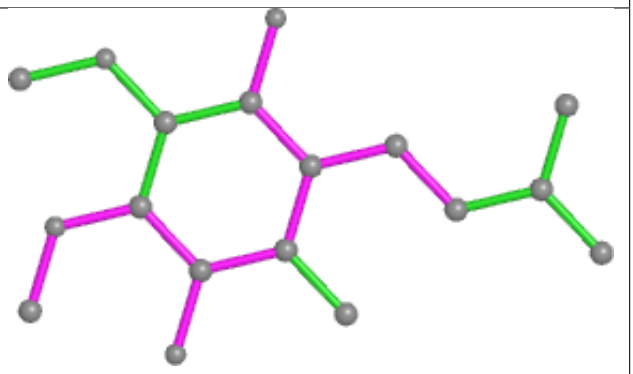


Rings

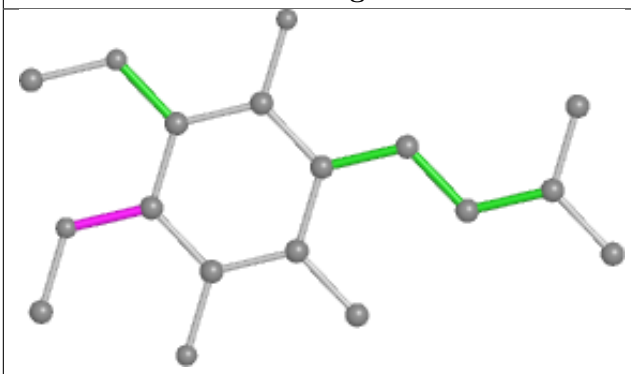
Ligand U10 R 2009



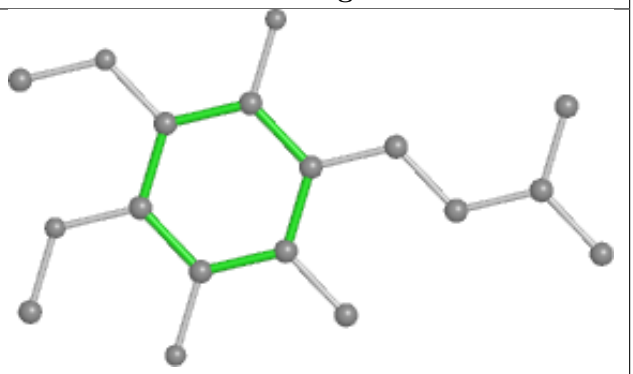
Bond lengths



Bond angles

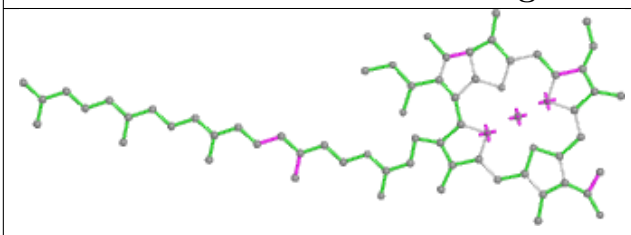


Torsions

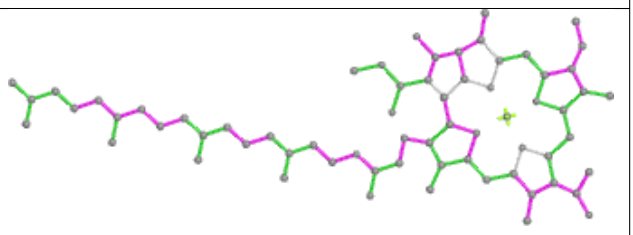


Rings

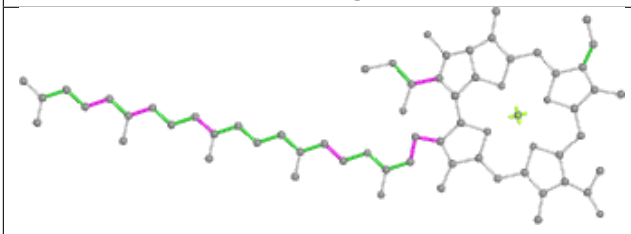
Ligand BCL L 1004



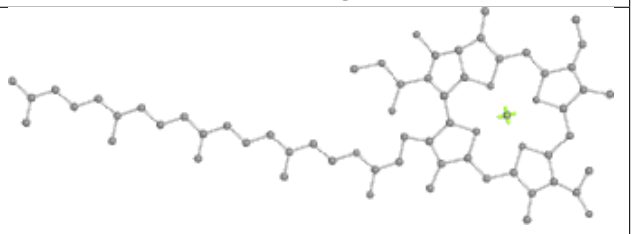
Bond lengths



Bond angles

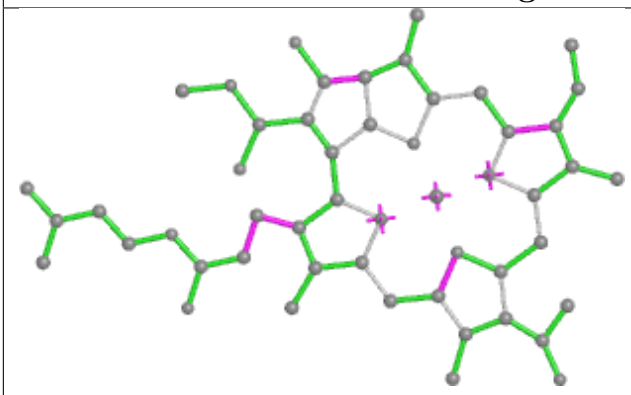


Torsions



Rings

Ligand BCL L 1001



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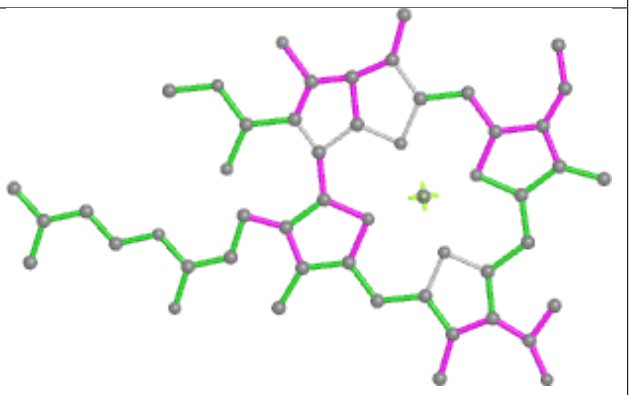
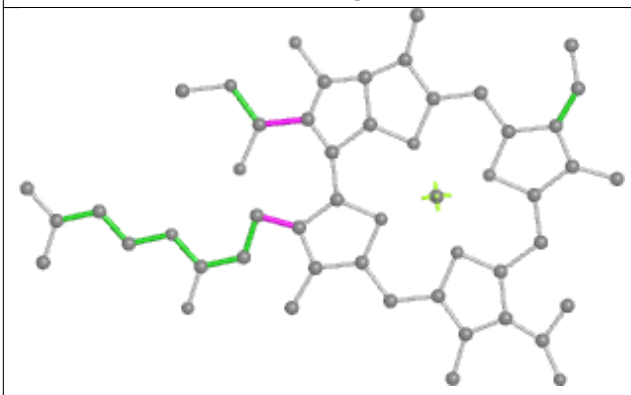


Bond angles



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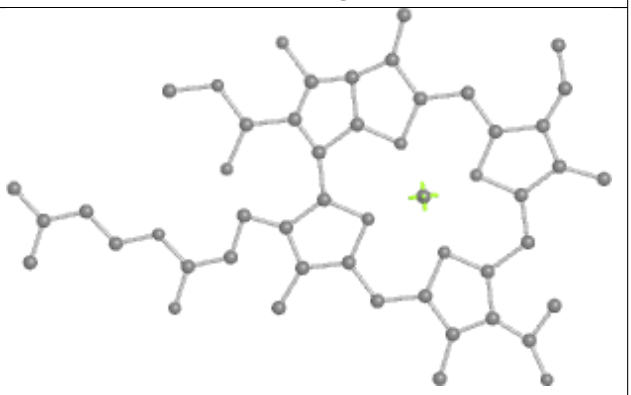
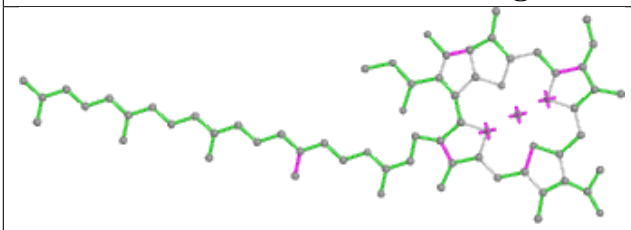
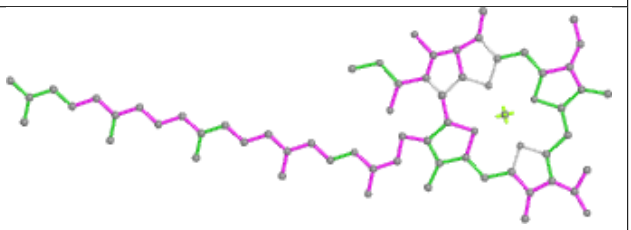


Rings

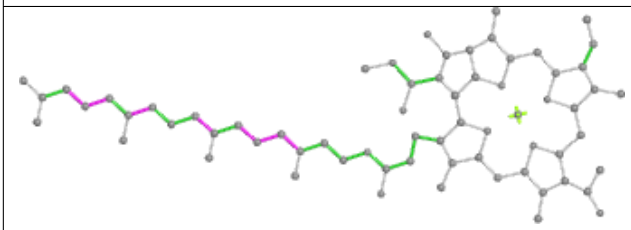
Ligand BCL M 1003



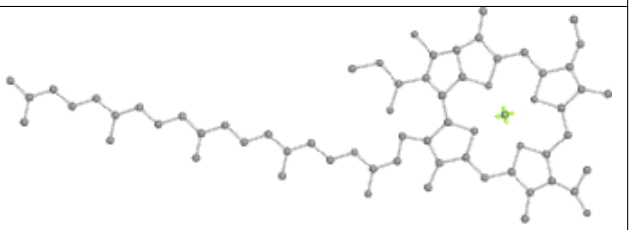
Bond lengths



Bond angles

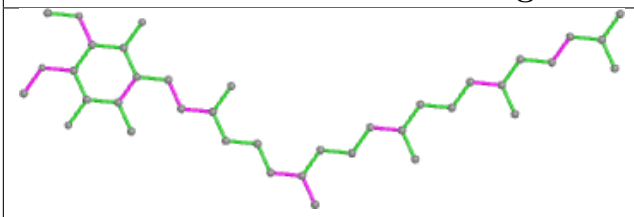


Torsions

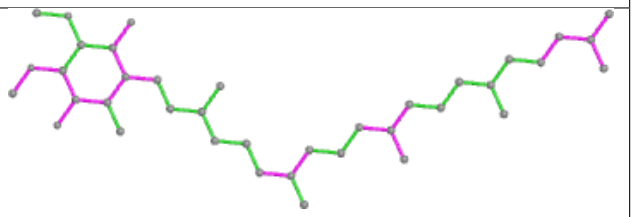


Rings

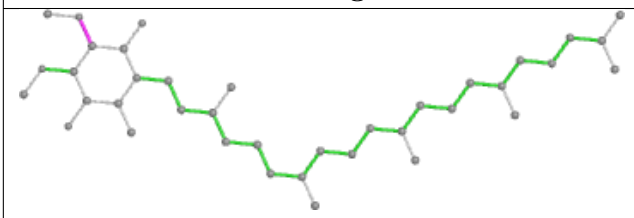
Ligand U10 M 1008



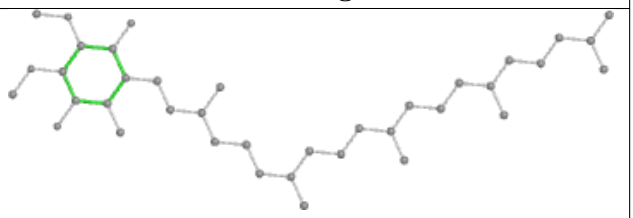
Bond lengths



Bond angles

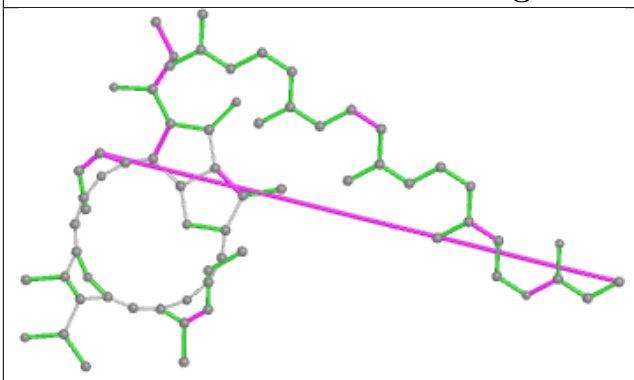


Torsions

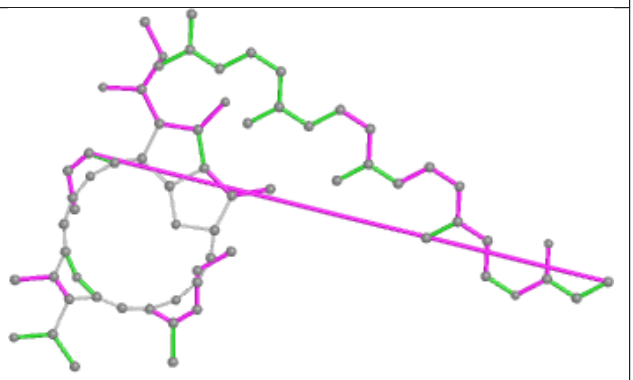


Rings

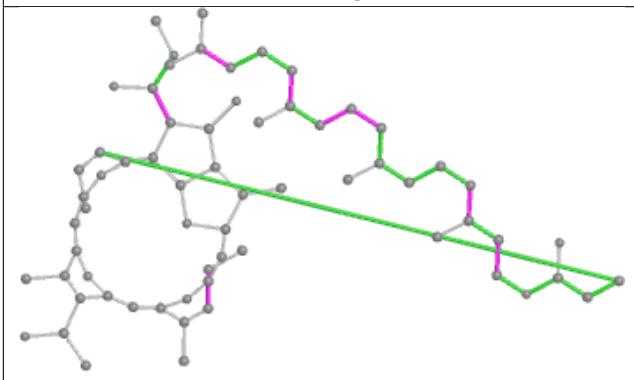
Ligand BPH R 2006



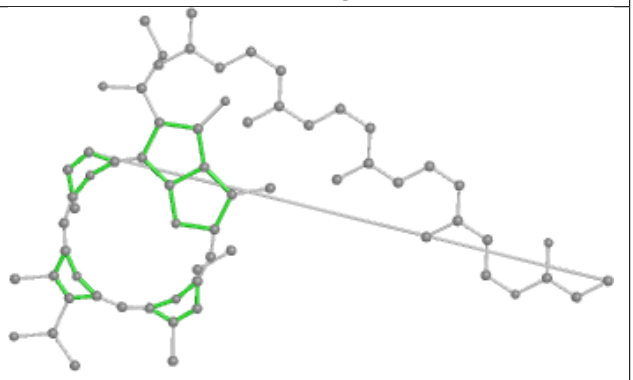
Bond lengths



Bond angles

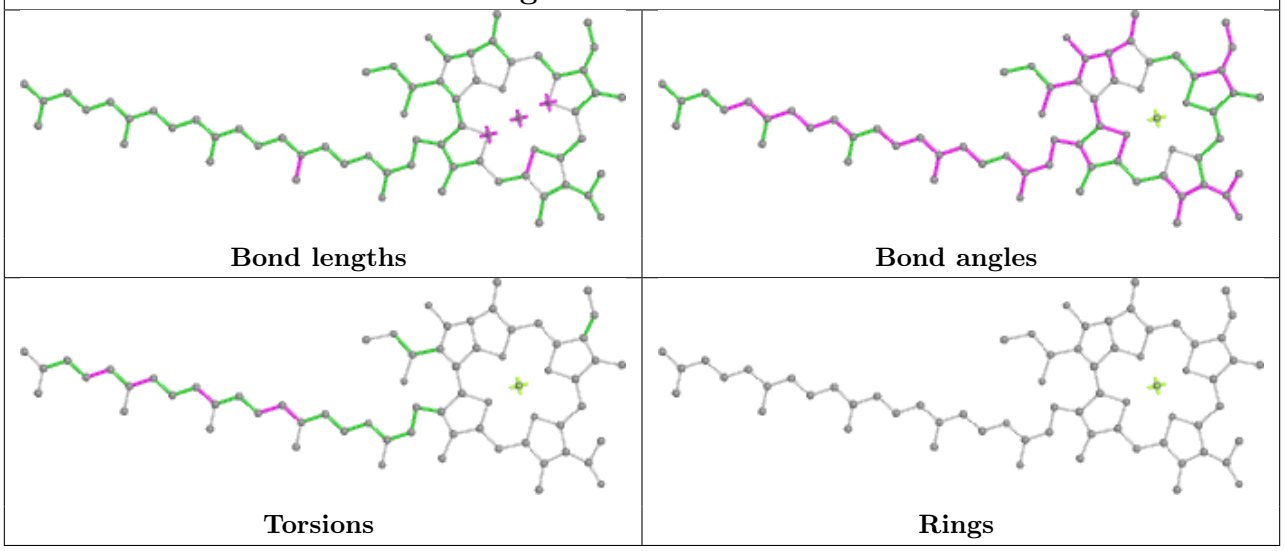


Torsions

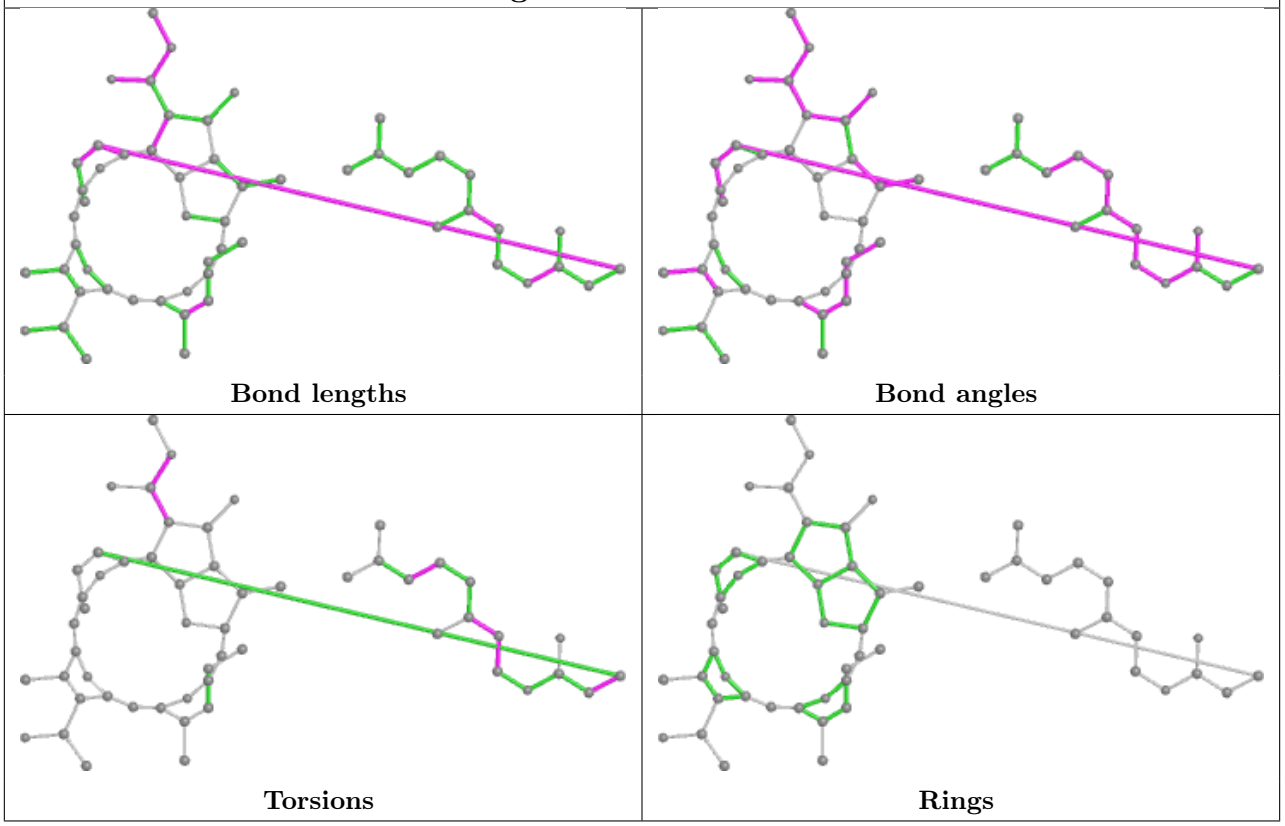


Rings

Ligand BCL S 2003



Ligand BPH M 1005



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%)	0.10	5 (1%) 68 66	17, 32, 49, 58	0
1	R	281/281 (100%)	0.29	16 (5%) 23 22	23, 41, 58, 69	0
2	M	299/307 (97%)	-0.04	12 (4%) 38 37	17, 27, 41, 67	0
2	S	299/307 (97%)	0.04	8 (2%) 54 52	24, 35, 48, 69	0
3	H	246/260 (94%)	0.08	10 (4%) 37 36	22, 34, 54, 88	0
3	T	246/260 (94%)	0.48	24 (9%) 7 7	31, 45, 70, 80	0
All	All	1652/1696 (97%)	0.15	75 (4%) 33 31	17, 36, 57, 88	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	252	VAL	6.1
3	H	254	ALA	5.6
3	H	255	MET	5.1
3	T	254	ALA	5.1
3	T	252	VAL	4.7

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 (i)

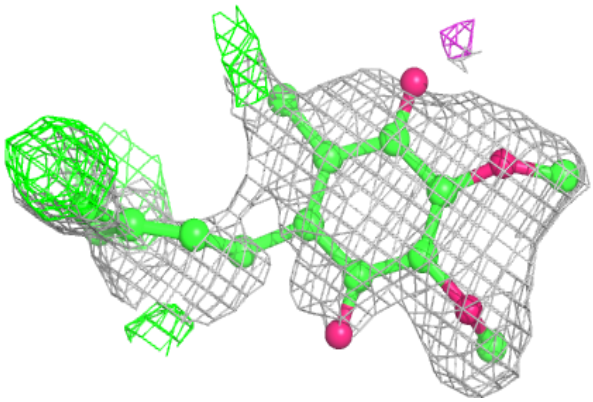
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

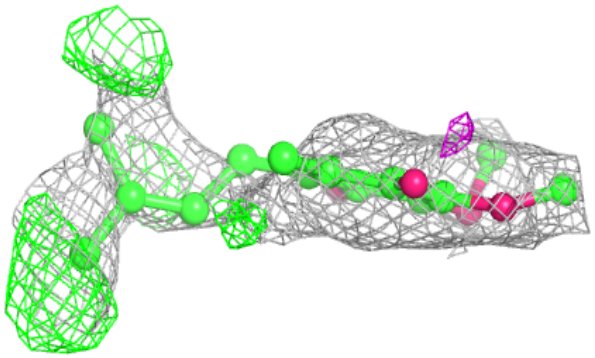
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	LDA	S	2011	16/16	0.60	0.42	74,79,85,85	0
9	LDA	M	1013	16/16	0.63	0.31	69,71,80,80	0
5	U10	R	2009	18/63	0.64	0.41	81,85,86,87	0
9	LDA	M	1011	16/16	0.64	0.26	49,57,74,74	0
5	U10	L	1009	44/63	0.66	0.34	66,72,79,79	0
9	LDA	M	1012	16/16	0.75	0.27	60,62,65,65	0
9	LDA	M	1014	16/16	0.78	0.34	50,55,59,60	0
8	SPO	S	2010	42/42	0.87	0.22	24,35,51,54	0
8	SPO	M	1010	42/42	0.87	0.21	16,28,47,51	0
4	BCL	R	2002	66/66	0.88	0.19	29,35,44,48	0
4	BCL	L	1001	51/66	0.90	0.22	17,24,51,55	0
4	BCL	S	2001	51/66	0.90	0.20	28,31,41,43	0
4	BCL	S	2003	66/66	0.90	0.21	27,33,48,55	0
4	BCL	L	1002	66/66	0.90	0.22	20,26,29,33	0
4	BCL	S	2004	66/66	0.91	0.21	26,34,58,60	0
4	BCL	L	1004	66/66	0.91	0.27	16,25,45,52	0
7	BPH	R	2006	65/65	0.92	0.19	31,38,45,46	0
5	U10	M	1008	38/63	0.92	0.30	23,30,53,53	0
4	BCL	M	1003	66/66	0.92	0.20	20,25,39,44	0
7	BPH	M	1006	65/65	0.92	0.25	23,28,37,40	0
7	BPH	M	1005	55/65	0.94	0.19	17,23,43,46	0
7	BPH	S	2005	55/65	0.94	0.17	25,30,55,58	0
5	U10	S	2008	32/63	0.94	0.34	36,42,51,54	0
6	FE2	S	2007	1/1	0.99	0.13	30,30,30,30	0
6	FE2	M	1007	1/1	0.99	0.14	20,20,20,20	0

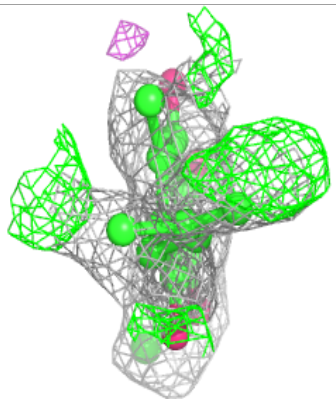
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 R 2009:

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

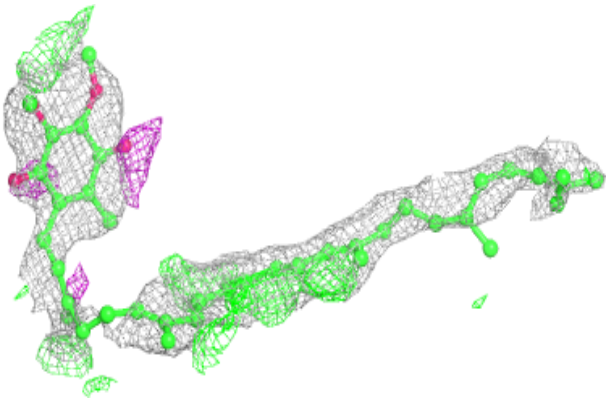


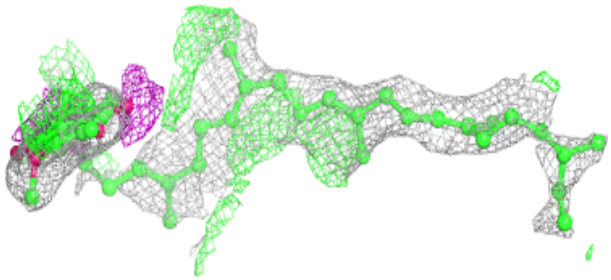


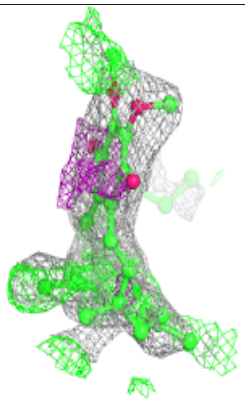


Electron density around U10 L 1009:

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

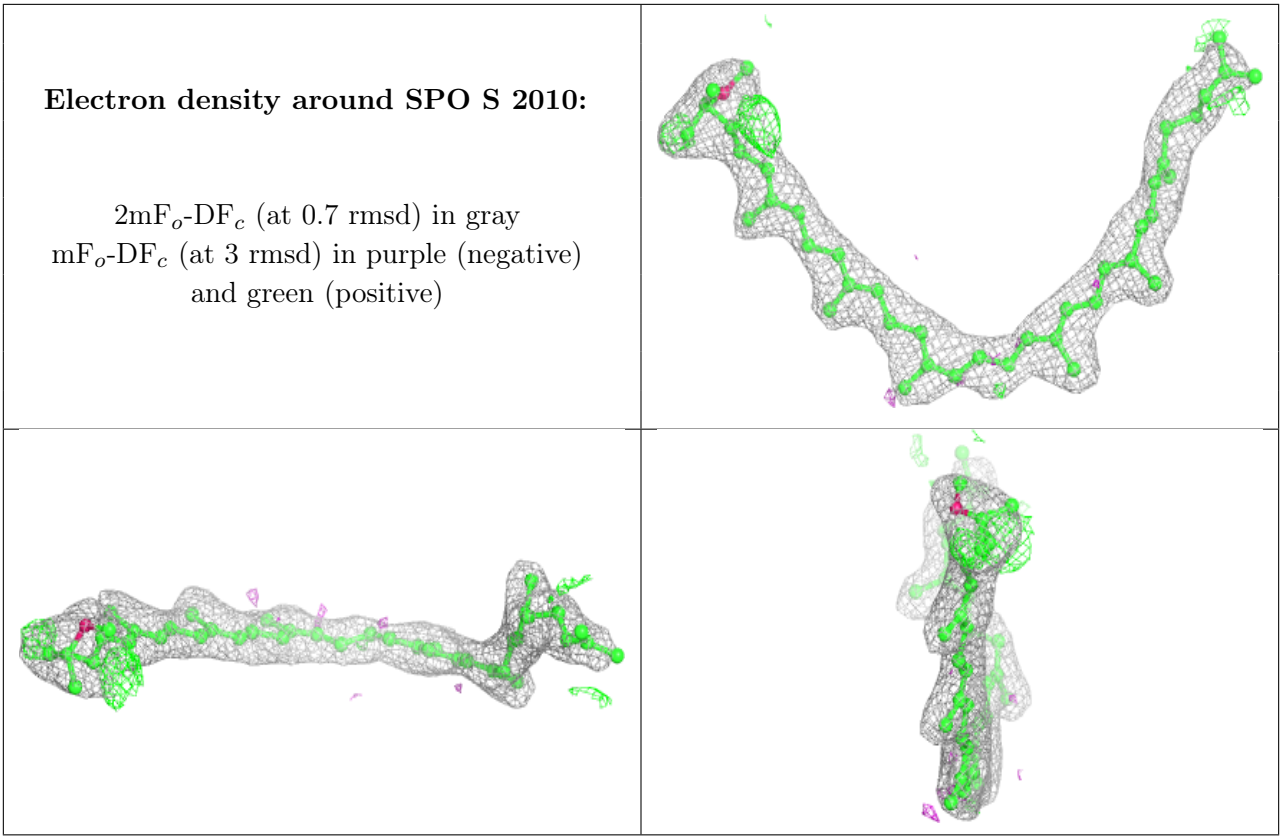






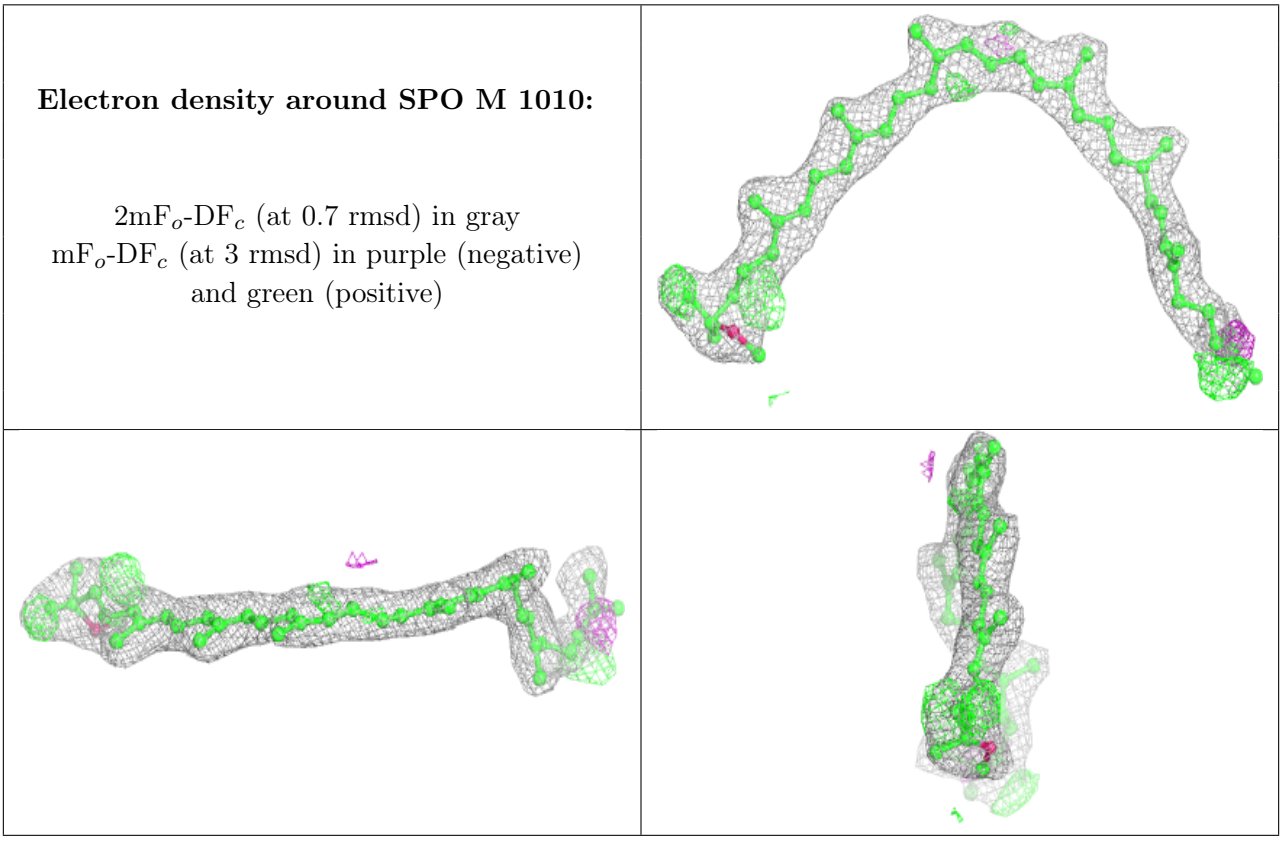
Electron density around SPO S 2010:

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



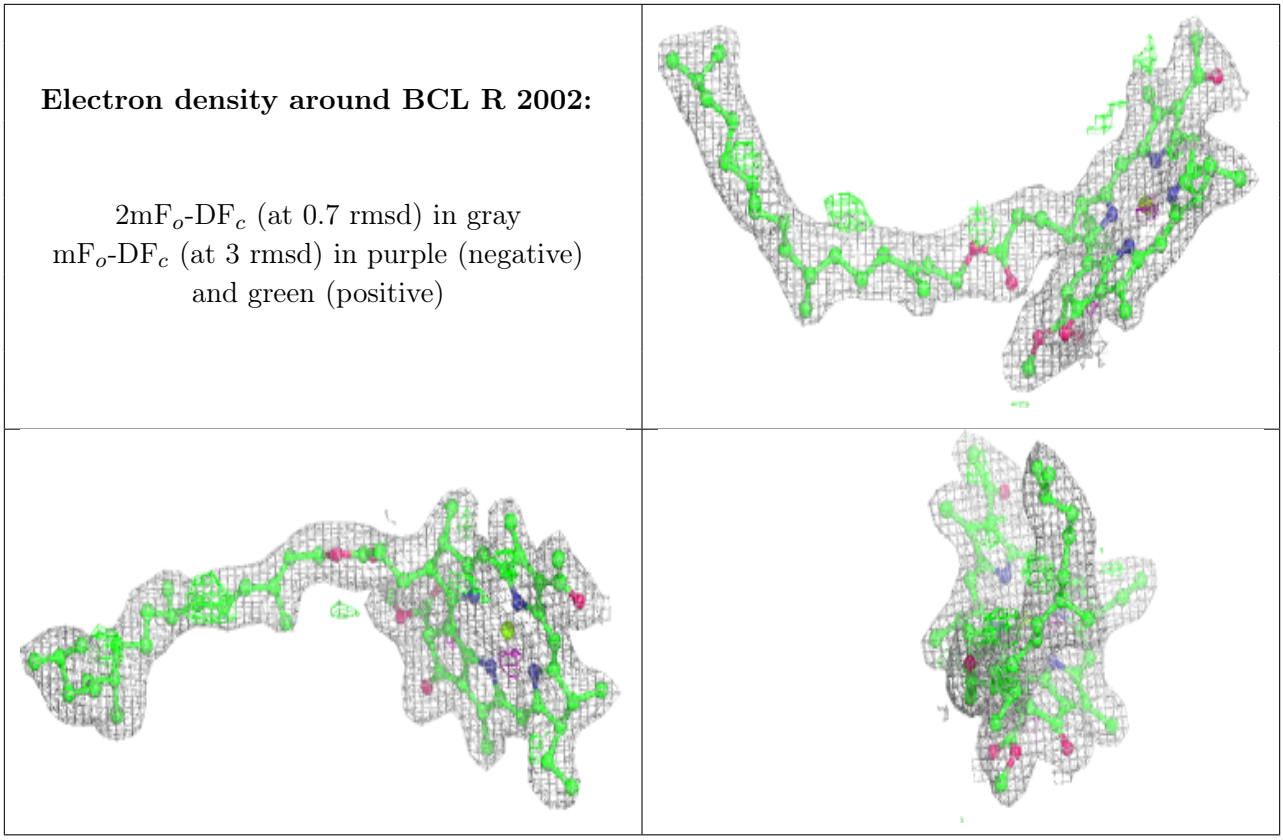
Electron density around SPO M 1010:

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



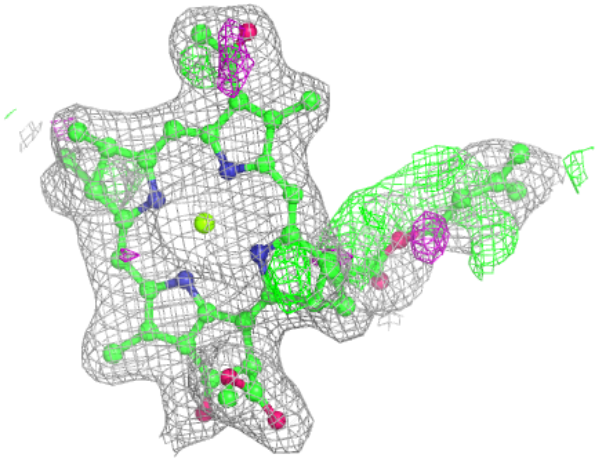
Electron density around BCL R 2002:

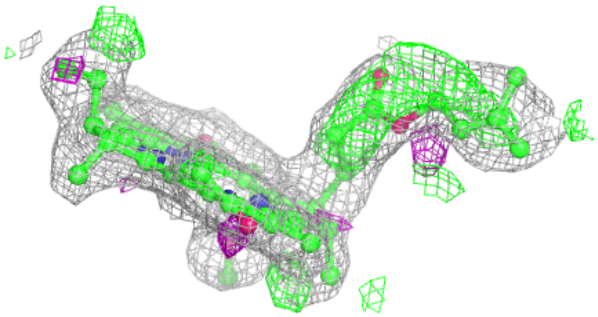
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

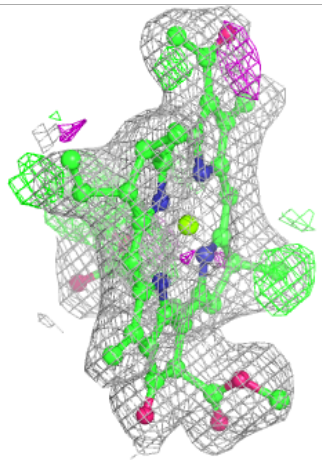


Electron density around BCL L 1001:

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

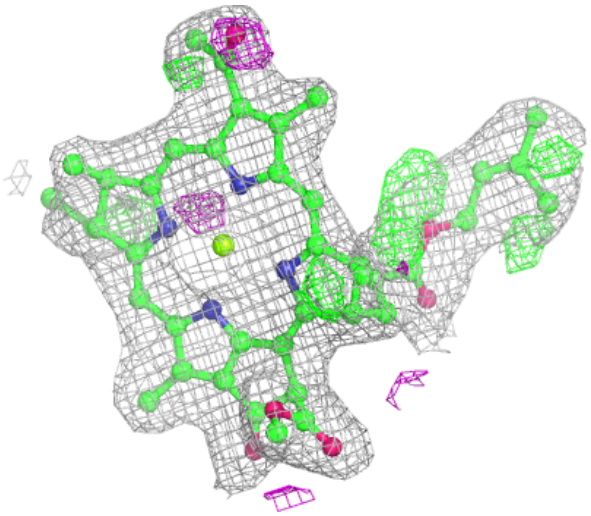


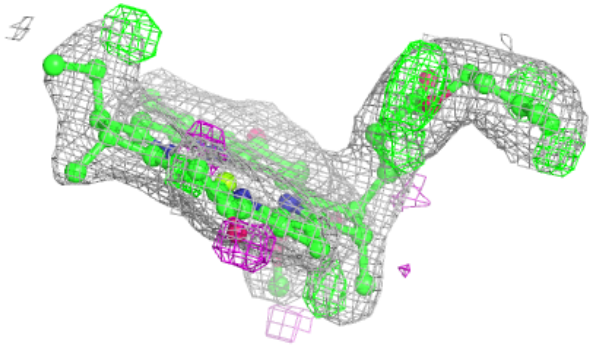


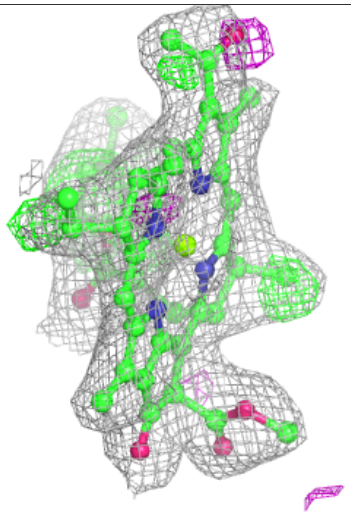


Electron density around BCL S 2001:

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

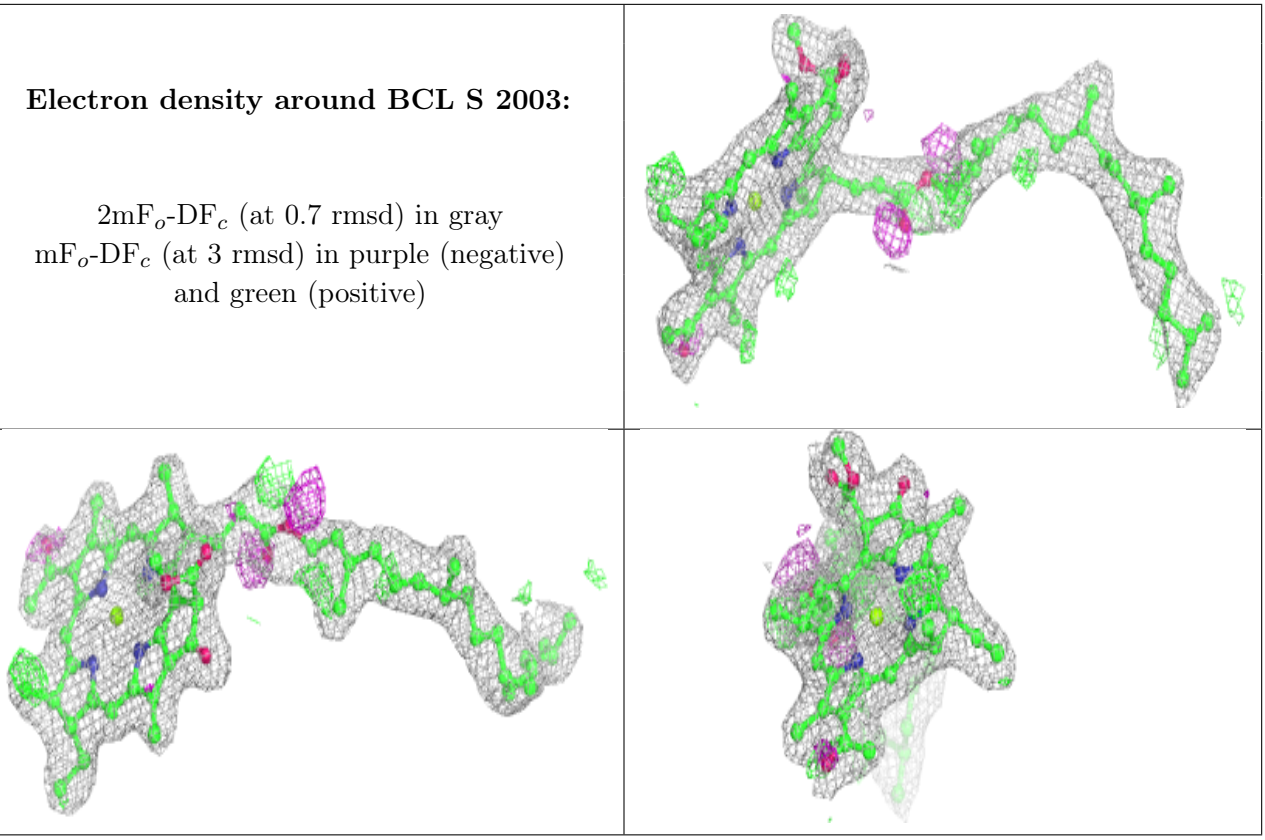






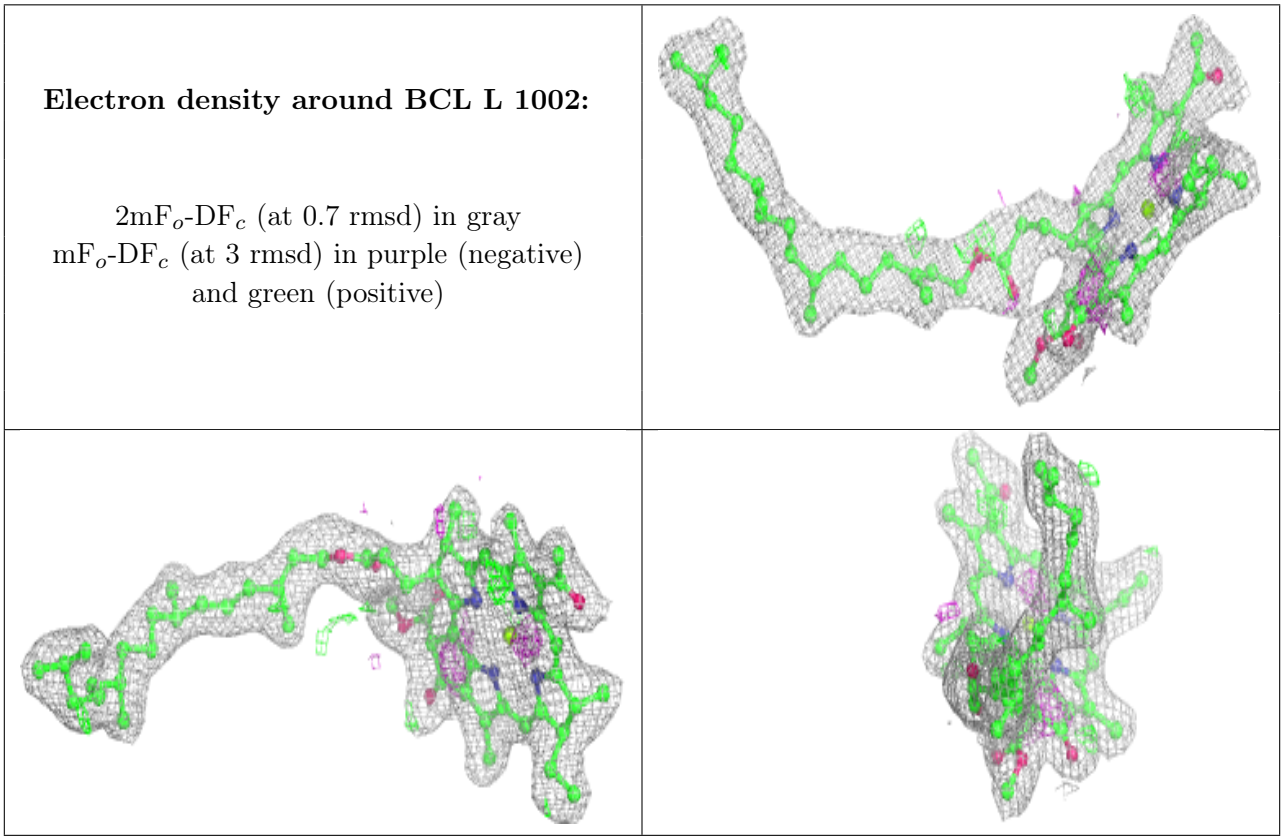
Electron density around BCL S 2003:

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



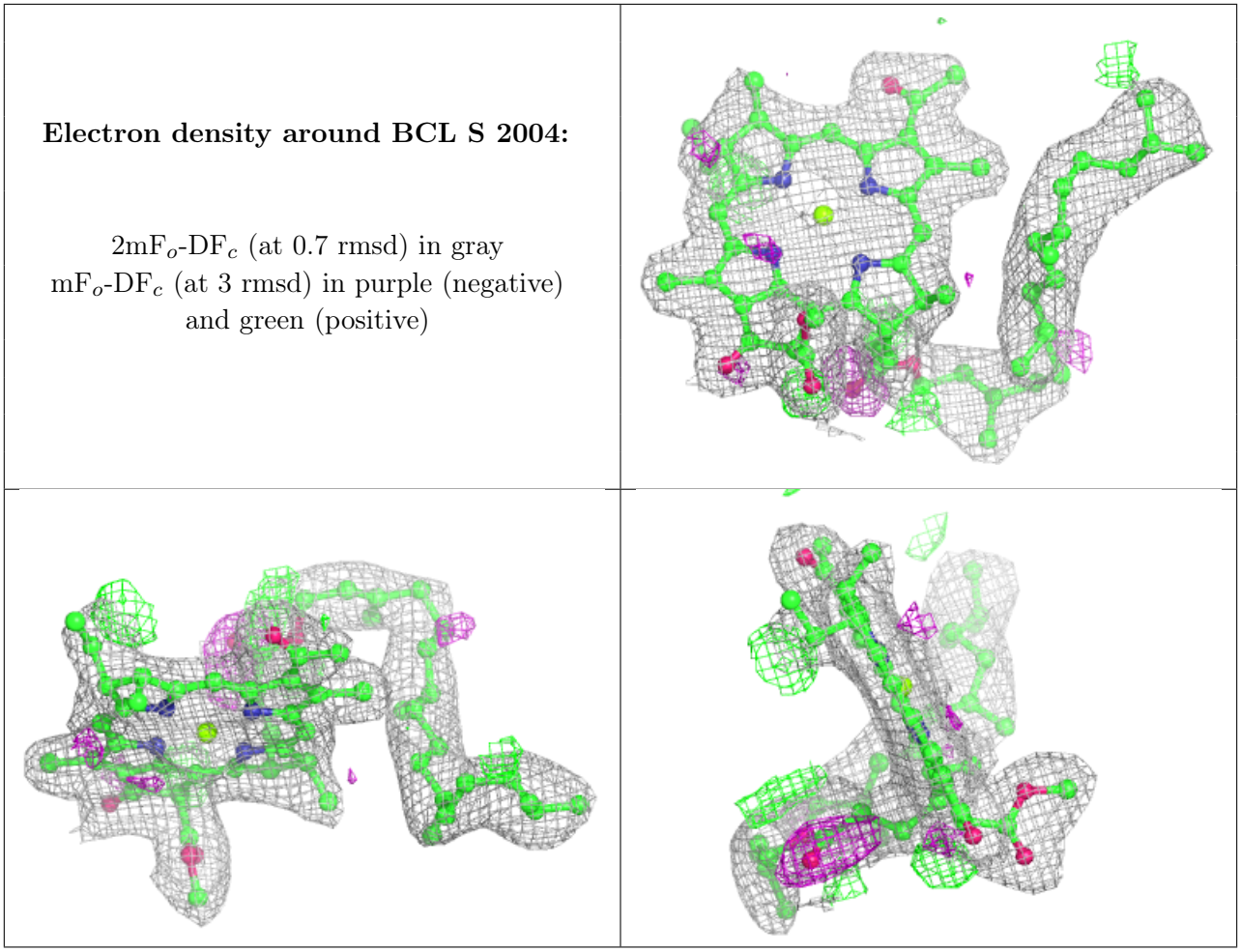
Electron density around BCL L 1002:

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



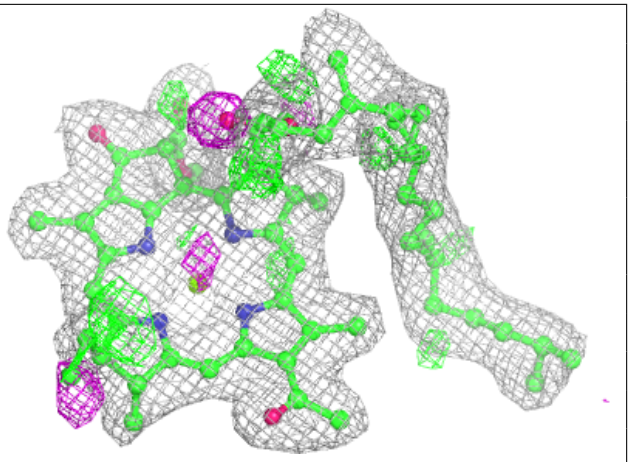
Electron density around BCL S 2004:

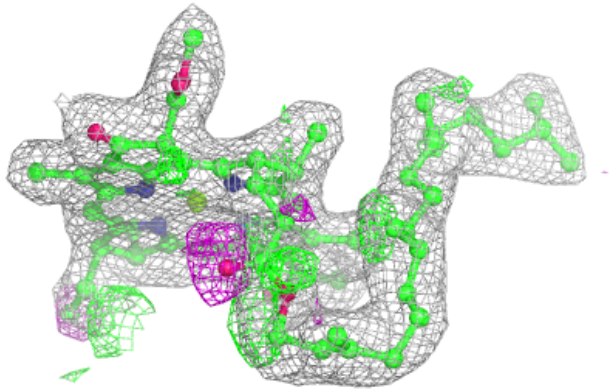
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

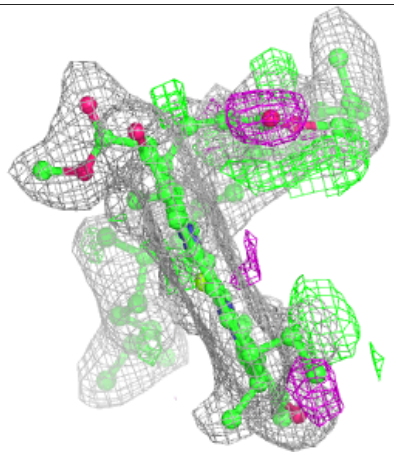


Electron density around BCL L 1004:

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

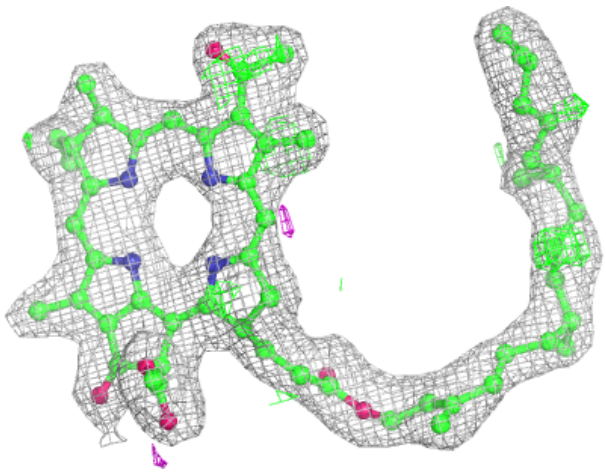


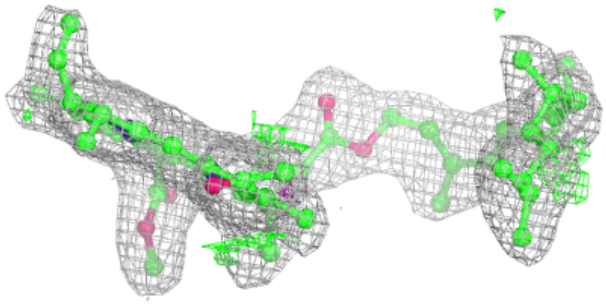


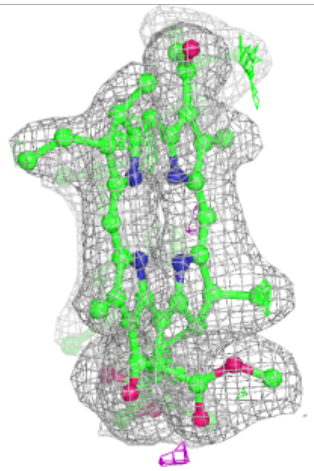


Electron density around BPH R 2006:

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

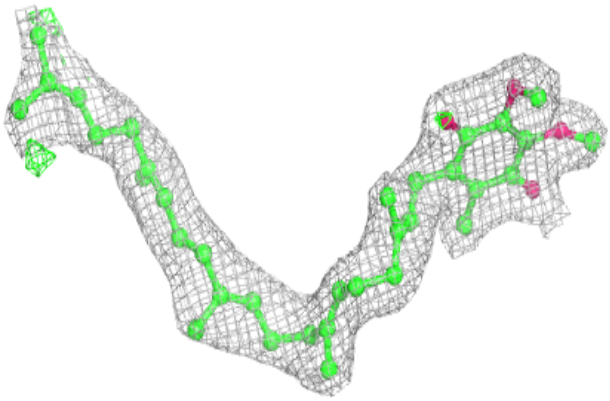


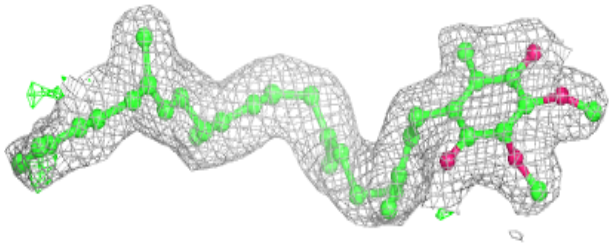




Electron density around U10 M 1008:

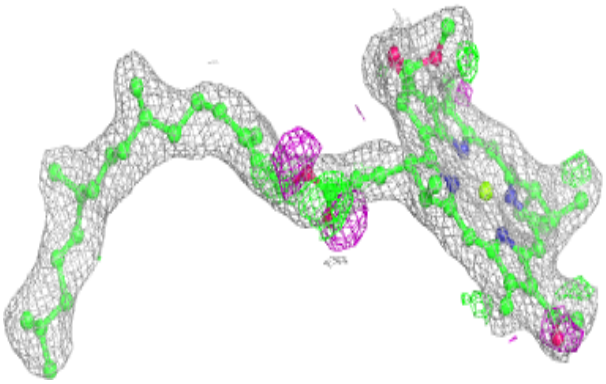
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

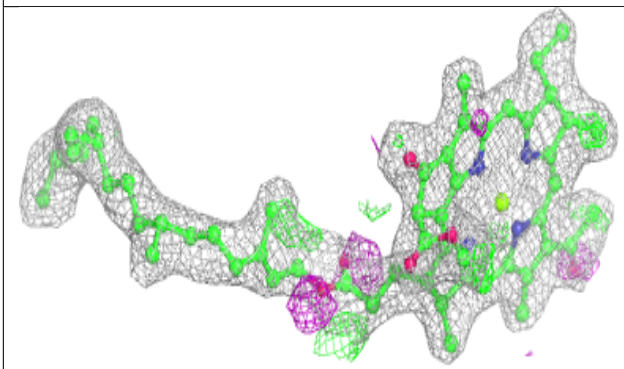


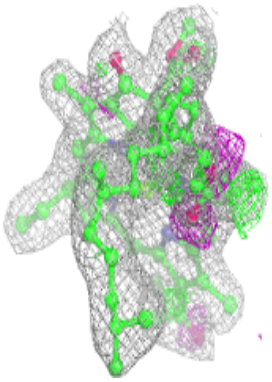


Electron density around BCL M 1003:

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

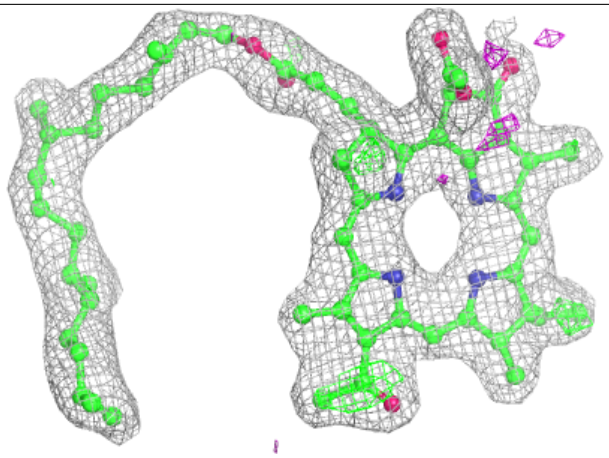


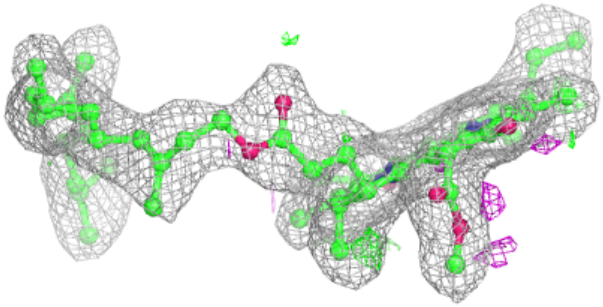


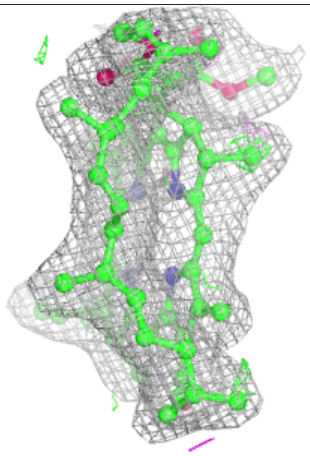


Electron density around BPH M 1006:

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

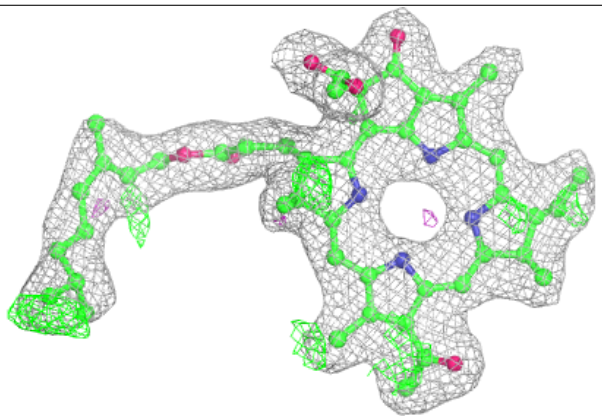


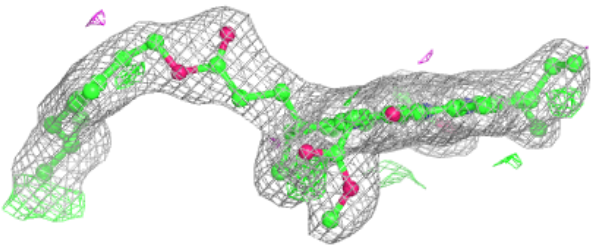




Electron density around BPH M 1005:

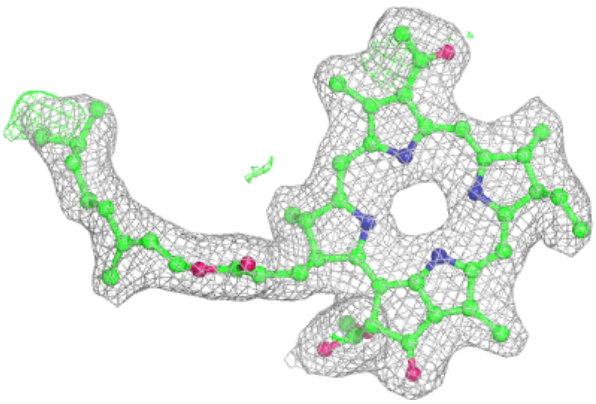
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

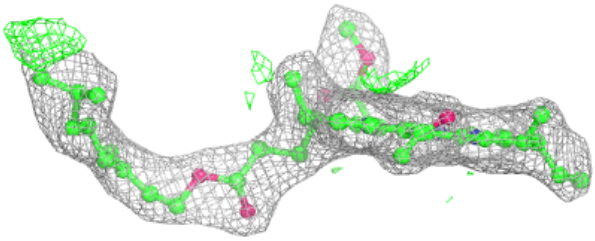


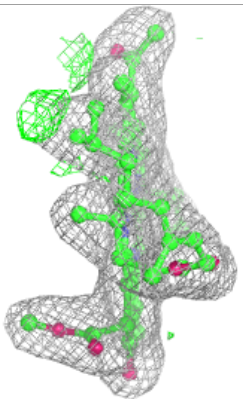


Electron density around BPH S 2005:

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

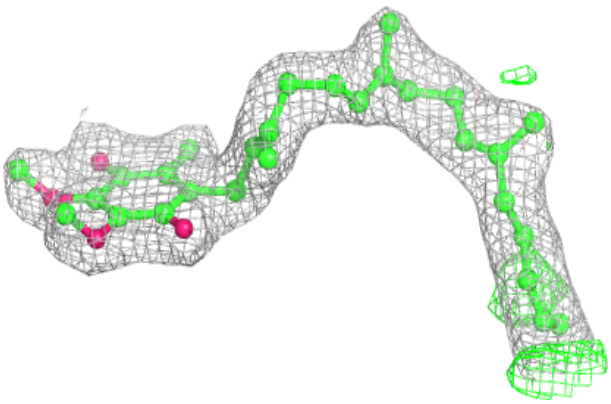


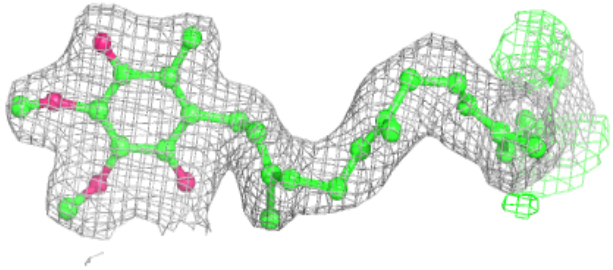


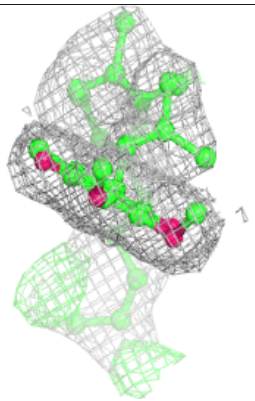


Electron density around U10 S 2008:

$2mF_o$-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.