



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:43 PM UTC

PDB ID : 7Q7Q / pdb_00007q7q
Title : LIPIDIC CUBIC PHASE SERIAL FEMTOSECOND CRYSTALLOGRA-
PHY STRUCTURE OF A PHOTOSYNTHETIC REACTION CENTRE
Authors : Baath, P.; Banacore, A.; Neutze, R.
Deposited on : 2021-11-09
Resolution : 2.25 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

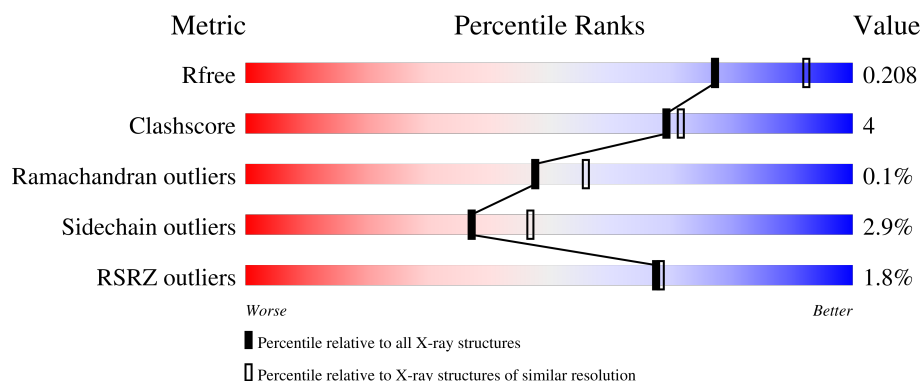
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. 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	336	% 91% 7% ..
2	HHH	258	5% 89% 6% 5%
3	LLL	273	% 92% 8%
4	MMM	323	% 92% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BPB	LLL	303	X	-	-	-
10	BPB	MMM	406	X	-	-	-
6	DGA	CCC	405	X	-	-	-
9	BCB	LLL	301	X	-	-	-
9	BCB	LLL	302	X	-	-	-
9	BCB	MMM	404	X	-	-	-
9	BCB	MMM	405	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 10609 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
1	CCC	332	Total	C	N	O	S	0	2	0
			2615	1648	470	479	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	HHH	246	Total	C	N	O	S	0	1	0
			1945	1243	335	365	2			

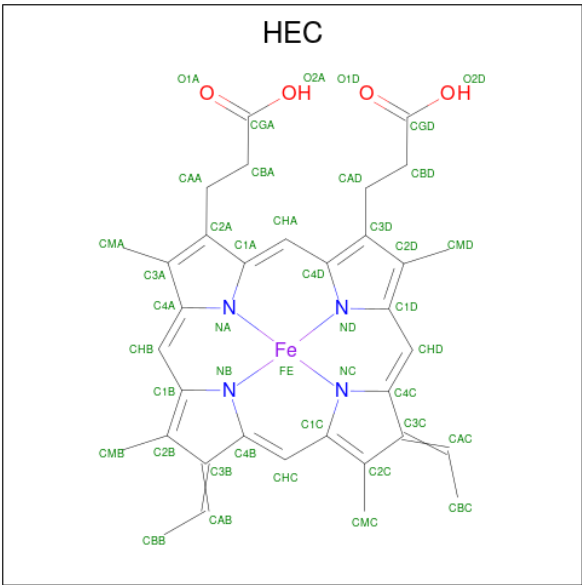
- Molecule 3 is a protein called Reaction center protein L chain.

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

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

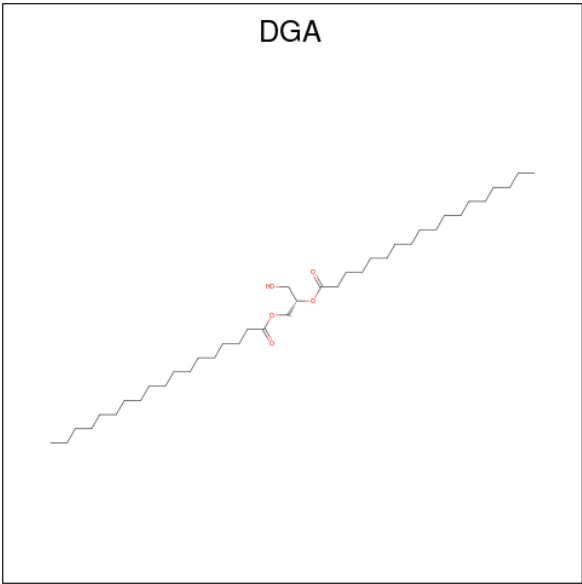
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	MMM	323	Total	C	N	O	S	0	1	0
			2565	1708	422	424	11			

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



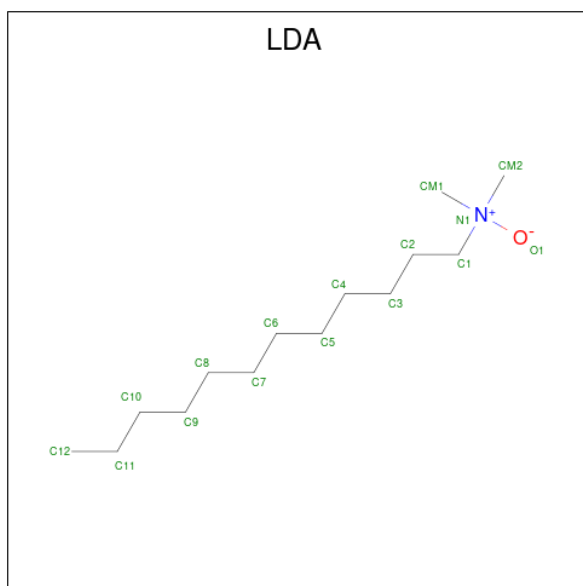
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	CCC	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	CCC	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	CCC	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	CCC	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



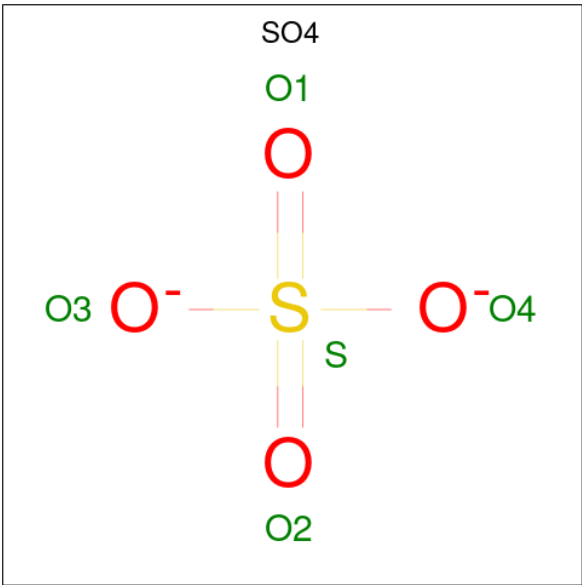
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	21	0
			44	39	5		

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



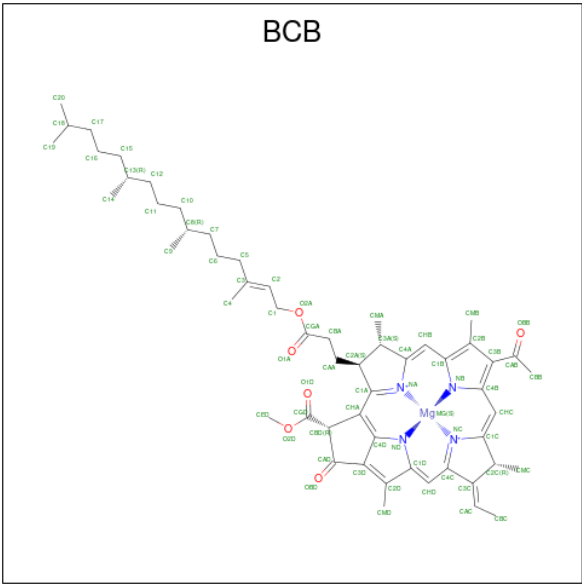
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	HHH	1	Total	C	N	O	0	0
			16	14	1	1		
7	HHH	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



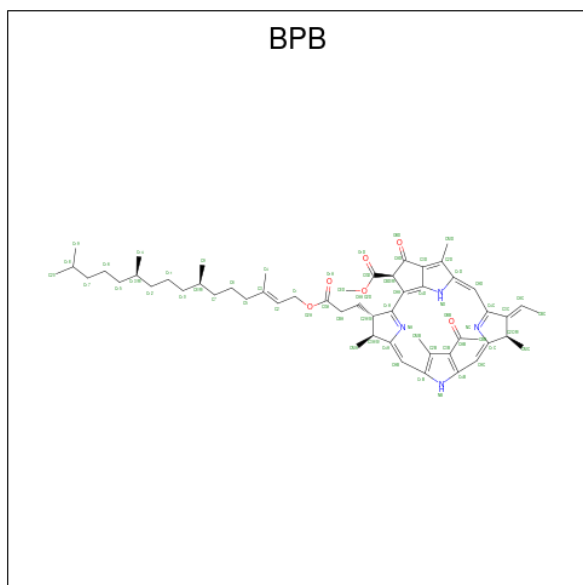
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	HHH	1	Total	O	S	0	0
			5	4	1		
8	MMM	1	Total	O	S	0	0
			5	4	1		
8	MMM	1	Total	O	S	0	0
			5	4	1		
8	MMM	1	Total	O	S	0	0
			5	4	1		
8	MMM	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆).



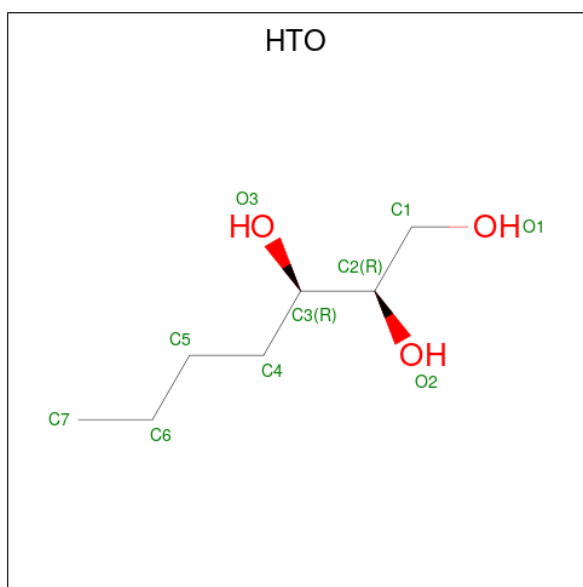
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	LLL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	LLL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	MMM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	MMM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



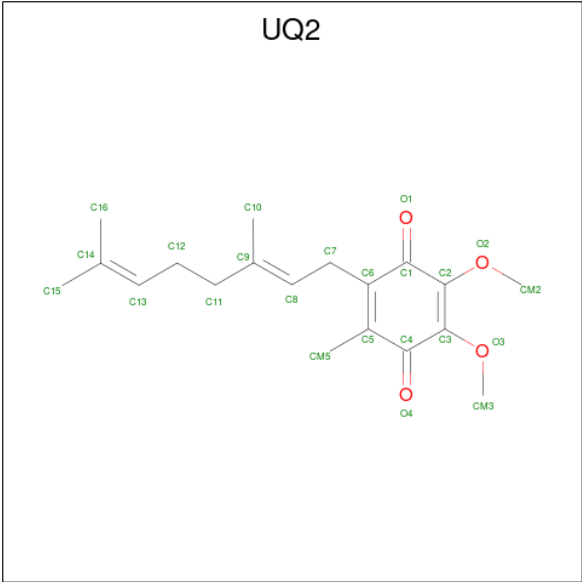
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	LLL	1	Total	C	N	O	0	0
			65	55	4	6		
10	MMM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 12 is UBIQUINONE-2 (CCD ID: UQ2) (formula: C₁₉H₂₆O₄).

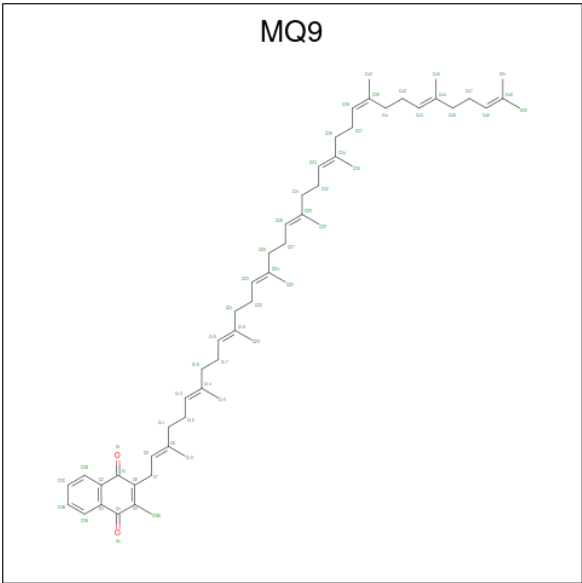


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	LLL	1	Total	C	O	0	0
			23	19	4		
12	MMM	1	Total	C	O	0	1
			46	38	8		

- Molecule 13 is FE (II) ION (CCD ID: FE2) (formula: Fe).

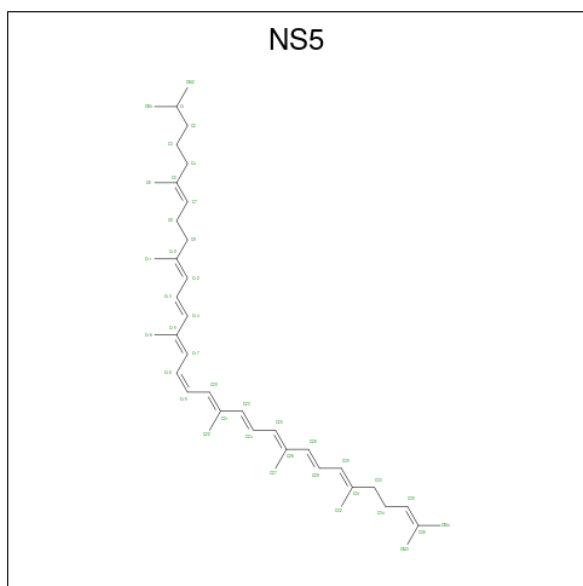
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	MMM	1	Total	Fe	0	0
			1	1		

- Molecule 14 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



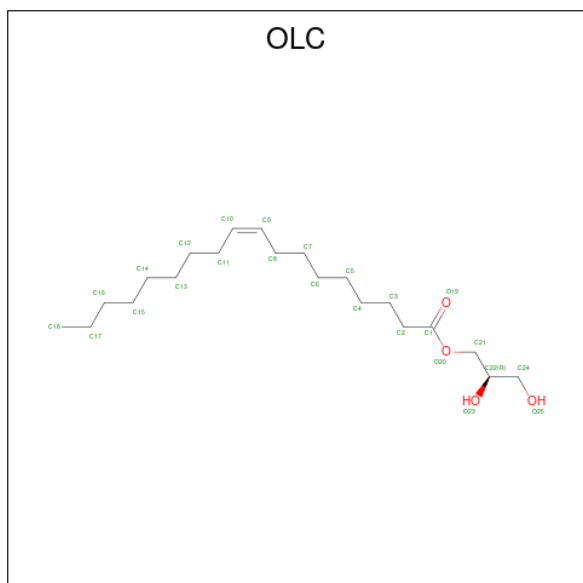
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	MMM	1	Total	C	O	0	0
			58	56	2		

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



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

- Molecule 16 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
16	MMM	1	Total	C	O	0	0
			25	21	4		
16	MMM	1	Total	C	O	0	0
			25	21	4		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	CCC	105	Total	O	0	0
			105	105		
17	HHH	48	Total	O	0	0
			48	48		
17	LLL	46	Total	O	0	0
			46	46		
17	MMM	68	Total	O	0	0
			68	68		

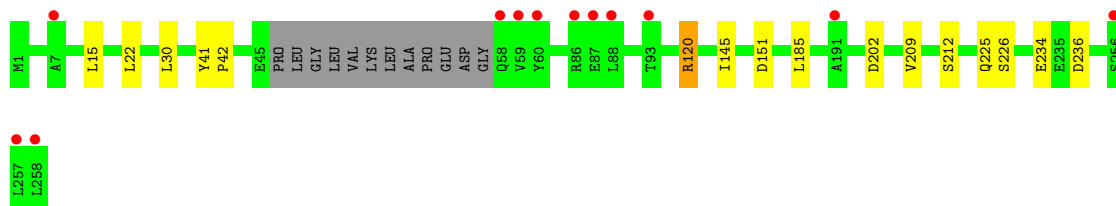
3 Residue-property plots [i](#)

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



- Molecule 2: Reaction center protein H chain



- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.66Å 125.13Å 182.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.70 – 2.25 23.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.70-2.25) 99.9 (23.70-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.203 0.177 , 0.208	Depositor DCC
R_{free} test set	24135 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	7.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10609	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FE2, HTO, UQ2, MQ9, HEC, BPB, FME, BCB, NS5, LDA, SO4, OLC, DGA

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	0.99	0/2688	1.33	0/3662
2	HHH	1.00	0/1979	1.32	0/2700
3	LLL	0.98	0/2267	1.41	3/3095 (0.1%)
4	MMM	0.96	0/2670	1.35	1/3652 (0.0%)
All	All	0.98	0/9604	1.35	4/13109 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LLL	153	HIS	CA-CB-CG	6.87	120.67	113.80
4	MMM	180	HIS	CA-CB-CG	5.99	119.79	113.80
3	LLL	201	GLY	CA-C-O	-5.71	117.43	121.88
3	LLL	164	TYR	CB-CA-C	5.09	119.33	111.13

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	2615	0	2597	16	0
2	HHH	1945	0	1941	6	0
3	LLL	2172	0	2097	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	MMM	2565	0	2458	17	0
5	CCC	172	0	120	4	0
6	CCC	44	0	72	1	0
7	HHH	32	0	62	1	0
7	MMM	80	0	155	6	0
8	HHH	5	0	0	0	0
8	MMM	20	0	0	1	0
9	LLL	132	0	144	3	0
9	MMM	132	0	144	3	0
10	LLL	65	0	74	1	0
10	MMM	65	0	74	5	0
11	LLL	60	0	96	0	0
11	MMM	20	0	32	1	0
12	LLL	23	0	26	4	0
12	MMM	46	0	52	6	0
13	MMM	1	0	0	0	0
14	MMM	58	0	80	0	0
15	MMM	40	0	60	6	0
16	MMM	50	0	80	0	0
17	CCC	105	0	0	0	0
17	HHH	48	0	0	2	0
17	LLL	46	0	0	0	0
17	MMM	68	0	0	2	0
All	All	10609	0	10364	73	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 4.

The worst 5 of 73 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:250:ALA:H	3:LLL:159:ASN:HD21	1.29	0.81
4:MMM:159:GLY:HA3	15:MMM:407:NS5:H272	1.64	0.80
10:MMM:406:BPB:HHC	10:MMM:406:BPB:HBBB	1.63	0.79
12:MMM:416[A]:UQ2:H101	12:MMM:416[A]:UQ2:H162	1.67	0.74
3:LLL:226:ALA:HA	12:LLL:309:UQ2:H3M2	1.70	0.73

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	332/336 (99%)	316 (95%)	16 (5%)	0	100	100
2	HHH	243/258 (94%)	237 (98%)	6 (2%)	0	100	100
3	LLL	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
4	MMM	322/323 (100%)	314 (98%)	7 (2%)	1 (0%)	36	40
All	All	1169/1190 (98%)	1132 (97%)	36 (3%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	MMM	193	ASN

5.3.2 Protein sidechains ⓘ

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	283/282 (100%)	275 (97%)	8 (3%)	38	48
2	HHH	204/212 (96%)	196 (96%)	8 (4%)	28	35
3	LLL	219/218 (100%)	213 (97%)	6 (3%)	39	49
4	MMM	250/249 (100%)	243 (97%)	7 (3%)	38	48
All	All	956/961 (100%)	927 (97%)	29 (3%)	37	45

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	HHH	226	SER
4	MMM	214	PHE
3	LLL	82	GLU
4	MMM	67	LEU
3	LLL	12	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.41	0	8,9,11	0.60	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	-	2/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	HHH	1	FME	O1-CN-N-CA
2	HHH	1	FME	CA-CB-CG-SD

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 39 ligands modelled in this entry, 1 is monoatomic - leaving 38 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	CCC	401	1	46,50,50	1.58	3 (6%)	58,82,82	2.25	9 (15%)
8	SO4	MMM	417	-	4,4,4	0.32	0	6,6,6	0.10	0
8	SO4	MMM	419	-	4,4,4	0.33	0	6,6,6	0.07	0
11	HTO	LLL	310	-	9,9,9	0.64	0	10,10,10	0.91	0
7	LDA	MMM	413	-	13,15,15	0.15	0	14,17,17	0.24	0
11	HTO	MMM	415	-	9,9,9	0.81	0	10,10,10	0.55	0
12	UQ2	MMM	416[A]	-	23,23,23	2.00	2 (8%)	30,31,31	1.60	7 (23%)
7	LDA	MMM	409	-	13,15,15	0.13	0	14,17,17	0.26	0
7	LDA	HHH	1301	-	13,15,15	0.20	0	14,17,17	0.18	0
7	LDA	MMM	402	-	13,15,15	0.22	0	14,17,17	0.30	0
5	HEC	CCC	403	1	46,50,50	1.55	3 (6%)	58,82,82	1.59	5 (8%)
11	HTO	LLL	305	-	9,9,9	1.02	1 (11%)	10,10,10	1.08	0
11	HTO	LLL	308	-	9,9,9	0.58	0	10,10,10	0.70	0
11	HTO	MMM	408	-	9,9,9	0.59	0	10,10,10	0.69	0
12	UQ2	MMM	416[B]	-	23,23,23	2.01	2 (8%)	30,31,31	1.30	4 (13%)
16	OLC	MMM	414	-	24,24,24	1.03	1 (4%)	25,25,25	1.10	2 (8%)
9	BCB	MMM	404	-	60,74,74	2.57	18 (30%)	59,115,115	2.76	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HTO	LLL	304	-	9,9,9	0.57	0	10,10,10	0.67	0
5	HEC	CCC	404	1	46,50,50	1.67	4 (8%)	58,82,82	1.64	9 (15%)
9	BCB	MMM	405	-	60,74,74	2.63	17 (28%)	59,115,115	2.60	16 (27%)
5	HEC	CCC	402	1	46,50,50	1.62	2 (4%)	58,82,82	1.29	4 (6%)
10	BPB	LLL	303	-	57,70,70	2.36	14 (24%)	55,101,101	2.04	11 (20%)
7	LDA	HHH	1302	-	13,15,15	0.12	0	14,17,17	0.25	0
6	DGA	CCC	405	-	43,43,43	2.84	3 (6%)	45,45,45	3.44	7 (15%)
8	SO4	HHH	1303	-	4,4,4	0.29	0	6,6,6	0.08	0
9	BCB	LLL	302	-	60,74,74	2.67	18 (30%)	59,115,115	2.70	15 (25%)
9	BCB	LLL	301	-	60,74,74	2.67	18 (30%)	59,115,115	2.77	20 (33%)
15	NS5	MMM	407	-	39,39,39	0.85	1 (2%)	46,46,46	1.75	10 (21%)
8	SO4	MMM	420	-	4,4,4	0.34	0	6,6,6	0.07	0
8	SO4	MMM	418	-	4,4,4	0.34	0	6,6,6	0.12	0
11	HTO	LLL	307	-	9,9,9	0.84	0	10,10,10	1.32	1 (10%)
10	BPB	MMM	406	-	57,70,70	2.49	14 (24%)	55,101,101	2.19	14 (25%)
16	OLC	MMM	410	-	24,24,24	0.96	1 (4%)	25,25,25	0.70	1 (4%)
14	MQ9	MMM	403	-	59,59,59	0.40	0	73,75,75	0.47	0
7	LDA	MMM	412	-	13,15,15	0.24	0	14,17,17	0.24	0
11	HTO	LLL	306	-	9,9,9	0.51	0	10,10,10	0.52	0
12	UQ2	LLL	309	-	23,23,23	1.97	2 (8%)	30,31,31	1.59	7 (23%)
7	LDA	MMM	411	-	13,15,15	0.21	0	14,17,17	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	CCC	401	1	-	6/14/54/54	-
11	HTO	LLL	310	-	-	6/10/10/10	-
11	HTO	MMM	415	-	-	4/10/10/10	-
7	LDA	MMM	413	-	-	7/13/13/13	-
12	UQ2	MMM	416[A]	-	-	4/15/39/39	0/1/1/1
7	LDA	MMM	409	-	-	9/13/13/13	-
7	LDA	HHH	1301	-	-	7/13/13/13	-
7	LDA	MMM	402	-	-	5/13/13/13	-
5	HEC	CCC	403	1	-	4/14/54/54	-
11	HTO	LLL	305	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HTO	LLL	308	-	-	3/10/10/10	-
11	HTO	MMM	408	-	-	7/10/10/10	-
12	UQ2	MMM	416[B]	-	-	6/15/39/39	0/1/1/1
16	OLC	MMM	414	-	-	11/24/24/24	-
9	BCB	MMM	404	-	3/3/21/26	11/37/137/137	-
11	HTO	LLL	304	-	-	2/10/10/10	-
5	HEC	CCC	404	1	-	4/14/54/54	-
9	BCB	MMM	405	-	3/3/21/26	6/37/137/137	-
5	HEC	CCC	402	1	-	7/14/54/54	-
10	BPB	LLL	303	-	1/1/18/23	4/37/105/105	0/5/6/6
7	LDA	HHH	1302	-	-	8/13/13/13	-
6	DGA	CCC	405	-	1/1/3/3	19/45/45/45	-
9	BCB	LLL	302	-	3/3/21/26	4/37/137/137	-
9	BCB	LLL	301	-	3/3/21/26	5/37/137/137	-
15	NS5	MMM	407	-	-	5/43/43/43	-
11	HTO	LLL	307	-	-	4/10/10/10	-
10	BPB	MMM	406	-	1/1/18/23	15/37/105/105	0/5/6/6
16	OLC	MMM	410	-	-	12/24/24/24	-
14	MQ9	MMM	403	-	-	4/53/73/73	0/2/2/2
7	LDA	MMM	412	-	-	8/13/13/13	-
11	HTO	LLL	306	-	-	3/10/10/10	-
12	UQ2	LLL	309	-	-	2/15/39/39	0/1/1/1
7	LDA	MMM	411	-	-	10/13/13/13	-

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	405	DGA	CG1-CG2	-16.99	0.97	1.50
10	LLL	303	BPB	C1D-C2D	8.90	1.49	1.39
10	MMM	406	BPB	C1B-C2B	8.83	1.49	1.39
10	MMM	406	BPB	C1D-C2D	8.56	1.48	1.39
12	MMM	416[B]	UQ2	C6-C5	8.29	1.50	1.35

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	CCC	405	DGA	CG1-CG2-CG3	20.16	158.34	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	LLL	301	BCB	C1B-CHB-C4A	11.59	128.78	121.32
5	CCC	401	HEC	CBB-CAB-C3B	-9.76	107.92	127.43
9	MMM	404	BCB	C4B-CHC-C1C	9.54	127.46	121.32
5	CCC	401	HEC	CBC-CAC-C3C	-9.51	108.43	127.43

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	CCC	405	DGA	CG2
9	LLL	301	BCB	NC
9	LLL	301	BCB	NA
9	LLL	301	BCB	ND
9	LLL	302	BCB	NC

5 of 218 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CCC	401	HEC	C2B-C3B-CAB-CBB
5	CCC	401	HEC	C4B-C3B-CAB-CBB
5	CCC	401	HEC	C2C-C3C-CAC-CBC
5	CCC	401	HEC	C4C-C3C-CAC-CBC
5	CCC	402	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

19 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	401	HEC	2	0
11	MMM	415	HTO	1	0
12	MMM	416[A]	UQ2	3	0
7	MMM	409	LDA	1	0
7	HHH	1301	LDA	1	0
7	MMM	402	LDA	1	0
5	CCC	403	HEC	1	0
12	MMM	416[B]	UQ2	3	0
9	MMM	404	BCB	3	0
5	CCC	404	HEC	1	0
10	LLL	303	BPB	1	0
6	CCC	405	DGA	1	0
9	LLL	302	BCB	1	0
9	LLL	301	BCB	2	0
15	MMM	407	NS5	6	0

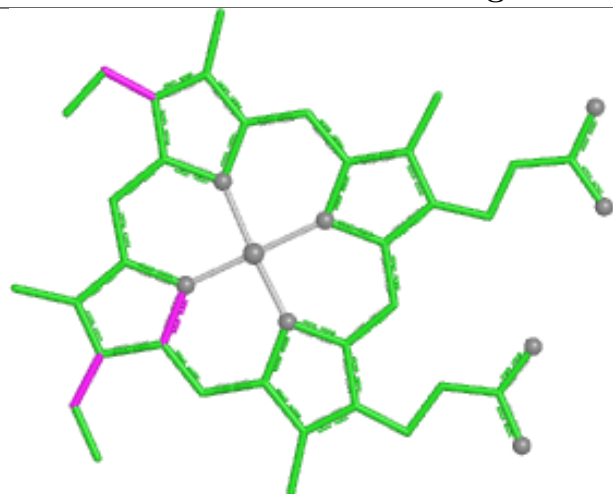
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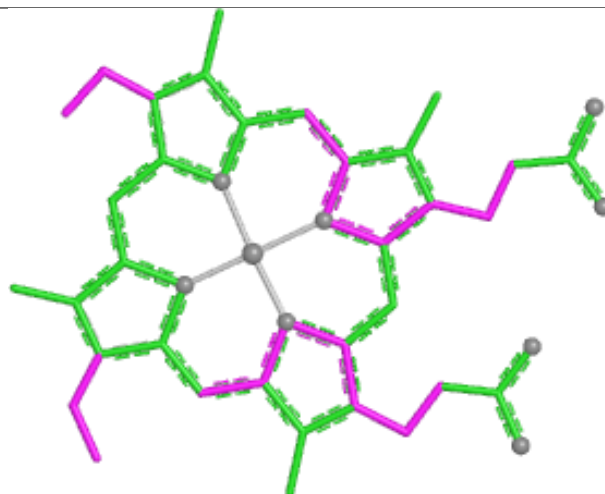
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	MMM	418	SO4	1	0
10	MMM	406	BPB	5	0
12	LLL	309	UQ2	4	0
7	MMM	411	LDA	4	0

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

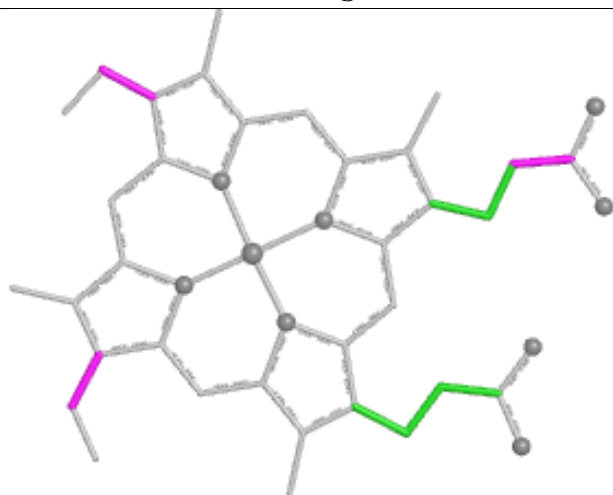
Ligand HEC CCC 401



Bond lengths



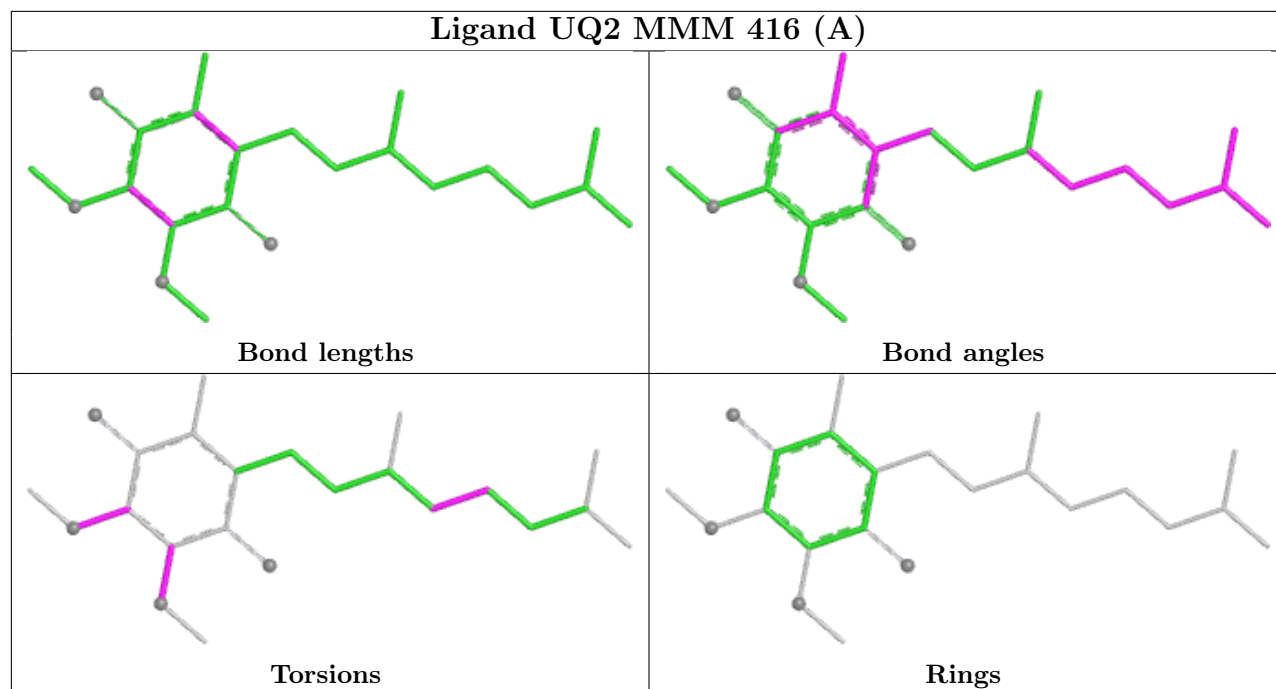
Bond angles



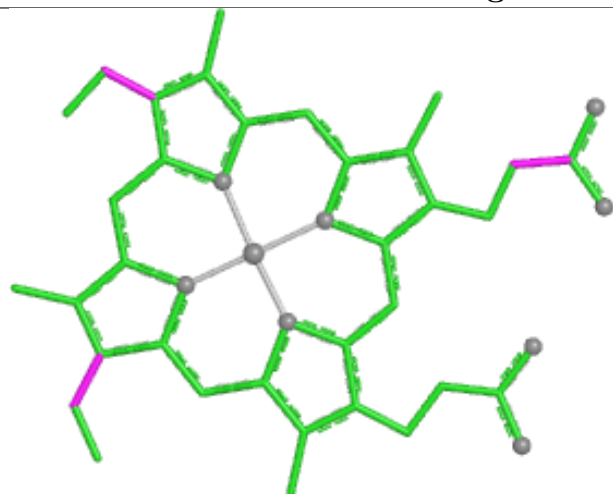
Torsions



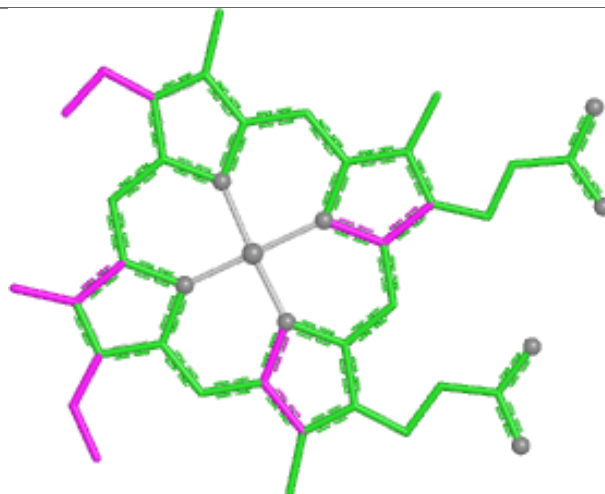
Rings



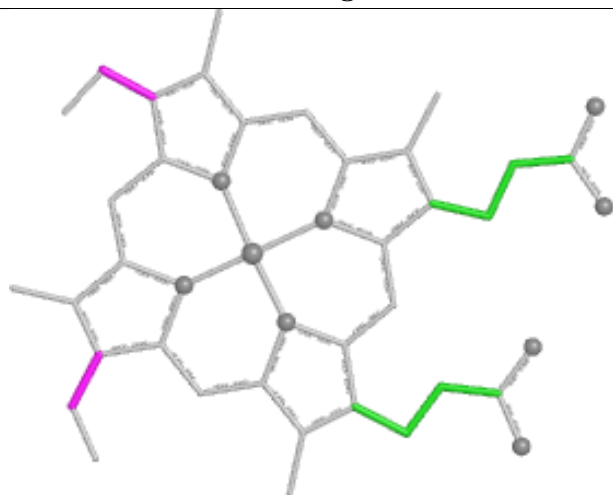
Ligand HEC CCC 403



Bond lengths



Bond angles

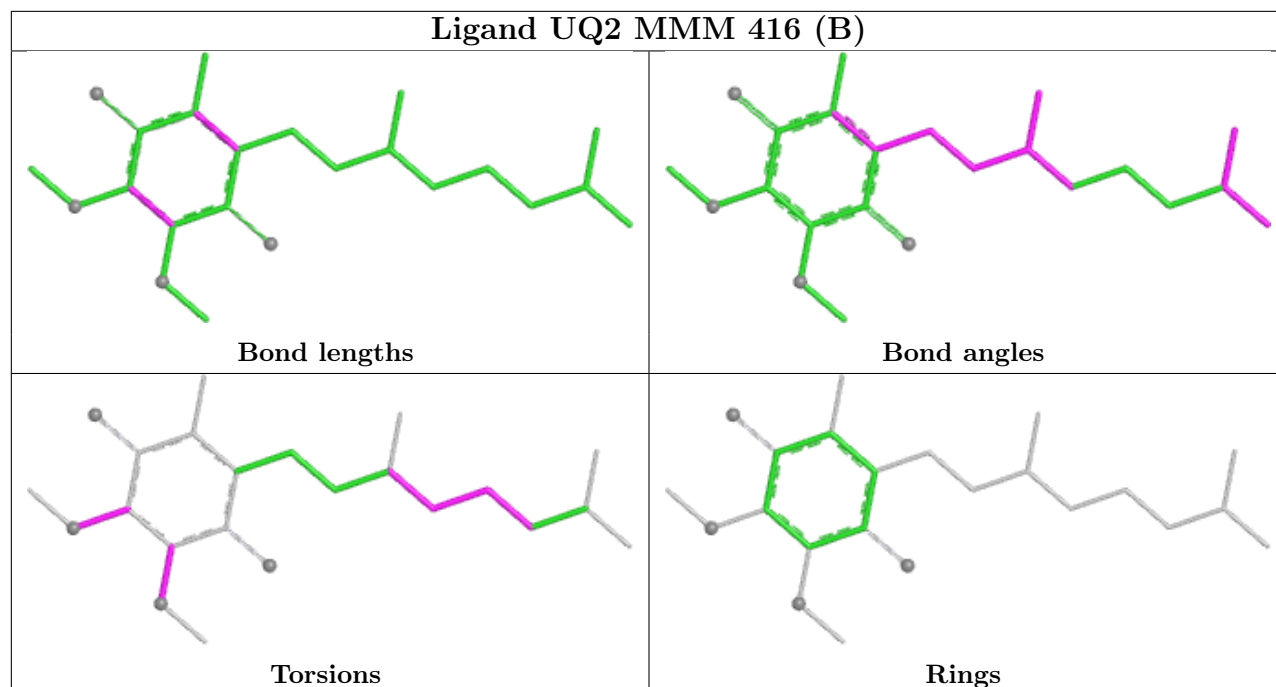


Torsions

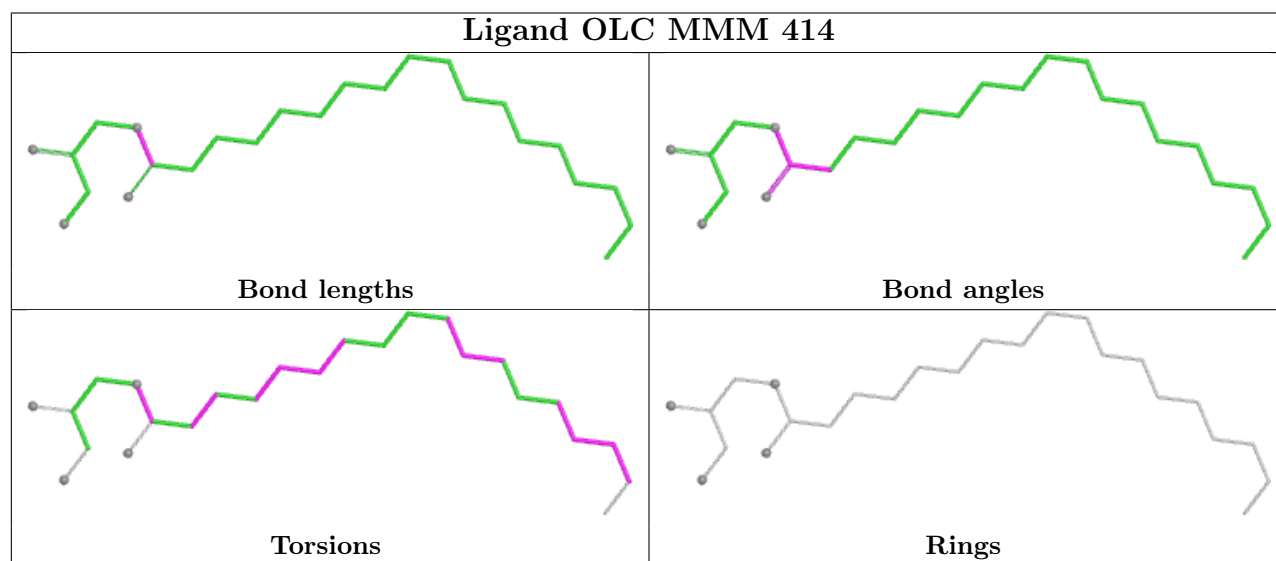


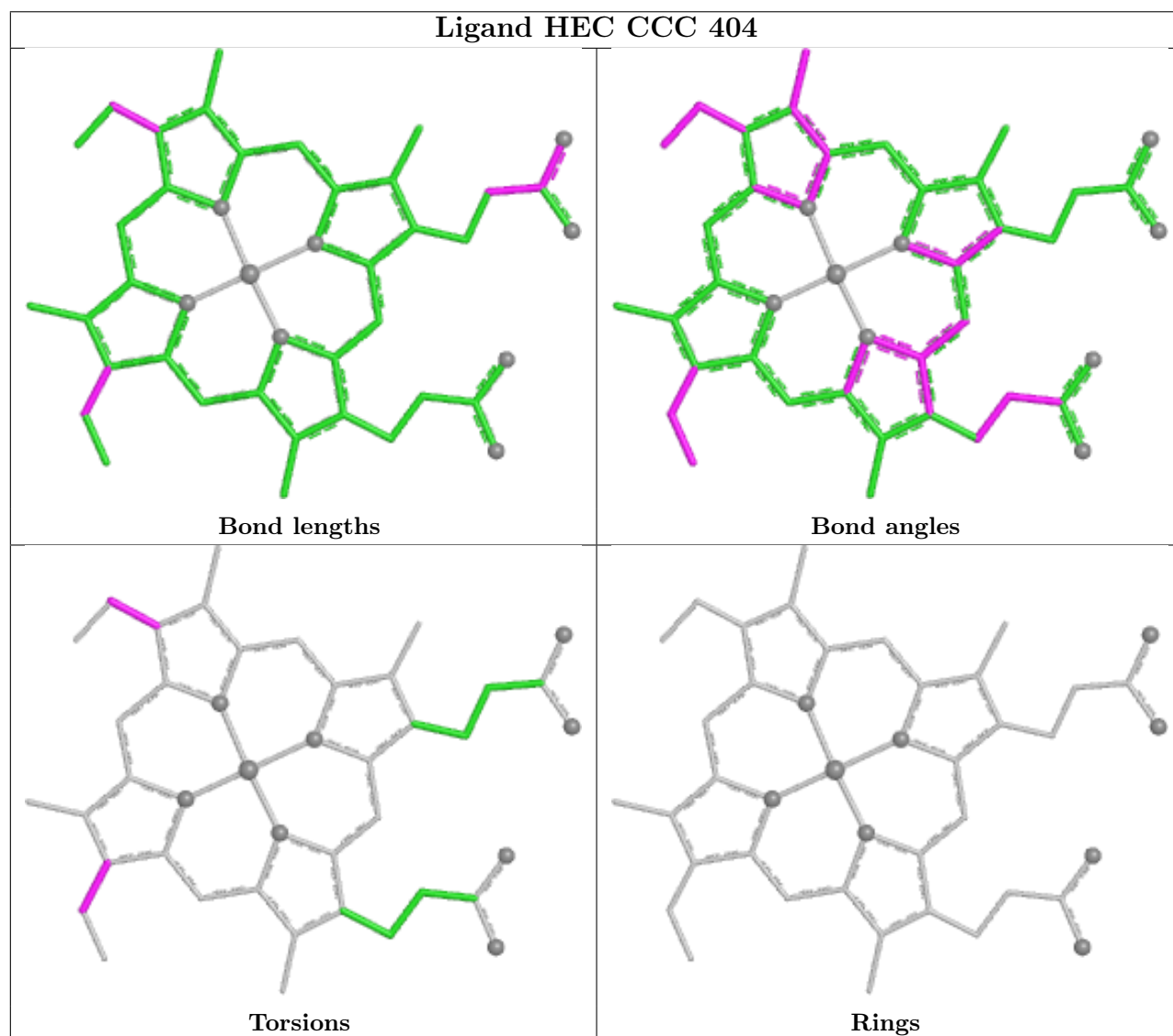
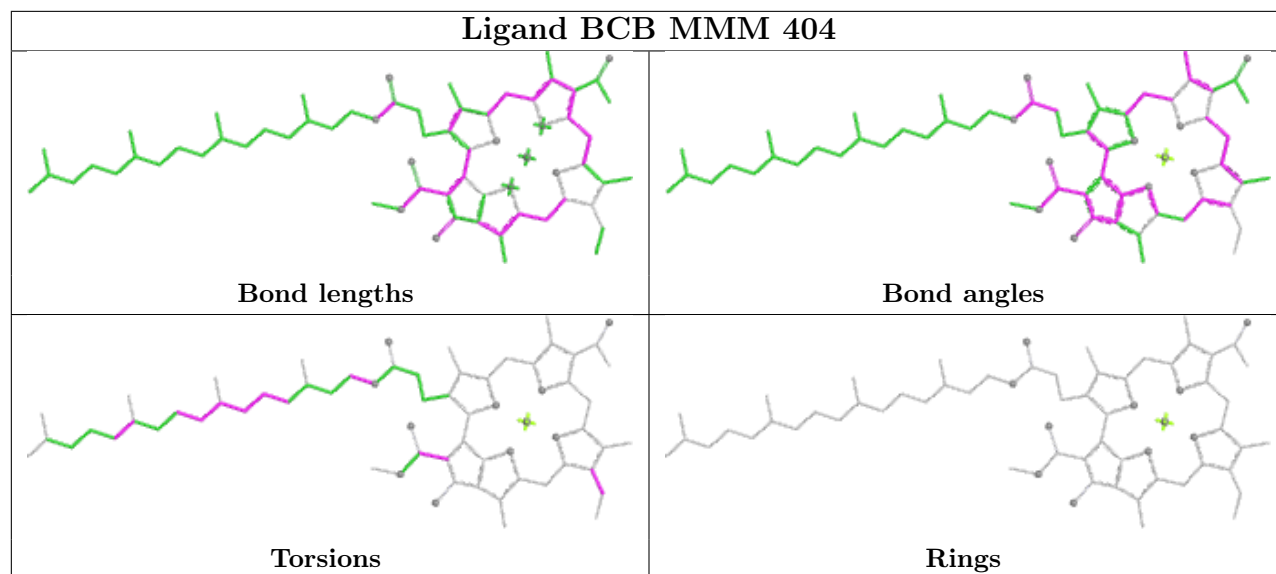
Rings

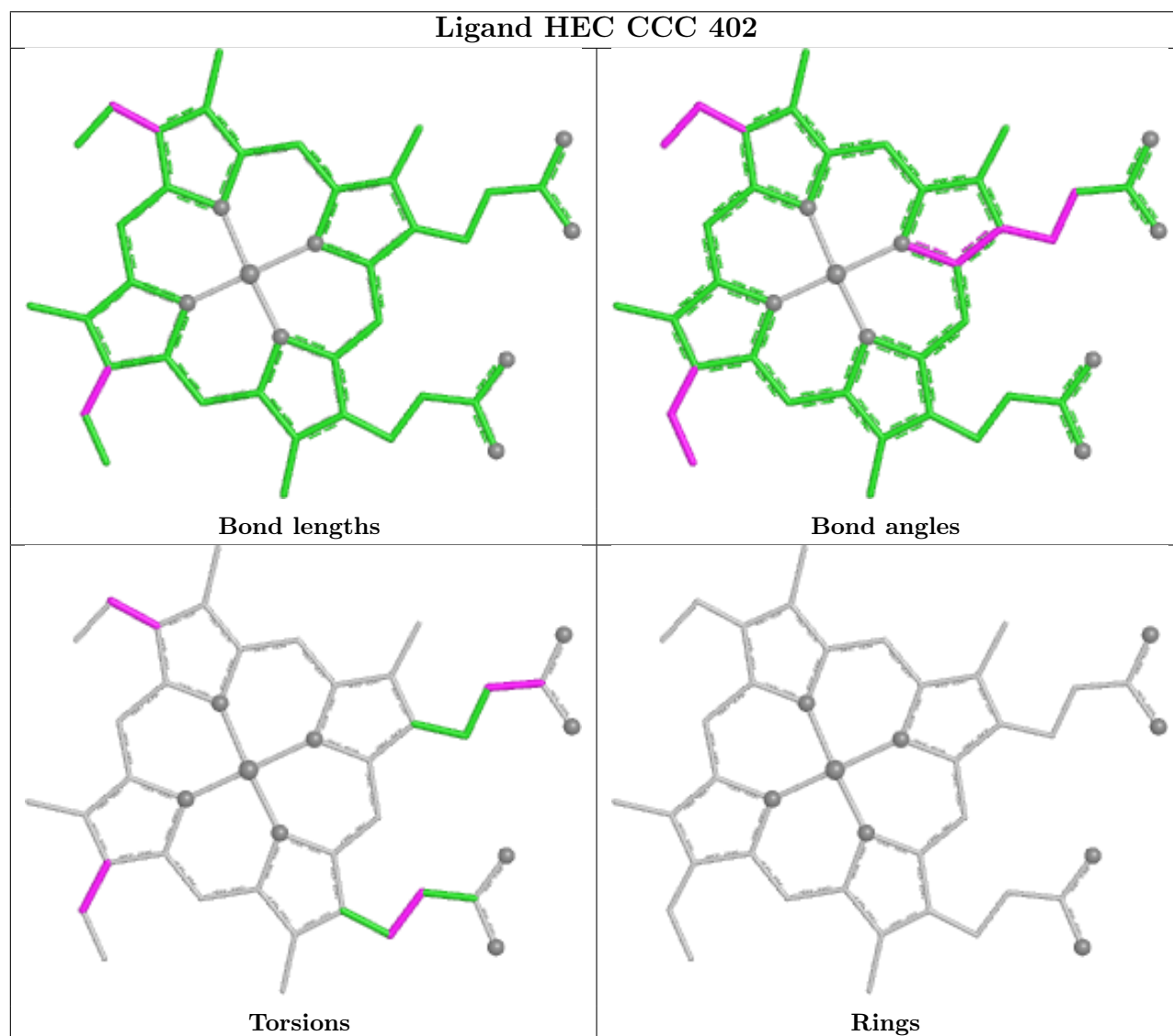
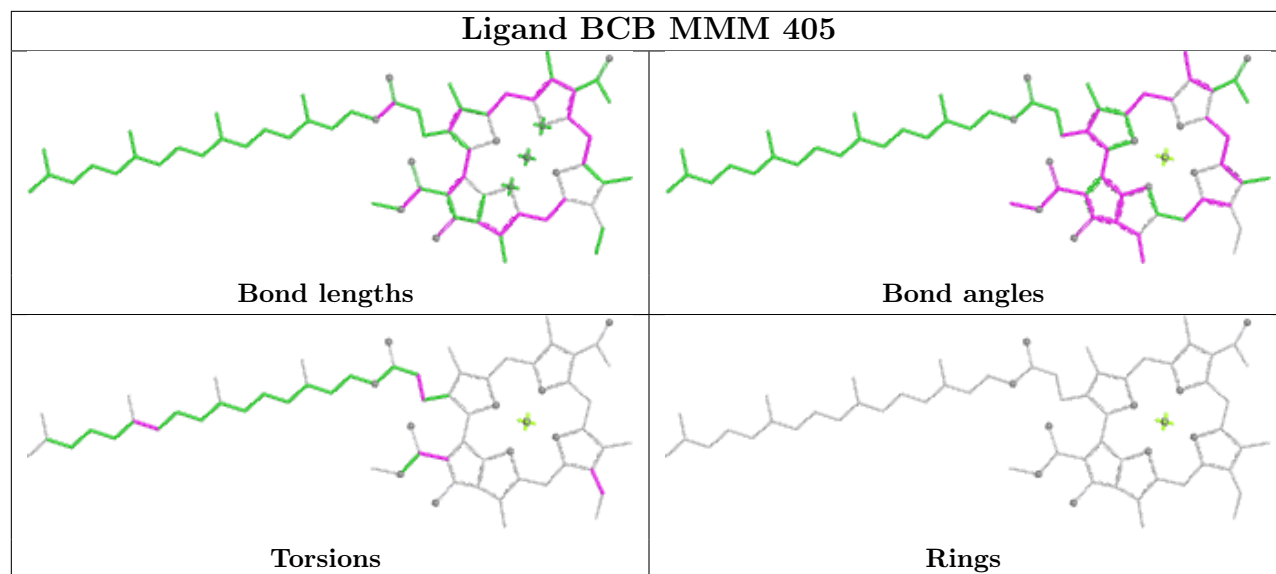
Ligand UQ2 MMM 416 (B)

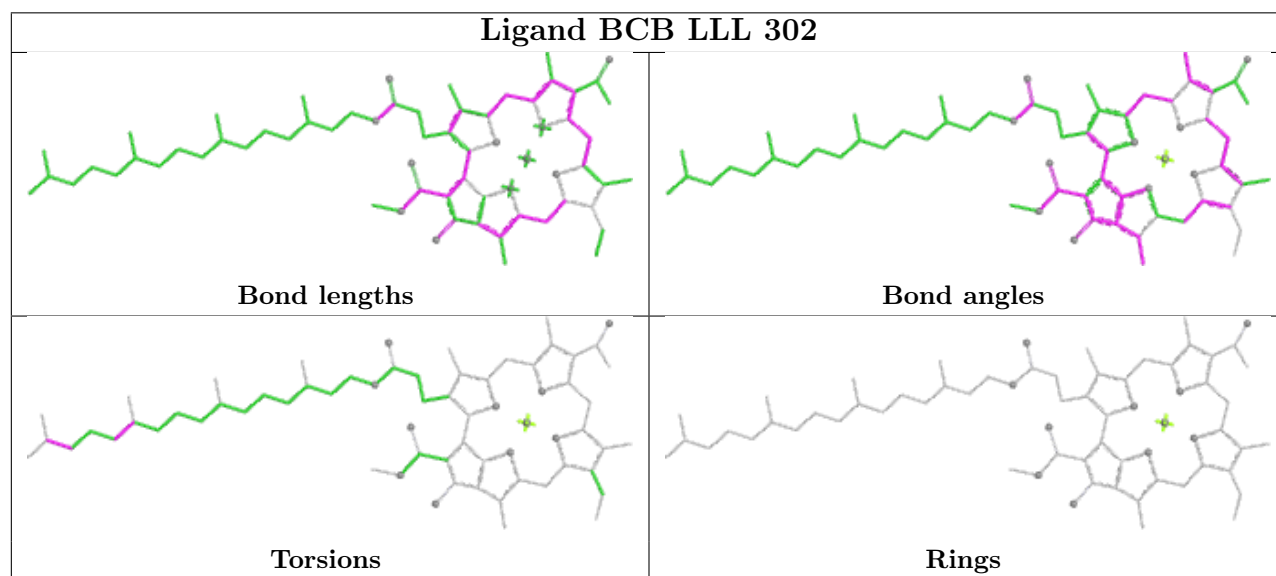
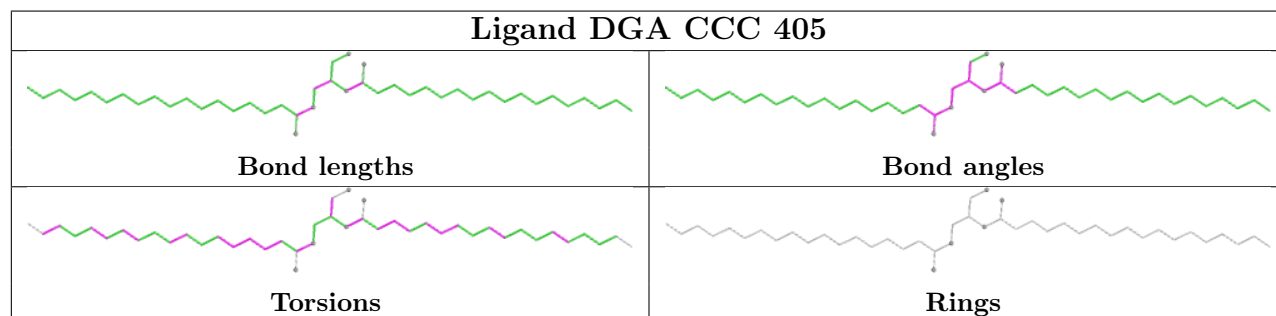
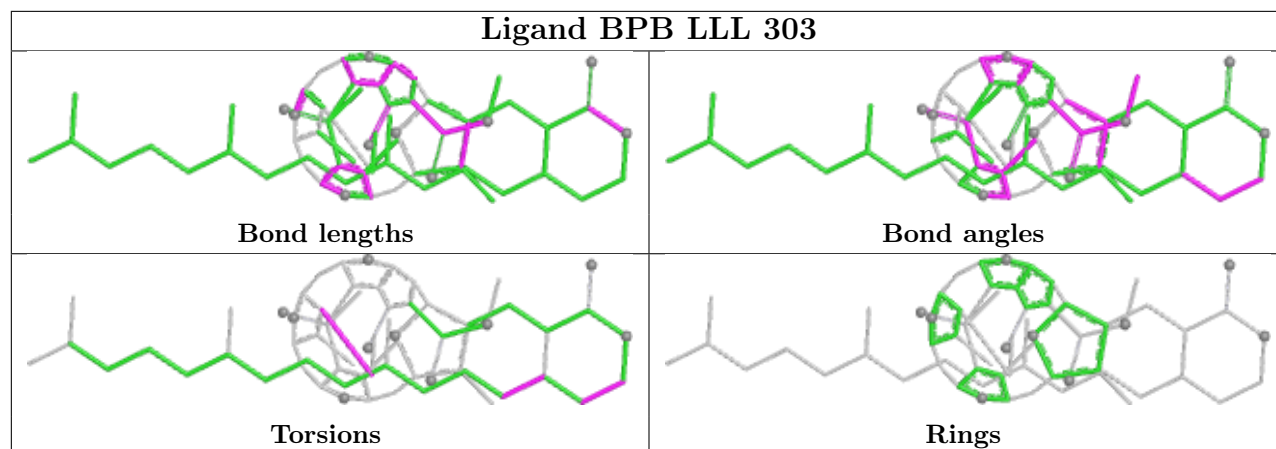


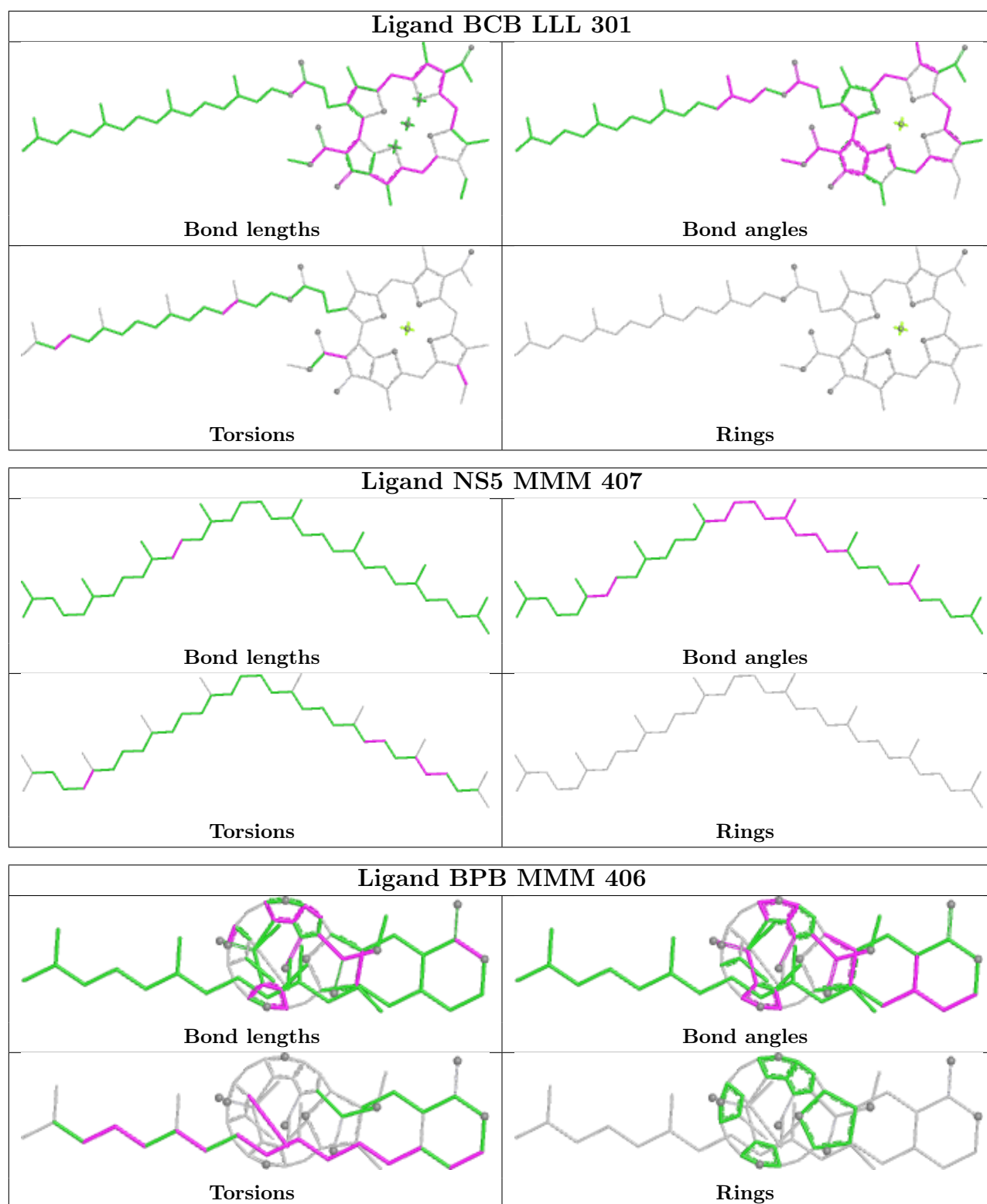
Ligand OLC MMM 414

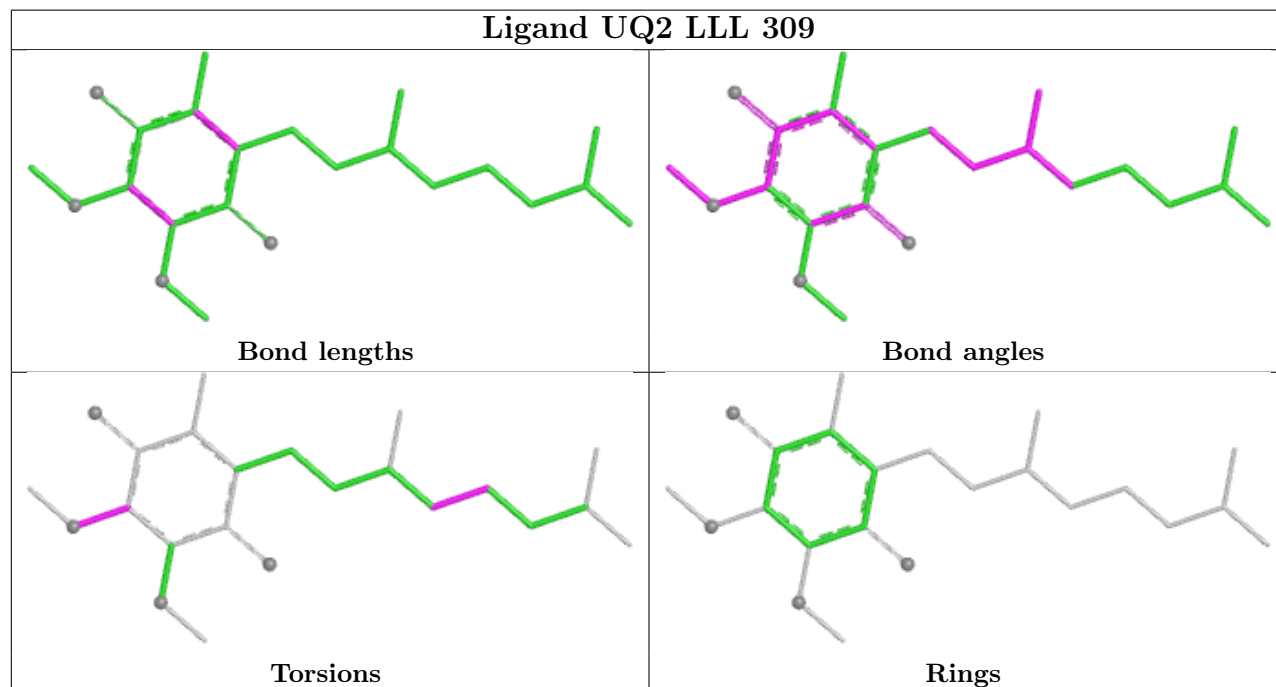
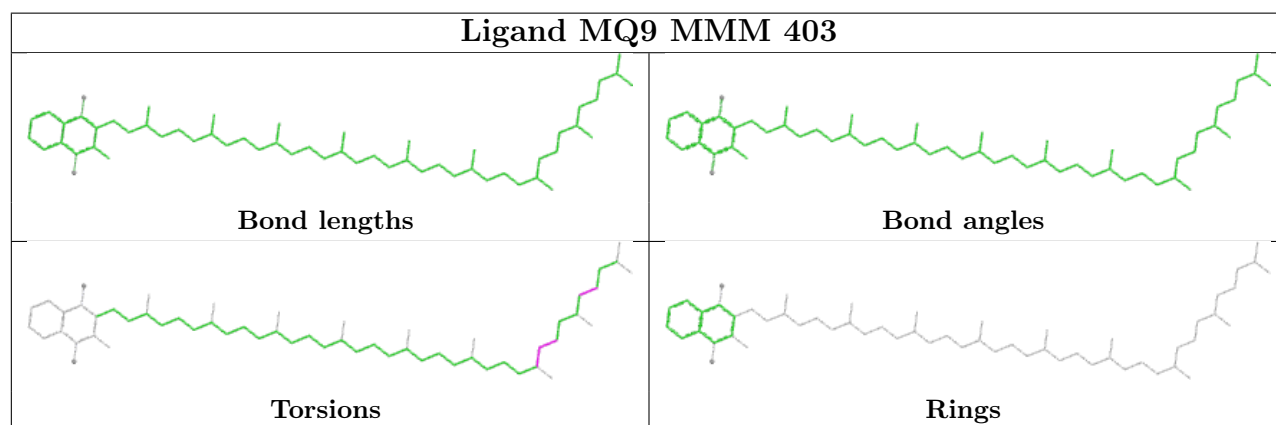
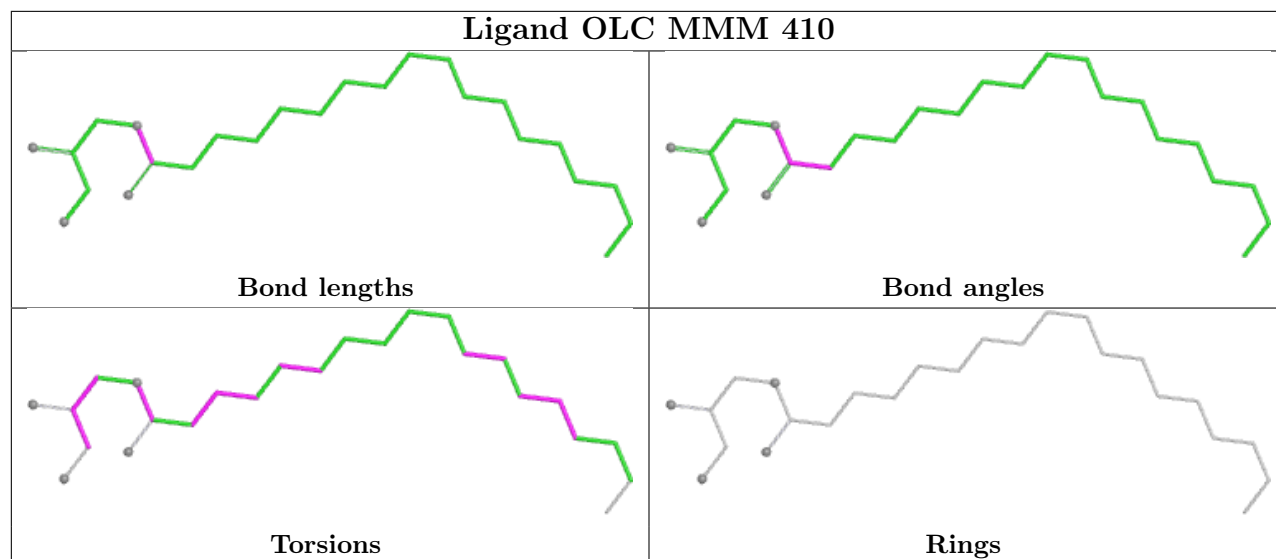












5.7 Other polymers [i](#)

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	332/336 (98%)	-0.26	2 (0%) 85 86	20, 44, 72, 109	2 (0%)
2	HHH	245/258 (94%)	0.09	12 (4%) 35 34	36, 55, 91, 128	1 (0%)
3	LLL	273/273 (100%)	-0.24	3 (1%) 78 79	31, 43, 70, 120	1 (0%)
4	MMM	323/323 (100%)	-0.32	4 (1%) 76 77	27, 42, 68, 92	1 (0%)
All	All	1173/1190 (98%)	-0.20	21 (1%) 67 68	20, 46, 79, 128	5 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HHH	59	VAL	3.9
2	HHH	257	LEU	3.6
2	HHH	258	LEU	3.3
3	LLL	59	TRP	3.0
2	HHH	60	TYR	3.0

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	0.13	60,94,117,121	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
8	SO4	MMM	420	5/5	0.60	0.21	203,207,209,213	5
11	HTO	MMM	415	10/10	0.63	0.21	79,89,97,103	0
11	HTO	LLL	305	10/10	0.69	0.21	67,82,93,95	0
12	UQ2	MMM	416[A]	23/23	0.69	0.26	62,73,85,87	23
12	UQ2	MMM	416[B]	23/23	0.69	0.26	74,82,90,98	23
11	HTO	LLL	306	10/10	0.71	0.20	91,102,111,119	0
11	HTO	LLL	307	10/10	0.71	0.20	91,100,103,105	0
11	HTO	LLL	308	10/10	0.71	0.21	91,108,118,120	0
11	HTO	LLL	304	10/10	0.72	0.19	83,90,91,93	0
7	LDA	HHH	1302	16/16	0.74	0.21	90,103,124,125	0
7	LDA	MMM	413	16/16	0.77	0.17	90,104,120,121	0
6	DGA	CCC	405	44/44	0.77	0.20	86,114,131,136	21
7	LDA	MMM	402	16/16	0.79	0.23	86,94,119,125	0
7	LDA	MMM	412	16/16	0.79	0.21	97,106,123,132	0
16	OLC	MMM	410	25/25	0.79	0.15	99,112,121,122	0
15	NS5	MMM	407	40/40	0.80	0.20	55,93,131,141	0
8	SO4	MMM	419	5/5	0.81	0.10	89,97,108,113	0
12	UQ2	LLL	309	23/23	0.81	0.17	52,65,85,89	0
8	SO4	HHH	1303	5/5	0.82	0.11	90,91,109,111	0
11	HTO	MMM	408	10/10	0.83	0.21	72,99,105,106	0
16	OLC	MMM	414	25/25	0.83	0.16	78,88,106,107	0
7	LDA	MMM	409	16/16	0.84	0.16	81,88,109,117	0
7	LDA	HHH	1301	16/16	0.85	0.17	76,84,103,110	0
11	HTO	LLL	310	10/10	0.88	0.18	89,96,97,97	0
8	SO4	MMM	418	5/5	0.90	0.12	88,96,105,115	0
7	LDA	MMM	411	16/16	0.91	0.18	66,78,110,116	0
14	MQ9	MMM	403	58/58	0.92	0.11	36,58,119,122	0
10	BPB	MMM	406	65/65	0.94	0.10	34,40,110,116	0
9	BCB	MMM	404	66/66	0.94	0.11	32,38,128,136	0
8	SO4	MMM	417	5/5	0.95	0.18	78,78,82,91	0
9	BCB	LLL	301	66/66	0.96	0.07	28,35,53,68	0
10	BPB	LLL	303	65/65	0.96	0.07	32,38,50,53	0
9	BCB	LLL	302	66/66	0.96	0.07	31,35,71,74	0
9	BCB	MMM	405	66/66	0.97	0.07	29,33,65,73	0
5	HEC	CCC	401	43/43	0.97	0.07	33,41,46,50	0
5	HEC	CCC	402	43/43	0.98	0.07	36,43,47,54	0
5	HEC	CCC	404	43/43	0.98	0.07	31,40,53,60	0

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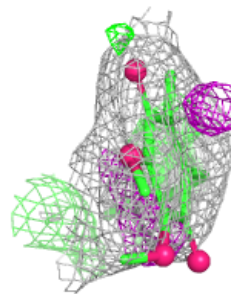
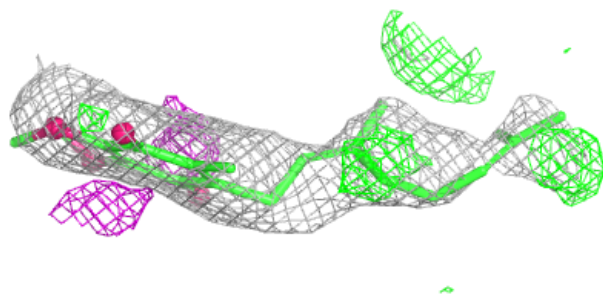
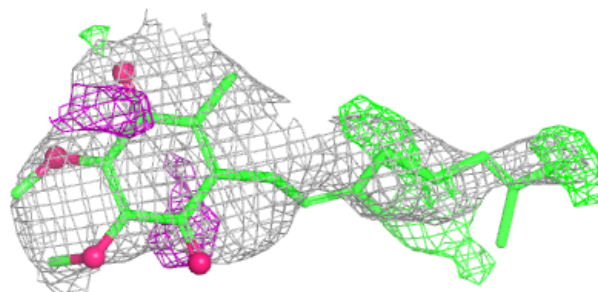
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	HEC	CCC	403	43/43	0.99	0.05	28,31,37,43	0
13	FE2	MMM	401	1/1	0.99	0.02	33,33,33,33	0

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.

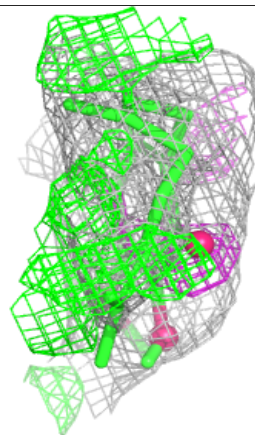
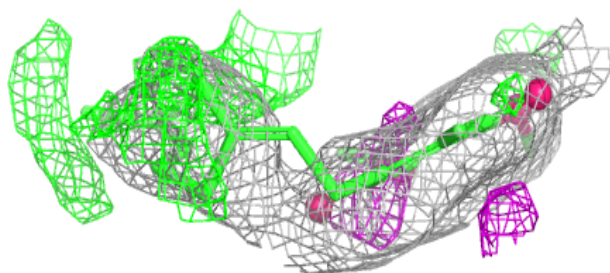
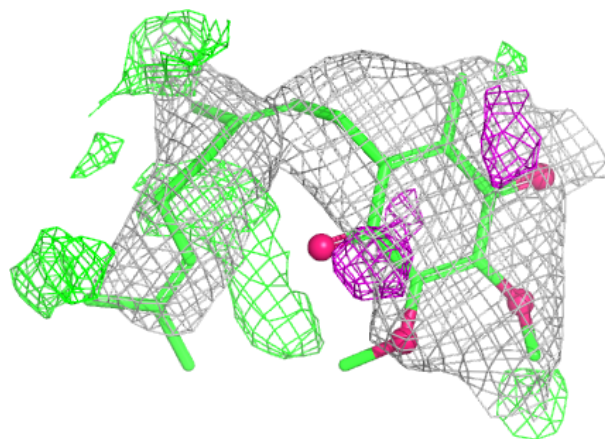
Electron density around UQ2 MMM 416 (A):

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

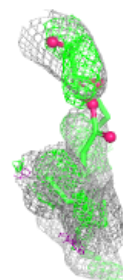
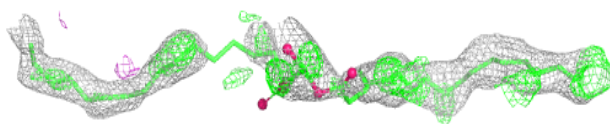
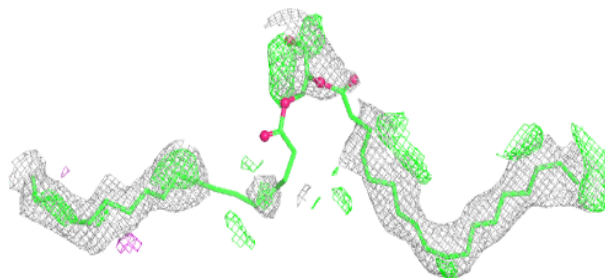


Electron density around UQ2 MMM 416 (B):

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

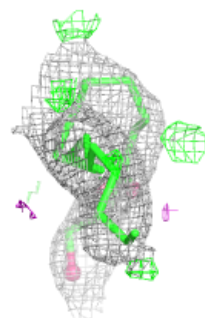
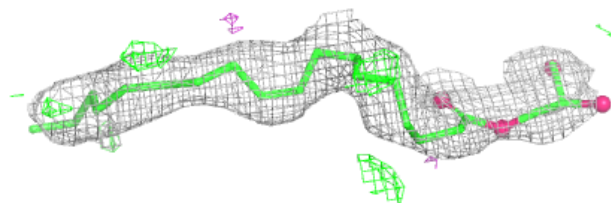
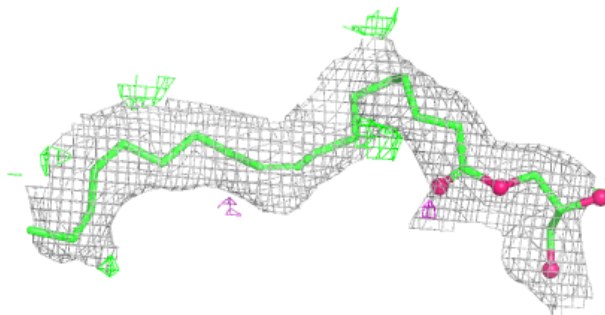
**Electron density around DGA CCC 405:**

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

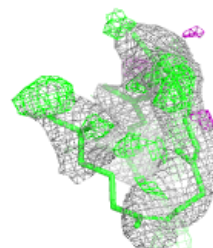
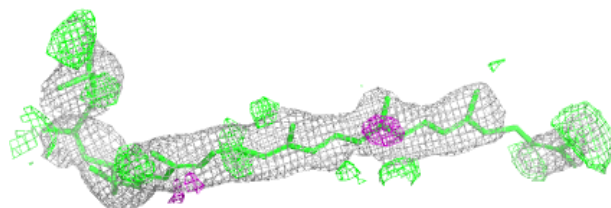
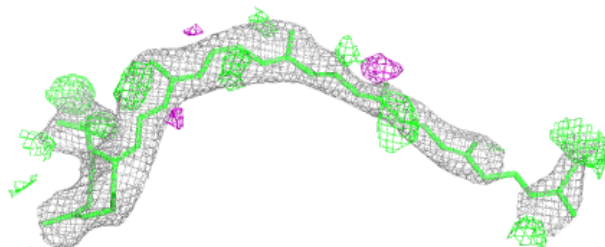


Electron density around OLC MMM 410:

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

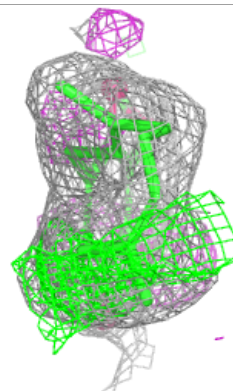
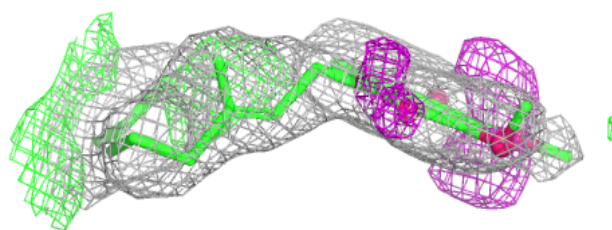
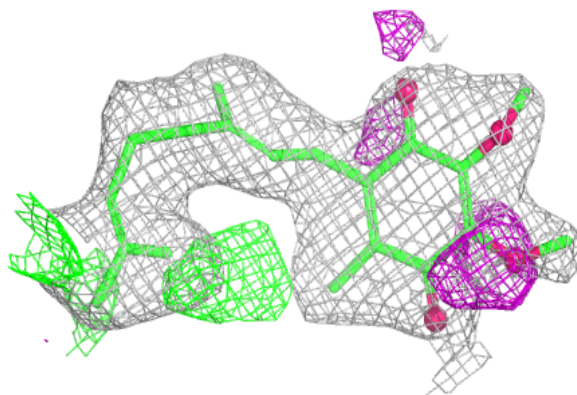
**Electron density around NS5 MMM 407:**

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

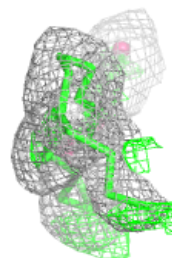
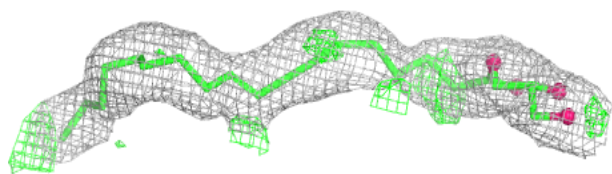
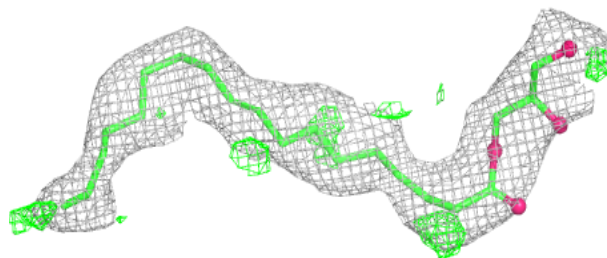


Electron density around UQ2 LLL 309:

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

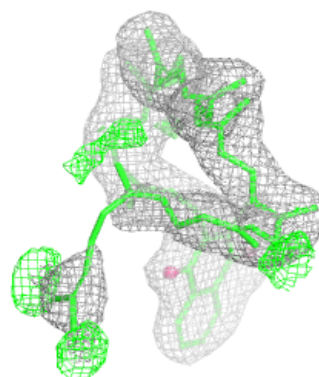
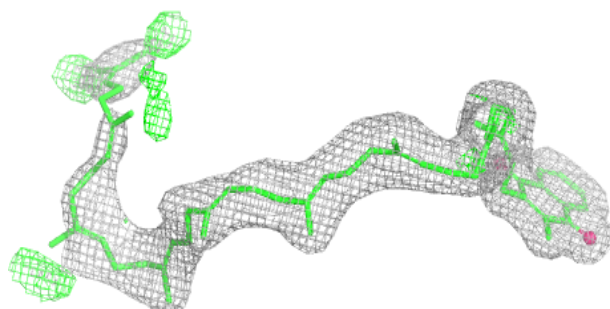
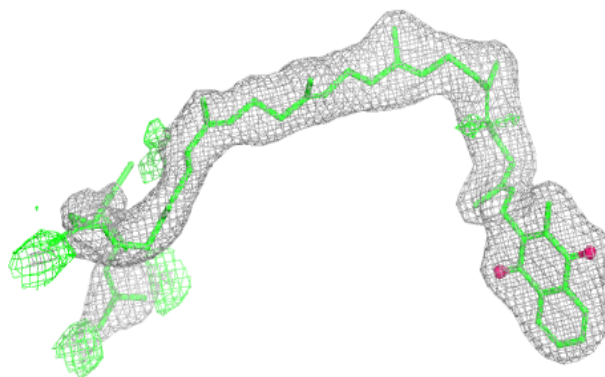
**Electron density around OLC MMM 414:**

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

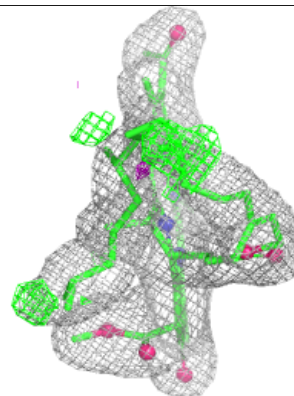
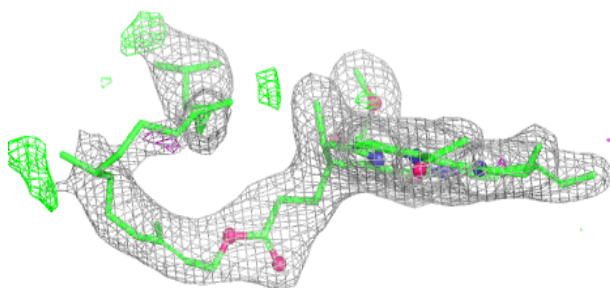
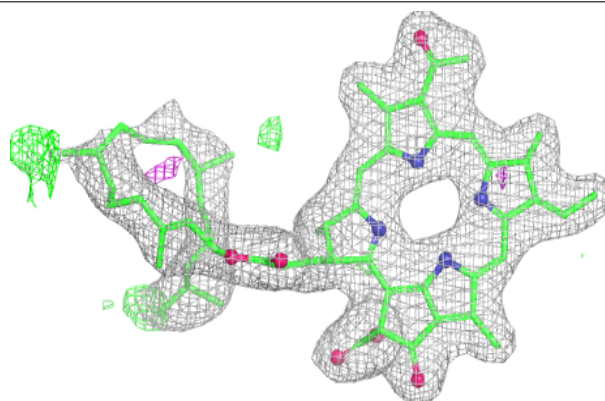


Electron density around MQ9 MMM 403:

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

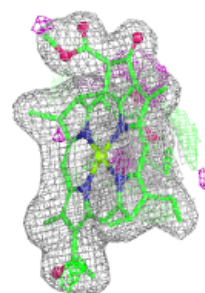
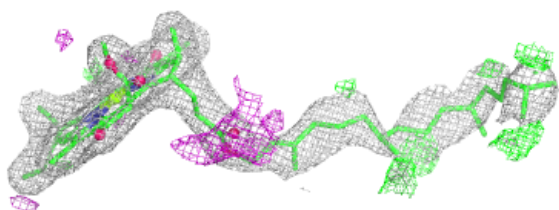
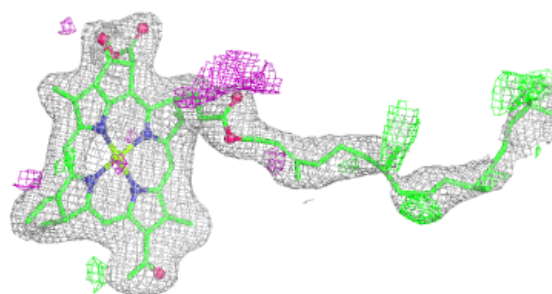
**Electron density around BPB MMM 406:**

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

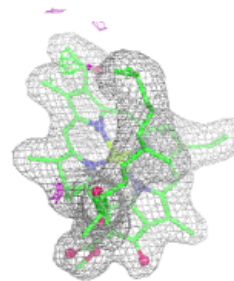
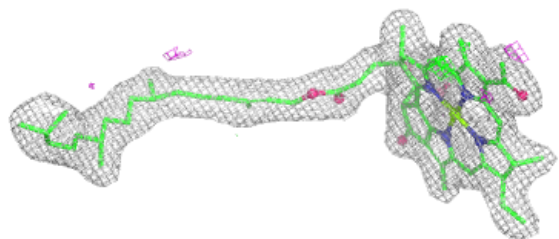


Electron density around BCB MMM 404:

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

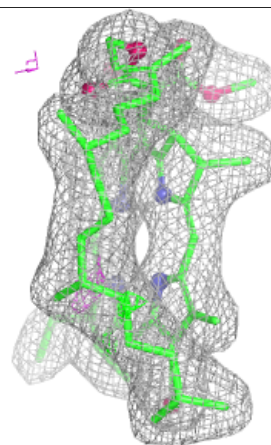
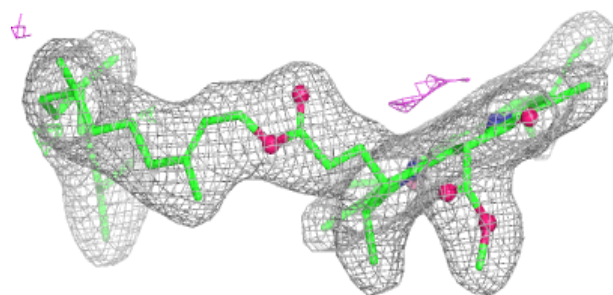
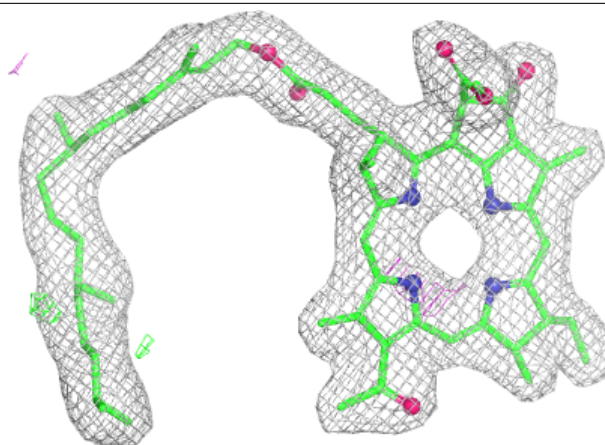
**Electron density around BCB LLL 301:**

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



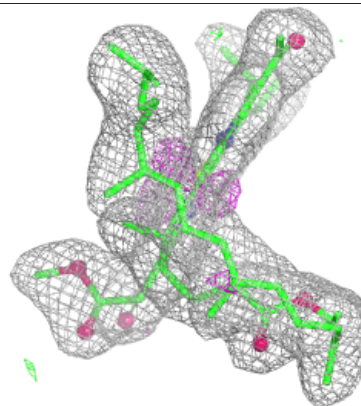
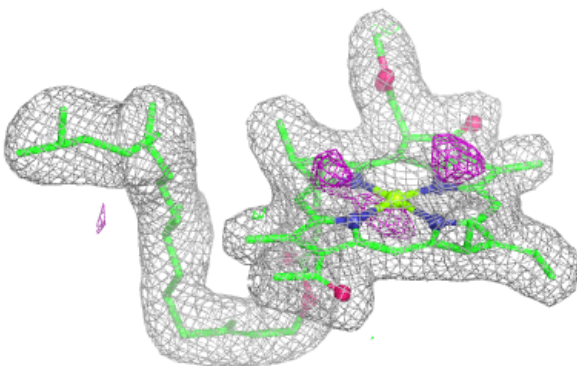
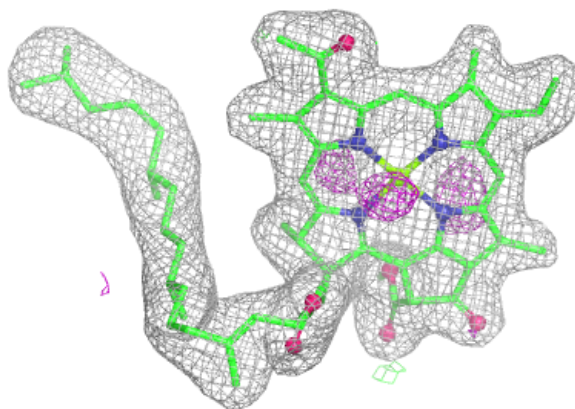
Electron density around BPB LLL 303:

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

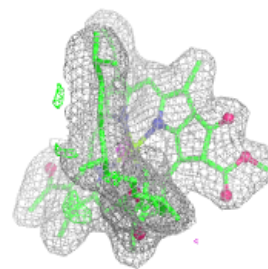
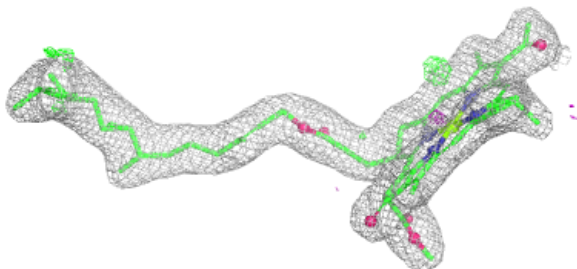
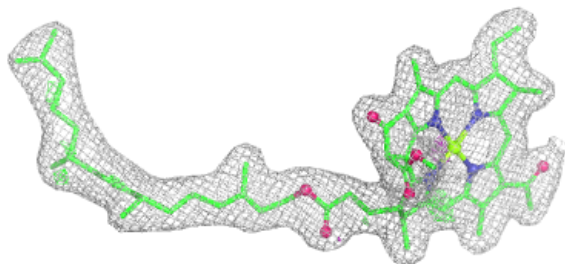


Electron density around BCB LLL 302:

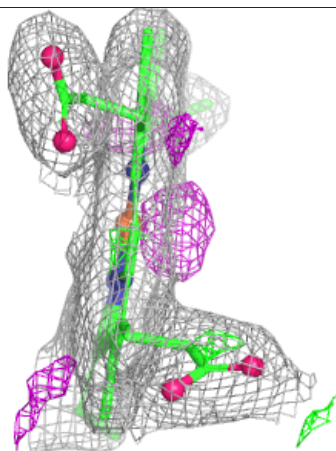
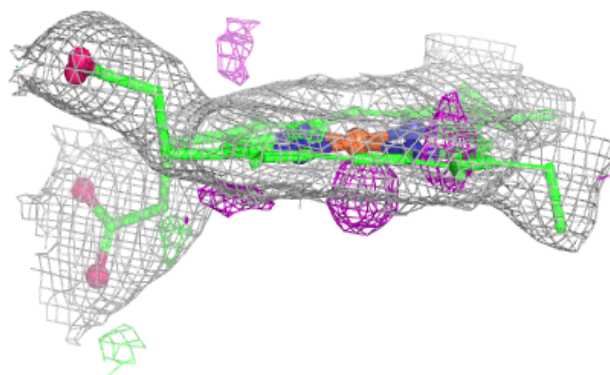
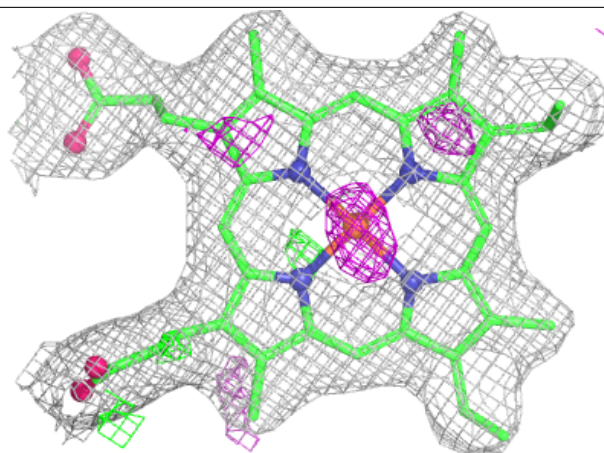
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCB 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)

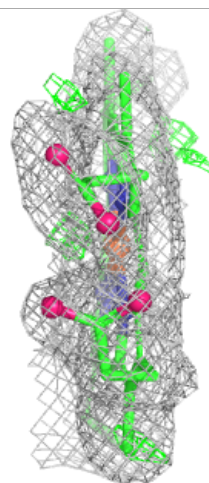
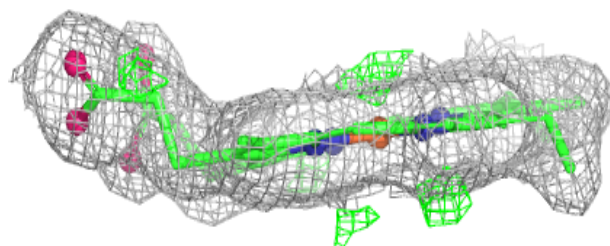
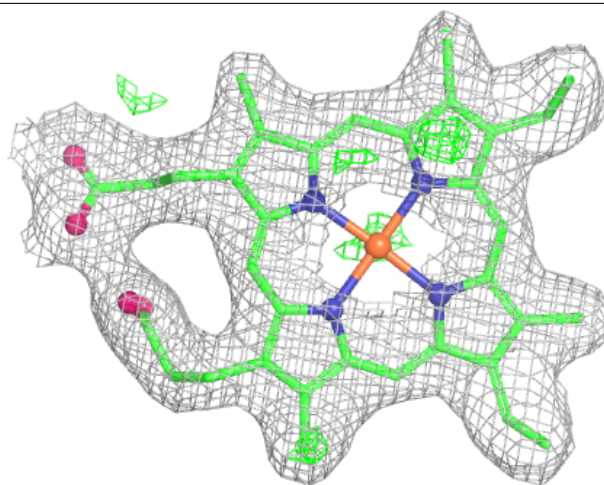


2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



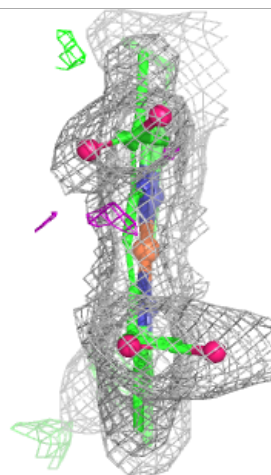
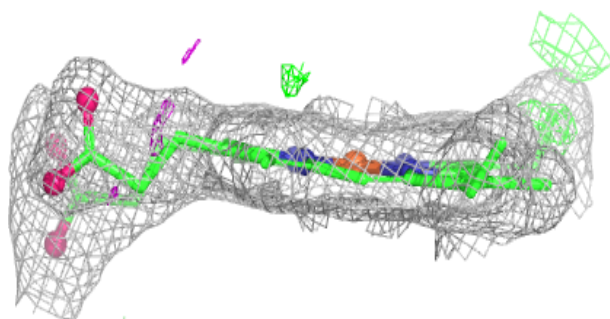
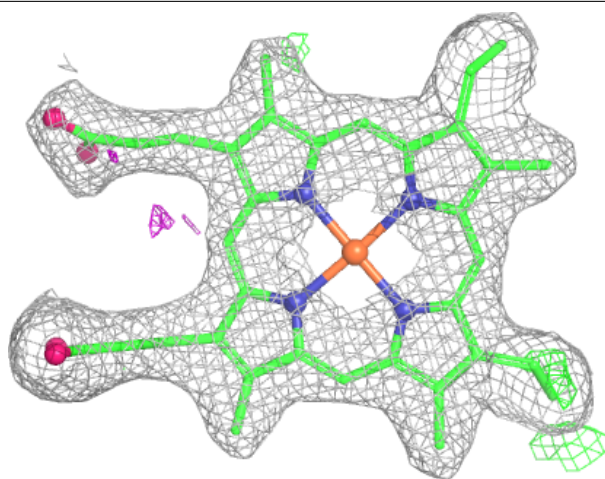
Electron density around HEC CCC 402:

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



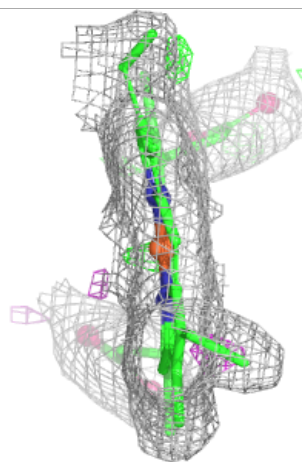
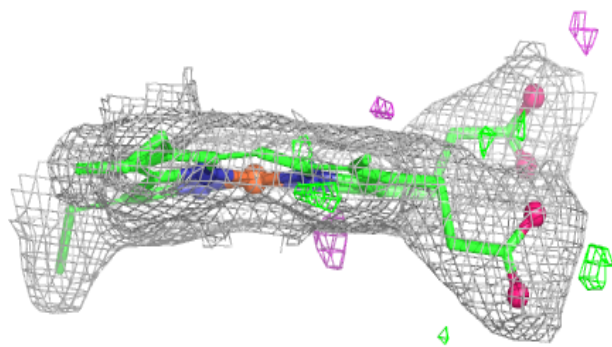
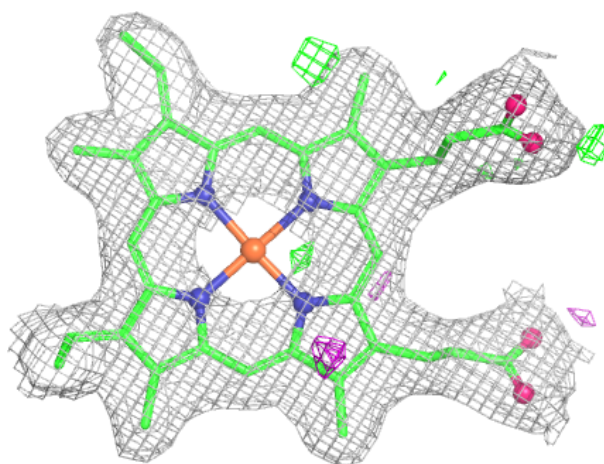
Electron density around HEC CCC 404:

$2mF_o-DF_c$ (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.