wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2024 – 08:42 AM EDT

PDB ID	:	1PRC
Title	:	CRYSTALLOGRAPHIC REFINEMENT AT 2.3 ANGSTROMS RESOLUTION AND REFINED MODEL OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS
Authors	:	Deisenhofer, J.; Epp, O.; Miki, K.; Huber, R.; Michel, H.
Deposited on	:	1988-02-04
Resolution	:	2.30 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:

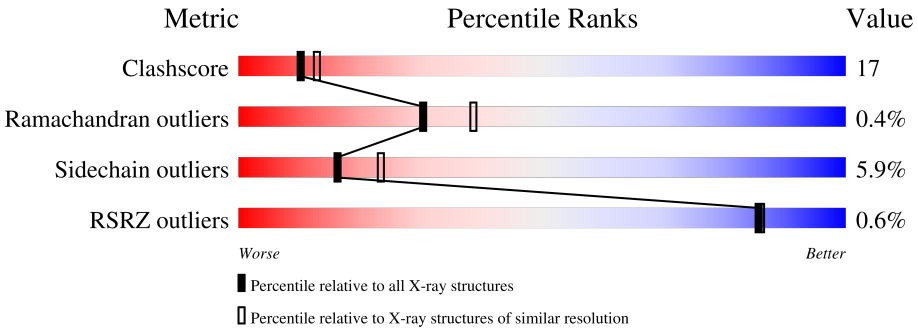
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 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))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	C	336	58% 35% 5%
2	L	273	65% 31%
3	M	323	66% 31%
4	H	258	3% 61% 32% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCB	L	602	X	-	-	-
6	BCB	L	604	X	-	-	-
6	BCB	M	601	X	-	-	-
6	BCB	M	603	X	-	-	-
8	UQ1	L	614	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10288 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	333	2603	1640	467	478	18	54	0	1

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	273	2171	1459	350	355	7	13	0	0

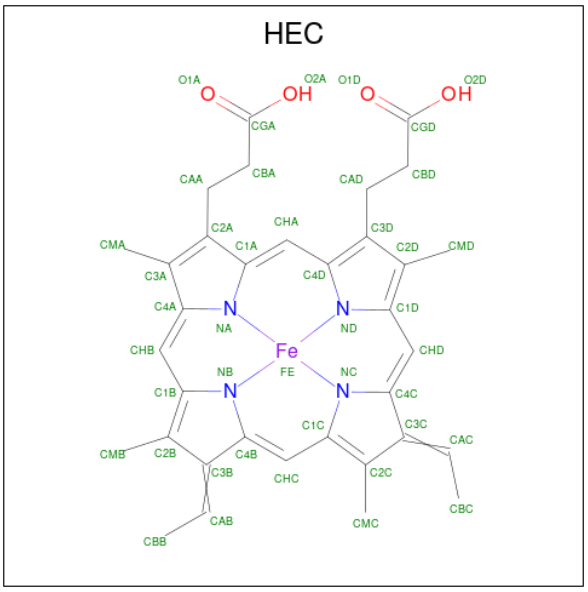
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	323	2555	1702	419	423	11	26	0	0

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

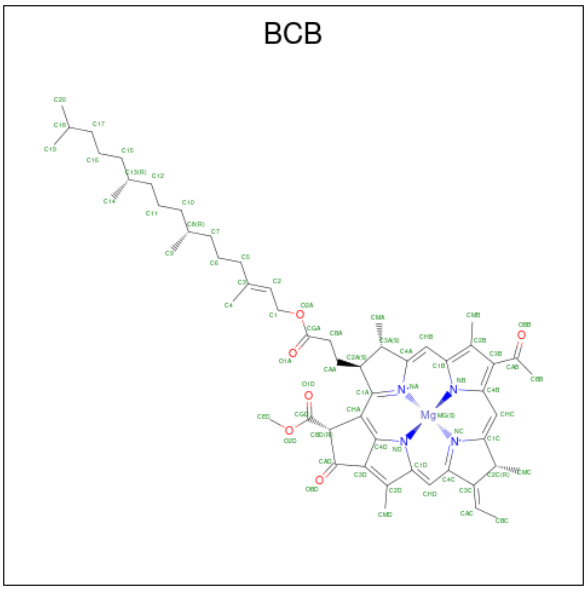
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2018	1292	344	380	2	106	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



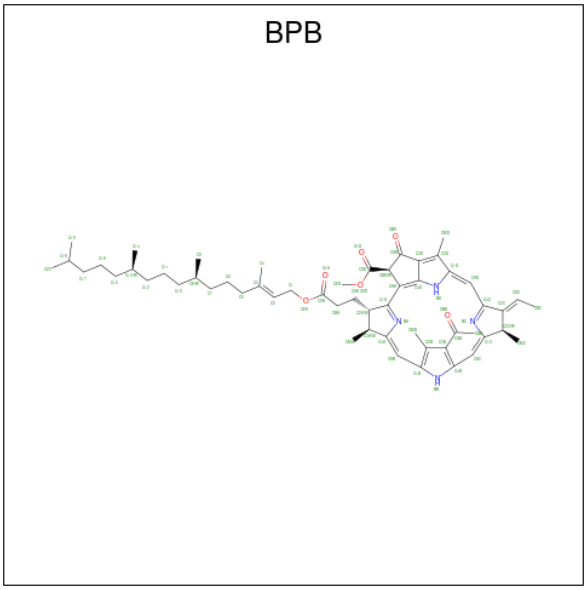
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



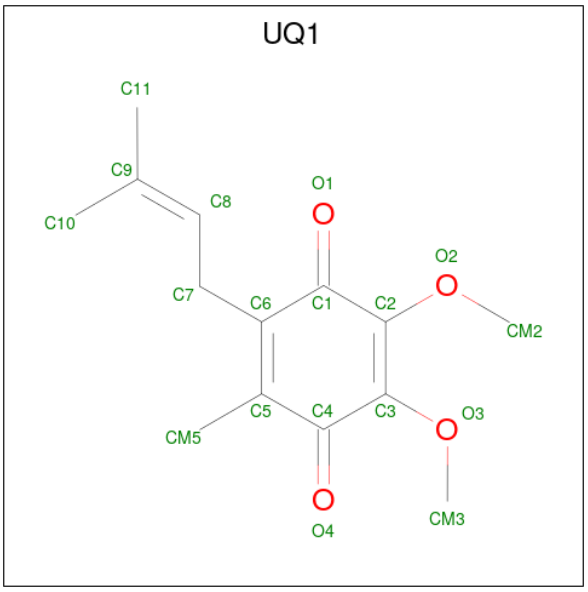
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	13	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



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

- Molecule 8 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).

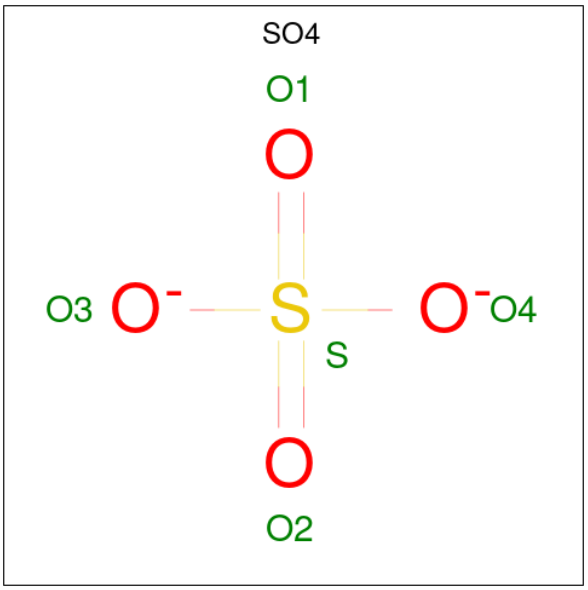


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 18 14 4	0	0

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

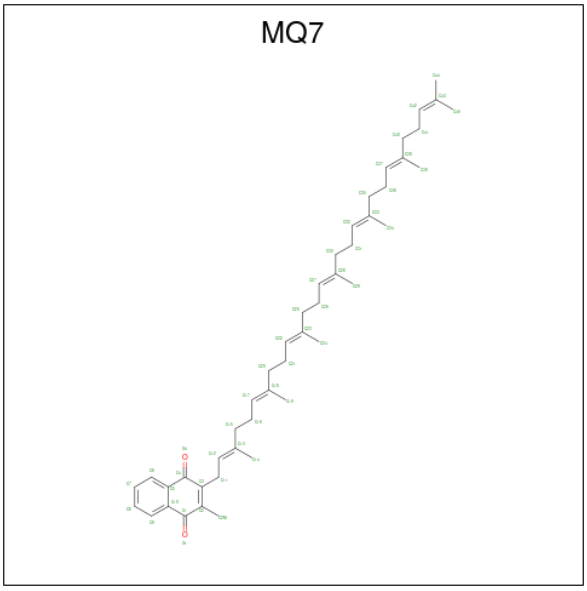
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



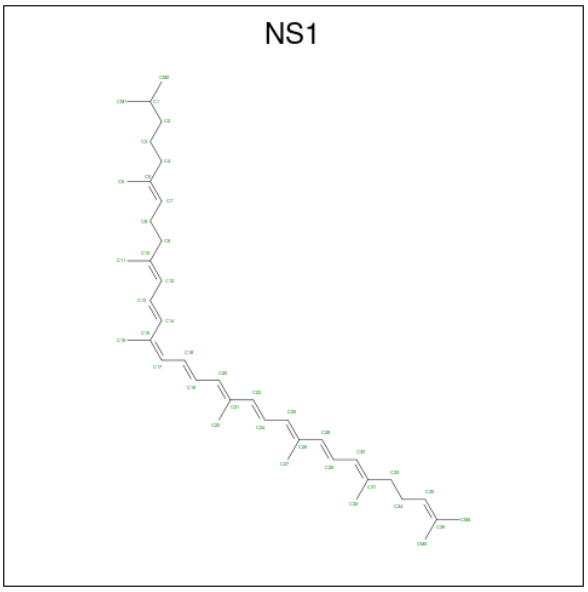
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



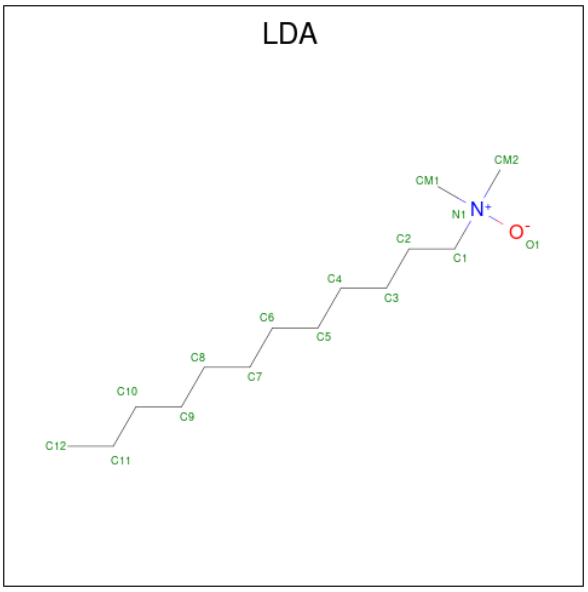
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 48 46 2	4	0

- Molecule 12 is 15-trans-1,2-dihydroneurosporene (three-letter code: NS1) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C 40 40	14	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C N O 16 14 1 1	0	0
13	H	1	Total C N O 16 14 1 1	6	0

- Molecule 14 is water.

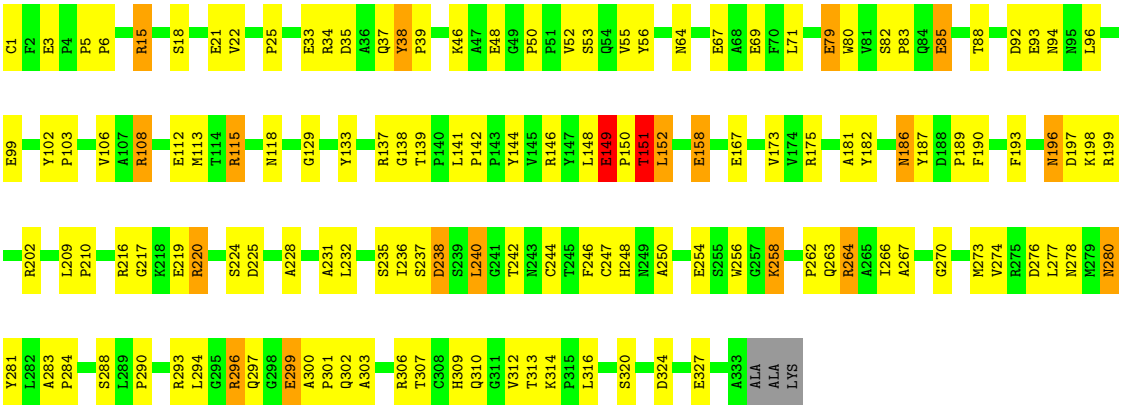
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	66	Total O 66 66	0	0
14	L	39	Total O 39 39	0	0
14	M	55	Total O 55 55	0	0
14	H	41	Total O 41 41	0	0

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.

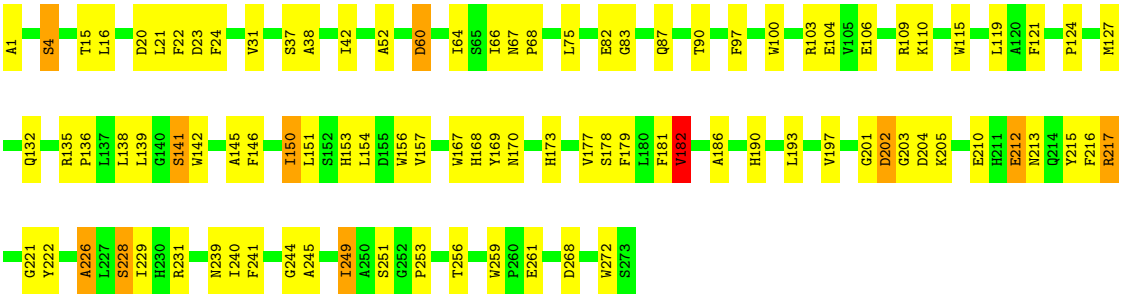
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



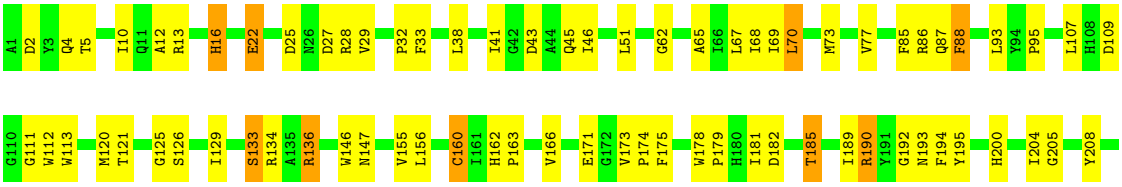
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

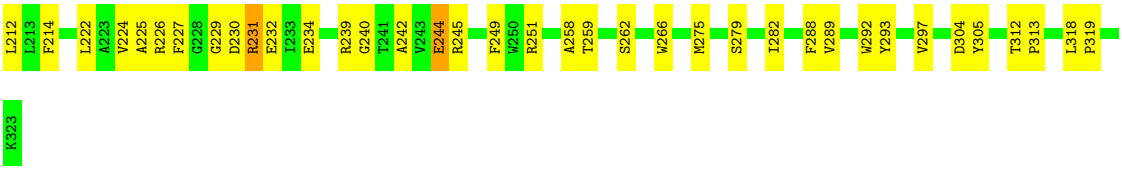
Chain L:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

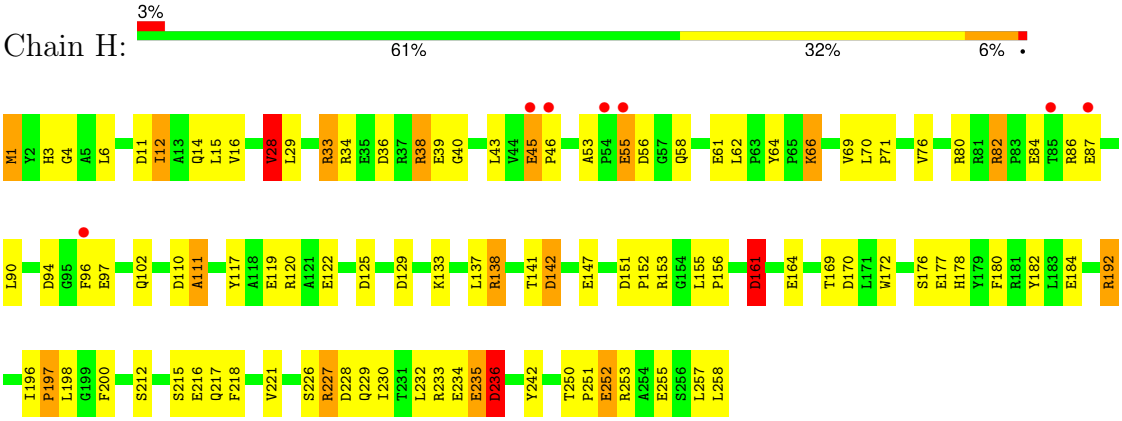
Chain M:





• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.99-2.30) 75.3 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.8	EDS
L-test for twinning[1]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]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: LDA, BPB, SO4, FE, BCB, UQ1, MQ7, FME, NS1, HEC

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	C	1.07	17/2670 (0.6%)	1.56	36/3639 (1.0%)
2	L	1.01	5/2259 (0.2%)	1.42	18/3084 (0.6%)
3	M	0.96	3/2659 (0.1%)	1.46	26/3637 (0.7%)
4	H	1.13	18/2055 (0.9%)	1.65	32/2807 (1.1%)
All	All	1.04	43/9643 (0.4%)	1.52	112/13167 (0.9%)

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	255	GLU	CD-OE2	9.06	1.35	1.25
1	C	299	GLU	CD-OE2	8.31	1.34	1.25
3	M	244	GLU	CD-OE2	8.03	1.34	1.25
2	L	261	GLU	CD-OE2	7.64	1.34	1.25
1	C	21	GLU	CD-OE2	7.48	1.33	1.25

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	38	ARG	NE-CZ-NH2	-18.45	111.08	120.30
3	M	245	ARG	NE-CZ-NH2	-11.45	114.57	120.30
3	M	25	ASP	CB-CG-OD2	-10.22	109.10	118.30
4	H	153	ARG	NE-CZ-NH2	-9.86	115.37	120.30
4	H	153	ARG	NE-CZ-NH1	9.74	125.17	120.30

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	C	2603	0	2579	82	0
2	L	2171	0	2098	83	0
3	M	2555	0	2452	78	0
4	H	2018	0	2020	58	0
5	C	172	0	122	20	0
6	L	132	0	144	22	0
6	M	132	0	144	22	0
7	L	65	0	74	8	0
7	M	65	0	74	11	0
8	L	18	0	18	10	0
9	M	1	0	0	0	0
10	H	15	0	0	0	0
10	M	20	0	0	0	0
11	M	48	0	64	1	0
12	M	40	0	59	4	0
13	H	16	0	31	2	0
13	M	16	0	31	1	0
14	C	66	0	0	5	0
14	H	41	0	0	1	0
14	L	39	0	0	3	0
14	M	55	0	0	3	0
All	All	10288	0	9910	327	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 17.

The worst 5 of 327 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)
3:M:120:MET:HE2	6:M:603:BCB:H172	1.41	1.00
3:M:136:ARG:HE	3:M:136:ARG:HA	1.31	0.93
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.90
7:L:606:BPB:HBBB	7:L:606:BPB:HHC	1.52	0.90
6:L:602:BCB:H61	6:L:604:BCB:HBB3	1.55	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	C	331/336 (98%)	306 (92%)	24 (7%)	1 (0%)	37 47
2	L	271/273 (99%)	252 (93%)	18 (7%)	1 (0%)	30 39
3	M	321/323 (99%)	300 (94%)	19 (6%)	2 (1%)	22 27
4	H	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	30 39
All	All	1179/1190 (99%)	1097 (93%)	77 (6%)	5 (0%)	30 39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	22	GLU
4	H	53	ALA
3	M	88	PHE
1	C	250	ALA
2	L	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	C	281/282 (100%)	261 (93%)	20 (7%)	12 17
2	L	218/218 (100%)	210 (96%)	8 (4%)	29 43
3	M	249/249 (100%)	235 (94%)	14 (6%)	17 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	212/212 (100%)	197 (93%)	15 (7%)	12 17
All	All	960/961 (100%)	903 (94%)	57 (6%)	16 23

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	16	HIS
4	H	236	ASP
3	M	147	ASN
4	H	217	GLN
4	H	169	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	239	ASN
4	H	3	HIS
4	H	229	GLN
4	H	225	GLN
2	L	144	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	H	1	4	8,9,10	0.96	1 (12%)	8,9,11	2.54	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	FME	CA-N	-2.45	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CA-N-CN	-4.40	116.05	122.82
4	H	1	FME	O1-CN-N	-4.10	114.72	125.32
4	H	1	FME	C-CA-N	3.01	115.31	109.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA
4	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	HEC	C	611	1	32,50,50	1.46	6 (18%)	30,82,82	1.86	7 (23%)
10	SO4	M	619	-	4,4,4	0.87	0	6,6,6	0.21	0
10	SO4	H	623	-	4,4,4	0.97	0	6,6,6	0.45	0
10	SO4	M	621	-	4,4,4	1.06	0	6,6,6	0.20	0
6	BCB	M	601	3	63,74,74	1.95	12 (19%)	72,115,115	1.56	14 (19%)
10	SO4	M	618	-	4,4,4	0.87	0	6,6,6	0.24	0
11	MQ7	M	608	-	49,49,49	1.44	5 (10%)	61,63,63	2.37	21 (34%)
6	BCB	L	602	2	63,74,74	1.88	6 (9%)	72,115,115	1.91	24 (33%)
7	BPB	M	605	-	49,70,70	1.59	10 (20%)	48,101,101	1.23	3 (6%)
10	SO4	H	617	-	4,4,4	0.94	0	6,6,6	0.18	0
13	LDA	H	616	-	13,15,15	2.84	2 (15%)	14,17,17	0.77	0
10	SO4	H	622	-	4,4,4	0.97	0	6,6,6	0.25	0
5	HEC	C	609	1	32,50,50	1.40	4 (12%)	30,82,82	2.38	9 (30%)
5	HEC	C	612	1	32,50,50	1.16	2 (6%)	30,82,82	2.26	7 (23%)
6	BCB	L	604	2	63,74,74	2.19	12 (19%)	72,115,115	1.73	17 (23%)
13	LDA	M	615	-	13,15,15	2.61	2 (15%)	14,17,17	1.77	5 (35%)
5	HEC	C	610	1	32,50,50	1.68	5 (15%)	30,82,82	2.25	3 (10%)
8	UQ1	L	614	-	18,18,18	0.80	1 (5%)	24,25,25	1.33	3 (12%)
12	NS1	M	613	-	39,39,39	2.09	11 (28%)	46,46,46	2.27	17 (36%)
6	BCB	M	603	3	63,74,74	2.21	17 (26%)	72,115,115	1.99	20 (27%)
7	BPB	L	606	-	49,70,70	1.71	7 (14%)	48,101,101	1.97	14 (29%)
10	SO4	M	620	-	4,4,4	0.71	0	6,6,6	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	611	1	-	4/10/54/54	-
5	HEC	C	609	1	-	4/10/54/54	-
5	HEC	C	612	1	-	1/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	L	602	2	3/3/21/26	11/37/137/137	-
6	BCB	L	604	2	3/3/21/26	4/37/137/137	-
12	NS1	M	613	-	-	15/43/43/43	-
7	BPB	M	605	-	-	10/37/105/105	0/5/6/6
13	LDA	M	615	-	-	7/13/13/13	-
6	BCB	M	603	3	3/3/21/26	7/37/137/137	-
5	HEC	C	610	1	-	2/10/54/54	-
6	BCB	M	601	3	1/1/21/26	2/37/137/137	-
8	UQ1	L	614	-	-	0/9/33/33	0/1/1/1
7	BPB	L	606	-	-	9/37/105/105	0/5/6/6
11	MQ7	M	608	-	-	4/41/61/61	0/2/2/2
13	LDA	H	616	-	-	1/13/13/13	-

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	603	BCB	CHC-C1C	10.19	1.42	1.33
6	L	602	BCB	CHC-C1C	9.76	1.42	1.33
6	L	604	BCB	CHC-C1C	9.56	1.42	1.33
6	M	601	BCB	CHC-C1C	8.61	1.41	1.33
13	M	615	LDA	O1-N1	-8.31	1.21	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	608	MQ7	C11-C3-C4	-9.46	108.61	118.58
5	C	610	HEC	CBC-CAC-C3C	-8.31	108.04	127.49
5	C	612	HEC	CBD-CAD-C3D	7.85	125.73	112.54
5	C	609	HEC	CBB-CAB-C3B	-7.62	109.66	127.49
5	C	610	HEC	CBB-CAB-C3B	-6.19	113.01	127.49

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	602	BCB	NA
6	L	602	BCB	NC
6	L	602	BCB	ND
6	L	604	BCB	NA
6	L	604	BCB	NC

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	611	HEC	C1A-C2A-CAA-CBA
5	C	611	HEC	C3A-C2A-CAA-CBA
6	M	601	BCB	C2C-C3C-CAC-CBC
6	M	603	BCB	CAD-CBD-CGD-O1D
6	M	603	BCB	CAD-CBD-CGD-O2D

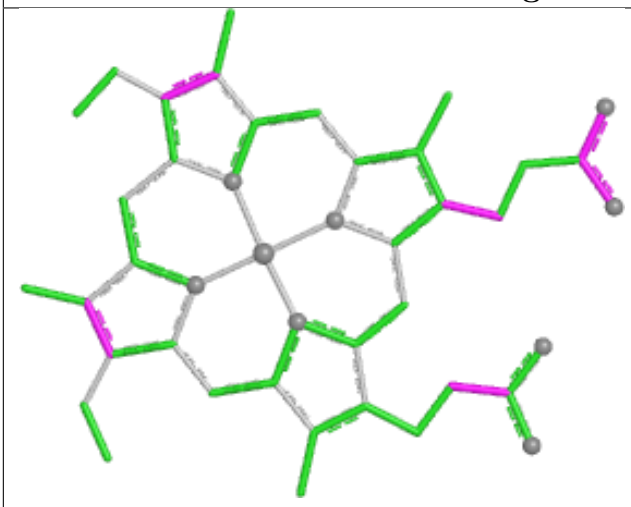
There are no ring outliers.

15 monomers are involved in 93 short contacts:

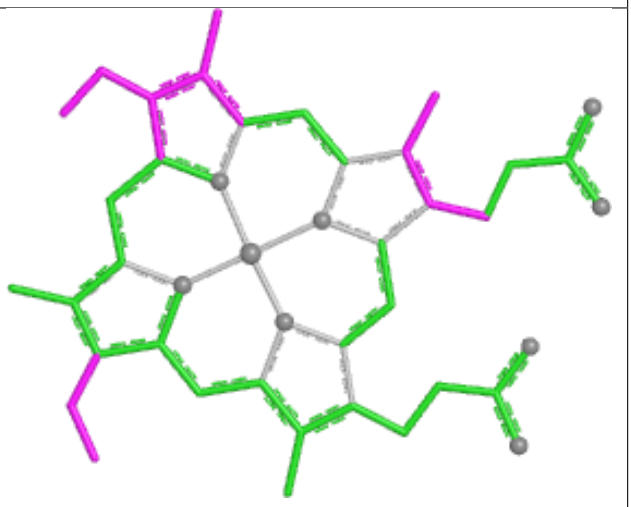
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	611	HEC	6	0
6	M	601	BCB	7	0
11	M	608	MQ7	1	0
6	L	602	BCB	16	0
7	M	605	BPB	11	0
13	H	616	LDA	2	0
5	C	609	HEC	6	0
5	C	612	HEC	3	0
6	L	604	BCB	11	0
13	M	615	LDA	1	0
5	C	610	HEC	5	0
8	L	614	UQ1	10	0
12	M	613	NS1	4	0
6	M	603	BCB	15	0
7	L	606	BPB	8	0

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.

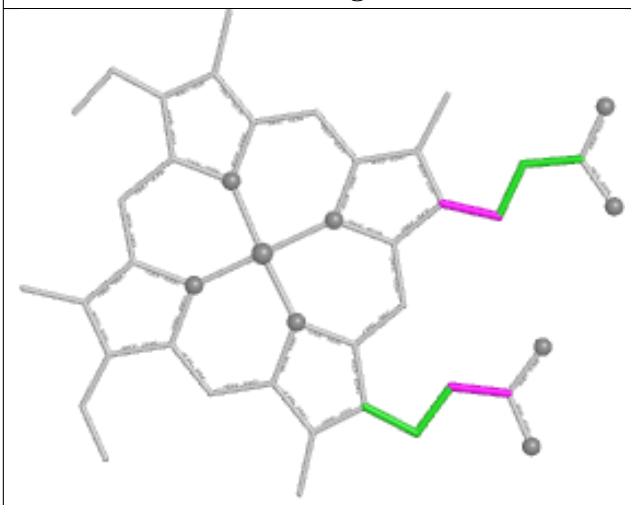
Ligand HEC C 611



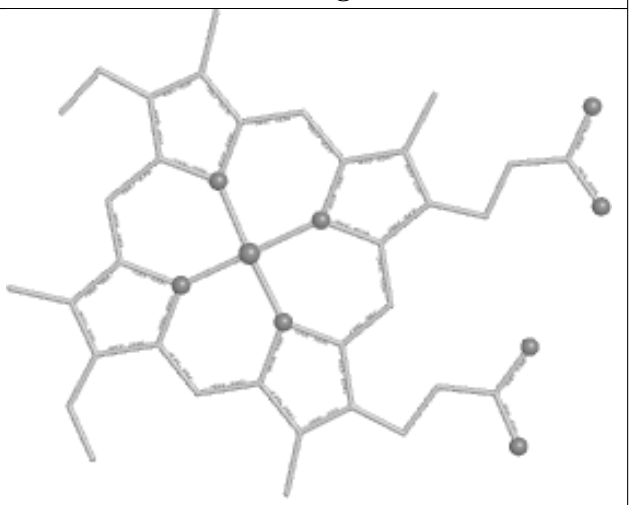
Bond lengths



Bond angles

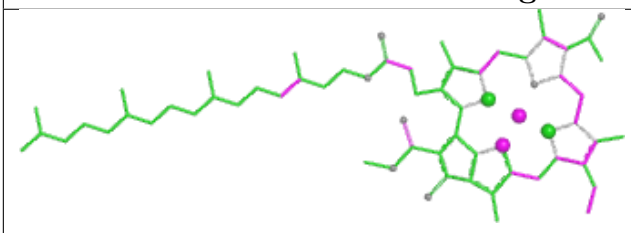


Torsions



Rings

Ligand BCB M 601



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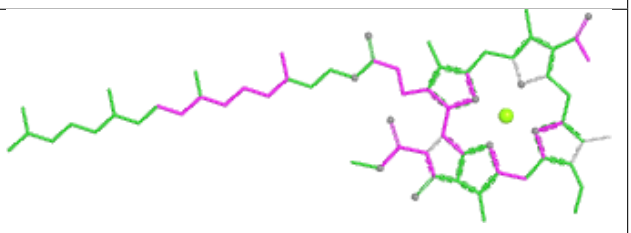

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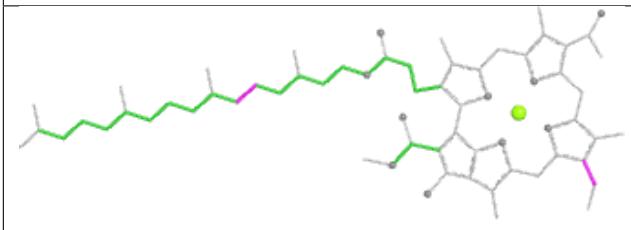

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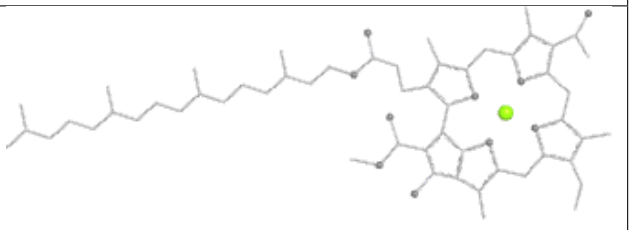
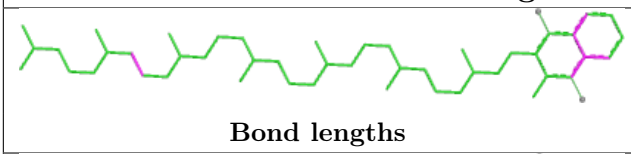


Rings

Ligand MQ7 M 608



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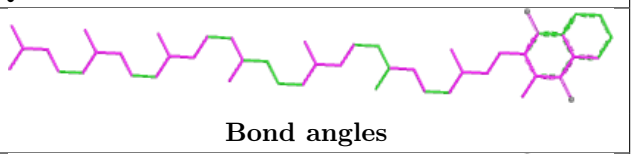
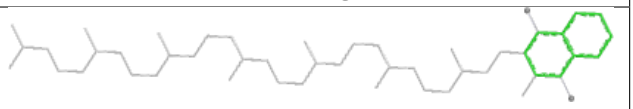


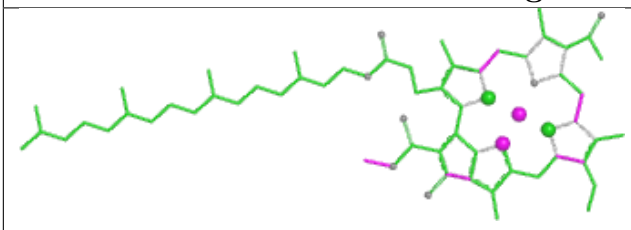
Bond angles

Torsions



Rings

Ligand BCB L 602



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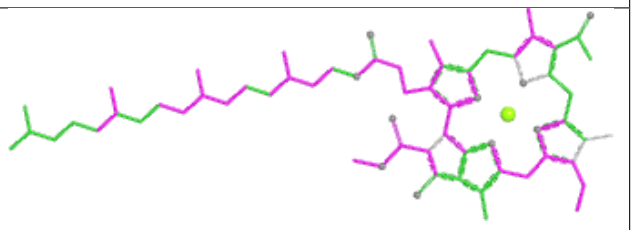
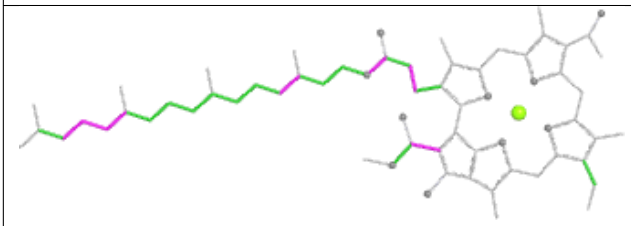
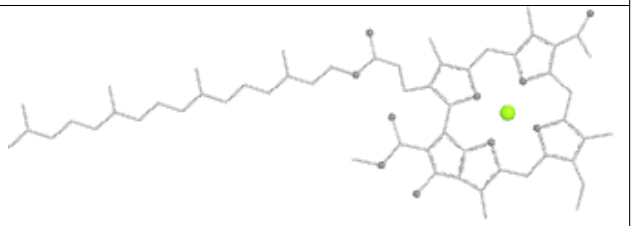


Bond angles

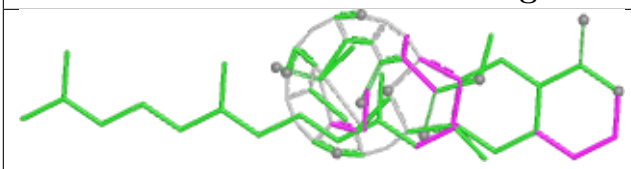


Torsions



Rings

Ligand BPB M 605



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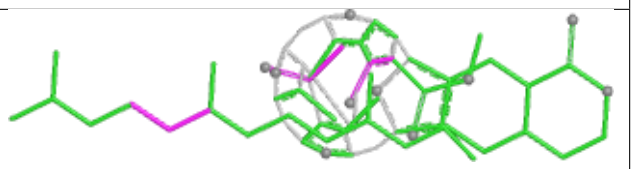
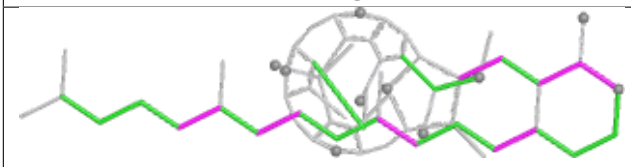


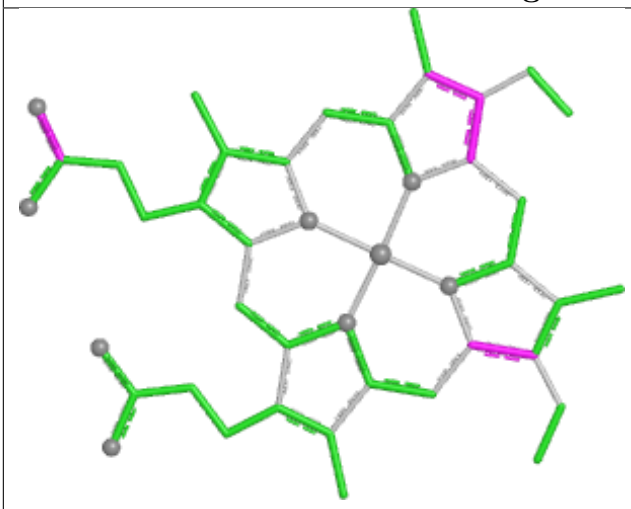
Bond angles



Torsions

Rings

Ligand HEC C 609



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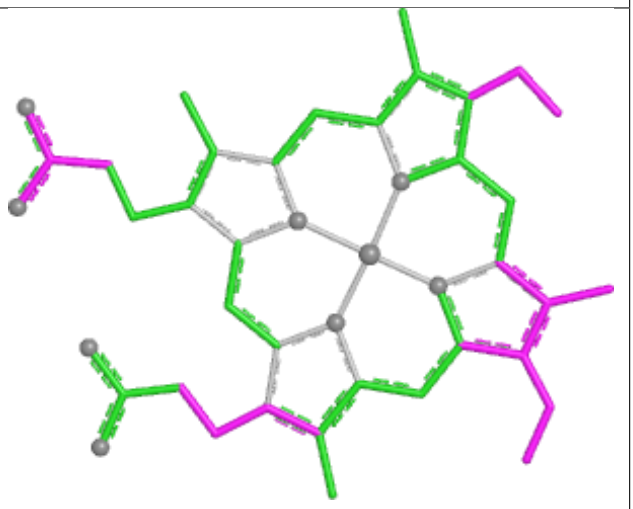
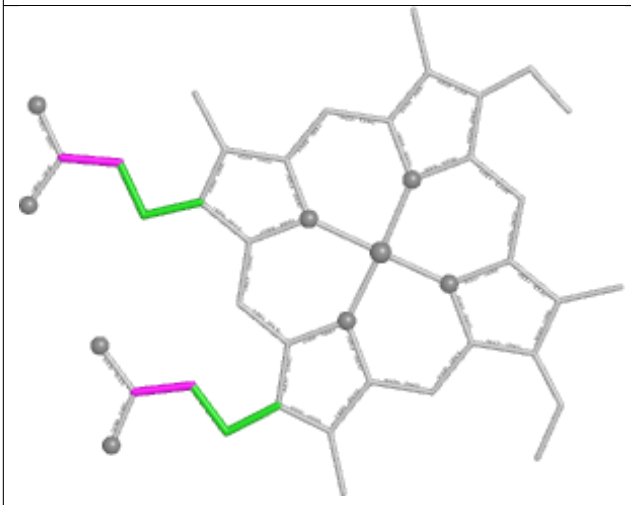
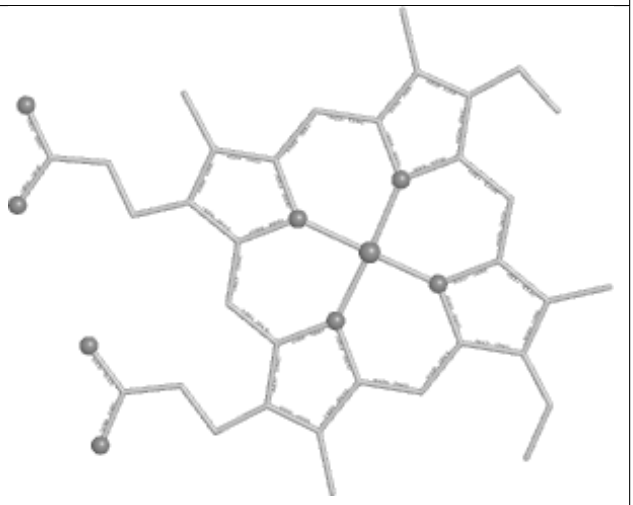


Bond angles

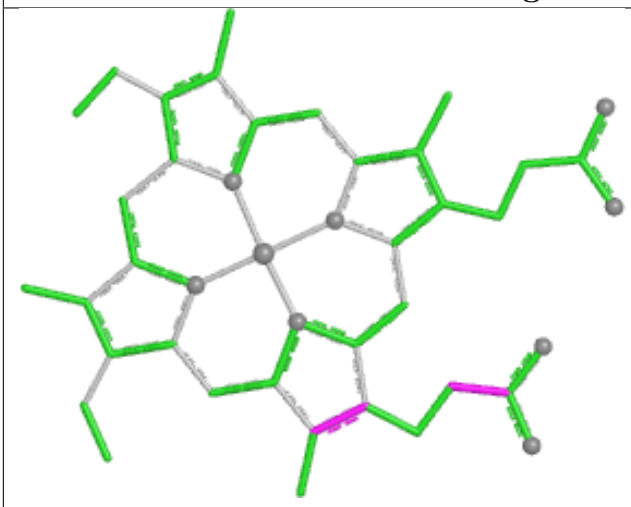


Torsions

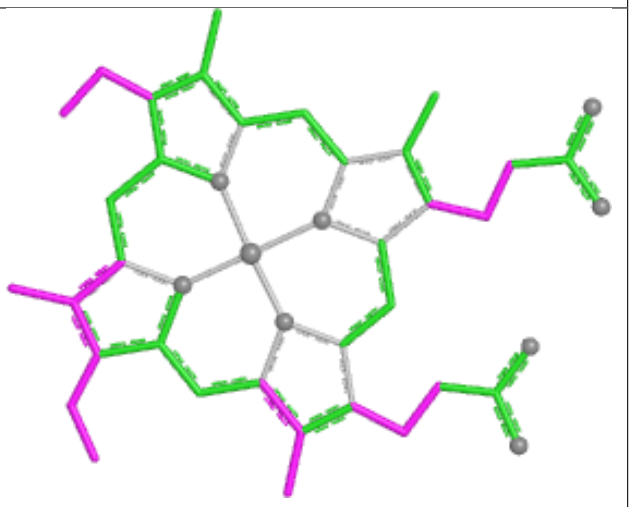


Rings

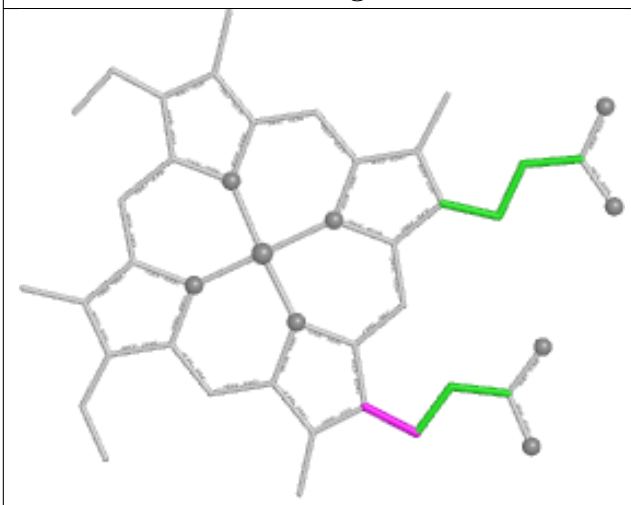
Ligand HEC C 612



Bond lengths



Bond angles



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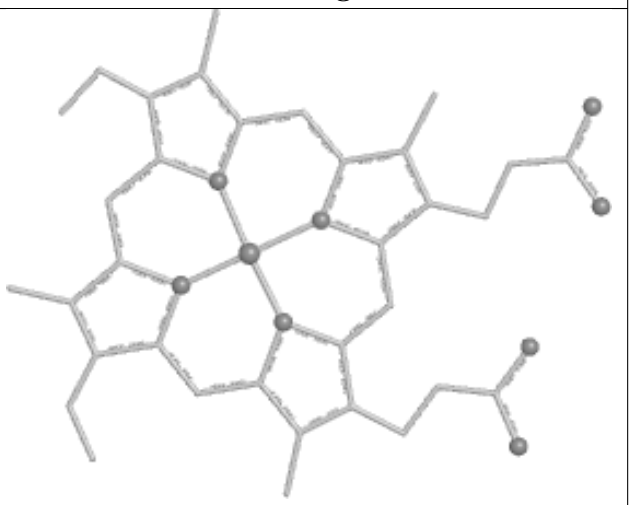
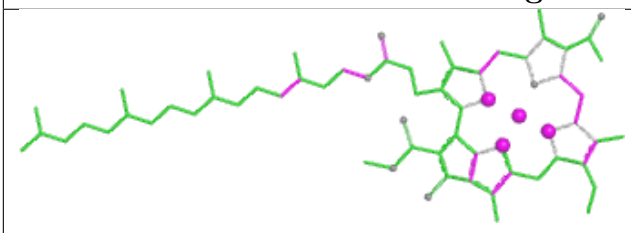
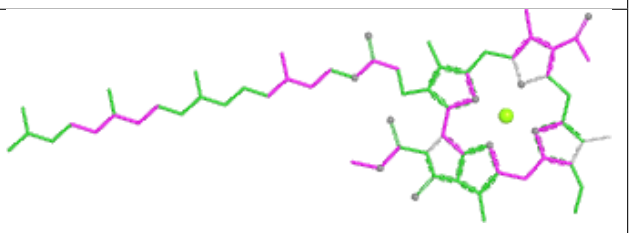


Rings

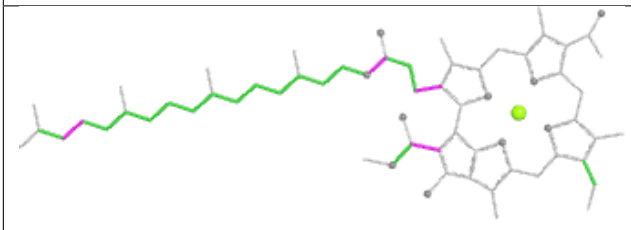
Ligand BCB L 604



Bond lengths



Bond angles



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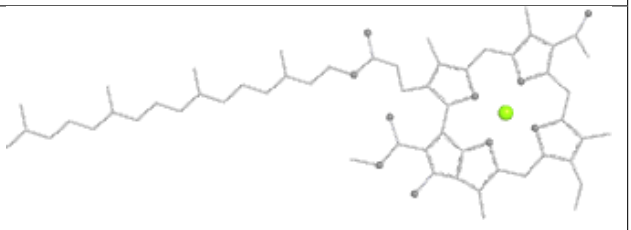
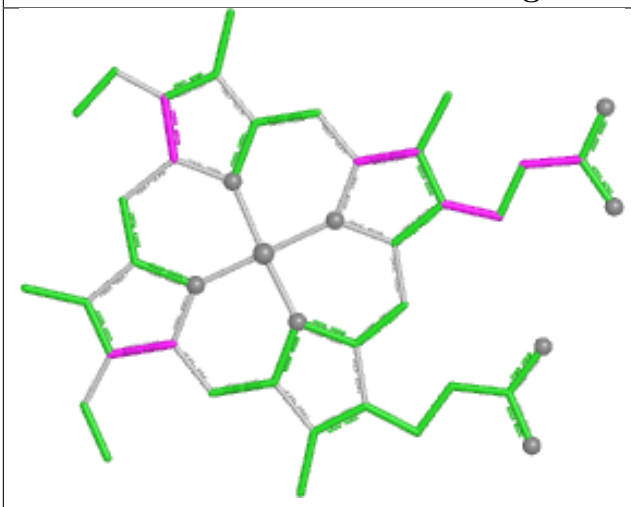


Rings

Ligand HEC C 610



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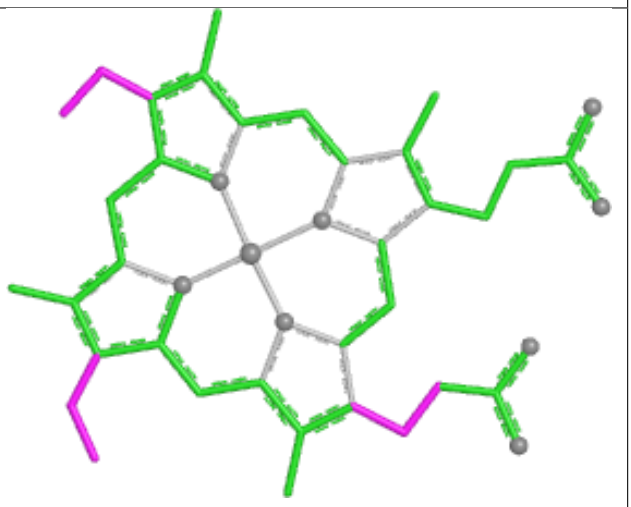
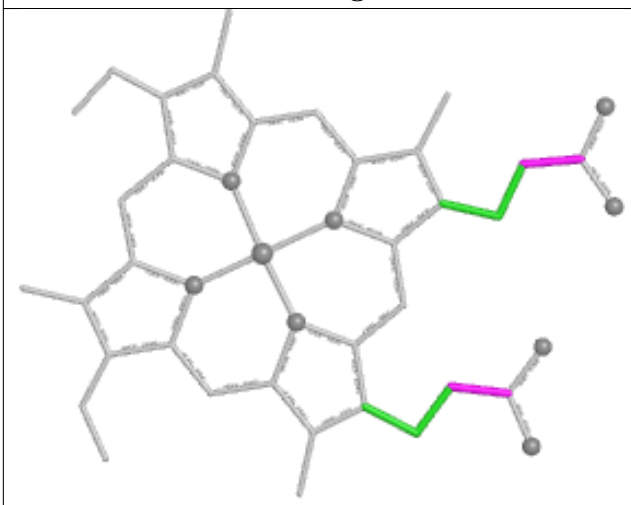
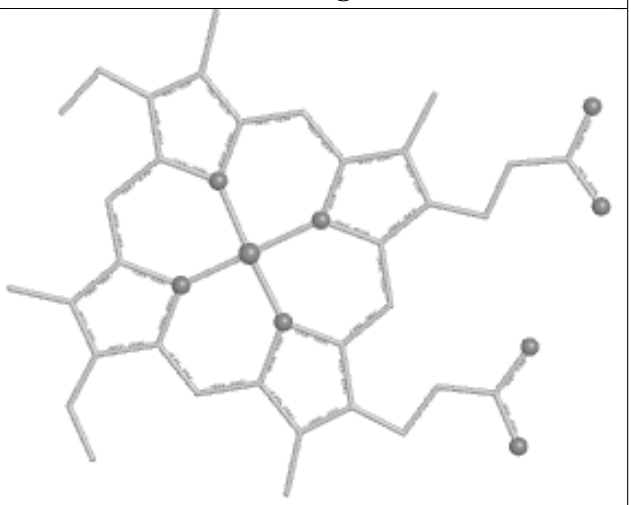


Bond angles

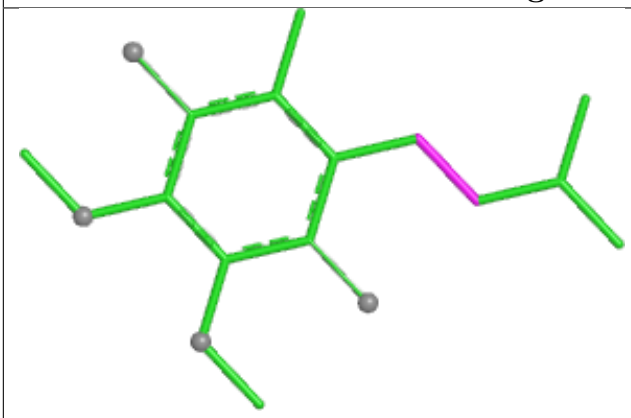


Torsions

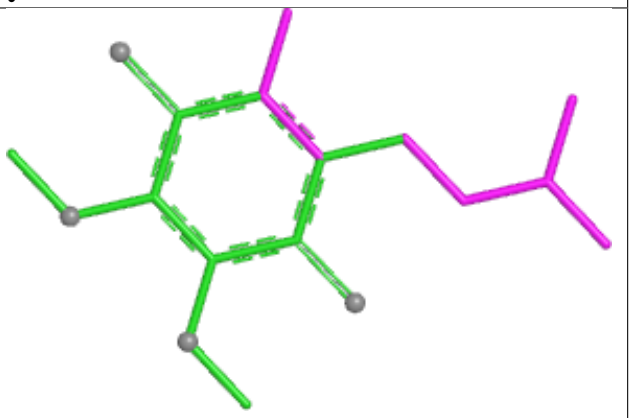


Rings

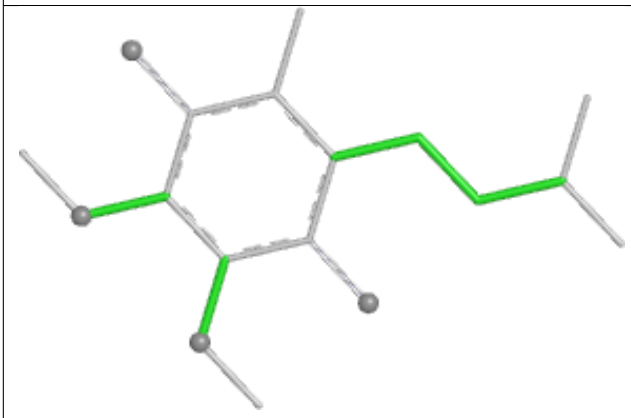
Ligand UQ1 L 614



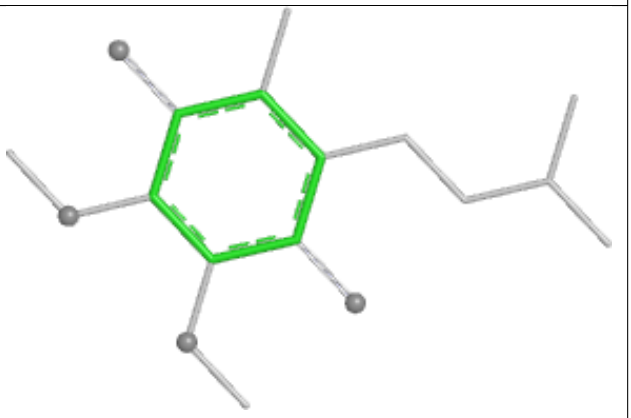
Bond lengths



Bond angles

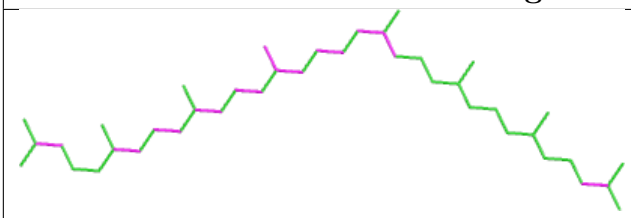


Torsions

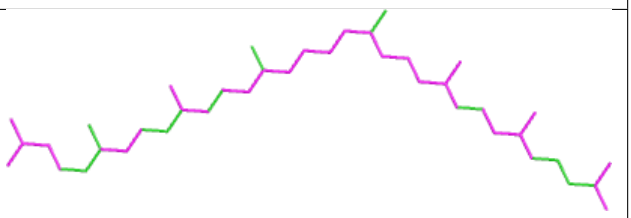


Rings

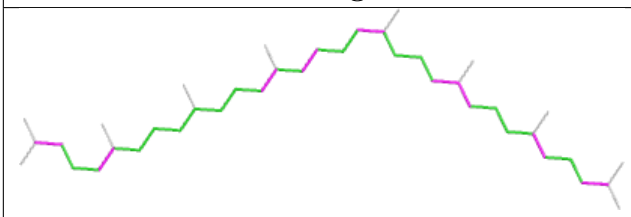
Ligand NS1 M 613



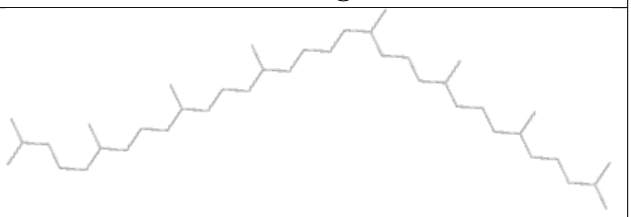
Bond lengths



Bond angles

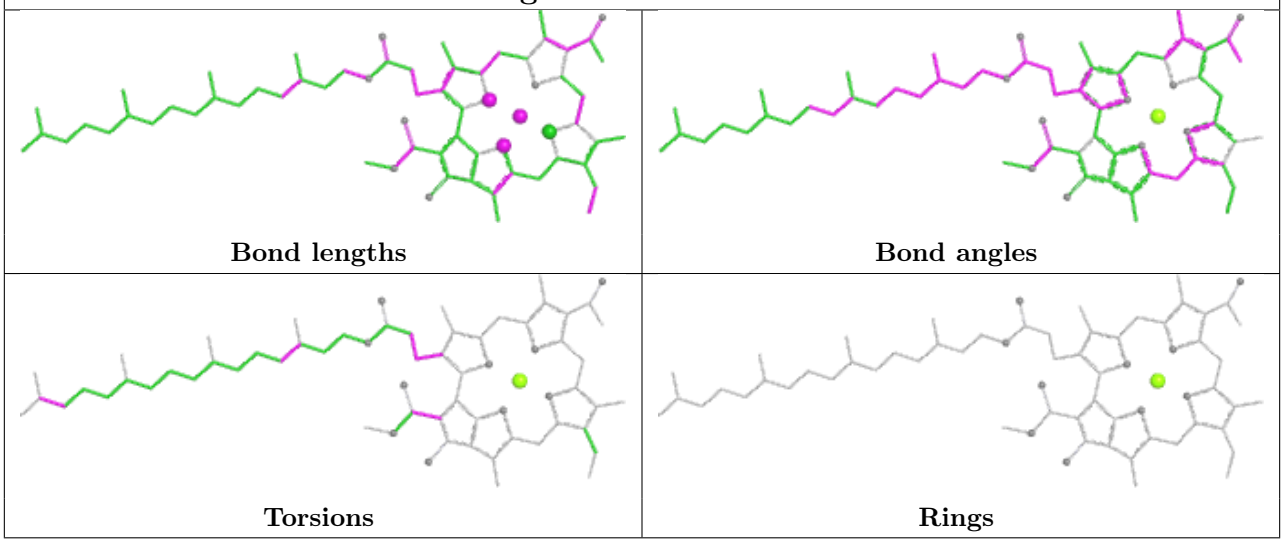


Torsions

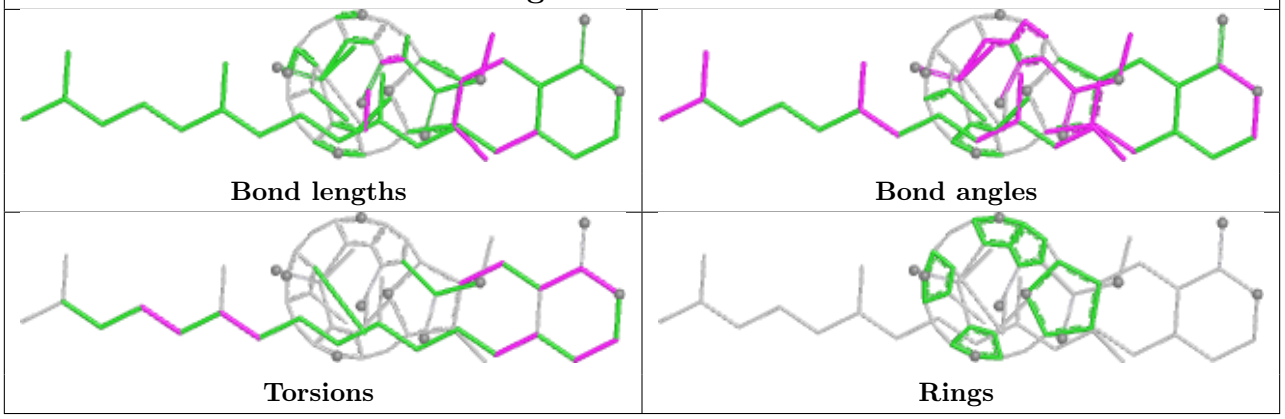


Rings

Ligand BCB M 603



Ligand BPB L 606



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	C	333/336 (99%)	-0.79	0	100	100	7, 21, 42, 73	17 (5%)
2	L	273/273 (100%)	-0.96	0	100	100	6, 16, 35, 47	6 (2%)
3	M	323/323 (100%)	-0.88	0	100	100	4, 18, 41, 58	8 (2%)
4	H	250/258 (96%)	-0.66	7 (2%)	55	56	8, 23, 46, 78	17 (6%)
All	All	1179/1190 (99%)	-0.83	7 (0%)	85	86	4, 19, 42, 78	48 (4%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.1
4	H	45	GLU	2.8
4	H	55	GLU	2.8
4	H	46	PRO	2.7
4	H	96	PHE	2.4

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

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
4	FME	H	1	10/11	0.96	0.07	21,32,41,45	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

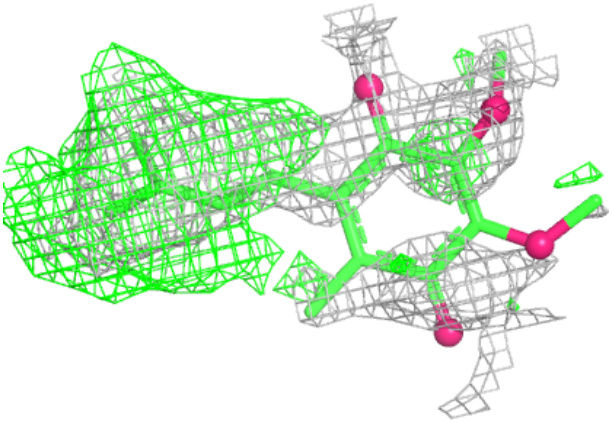
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

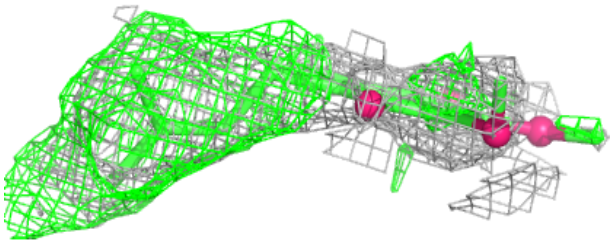
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UQ1	L	614	18/18	0.81	0.37	19,26,29,30	18
10	SO4	H	622	5/5	0.84	0.17	73,74,85,89	0
13	LDA	H	616	16/16	0.85	0.14	0,27,42,46	6
10	SO4	H	623	5/5	0.89	0.12	58,59,62,64	5
10	SO4	M	621	5/5	0.89	0.15	68,78,81,82	0
12	NS1	M	613	40/40	0.92	0.10	0,25,39,49	14
13	LDA	M	615	16/16	0.94	0.07	17,25,36,37	0
10	SO4	H	617	5/5	0.94	0.09	47,50,59,61	0
11	MQ7	M	608	48/48	0.97	0.05	0,10,20,32	4
6	BCB	M	601	66/66	0.97	0.06	0,12,40,61	13
10	SO4	M	619	5/5	0.97	0.10	39,43,50,59	0
7	BPB	M	605	65/65	0.97	0.07	0,21,62,71	7
7	BPB	L	606	65/65	0.98	0.04	3,10,19,22	0
6	BCB	L	604	66/66	0.98	0.04	3,10,27,35	0
6	BCB	L	602	66/66	0.98	0.04	3,10,19,21	0
6	BCB	M	603	66/66	0.98	0.05	3,10,20,21	0
5	HEC	C	611	43/43	0.99	0.04	5,16,25,38	0
10	SO4	M	618	5/5	0.99	0.04	22,23,35,37	0
5	HEC	C	612	43/43	0.99	0.05	3,22,31,46	0
10	SO4	M	620	5/5	0.99	0.04	31,34,40,41	0
5	HEC	C	609	43/43	0.99	0.06	7,22,32,36	0
5	HEC	C	610	43/43	0.99	0.05	3,21,29,37	0
9	FE	M	607	1/1	1.00	0.01	19,19,19,19	0

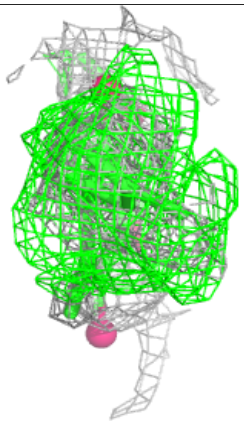
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ1 L 614:

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

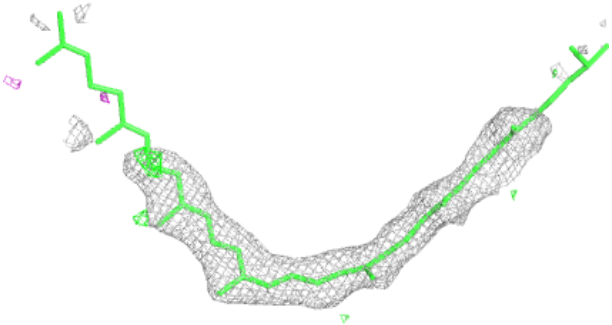


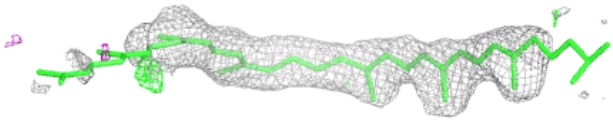


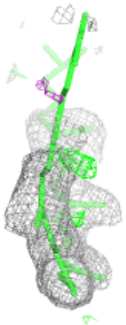


Electron density around NS1 M 613:

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

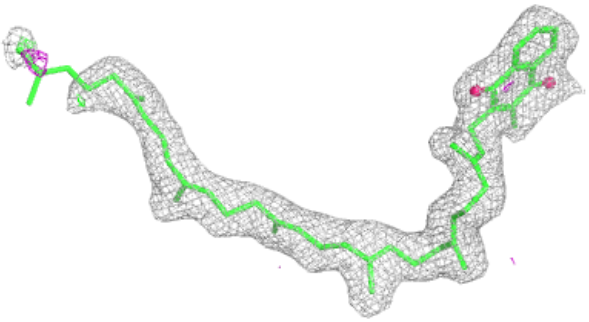


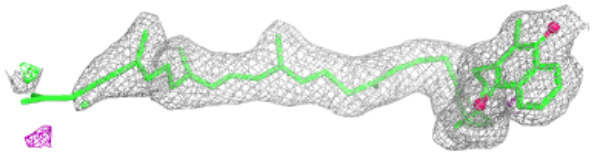


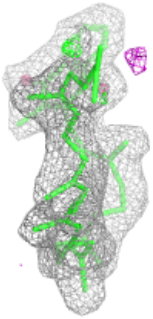


Electron density around MQ7 M 608:

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

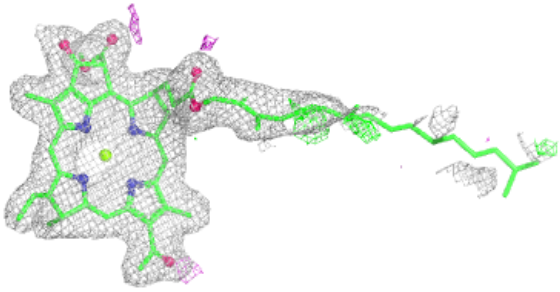


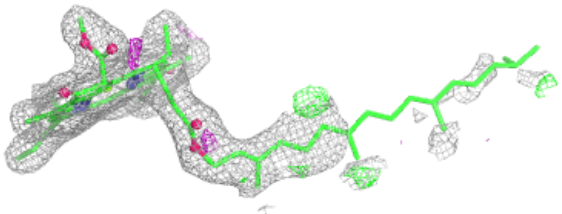


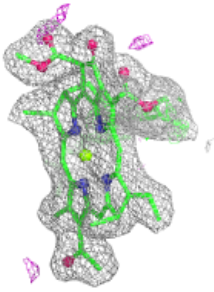


Electron density around BCB M 601:

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

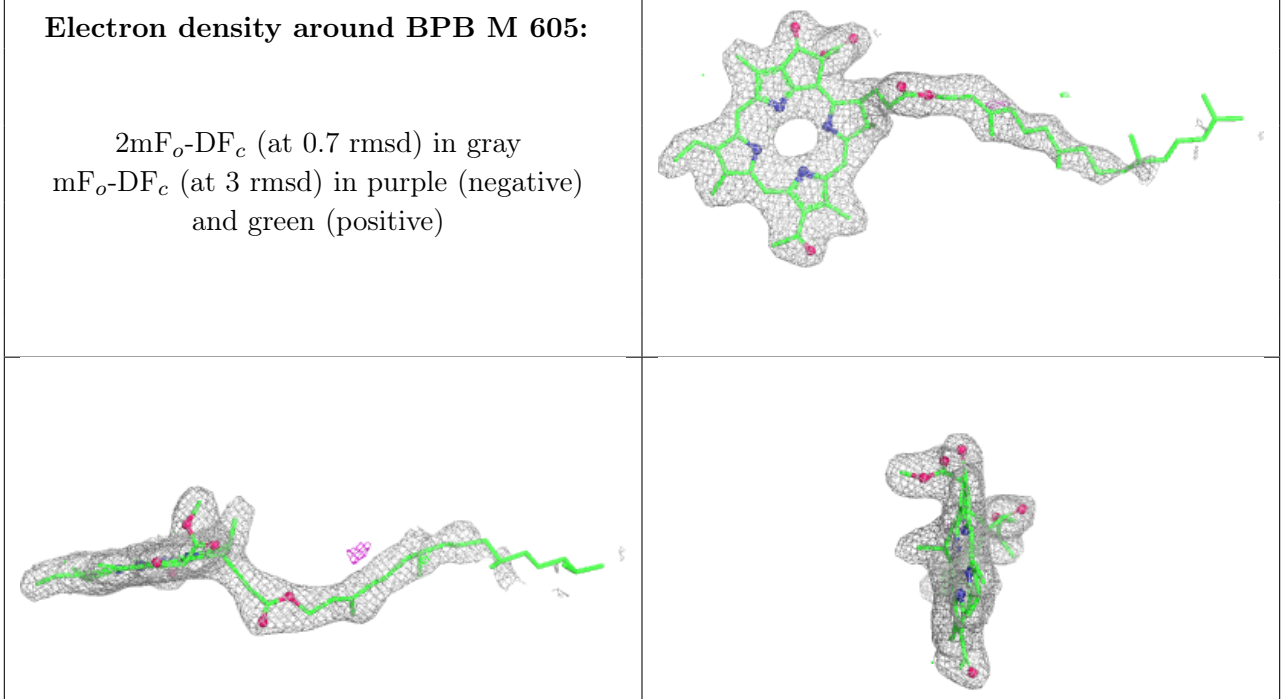






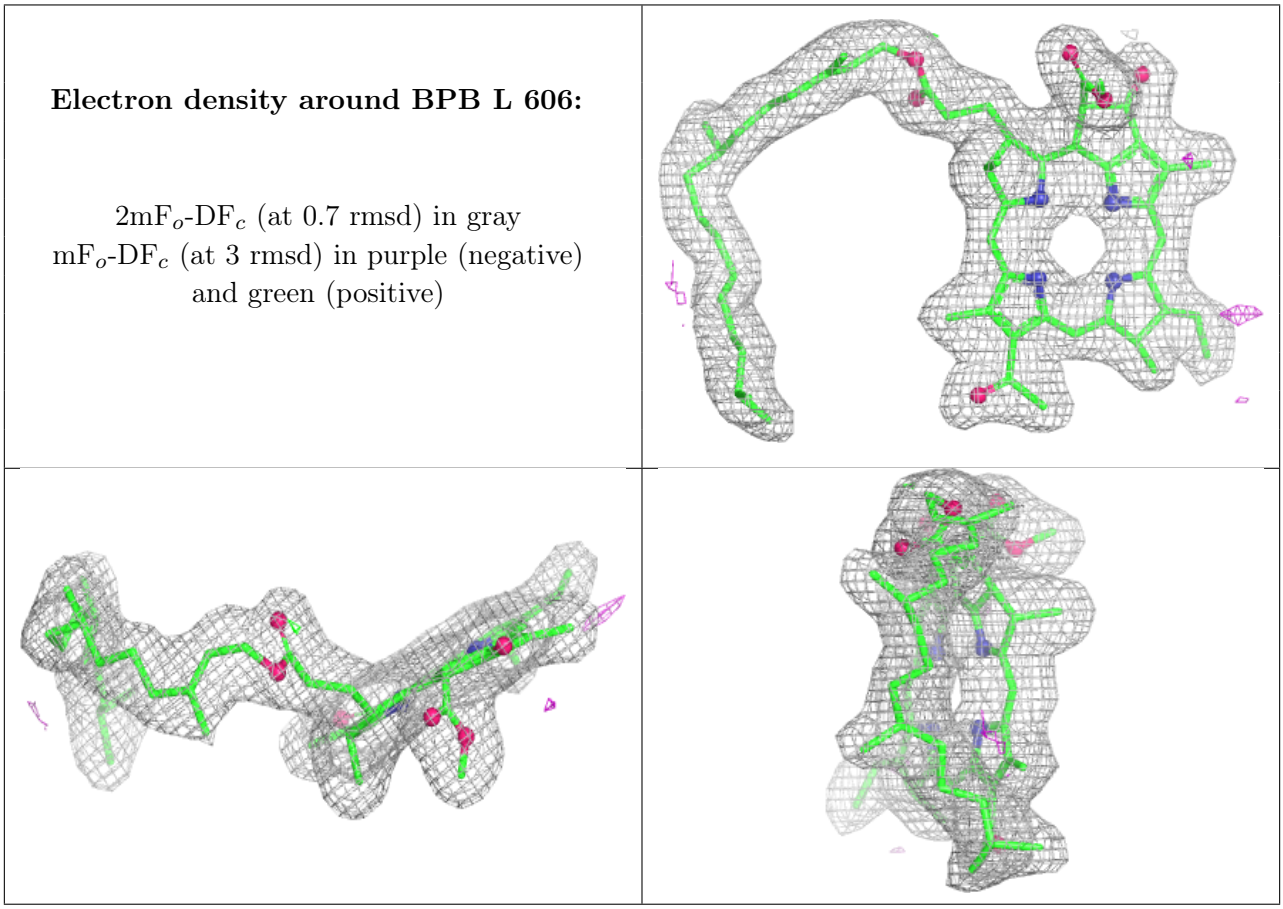
Electron density around BPB M 605:

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



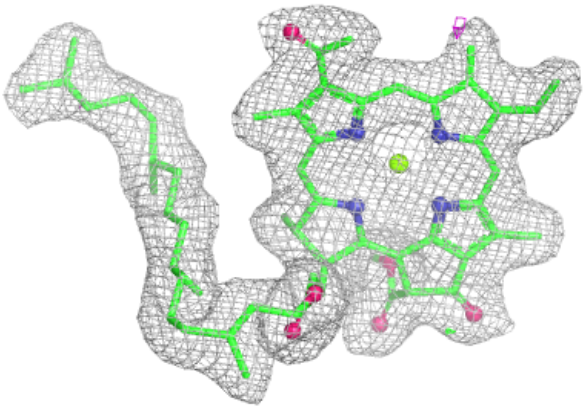
Electron density around BPB L 606:

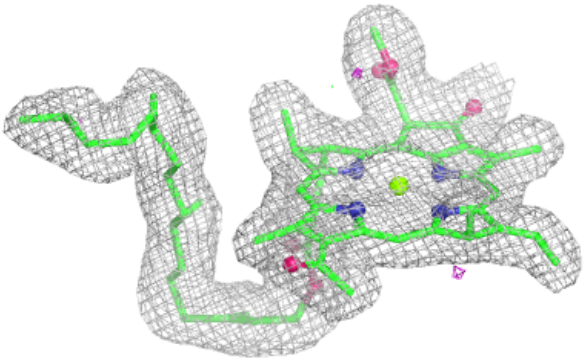
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

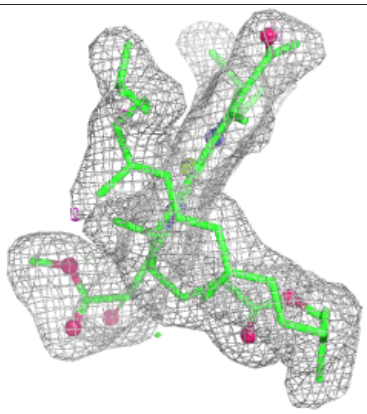


Electron density around BCB L 604:

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

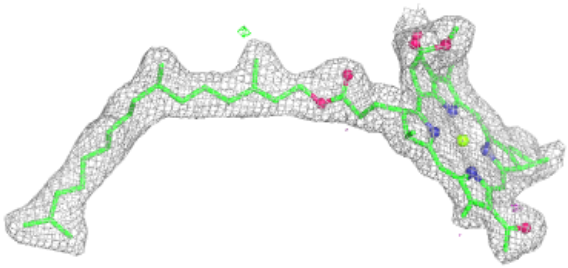


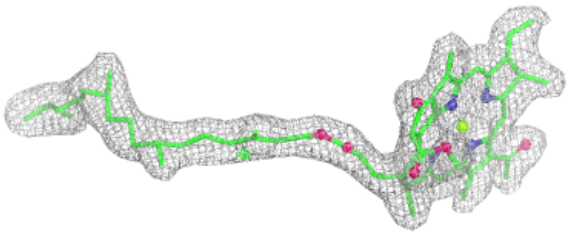


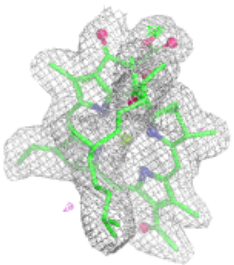


Electron density around BCB L 602:

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







Electron density around BCB M 603:

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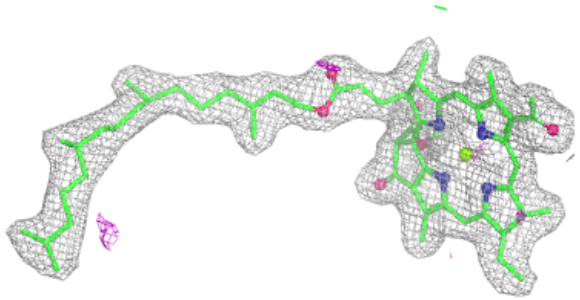
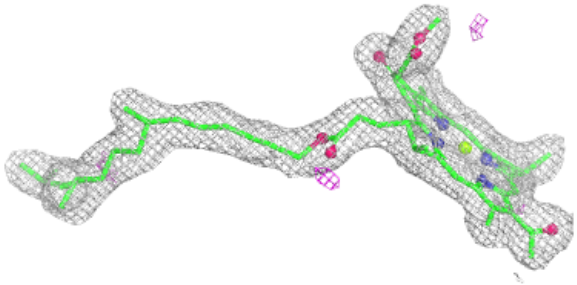
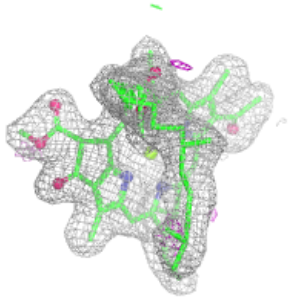
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

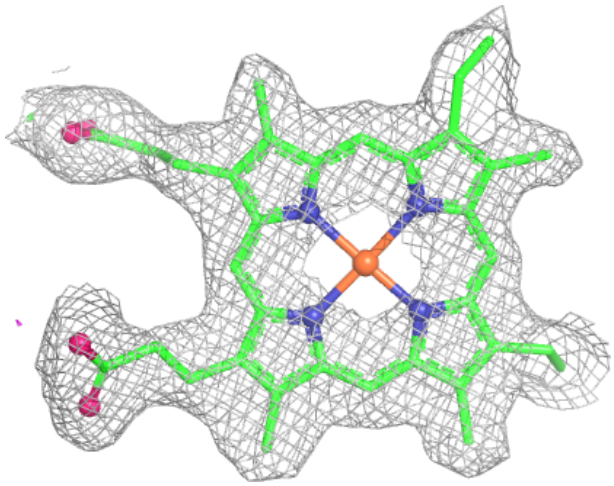


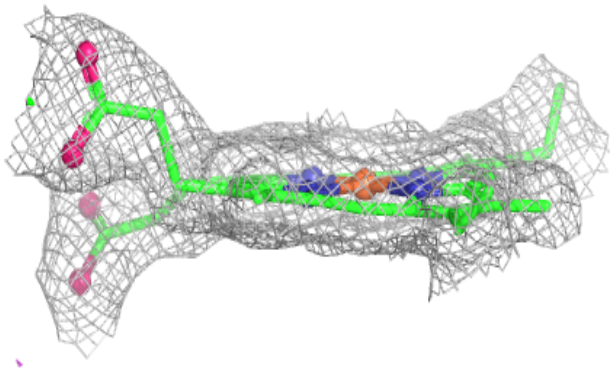


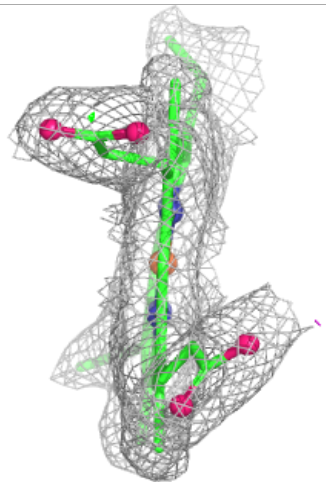


Electron density around HEC C 611:

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

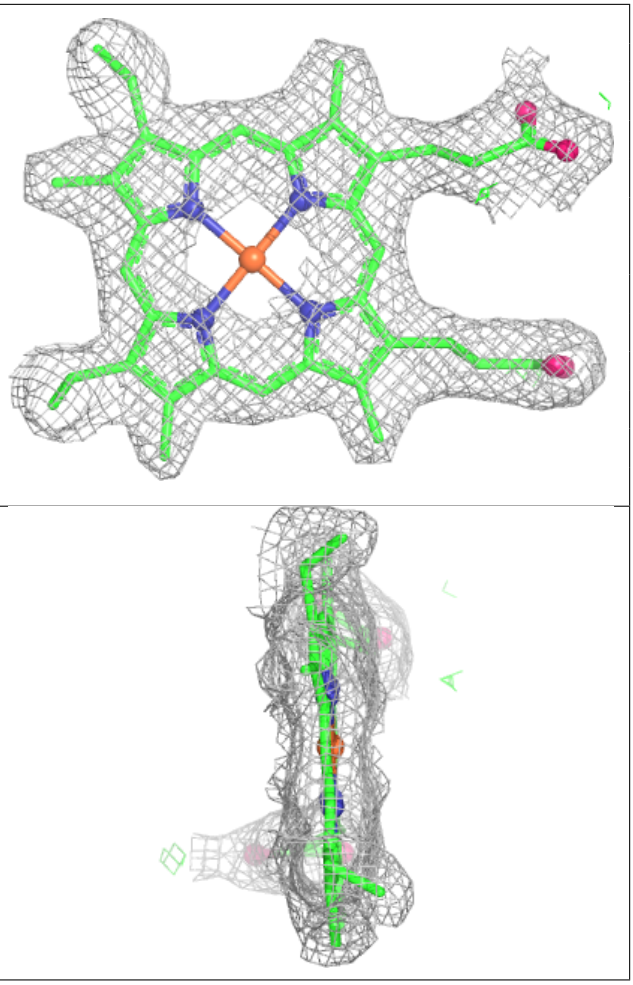






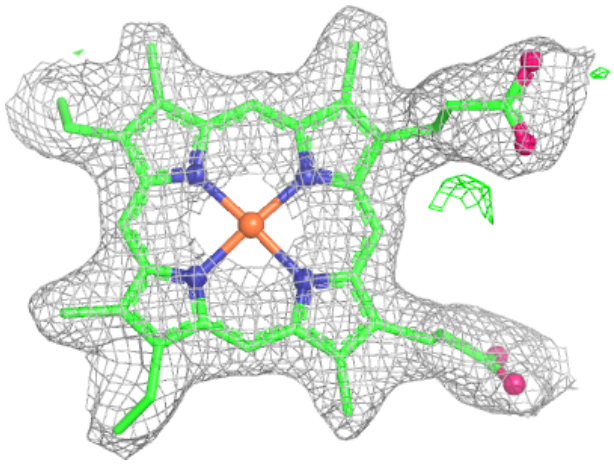
Electron density around HEC C 612:

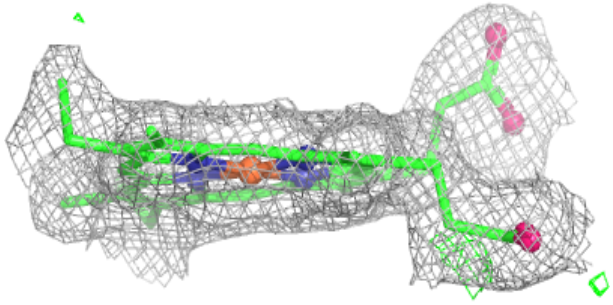
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

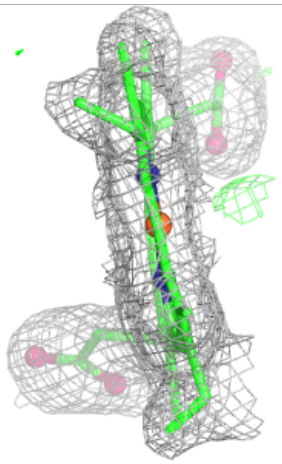


Electron density around HEC C 609:

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

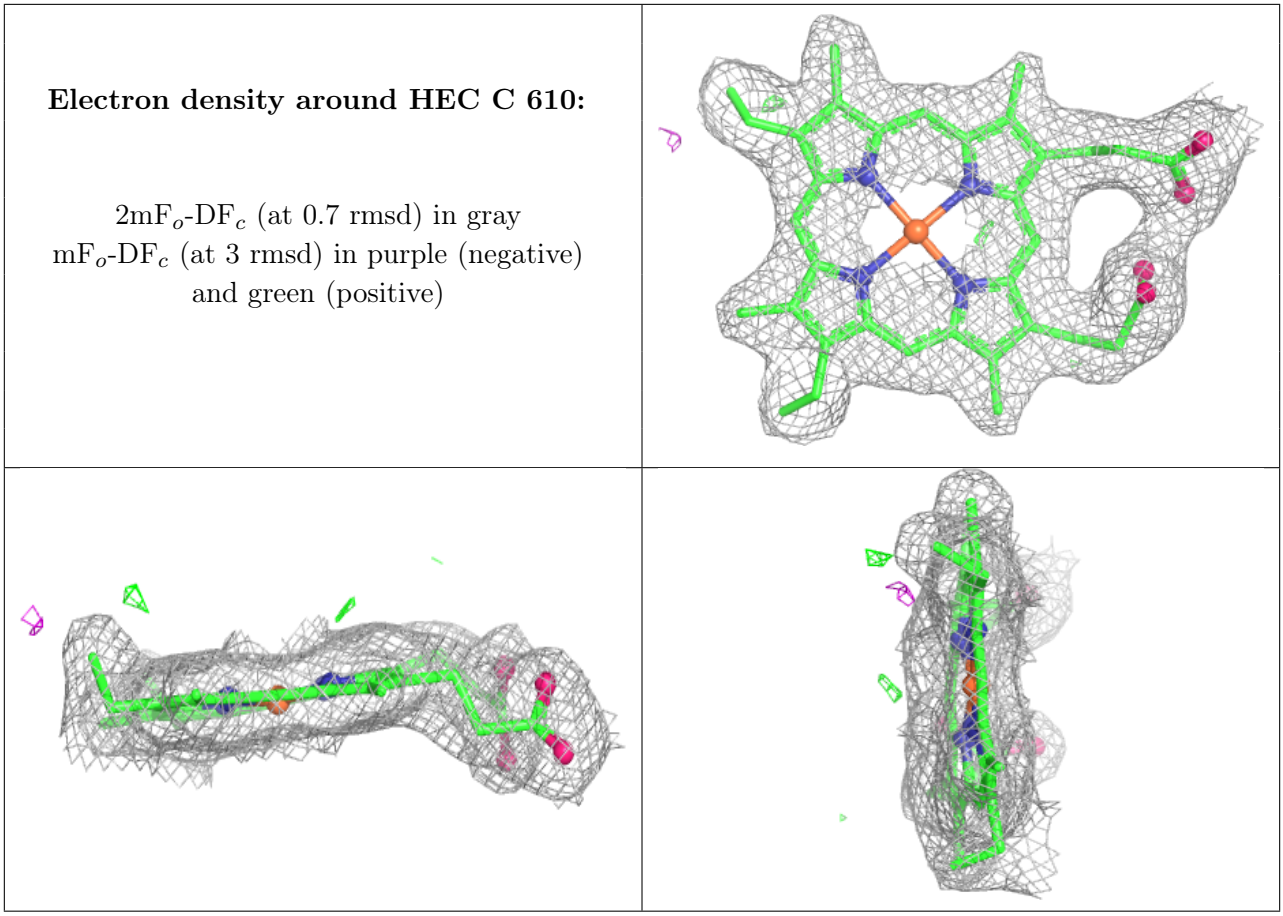






Electron density around HEC C 610:

$2mF_o$-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

There are no such residues in this entry.