WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 06:46 PM EDT

PDB ID	:	3D38
Title	:	Crystal structure of new trigonal form of photosynthetic reaction center from Blastochloris viridis. Crystals grown in microfluidics by detergent capture.
Authors	:	Li, L.; Nachtergaele, S.H.M.; Seddon, A.M.; Tereshko, V.; Ponomarenko, N.; Ismagilov, R.F.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)
Deposited on	:	2008-05-09
Resolution	:	3.21 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

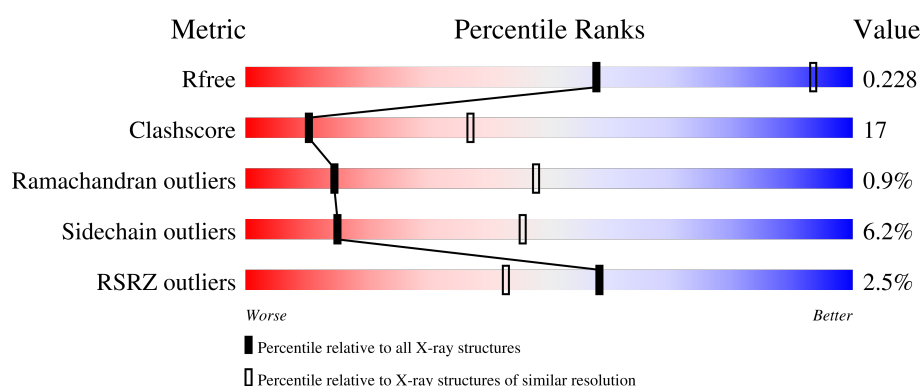|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh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

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.21 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		17
Ramachandran outliers		0.9%
Sidechain outliers		6.2%
RSRZ outliers		2.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1638 (3.24-3.20)
Clashscore	180529	1778 (3.24-3.20)
Ramachandran outliers	177936	1751 (3.24-3.20)
Sidechain outliers	177891	1750 (3.24-3.20)
RSRZ outliers	164620	1639 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	4% / 73% / 24% / ··
2	H	258	3% / 67% / 27% / · ·
3	L	273	% / 72% / 26% / ·
4	M	323	% / 72% / 25% / ·

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
7	HTO	C	706	-	-	-	X
7	HTO	C	707	-	-	-	X
7	HTO	H	705	-	-	-	X
9	BCB	L	400	X	-	-	-
9	BCB	L	401	X	-	-	-
9	BCB	M	400	X	-	-	-
9	BCB	M	401	X	-	-	-

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 10311 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	C	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1958	1251	335	370	2			

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

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

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

HEC

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

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

HTO
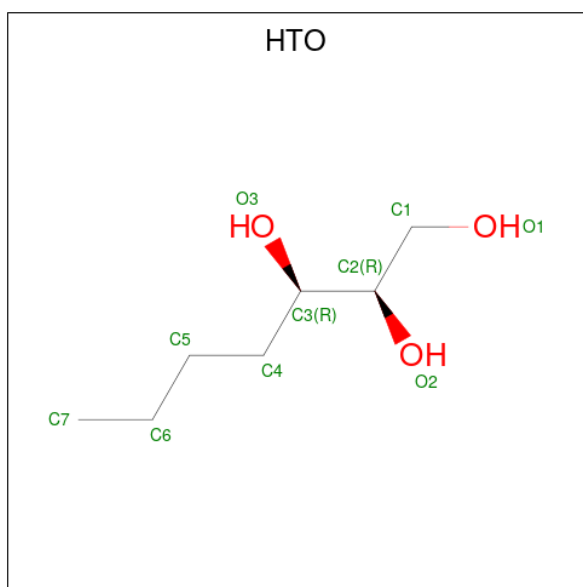
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total 10	C 7	O 3	0	0
7	C	1	Total 10	C 7	O 3	0	0
7	H	1	Total 10	C 7	O 3	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

LDA
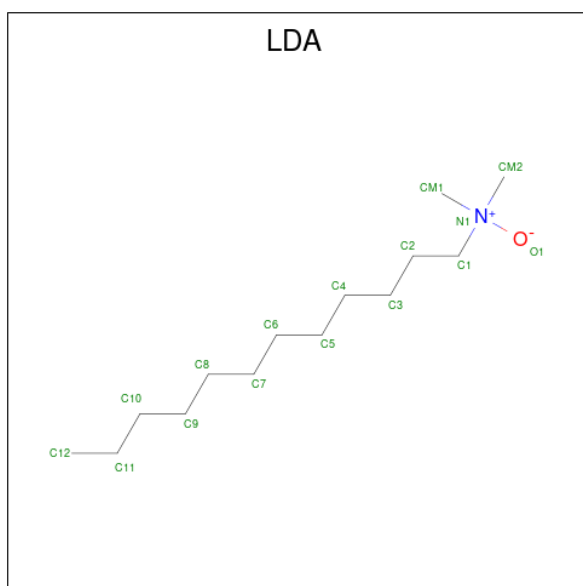
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).
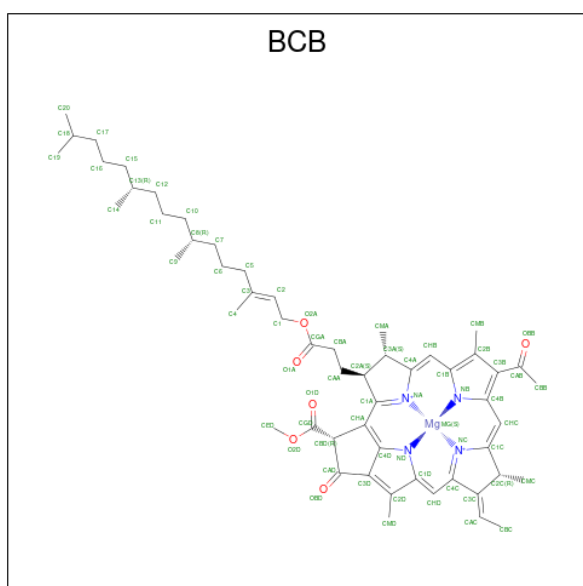
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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

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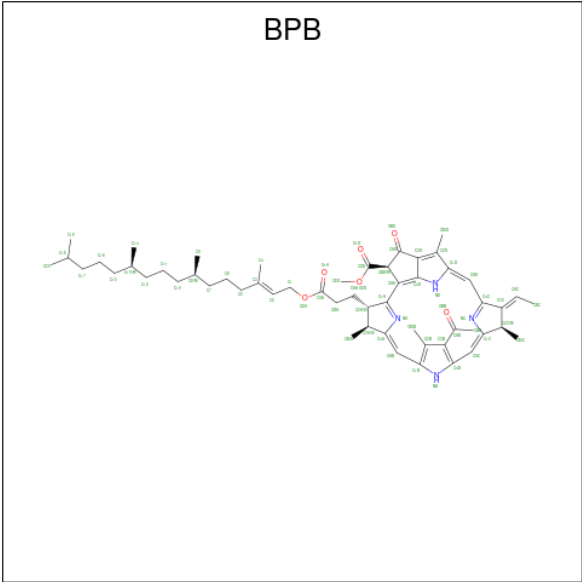
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

• Molecule 11 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).

UQ1
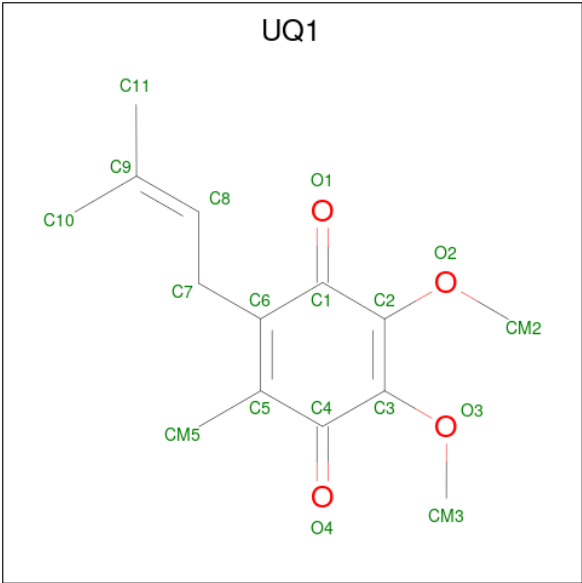
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			18	14	4		
11	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).
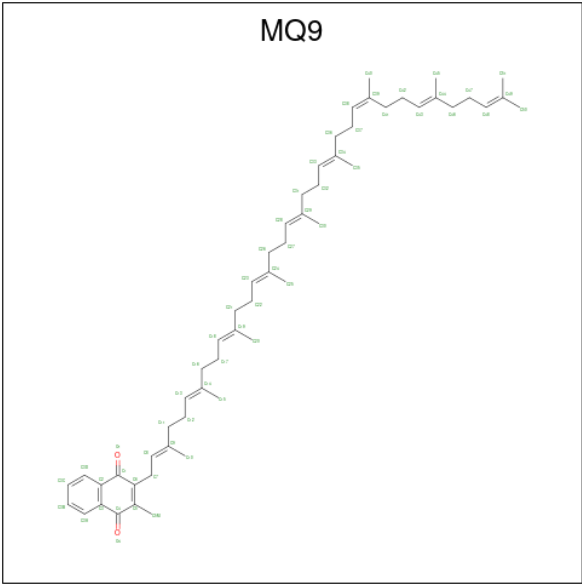
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).
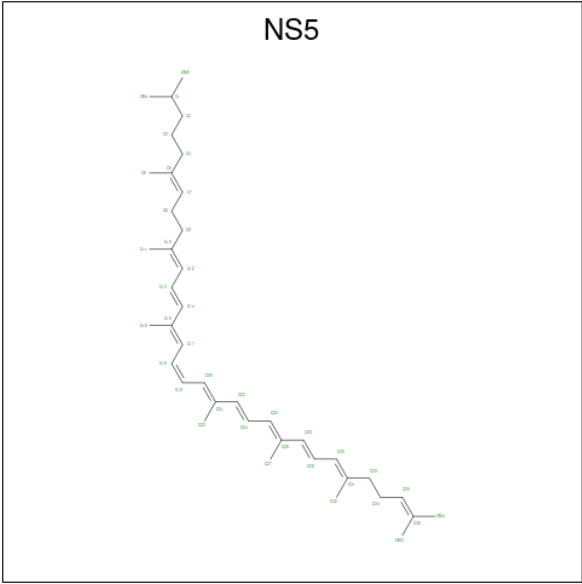
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total 40	C 40	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	47	Total 47	O 47	0	0
15	H	28	Total 28	O 28	0	0
15	L	38	Total 38	O 38	0	0
15	M	46	Total 46	O 46	0	0

3 Residue-property plots ⓘ

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
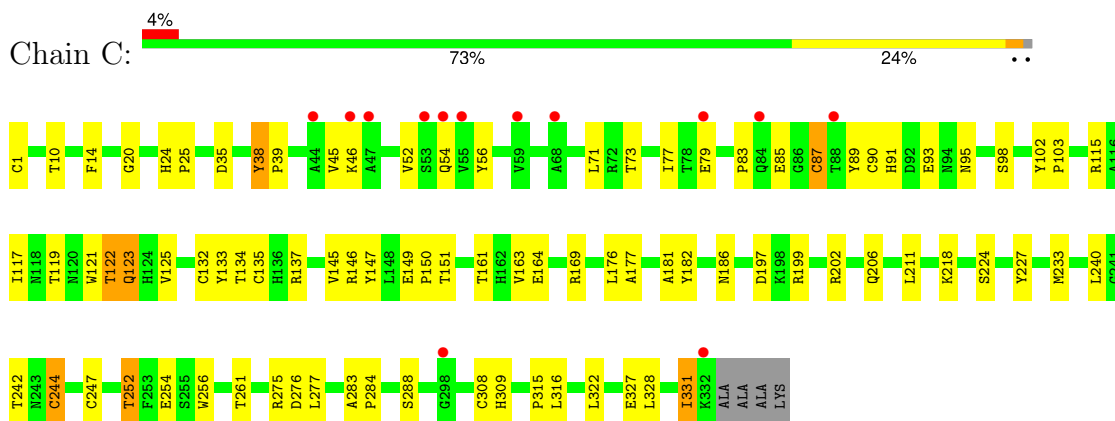
• Molecule 2: Reaction center protein H chain
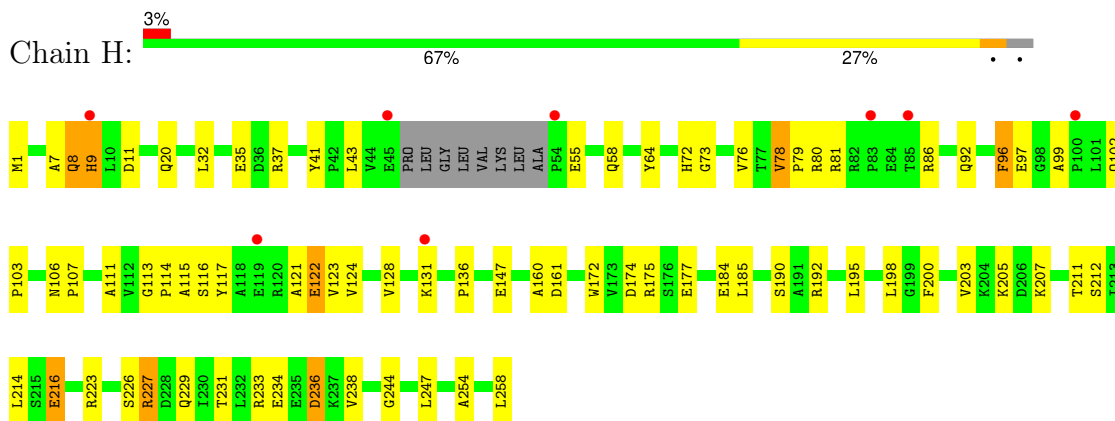
• Molecule 3: Reaction center protein L chain

W259 P260 E261 F271 W272 S273
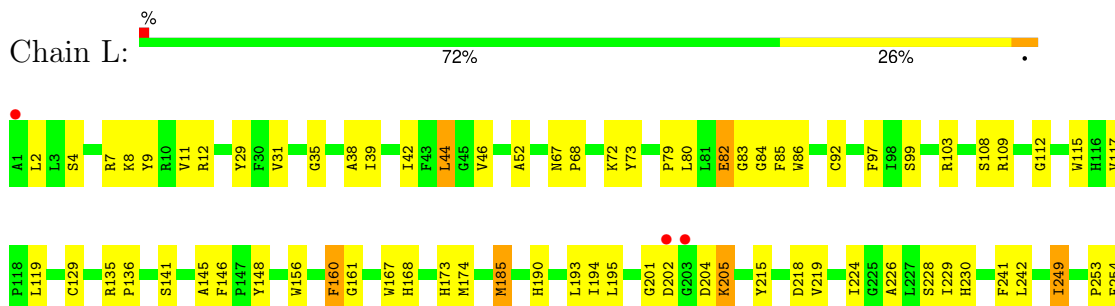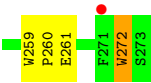
• Molecule 4: Reaction center protein M chain

Chain M:

%

72% 25%

A1 D2 Y3 Q4 I10 Q11 A12 R13 G21 D25 N26 V29 G30 K31 P32 F33 Y34 W37 L38 G39 K40 L51 I56 F59 I66 L70 H78 F79 D80 P81 L82 Q83 Q87 L91 P95 P96 L107 G110 G111 W112 W113 L114 M115 A116

G117 M120 L124 W127 Y132 S133 R134 T142 H143 W146 N147 F148 A149 I152 C157 I158 G159 C160 I161 H162 P163 T164 F175 G176 I177 W178 P179 L184 G192 N193 H200 G201 F202 S203 I204 G205 F206 F214 I221 R226 D230 E234

R239 G240 T241 E244 R245 F249 W250 R251 I254 G255 F256 N257 A258 T259 I260 E261 S262 V263 H264 R265 W266 M273 D290 P306 T312 P313 L318 P319 G320 A321 P322 K323

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.17Å 241.17Å 113.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.21 50.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.21) 99.8 (50.00-3.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.192 , 0.224 0.196 , 0.228	Depositor DCC
R_{free} test set	3141 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.6	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10311	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, HTO, BPB, HEC, LDA, FME, UQ1, MQ9, BCB, SO4, NS5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	C	0.53	1/2665 (0.0%)	0.64	0/3633
2	H	0.59	0/1993	0.68	0/2720
3	L	0.60	1/2259 (0.0%)	0.66	0/3084
4	M	0.57	0/2659	0.65	1/3637 (0.0%)
All	All	0.57	2/9576 (0.0%)	0.66	1/13074 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	CYS	CB-SG	-5.84	1.72	1.81
3	L	129	CYS	CB-SG	-5.38	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	70	LEU	CA-CB-CG	7.57	132.71	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2573	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1958	0	1946	65	0
3	L	2171	0	2098	64	0
4	M	2555	0	2452	76	0
5	C	35	0	0	0	0
5	H	20	0	0	1	0
5	M	20	0	0	1	0
6	C	172	0	125	31	0
7	C	20	0	32	1	0
7	H	10	0	16	2	0
8	H	32	0	62	6	0
8	L	16	0	31	2	0
8	M	16	0	31	0	0
9	L	132	0	144	24	0
9	M	132	0	144	27	0
10	L	65	0	74	9	0
10	M	65	0	74	20	0
11	L	36	0	36	4	0
12	M	1	0	0	0	0
13	M	58	0	80	3	0
14	M	40	0	60	11	0
15	C	47	0	0	9	0
15	H	28	0	0	5	0
15	L	38	0	0	3	0
15	M	46	0	0	7	0
All	All	10311	0	9978	337	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 337 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:C:90:CYS:SG	6:C:401:HEC:HAC	1.31	1.69
1:C:132:CYS:SG	6:C:402:HEC:HAB	1.48	1.52
1:C:244:CYS:SG	6:C:403:HEC:HAB	1.54	1.47
1:C:132:CYS:SG	6:C:402:HEC:CAB	2.08	1.39
1:C:135:CYS:SG	6:C:402:HEC:CAC	2.12	1.37

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	C	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	37	68
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	8	36
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	30	63
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	8	36
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	14	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	147	GLU
2	H	73	GLY
4	M	32	PRO
4	M	51	LEU
4	M	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	C	280/282 (99%)	266 (95%)	14 (5%)	20	52
2	H	205/212 (97%)	188 (92%)	17 (8%)	9	34
3	L	218/218 (100%)	203 (93%)	15 (7%)	13	41
4	M	249/249 (100%)	236 (95%)	13 (5%)	19	50
All	All	952/961 (99%)	893 (94%)	59 (6%)	15	45

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	227	ARG
4	M	230	ASP
3	L	44	LEU
4	M	214	PHE
4	M	40	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	4	GLN
4	M	147	ASN
4	M	78	HIS
2	H	106	ASN
3	L	239	ASN

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	H	1	2	8,9,10	0.83	0	8,9,11	3.48	1 (12%)

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	H	1	2	-	4/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-9.15	108.76	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	SO4	H	807	-	4,4,4	0.23	0	6,6,6	0.32	0
5	SO4	H	803	-	4,4,4	0.27	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	UQ1	L	502	-	18,18,18	2.26	2 (11%)	24,25,25	1.53	5 (20%)
8	LDA	H	703	-	13,15,15	2.49	2 (15%)	14,17,17	0.53	0
5	SO4	C	809	-	4,4,4	0.25	0	6,6,6	0.11	0
8	LDA	M	704	-	13,15,15	2.39	2 (15%)	14,17,17	0.44	0
10	BPB	M	402	-	49,70,70	1.43	6 (12%)	48,101,101	2.04	9 (18%)
5	SO4	H	812	-	4,4,4	0.27	0	6,6,6	0.19	0
13	MQ9	M	501	-	59,59,59	1.80	18 (30%)	73,75,75	1.57	21 (28%)
14	NS5	M	600	-	39,39,39	1.52	3 (7%)	46,46,46	1.99	14 (30%)
5	SO4	C	815	-	4,4,4	0.27	0	6,6,6	0.15	0
5	SO4	M	801	-	4,4,4	0.31	0	6,6,6	0.56	0
5	SO4	C	813	-	4,4,4	0.19	0	6,6,6	0.26	0
7	HTO	C	707	-	9,9,9	0.69	0	10,10,10	0.58	0
5	SO4	C	808	-	4,4,4	0.22	0	6,6,6	0.20	0
5	SO4	M	802	-	4,4,4	0.29	0	6,6,6	0.24	0
9	BCB	L	401	3	63,74,74	1.96	10 (15%)	72,115,115	2.04	15 (20%)
6	HEC	C	404	1	32,50,50	1.65	2 (6%)	30,82,82	2.26	5 (16%)
5	SO4	M	804	-	4,4,4	0.26	0	6,6,6	0.29	0
6	HEC	C	401	1	32,50,50	1.85	3 (9%)	30,82,82	2.31	3 (10%)
5	SO4	C	810	-	4,4,4	0.26	0	6,6,6	0.08	0
7	HTO	C	706	-	9,9,9	0.28	0	10,10,10	0.77	0
9	BCB	M	401	4	63,74,74	2.06	12 (19%)	72,115,115	1.96	20 (27%)
6	HEC	C	402	1	32,50,50	1.69	2 (6%)	30,82,82	2.36	5 (16%)
5	SO4	C	811	-	4,4,4	0.28	0	6,6,6	0.24	0
5	SO4	H	806	-	4,4,4	0.27	0	6,6,6	0.22	0
7	HTO	H	705	-	9,9,9	0.73	0	10,10,10	0.86	0
6	HEC	C	403	1	32,50,50	1.69	3 (9%)	30,82,82	2.17	4 (13%)
5	SO4	C	814	-	4,4,4	0.24	0	6,6,6	0.35	0
9	BCB	L	400	3	63,74,74	2.22	12 (19%)	72,115,115	2.15	17 (23%)
11	UQ1	L	503	-	18,18,18	2.31	2 (11%)	24,25,25	1.37	4 (16%)
8	LDA	H	701	-	13,15,15	2.22	2 (15%)	14,17,17	0.47	0
8	LDA	L	702	-	13,15,15	2.26	2 (15%)	14,17,17	0.62	0
5	SO4	M	805	-	4,4,4	0.27	0	6,6,6	0.40	0
9	BCB	M	400	4	63,74,74	2.07	11 (17%)	72,115,115	1.95	17 (23%)
10	BPB	L	402	-	49,70,70	1.53	6 (12%)	48,101,101	1.99	13 (27%)

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
11	UQ1	L	502	-	-	3/9/33/33	0/1/1/1
8	LDA	H	703	-	-	6/13/13/13	-
8	LDA	M	704	-	-	9/13/13/13	-
10	BPB	M	402	-	-	15/37/105/105	0/5/6/6
13	MQ9	M	501	-	-	16/53/73/73	0/2/2/2
14	NS5	M	600	-	-	14/43/43/43	-
7	HTO	C	707	-	-	8/10/10/10	-
9	BCB	L	401	3	2/2/21/26	9/37/137/137	-
6	HEC	C	404	1	-	4/10/54/54	-
6	HEC	C	401	1	-	2/10/54/54	-
9	BCB	M	401	4	2/2/21/26	16/37/137/137	-
7	HTO	C	706	-	-	5/10/10/10	-
6	HEC	C	402	1	-	4/10/54/54	-
7	HTO	H	705	-	-	8/10/10/10	-
6	HEC	C	403	1	-	3/10/54/54	-
9	BCB	L	400	3	3/3/21/26	14/37/137/137	-
11	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
8	LDA	H	701	-	-	8/13/13/13	-
8	LDA	L	702	-	-	11/13/13/13	-
9	BCB	M	400	4	2/2/21/26	12/37/137/137	-
10	BPB	L	402	-	-	14/37/105/105	0/5/6/6

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	400	BCB	CHC-C1C	9.93	1.42	1.33
9	M	400	BCB	CHB-C4A	8.61	1.41	1.33
11	L	502	UQ1	C6-C5	8.27	1.50	1.35
11	L	503	UQ1	C6-C5	8.23	1.50	1.35
9	M	401	BCB	CHC-C1C	8.03	1.40	1.33

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	402	BPB	O2D-CGD-CBD	9.48	121.37	110.95
9	L	400	BCB	C1C-NC-C4C	9.07	110.82	106.68
6	C	402	HEC	CBB-CAB-C3B	-8.32	108.01	127.49
6	C	401	HEC	CBC-CAC-C3C	-8.26	108.15	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	402	BPB	O2D-CGD-CBD	7.98	119.71	110.95

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	L	400	BCB	ND
9	L	400	BCB	NA
9	L	400	BCB	NC
9	L	401	BCB	NA
9	L	401	BCB	NC

5 of 181 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	404	HEC	C2D-C3D-CAD-CBD
6	C	404	HEC	C4D-C3D-CAD-CBD
7	C	706	HTO	C1-C2-C3-O3
7	C	706	HTO	O2-C2-C3-O3
7	C	706	HTO	O2-C2-C3-C4

There are no ring outliers.

19 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	807	SO4	1	0
11	L	502	UQ1	4	0
8	H	703	LDA	6	0
10	M	402	BPB	20	0
13	M	501	MQ9	3	0
14	M	600	NS5	11	0
9	L	401	BCB	10	0
6	C	404	HEC	2	0
6	C	401	HEC	13	0
7	C	706	HTO	1	0
9	M	401	BCB	17	0
6	C	402	HEC	10	0
7	H	705	HTO	2	0
6	C	403	HEC	6	0
9	L	400	BCB	17	0
8	L	702	LDA	2	0
5	M	805	SO4	1	0
9	M	400	BCB	11	0
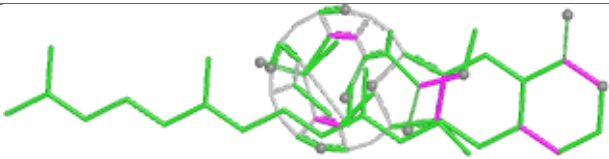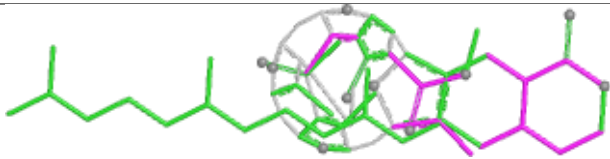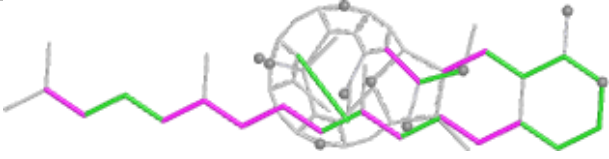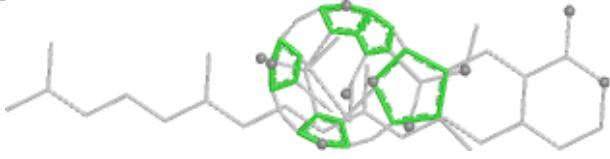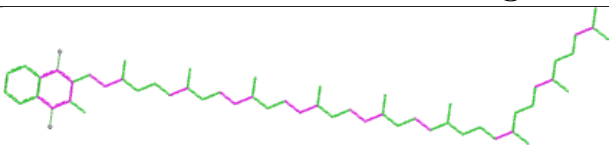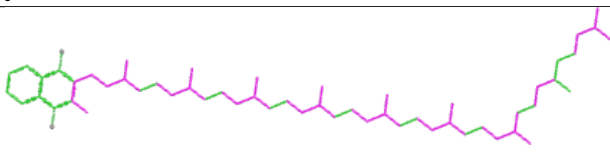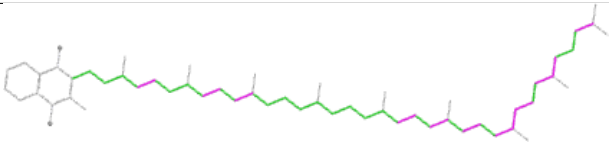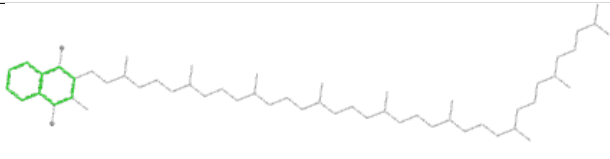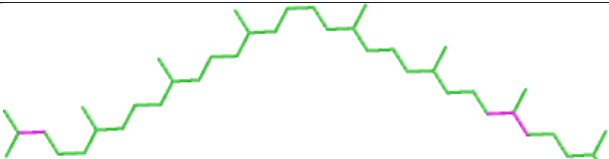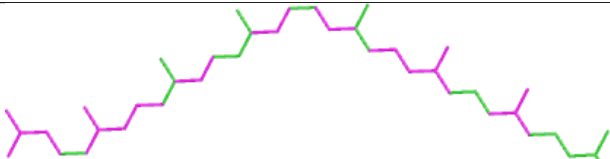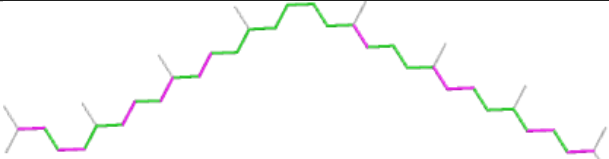
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	402	BPB	9	0

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 L 502

Bond lengths

Bond angles
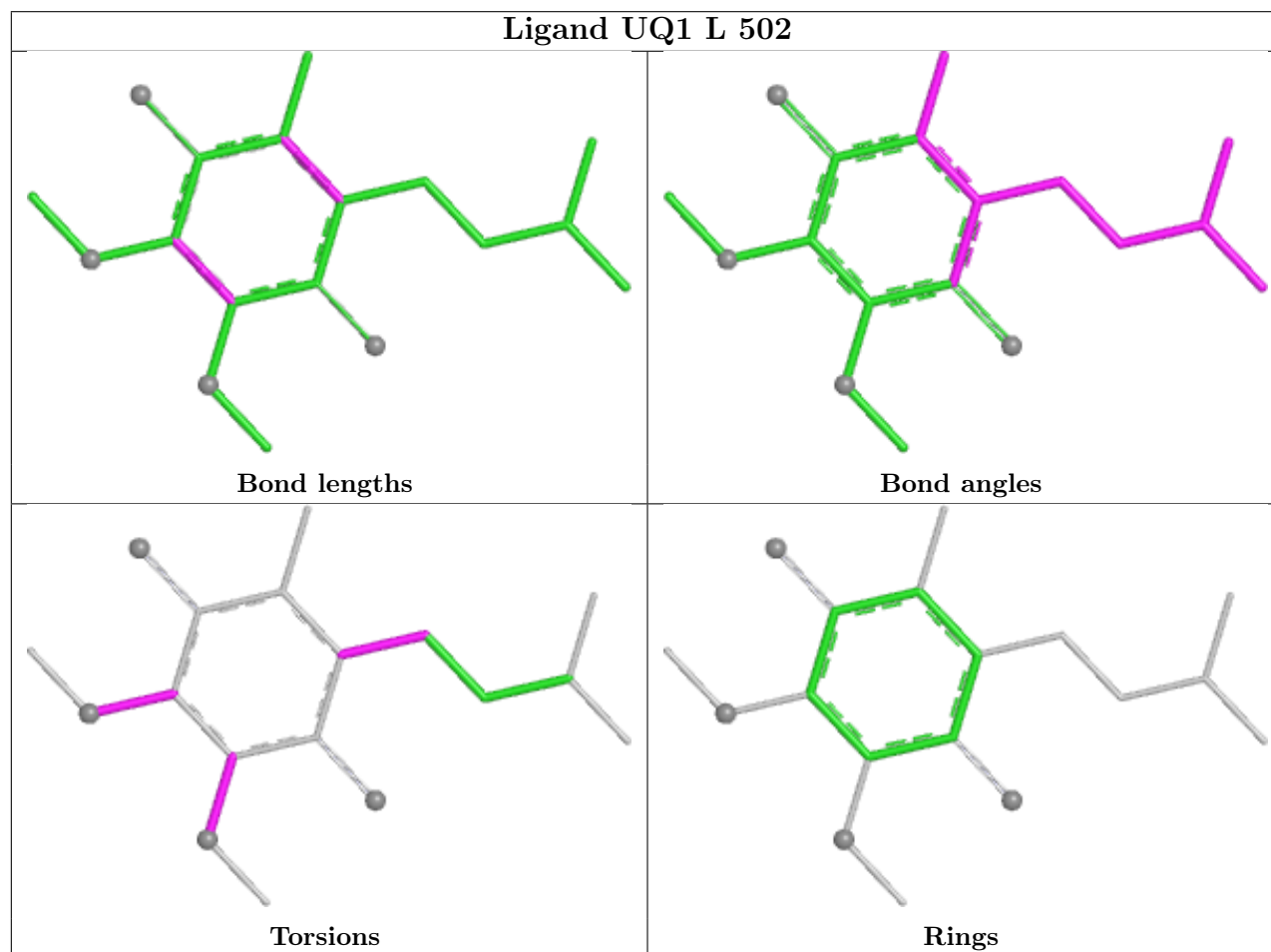
Torsions

Rings

Ligand BPB M 402

Bond lengths

Bond angles

Torsions

Rings

Ligand MQ9 M 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NS5 M 600

Bond lengths

Bond angles

Torsions

Rings

Ligand BCB L 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC C 404

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand BCB M 401

Bond lengths

Bond angles
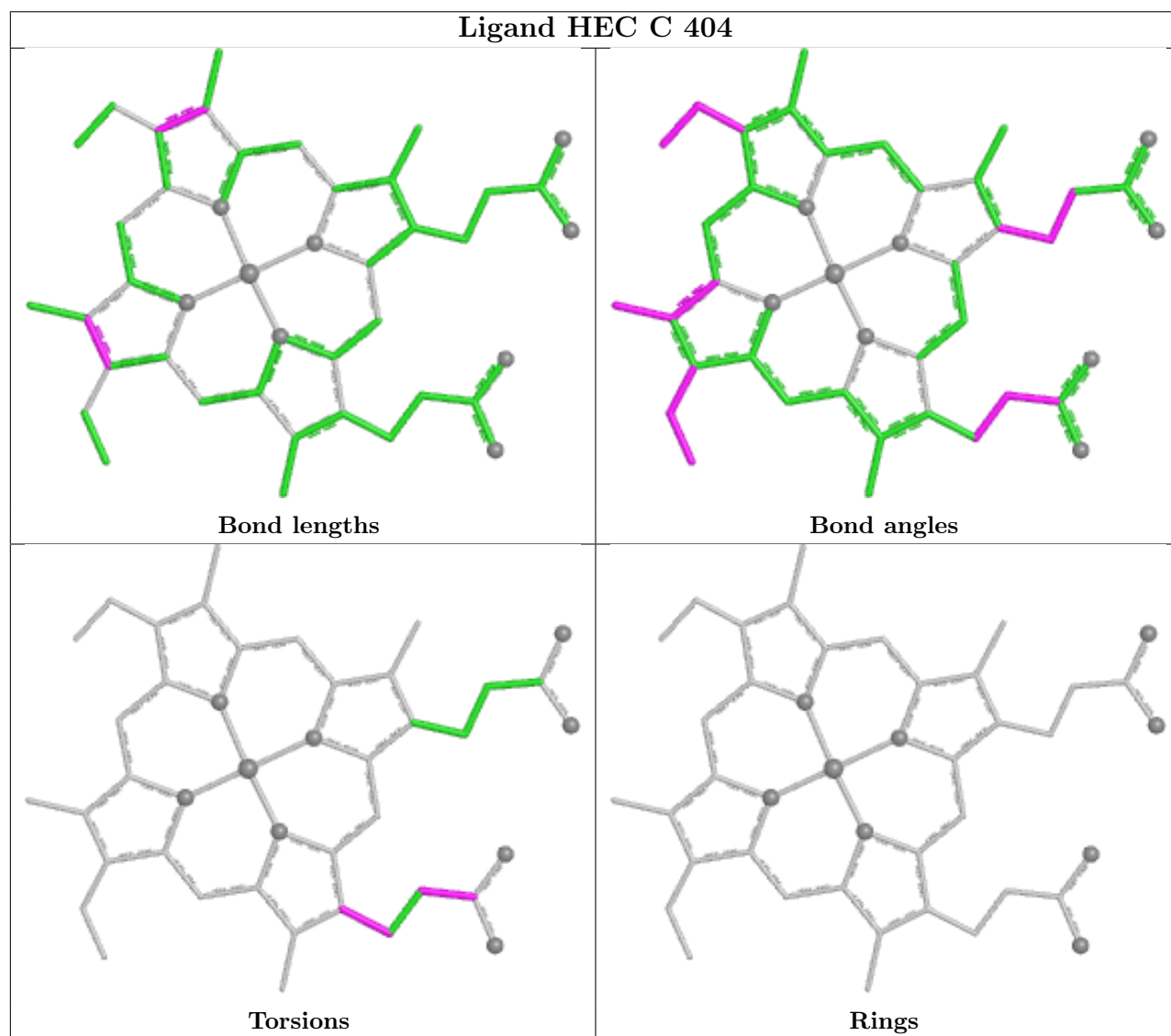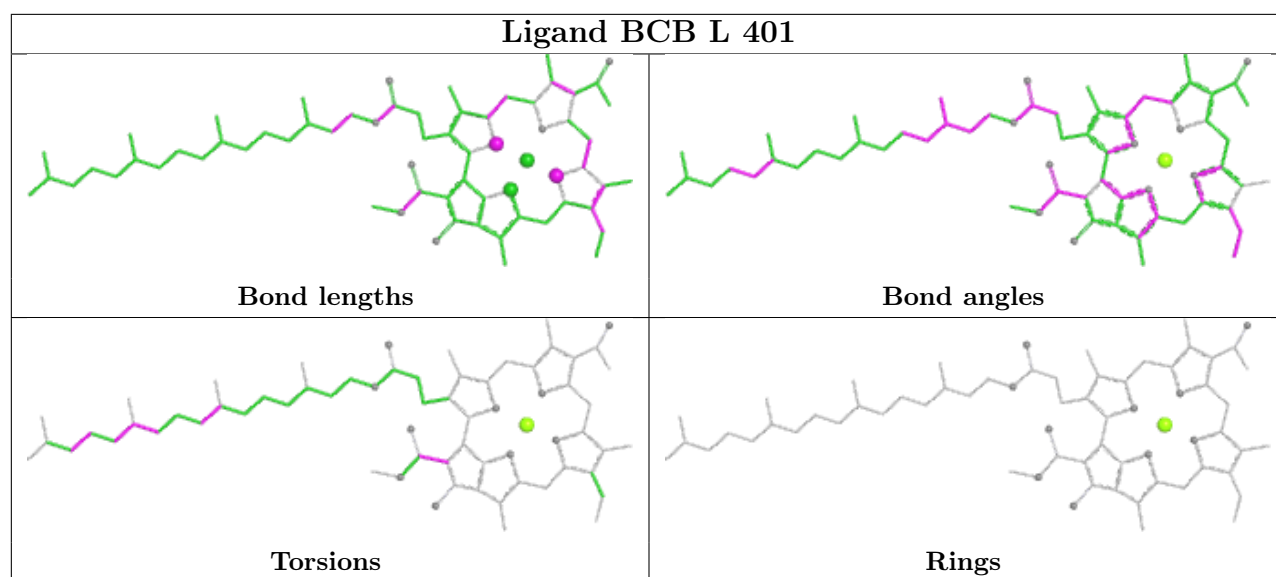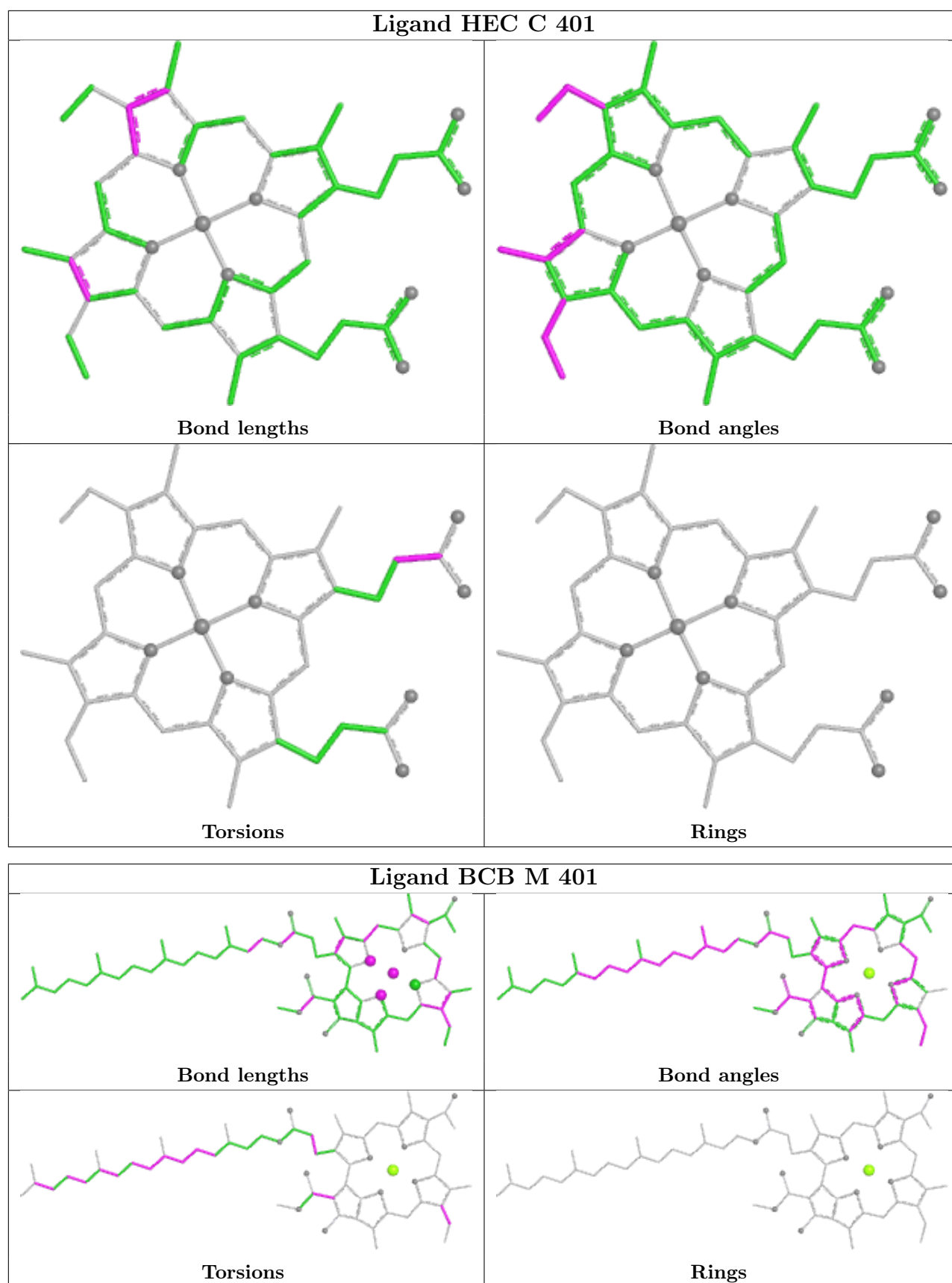
Torsions

Rings

Ligand HEC C 402

Bond lengths
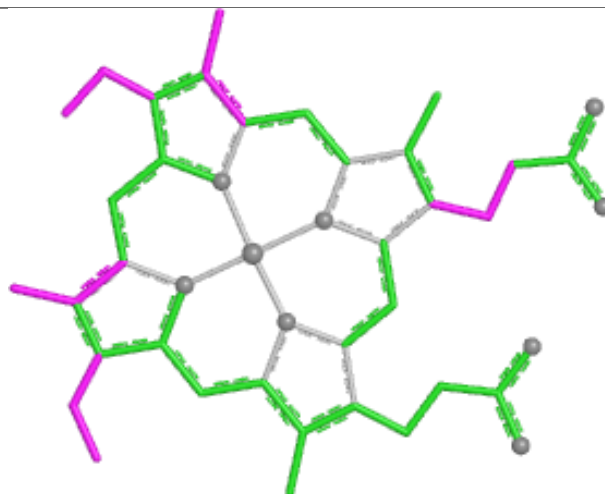
Bond angles
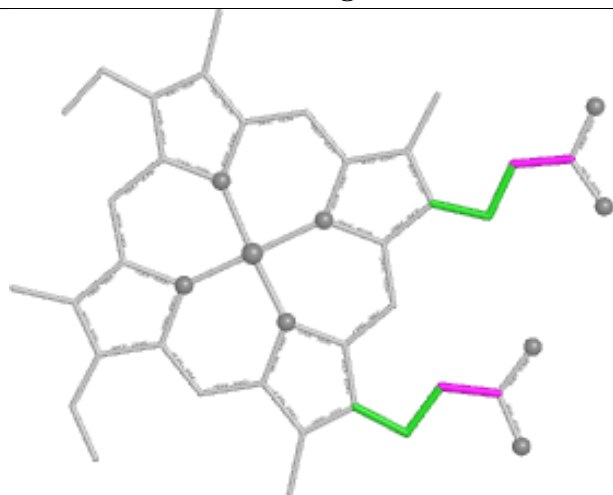
Torsions

Rings

Ligand HEC C 403
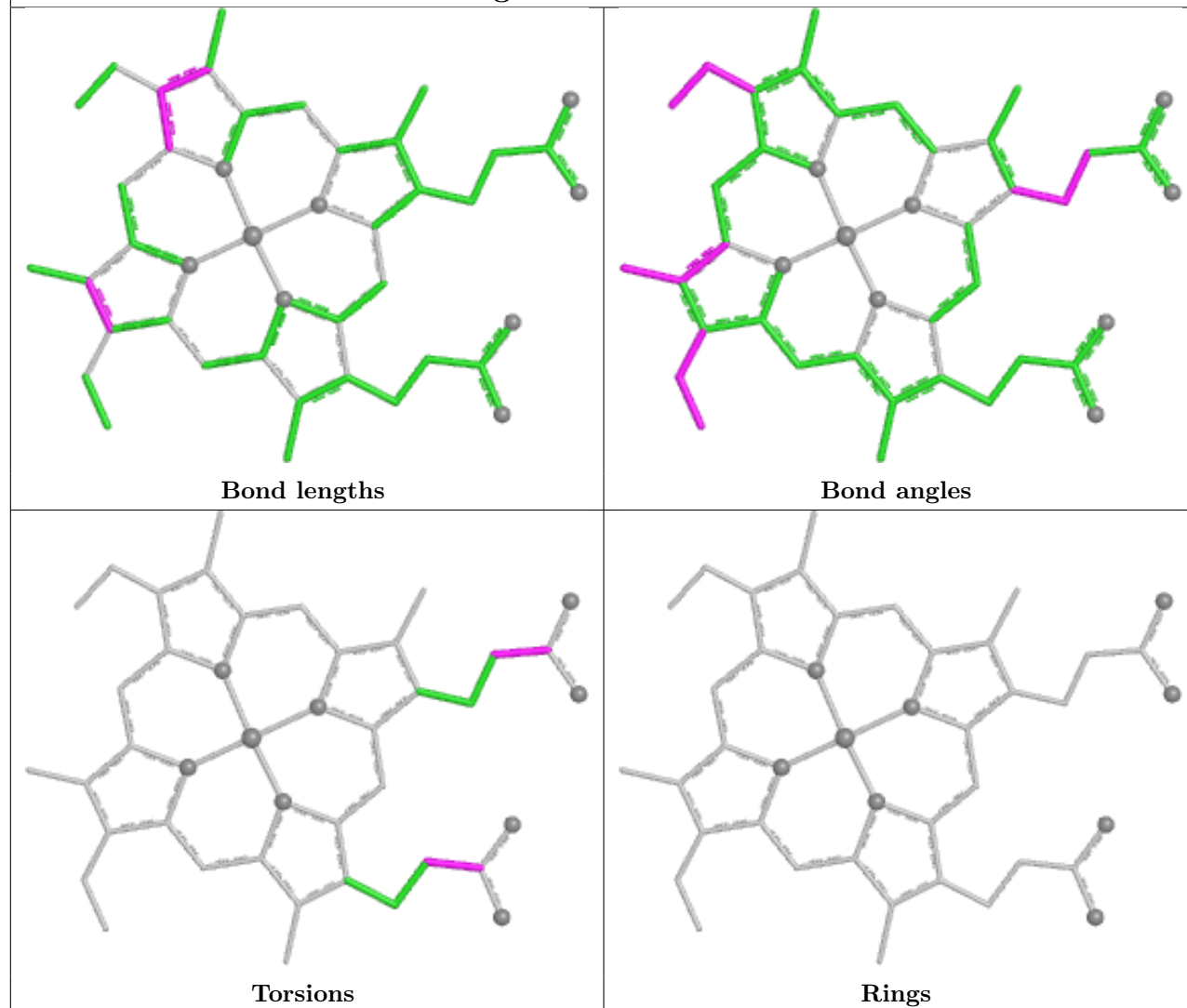
Bond lengths

Bond angles

Torsions

Rings

Ligand BCB L 400

Bond lengths

Bond angles

Torsions

Rings

Ligand UQ1 L 503

Bond lengths

Bond angles

Torsions

Rings

Ligand BCB M 400

Bond lengths

Bond angles

Torsions

Rings

Ligand BPB L 402

Bond lengths

Bond angles

Torsions

Rings
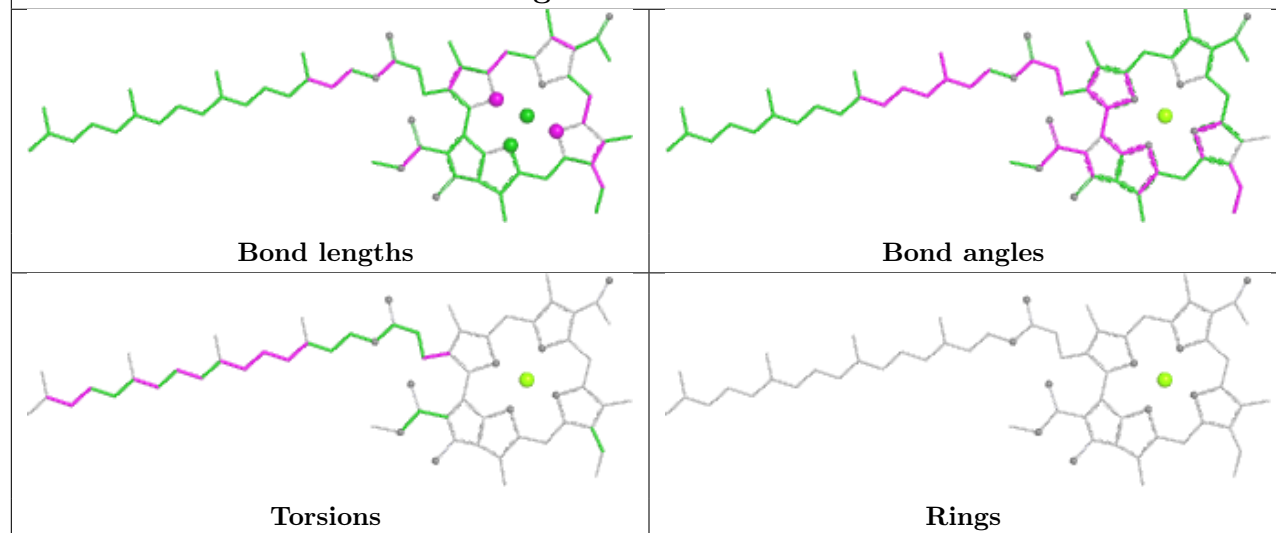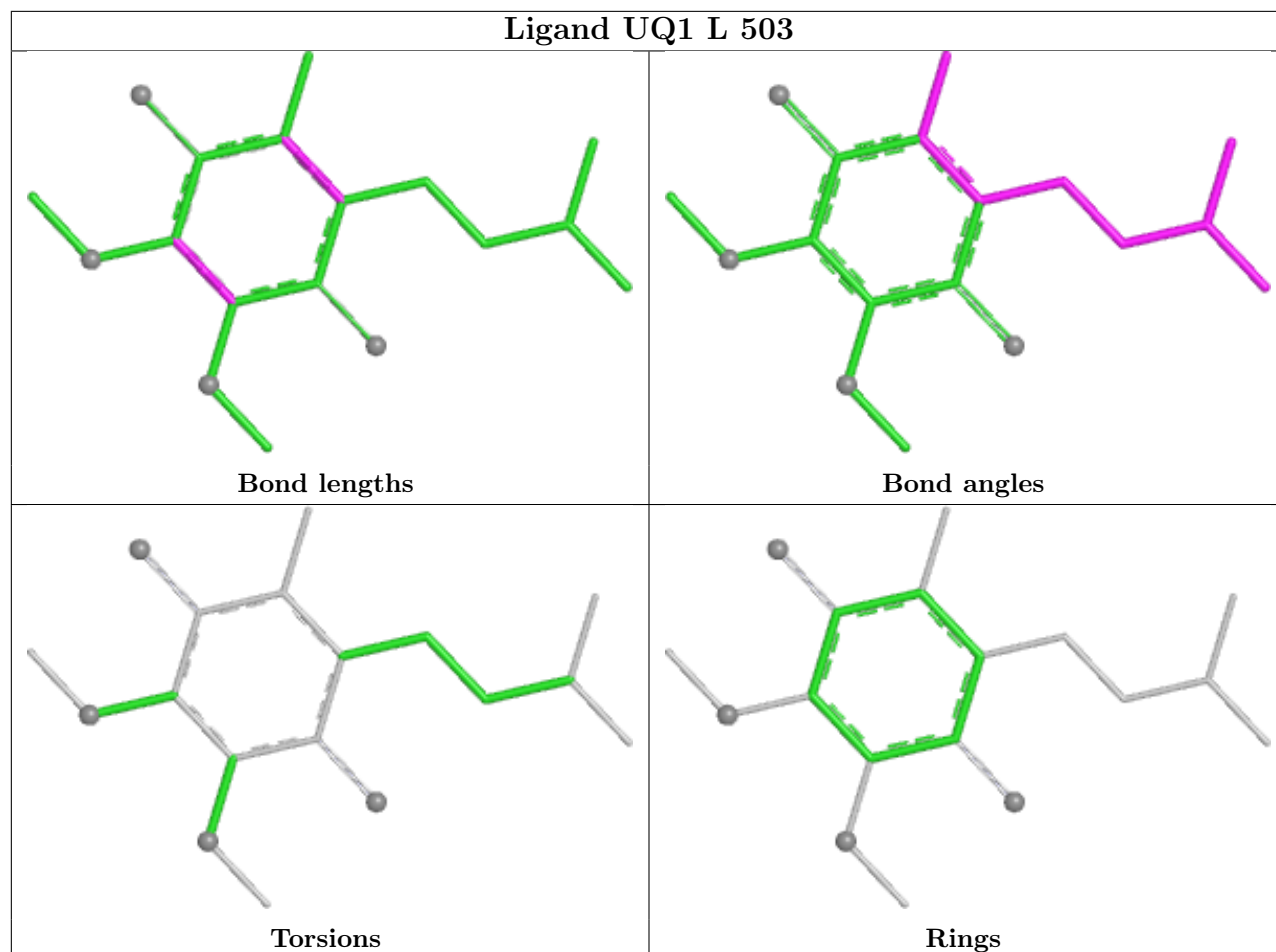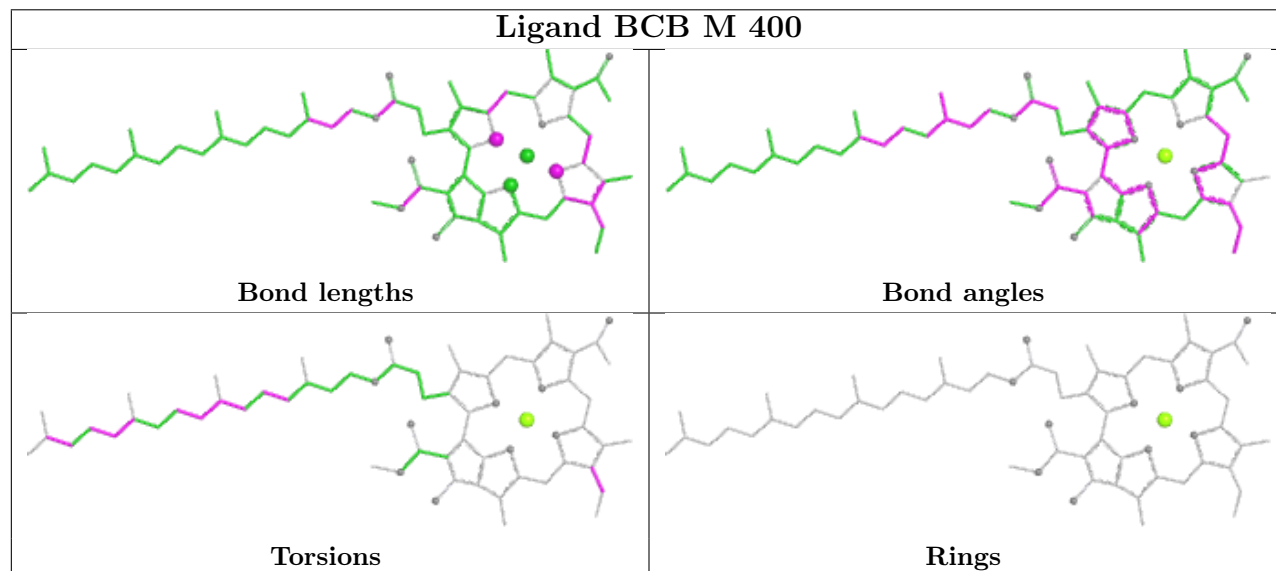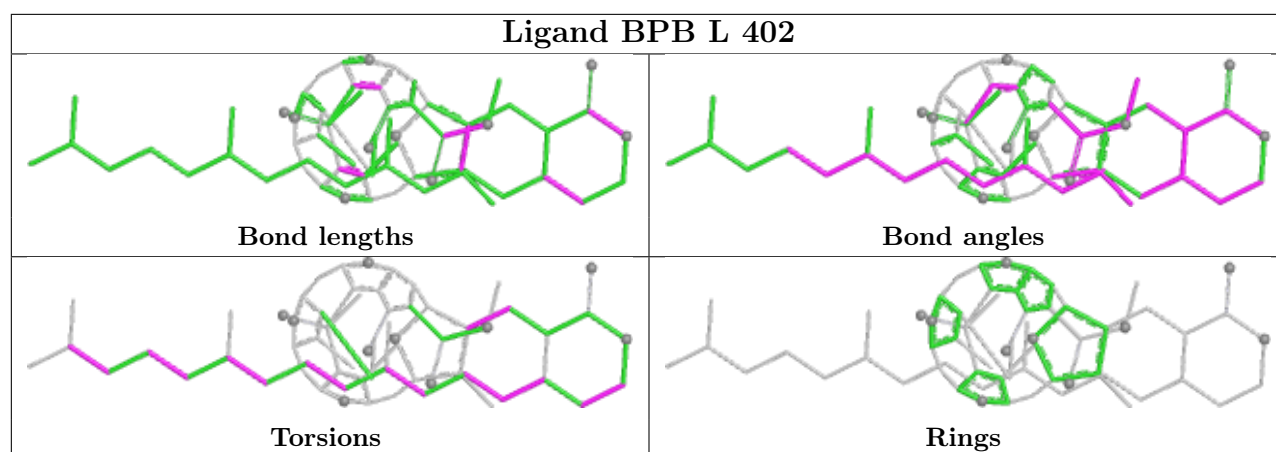
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	332/336 (98%)	-0.09	13 (3%)	44	30	46, 74, 113, 124	0
2	H	249/258 (96%)	-0.00	8 (3%)	50	35	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.46	4 (1%)	71	57	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.42	4 (1%)	76	62	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.25	29 (2%)	58	43	37, 66, 102, 124	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	4.1
2	H	54	PRO	4.0
3	L	1	ALA	3.8
2	H	45	GLU	3.6
4	M	321	ALA	3.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	H	1	10/11	0.75	0.22	104,105,115,117	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

wwPDB X-ray Structure Validation Summary Report

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
5	SO4	C	808	5/5	0.48	0.31	104,104,104,104	5
7	HTO	H	705	10/10	0.60	1.17	56,59,61,61	10
7	HTO	C	706	10/10	0.66	1.28	56,57,58,58	10
7	HTO	C	707	10/10	0.75	0.76	44,48,49,49	10
5	SO4	H	812	5/5	0.76	0.23	92,92,93,93	5
5	SO4	H	803	5/5	0.76	0.23	82,82,83,83	5
5	SO4	C	809	5/5	0.81	0.21	109,110,110,110	5
5	SO4	H	807	5/5	0.84	0.17	108,108,108,109	5
5	SO4	C	814	5/5	0.86	0.18	48,48,49,50	5
5	SO4	C	813	5/5	0.87	0.18	79,79,80,80	5
5	SO4	C	810	5/5	0.87	0.18	88,88,88,88	5
11	UQ1	L	503	18/18	0.87	0.42	73,76,78,78	18
5	SO4	M	805	5/5	0.91	0.14	64,65,65,67	5
14	NS5	M	600	40/40	0.91	0.22	65,71,100,101	4
5	SO4	H	806	5/5	0.92	0.10	72,72,73,73	5
8	LDA	M	704	16/16	0.92	0.25	68,70,73,73	16
5	SO4	C	811	5/5	0.93	0.19	76,76,76,77	5
10	BPB	M	402	65/65	0.93	0.17	61,67,123,124	0
5	SO4	M	802	5/5	0.93	0.14	89,89,90,90	0
8	LDA	H	703	16/16	0.93	0.19	54,58,60,61	16
11	UQ1	L	502	18/18	0.94	0.22	63,65,66,66	18
5	SO4	M	804	5/5	0.95	0.07	94,95,96,96	0
5	SO4	M	801	5/5	0.96	0.08	61,62,63,63	0
9	BCB	M	400	66/66	0.96	0.12	37,48,107,108	0
13	MQ9	M	501	58/58	0.96	0.12	40,64,102,103	0
6	HEC	C	401	43/43	0.96	0.13	99,110,118,120	0
5	SO4	C	815	5/5	0.97	0.10	40,40,41,41	5
8	LDA	L	702	16/16	0.97	0.12	67,73,79,80	0
8	LDA	H	701	16/16	0.97	0.11	54,57,68,68	0
9	BCB	L	400	66/66	0.98	0.08	37,40,45,49	0
9	BCB	M	401	66/66	0.98	0.09	36,41,63,68	0
10	BPB	L	402	65/65	0.98	0.08	38,51,60,60	0
9	BCB	L	401	66/66	0.98	0.08	41,44,59,64	0
6	HEC	C	404	43/43	0.99	0.06	52,55,68,73	0
6	HEC	C	402	43/43	0.99	0.08	73,76,80,81	0
6	HEC	C	403	43/43	0.99	0.07	46,48,52,54	0
12	FE2	M	500	1/1	1.00	0.01	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
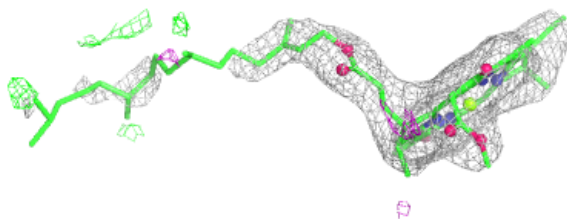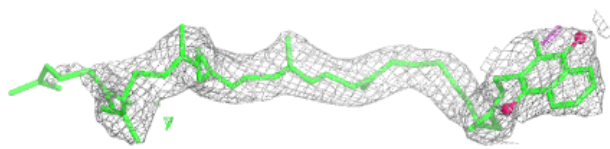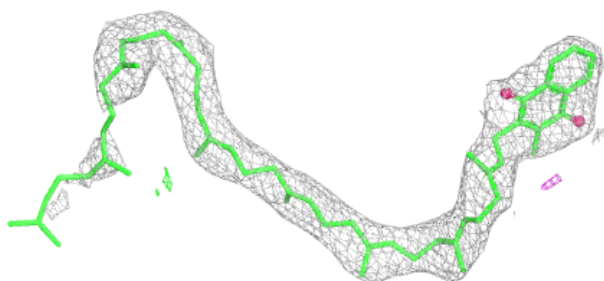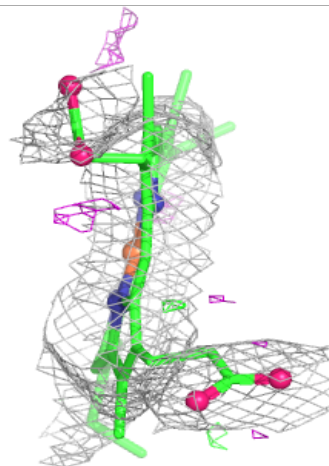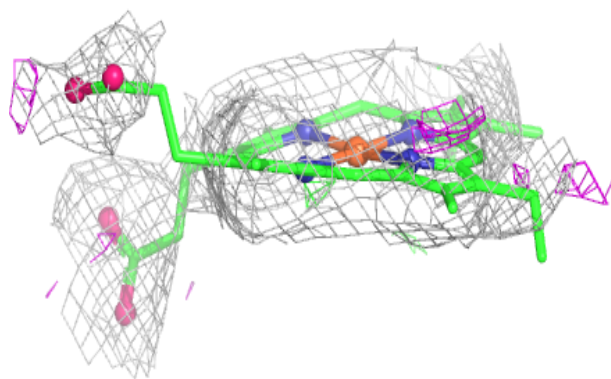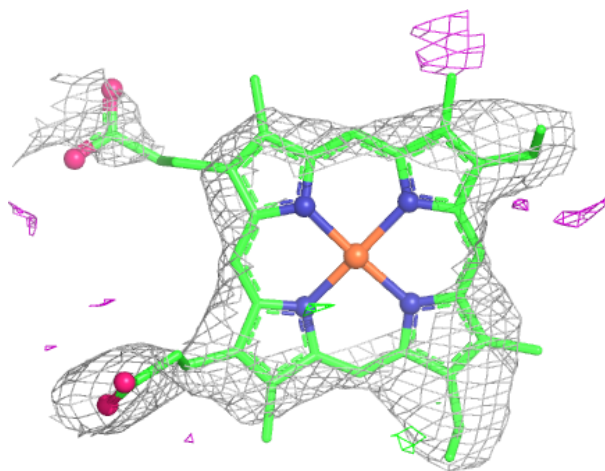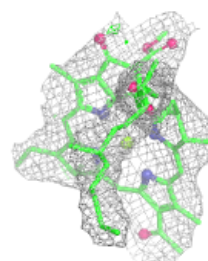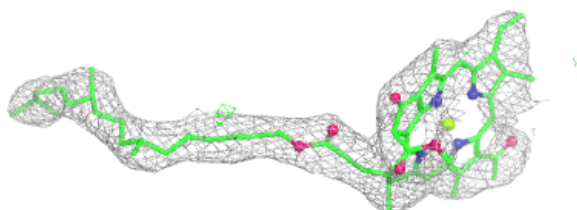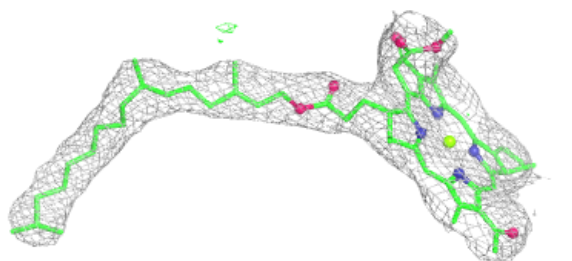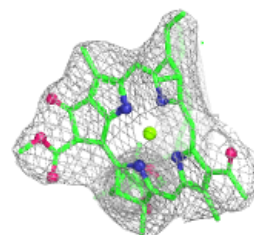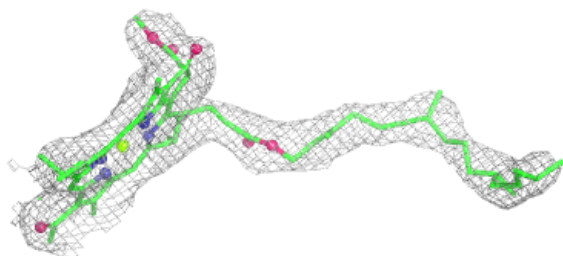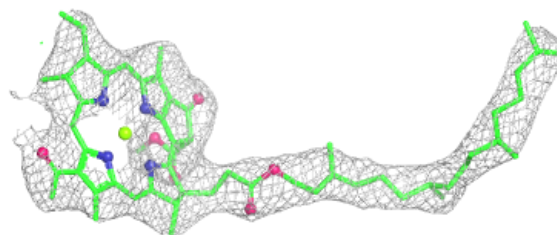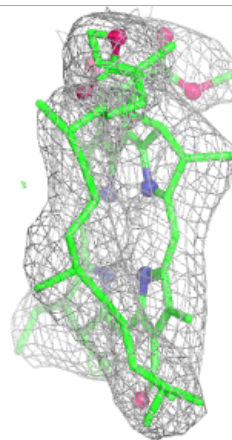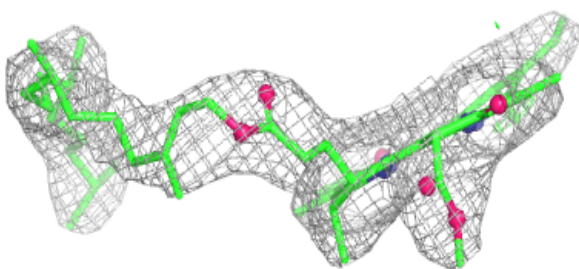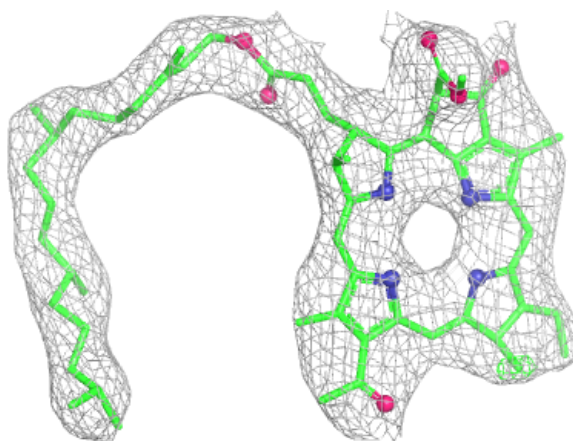
Electron density around UQ1 L 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
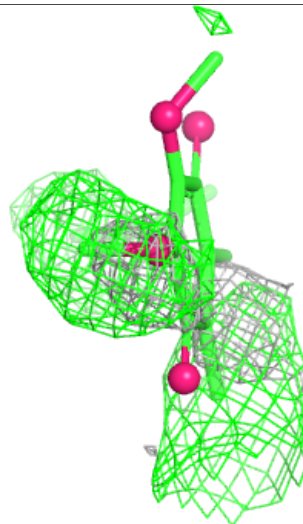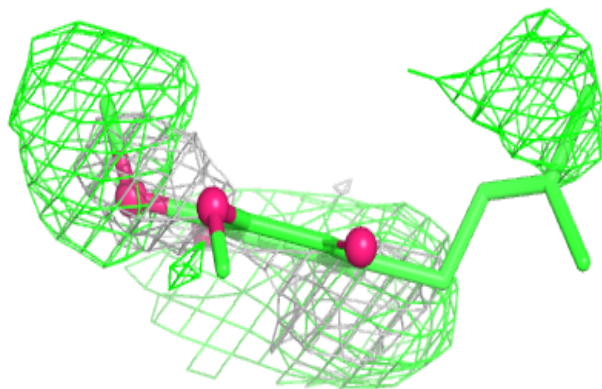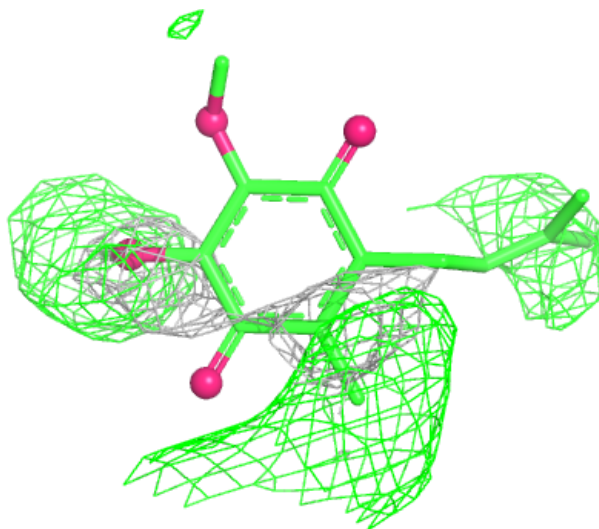
Electron density around NS5 M 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
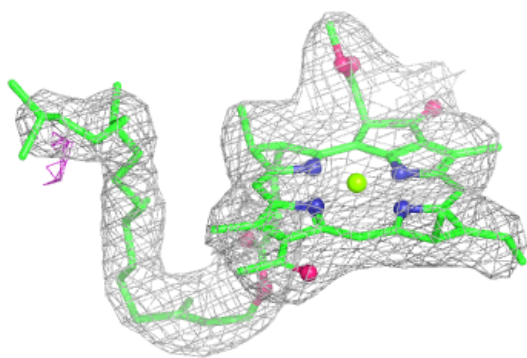mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
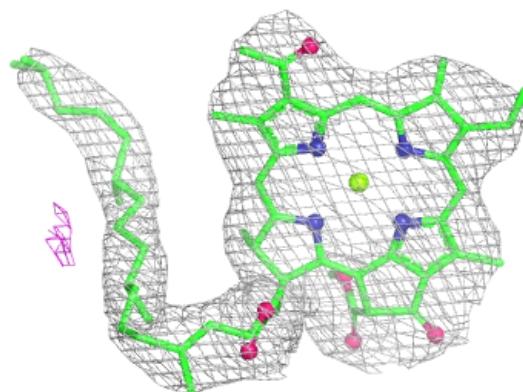and green (positive)
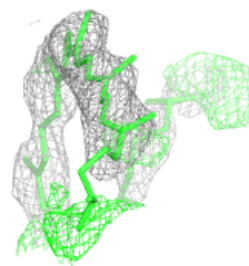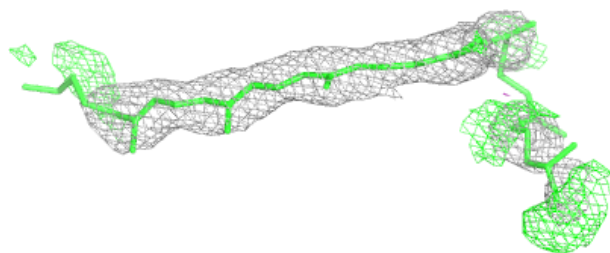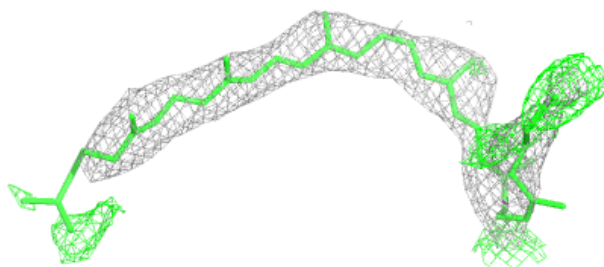
Electron density around BPB M 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
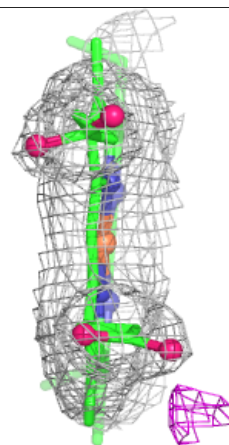mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
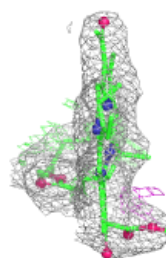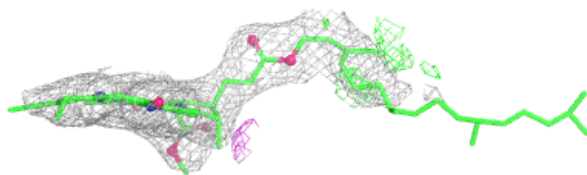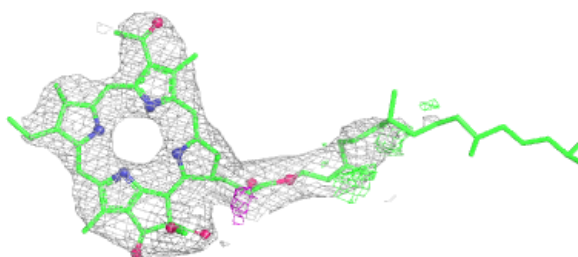
Electron density around UQ1 L 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
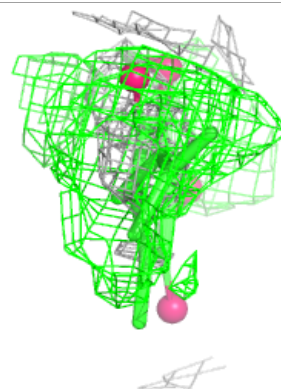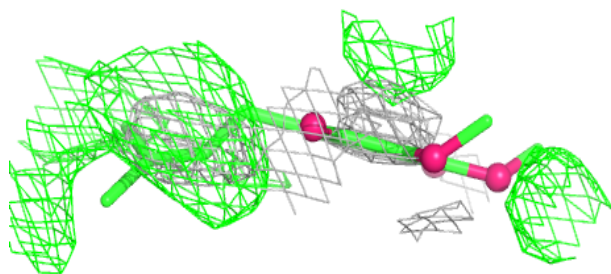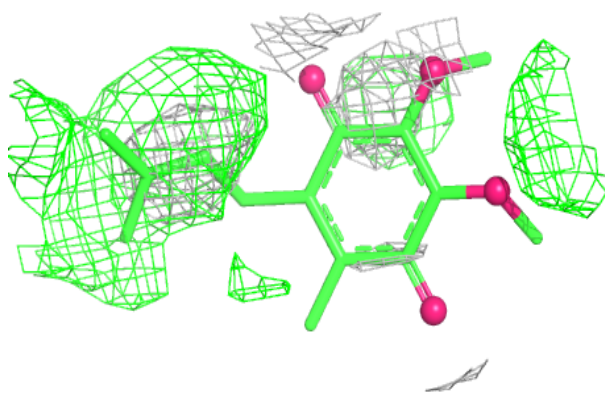
Electron density around BCB M 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
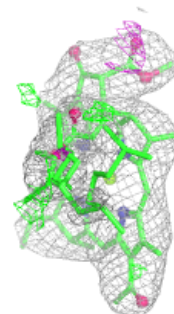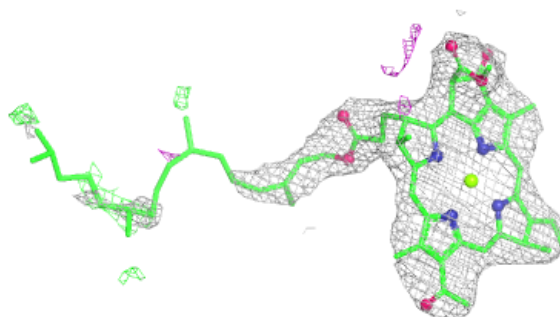
Electron density around MQ9 M 501:

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

Electron density around HEC C 401:

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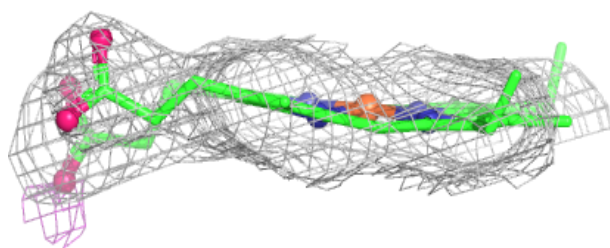$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
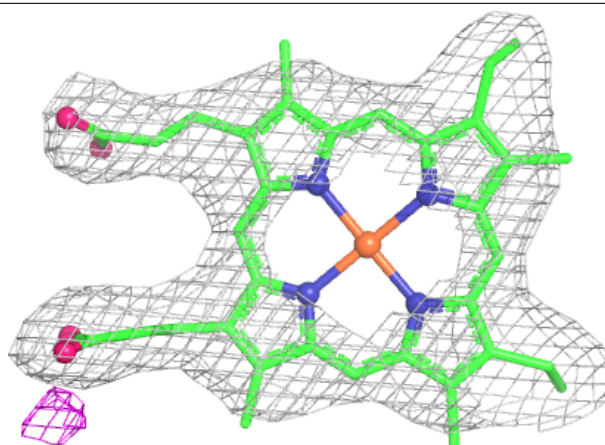and green (positive)

Electron density around BCB L 400:

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

Electron density around BCB M 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 BPB L 402:

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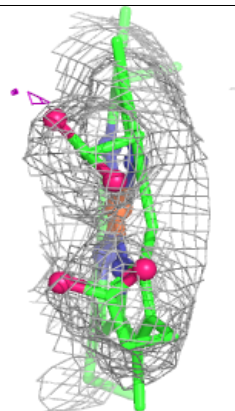mF_o-DF_c (at 3 rmsd) in purple (negative)
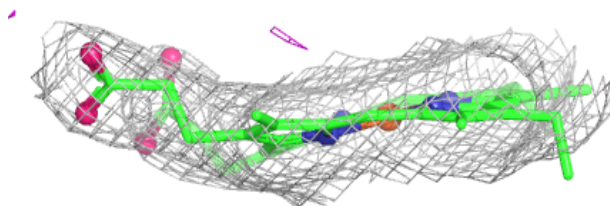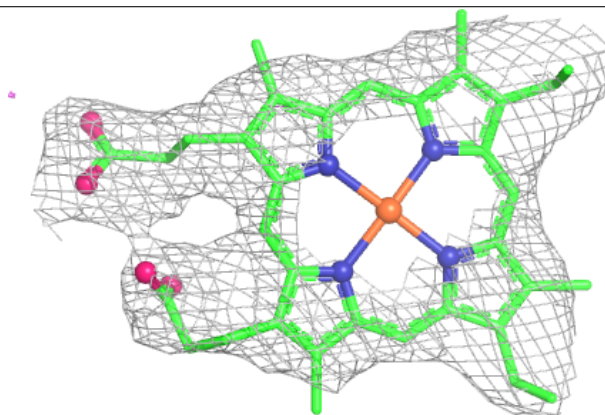and green (positive)

Electron density around BCB L 401:

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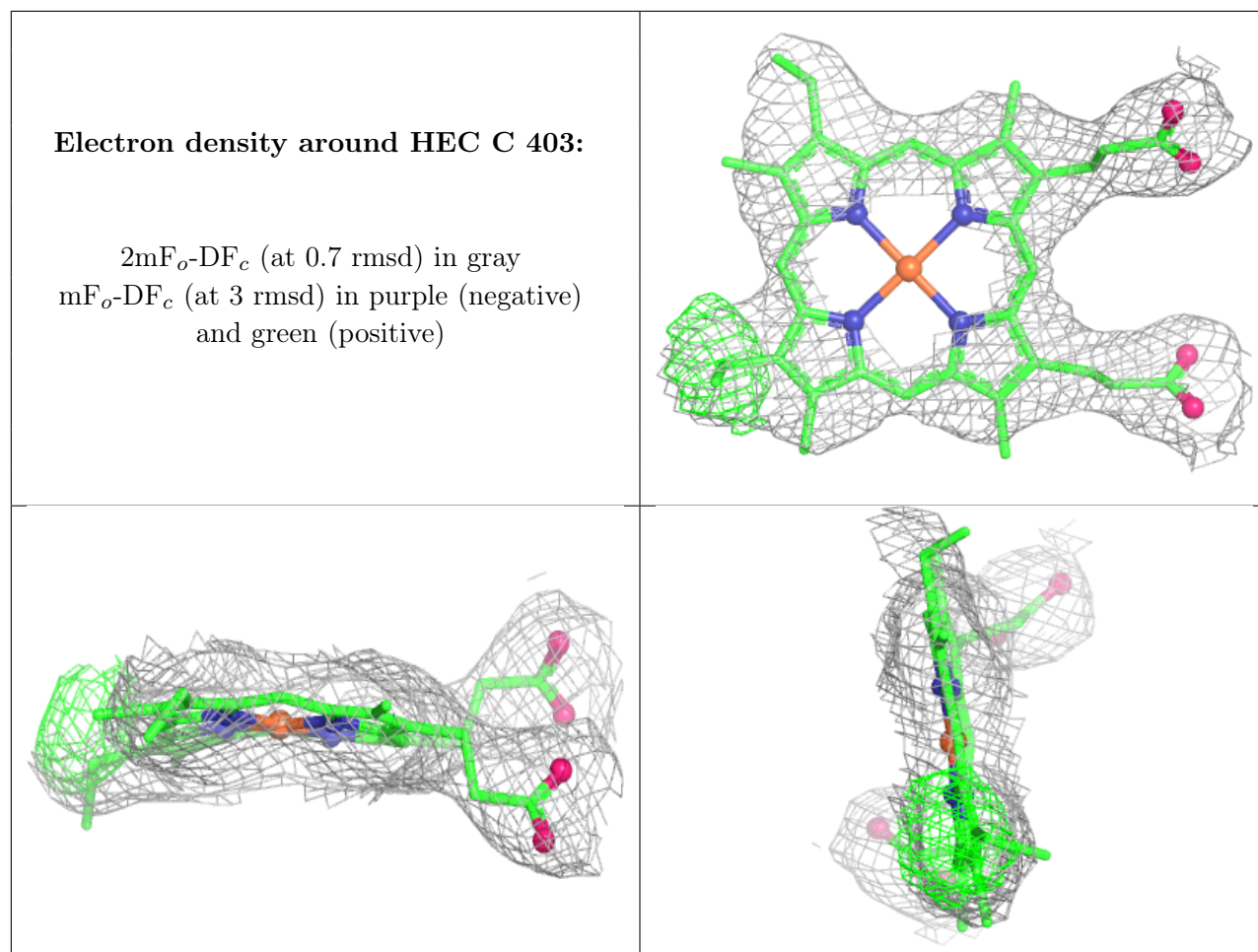mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEC C 404:

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

Electron density around HEC C 402:

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

Electron density around HEC C 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 ⓘ

There are no such residues in this entry.