wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 04:48 am BST

PDB ID	:	7Q7P / pdb_00007q7p
Title	:	LIPIDIC CUBIC PHASE SERIAL FEMTOSECOND CRYSTALLOGRAPHY STRUCTURE OF A PHOTOSYNTHETIC REACTION CENTRE
Authors	:	Baath, P.; Banacore, A.; Neutze, R.
Deposited on	:	2021-11-09
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:

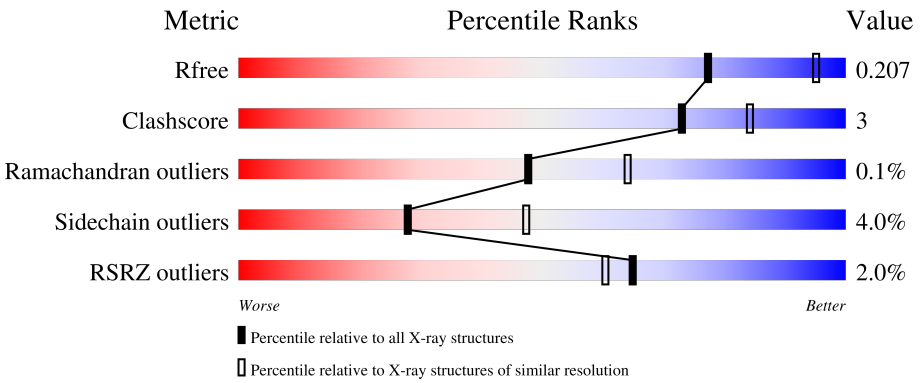
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	CCC	356	.% 86% 7% 7%
2	HHH	258	5% 82% 13% • •
3	LLL	273	2% 92% 7% •
4	MMM	323	.% 93% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BCB	LLL	301	X	-	-	-
10	BCB	LLL	302	X	-	-	-
10	BCB	MMM	403	X	-	-	-
10	BCB	MMM	404	X	-	-	-
11	BPB	LLL	303	X	-	-	-
11	BPB	MMM	405	X	-	-	-
5	HEC	CCC	401	X	-	-	-
5	HEC	CCC	402	X	-	-	-
5	HEC	CCC	403	X	-	-	-
5	HEC	CCC	404	X	-	-	-
6	DGA	CCC	405	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 10442 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 cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CCC	332	2618	1649	471	480	18	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	HHH	247	1941	1242	332	365	2	0	0	0

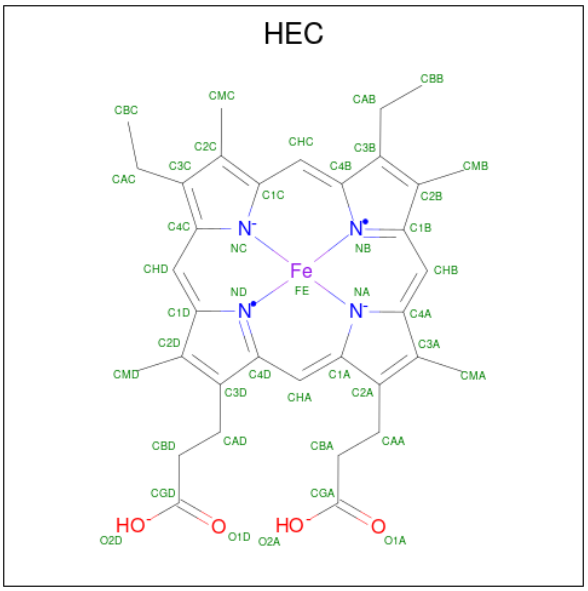
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	LLL	273	2172	1460	350	355	7	0	1	0

- Molecule 4 is a protein called Reaction center protein M chain.

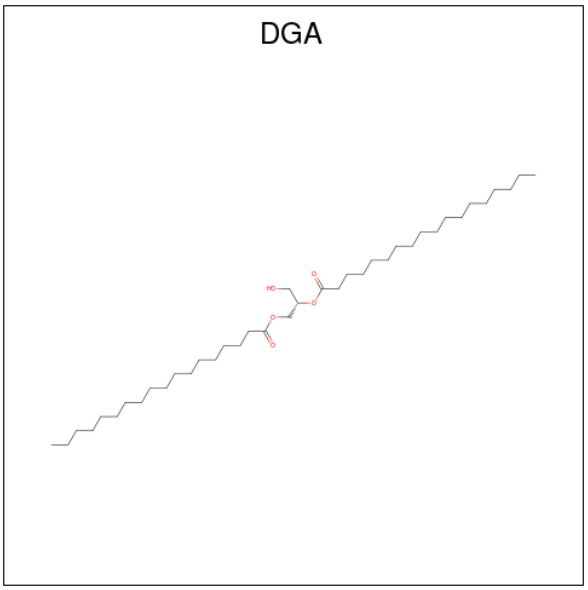
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	MMM	323	2555	1702	419	423	11	0	0	0

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



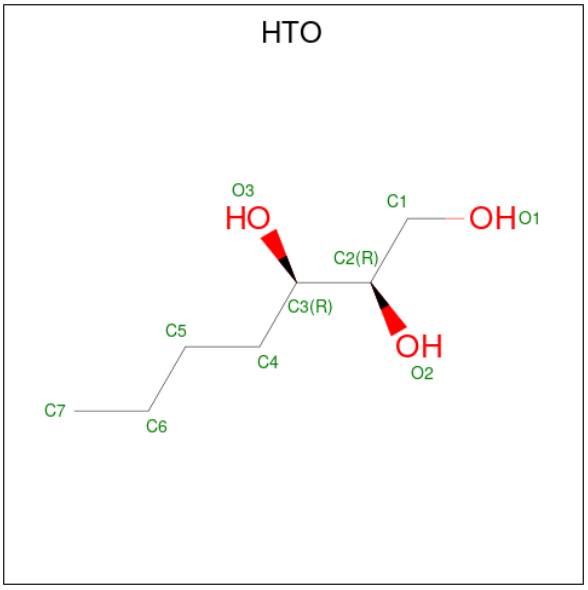
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	CCC	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	CCC	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	CCC	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	CCC	1	43	34	1	4	4	0	0

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



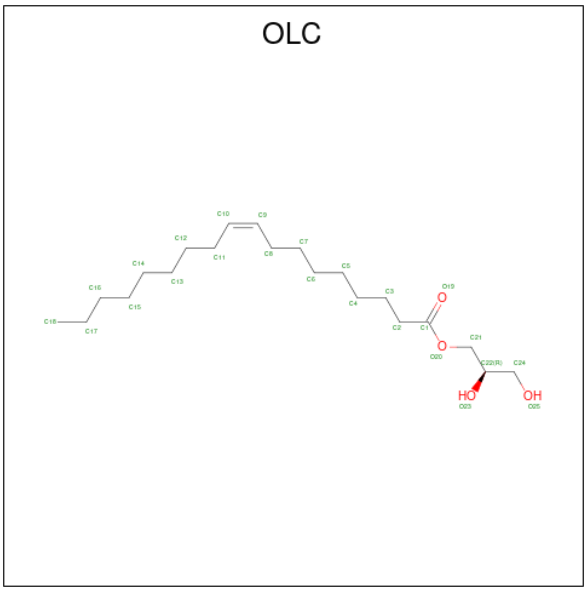
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	CCC	1	44	39	5	41	0

- Molecule 7 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



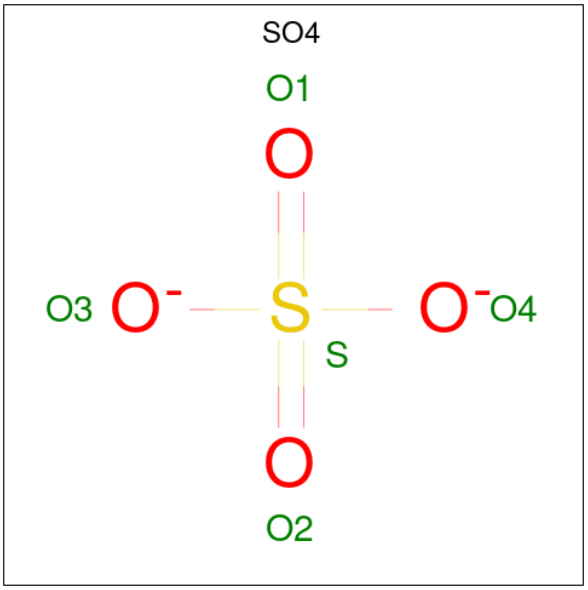
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	HHH	1	10	7	3	0	0
7	LLL	1	10	7	3	0	0
7	LLL	1	10	7	3	0	0
7	LLL	1	10	7	3	0	0
7	LLL	1	10	7	3	0	0
7	LLL	1	10	7	3	0	0
7	MMM	1	10	7	3	0	0
7	MMM	1	10	7	3	0	0
7	MMM	1	10	7	3	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	HHH	1	25	21	4	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	HHH	1	5	4	1	0	0
9	LLL	1	Total	O	S	0	0
			5	4	1		
9	MMM	1	Total	O	S	0	0
			5	4	1		

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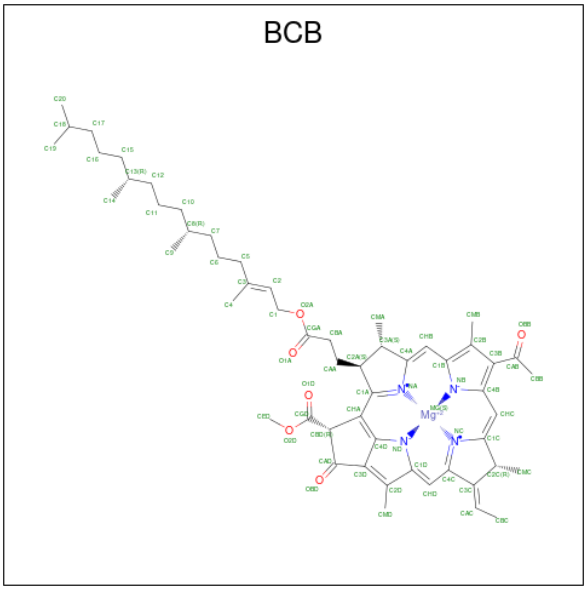
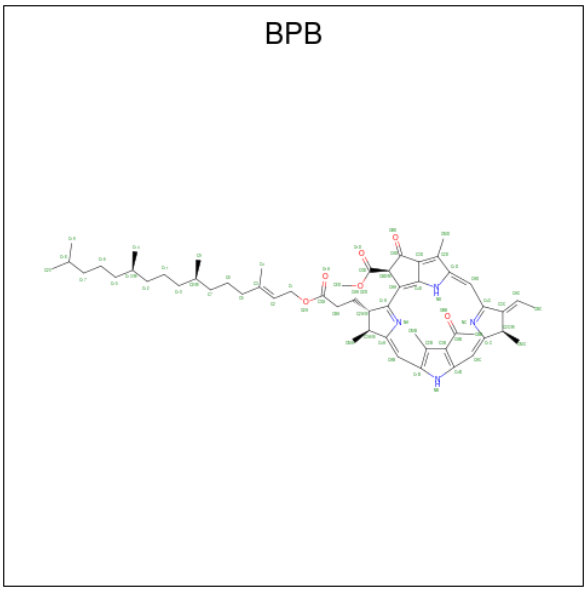
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	MMM	1	5	4	1	0	0
			Total	O	S		
9	MMM	1	5	4	1	0	0
			Total	O	S		
9	MMM	1	5	4	1	0	0

- Molecule 10 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



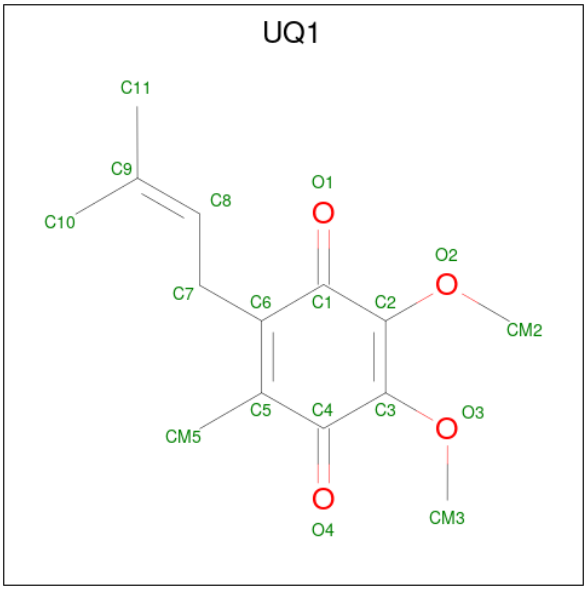
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
10	LLL	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
10	LLL	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
10	MMM	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
10	MMM	1	66	55	1	4	6	0	0

- Molecule 11 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



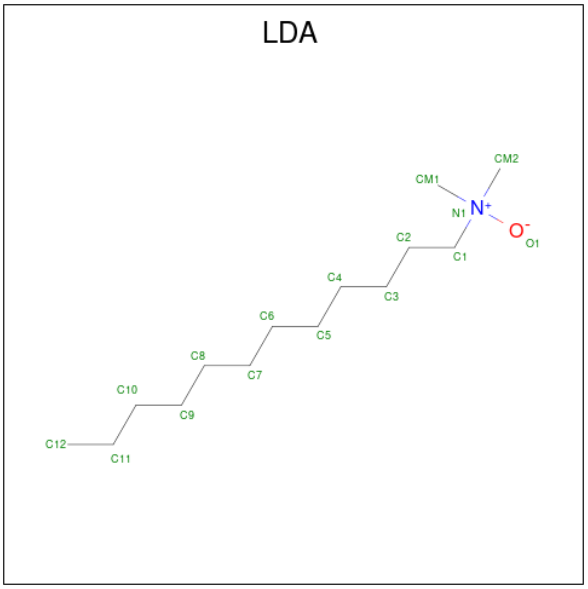
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	LLL	1	65	55	4	6	0	0
			Total	C	N	O		
11	MMM	1	65	55	4	6	0	0

- Molecule 12 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	LLL	1	18	14	4	0	0
			Total	C	O		
12	LLL	1	18	14	4	0	0

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

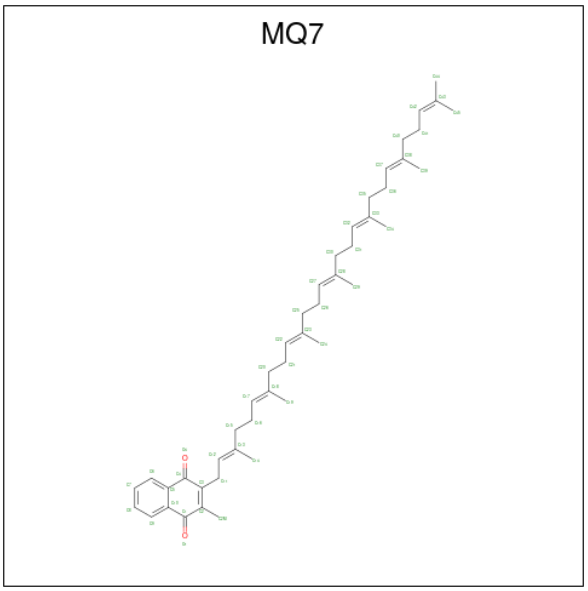


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	LLL	1	16	14	1	1	0	0
			Total	C	N	O		
13	MMM	1	16	14	1	1	0	0

- Molecule 14 is FE (II) ION (CCD ID: FE2) (formula: Fe).

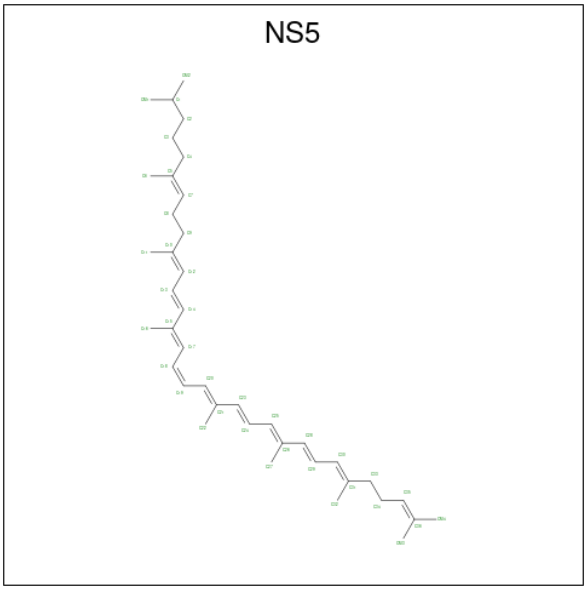
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
14	MMM	1	1	1	0	0

- Molecule 15 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	MMM	1	48	46	2	0	0

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
16	MMM	1	40	40	0	0

- Molecule 17 is water.

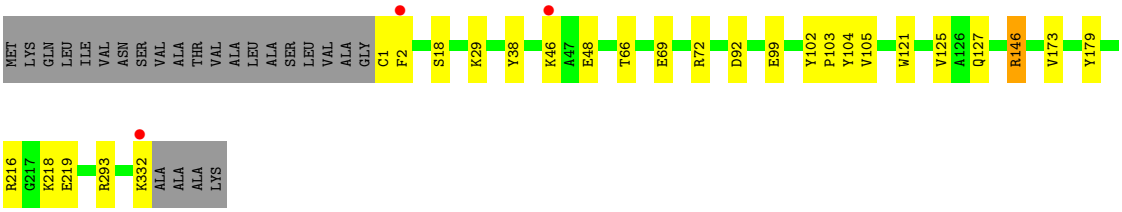
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	CCC	95	95	95	0	0
			Total	O		
17	HHH	43	43	43	0	0
			Total	O		
17	LLL	42	42	42	0	0
			Total	O		
17	MMM	64	64	64	0	0

3 Residue-property plots (i)

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

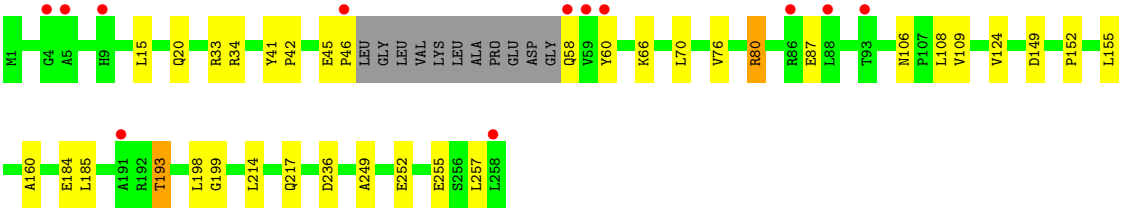
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain CCC:



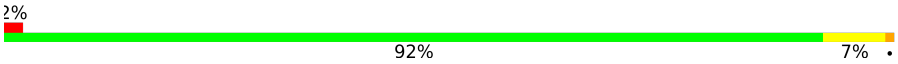
• Molecule 2: Reaction center protein H chain

Chain HHH:



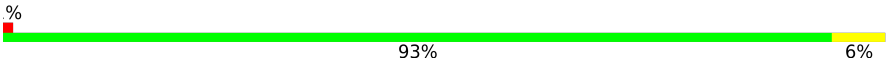
• Molecule 3: Reaction center protein L chain

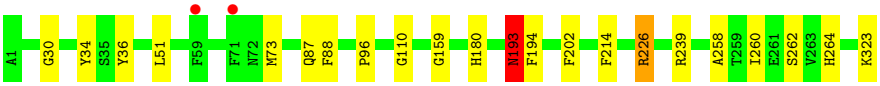
Chain LLL:



• Molecule 4: Reaction center protein M chain

Chain MMM:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.90Å 125.30Å 182.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.92 – 2.40 73.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.92-2.40) 99.9 (73.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.165 , 0.204 0.175 , 0.207	Depositor DCC
R_{free} test set	10006 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.3	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10442	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[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: NS5, SO4, LDA, HTO, FME, MQ7, DGA, FE2, UQ1, BPB, OLC, BCB, 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	CCC	1.02	0/2688	1.36	0/3662
2	HHH	1.01	0/1976	1.36	0/2698
3	LLL	0.99	0/2267	1.40	4/3095 (0.1%)
4	MMM	0.97	0/2659	1.39	2/3637 (0.1%)
All	All	1.00	0/9590	1.38	6/13092 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	LLL	201	GLY	CA-C-O	-6.23	117.24	122.29
4	MMM	30	GLY	CA-C-O	-5.84	118.42	122.22
3	LLL	271	PHE	CA-CB-CG	5.71	119.51	113.80
3	LLL	248	THR	CA-C-N	5.16	127.81	120.53
3	LLL	248	THR	C-N-CA	5.16	127.81	120.53

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	CCC	2618	0	2596	11	0
2	HHH	1941	0	1936	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	LLL	2172	0	2097	14	0
4	MMM	2555	0	2452	12	0
5	CCC	172	0	120	1	0
6	CCC	44	0	69	0	0
7	HHH	10	0	16	0	0
7	LLL	50	0	80	0	0
7	MMM	30	0	48	0	0
8	HHH	25	0	40	3	0
9	HHH	5	0	0	0	0
9	LLL	5	0	0	0	0
9	MMM	20	0	0	0	0
10	LLL	132	0	144	5	0
10	MMM	132	0	144	1	0
11	LLL	65	0	74	1	0
11	MMM	65	0	74	6	0
12	LLL	36	0	36	2	0
13	LLL	16	0	31	0	0
13	MMM	16	0	31	0	0
14	MMM	1	0	0	0	0
15	MMM	48	0	64	2	0
16	MMM	40	0	60	5	0
17	CCC	95	0	0	0	0
17	HHH	43	0	0	1	0
17	LLL	42	0	0	0	0
17	MMM	64	0	0	2	0
All	All	10442	0	10112	64	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 3.

The worst 5 of 64 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)
11:MMM:405:BPB:HHC	11:MMM:405:BPB:HBBB	1.62	0.80
4:MMM:159:GLY:HA3	16:MMM:406:NS5:H272	1.68	0.76
3:LLL:181:PHE:HB3	11:MMM:405:BPB:HBBA	1.69	0.74
3:LLL:132:GLN:HE22	3:LLL:146:PHE:H	1.32	0.73
10:MMM:403:BCB:HBB2	10:MMM:403:BCB:HHC	1.74	0.69

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	CCC	332/356 (93%)	317 (96%)	15 (4%)	0	100	100
2	HHH	243/258 (94%)	233 (96%)	10 (4%)	0	100	100
3	LLL	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
4	MMM	321/323 (99%)	313 (98%)	7 (2%)	1 (0%)	36	50
All	All	1168/1210 (96%)	1128 (97%)	39 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	MMM	193	ASN

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	CCC	283/297 (95%)	269 (95%)	14 (5%)	22	39
2	HHH	204/212 (96%)	191 (94%)	13 (6%)	16	28
3	LLL	219/218 (100%)	214 (98%)	5 (2%)	44	66
4	MMM	249/249 (100%)	242 (97%)	7 (3%)	38	60
All	All	955/976 (98%)	916 (96%)	39 (4%)	28	46

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LLL	20	ASP
4	MMM	194	PHE
3	LLL	21	LEU
4	MMM	51	LEU
4	MMM	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\#\|Z\| > 2$
2	FME	HHH	1	2	8,9,10	0.45	0	7,9,11	0.89	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
2	FME	HHH	1	2	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	HHH	1	FME	N-CA-CB-CG
2	HHH	1	FME	C-CA-CB-CG
2	HHH	1	FME	CA-CB-CG-SD
2	HHH	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	HTO	MMM	409	-	9,9,9	0.88	0	10,10,10	1.01	1 (10%)
12	UQ1	LLL	310	-	18,18,18	2.57	3 (16%)	22,25,25	1.46	6 (27%)
7	HTO	LLL	312	-	9,9,9	0.94	0	10,10,10	1.49	2 (20%)
9	SO4	MMM	411	-	4,4,4	0.33	0	6,6,6	0.07	0
5	HEC	CCC	403	1	50,50,50	1.33	5 (10%)	68,82,82	1.47	13 (19%)
7	HTO	LLL	304	-	9,9,9	0.81	0	10,10,10	0.76	0
9	SO4	MMM	413	-	4,4,4	0.36	0	6,6,6	0.07	0
12	UQ1	LLL	309	-	18,18,18	2.32	3 (16%)	22,25,25	1.64	4 (18%)
16	NS5	MMM	406	-	39,39,39	0.95	0	44,46,46	1.68	10 (22%)
10	BCB	LLL	301	3	68,74,74	1.91	17 (25%)	79,115,115	3.05	27 (34%)
15	MQ7	MMM	402	-	49,49,49	1.36	3 (6%)	60,63,63	1.07	3 (5%)
8	OLC	HHH	402	-	24,24,24	1.19	1 (4%)	25,25,25	1.37	3 (12%)
5	HEC	CCC	401	1	50,50,50	1.38	5 (10%)	68,82,82	1.45	14 (20%)
9	SO4	MMM	412	-	4,4,4	0.34	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SO4	MMM	414	-	4,4,4	0.37	0	6,6,6	0.07	0
9	SO4	LLL	308	-	4,4,4	0.37	0	6,6,6	0.04	0
5	HEC	CCC	404	1	50,50,50	1.45	5 (10%)	68,82,82	1.77	15 (22%)
5	HEC	CCC	402	1	50,50,50	1.45	5 (10%)	68,82,82	1.54	10 (14%)
7	HTO	LLL	306	-	9,9,9	0.69	0	10,10,10	0.95	0
13	LDA	LLL	311	-	12,15,15	0.29	0	14,17,17	0.34	0
13	LDA	MMM	410	-	12,15,15	0.28	0	14,17,17	0.34	0
9	SO4	HHH	403	-	4,4,4	0.37	0	6,6,6	0.13	0
7	HTO	LLL	305	-	9,9,9	0.73	0	10,10,10	1.20	1 (10%)
7	HTO	HHH	401	-	9,9,9	0.94	0	10,10,10	0.70	0
10	BCB	LLL	302	3	68,74,74	1.85	16 (23%)	79,115,115	2.99	19 (24%)
7	HTO	LLL	307	-	9,9,9	0.98	0	10,10,10	1.01	2 (20%)
10	BCB	MMM	403	4	68,74,74	1.82	17 (25%)	79,115,115	2.93	29 (36%)
11	BPB	LLL	303	-	57,70,70	2.38	16 (28%)	56,101,101	2.40	15 (26%)
7	HTO	MMM	408	-	9,9,9	0.72	0	10,10,10	0.99	1 (10%)
6	DGA	CCC	405	1	43,43,43	4.46	4 (9%)	45,45,45	4.51	8 (17%)
10	BCB	MMM	404	4	68,74,74	1.84	15 (22%)	79,115,115	3.03	27 (34%)
11	BPB	MMM	405	-	57,70,70	2.46	14 (24%)	56,101,101	2.77	21 (37%)
7	HTO	MMM	407	-	9,9,9	0.97	0	10,10,10	1.29	2 (20%)

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
7	HTO	MMM	409	-	-	5/10/10/10	-
12	UQ1	LLL	310	-	-	3/9/33/33	0/1/1/1
7	HTO	LLL	312	-	-	3/10/10/10	-
5	HEC	CCC	403	1	1/1/3/7	4/14/54/54	-
7	HTO	LLL	304	-	-	4/10/10/10	-
12	UQ1	LLL	309	-	-	0/9/33/33	0/1/1/1
16	NS5	MMM	406	-	-	6/43/43/43	-
10	BCB	LLL	301	3	3/3/21/26	8/41/137/137	-
15	MQ7	MMM	402	-	-	2/41/61/61	0/2/2/2
8	OLC	HHH	402	-	-	8/24/24/24	-
5	HEC	CCC	401	1	1/1/3/7	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	CCC	404	1	1/1/3/7	7/14/54/54	-
5	HEC	CCC	402	1	1/1/3/7	9/14/54/54	-
7	HTO	LLL	306	-	-	6/10/10/10	-
13	LDA	LLL	311	-	-	5/13/13/13	-
13	LDA	MMM	410	-	-	11/13/13/13	-
7	HTO	LLL	305	-	-	6/10/10/10	-
7	HTO	HHH	401	-	-	5/10/10/10	-
10	BCB	LLL	302	3	3/3/21/26	7/41/137/137	-
7	HTO	LLL	307	-	-	6/10/10/10	-
10	BCB	MMM	403	4	3/3/21/26	13/41/137/137	-
11	BPB	LLL	303	-	1/1/18/23	9/37/105/105	0/5/6/6
7	HTO	MMM	408	-	-	4/10/10/10	-
6	DGA	CCC	405	1	1/1/3/3	28/45/45/45	-
10	BCB	MMM	404	4	3/3/21/26	11/41/137/137	-
11	BPB	MMM	405	-	1/1/18/23	11/37/105/105	0/5/6/6
7	HTO	MMM	407	-	-	6/10/10/10	-

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	405	DGA	OG1-CG1	-20.66	0.98	1.45
6	CCC	405	DGA	CG1-CG2	-13.44	1.09	1.50
6	CCC	405	DGA	OG2-CG2	-12.10	1.16	1.46
6	CCC	405	DGA	CB2-CB1	-9.70	1.22	1.50
12	LLL	310	UQ1	C6-C5	8.95	1.51	1.35

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	LLL	302	BCB	C1C-NC-C4C	-18.18	98.53	106.71
10	LLL	301	BCB	C1C-NC-C4C	-17.82	98.70	106.71
10	MMM	404	BCB	C1C-NC-C4C	-15.67	99.66	106.71
10	MMM	403	BCB	C1C-NC-C4C	-15.45	99.76	106.71
6	CCC	405	DGA	OG2-CG2-CG3	-14.69	55.66	108.36

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	CCC	401	HEC	NA
5	CCC	402	HEC	NA
5	CCC	403	HEC	NA
5	CCC	404	HEC	NA
6	CCC	405	DGA	CG2

5 of 195 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	CCC	405	DGA	CB2-CB1-OG2-CG2
6	CCC	405	DGA	CG1-CG2-CG3-OXT
7	HHH	401	HTO	C1-C2-C3-O3
7	HHH	401	HTO	C1-C2-C3-C4
7	HHH	401	HTO	O2-C2-C3-O3

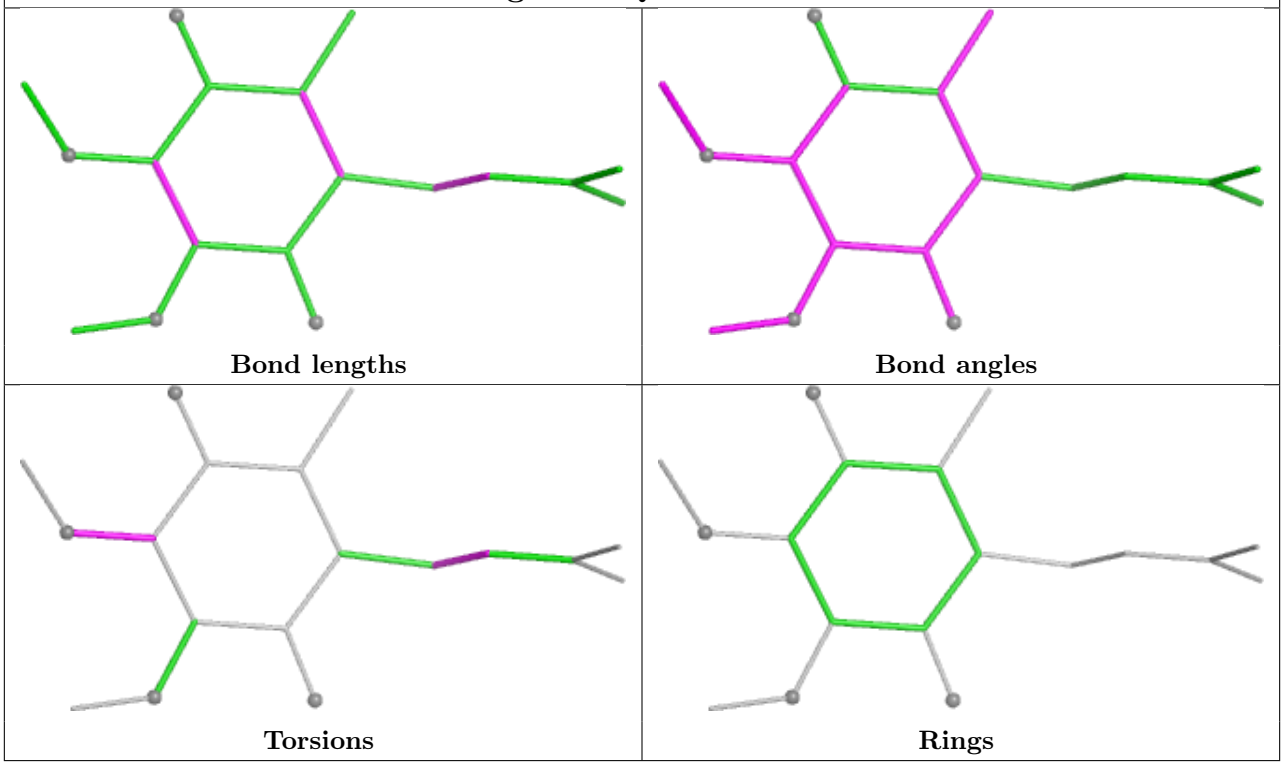
There are no ring outliers.

10 monomers are involved in 24 short contacts:

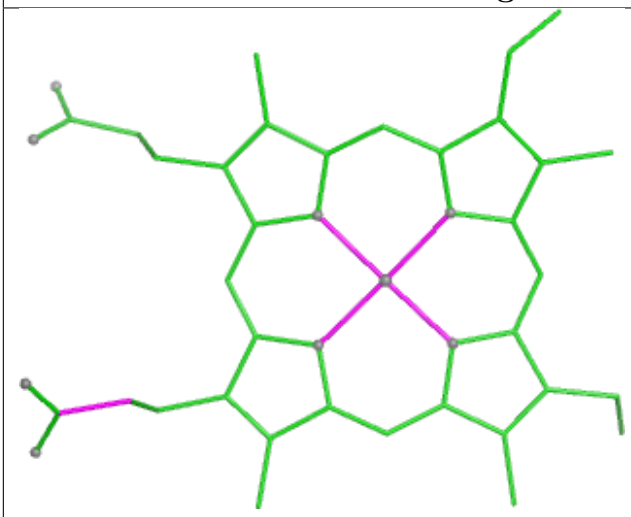
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	LLL	309	UQ1	2	0
16	MMM	406	NS5	5	0
10	LLL	301	BCB	4	0
15	MMM	402	MQ7	2	0
8	HHH	402	OLC	3	0
5	CCC	402	HEC	1	0
10	LLL	302	BCB	1	0
10	MMM	403	BCB	1	0
11	LLL	303	BPB	1	0
11	MMM	405	BPB	6	0

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.

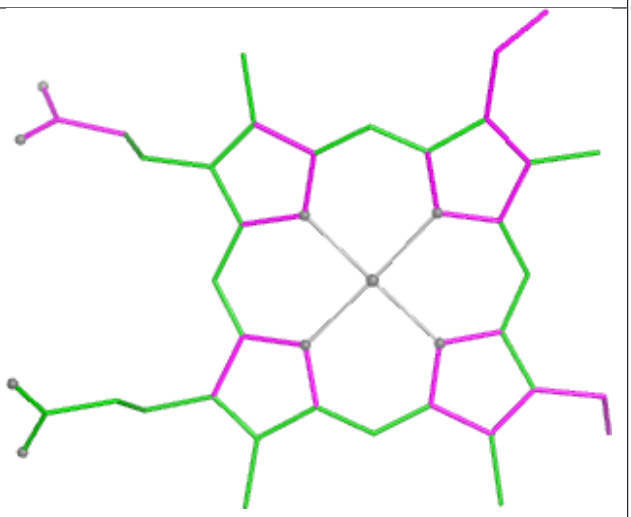
Ligand UQ1 LLL 310



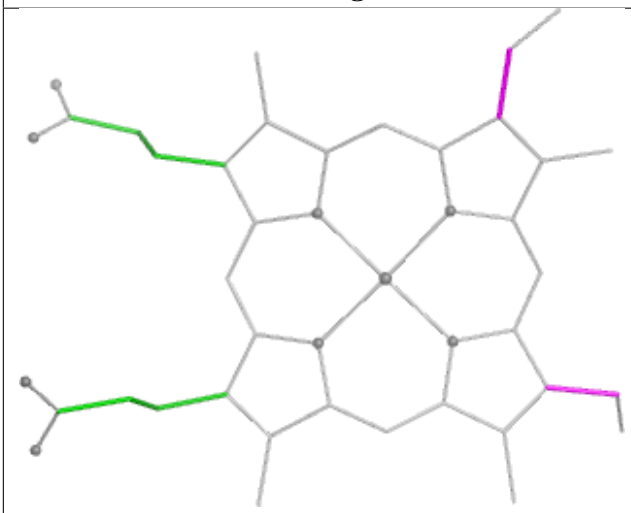
Ligand HEC CCC 403



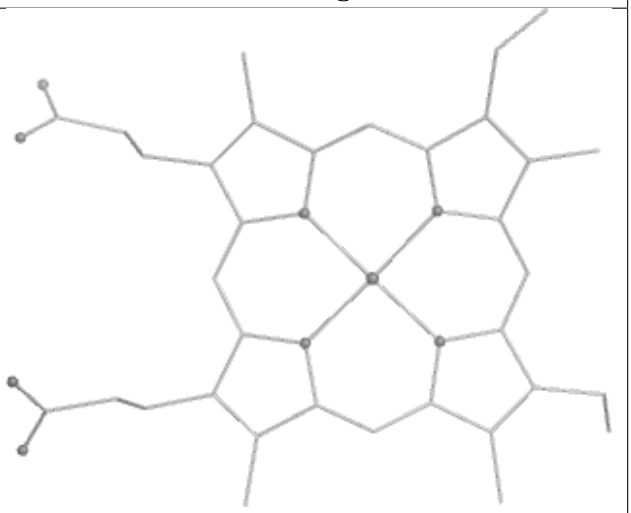
Bond lengths



Bond angles

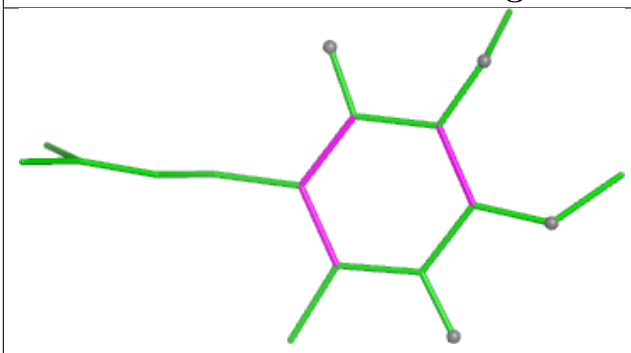


Torsions



Rings

Ligand UQ1 LLL 309



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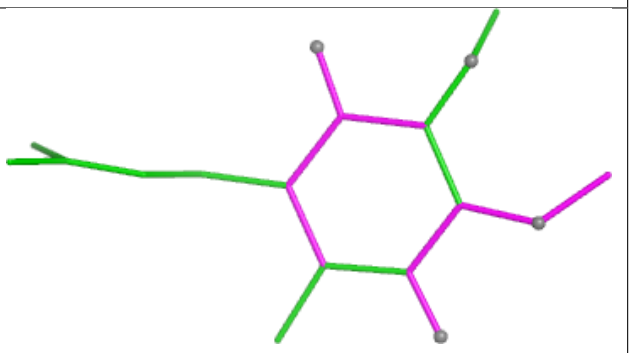

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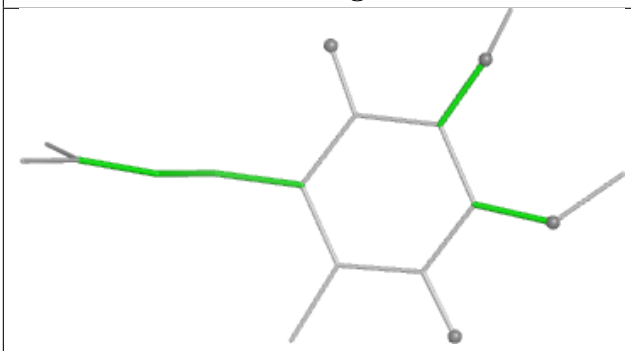
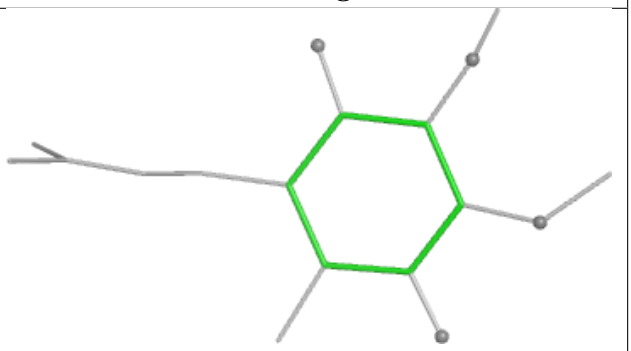
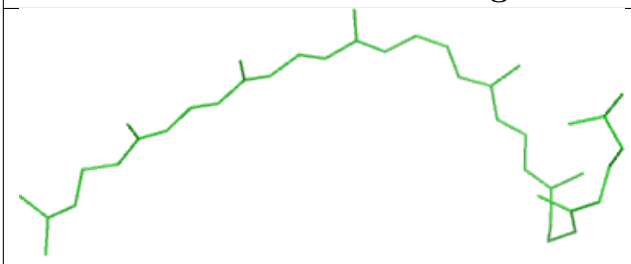


Torsions



Rings

Ligand NS5 MMM 406



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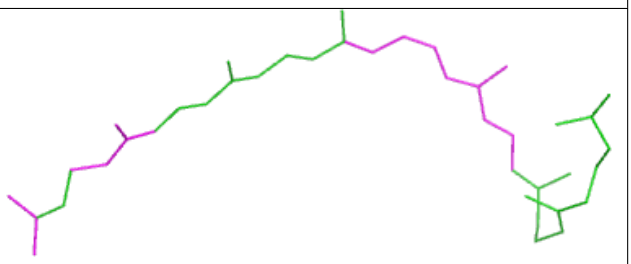
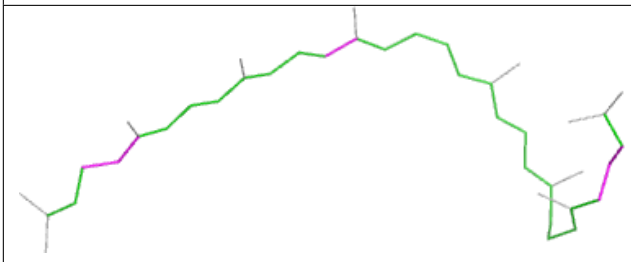


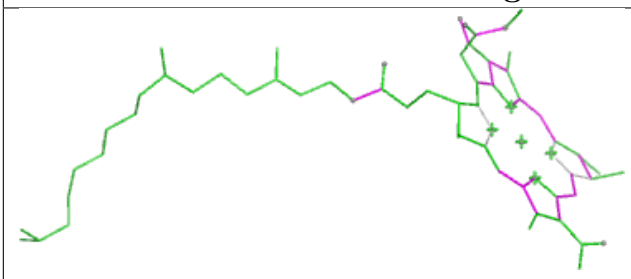
Bond angles



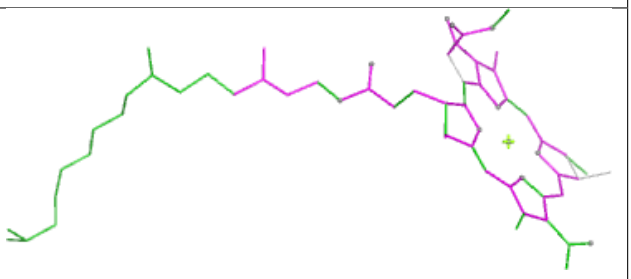
Torsions

Rings

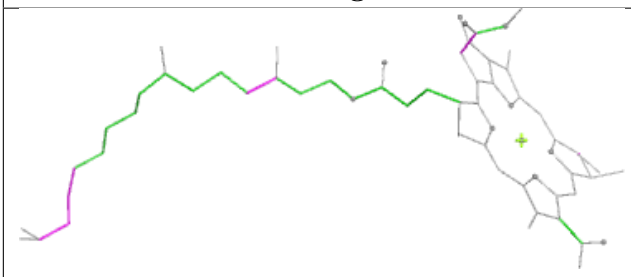
Ligand BCB LLL 301



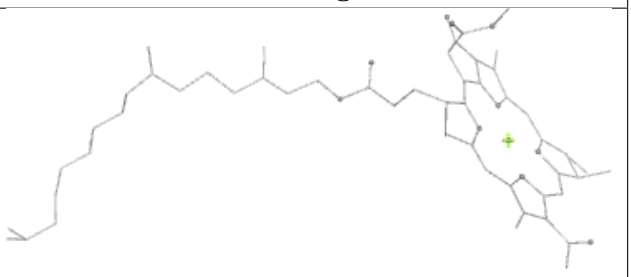
Bond lengths



Bond angles



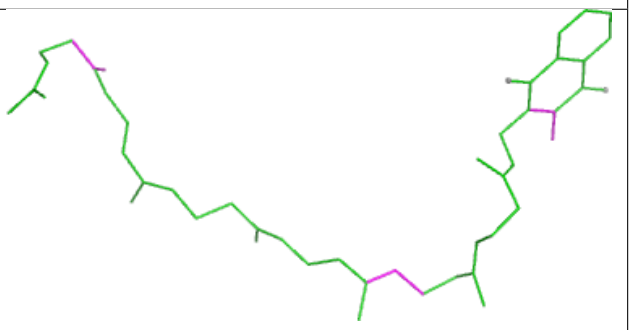
Torsions



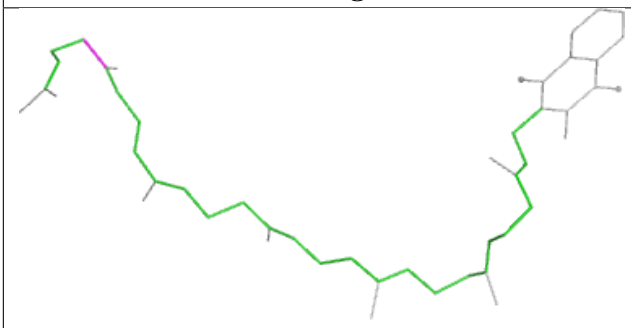
Rings

Ligand MQ7 MMM 402

Bond lengths



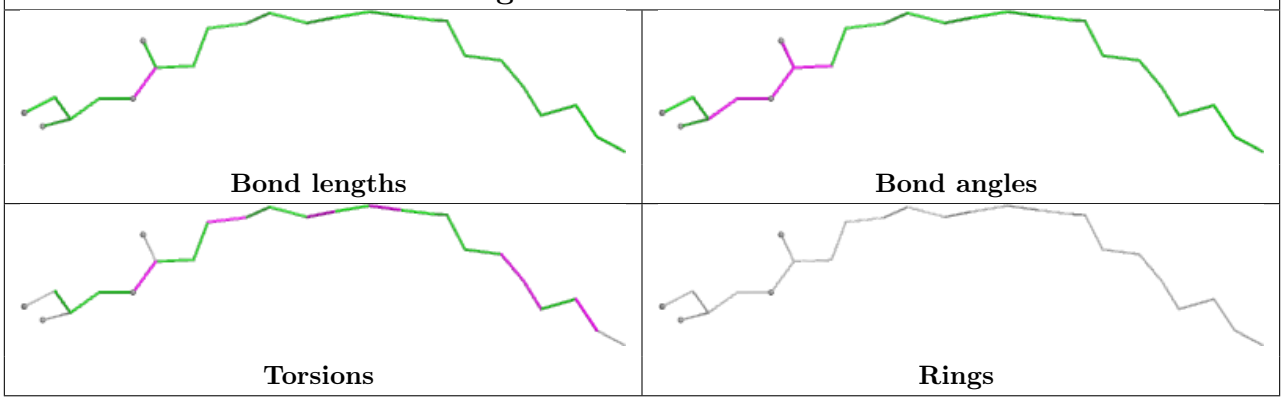
Bond angles



Torsions

Rings

Ligand OLC HHH 402



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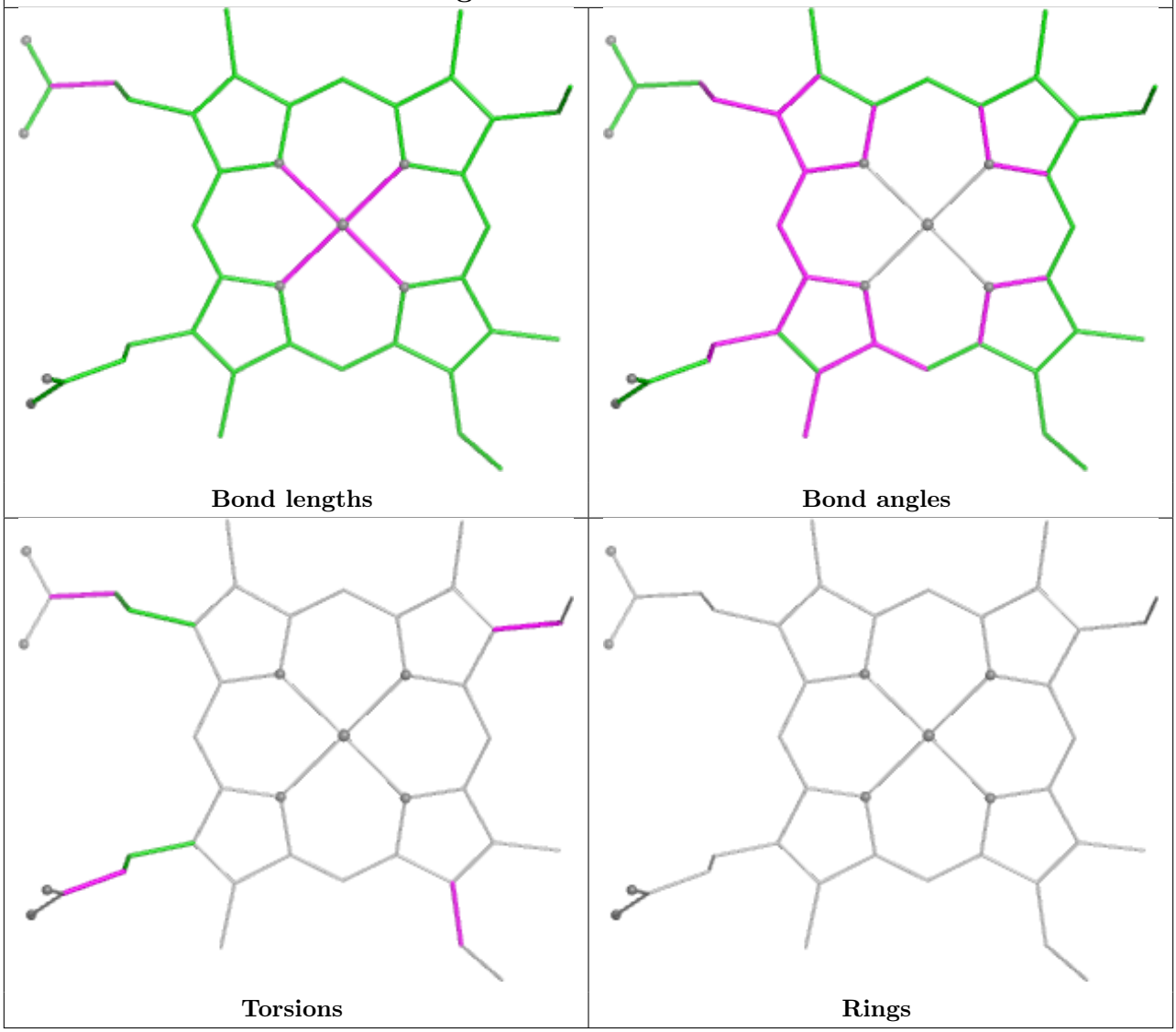

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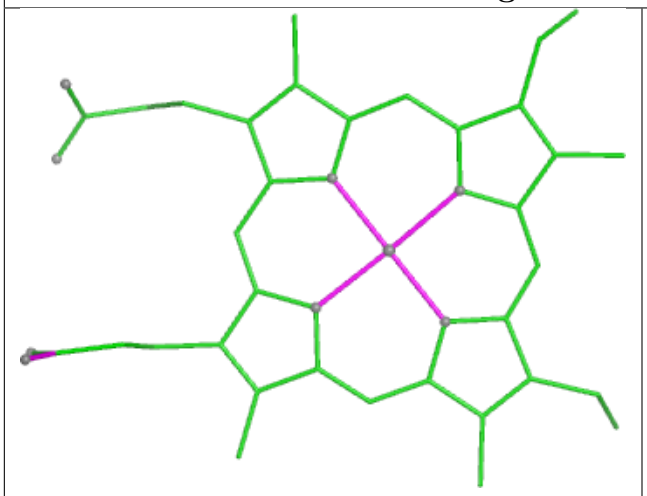
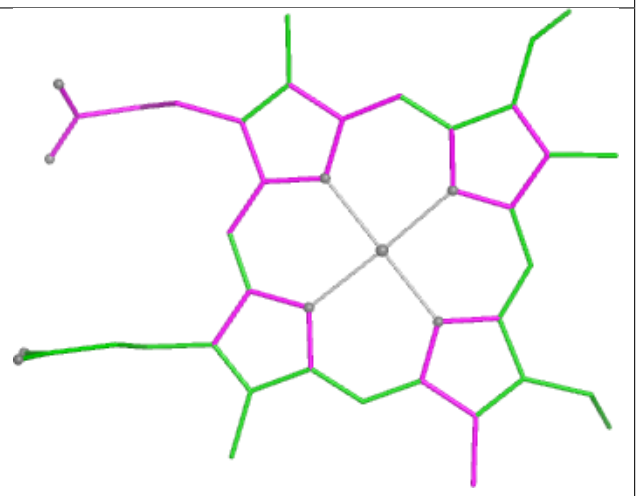
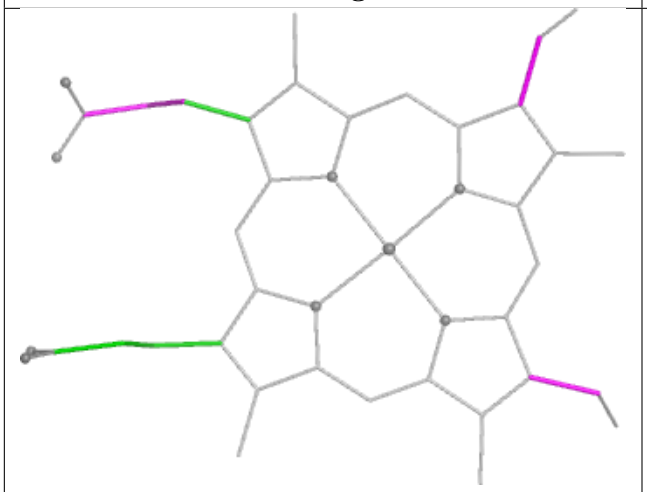


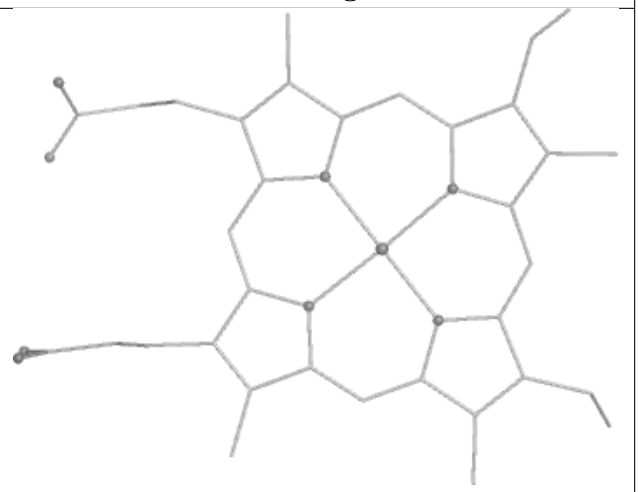
Bond lengths



Bond angles

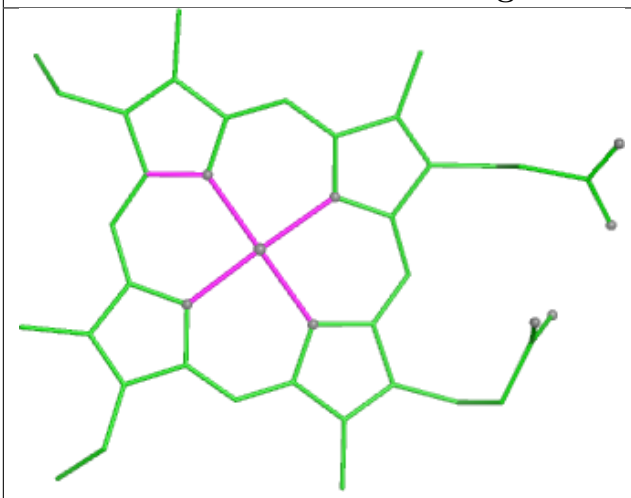


Torsions

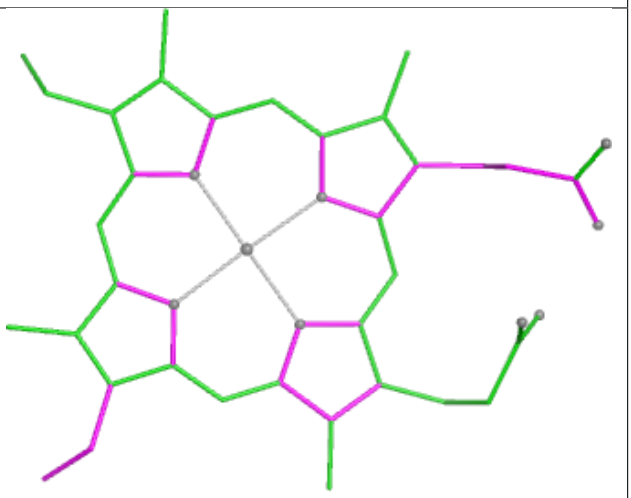


Rings

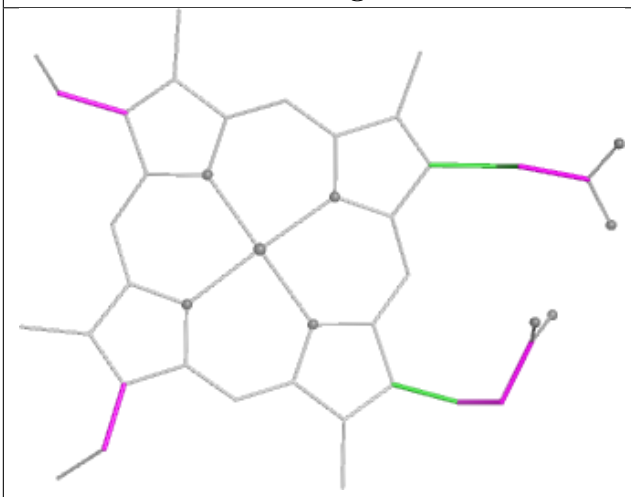
Ligand HEC CCC 402



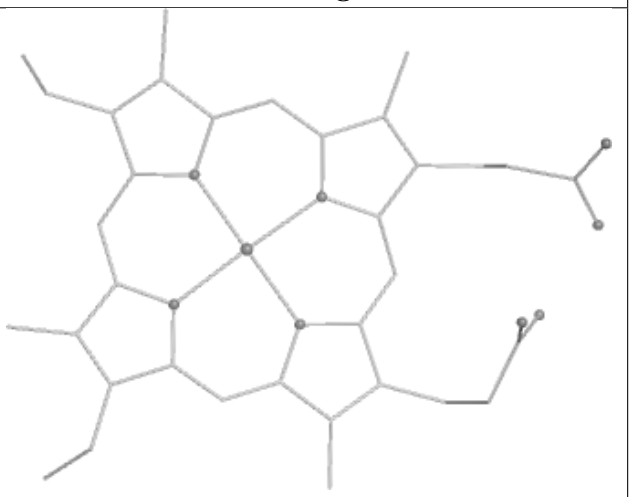
Bond lengths



Bond angles

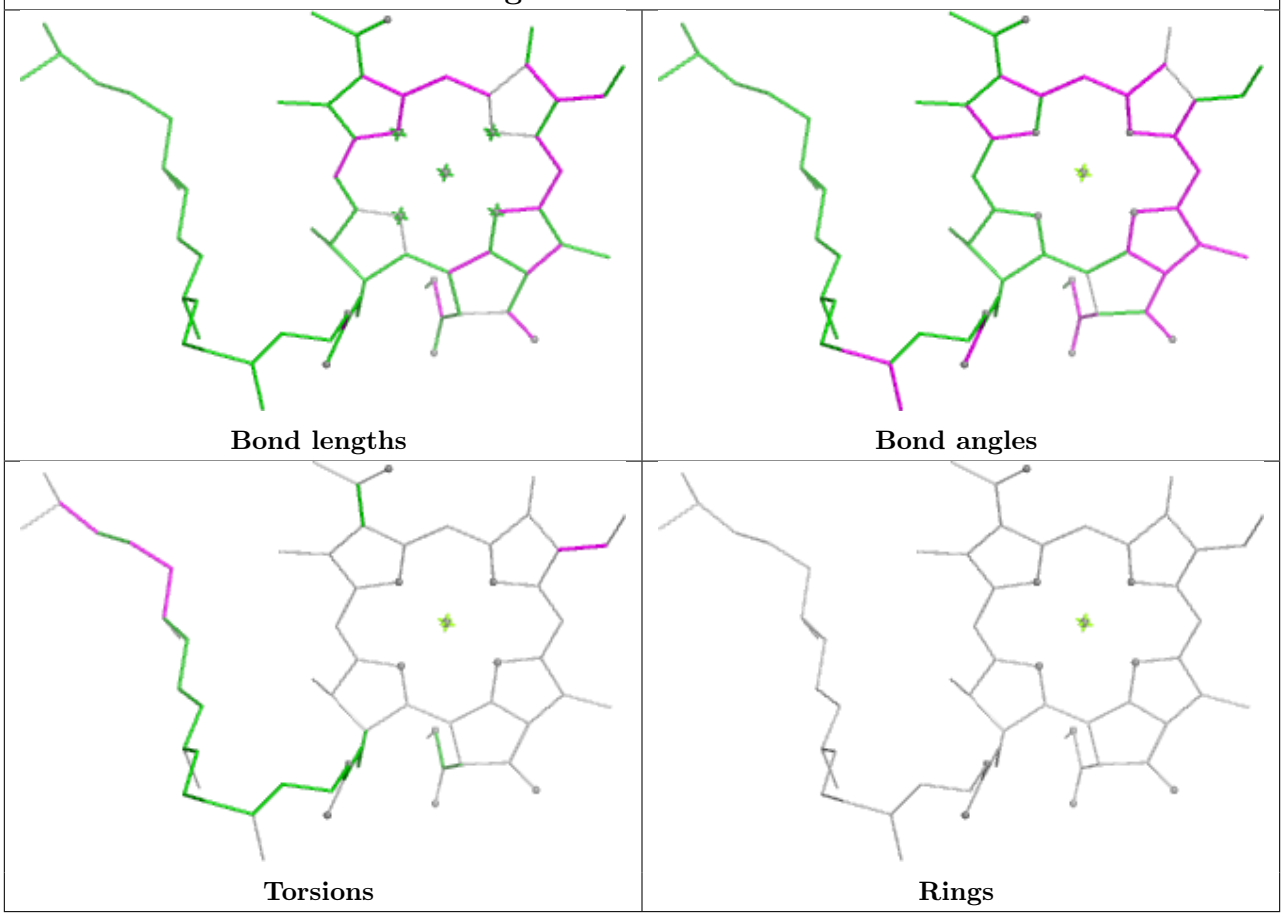


Torsions

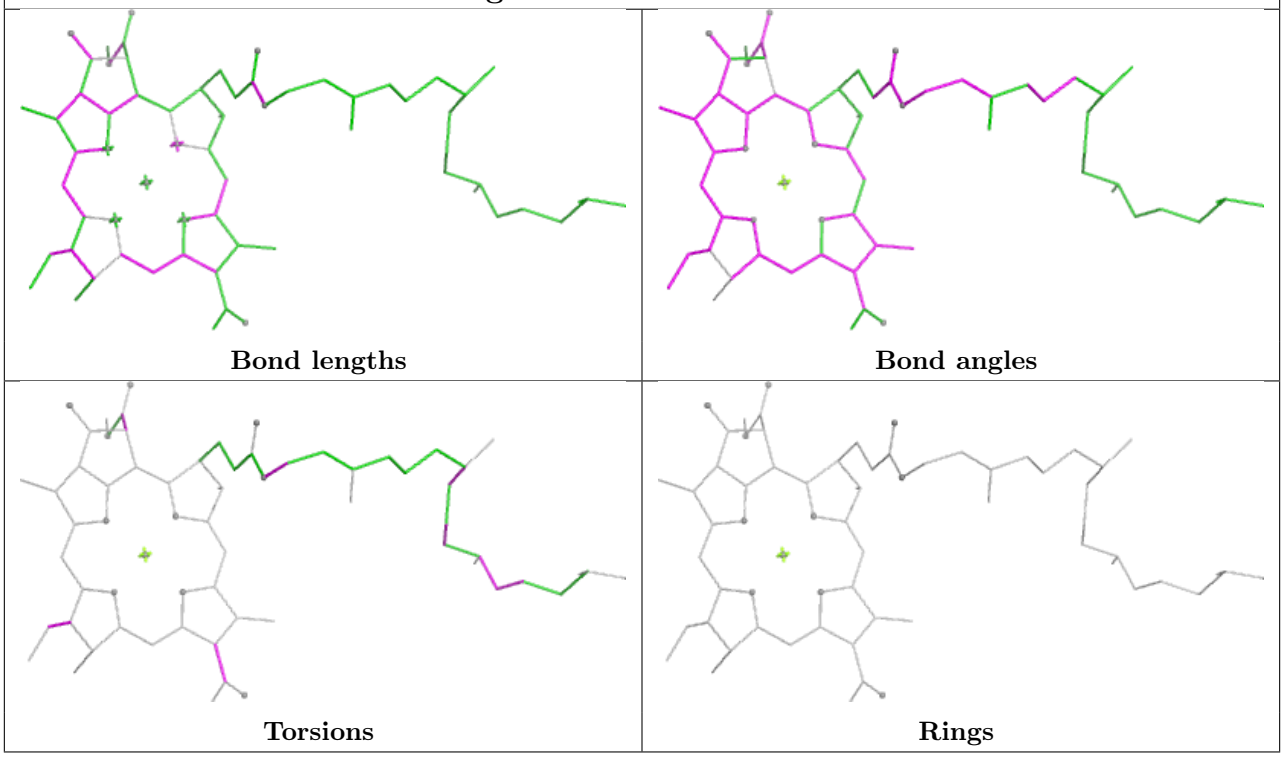


Rings

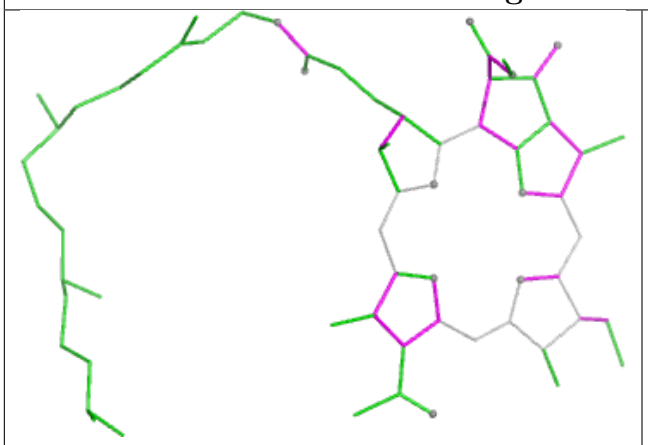
Ligand BCB LLL 302



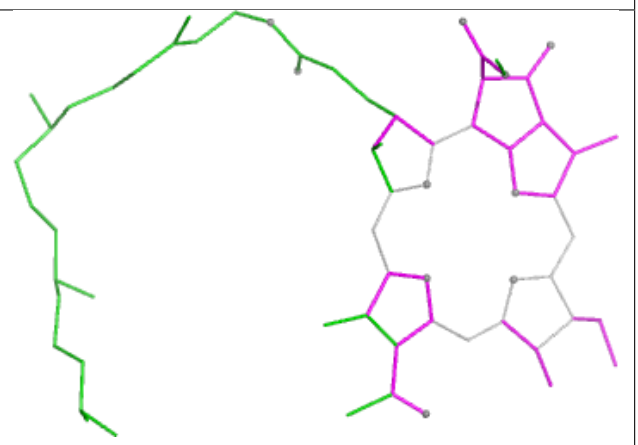
Ligand BCB MMM 403



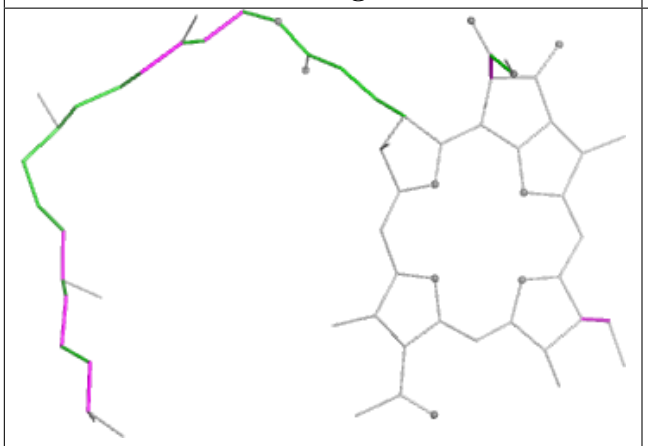
Ligand BPB LLL 303



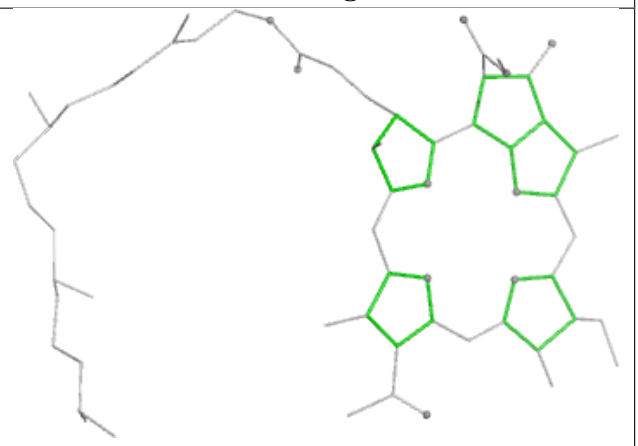
Bond lengths



Bond angles



Torsions



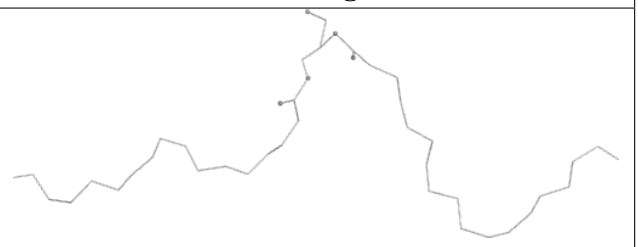
Rings

Ligand DGA CCC 405

Bond lengths

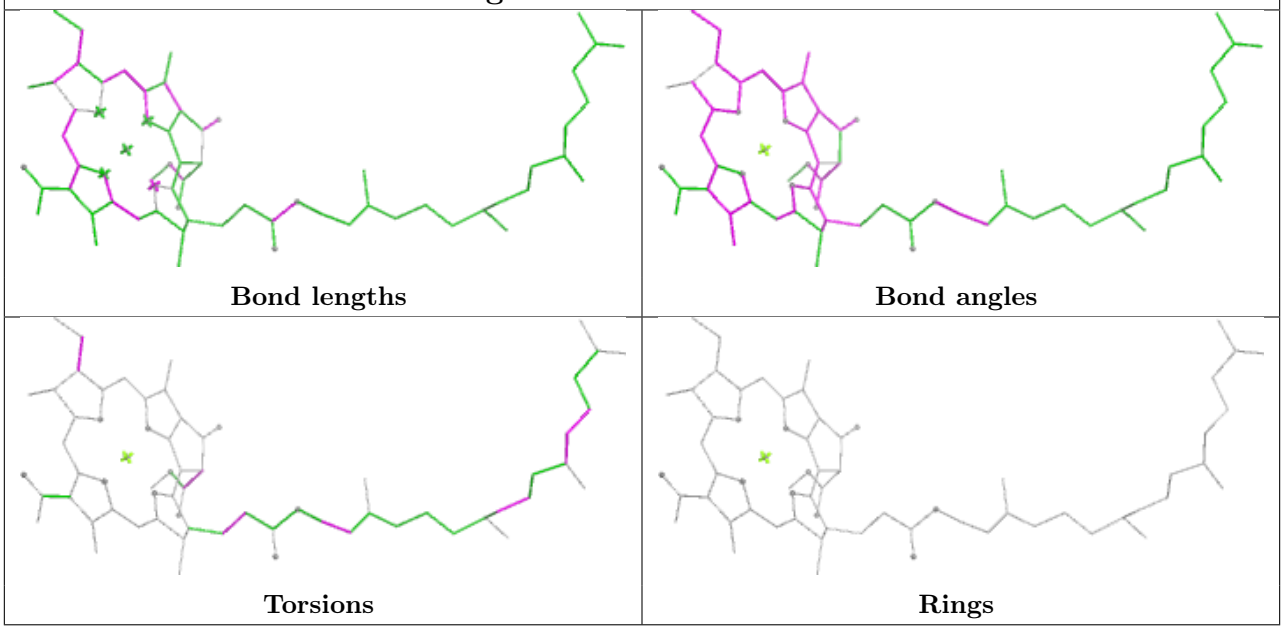
Bond angles

Torsions

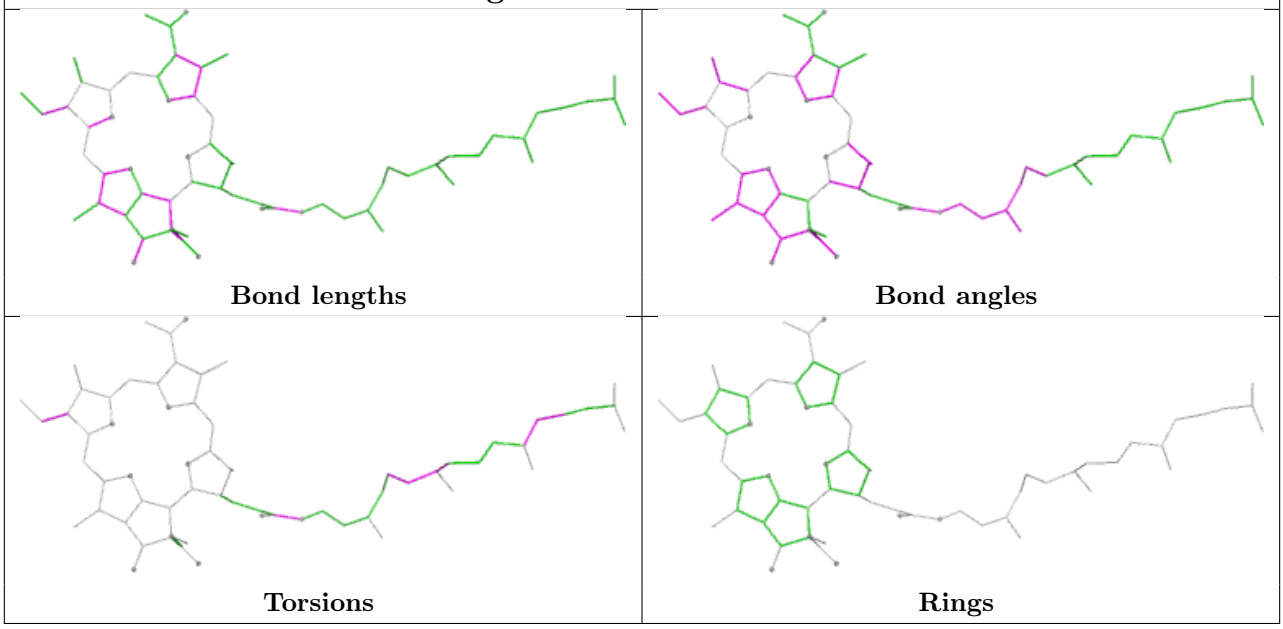


Rings

Ligand BCB MMM 404



Ligand BPB MMM 405



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	CCC	332/356 (93%)	-0.38	3 (0%)	81	78	18, 43, 71, 106	2 (0%)
2	HHH	246/258 (95%)	0.06	12 (4%)	35	31	37, 55, 94, 123	0
3	LLL	273/273 (100%)	-0.20	6 (2%)	62	58	31, 43, 70, 118	1 (0%)
4	MMM	323/323 (100%)	-0.33	2 (0%)	85	83	30, 42, 65, 92	0
All	All	1174/1210 (97%)	-0.23	23 (1%)	65	60	18, 45, 77, 123	3 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HHH	59	VAL	4.3
2	HHH	46	PRO	4.1
2	HHH	60	TYR	3.7
2	HHH	5	ALA	3.5
2	HHH	258	LEU	3.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FME	HHH	1	10/11	0.86	0.19	59,96,117,117	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

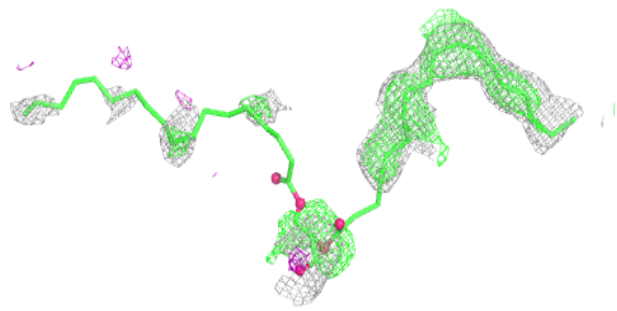
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SO4	MMM	413	5/5	0.67	0.17	147,157,162,179	0
7	HTO	MMM	409	10/10	0.70	0.27	78,92,112,116	0
6	DGA	CCC	405	44/44	0.72	0.32	69,106,143,189	41
7	HTO	LLL	305	10/10	0.77	0.25	82,85,101,105	0
7	HTO	LLL	307	10/10	0.78	0.21	88,97,101,103	0
7	HTO	MMM	408	10/10	0.78	0.20	76,90,96,97	0
9	SO4	MMM	411	5/5	0.79	0.11	97,101,104,116	0
7	HTO	HHH	401	10/10	0.79	0.23	84,97,104,106	0
7	HTO	MMM	407	10/10	0.82	0.20	73,88,96,103	0
13	LDA	MMM	410	16/16	0.82	0.26	75,81,132,147	0
12	UQ1	LLL	310	18/18	0.83	0.20	69,82,98,99	0
13	LDA	LLL	311	16/16	0.83	0.31	83,95,116,124	0
7	HTO	LLL	312	10/10	0.83	0.26	69,93,103,114	0
9	SO4	HHH	403	5/5	0.85	0.12	89,99,105,111	0
7	HTO	LLL	304	10/10	0.88	0.23	72,87,99,101	0
8	OLC	HHH	402	25/25	0.88	0.18	63,71,91,106	0
16	NS5	MMM	406	40/40	0.89	0.22	47,71,130,133	0
9	SO4	MMM	414	5/5	0.90	0.13	98,100,115,120	0
12	UQ1	LLL	309	18/18	0.90	0.17	57,63,73,73	0
9	SO4	LLL	308	5/5	0.91	0.19	124,131,134,144	0
9	SO4	MMM	412	5/5	0.92	0.09	76,80,90,93	0
7	HTO	LLL	306	10/10	0.93	0.15	84,89,93,95	0
11	BPB	MMM	405	65/65	0.95	0.12	31,37,119,125	0
10	BCB	LLL	301	66/66	0.95	0.09	27,34,51,64	0
15	MQ7	MMM	402	48/48	0.95	0.10	32,45,79,84	0
10	BCB	MMM	403	66/66	0.95	0.13	29,34,114,127	0
10	BCB	MMM	404	66/66	0.96	0.09	29,33,56,65	0
11	BPB	LLL	303	65/65	0.96	0.07	30,36,45,51	0
10	BCB	LLL	302	66/66	0.96	0.08	28,33,67,68	0
5	HEC	CCC	402	43/43	0.98	0.07	32,42,49,53	0
5	HEC	CCC	401	43/43	0.98	0.06	33,39,44,45	0
5	HEC	CCC	404	43/43	0.99	0.06	29,40,55,76	0
5	HEC	CCC	403	43/43	0.99	0.05	27,30,37,39	0
14	FE2	MMM	401	1/1	1.00	0.01	34,34,34,34	0

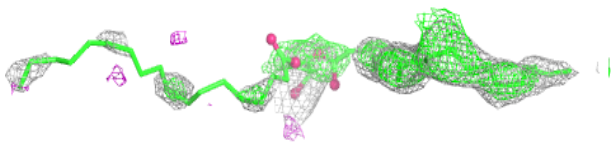
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

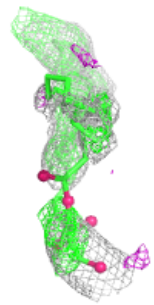
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DGA CCC 405:

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

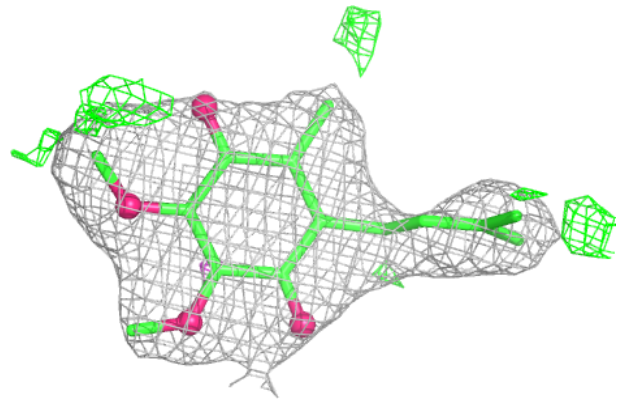


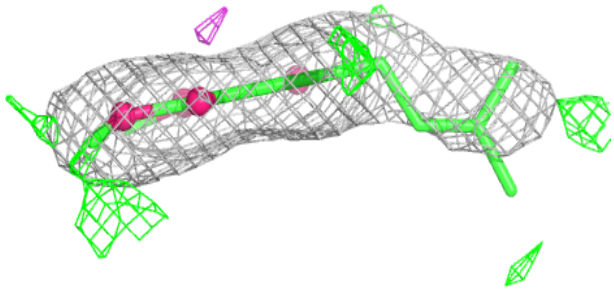


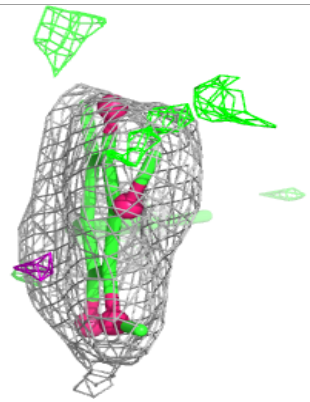


Electron density around UQ1 LLL 310:

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

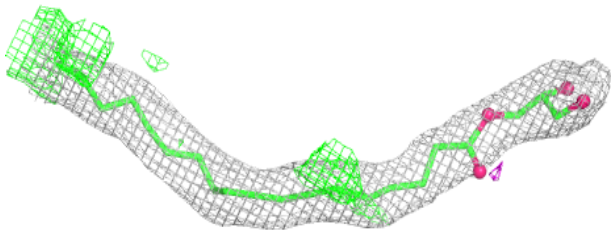


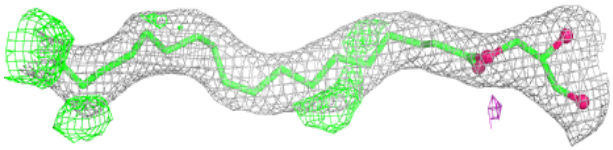


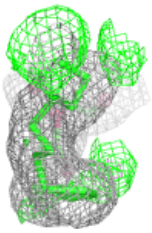


Electron density around OLC HHH 402:

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

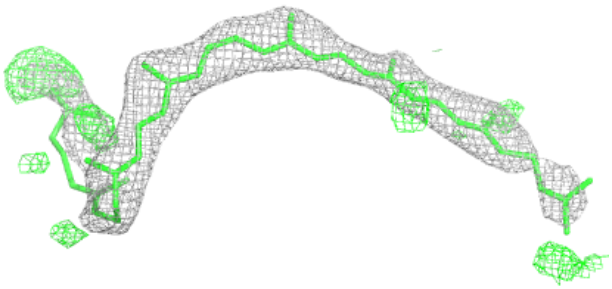


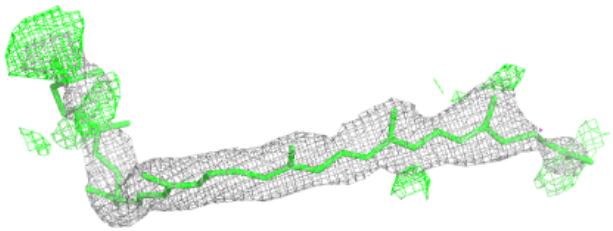


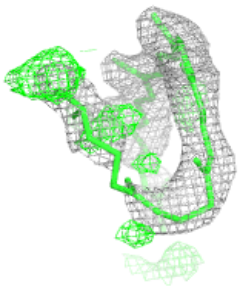


Electron density around NS5 MMM 406:

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

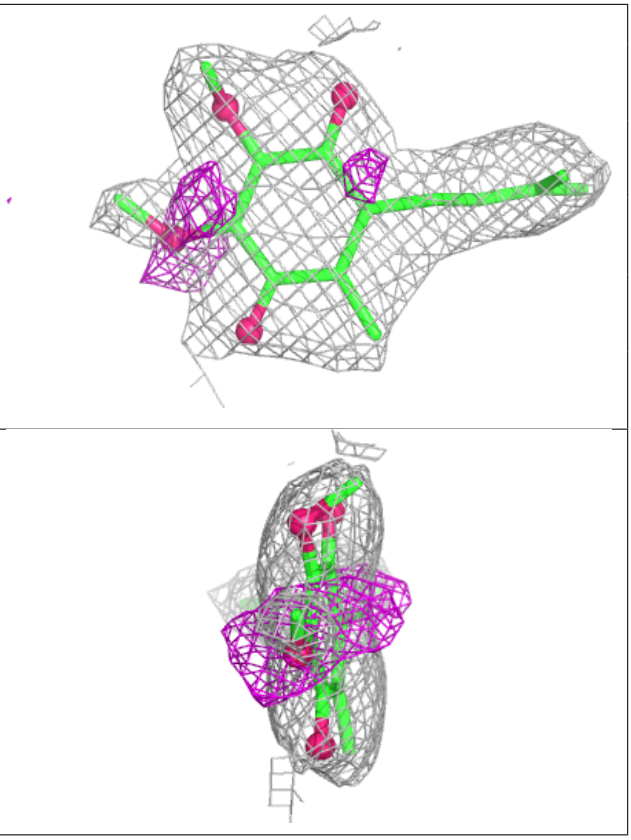






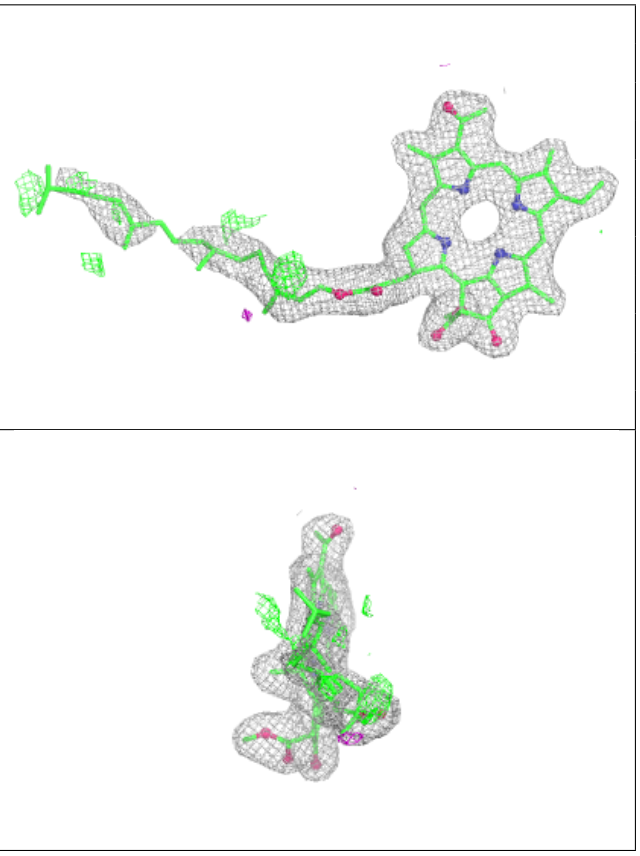
Electron density around UQ1 LLL 309:

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



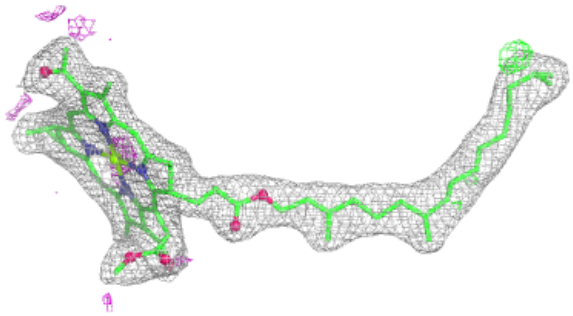
Electron density around BPB MMM 405:

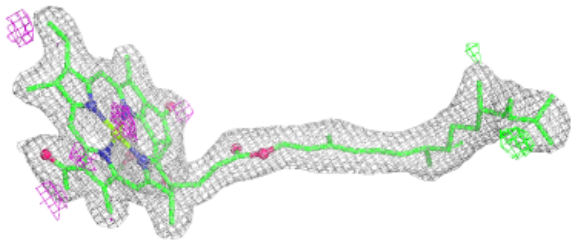
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

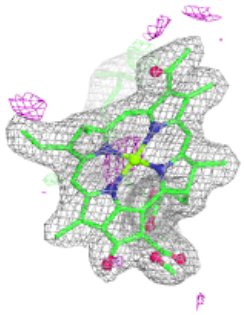


Electron density around BCB LLL 301:

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

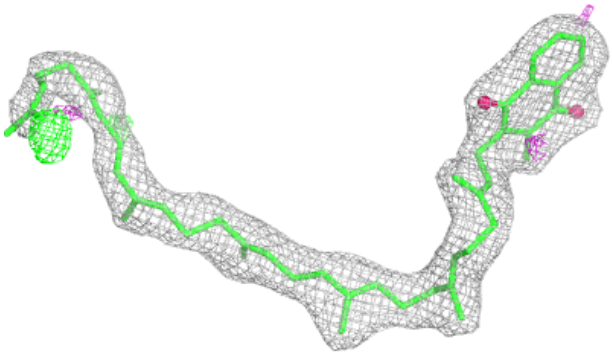


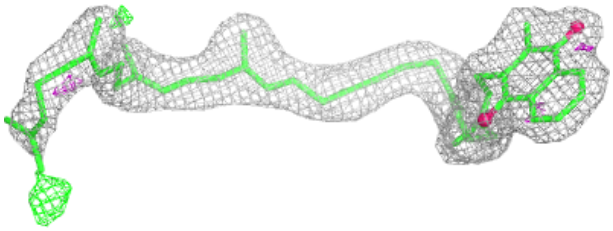


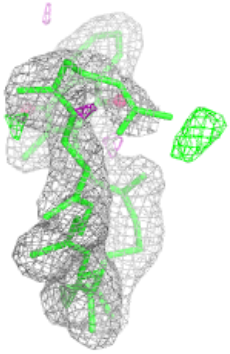


Electron density around MQ7 MMM 402:

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

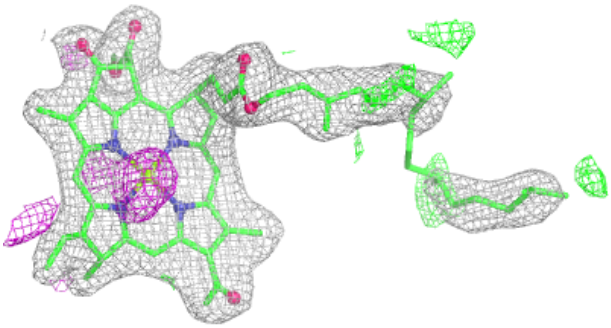


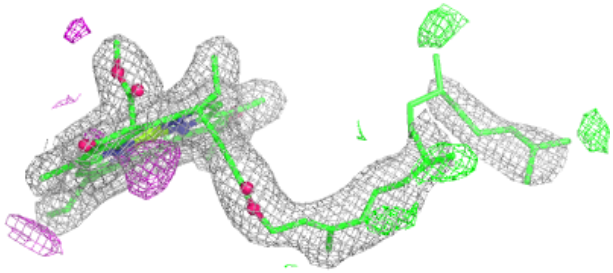


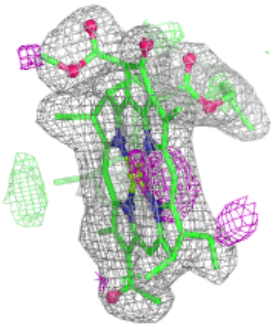


Electron density around BCB MMM 403:

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

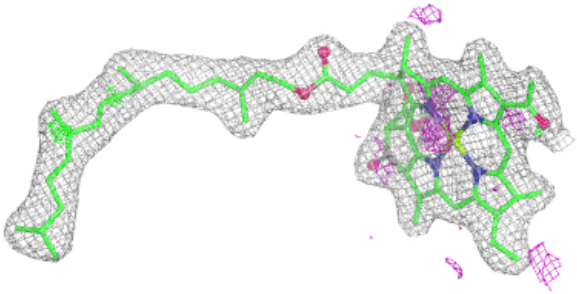


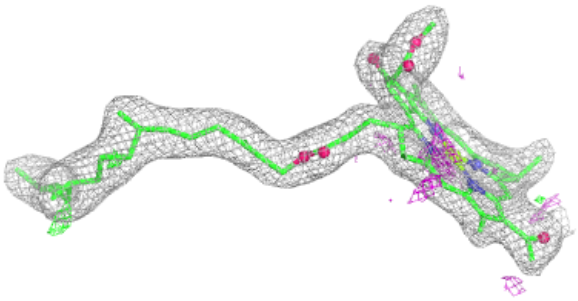


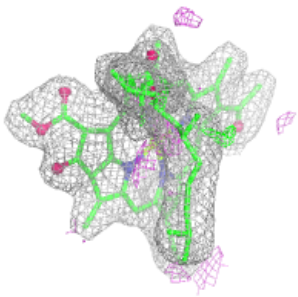


Electron density around BCB MMM 404:

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

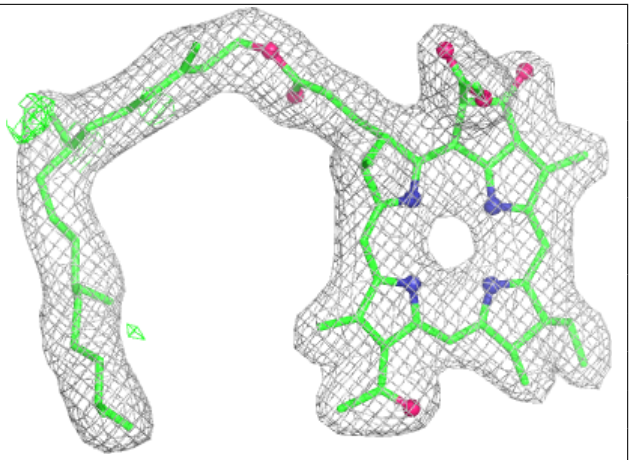


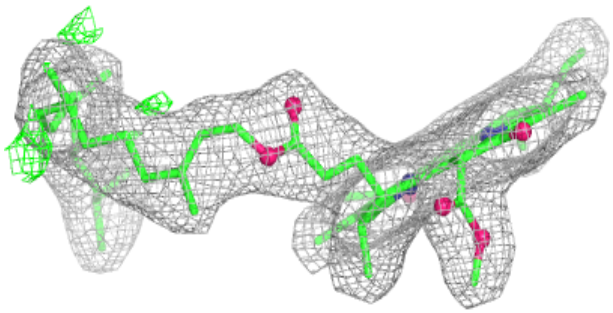


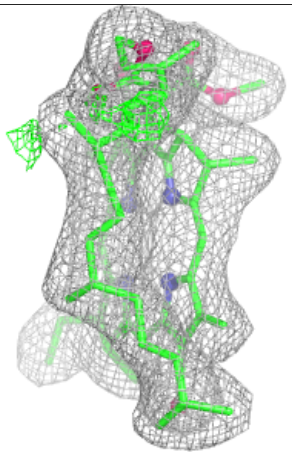


Electron density around BPB LLL 303:

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

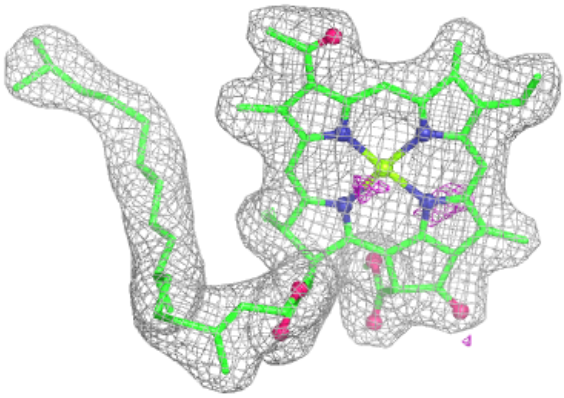


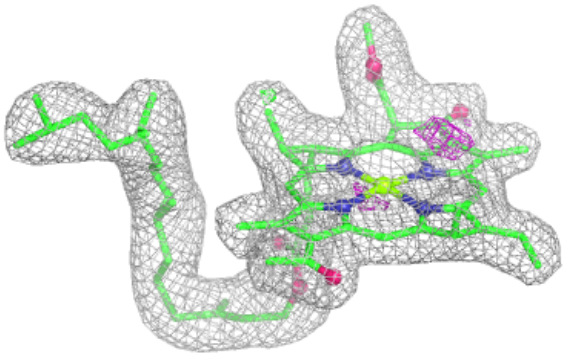


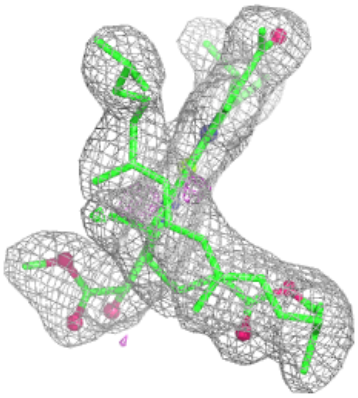


Electron density around BCB LLL 302:

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

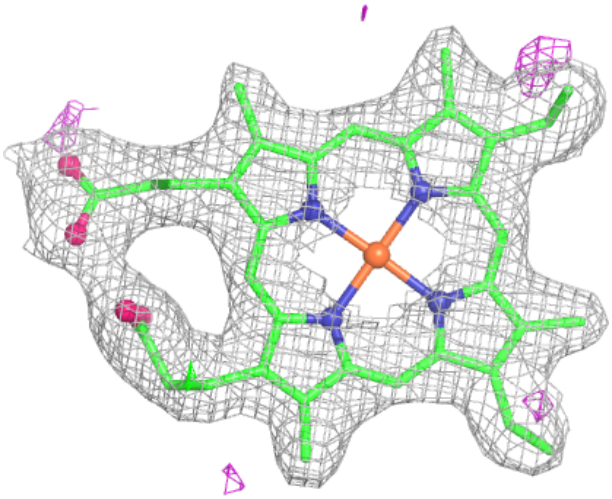


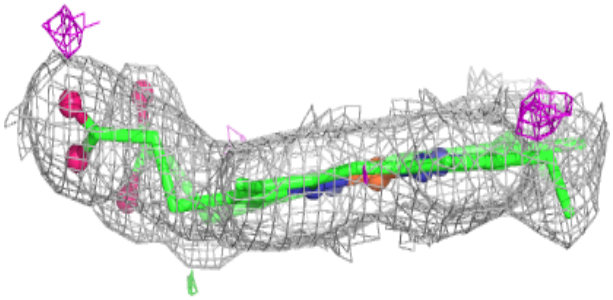


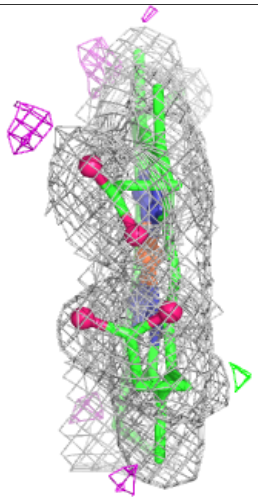


Electron density around HEC CCC 402:

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

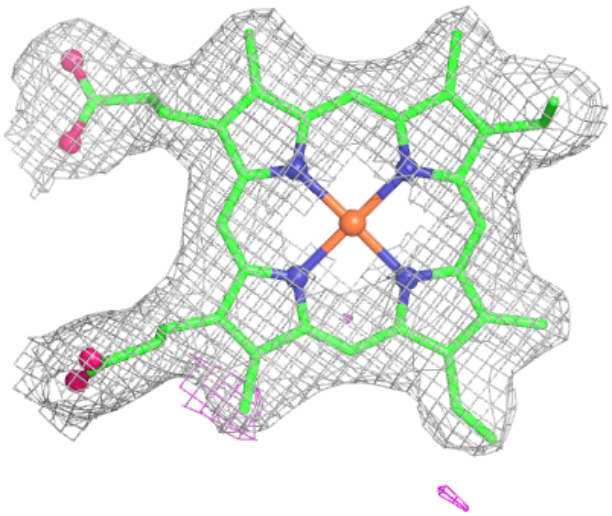


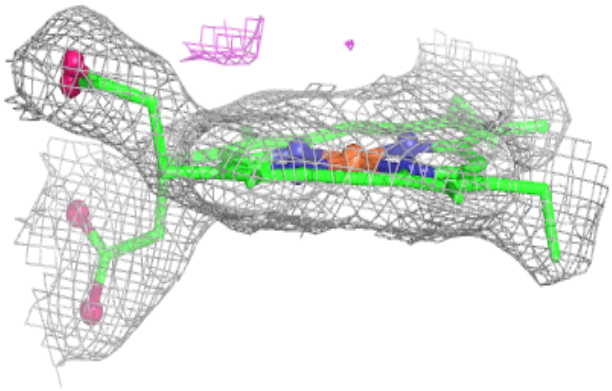


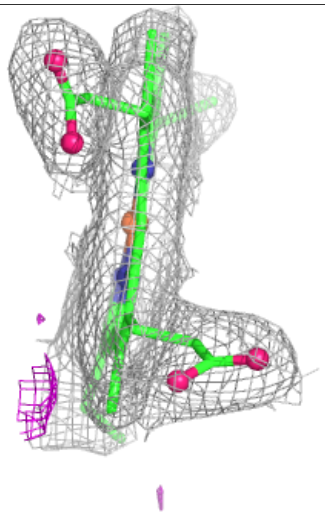


Electron density around HEC CCC 401:

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

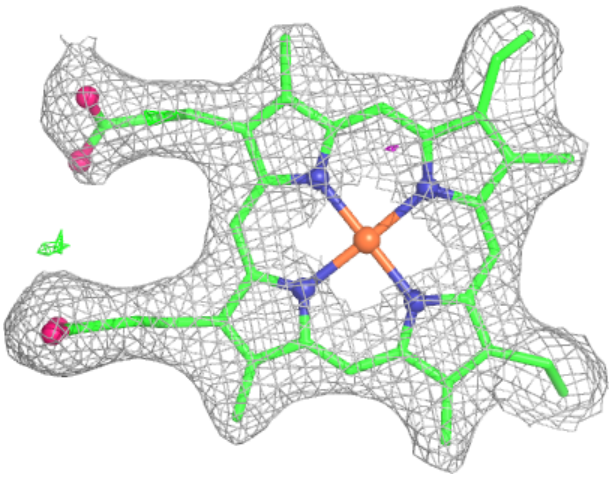


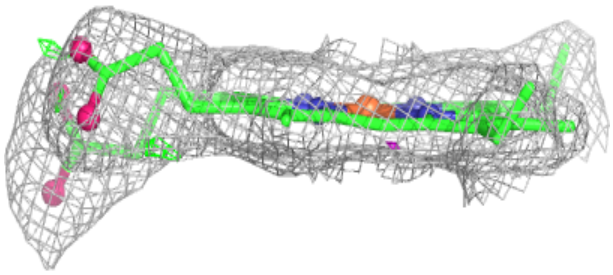


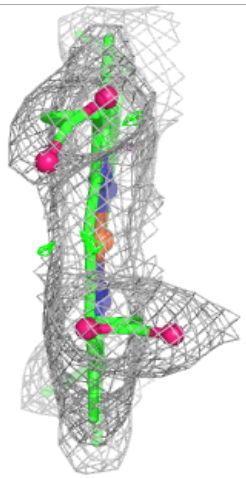


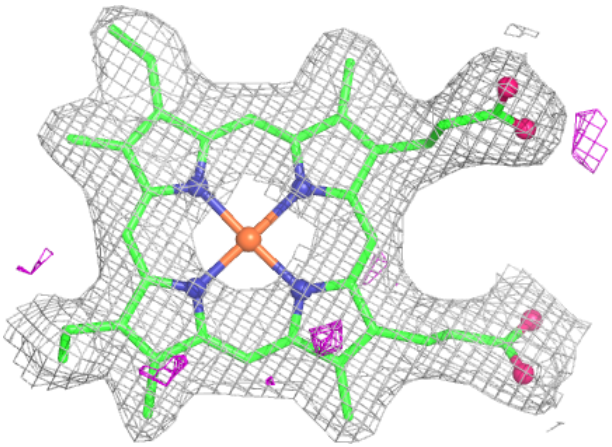
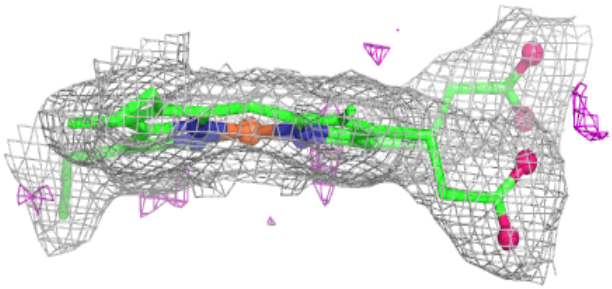
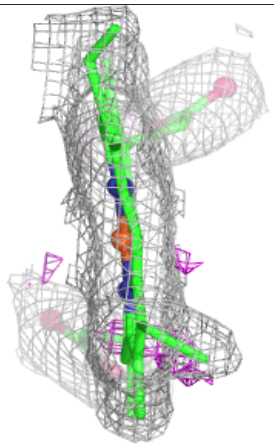
Electron density around HEC CCC 404:

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







Electron density around HEC CCC 403: $2mF_o$-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.