



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2024 – 07:32 pm GMT

PDB ID : 7Q7Q
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

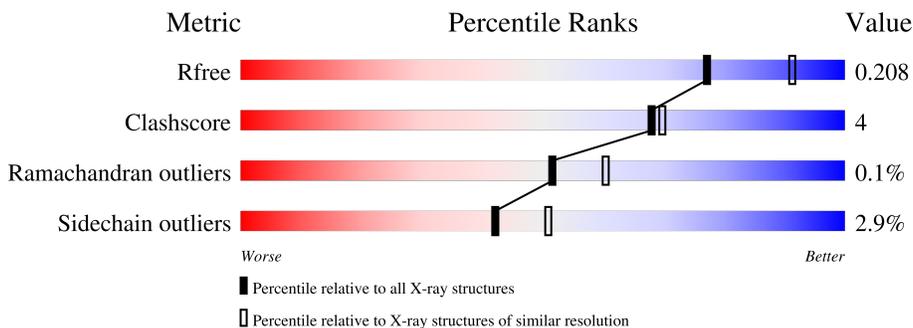
1 Overall quality at a glance

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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	CCC	336	91% 7% ..
2	HHH	258	89% 6% 5%
3	LLL	273	93% 7%
4	MMM	323	92% 7% .

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 [i](#)

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
			Total	C	N	O	S			
1	CCC	332	2615	1648	470	479	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	246	1945	1243	335	365	2	0	1	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

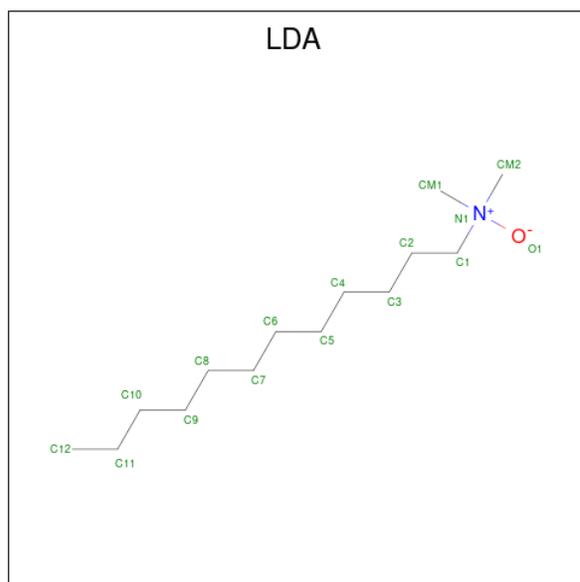
- Molecule 4 is a protein called Reaction center protein M chain.

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

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

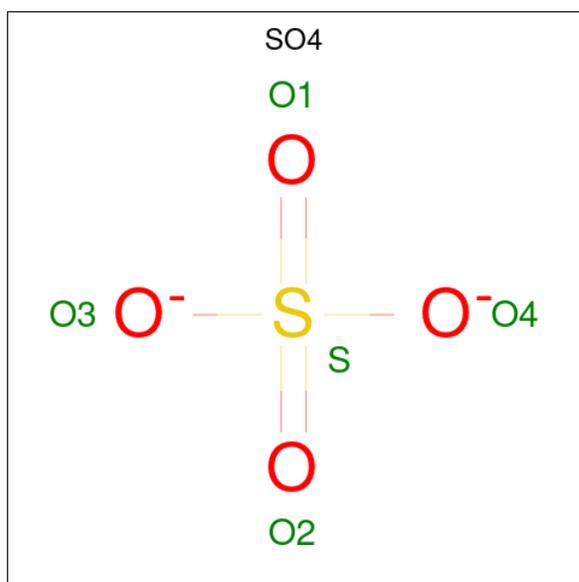
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	21	0
			44	39	5		

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



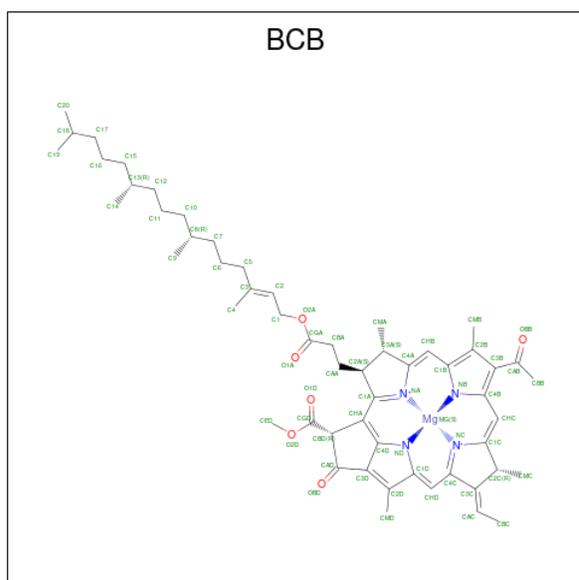
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	HHH	1	Total	C	N	O	0	0
			16	14	1	1		
7	HHH	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		
7	MMM	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



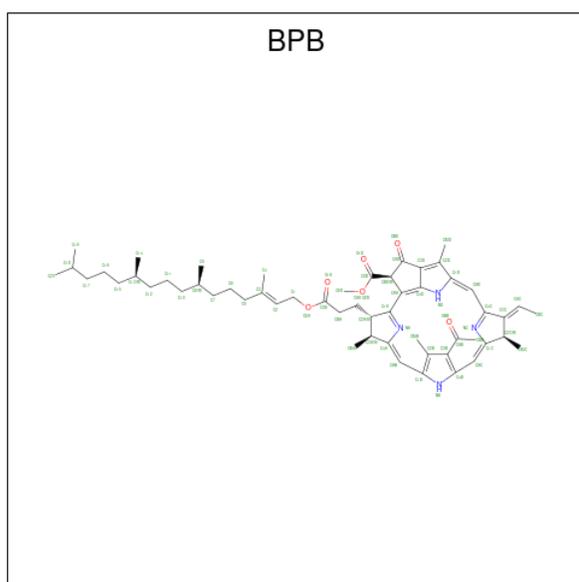
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	HHH	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



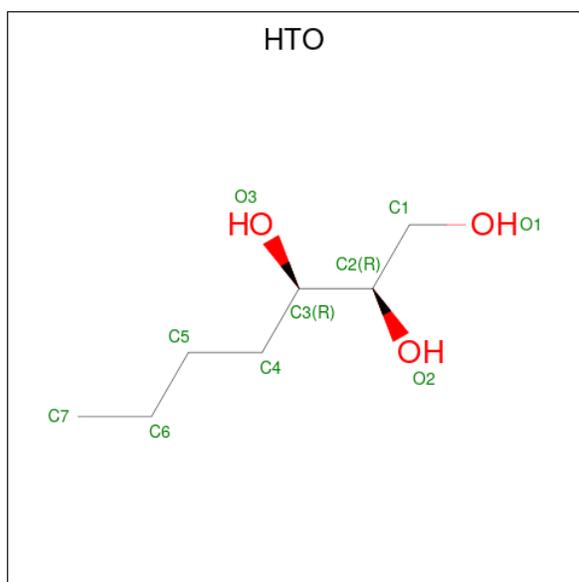
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	LLL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	LLL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	MMM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	MMM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).



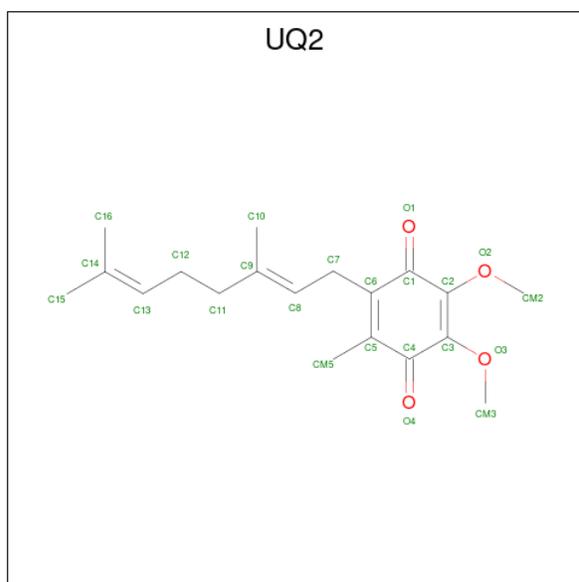
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
10	LLL	1	Total	C	N	O	0	0
			65	55	4	6		
10	MMM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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

- Molecule 12 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C₁₉H₂₆O₄).

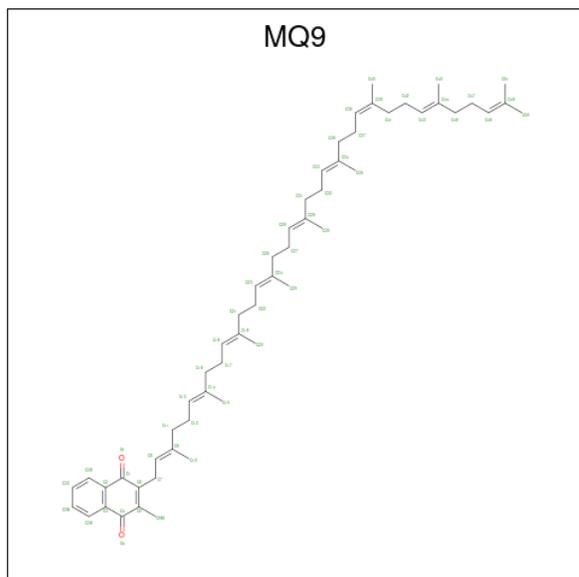


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	LLL	1	Total	C O	0	0
			23	19 4		
12	MMM	1	Total	C O	0	1
			46	38 8		

- Molecule 13 is FE (II) ION (three-letter code: FE2) (formula: Fe).

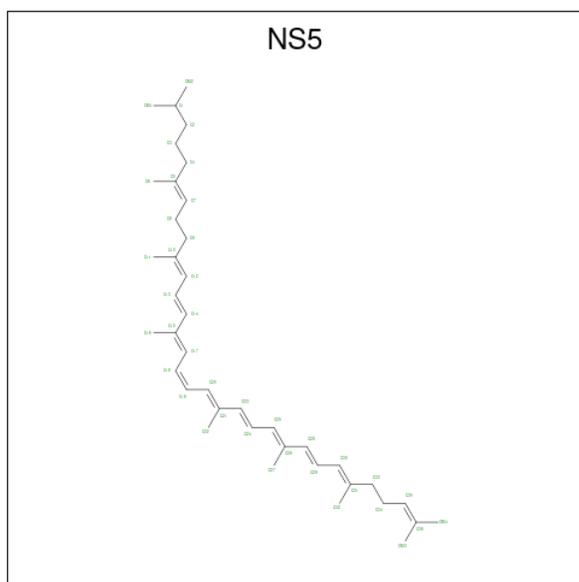
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	MMM	1	Total	Fe	0	0
			1	1		

- Molecule 14 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂).



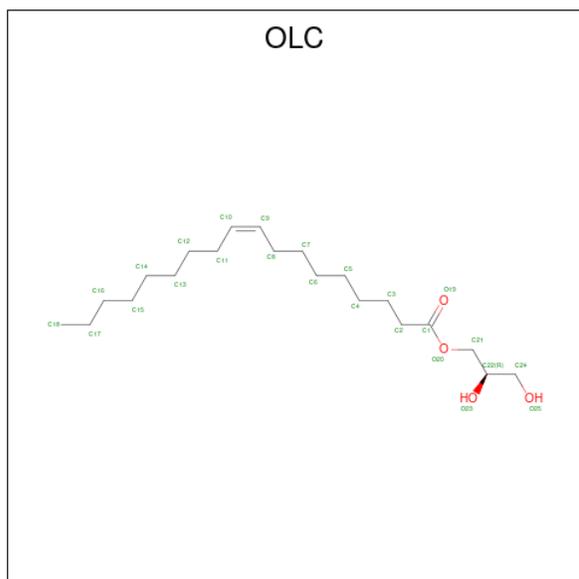
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	MMM	1	Total	C O	0	0
			58	56 2		

- Molecule 15 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C₄₀H₆₀).



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 (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



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. 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. 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:  91% 7% ..

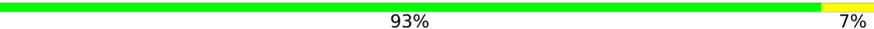


- Molecule 2: Reaction center protein H chain

Chain HHH:  89% 6% 5%



- Molecule 3: Reaction center protein L chain

Chain LLL:  93% 7%



- Molecule 4: Reaction center protein M chain

Chain MMM:  92% 7%



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 23.69 – 1.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.70-2.25) 96.3 (23.69-1.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.27Å)	Xtrriage
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	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10609	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage'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: BCB, NS5, UQ2, DGA, HEC, FME, SO4, BPB, FE2, HTO, MQ9, OLC, LDA

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	0.66	0/2688	0.77	0/3662
2	HHH	0.64	0/1979	0.78	0/2700
3	LLL	0.64	0/2267	0.74	0/3095
4	MMM	0.62	0/2670	0.73	0/3652
All	All	0.64	0/9604	0.75	0/13109

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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
4	MMM	2565	0	2458	16	0
5	CCC	172	0	120	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	MMM	20	0	0	1	0
9	LLL	132	0	144	6	0
9	MMM	132	0	144	4	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	7	0
13	MMM	1	0	0	0	0
14	MMM	58	0	80	0	0
15	MMM	40	0	60	5	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	78	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 78 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
5:CCC:401:HEC:HBC3	5:CCC:401:HEC:HMC1	1.65	0.78
12:MMM:416[A]:UQ2:H101	12:MMM:416[A]:UQ2:H162	1.67	0.74

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	332/336 (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%)	41	46
All	All	1169/1190 (98%)	1132 (97%)	36 (3%)	1 (0%)	51	60

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	283/282 (100%)	275 (97%)	8 (3%)	43	52
2	HHH	204/212 (96%)	196 (96%)	8 (4%)	32	38
3	LLL	219/218 (100%)	213 (97%)	6 (3%)	44	54
4	MMM	250/249 (100%)	243 (97%)	7 (3%)	43	52
All	All	956/961 (100%)	927 (97%)	29 (3%)	42	50

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 [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	0.37	0	7,9,11	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 monosaccharides 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
14	MQ9	MMM	403	-	59,59,59	0.38	0	72,75,75	0.44	0
12	UQ2	MMM	416[A]	-	23,23,23	1.94	2 (8%)	28,31,31	1.54	5 (17%)
11	HTO	LLL	306	-	9,9,9	0.48	0	10,10,10	0.52	0
7	LDA	MMM	413	-	12,15,15	0.17	0	14,17,17	0.24	0
11	HTO	MMM	408	-	9,9,9	0.56	0	10,10,10	0.65	0
11	HTO	MMM	415	-	9,9,9	0.77	0	10,10,10	0.55	0
5	HEC	CCC	402	1	32,50,50	1.66	4 (12%)	24,82,82	1.82	4 (16%)
8	SO4	MMM	417	-	4,4,4	0.35	0	6,6,6	0.07	0
8	SO4	MMM	418	-	4,4,4	0.39	0	6,6,6	0.12	0
7	LDA	HHH	1301	-	12,15,15	0.16	0	14,17,17	0.18	0
9	BCB	MMM	404	-	63,74,74	1.70	14 (22%)	74,115,115	3.06	22 (29%)
5	HEC	CCC	404	1	32,50,50	1.63	5 (15%)	24,82,82	1.85	6 (25%)
11	HTO	LLL	307	-	9,9,9	0.80	0	10,10,10	1.29	1 (10%)
9	BCB	MMM	405	-	63,74,74	1.79	14 (22%)	74,115,115	2.87	26 (35%)
8	SO4	MMM	419	-	4,4,4	0.35	0	6,6,6	0.08	0
7	LDA	MMM	402	-	12,15,15	0.21	0	14,17,17	0.31	0
11	HTO	LLL	305	-	9,9,9	0.97	1 (11%)	10,10,10	1.05	0
7	LDA	MMM	412	-	12,15,15	0.24	0	14,17,17	0.24	0
7	LDA	MMM	409	-	12,15,15	0.11	0	14,17,17	0.28	0
11	HTO	LLL	308	-	9,9,9	0.55	0	10,10,10	0.69	0
9	BCB	LLL	301	-	63,74,74	1.73	13 (20%)	74,115,115	3.04	28 (37%)
8	SO4	HHH	1303	-	4,4,4	0.35	0	6,6,6	0.07	0
11	HTO	LLL	304	-	9,9,9	0.54	0	10,10,10	0.68	0
9	BCB	LLL	302	-	63,74,74	1.71	14 (22%)	74,115,115	2.88	20 (27%)
16	OLC	MMM	414	-	24,24,24	1.02	1 (4%)	25,25,25	1.08	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEC	CCC	403	1	32,50,50	1.63	5 (15%)	24,82,82	1.76	5 (20%)
10	BPB	MMM	406	-	49,70,70	1.88	9 (18%)	47,101,101	1.95	8 (17%)
10	BPB	LLL	303	-	49,70,70	1.88	9 (18%)	47,101,101	1.61	8 (17%)
15	NS5	MMM	407	-	39,39,39	0.95	1 (2%)	44,46,46	1.64	8 (18%)
7	LDA	HHH	1302	-	12,15,15	0.11	0	14,17,17	0.25	0
16	OLC	MMM	410	-	24,24,24	0.96	1 (4%)	25,25,25	0.69	0
8	SO4	MMM	420	-	4,4,4	0.38	0	6,6,6	0.05	0
7	LDA	MMM	411	-	12,15,15	0.16	0	14,17,17	0.18	0
11	HTO	LLL	310	-	9,9,9	0.62	0	10,10,10	0.88	0
5	HEC	CCC	401	1	32,50,50	1.68	4 (12%)	24,82,82	2.19	5 (20%)
12	UQ2	LLL	309	-	23,23,23	1.92	2 (8%)	28,31,31	1.51	5 (17%)
6	DGA	CCC	405	-	43,43,43	2.88	3 (6%)	45,45,45	3.40	7 (15%)
12	UQ2	MMM	416[B]	-	23,23,23	1.95	2 (8%)	28,31,31	1.24	3 (10%)

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
14	MQ9	MMM	403	-	-	4/53/73/73	0/2/2/2
12	UQ2	MMM	416[A]	-	-	3/15/39/39	0/1/1/1
11	HTO	LLL	306	-	-	4/10/10/10	-
7	LDA	MMM	413	-	-	7/13/13/13	-
11	HTO	MMM	408	-	-	7/10/10/10	-
11	HTO	MMM	415	-	-	4/10/10/10	-
5	HEC	CCC	402	1	-	4/10/54/54	-
9	BCB	MMM	404	-	3/3/21/26	11/37/137/137	-
7	LDA	HHH	1301	-	-	7/13/13/13	-
5	HEC	CCC	404	1	-	0/10/54/54	-
11	HTO	LLL	307	-	-	2/10/10/10	-
9	BCB	MMM	405	-	3/3/21/26	9/37/137/137	-
7	LDA	MMM	402	-	-	5/13/13/13	-
11	HTO	LLL	305	-	-	6/10/10/10	-
7	LDA	MMM	412	-	-	8/13/13/13	-
7	LDA	MMM	409	-	-	9/13/13/13	-
11	HTO	LLL	308	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCB	LLL	301	-	3/3/21/26	5/37/137/137	-
11	HTO	LLL	304	-	-	2/10/10/10	-
9	BCB	LLL	302	-	3/3/21/26	5/37/137/137	-
16	OLC	MMM	414	-	-	11/24/24/24	-
5	HEC	CCC	403	1	-	0/10/54/54	-
10	BPB	MMM	406	-	1/1/18/23	16/37/105/105	0/5/6/6
10	BPB	LLL	303	-	1/1/18/23	5/37/105/105	0/5/6/6
15	NS5	MMM	407	-	-	5/43/43/43	-
7	LDA	HHH	1302	-	-	8/13/13/13	-
16	OLC	MMM	410	-	-	12/24/24/24	-
7	LDA	MMM	411	-	-	10/13/13/13	-
11	HTO	LLL	310	-	-	6/10/10/10	-
5	HEC	CCC	401	1	-	2/10/54/54	-
12	UQ2	LLL	309	-	-	3/15/39/39	0/1/1/1
6	DGA	CCC	405	-	1/1/3/3	19/45/45/45	-
12	UQ2	MMM	416[B]	-	-	6/15/39/39	0/1/1/1

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	405	DGA	CG1-CG2	-17.30	0.97	1.50
12	MMM	416[B]	UQ2	C6-C5	8.14	1.50	1.35
12	LLL	309	UQ2	C6-C5	7.95	1.49	1.35
12	MMM	416[A]	UQ2	C6-C5	7.82	1.49	1.35
10	LLL	303	BPB	CAC-C3C	7.30	1.52	1.33

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	CCC	405	DGA	CG1-CG2-CG3	19.88	158.34	111.80
9	MMM	404	BCB	C1C-NC-C4C	-18.43	98.42	106.71
9	LLL	302	BCB	C1C-NC-C4C	-18.08	98.58	106.71
9	LLL	301	BCB	C1C-NC-C4C	-17.53	98.82	106.71
9	MMM	405	BCB	C1C-NC-C4C	-15.06	99.93	106.71

5 of 15 chirality outliers are listed below:

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

5 of 208 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	CCC	405	DGA	CA2-CA1-OG1-CG1
6	CCC	405	DGA	OA1-CA1-OG1-CG1
7	HHH	1302	LDA	C2-C1-N1-O1
7	HHH	1302	LDA	C2-C1-N1-CM2
7	MMM	402	LDA	C2-C1-N1-CM1

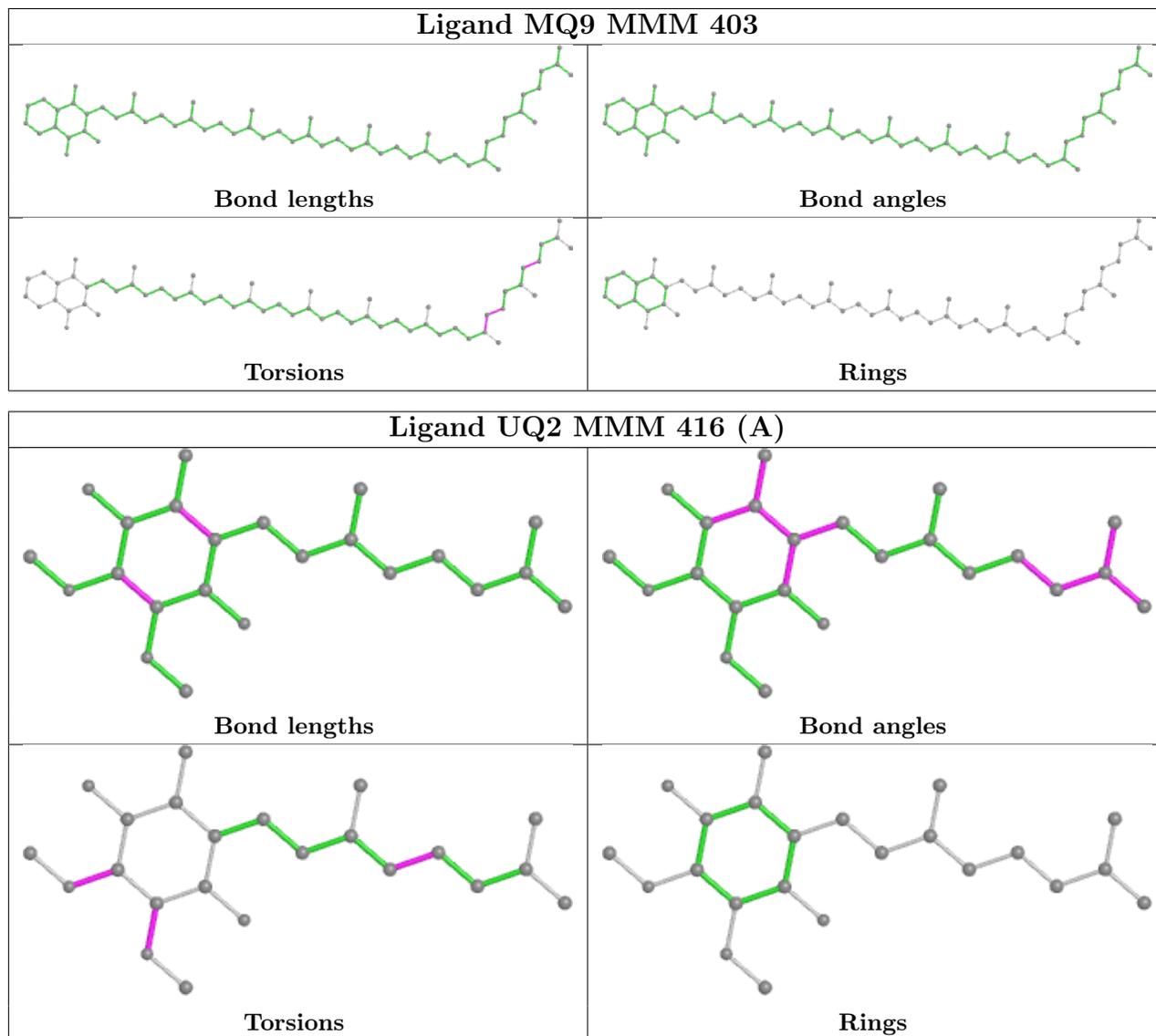
There are no ring outliers.

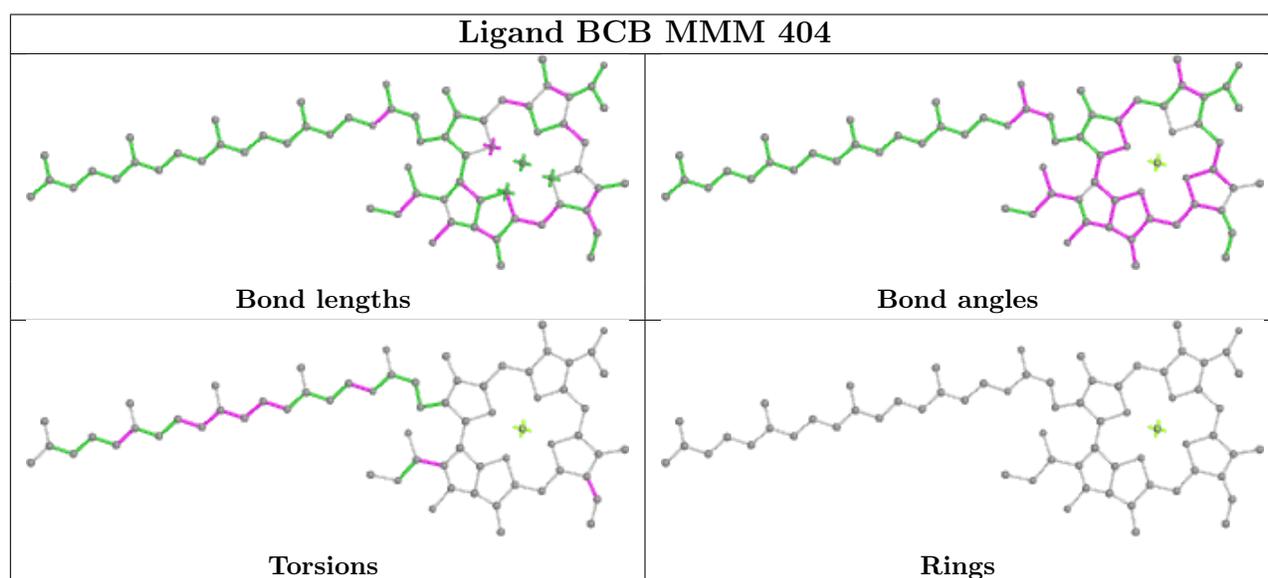
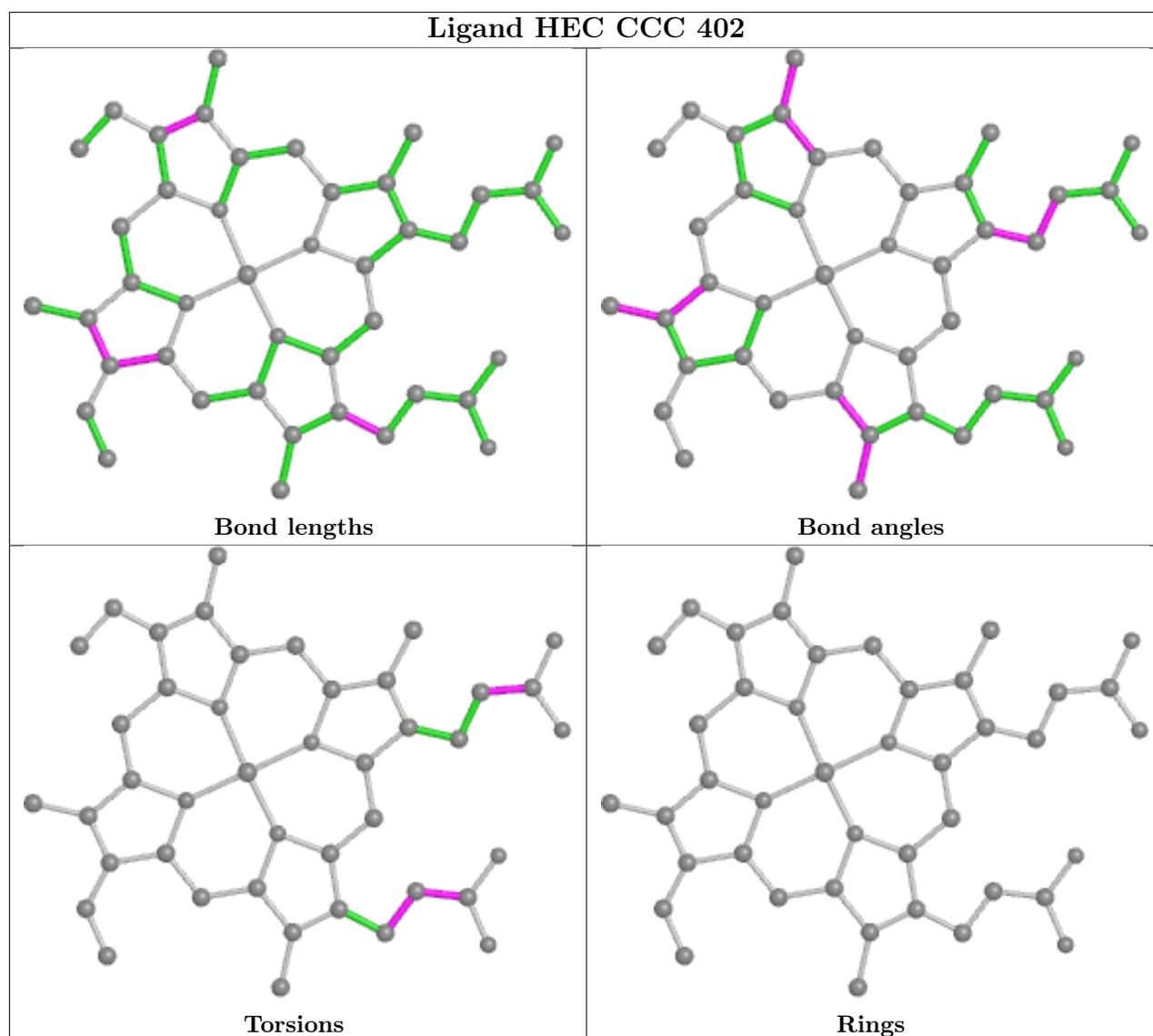
20 monomers are involved in 45 short contacts:

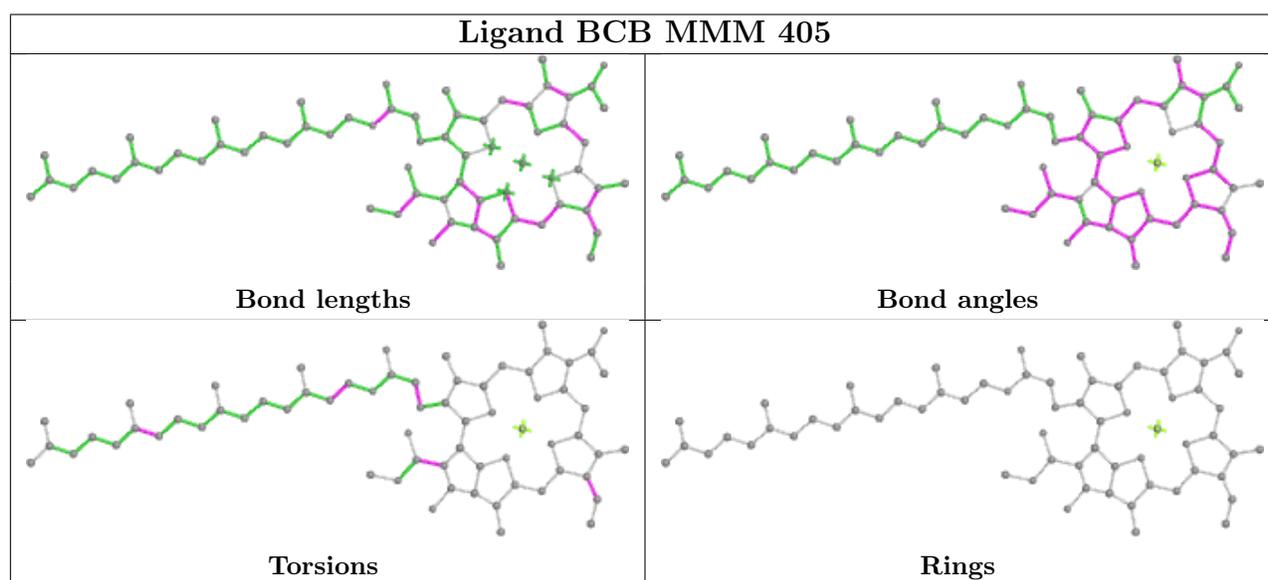
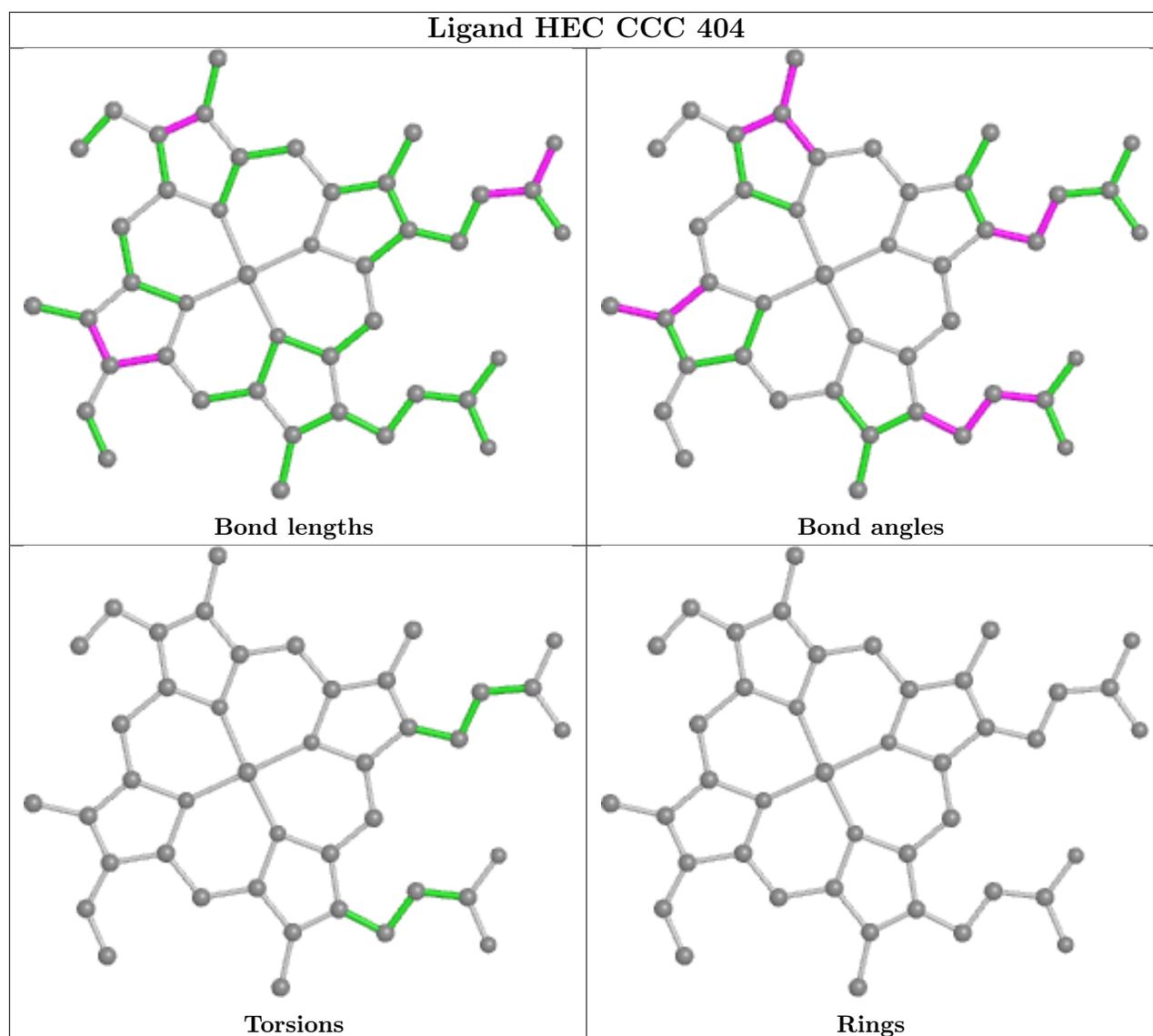
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	MMM	416[A]	UQ2	4	0
11	MMM	415	HTO	1	0
8	MMM	418	SO4	1	0
7	HHH	1301	LDA	1	0
9	MMM	404	BCB	3	0
5	CCC	404	HEC	1	0
9	MMM	405	BCB	1	0
7	MMM	402	LDA	1	0
7	MMM	409	LDA	1	0
9	LLL	301	BCB	4	0
9	LLL	302	BCB	2	0
5	CCC	403	HEC	2	0
10	MMM	406	BPB	5	0
10	LLL	303	BPB	1	0
15	MMM	407	NS5	5	0
7	MMM	411	LDA	4	0
5	CCC	401	HEC	2	0
12	LLL	309	UQ2	4	0
6	CCC	405	DGA	1	0
12	MMM	416[B]	UQ2	3	0

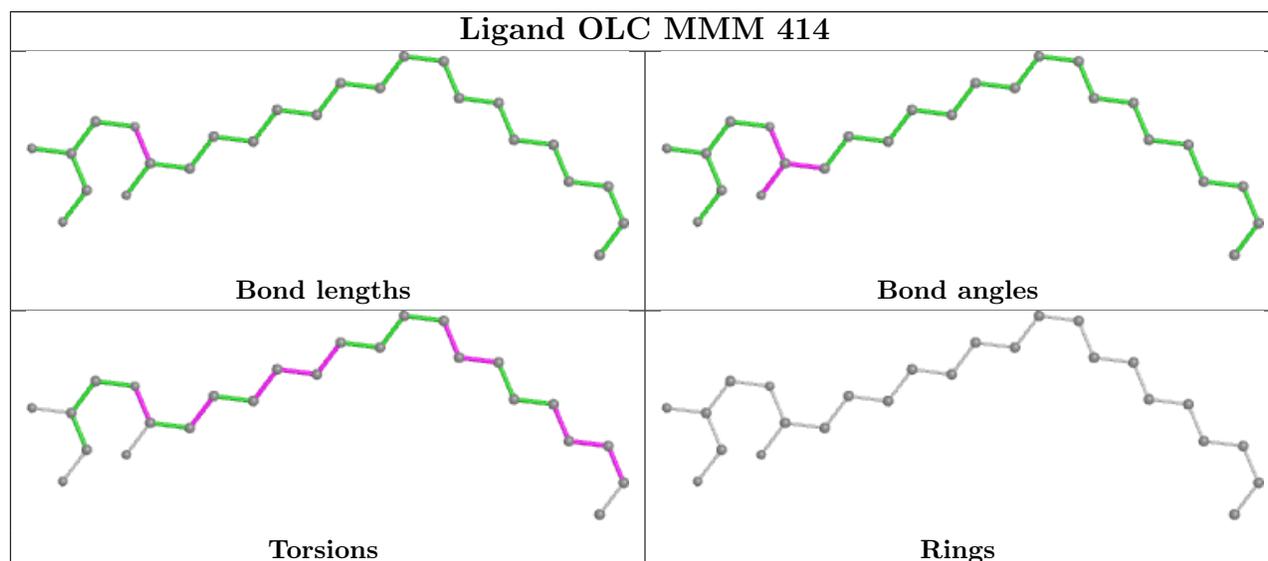
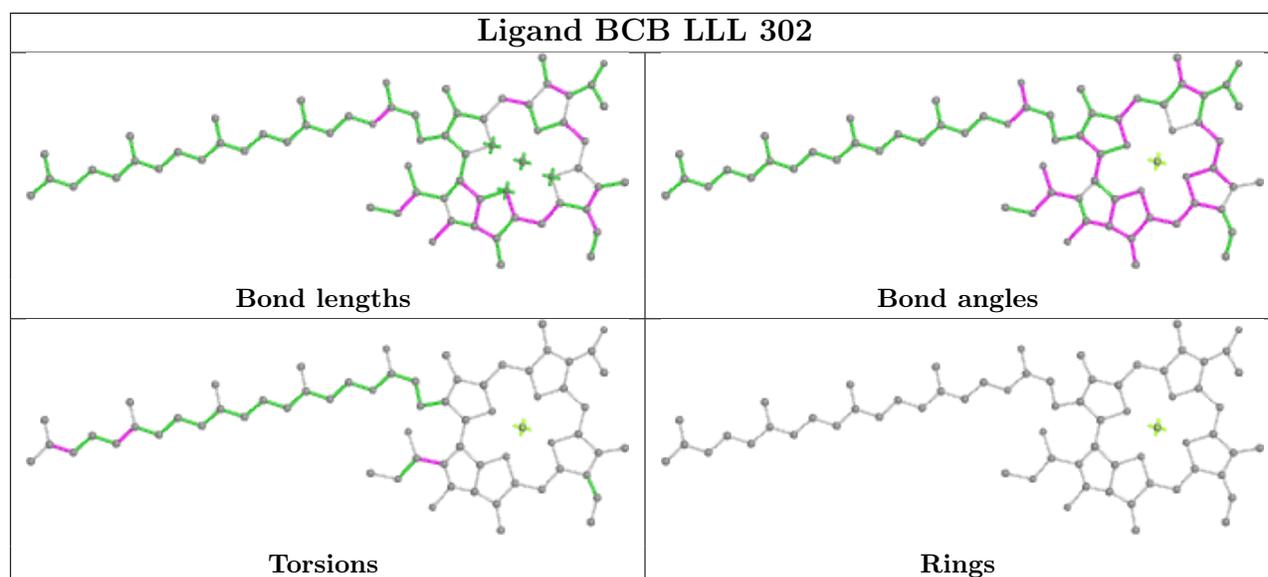
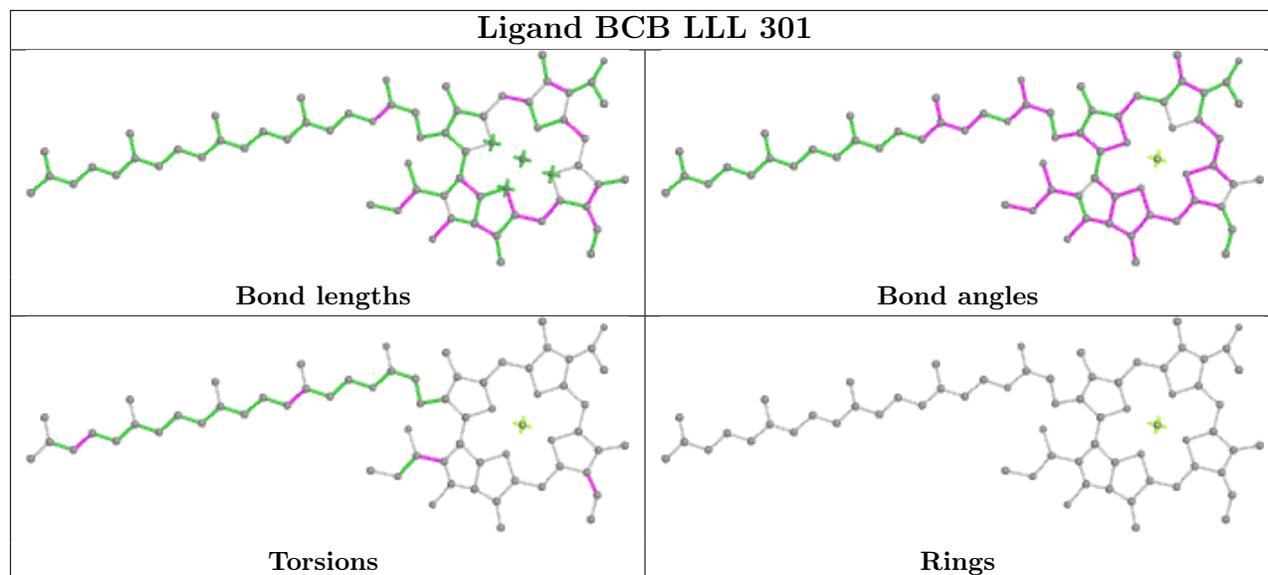
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

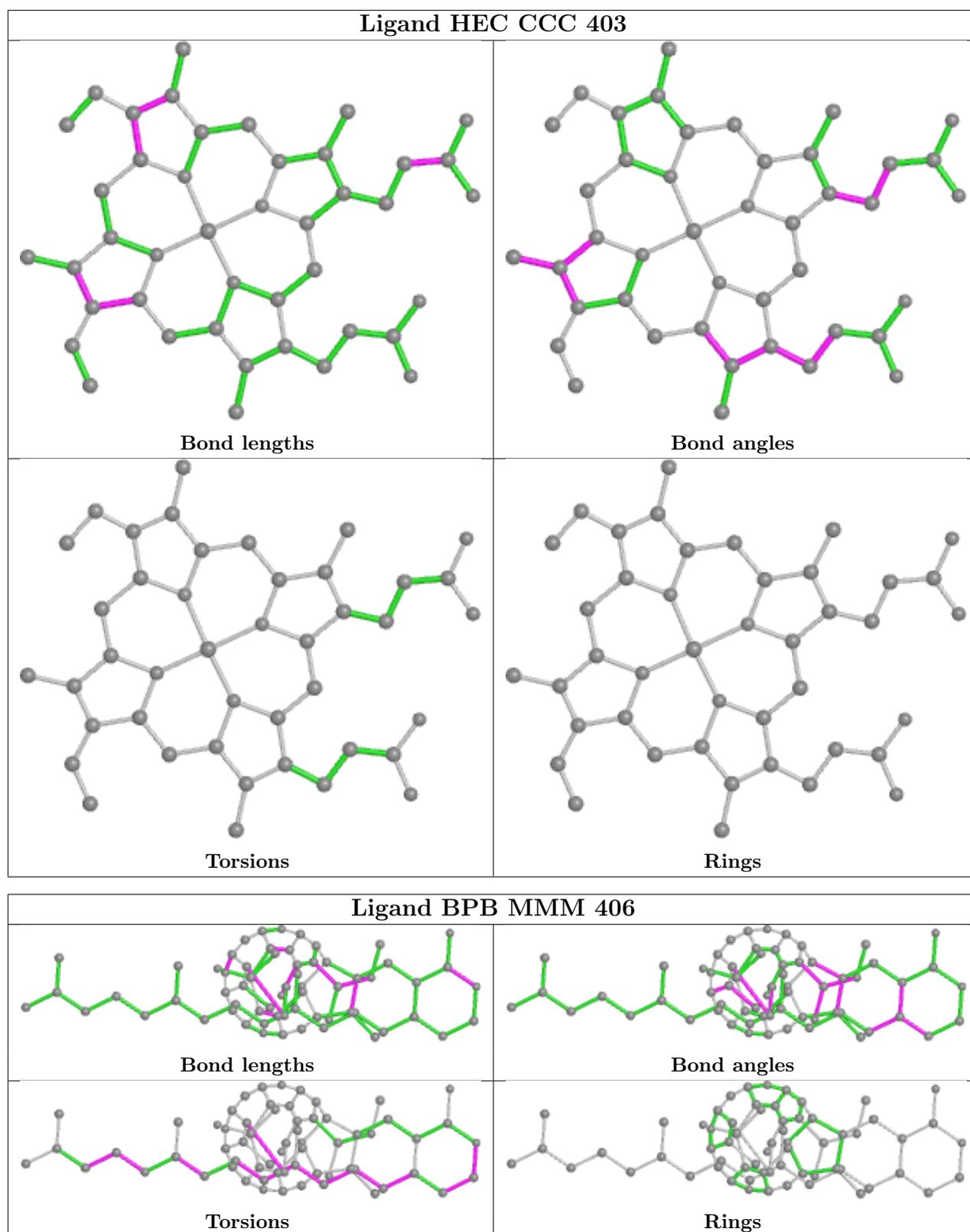
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

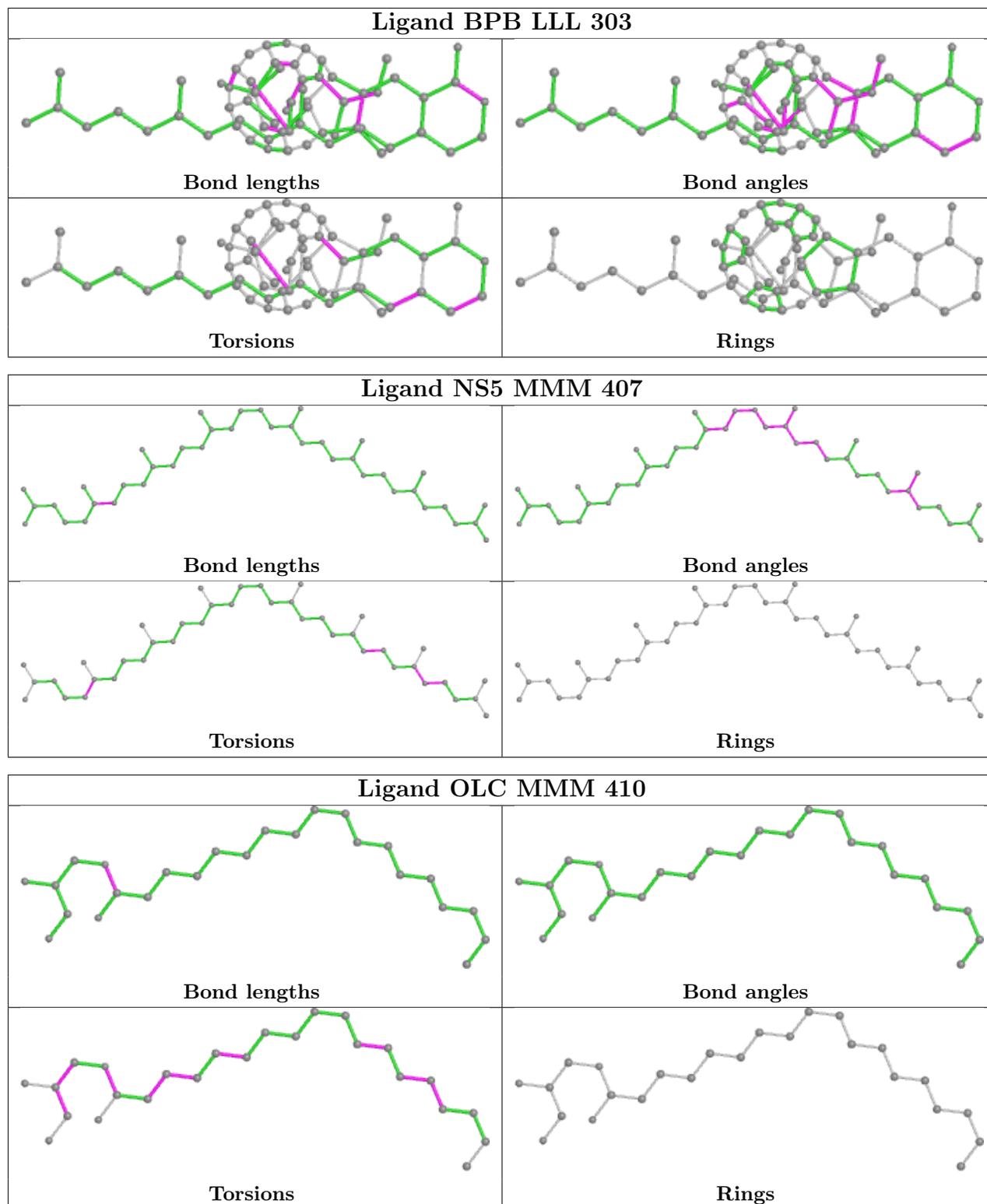


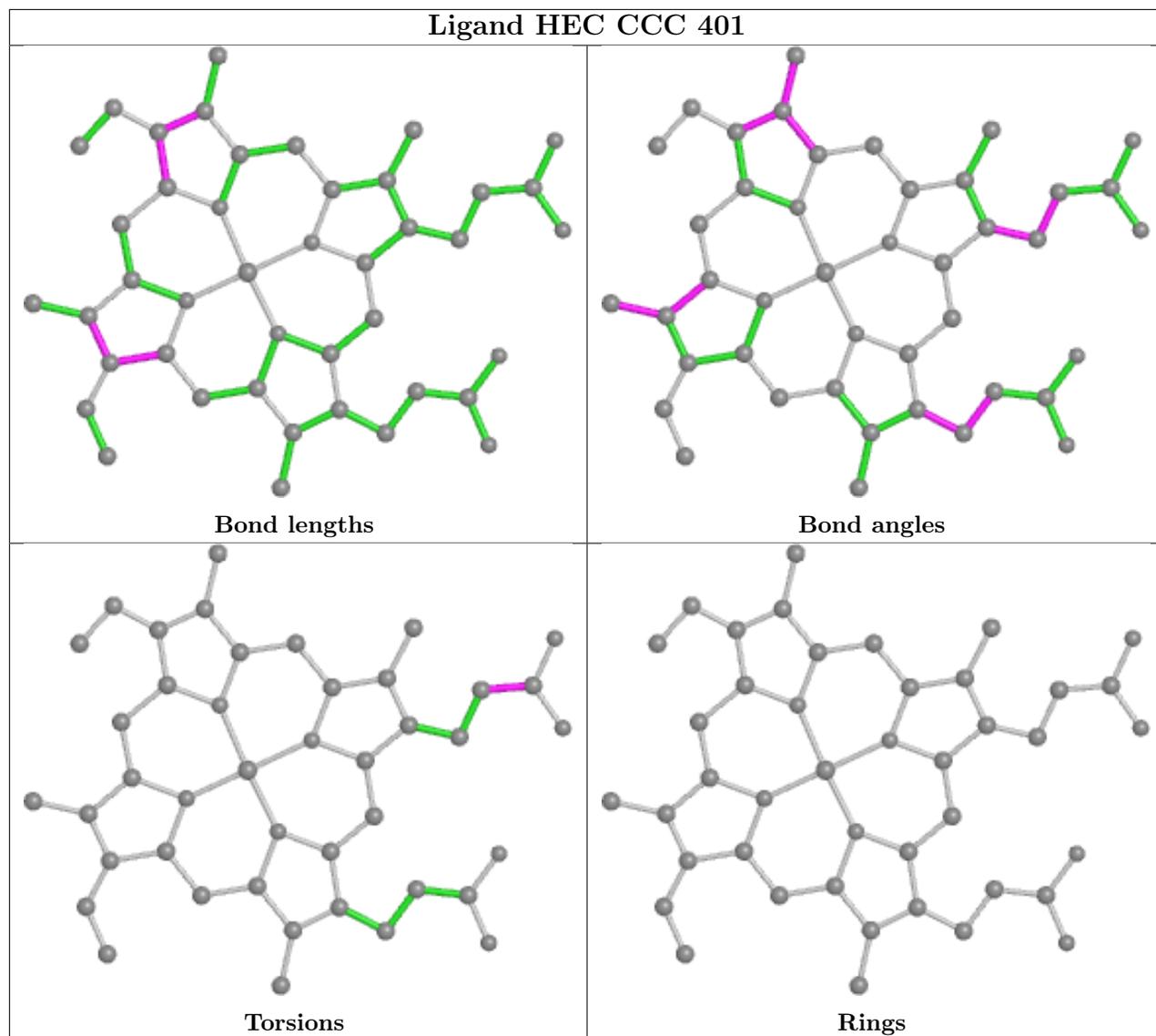


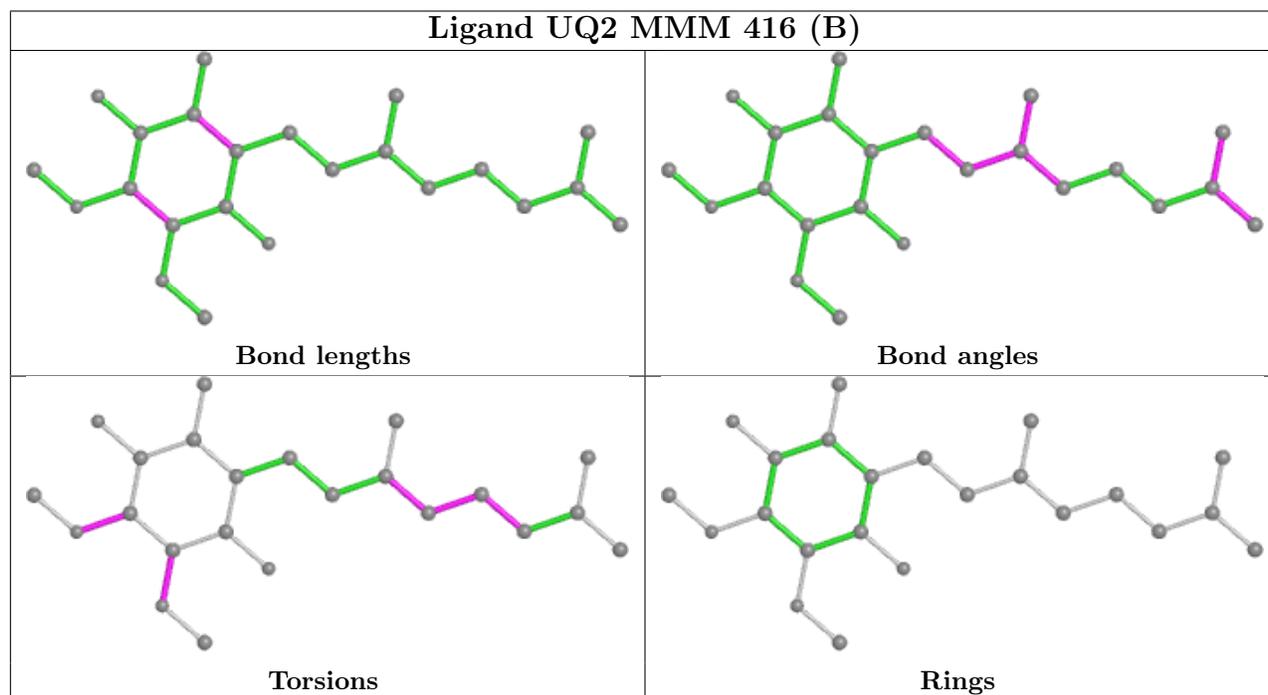
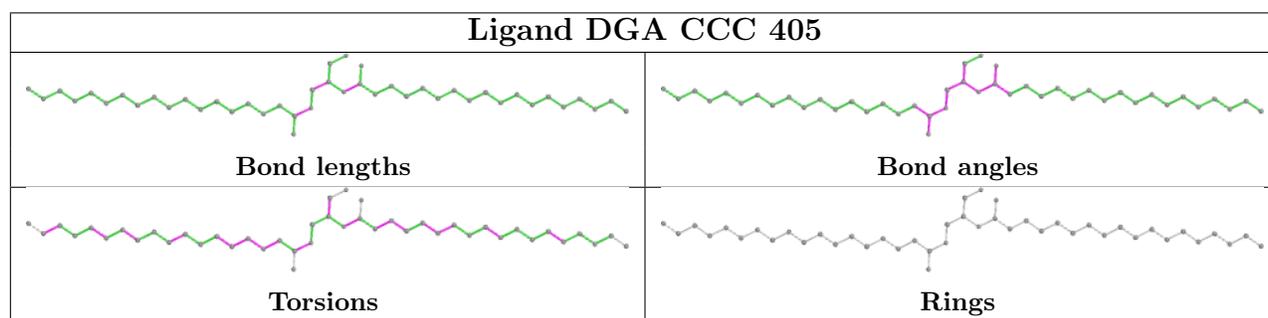
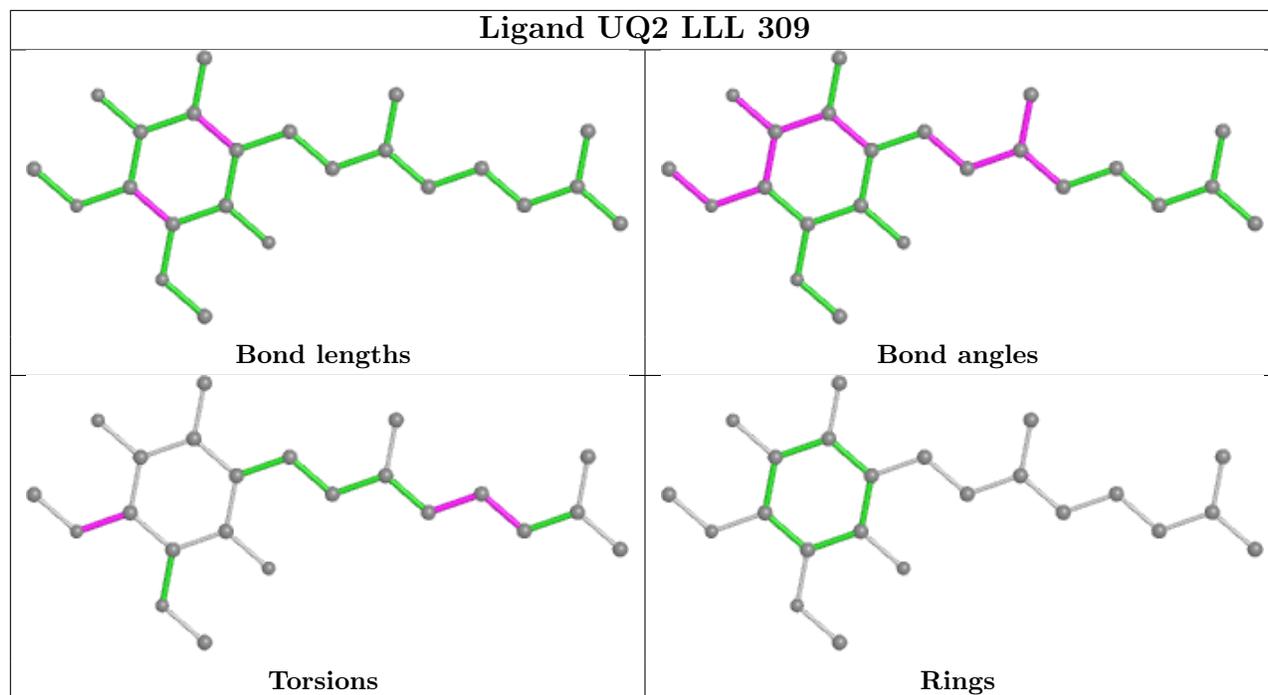












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

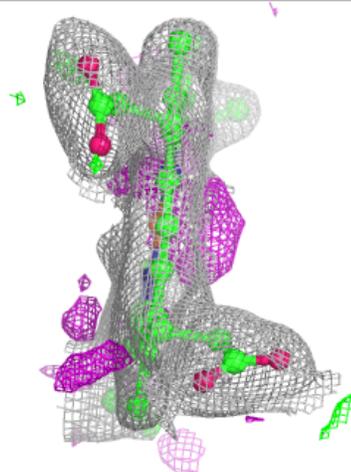
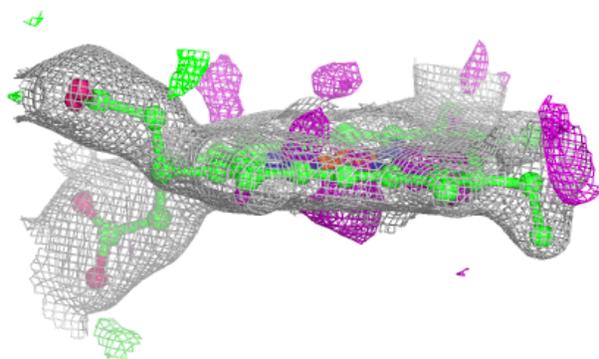
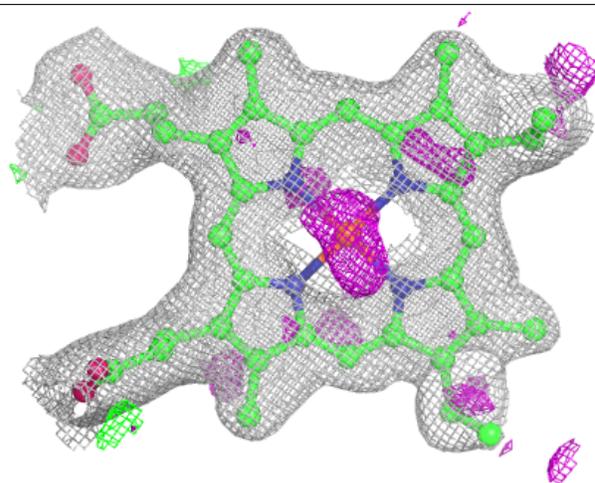
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

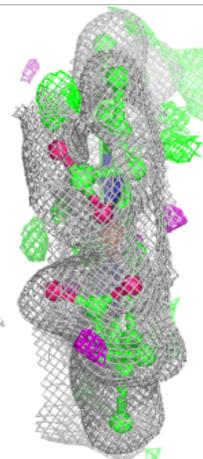
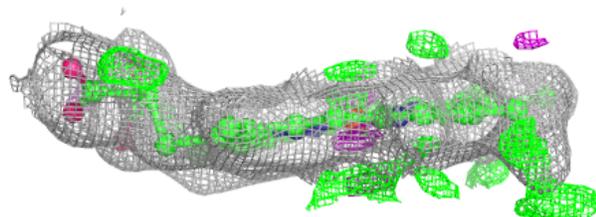
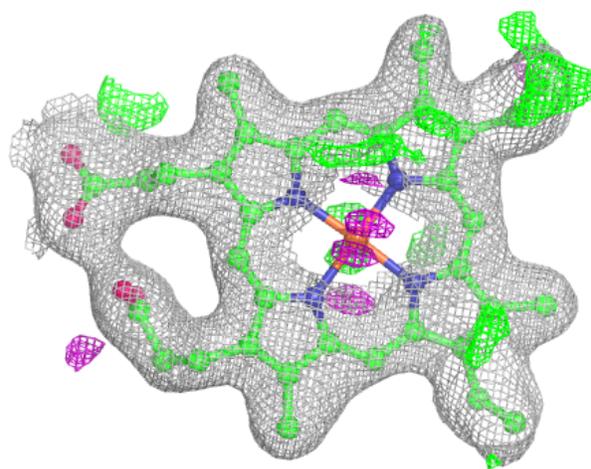
Electron density around HEC CCC 401:

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



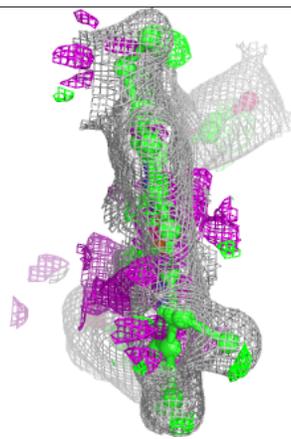
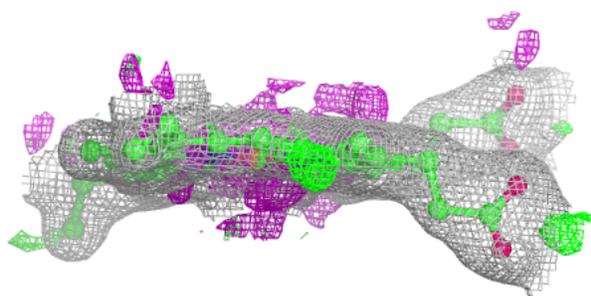
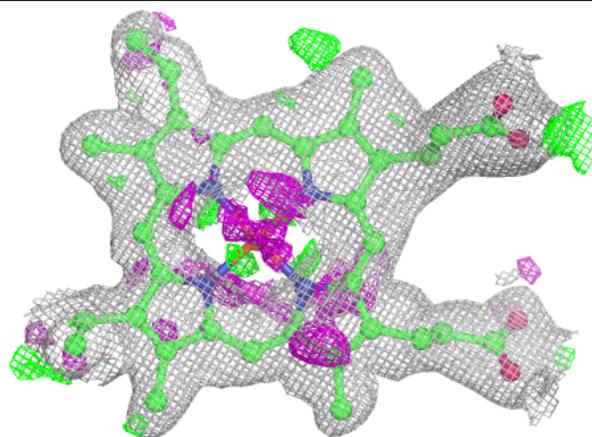
Electron density around HEC CCC 402:

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



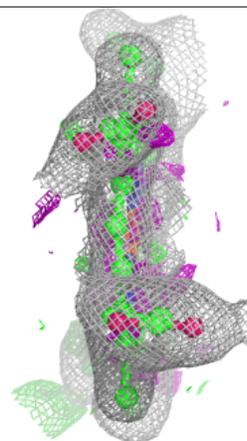
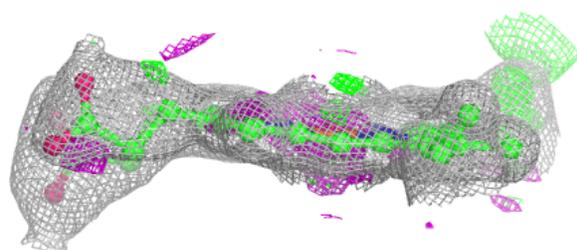
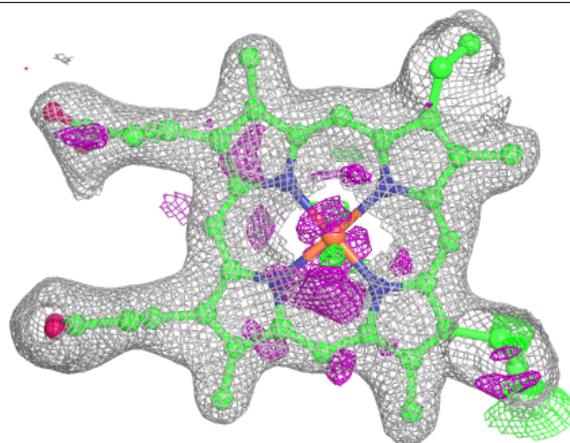
Electron density around HEC CCC 403:

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

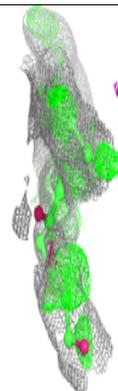
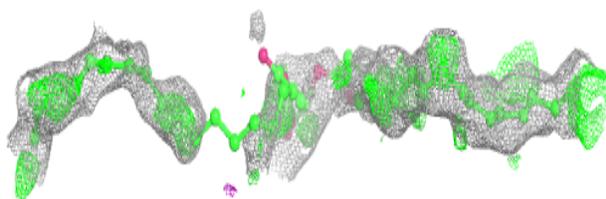
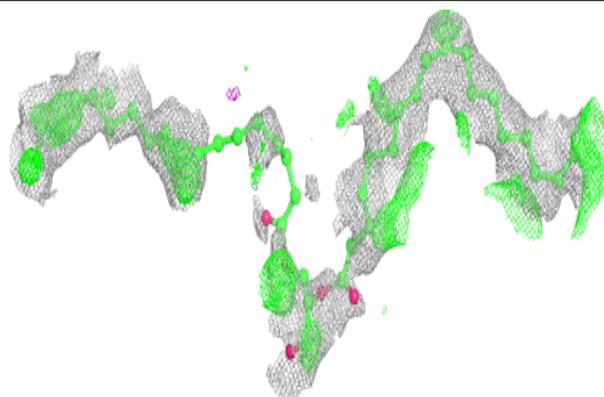


Electron density around HEC CCC 404:

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

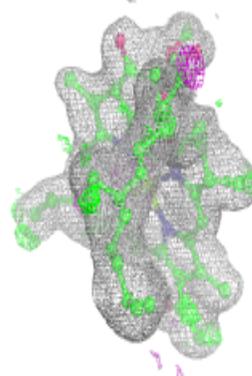
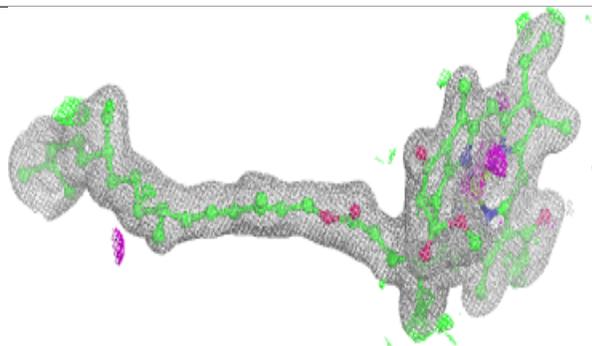
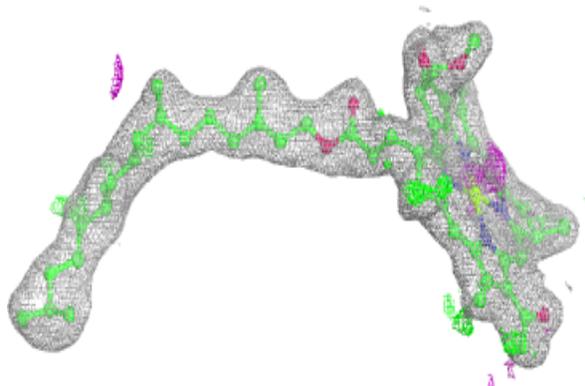
**Electron density around DGA CCC 405:**

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

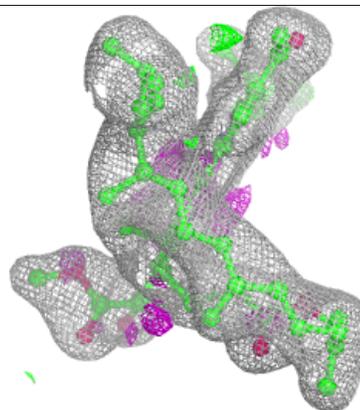
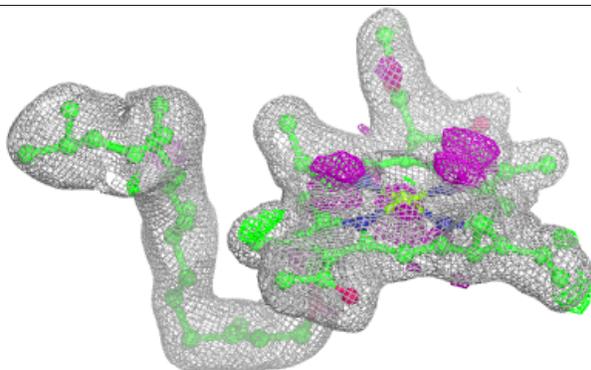
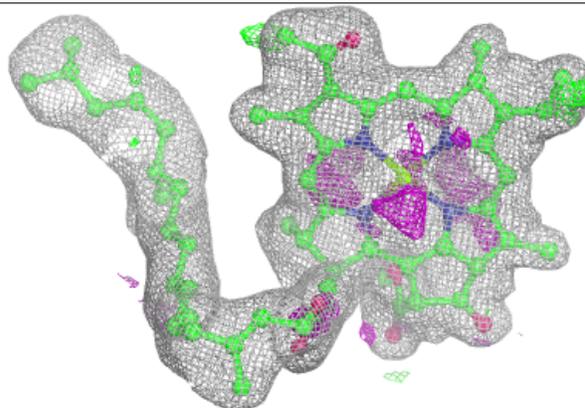


Electron density around BCB LLL 301:

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

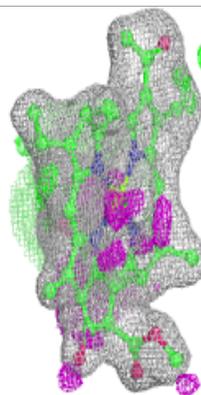
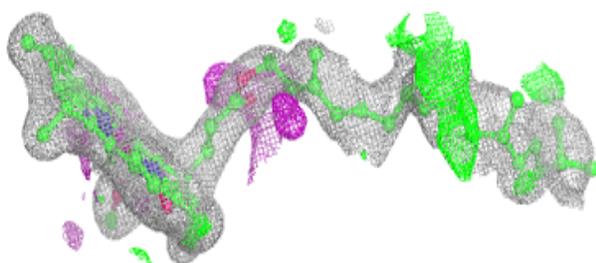
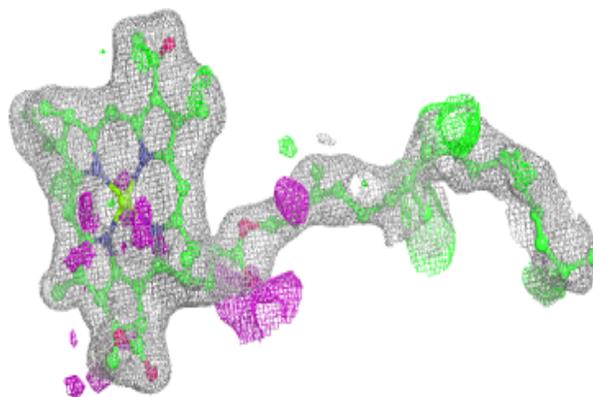
**Electron density around BCB LLL 302:**

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

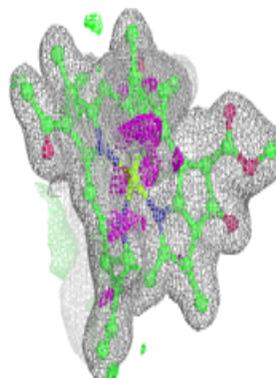
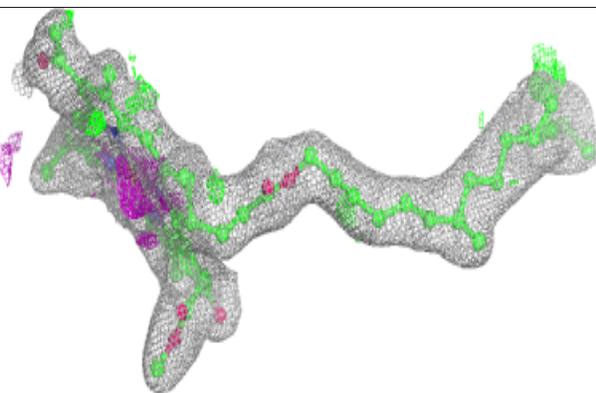
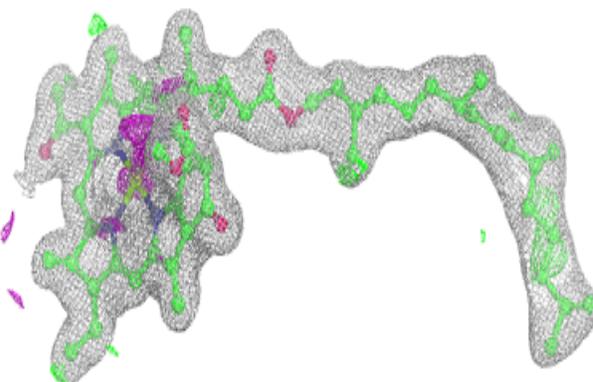


Electron density around BCB MMM 404:

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

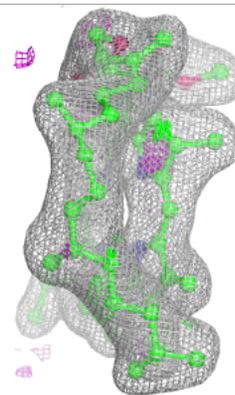
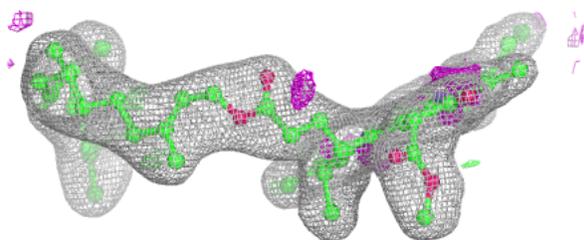
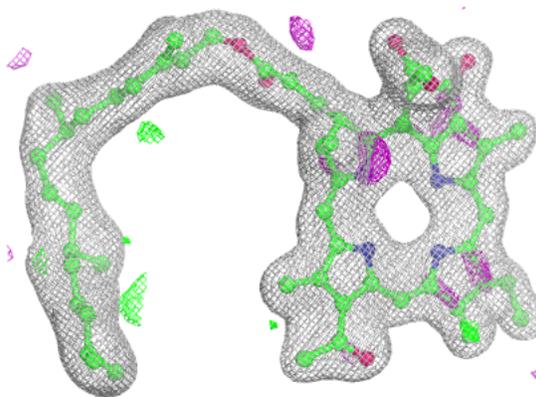
**Electron density around BCB MMM 405:**

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

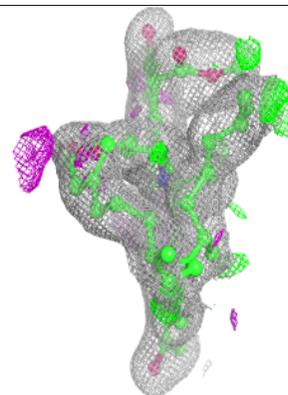
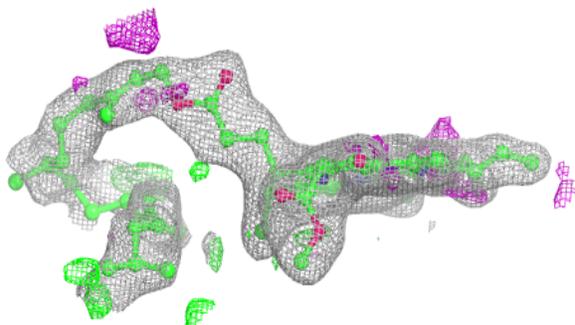
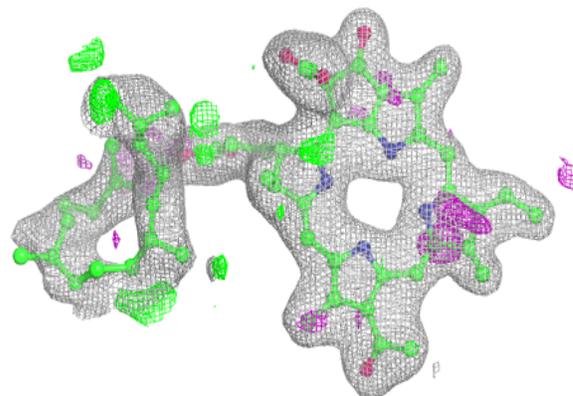


Electron density around BPB LLL 303:

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

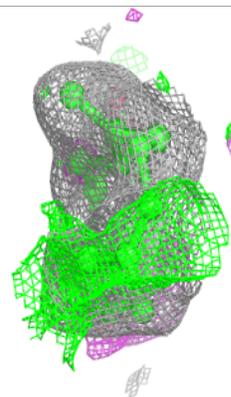
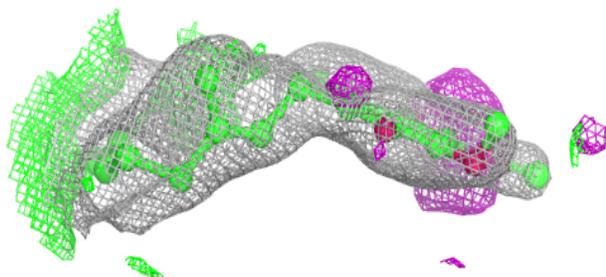
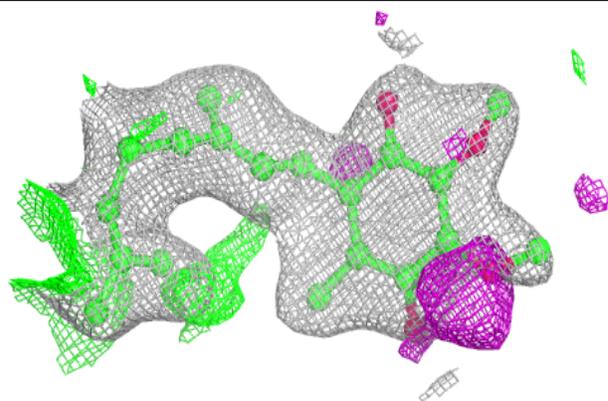
**Electron density around BPB MMM 406:**

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

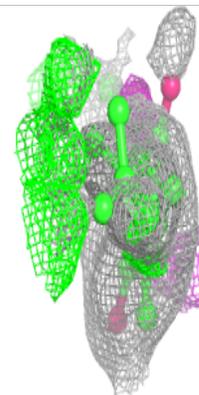
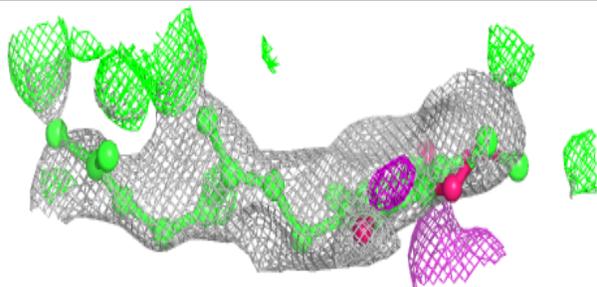
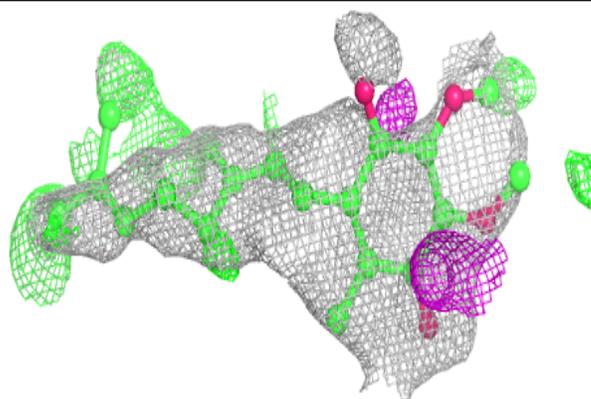


Electron density around UQ2 LLL 309:

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

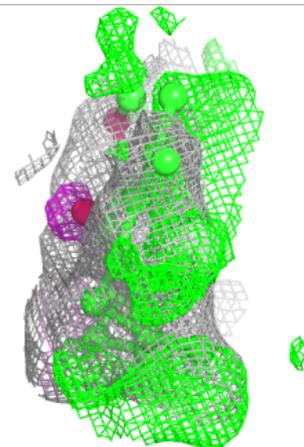
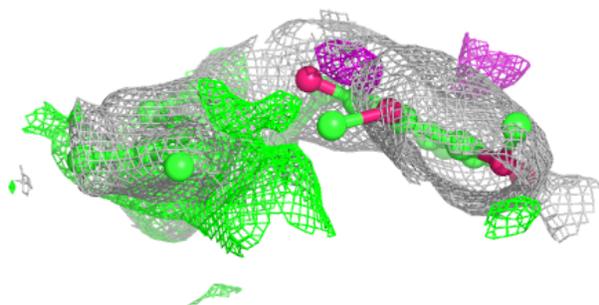
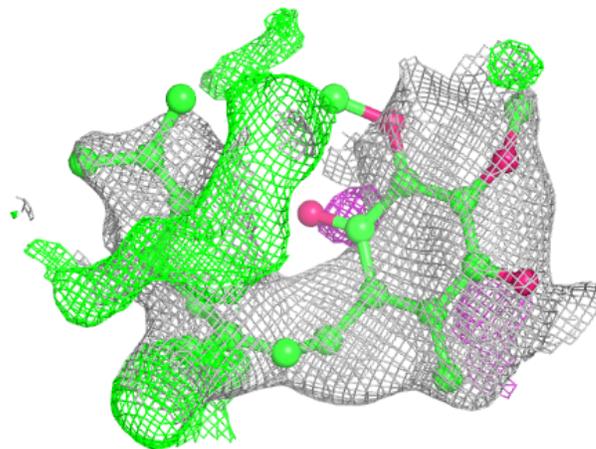
**Electron density around UQ2 MMM 416 (A):**

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



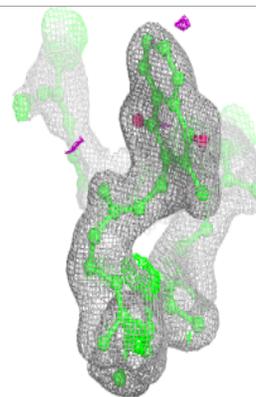
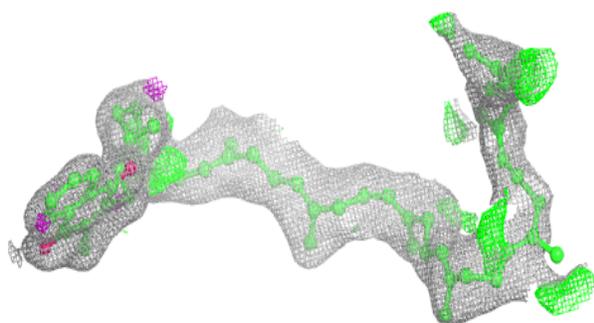
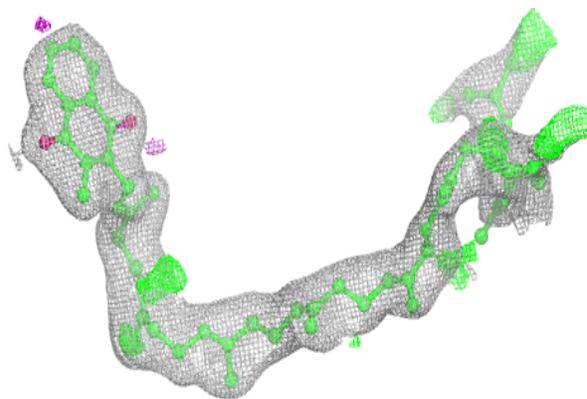
Electron density around UQ2 MMM 416 (B):

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

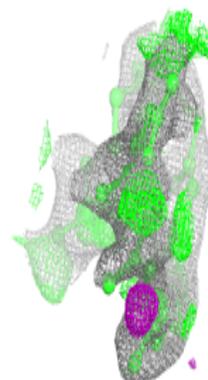
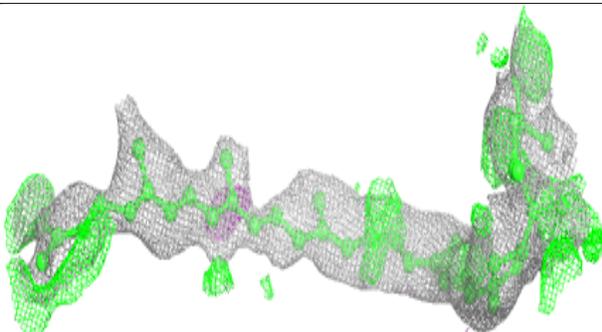
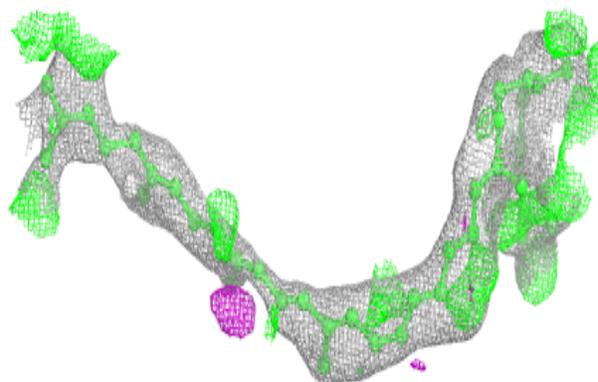


Electron density around MQ9 MMM 403:

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

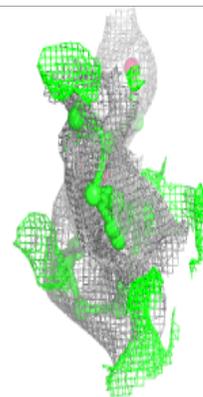
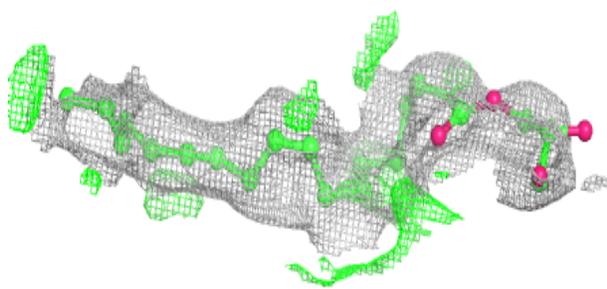
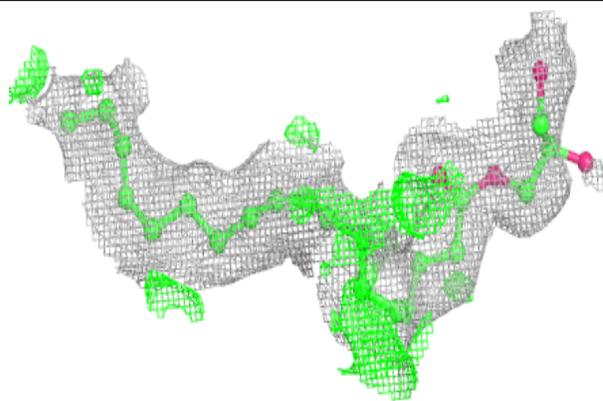
**Electron density around NS5 MMM 407:**

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

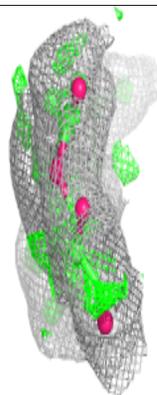
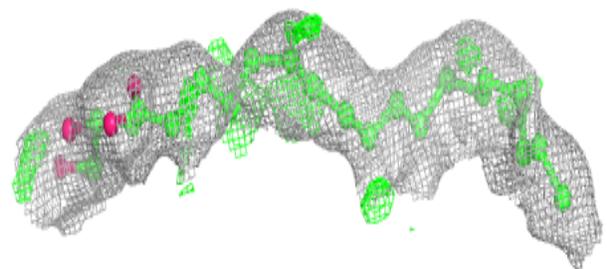
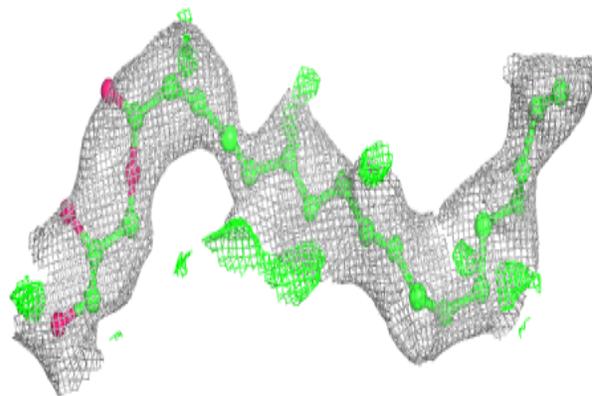


Electron density around OLC MMM 410:

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

**Electron density around 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)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.