



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 1R2C / pdb_00001r2c
Title : PHOTOSYNTHETIC REACTION CENTER BLASTOCHLORIS VIRIDIS (ATCC)
Authors : Baxter, R.H.; Ponomarenko, N.; Pahl, R.; Srajer, V.; Moffat, K.; Norris, J.R.
Deposited on : 2003-09-26
Resolution : 2.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

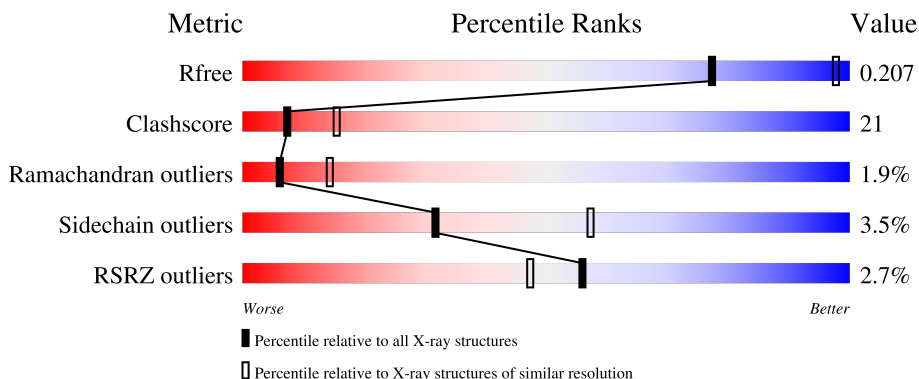
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	9% 65% 33% ..
2	L	273	65% 32% .
3	M	323	64% 33% .
4	H	258	9% 52% 41% 6% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCB	L	302	X	-	-	-
6	BCB	L	304	X	-	-	-
6	BCB	M	1301	X	-	-	-
6	BCB	M	1303	X	-	-	-
7	BPB	M	401	X	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10140 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 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	41	0	0
			2602	1640	466	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	10	0	0
			2171	1459	350	355	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	15	0	0
			2555	1702	419	423	11			

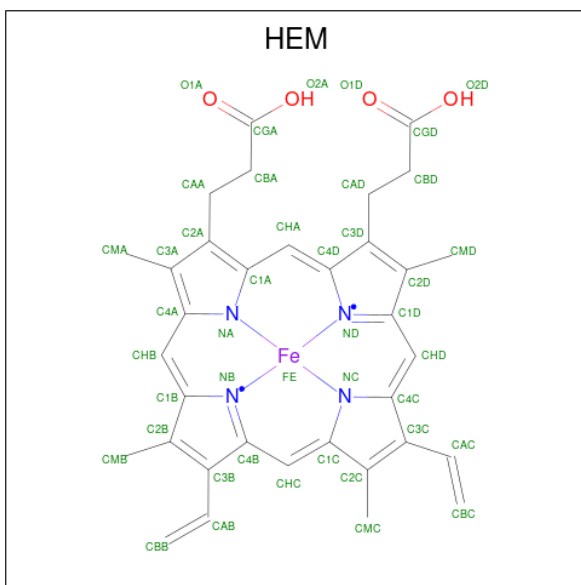
- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	98	0	0
			2018	1292	344	380	2			

There is a discrepancy between the modelled and reference sequences:

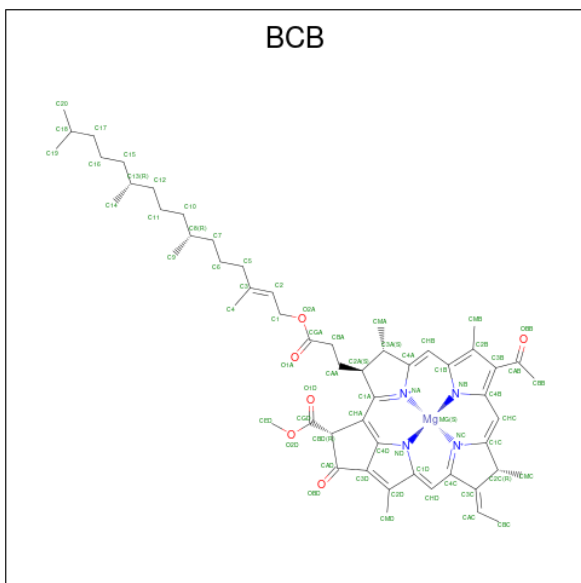
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	modified residue	UNP P06008

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



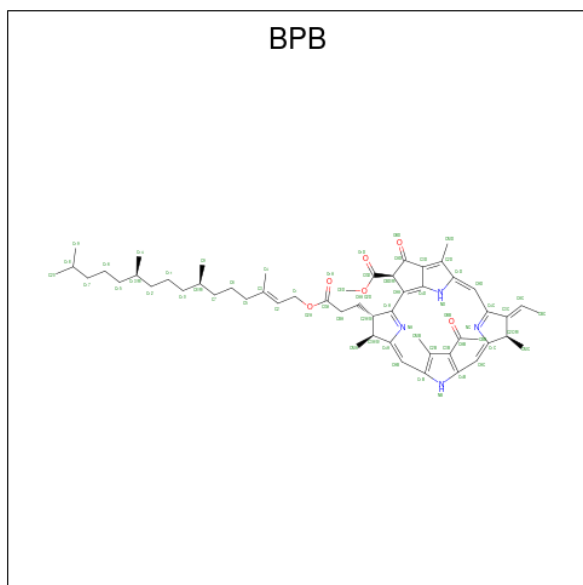
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



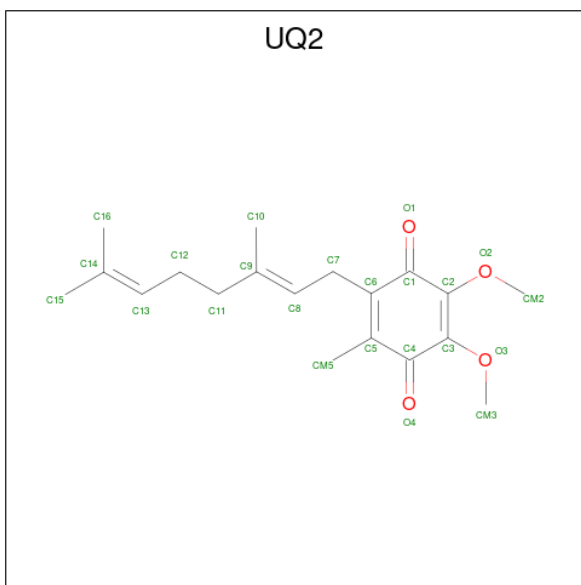
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	15	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



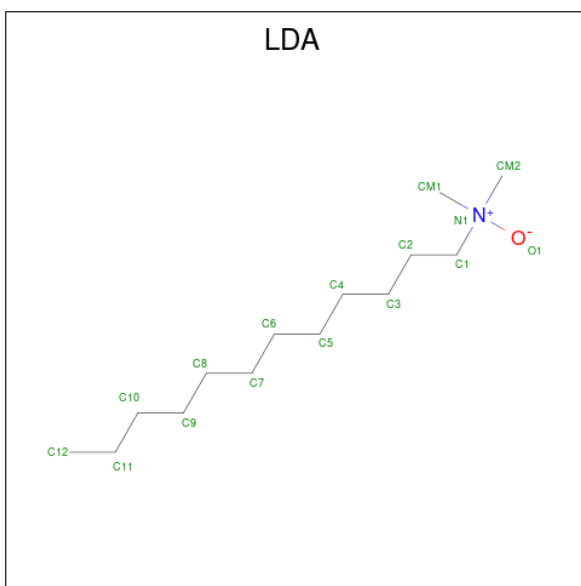
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	3	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

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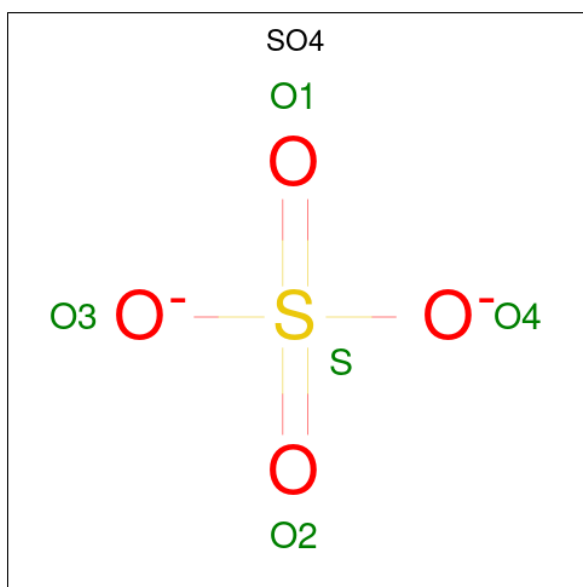
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	3	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

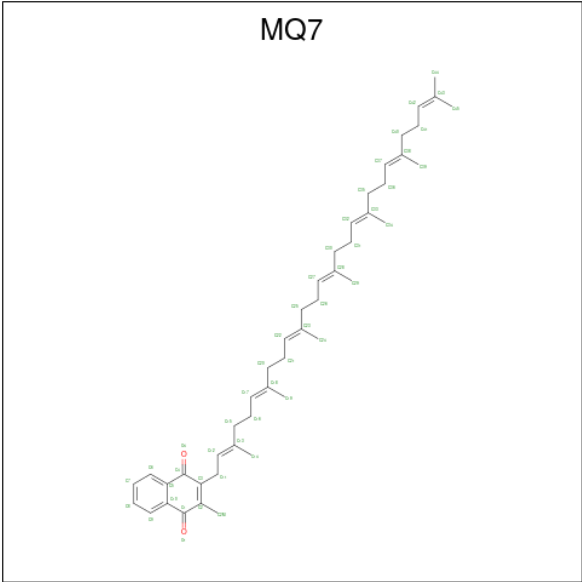
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



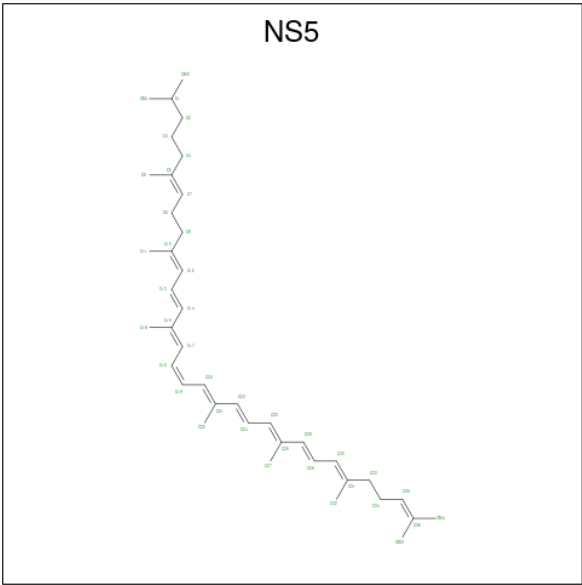
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	O	S	0	0
			5	4	1		
11	M	1	Total	O	S	0	0
			5	4	1		
11	M	1	Total	O	S	0	0
			5	4	1		
11	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).

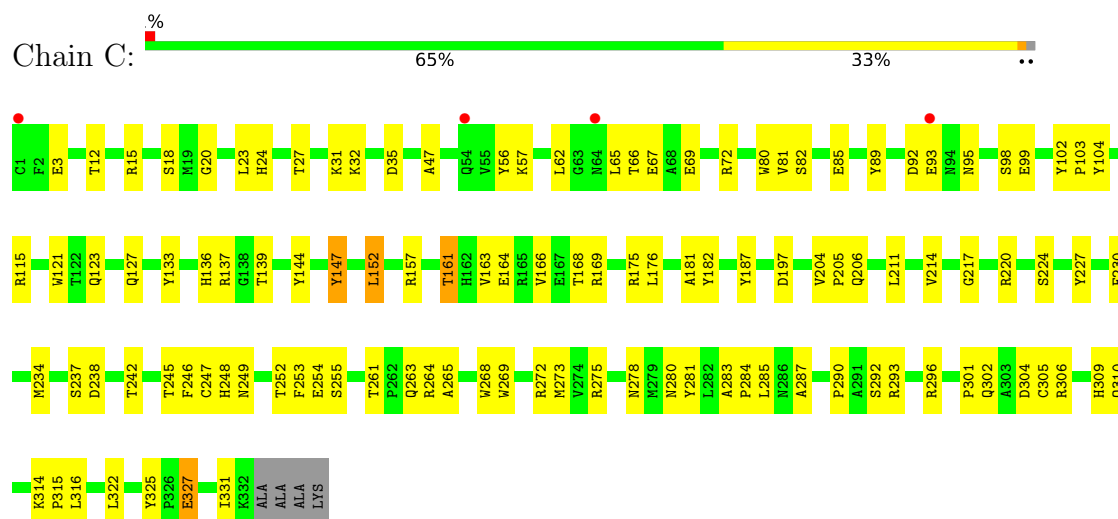


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C	11	0
			40	40		

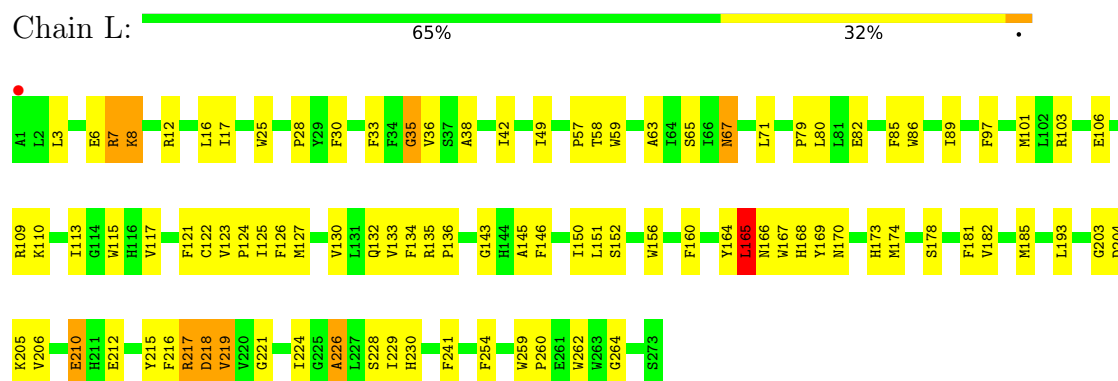
3 Residue-property plots [i](#)

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.

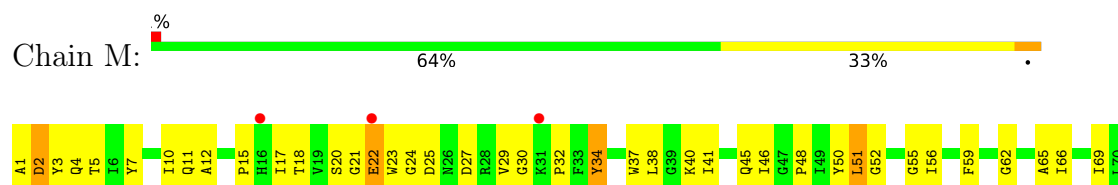
- Molecule 1: Photosynthetic reaction center cytochrome C subunit precursor

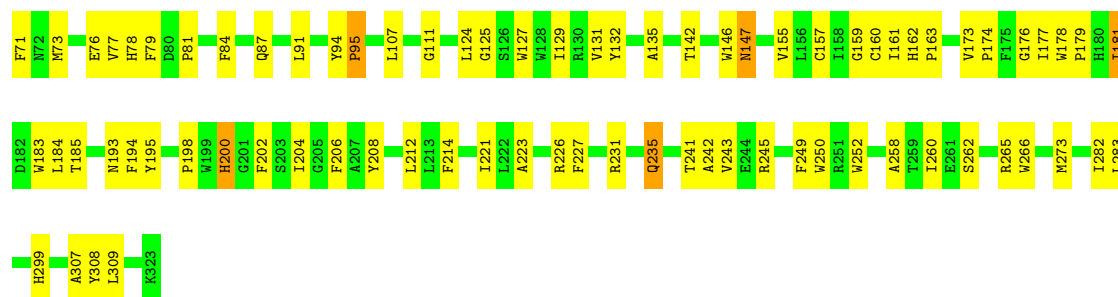


- Molecule 2: Reaction center protein L chain

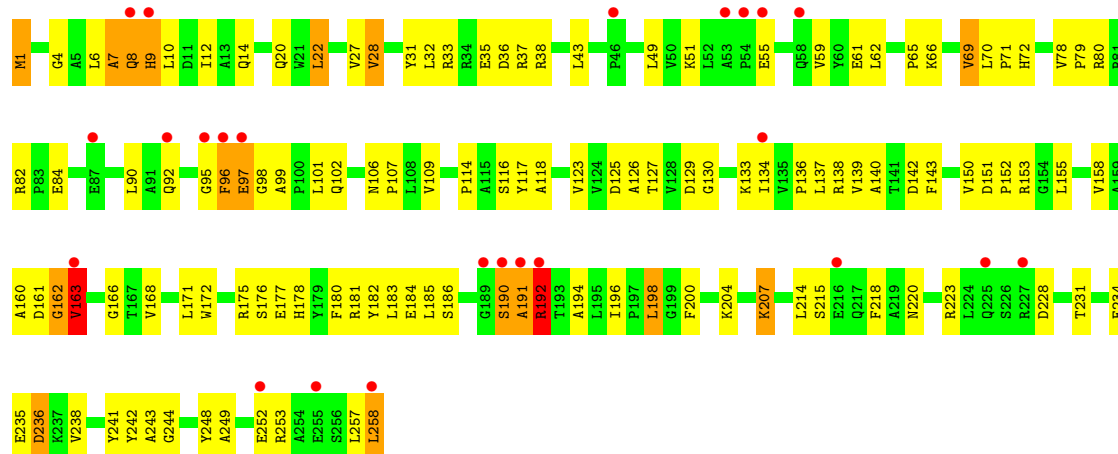


- Molecule 3: Reaction center protein M chain





• Molecule 4: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50Å 223.50Å 112.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.86 48.83 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.83-2.86) 97.4 (48.83-2.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.228 0.187 , 0.207	Depositor DCC
R_{free} test set	6311 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: NS5, LDA, FE2, BCB, FME, UQ2, SO4, BPB, HEM, MQ7

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	0.46	0/2669	0.95	6/3637 (0.2%)
2	L	0.47	0/2259	0.99	11/3084 (0.4%)
3	M	0.47	0/2659	0.94	8/3637 (0.2%)
4	H	0.41	0/2055	0.91	3/2807 (0.1%)
All	All	0.45	0/9642	0.95	28/13165 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	308	TYR	N-CA-C	-8.87	99.98	112.13
3	M	309	LEU	N-CA-C	-7.25	100.64	110.36
1	C	249	ASN	N-CA-C	-7.20	93.44	107.62
2	L	35	GLY	N-CA-C	-7.12	103.65	112.77
2	L	133	VAL	N-CA-C	7.00	118.06	111.48

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	2602	0	2579	78	0
2	L	2171	0	2098	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	2555	0	2452	114	0
4	H	2018	0	2020	121	0
5	C	172	0	120	7	0
6	L	132	0	144	18	0
6	M	132	0	143	26	0
7	L	65	0	74	12	0
7	M	65	0	74	21	0
8	L	23	0	26	4	0
9	H	16	0	31	4	0
9	L	16	0	31	2	0
9	M	64	0	124	11	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	0	0
12	M	48	0	64	0	0
13	M	40	0	60	5	0
All	All	10140	0	10040	404	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 21.

The worst 5 of 404 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)
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.31	1.05
7:M:401:BPB:H14	7:M:401:BPB:H17	1.39	1.03
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.39	1.02
6:L:302:BCB:HBD	6:L:302:BCB:HBA1	1.46	0.94
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.47	0.94

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%)	299 (91%)	30 (9%)	1 (0%)	36	54
2	L	271/273 (99%)	251 (93%)	17 (6%)	3 (1%)	11	24
3	M	321/323 (99%)	299 (93%)	19 (6%)	3 (1%)	14	28
4	H	256/258 (99%)	216 (84%)	25 (10%)	15 (6%)	1	2
All	All	1178/1190 (99%)	1065 (90%)	91 (8%)	22 (2%)	6	14

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	57	PRO
4	H	7	ALA
4	H	8	GLN
4	H	9	HIS
4	H	96	PHE

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	281/282 (100%)	276 (98%)	5 (2%)	51	73
2	L	218/218 (100%)	211 (97%)	7 (3%)	34	59
3	M	249/249 (100%)	241 (97%)	8 (3%)	34	59
4	H	212/212 (100%)	198 (93%)	14 (7%)	15	32
All	All	960/961 (100%)	926 (96%)	34 (4%)	32	57

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	192	ARG
4	H	198	LEU
4	H	252	GLU

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Mol	Chain	Res	Type
3	M	22	GLU
2	L	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	58	GLN
4	H	220	ASN
4	H	229	GLN
4	H	106	ASN
2	L	183	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	$\# Z > 2$
4	FME	H	1	4	8,9,10	0.67	0	8,9,11	3.14	3 (37%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	CA-N-CN	-7.21	111.74	122.82
4	H	1	FME	O1-CN-N	-4.09	114.75	125.32
4	H	1	FME	CE-SD-CG	-2.17	89.07	100.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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
11	SO4	H	801	-	4,4,4	0.31	0	6,6,6	0.37	0
5	HEM	C	1202	1	50,50,50	1.38	5 (10%)	67,82,82	1.18	8 (11%)
12	MQ7	M	501	-	49,49,49	1.67	17 (34%)	61,63,63	1.50	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LDA	M	701	-	13,15,15	2.37	2 (15%)	14,17,17	0.64	0
6	BCB	M	1303	3	60,74,74	1.74	9 (15%)	59,115,115	2.67	18 (30%)
5	HEM	C	1201	1	50,50,50	1.42	6 (12%)	67,82,82	1.10	6 (8%)
9	LDA	M	706	-	13,15,15	2.54	2 (15%)	14,17,17	0.51	0
8	UQ2	L	502	-	23,23,23	1.78	5 (21%)	30,31,31	1.29	3 (10%)
9	LDA	M	704	-	13,15,15	2.61	2 (15%)	14,17,17	0.54	0
9	LDA	L	705	-	13,15,15	2.44	2 (15%)	14,17,17	0.57	0
7	BPB	M	401	-	57,70,70	1.72	12 (21%)	55,101,101	2.86	18 (32%)
5	HEM	C	1203	1	50,50,50	1.38	5 (10%)	67,82,82	0.91	2 (2%)
6	BCB	L	302	2	60,74,74	1.79	10 (16%)	59,115,115	3.15	20 (33%)
13	NS5	M	600	-	39,39,39	0.70	0	46,46,46	1.06	4 (8%)
6	BCB	L	304	2	60,74,74	1.70	10 (16%)	59,115,115	3.10	17 (28%)
11	SO4	M	803	-	4,4,4	0.42	0	6,6,6	0.07	0
11	SO4	M	802	-	4,4,4	0.45	0	6,6,6	0.54	0
5	HEM	C	1204	1	50,50,50	1.43	6 (12%)	67,82,82	1.25	6 (8%)
11	SO4	M	804	-	4,4,4	0.45	0	6,6,6	0.41	0
9	LDA	H	703	-	13,15,15	2.73	2 (15%)	14,17,17	0.49	0
6	BCB	M	1301	3	60,74,74	1.61	8 (13%)	59,115,115	2.91	15 (25%)
9	LDA	M	702	-	13,15,15	2.18	2 (15%)	14,17,17	0.51	0
7	BPB	L	402	-	57,70,70	1.64	9 (15%)	55,101,101	3.29	19 (34%)

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	HEM	C	1202	1	-	8/14/54/54	-
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
9	LDA	M	701	-	-	0/13/13/13	-
6	BCB	M	1303	3	4/4/21/26	7/37/137/137	-
5	HEM	C	1201	1	-	4/14/54/54	-
9	LDA	M	706	-	-	0/13/13/13	-
8	UQ2	L	502	-	-	3/15/39/39	0/1/1/1
9	LDA	M	704	-	-	3/13/13/13	-
9	LDA	L	705	-	-	0/13/13/13	-
7	BPB	M	401	-	1/1/18/23	12/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	C	1203	1	-	8/14/54/54	-
6	BCB	L	302	2	2/2/21/26	9/37/137/137	-
13	NS5	M	600	-	-	8/43/43/43	-
6	BCB	L	304	2	4/4/21/26	12/37/137/137	-
5	HEM	C	1204	1	-	7/14/54/54	-
9	LDA	H	703	-	-	1/13/13/13	-
6	BCB	M	1301	3	3/3/21/26	5/37/137/137	-
9	LDA	M	702	-	-	0/13/13/13	-
7	BPB	L	402	-	-	5/37/105/105	0/5/6/6

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	703	LDA	O1-N1	-8.24	1.22	1.42
9	M	704	LDA	O1-N1	-8.12	1.22	1.42
9	M	701	LDA	O1-N1	-7.98	1.22	1.42
9	M	706	LDA	O1-N1	-7.88	1.22	1.42
9	M	702	LDA	O1-N1	-7.41	1.24	1.42

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	402	BPB	O2D-CGD-CBD	11.78	123.89	110.95
7	L	402	BPB	C1-C2-C3	11.36	144.81	126.20
6	L	304	BCB	O2D-CGD-CBD	11.28	123.34	110.95
7	M	401	BPB	O2D-CGD-CBD	11.17	123.22	110.95
6	M	1301	BCB	O2D-CGD-CBD	10.91	122.94	110.95

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	302	BCB	NA
6	L	302	BCB	ND
6	L	304	BCB	NA
6	L	304	BCB	C8
6	L	304	BCB	NC

5 of 94 torsion outliers are listed below:

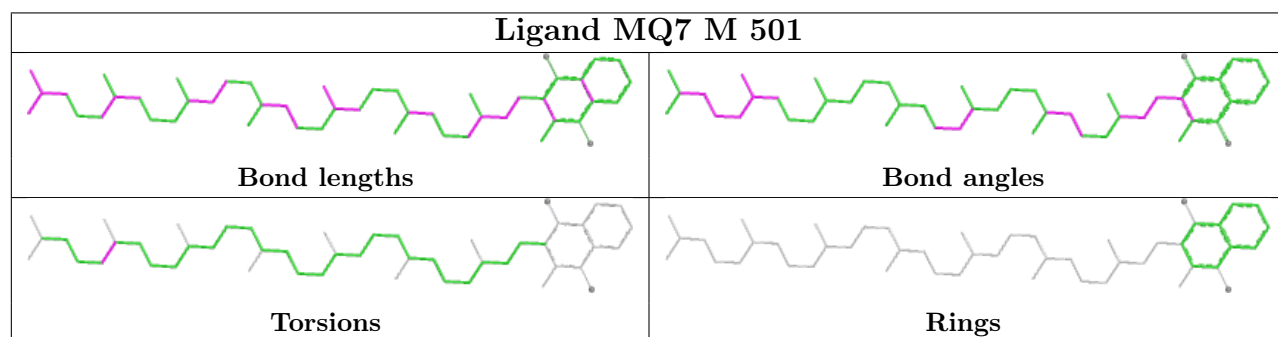
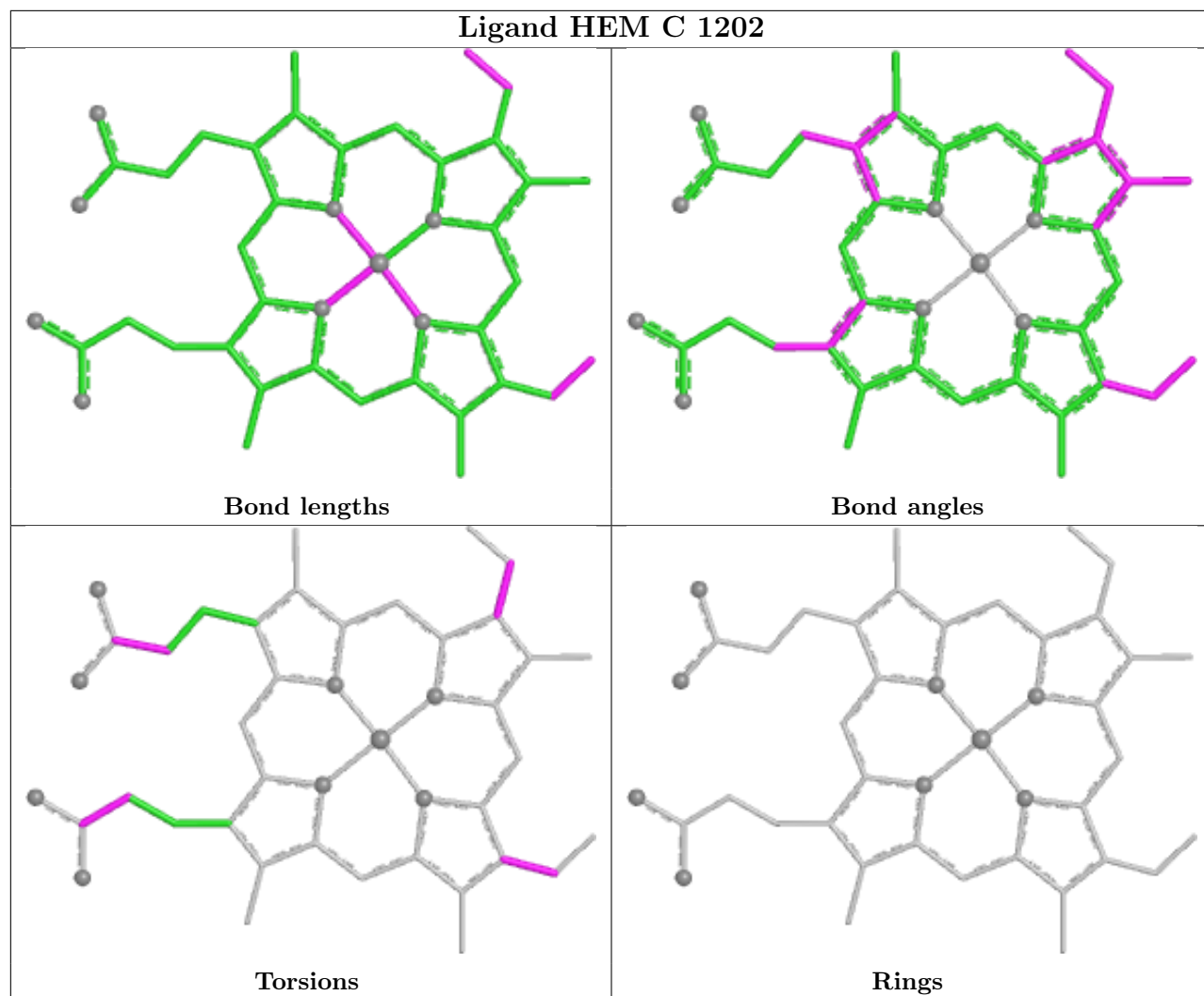
Mol	Chain	Res	Type	Atoms
6	L	302	BCB	CAD-CBD-CGD-O1D
6	L	302	BCB	CAD-CBD-CGD-O2D
6	M	1301	BCB	C4C-C3C-CAC-CBC
6	M	1303	BCB	CAD-CBD-CGD-O1D
6	M	1303	BCB	CAD-CBD-CGD-O2D

There are no ring outliers.

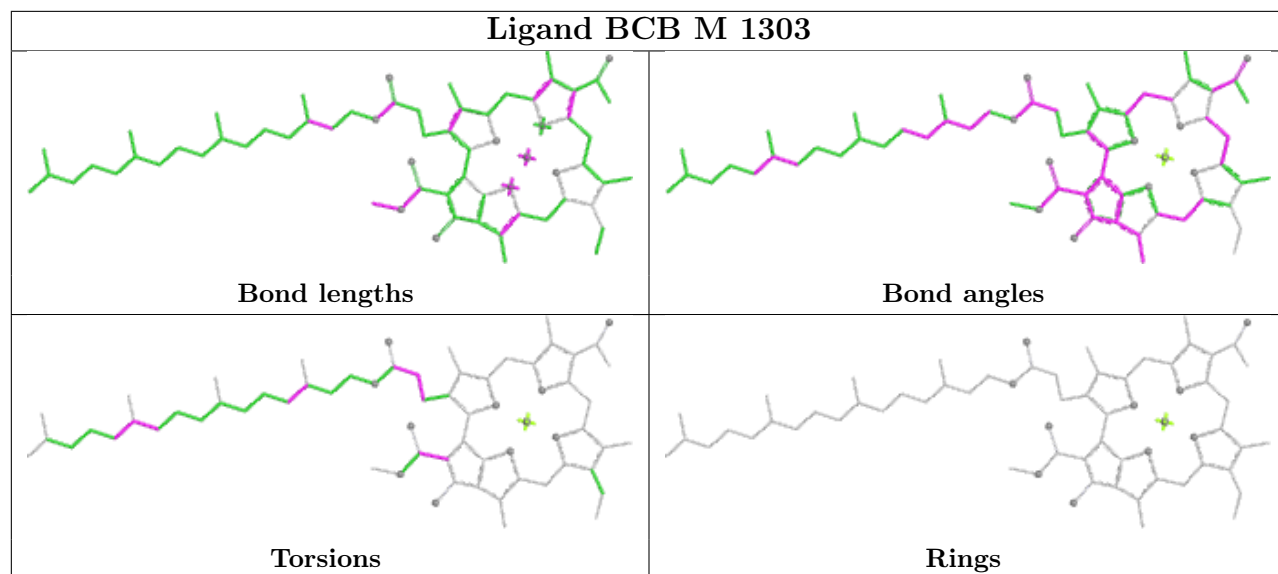
17 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1202	HEM	1	0
9	M	701	LDA	3	0
6	M	1303	BCB	16	0
5	C	1201	HEM	2	0
9	M	706	LDA	1	0
8	L	502	UQ2	4	0
9	L	705	LDA	2	0
7	M	401	BPB	21	0
5	C	1203	HEM	1	0
6	L	302	BCB	14	0
13	M	600	NS5	5	0
6	L	304	BCB	5	0
5	C	1204	HEM	3	0
9	H	703	LDA	4	0
6	M	1301	BCB	12	0
9	M	702	LDA	7	0
7	L	402	BPB	12	0

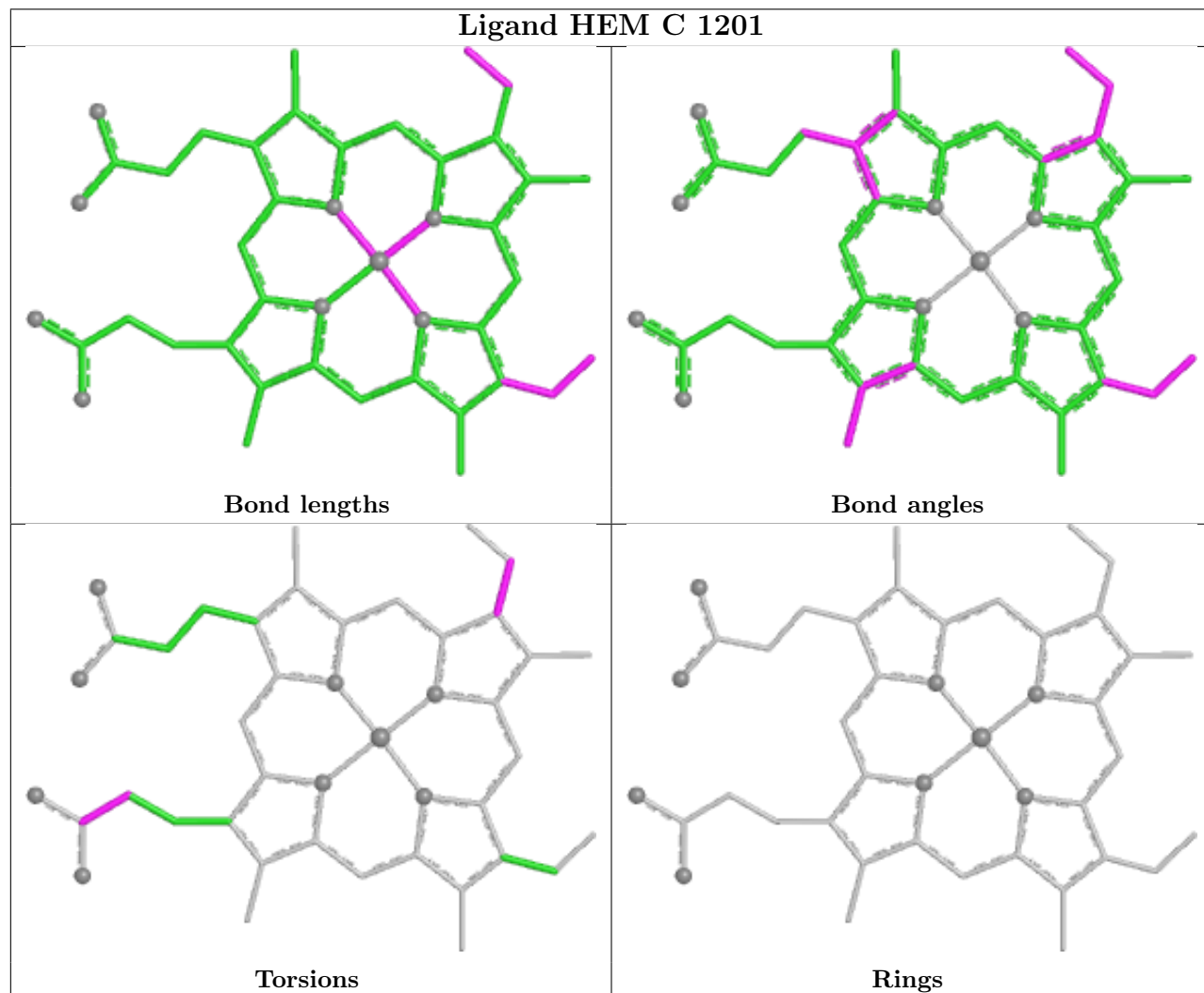
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



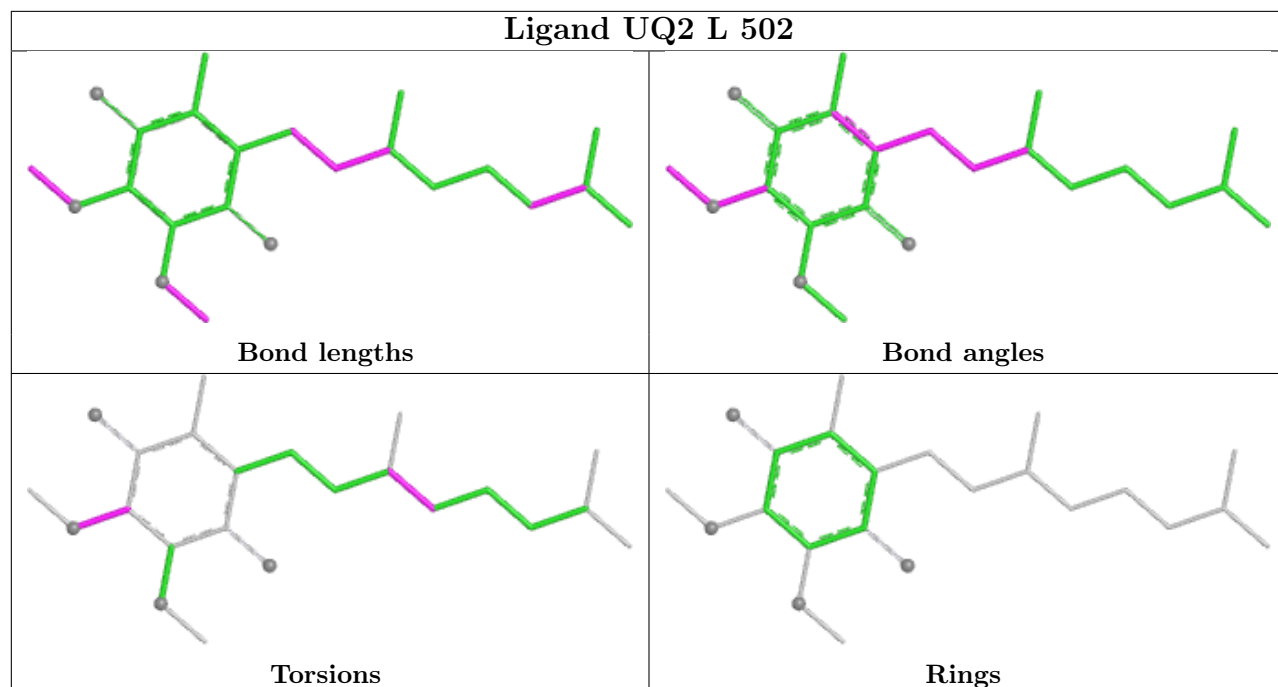
Ligand BCB M 1303



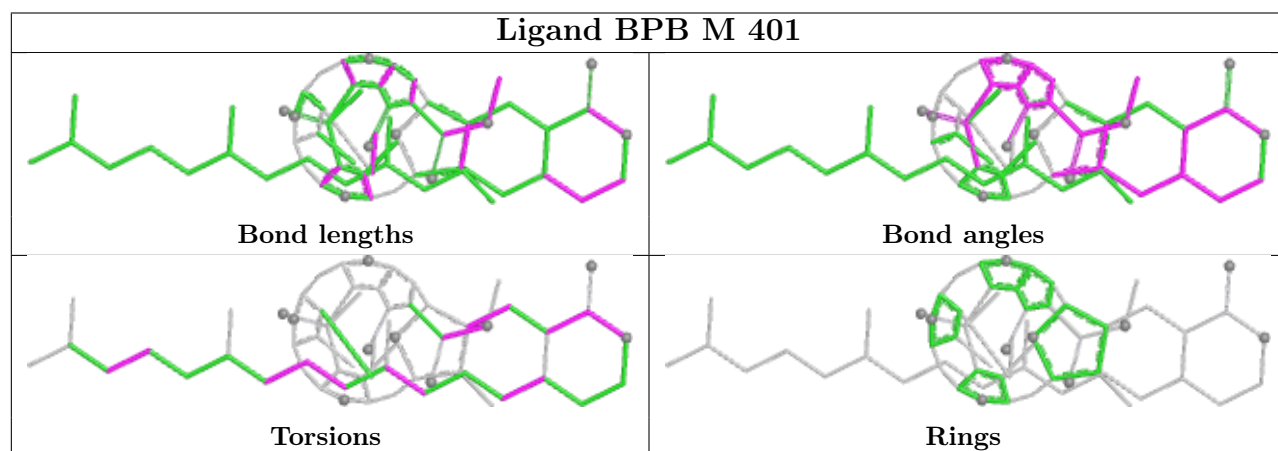
Ligand HEM C 1201



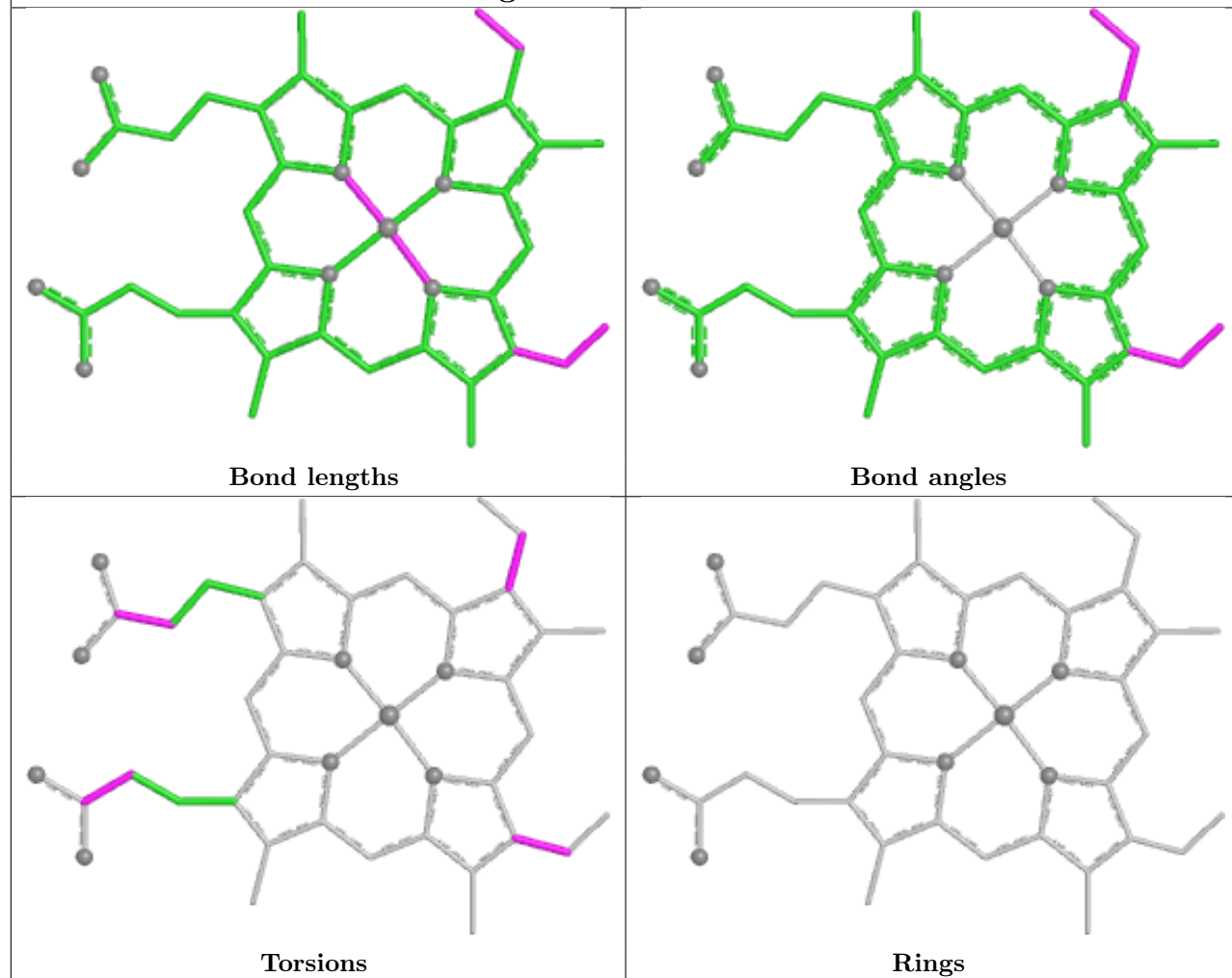
Ligand UQ2 L 502



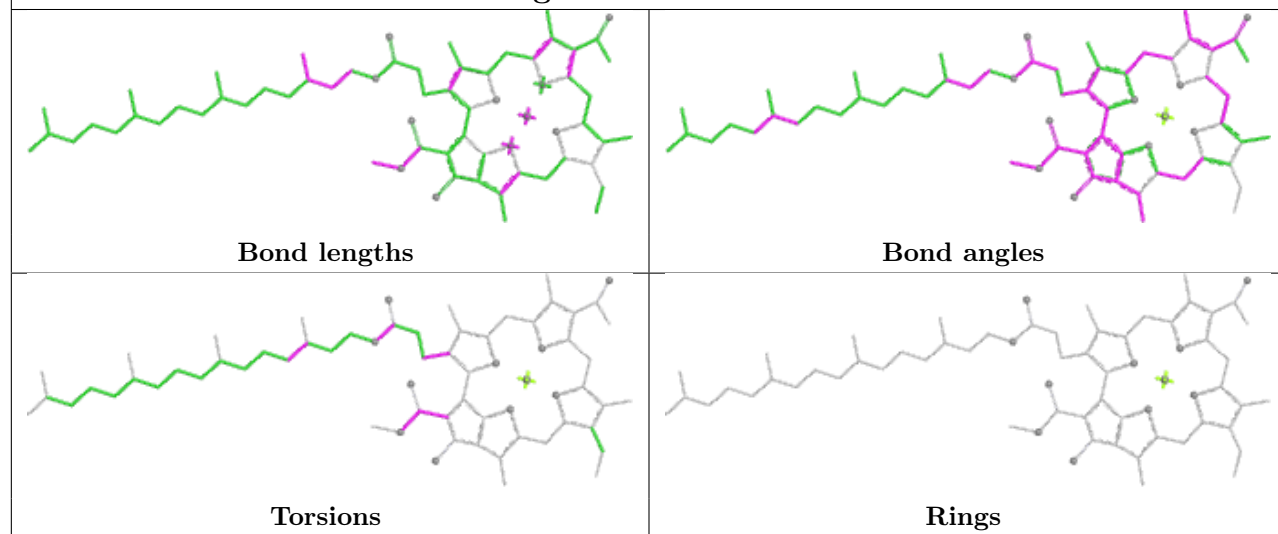
Ligand BPB M 401

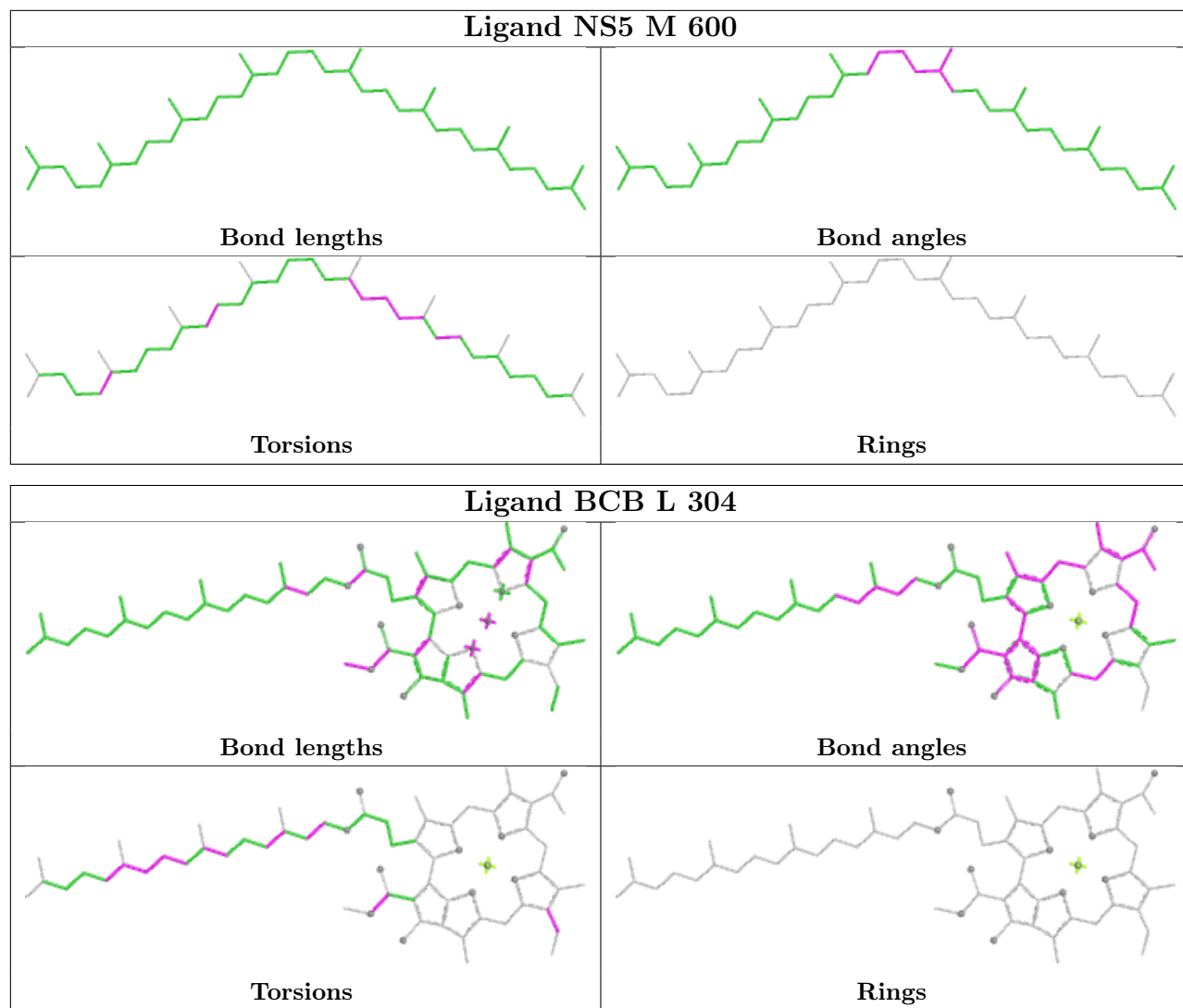


Ligand HEM C 1203

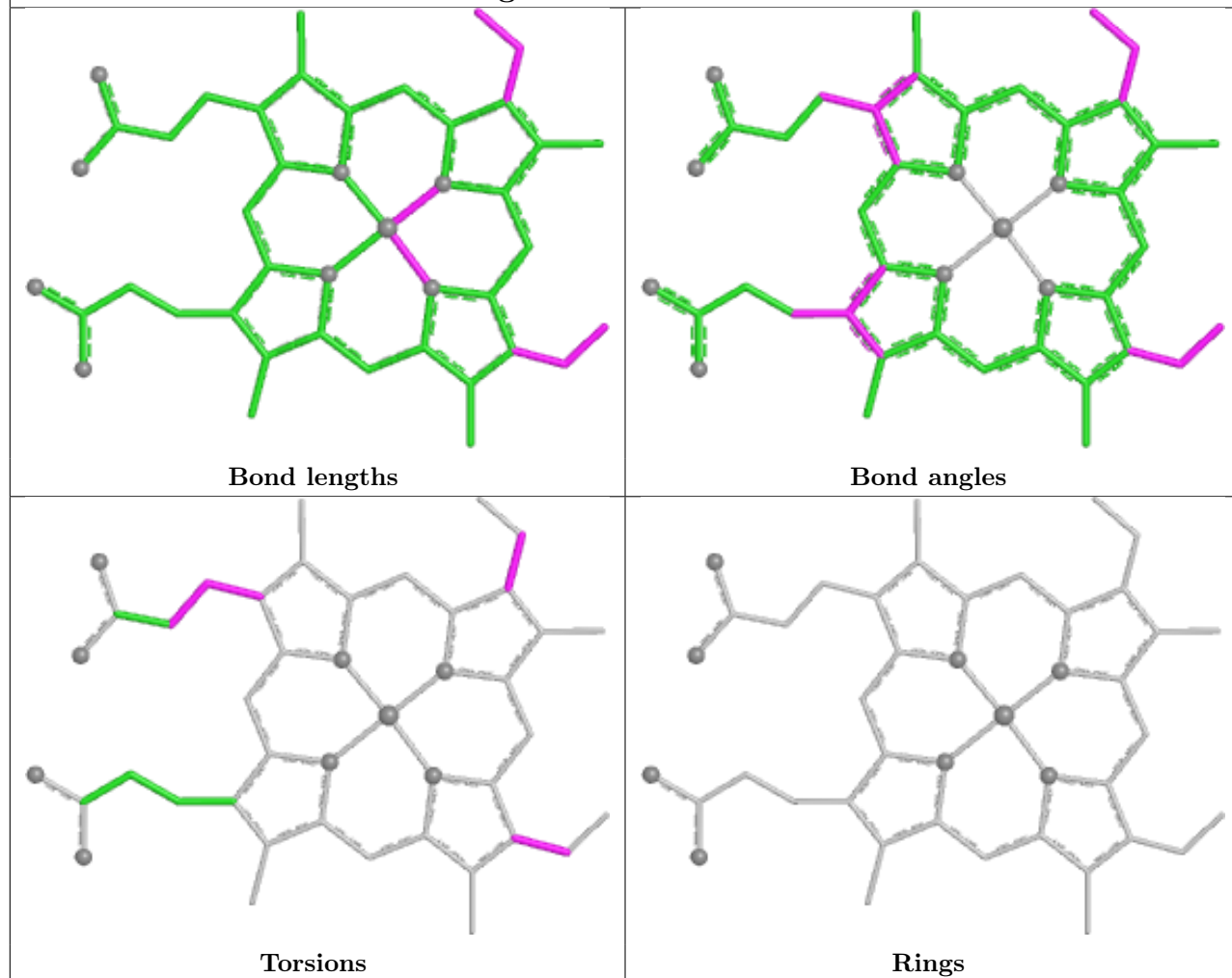


Ligand BCB L 302

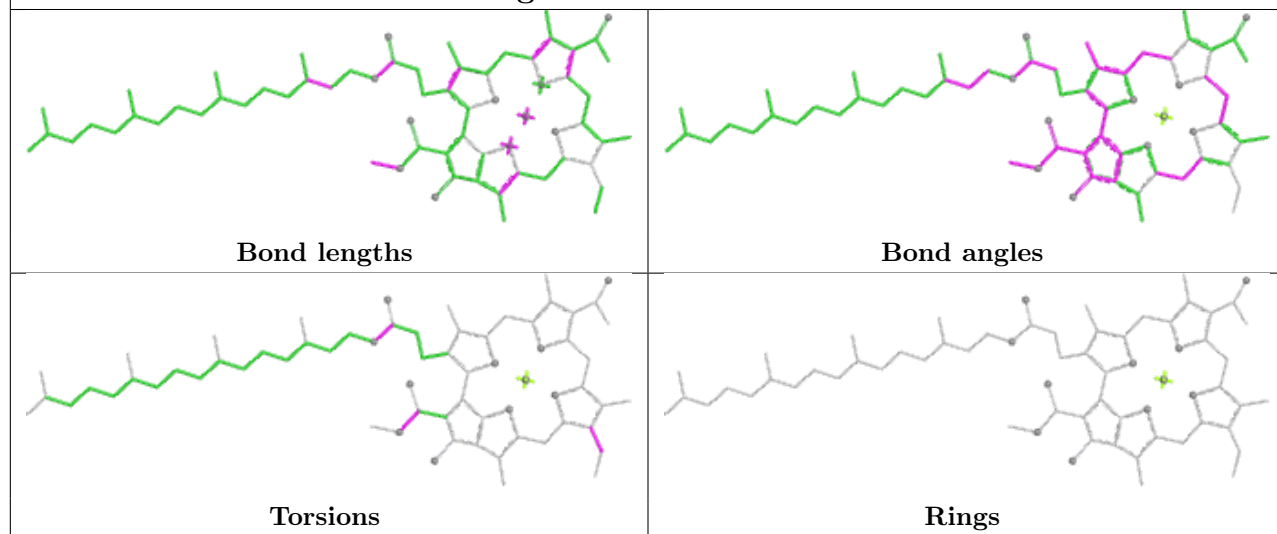


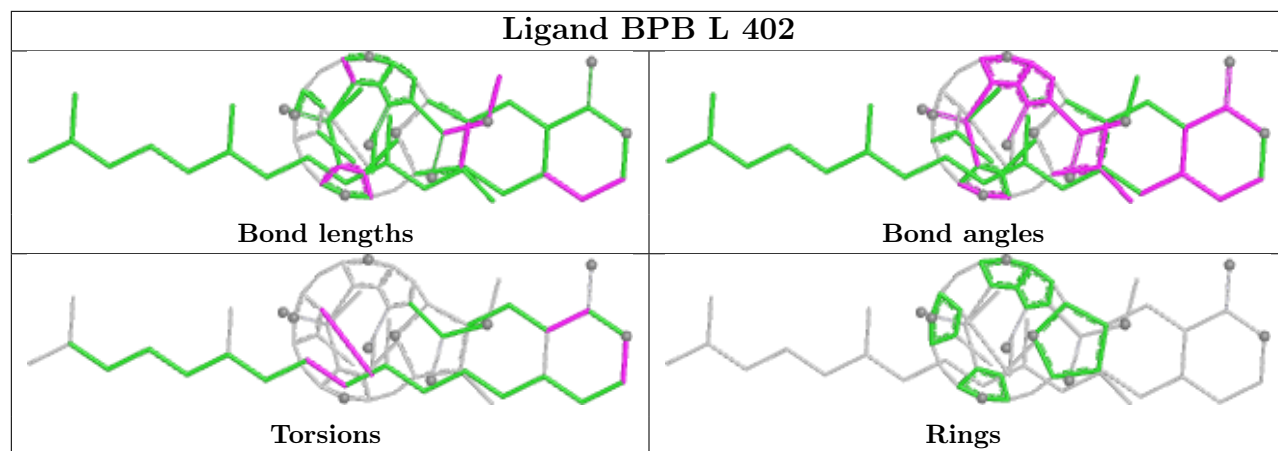


Ligand HEM C 1204



Ligand BCB M 1301





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%)	-0.15	4 (1%) 76 71	23, 44, 65, 78	15 (4%)
2	L	273/273 (100%)	-0.27	1 (0%) 88 87	25, 42, 65, 76	6 (2%)
3	M	323/323 (100%)	-0.17	3 (0%) 81 76	25, 42, 66, 76	8 (2%)
4	H	251/258 (97%)	0.56	24 (9%) 13 11	27, 54, 83, 93	19 (7%)
All	All	1179/1190 (99%)	-0.03	32 (2%) 56 47	23, 46, 70, 93	48 (4%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	46	PRO	5.7
4	H	92	GLN	5.3
4	H	55	GLU	4.8
4	H	54	PRO	4.4
1	C	93	GLU	4.3

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
4	FME	H	1	10/11	0.93	0.13	53,55,63,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

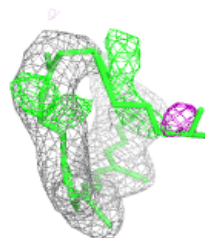
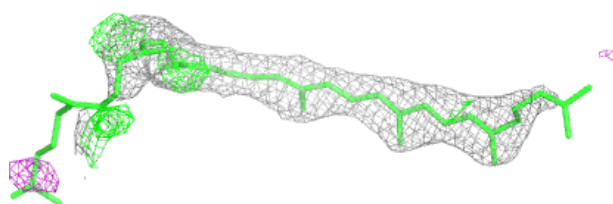
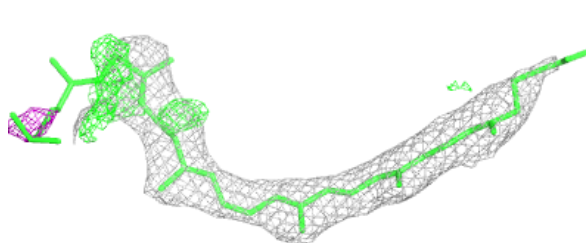
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	LDA	L	705	16/16	0.83	0.30	71,78,94,95	3
9	LDA	M	702	16/16	0.83	0.32	73,87,100,101	0
9	LDA	M	706	16/16	0.85	0.33	99,105,114,114	0
11	SO4	M	804	5/5	0.86	0.17	81,82,82,83	0
9	LDA	H	703	16/16	0.88	0.26	74,79,85,85	0
9	LDA	M	704	16/16	0.88	0.27	79,82,83,84	3
13	NS5	M	600	40/40	0.92	0.15	39,58,67,68	11
7	BPB	M	401	65/65	0.93	0.14	37,45,94,95	0
11	SO4	M	803	5/5	0.93	0.12	102,102,103,103	0
11	SO4	H	801	5/5	0.94	0.08	73,76,76,77	0
8	UQ2	L	502	23/23	0.95	0.20	48,49,50,50	23
9	LDA	M	701	16/16	0.95	0.13	48,50,52,52	0
6	BCB	M	1301	66/66	0.96	0.09	33,43,59,63	15
12	MQ7	M	501	48/48	0.96	0.11	36,45,67,70	0
7	BPB	L	402	65/65	0.96	0.10	31,41,45,47	0
6	BCB	L	302	66/66	0.97	0.08	10,20,42,43	0
6	BCB	M	1303	66/66	0.97	0.08	17,25,46,48	0
11	SO4	M	802	5/5	0.97	0.08	57,59,61,61	0
6	BCB	L	304	66/66	0.97	0.09	23,29,54,57	0
5	HEM	C	1201	43/43	0.98	0.08	47,51,61,65	0
5	HEM	C	1203	43/43	0.99	0.06	26,33,41,44	0
5	HEM	C	1204	43/43	0.99	0.07	32,36,48,53	0
5	HEM	C	1202	43/43	0.99	0.06	39,43,55,58	0
10	FE2	M	500	1/1	1.00	0.05	33,33,33,33	0

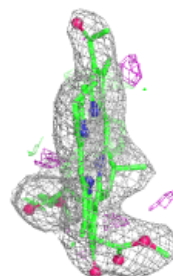
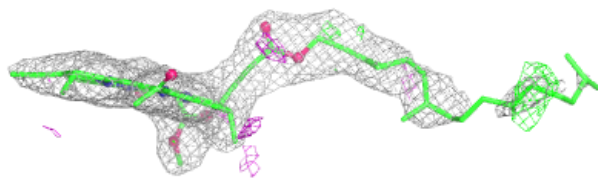
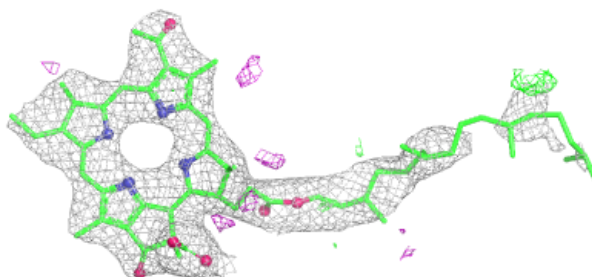
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

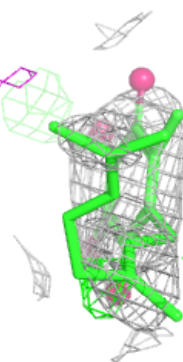
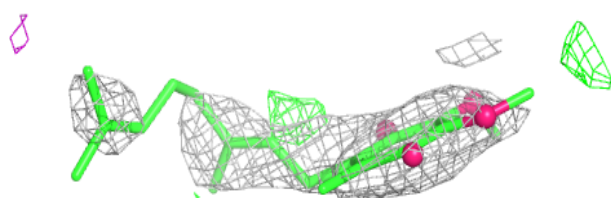
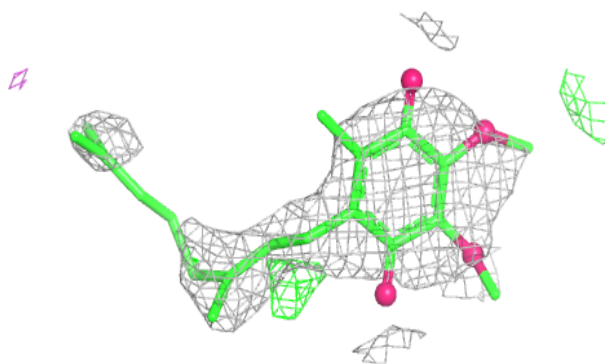
**Electron density around BPB M 401:**

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

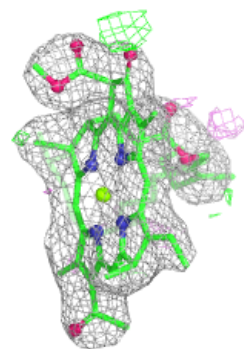
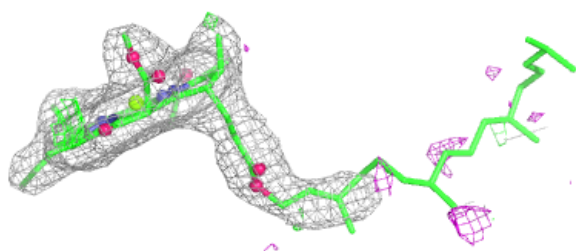
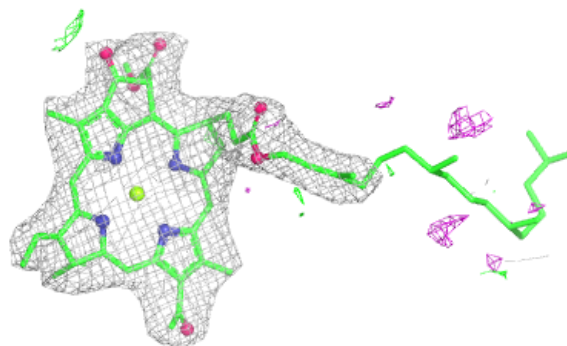


Electron density around UQ2 L 502:

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

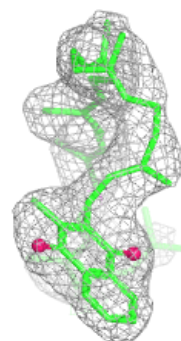
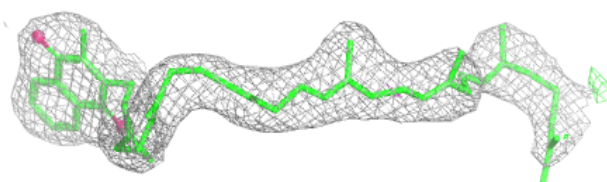
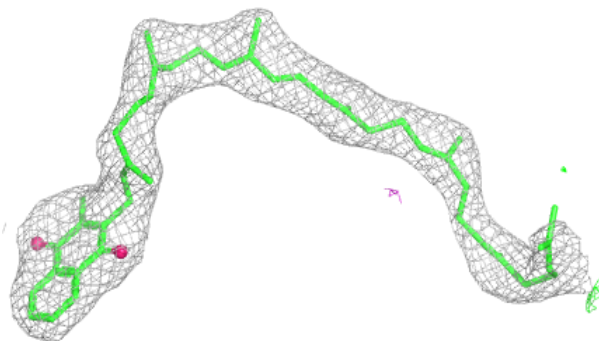
**Electron density around BCB M 1301:**

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

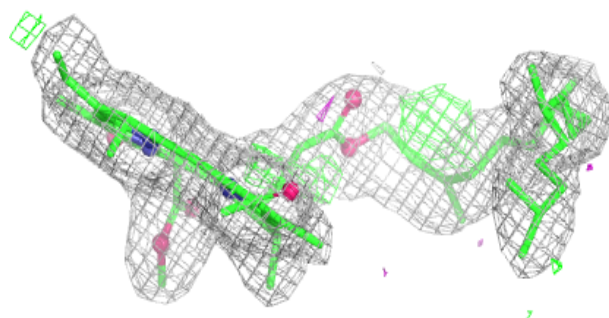
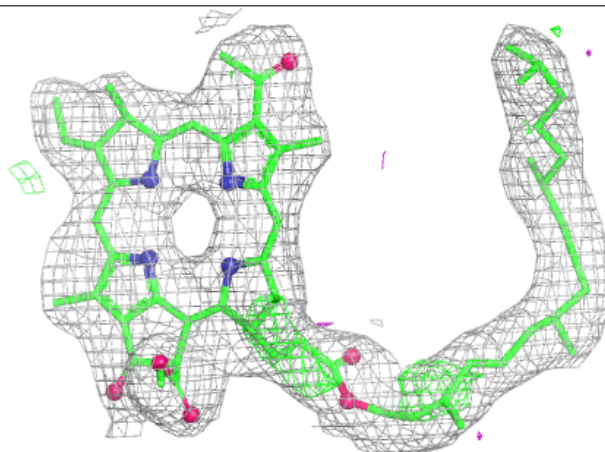


Electron density around MQ7 M 501:

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

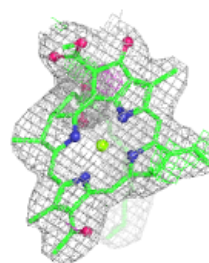
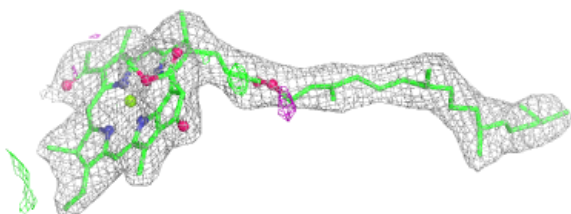
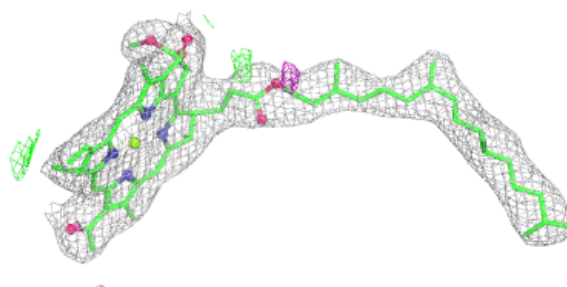
**Electron density around BPB L 402:**

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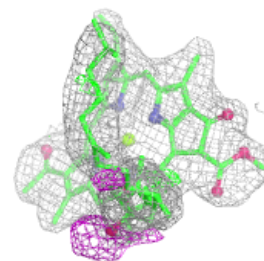
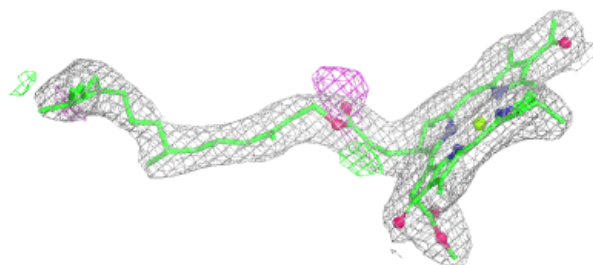
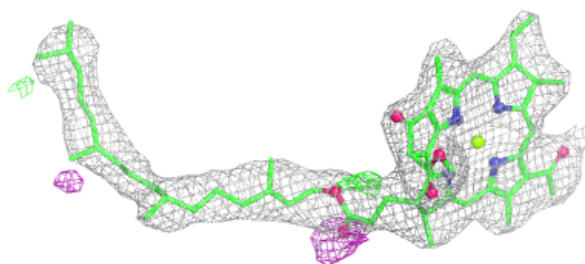


Electron density around BCB L 302:

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and green (positive)

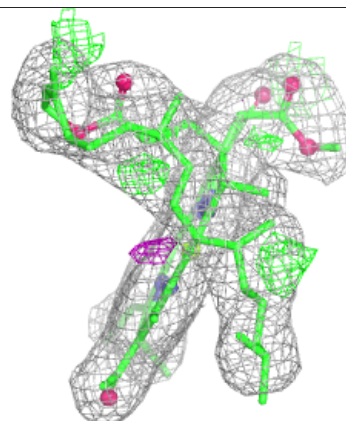
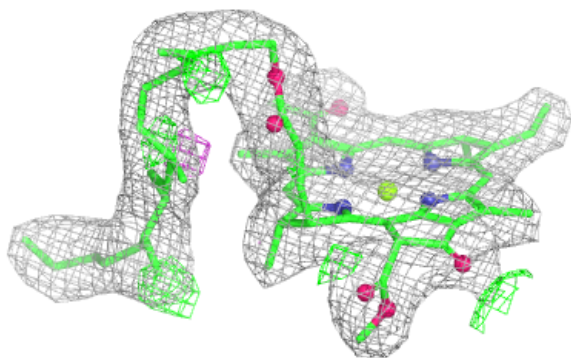
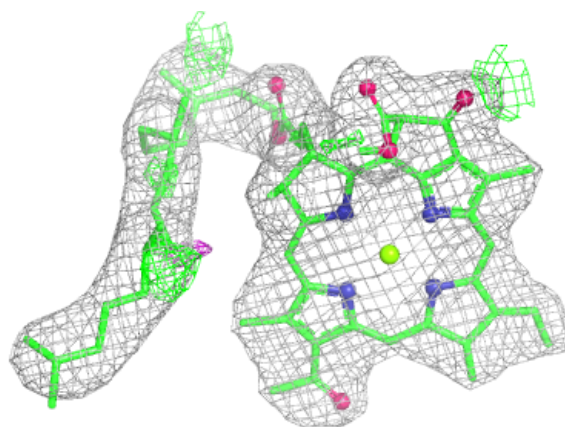
**Electron density around BCB M 1303:**

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



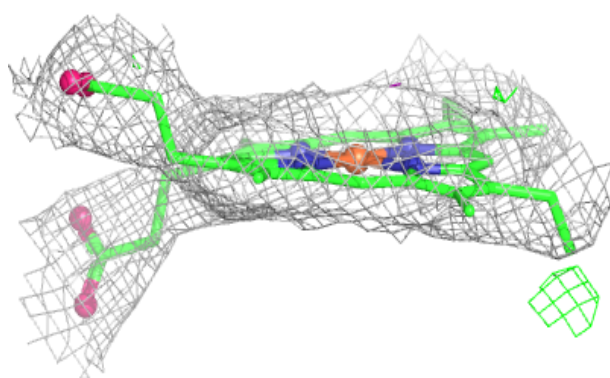
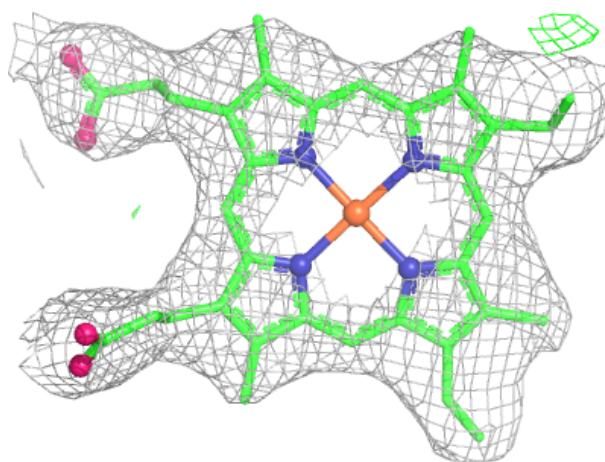
Electron density around BCB L 304:

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



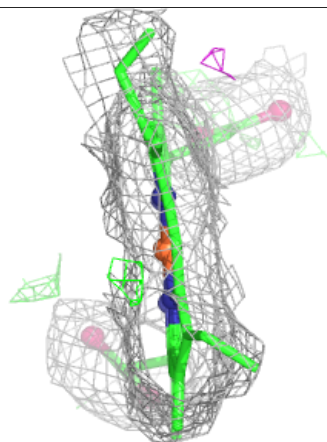
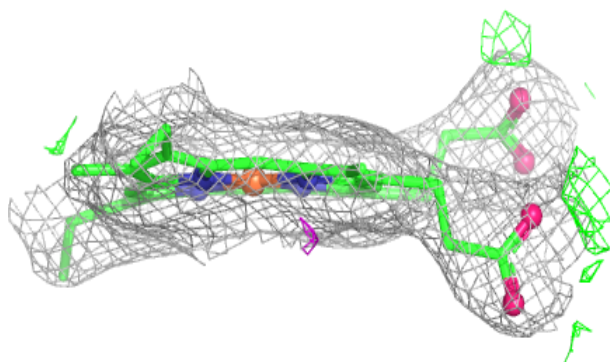
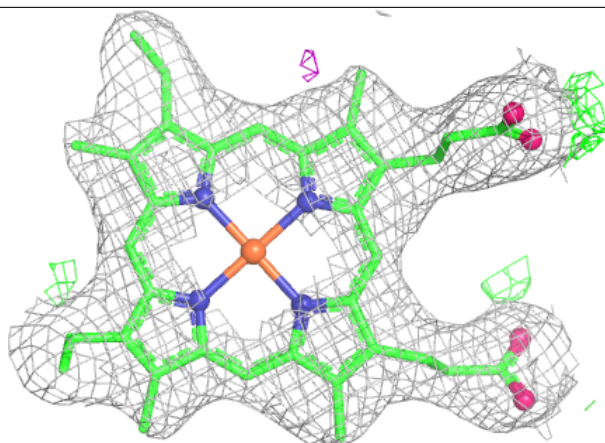
Electron density around HEM C 1201:

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

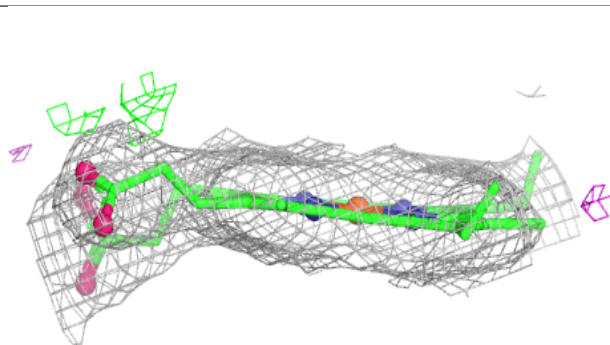
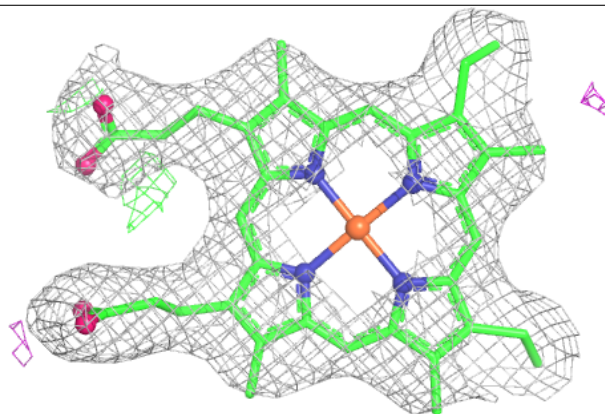


Electron density around HEM C 1203:

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

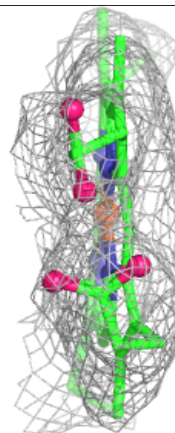
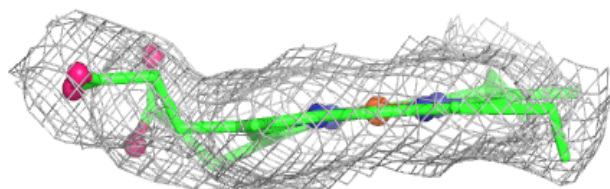
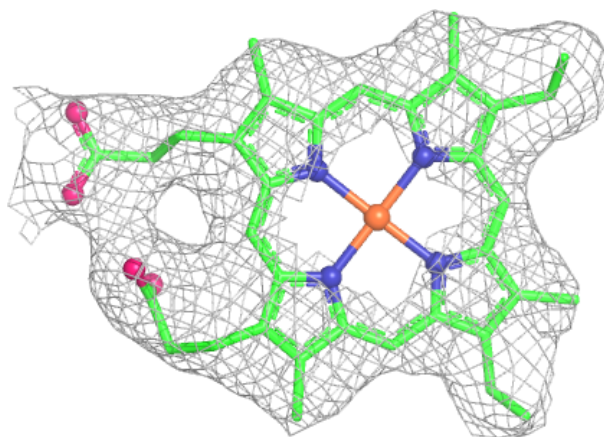
**Electron density around HEM C 1204:**

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



Electron density around HEM C 1202:

$2mF_o - DF_c$ (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.