



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 10:49 AM EST

PDB ID : 3G7F
Title : Crystal structure of Blastochloris viridis heterodimer mutant reaction center
Authors : Ponomarenko, N.S.; Li, L.; Tereshko, V.; Ismagilov, R.F.; Norris Jr., J.R.
Deposited on : 2009-02-09
Resolution : 2.50 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

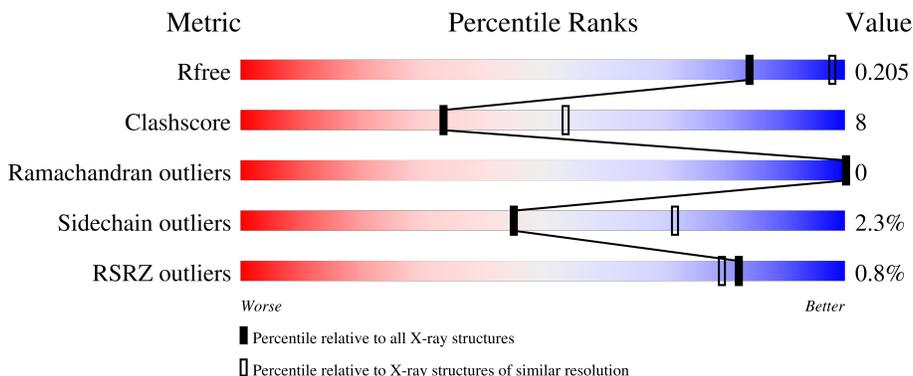
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	C	336	 92% 7%
2	H	258	 2% 88% 9%
3	L	273	 92% 7%
4	M	323	 86% 14%

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	M	401	-	-	X	-
6	SO4	C	815	-	-	-	X
6	SO4	C	817	-	-	-	X
6	SO4	L	814	-	-	-	X
6	SO4	M	816	-	-	-	X
6	SO4	M	818	-	-	-	X
6	SO4	M	819	-	-	-	X
7	HTO	L	708	-	-	-	X
7	HTO	L	709	-	-	-	X
9	BCB	L	400	X	-	-	-
9	BCB	L	401	X	-	-	-
9	BCB	M	400	X	-	-	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 10922 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	C	332	2598	1637	465	478	18	0	0	0

- Molecule 2 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	250	1956	1250	335	369	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ASP	GLU	variant	UNP P06008
H	256	ALA	SER	variant	UNP P06008

- Molecule 3 is a protein called Photosynthetic reaction center L subunit.

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

- Molecule 4 is a protein called Photosynthetic reaction center M subunit.

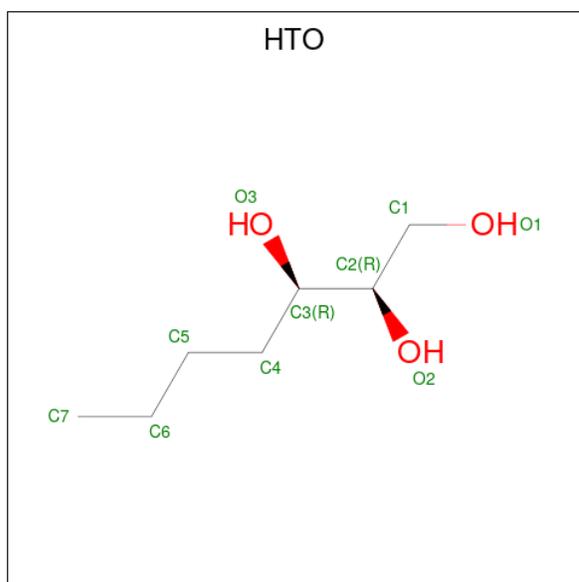
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2557	1704	417	424	12	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	200	LEU	HIS	variant	UNP P06010

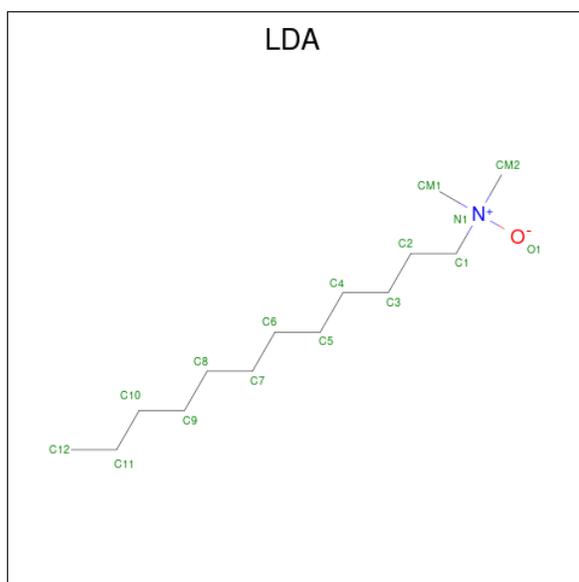
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total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

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



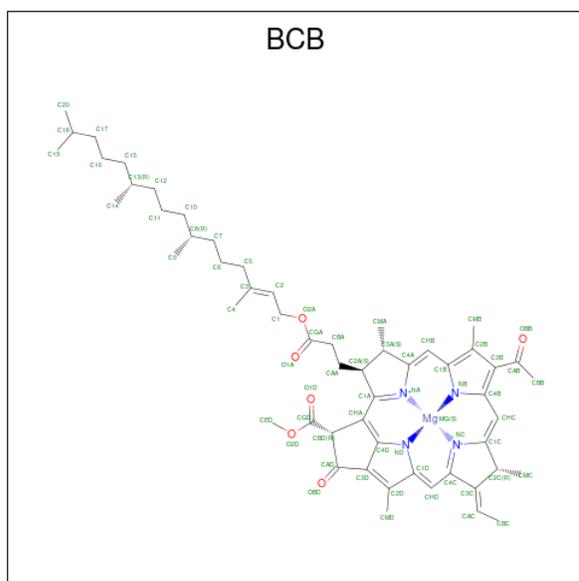
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 10 7 3	0	0
7	C	1	Total C O 10 7 3	0	0
7	H	1	Total C O 10 7 3	0	0
7	L	1	Total C O 10 7 3	0	0
7	L	1	Total C O 10 7 3	0	0

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



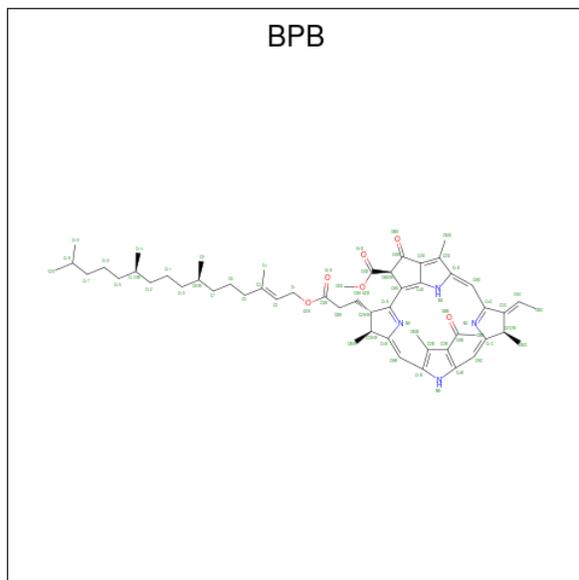
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



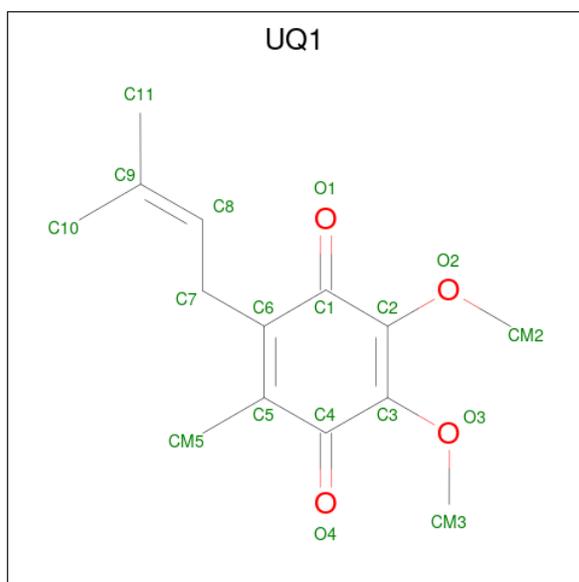
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

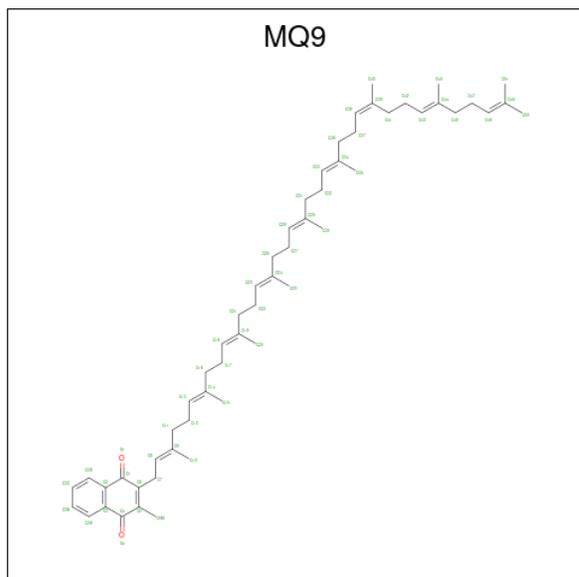


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	C O	0	0
			18	14 4		
11	M	1	Total	C O	0	0
			18	14 4		

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

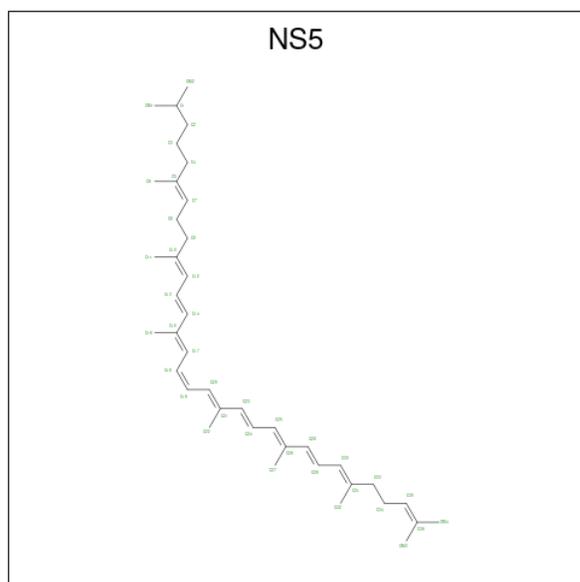
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂).



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: C₄₀H₆₀).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	292	Total	O	0	0
			292	292		
15	H	172	Total	O	1	0
			172	172		
15	L	94	Total	O	0	0
			94	94		
15	M	172	Total	O	2	0
			172	172		

3 Residue-property plots [i](#)

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

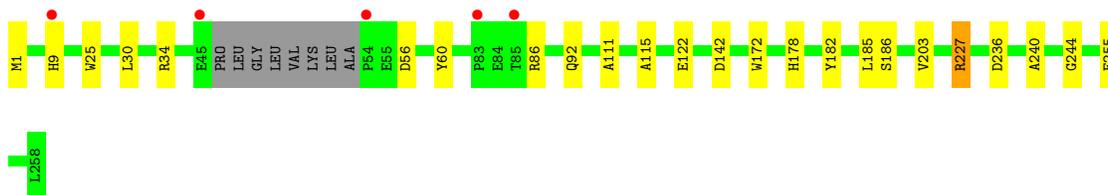
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 



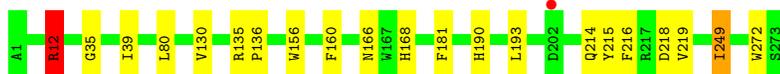
- Molecule 2: Photosynthetic reaction center H subunit

Chain H: 



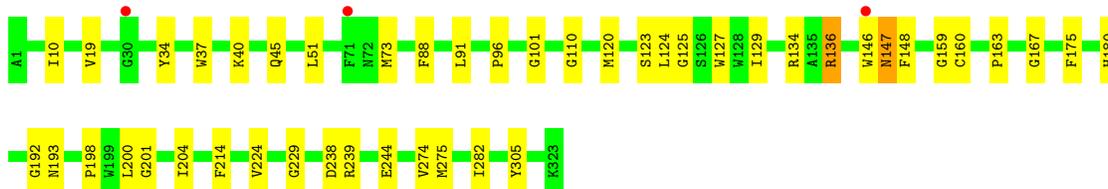
- Molecule 3: Photosynthetic reaction center L subunit

Chain L: 



- Molecule 4: Photosynthetic reaction center M subunit

Chain M: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.13Å 220.13Å 112.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.50) 99.1 (20.00-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.206 0.175 , 0.205	Depositor DCC
R_{free} test set	4754 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: LDA, SO4, BCB, UQ1, HTO, NS5, FE2, MQ9, FME, BPB, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.62	0/2665	0.66	0/3633
2	H	0.65	0/1991	0.65	0/2718
3	L	0.72	0/2267	0.68	2/3095 (0.1%)
4	M	0.71	0/2670	0.63	0/3651
All	All	0.67	0/9593	0.65	2/13097 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	12	ARG	NE-CZ-NH2	-6.70	116.95	120.30
3	L	12	ARG	CG-CD-NE	-5.23	100.82	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2568	16	0
2	H	1956	0	1944	14	0
3	L	2172	0	2097	22	0
4	M	2557	0	2462	48	0
5	C	172	0	120	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	35	0	0	1	0
6	H	20	0	0	0	0
6	L	5	0	0	0	0
6	M	35	0	0	1	0
7	C	20	0	32	2	0
7	H	10	0	16	1	0
7	L	20	0	32	0	0
8	H	32	0	62	0	0
8	M	32	0	62	3	0
9	L	132	0	144	27	0
9	M	66	0	72	7	0
10	L	65	0	74	6	0
10	M	130	0	148	40	0
11	L	18	0	18	4	0
11	M	18	0	18	0	0
12	M	1	0	0	0	0
13	M	58	0	80	4	0
14	M	40	0	60	4	0
15	C	292	0	0	2	0
15	H	172	0	0	4	0
15	L	94	0	0	0	0
15	M	172	0	0	3	0
All	All	10922	0	10009	152	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 8.

The worst 5 of 152 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)
10:M:401:BPB:H4A	10:M:402:BPB:CBB	1.98	0.92
10:M:401:BPB:H4A	10:M:402:BPB:HB BB	1.53	0.90
10:M:402:BPB:CBB	10:M:402:BPB:HHC	2.04	0.88
4:M:204:ILE:HG12	10:M:401:BPB:CHB	2.03	0.87
4:M:200:LEU:HD13	4:M:204:ILE:HD12	1.60	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	318 (96%)	12 (4%)	0	100	100
2	H	246/258 (95%)	240 (98%)	6 (2%)	0	100	100
3	L	272/273 (100%)	267 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	9 (3%)	0	100	100
All	All	1171/1190 (98%)	1139 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	280/282 (99%)	275 (98%)	5 (2%)	54	78
2	H	204/211 (97%)	198 (97%)	6 (3%)	37	64
3	L	219/218 (100%)	215 (98%)	4 (2%)	54	78
4	M	251/249 (101%)	244 (97%)	7 (3%)	38	65
All	All	954/960 (99%)	932 (98%)	22 (2%)	45	72

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	272	TRP
4	M	124	LEU
4	M	51	LEU

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Mol	Chain	Res	Type
4	M	136	ARG
2	H	178	HIS

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

Mol	Chain	Res	Type
3	L	183	ASN
3	L	214	GLN
4	M	147	ASN
3	L	239	ASN
2	H	58	GLN

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	H	1	2	8,9,10	0.83	0	8,9,11	3.01	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	-	3/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.98	110.55	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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 43 ligands modelled in this entry, 1 is monoatomic - leaving 42 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEC	C	403	1	32,50,50	1.65	5 (15%)	30,82,82	2.17	5 (16%)
6	SO4	H	807	-	4,4,4	0.22	0	6,6,6	0.24	0
6	SO4	C	813	-	4,4,4	0.28	0	6,6,6	0.47	0
8	LDA	M	702	-	13,15,15	2.10	2 (15%)	14,17,17	0.71	0
7	HTO	L	709	-	9,9,9	0.23	0	10,10,10	0.75	0
10	BPB	M	402	-	49,70,70	1.37	5 (10%)	48,101,101	2.07	9 (18%)
8	LDA	M	704	-	13,15,15	2.11	2 (15%)	14,17,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	M	818	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	M	805	-	4,4,4	0.21	0	6,6,6	0.30	0
6	SO4	H	803	-	4,4,4	0.23	0	6,6,6	0.23	0
7	HTO	C	707	-	9,9,9	0.82	0	10,10,10	1.00	0
6	SO4	M	801	-	4,4,4	0.29	0	6,6,6	0.34	0
7	HTO	L	708	-	9,9,9	0.23	0	10,10,10	0.79	0
6	SO4	C	809	-	4,4,4	0.25	0	6,6,6	0.17	0
5	HEC	C	402	1	32,50,50	1.71	4 (12%)	30,82,82	2.02	5 (16%)
9	BCB	L	400	3	63,74,74	2.11	9 (14%)	72,115,115	2.01	15 (20%)
5	HEC	C	404	1	32,50,50	1.49	2 (6%)	30,82,82	2.13	6 (20%)
9	BCB	M	400	4	63,74,74	2.03	9 (14%)	72,115,115	1.74	14 (19%)
6	SO4	C	817	-	4,4,4	0.23	0	6,6,6	0.06	0
5	HEC	C	401	1	32,50,50	1.81	4 (12%)	30,82,82	2.25	5 (16%)
7	HTO	H	705	-	9,9,9	0.42	0	10,10,10	0.87	0
6	SO4	M	816	-	4,4,4	0.23	0	6,6,6	0.07	0
10	BPB	L	402	-	49,70,70	1.30	5 (10%)	48,101,101	1.99	10 (20%)
8	LDA	H	701	-	13,15,15	1.96	2 (15%)	14,17,17	0.74	0
9	BCB	L	401	3	63,74,74	2.08	8 (12%)	72,115,115	1.91	14 (19%)
6	SO4	C	815	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	M	802	-	4,4,4	0.21	0	6,6,6	0.38	0
6	SO4	H	806	-	4,4,4	0.27	0	6,6,6	0.28	0
11	UQ1	M	503	-	18,18,18	2.39	2 (11%)	24,25,25	1.30	3 (12%)
6	SO4	M	819	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	C	811	-	4,4,4	0.24	0	6,6,6	0.21	0
7	HTO	C	706	-	9,9,9	0.45	0	10,10,10	0.64	0
11	UQ1	L	502	-	18,18,18	2.31	2 (11%)	24,25,25	1.22	2 (8%)
8	LDA	H	703	-	13,15,15	2.16	2 (15%)	14,17,17	0.68	0
6	SO4	M	804	-	4,4,4	0.17	0	6,6,6	0.17	0
10	BPB	M	401	-	49,70,70	1.51	6 (12%)	48,101,101	2.09	12 (25%)
13	MQ9	M	501	-	59,59,59	1.85	18 (30%)	73,75,75	1.40	16 (21%)
6	SO4	C	810	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	H	812	-	4,4,4	0.20	0	6,6,6	0.17	0
14	NS5	M	600	-	39,39,39	1.44	3 (7%)	46,46,46	1.98	12 (26%)
6	SO4	C	808	-	4,4,4	0.35	0	6,6,6	0.37	0
6	SO4	L	814	-	4,4,4	0.23	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	403	1	-	0/10/54/54	-
8	LDA	M	702	-	-	5/13/13/13	-
7	HTO	L	709	-	-	6/10/10/10	-
10	BPB	M	402	-	-	17/37/105/105	0/5/6/6
8	LDA	M	704	-	-	9/13/13/13	-
7	HTO	C	707	-	-	7/10/10/10	-
7	HTO	L	708	-	-	6/10/10/10	-
5	HEC	C	402	1	-	5/10/54/54	-
9	BCB	L	400	3	3/3/21/26	10/37/137/137	-
5	HEC	C	404	1	-	0/10/54/54	-
9	BCB	M	400	4	2/2/21/26	10/37/137/137	-
5	HEC	C	401	1	-	2/10/54/54	-
7	HTO	H	705	-	-	7/10/10/10	-
10	BPB	L	402	-	-	5/37/105/105	0/5/6/6
8	LDA	H	701	-	-	8/13/13/13	-
9	BCB	L	401	3	2/2/21/26	4/37/137/137	-
11	UQ1	M	503	-	-	0/9/33/33	0/1/1/1
7	HTO	C	706	-	-	3/10/10/10	-
11	UQ1	L	502	-	-	2/9/33/33	0/1/1/1
8	LDA	H	703	-	-	8/13/13/13	-
10	BPB	M	401	-	-	17/37/105/105	0/5/6/6
13	MQ9	M	501	-	-	13/53/73/73	0/2/2/2
14	NS5	M	600	-	-	10/43/43/43	-

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	502	UQ1	C6-C5	8.46	1.50	1.35
11	M	503	UQ1	C6-C5	8.40	1.50	1.35
9	L	400	BCB	CHC-C1C	8.39	1.40	1.33
9	L	401	BCB	CHC-C1C	8.20	1.40	1.33
9	L	401	BCB	CAC-C3C	7.94	1.53	1.33

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	402	BPB	O2D-CGD-CBD	9.17	121.03	110.95
10	L	402	BPB	O2D-CGD-CBD	8.89	120.71	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	401	BPB	O2D-CGD-CBD	8.79	120.60	110.95
9	L	401	BCB	C4A-NA-C1A	7.74	110.21	106.68
5	C	403	HEC	CBB-CAB-C3B	-7.62	109.66	127.49

5 of 7 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 154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	707	HTO	O1-C1-C2-O2
7	C	707	HTO	O1-C1-C2-C3
7	C	707	HTO	O3-C3-C4-C5
7	H	705	HTO	O2-C2-C3-C4
7	L	708	HTO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 89 short contacts:

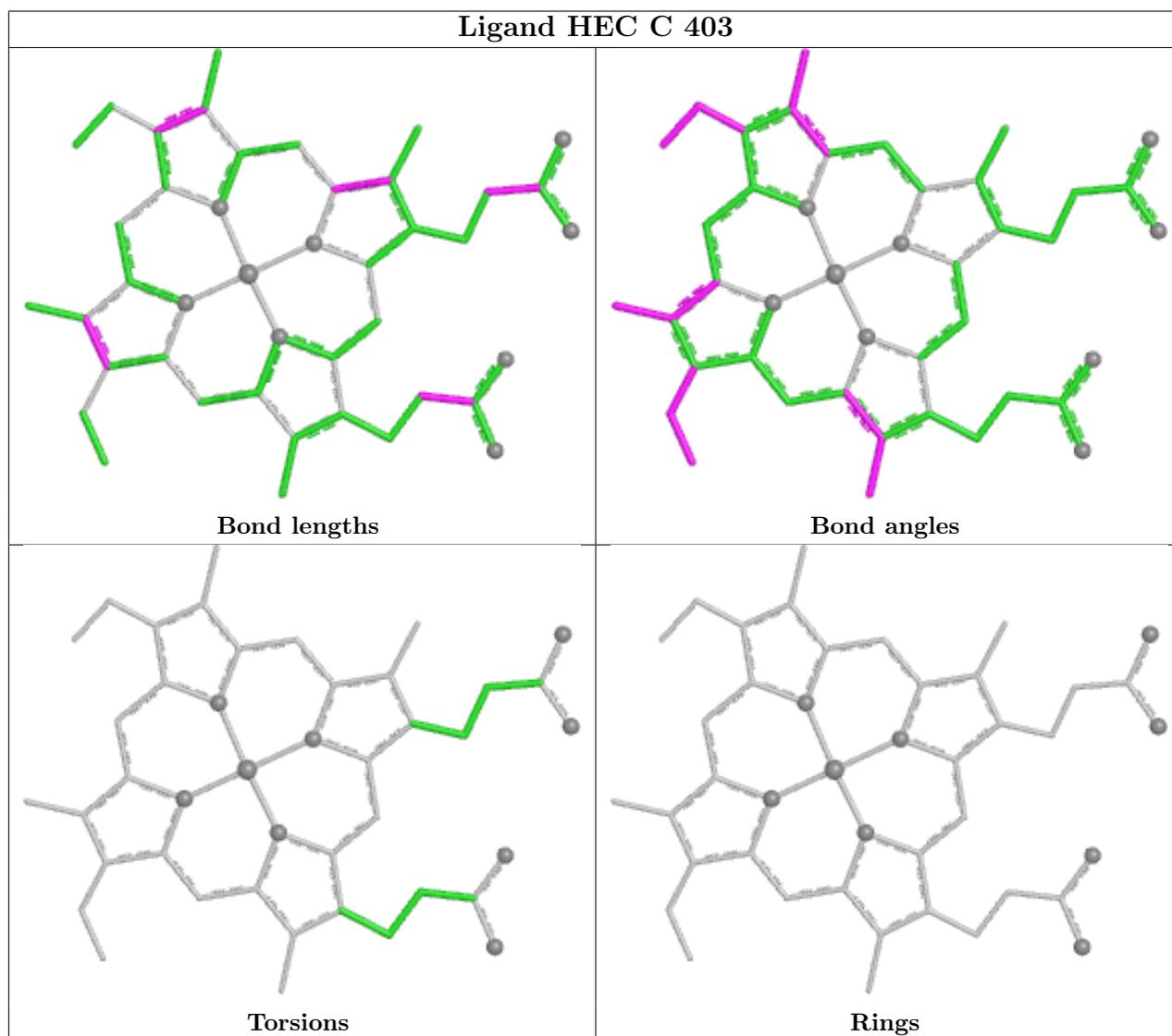
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	HEC	2	0
6	C	813	SO4	1	0
8	M	702	LDA	2	0
10	M	402	BPB	17	0
8	M	704	LDA	1	0
6	M	805	SO4	1	0
7	C	707	HTO	1	0
9	L	400	BCB	20	0
5	C	404	HEC	1	0
9	M	400	BCB	7	0
7	H	705	HTO	1	0
10	L	402	BPB	6	0
9	L	401	BCB	8	0
7	C	706	HTO	1	0
11	L	502	UQ1	4	0
10	M	401	BPB	27	0

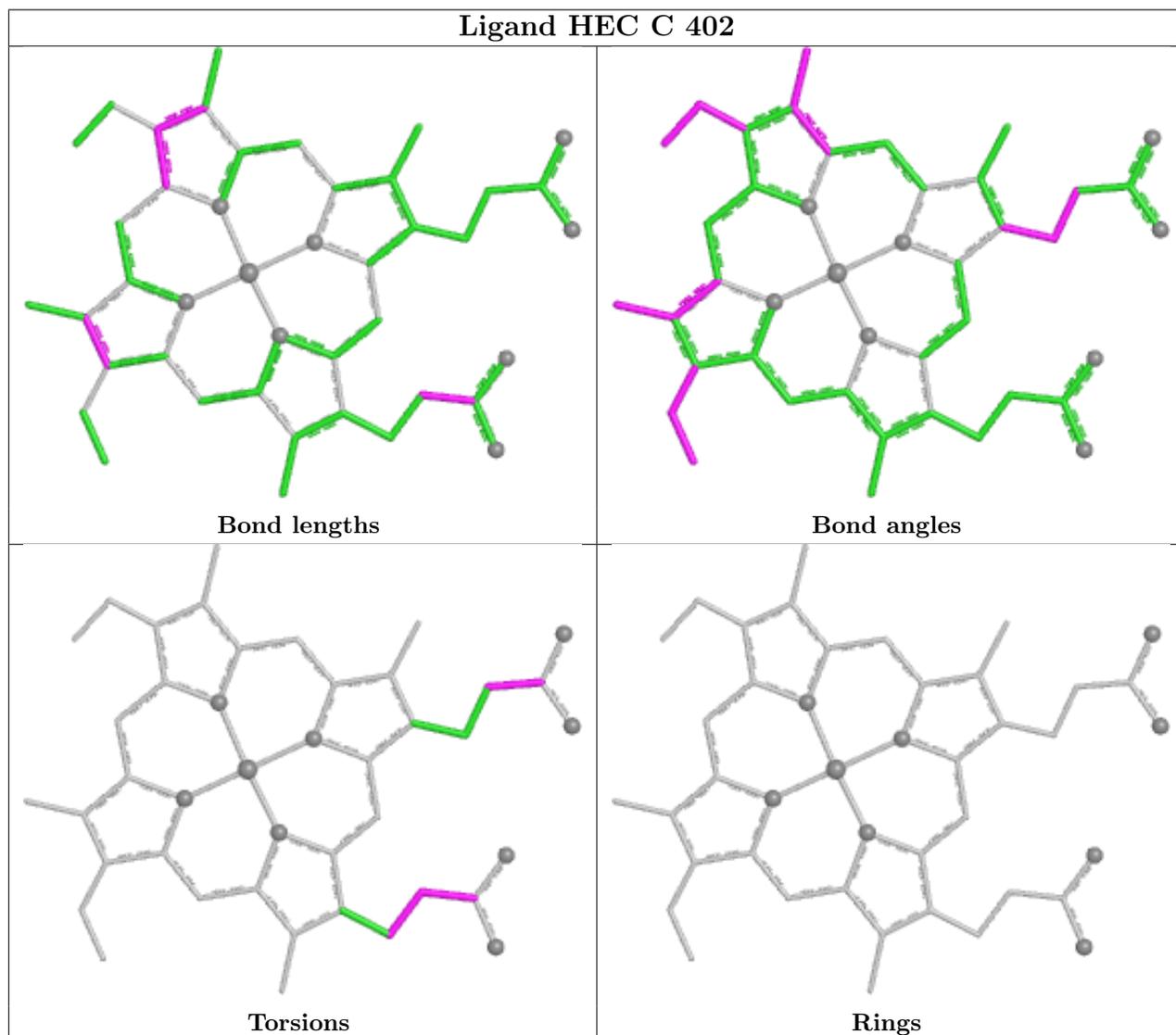
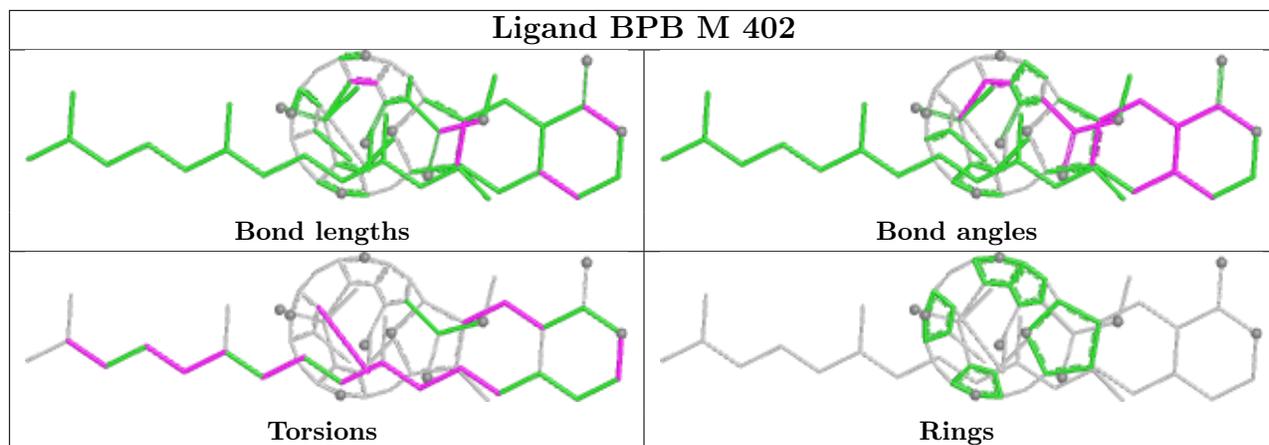
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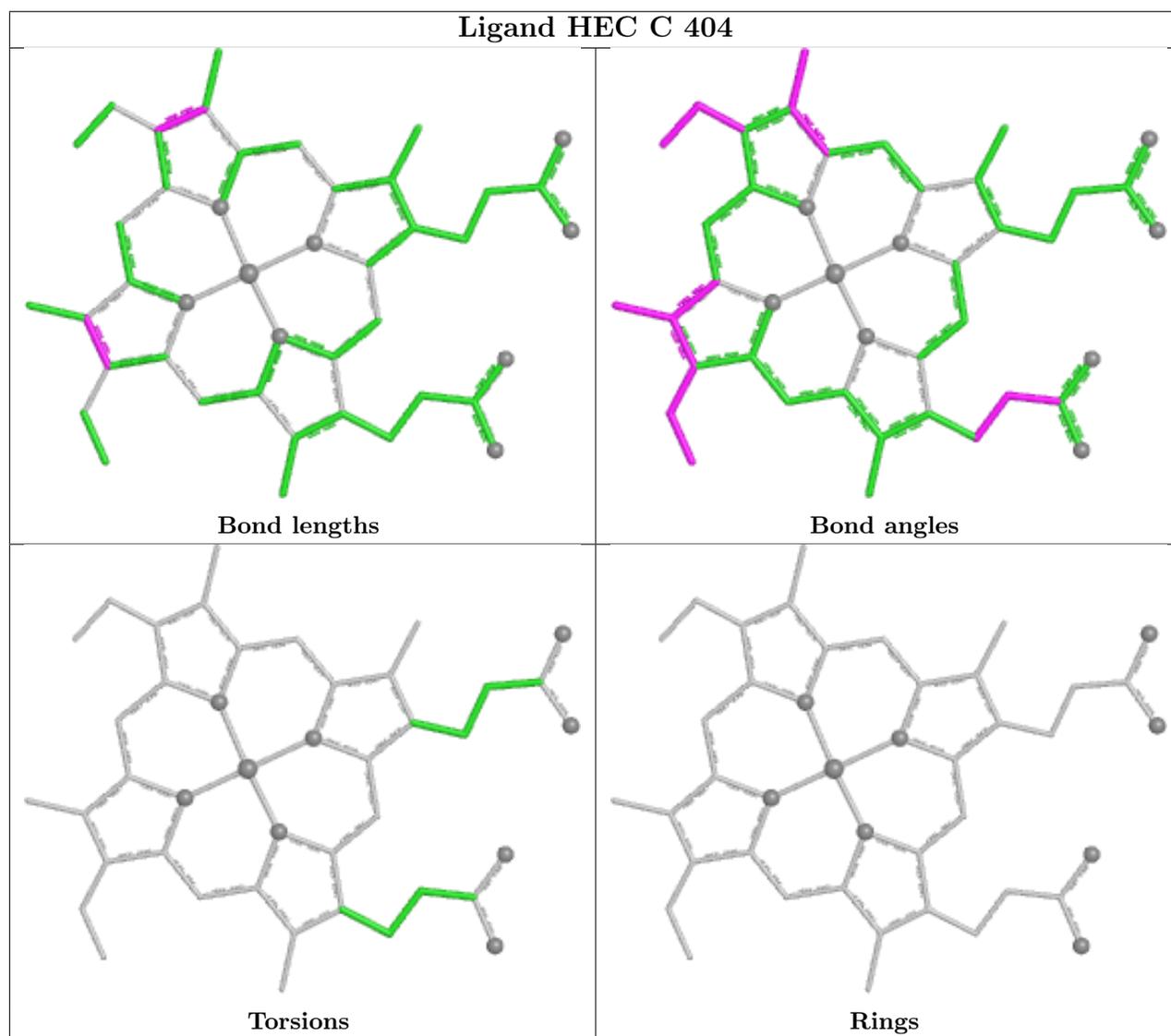
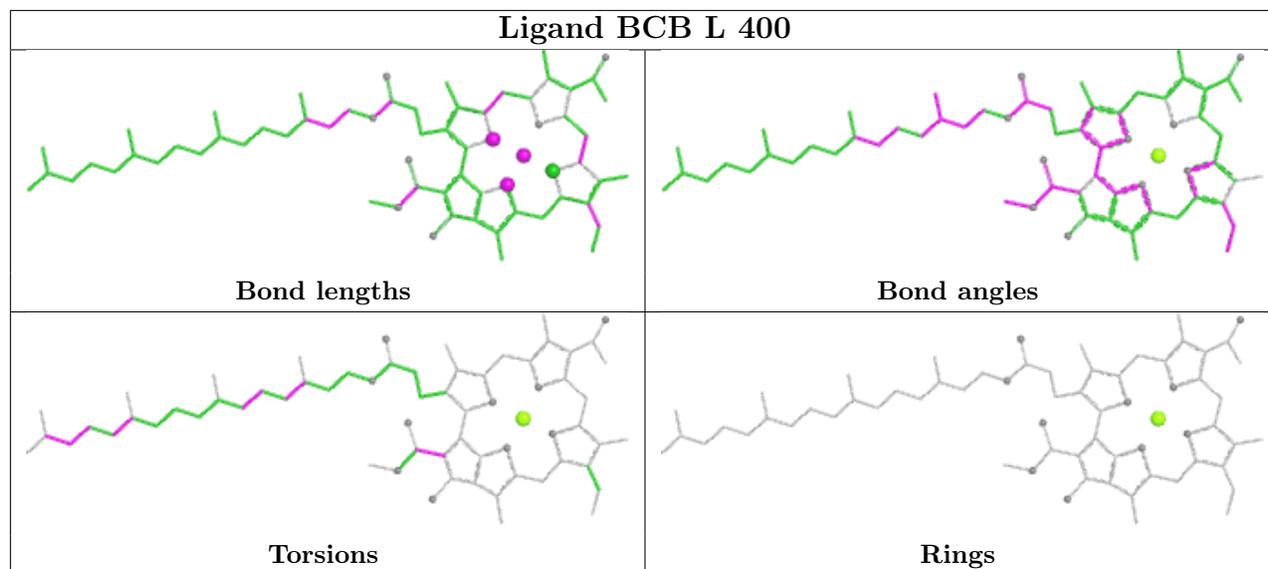
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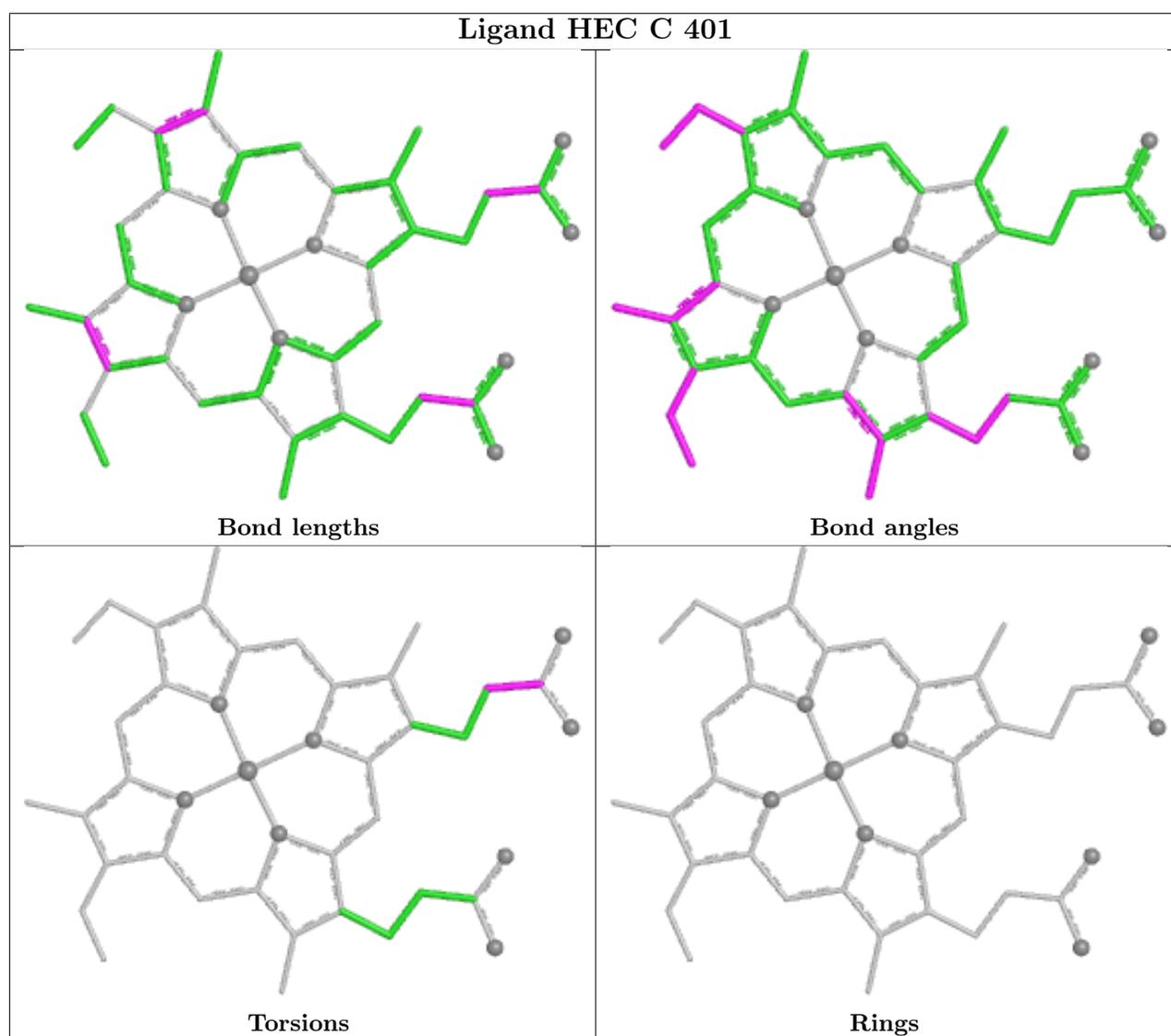
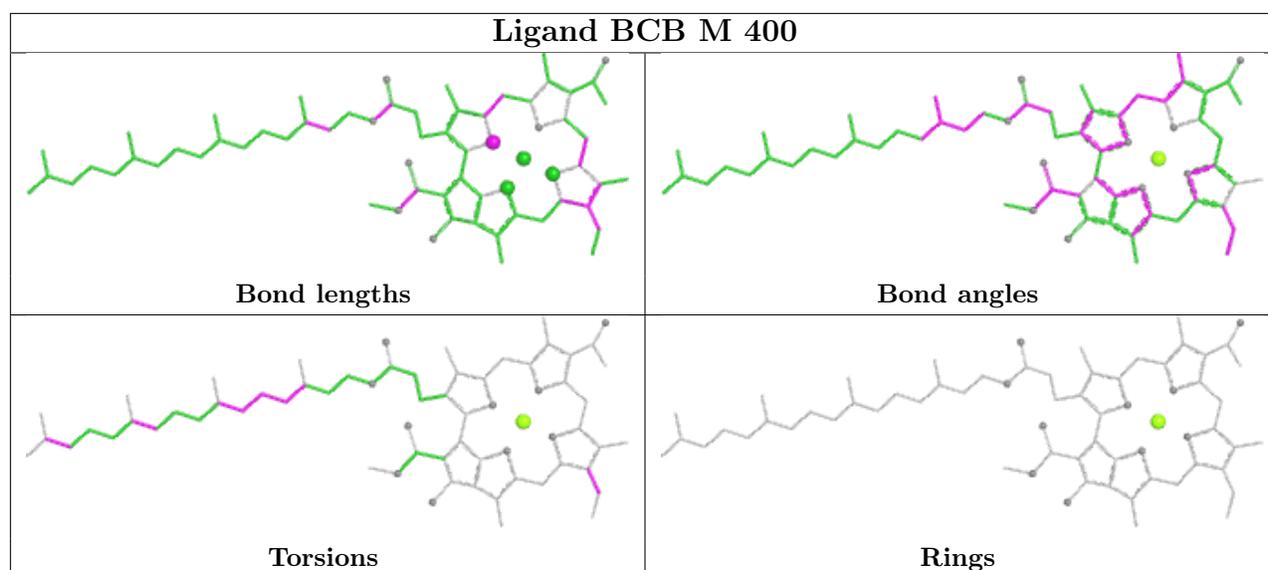
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	501	MQ9	4	0
14	M	600	NS5	4	0

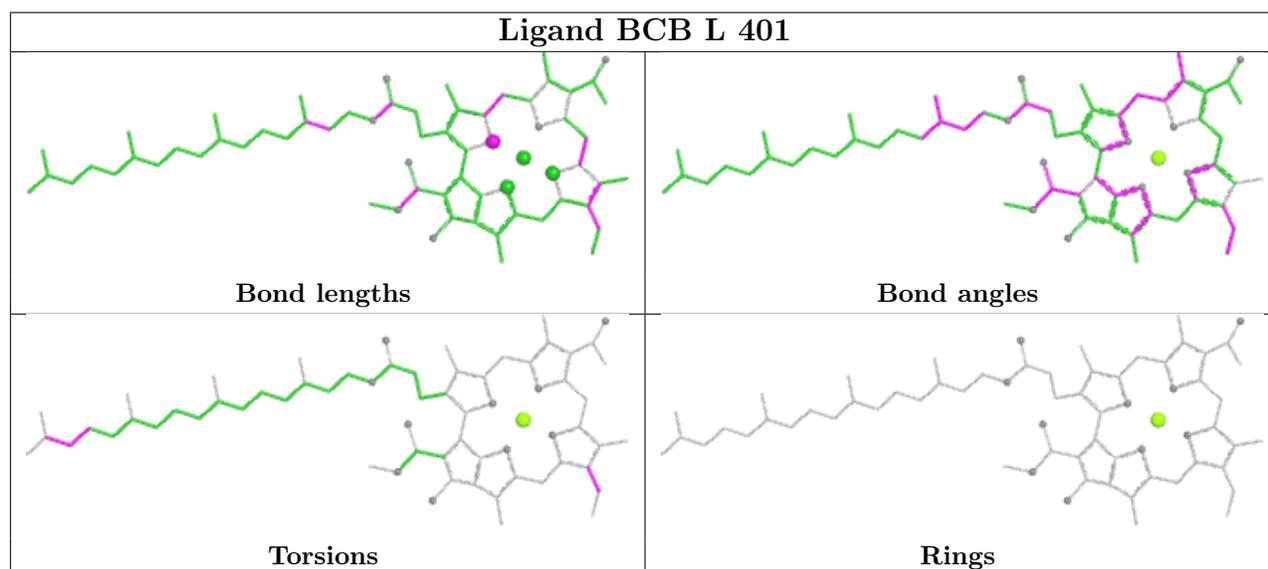
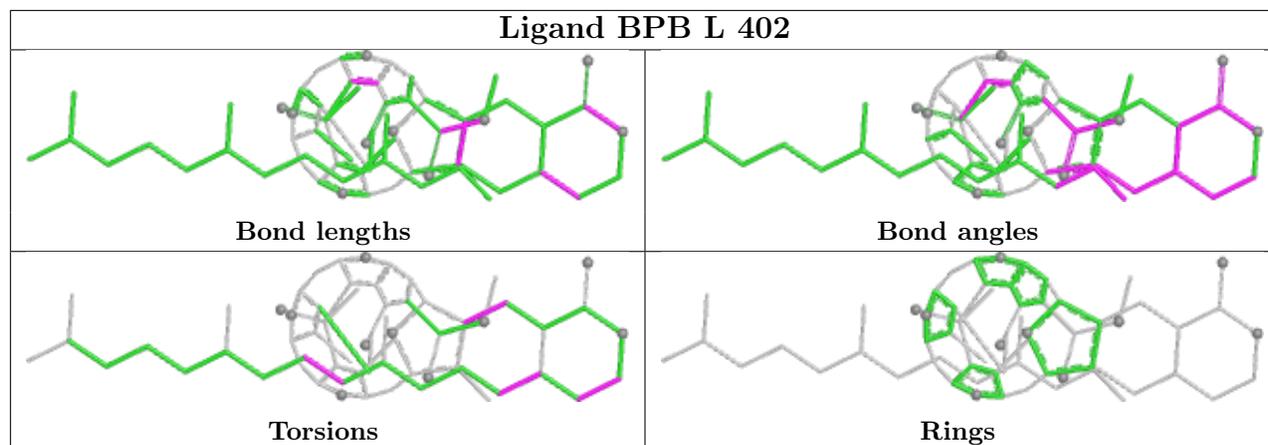
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

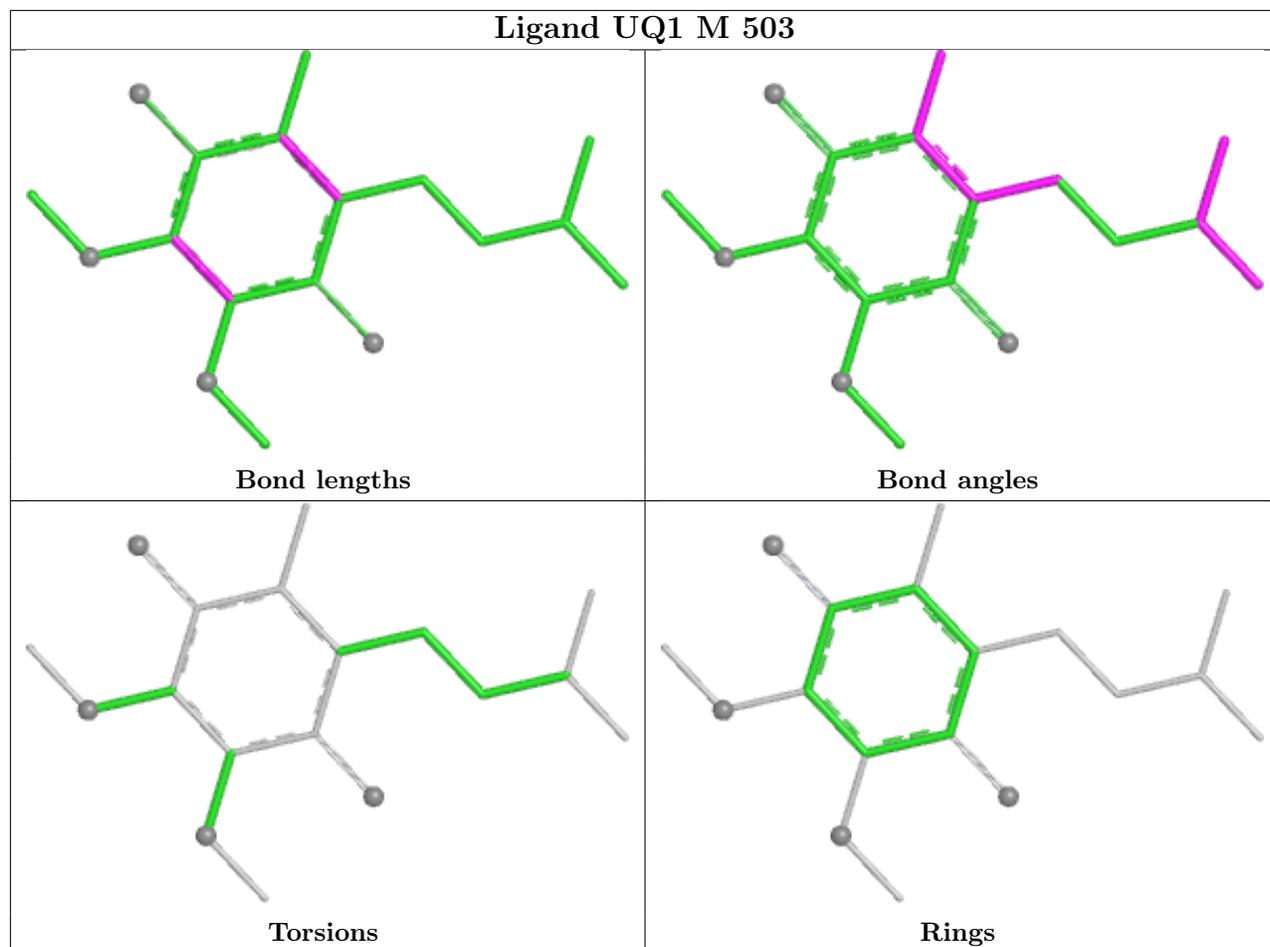


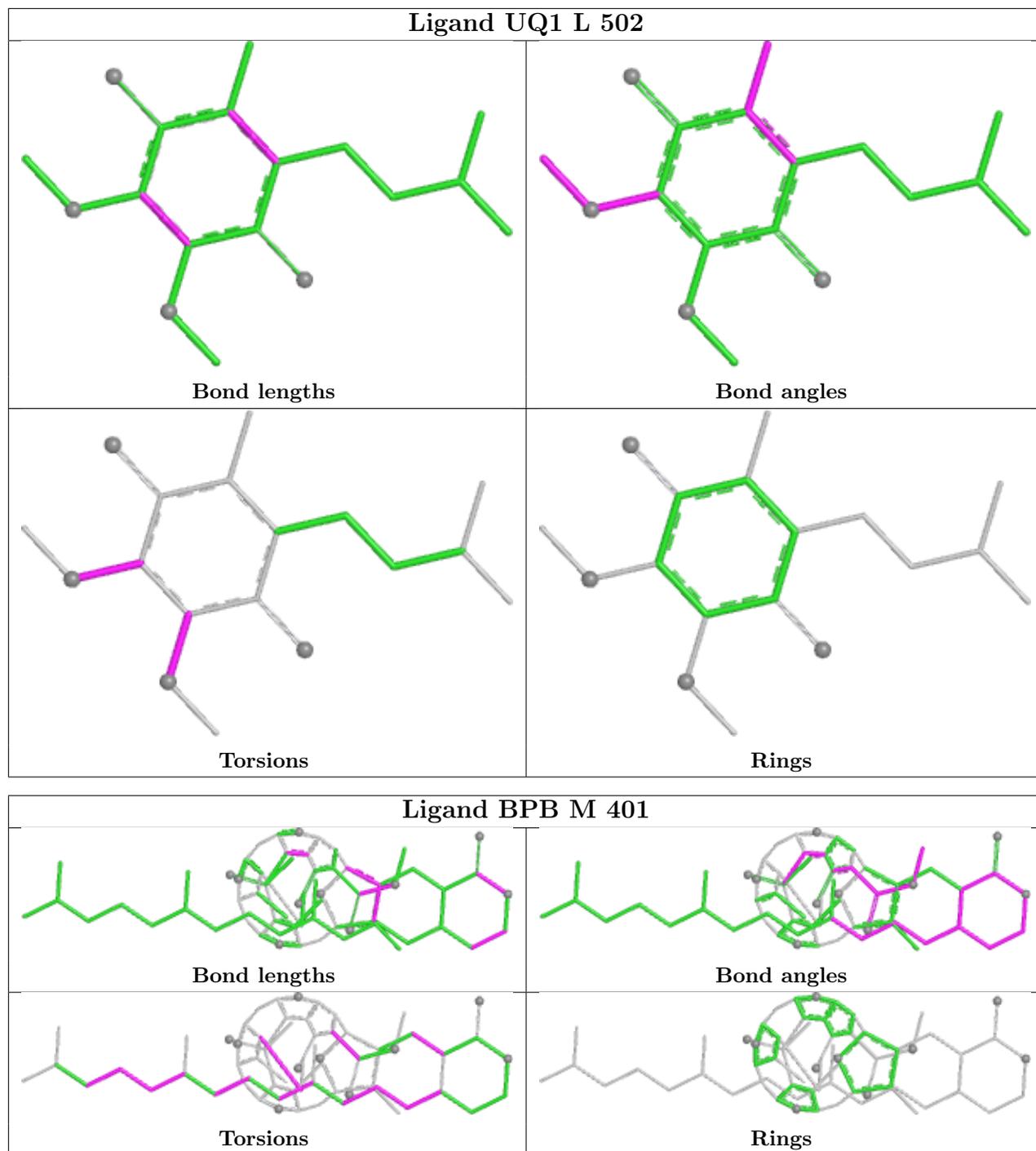


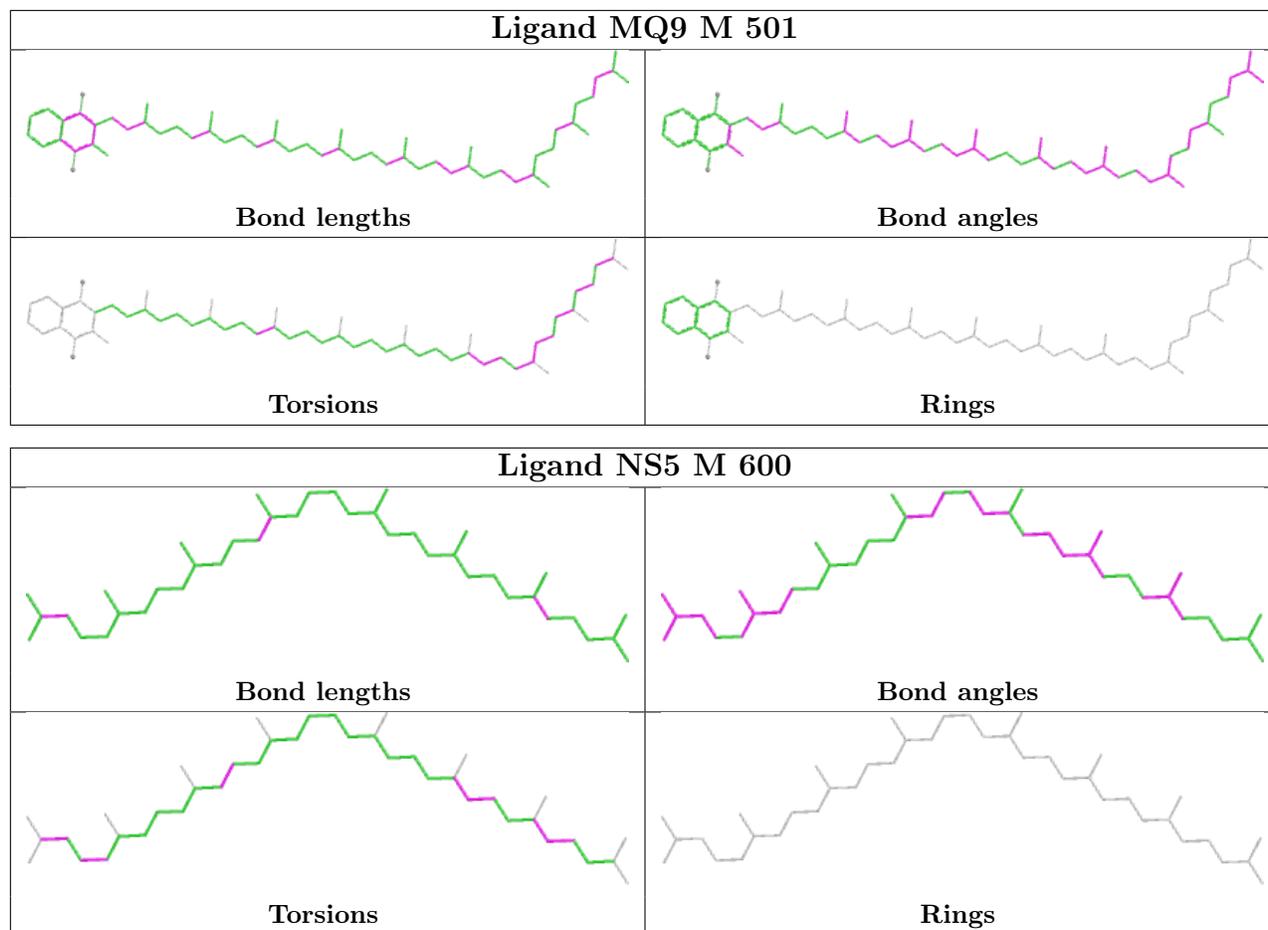












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	332/336 (98%)	-0.67	0 100 100	21, 31, 49, 61	0
2	H	249/258 (96%)	-0.52	5 (2%) 64 62	18, 32, 50, 60	0
3	L	273/273 (100%)	-0.82	1 (0%) 89 86	20, 26, 41, 47	1 (0%)
4	M	323/323 (100%)	-0.69	3 (0%) 81 78	17, 28, 45, 50	2 (0%)
All	All	1177/1190 (98%)	-0.68	9 (0%) 82 79	17, 29, 46, 61	3 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	4.5
2	H	9	HIS	2.8
2	H	83	PRO	2.5
2	H	45	GLU	2.4
3	L	202	ASP	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	H	1	10/11	0.95	0.08	36,38,49,53	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

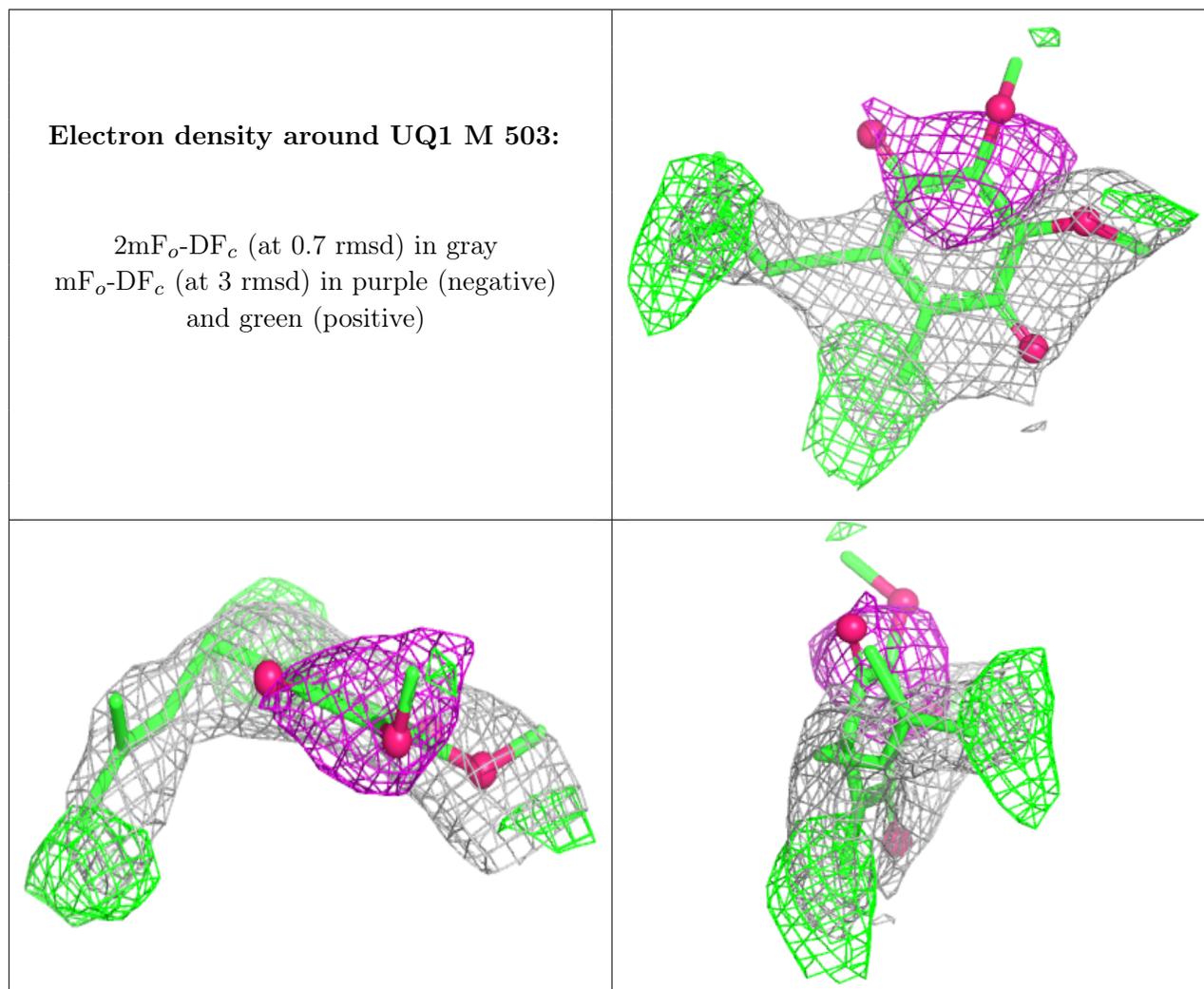
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	M	816	5/5	-0.41	2.74	2,2,2,2	5
6	SO4	L	814	5/5	-0.28	2.40	2,2,2,2	5
6	SO4	M	819	5/5	-0.20	2.54	2,2,2,2	5
6	SO4	C	817	5/5	-0.19	2.65	2,2,2,2	5
6	SO4	M	818	5/5	-0.15	2.39	2,2,2,2	5
7	HTO	L	708	10/10	-0.11	1.91	2,2,2,2	10
6	SO4	C	815	5/5	-0.08	2.50	2,2,2,2	5
7	HTO	L	709	10/10	0.11	2.71	2,2,2,2	10
11	UQ1	M	503	18/18	0.63	0.34	93,94,95,95	0
10	BPB	M	401	65/65	0.77	0.25	28,39,45,47	65
14	NS5	M	600	40/40	0.82	0.19	35,45,74,74	4
11	UQ1	L	502	18/18	0.83	0.15	45,46,49,50	0
8	LDA	M	704	16/16	0.84	0.21	55,58,68,69	0
7	HTO	C	707	10/10	0.86	0.20	50,54,57,57	0
6	SO4	C	808	5/5	0.86	0.14	55,56,57,58	5
6	SO4	C	810	5/5	0.86	0.22	46,47,47,47	5
6	SO4	C	813	5/5	0.86	0.15	39,39,41,41	5
7	HTO	C	706	10/10	0.87	0.18	45,50,51,51	0
8	LDA	M	702	16/16	0.91	0.15	47,57,67,67	0
6	SO4	C	811	5/5	0.91	0.19	42,43,44,44	5
6	SO4	C	809	5/5	0.91	0.15	66,67,67,68	5
6	SO4	H	812	5/5	0.92	0.20	47,47,48,48	5
6	SO4	H	803	5/5	0.92	0.15	67,68,68,69	0
10	BPB	M	402	65/65	0.92	0.13	21,27,97,99	0
7	HTO	H	705	10/10	0.93	0.10	41,42,44,45	0
6	SO4	H	807	5/5	0.93	0.13	64,65,66,66	5
9	BCB	M	400	66/66	0.94	0.10	23,27,85,86	0
6	SO4	M	805	5/5	0.94	0.10	48,49,49,50	5
8	LDA	H	703	16/16	0.95	0.13	47,53,60,62	0
6	SO4	H	806	5/5	0.95	0.10	48,49,50,50	5
8	LDA	H	701	16/16	0.95	0.08	36,41,47,48	0
13	MQ9	M	501	58/58	0.96	0.08	16,22,74,75	0
6	SO4	M	804	5/5	0.97	0.15	53,54,55,56	0
10	BPB	L	402	65/65	0.97	0.05	14,20,28,29	0
9	BCB	L	400	66/66	0.97	0.06	23,26,33,38	0
9	BCB	L	401	66/66	0.97	0.05	18,24,40,44	0

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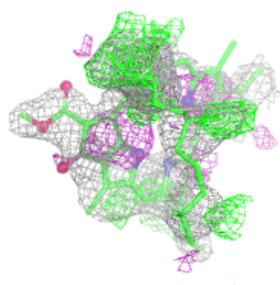
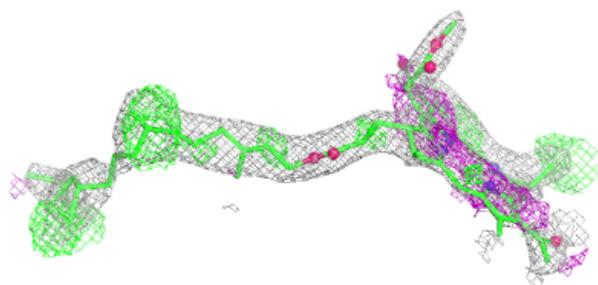
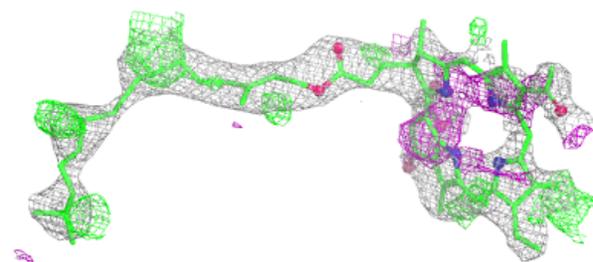
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	HEC	C	402	43/43	0.98	0.07	26,30,37,39	0
6	SO4	M	802	5/5	0.98	0.06	47,48,49,50	0
5	HEC	C	403	43/43	0.99	0.05	14,21,27,31	0
5	HEC	C	404	43/43	0.99	0.06	21,24,34,41	0
6	SO4	M	801	5/5	0.99	0.06	29,29,32,32	0
5	HEC	C	401	43/43	0.99	0.06	30,33,45,51	0
12	FE2	M	500	1/1	1.00	0.01	21,21,21,21	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.

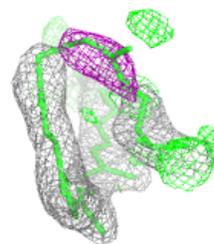
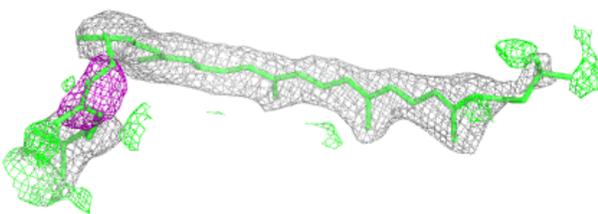
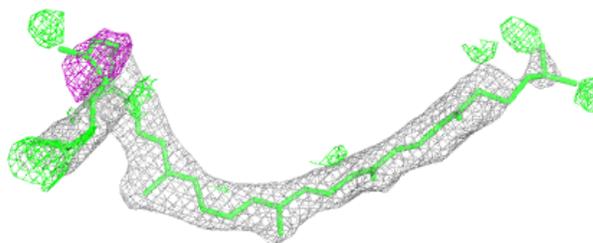


Electron density around BPB M 401:

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

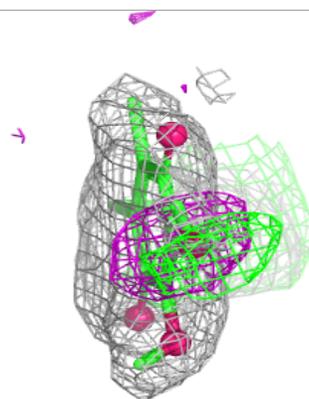
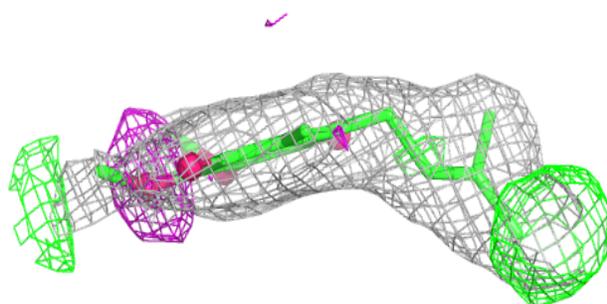
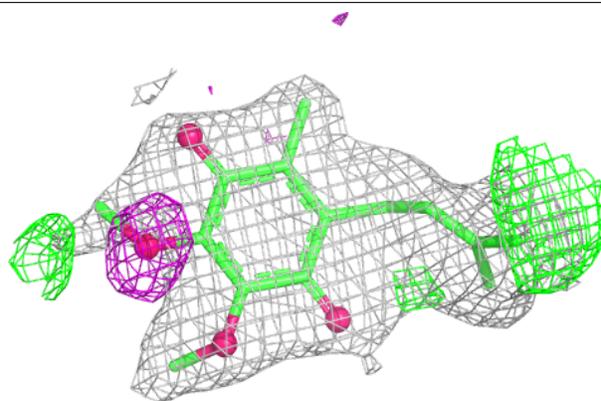
**Electron density around NS5 M 600:**

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

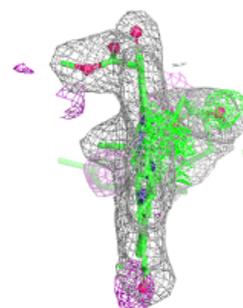
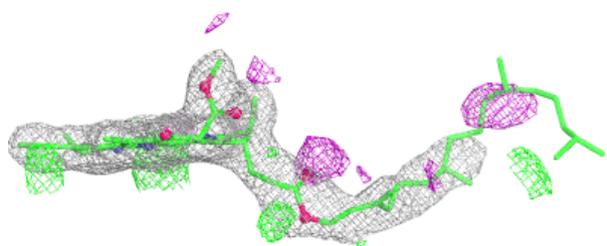
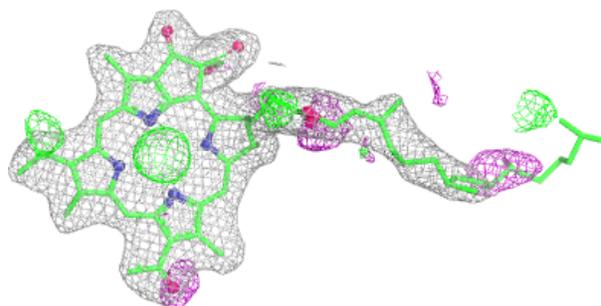


Electron density around UQ1 L 502:

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

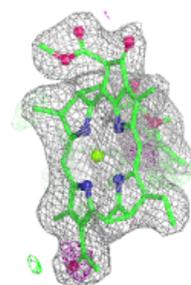
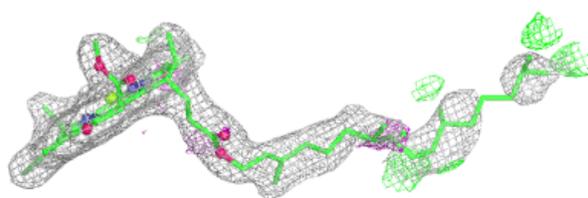
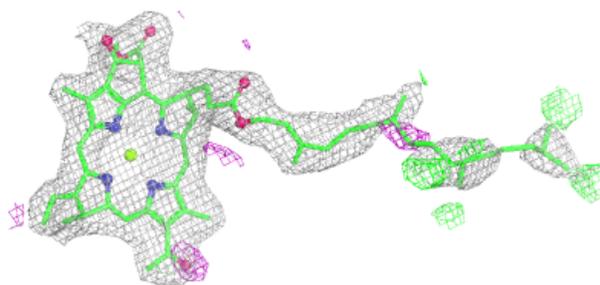
**Electron density around BPB M 402:**

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

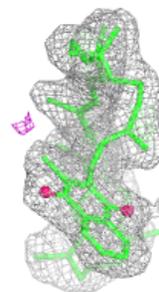
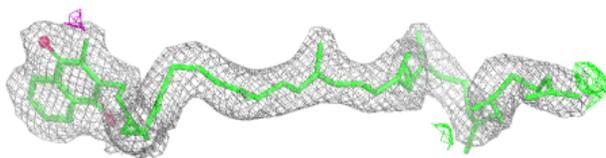
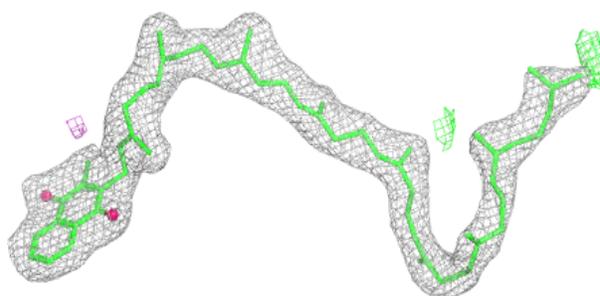


Electron density around BCB M 400:

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

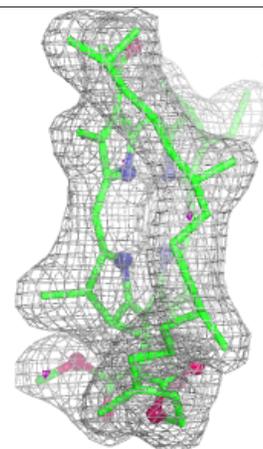
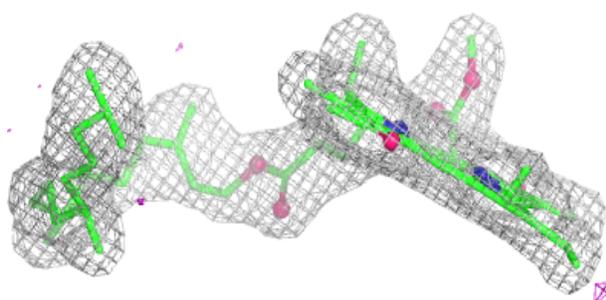
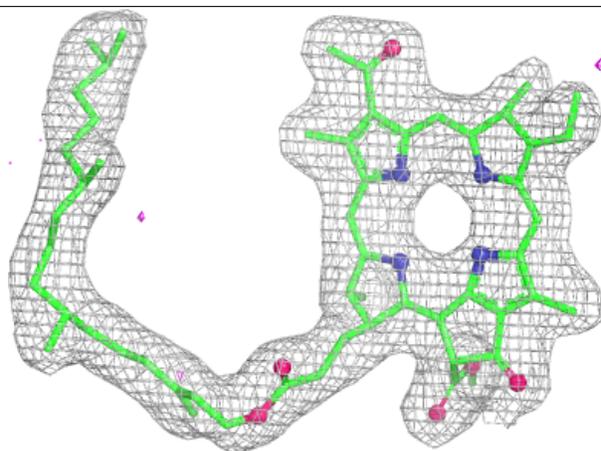
**Electron density around MQ9 M 501:**

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



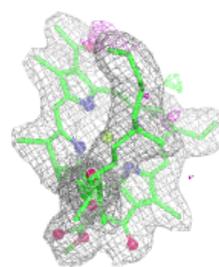
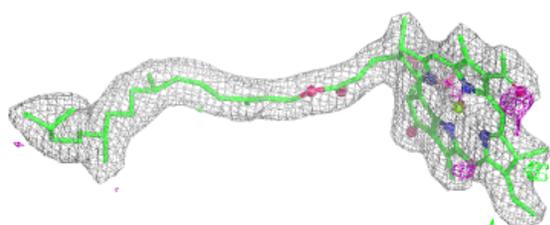
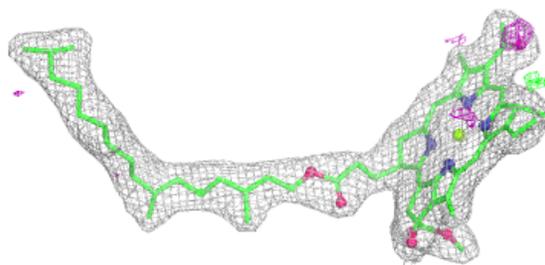
Electron density around BPB L 402:

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

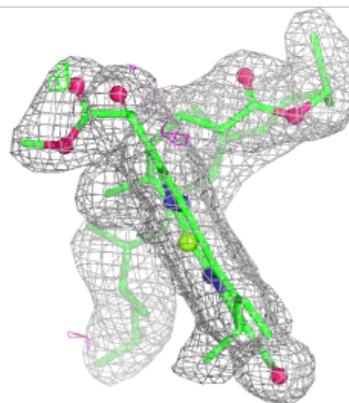
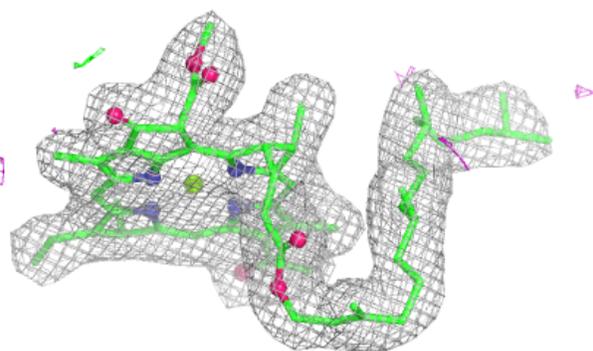
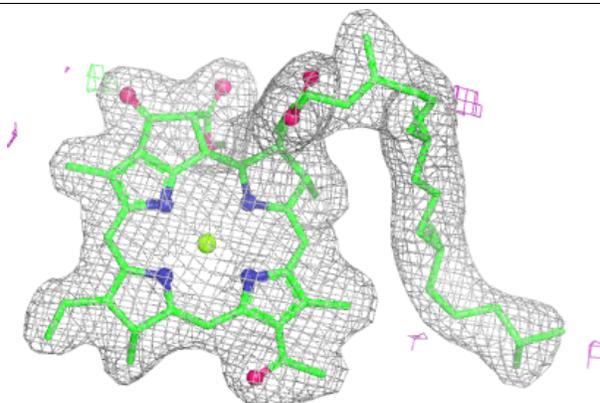


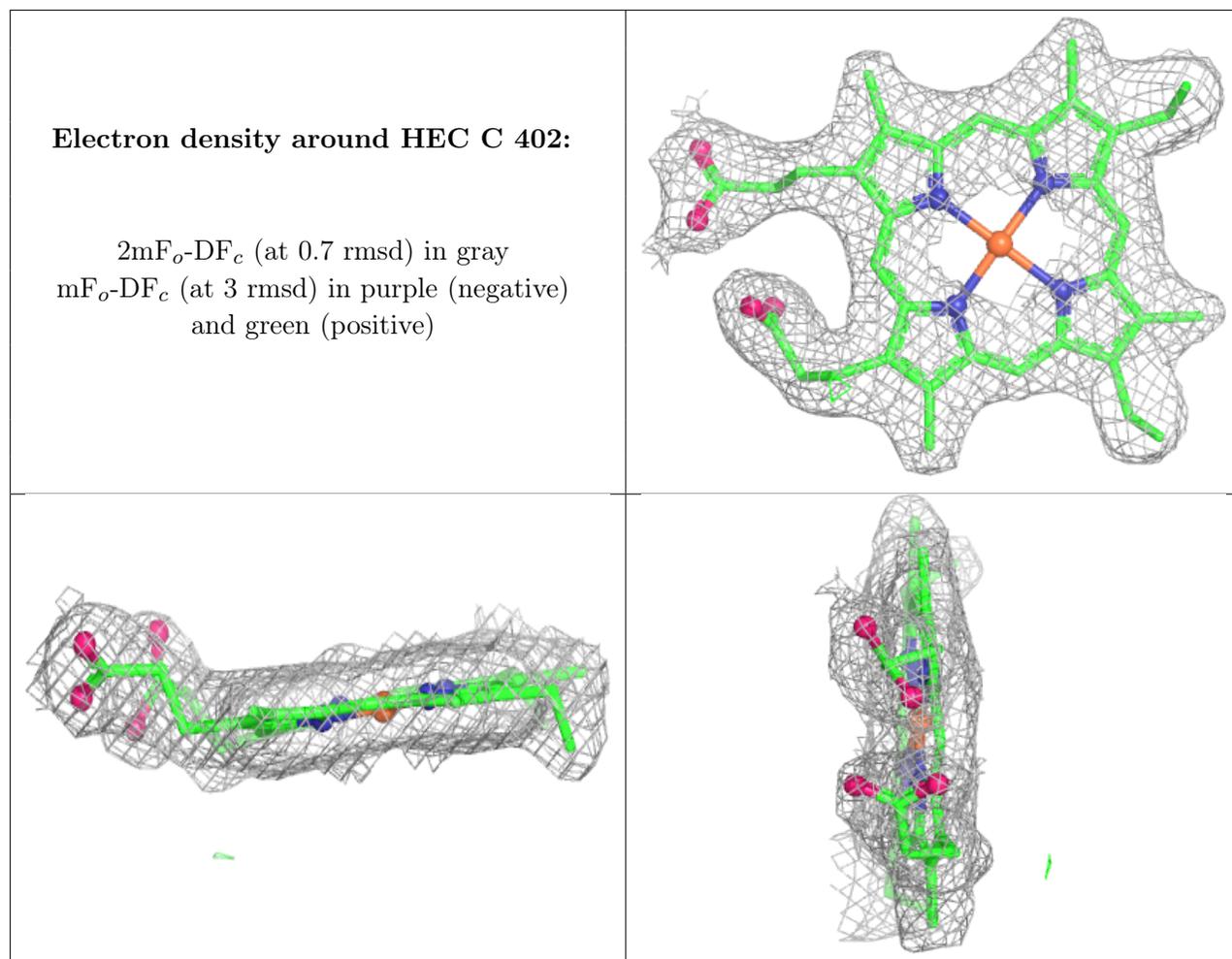
Electron density around BCB L 400:

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

**Electron density around BCB L 401:**

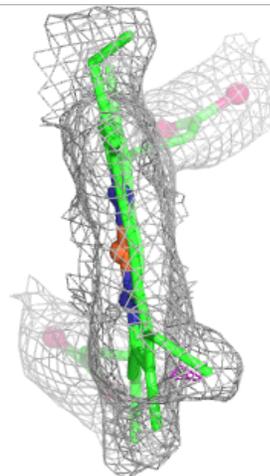
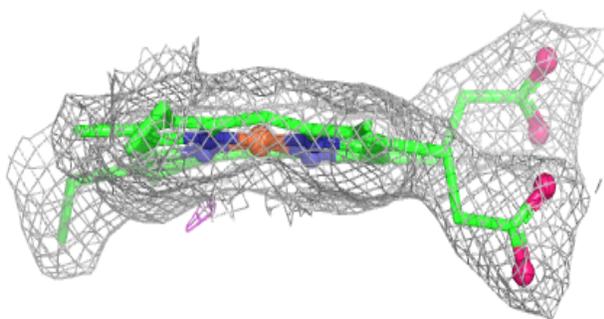
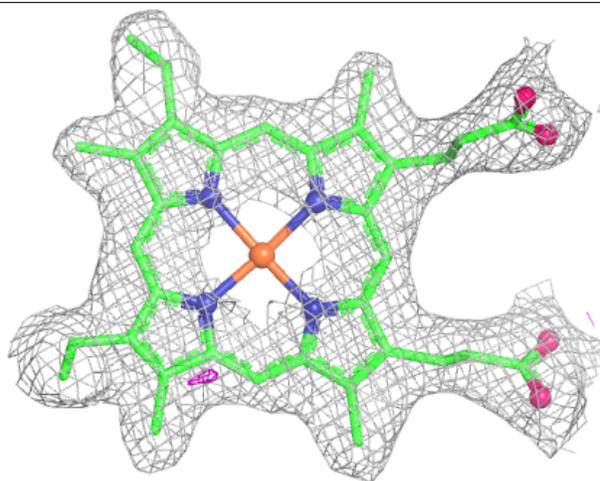
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

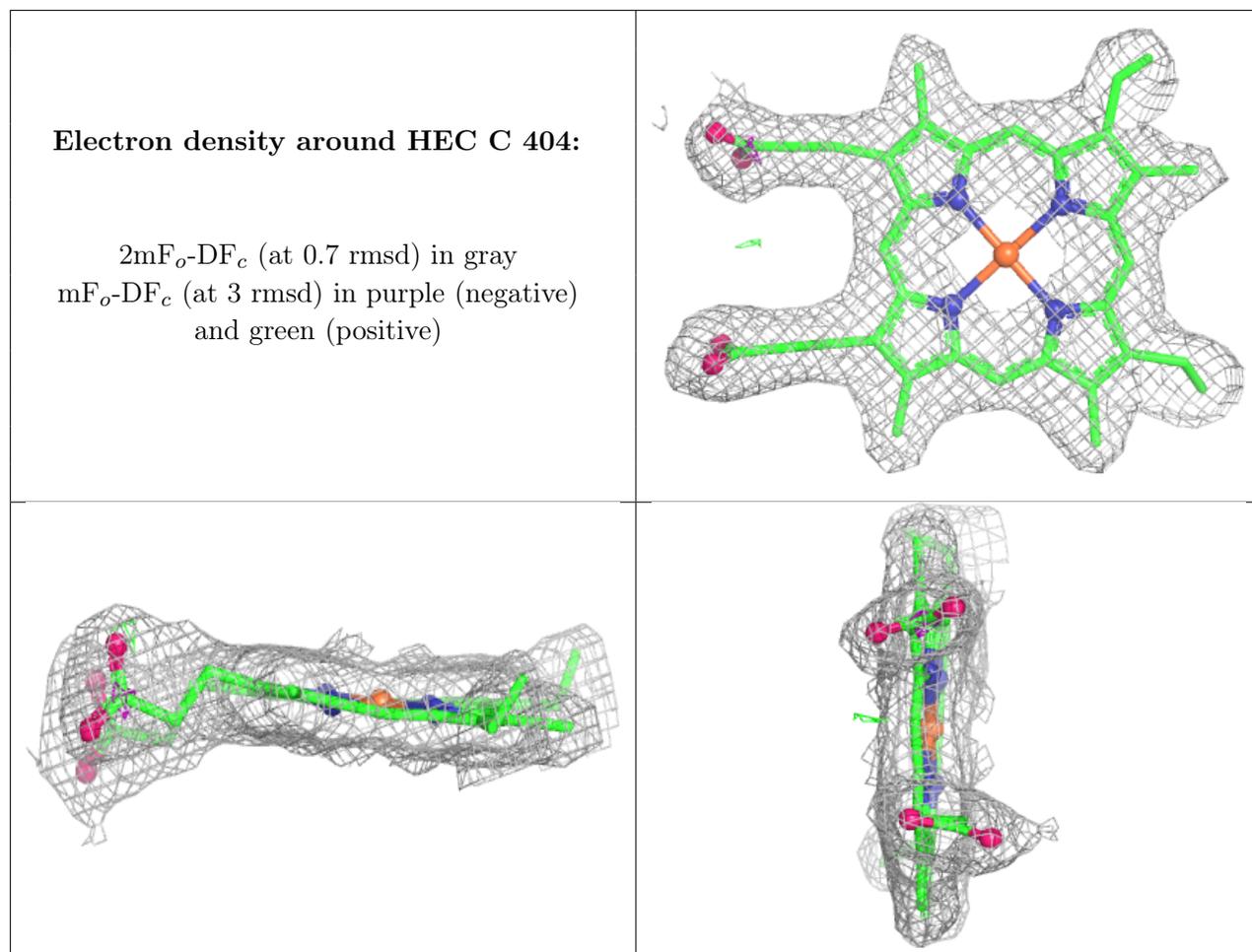


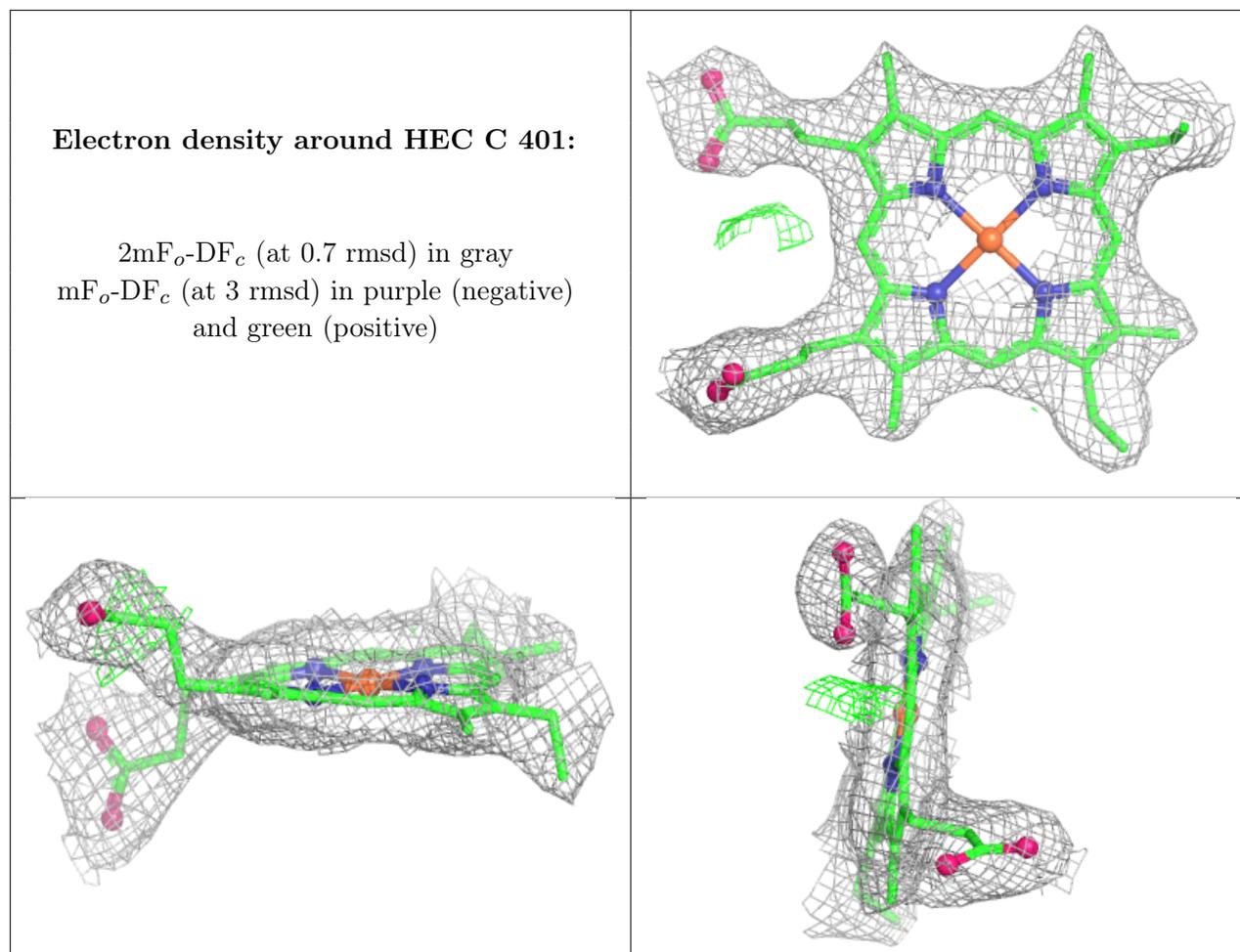


Electron density around HEC C 403:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.