



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 07:39 PM EDT

PDB ID : 2X5V
Title : 80 microsecond laue diffraction snapshot from crystals of a photosynthetic reaction centre 3 millisecond following photoactivation.
Authors : Wohri, A.B.; Katona, G.; Johansson, L.C.; Fritz, E.; Malmerberg, E.; Andersson, M.; Vincent, J.; Eklund, M.; Cammarata, M.; Wulff, M.; Davidsson, J.; Groenhof, G.; Neutze, R.
Deposited on : 2010-02-10
Resolution : 3.00 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](#) 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	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

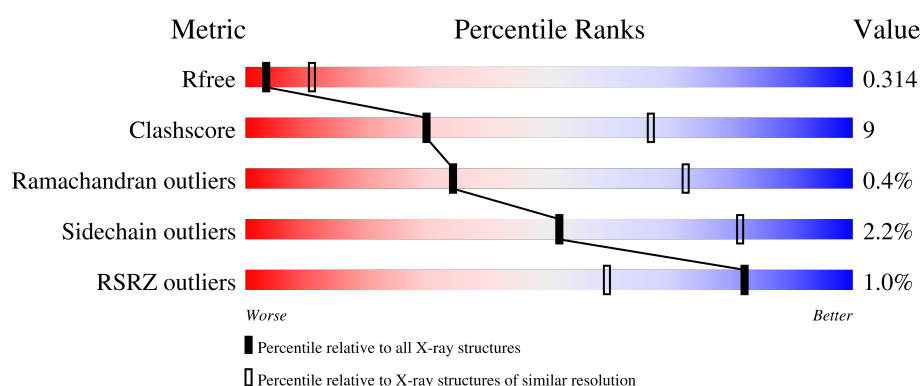
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	
2	H	258	
3	L	274	
4	M	324	

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	1274	X	-	-	-
6	BCB	L	1275	X	-	-	-
6	BCB	M	1324	X	-	-	-
6	BCB	M	1325	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9871 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	4	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	243	Total	C	N	O	S	26	0	0
			1906	1218	327	359	2			

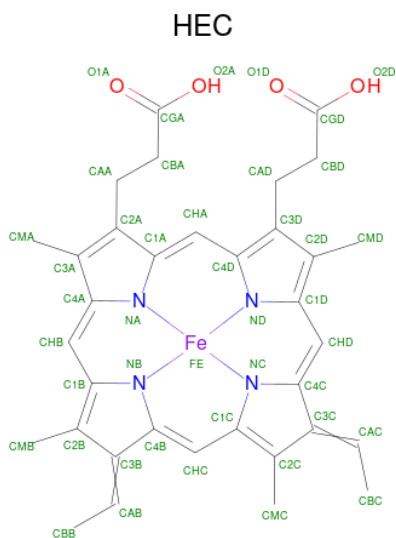
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	10	4	0
			2196	1476	352	361	7			

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

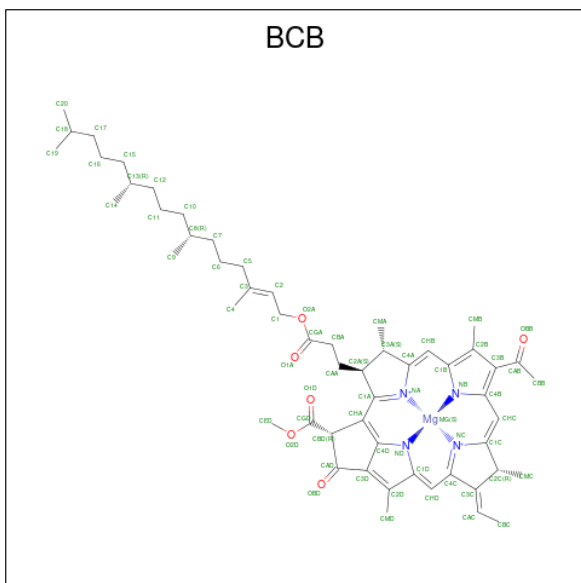
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	7	0	0
			2555	1702	419	423	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



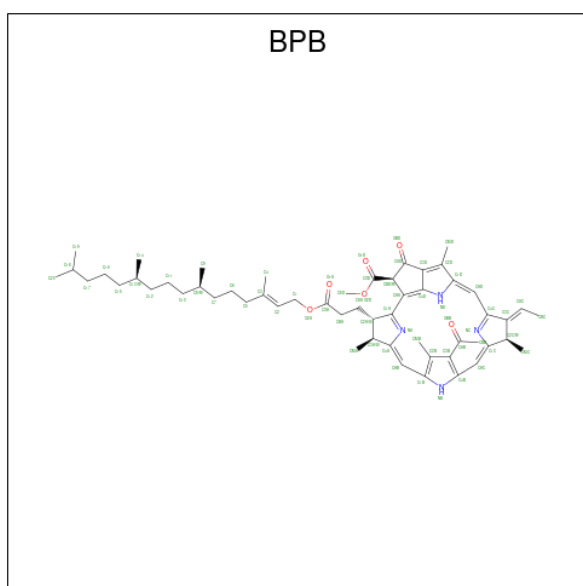
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	
6	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	
6	M	1	Total	C	Mg	N	O	
			65	54	1	4	6	
6	M	1	Total	C	Mg	N	O	
			66	55	1	4	6	

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

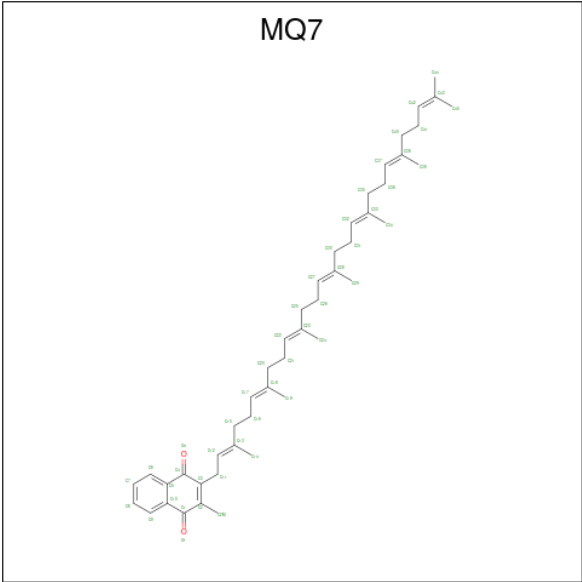


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O		
			65	55	4	6	0	0
7	M	1	Total	C	N	O		
			61	51	4	6	0	0

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



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

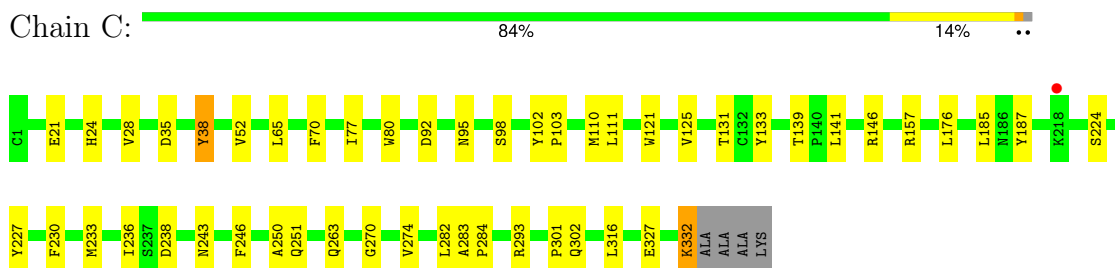
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	1	Total	O	0	0
			1	1		
10	M	1	Total	O	0	0
			1	1		

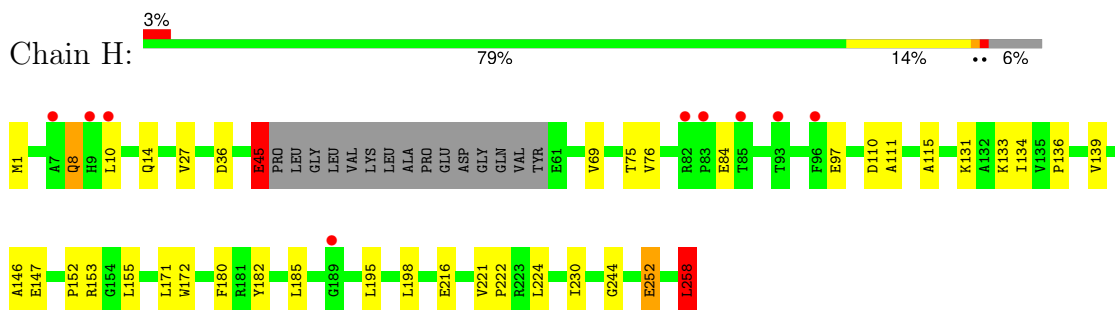
3 Residue-property plots [i](#)

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

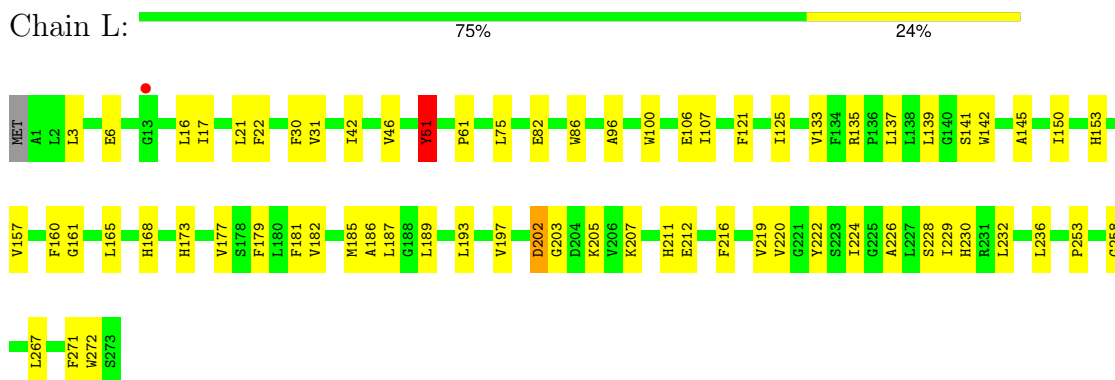
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



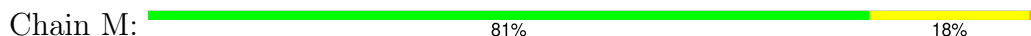
• Molecule 2: REACTION CENTER PROTEIN H CHAIN

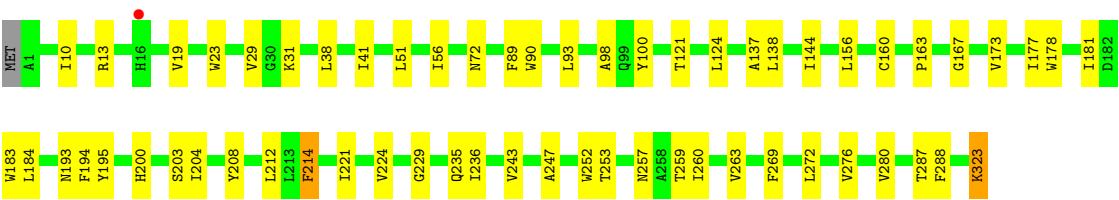


• Molecule 3: REACTION CENTER PROTEIN L CHAIN



• Molecule 4: REACTION CENTER PROTEIN M CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.69Å 143.47Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 3.00 46.18 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (46.18-3.00) 90.6 (46.18-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.79 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.277 , 0.319 0.277 , 0.314	Depositor DCC
R_{free} test set	2049 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	9871	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCB, HEC, BPB, FE2, FME, 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	0.73	1/2669 (0.0%)	0.56	1/3637 (0.0%)
2	H	1.37	7/1939 (0.4%)	0.90	9/2646 (0.3%)
3	L	1.16	2/2291 (0.1%)	1.02	4/3127 (0.1%)
4	M	0.71	2/2659 (0.1%)	0.56	3/3637 (0.1%)
All	All	1.00	12/9558 (0.1%)	0.76	17/13047 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2
3	L	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	51	TYR	CB-CG	42.20	2.15	1.51
2	H	216	GLU	CB-CG	40.41	2.29	1.52
1	C	332	LYS	CB-CG	31.18	2.36	1.52
3	L	202	ASP	CB-CG	29.64	2.13	1.51
2	H	131	LYS	CD-CE	23.83	2.10	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	51	TYR	CB-CG-CD2	-36.12	99.33	121.00
3	L	51	TYR	CB-CG-CD1	28.92	138.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	GLU	CA-CB-CG	-23.31	62.13	113.40
2	H	45	GLU	CG-CD-OE1	-16.25	85.80	118.30
2	H	97	GLU	CB-CG-CD	-13.54	77.64	114.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	252	GLU	Sidechain
2	H	45	GLU	Sidechain
3	L	51	TYR	Sidechain

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	35	0
2	H	1906	0	1903	27	0
3	L	2196	0	2120	59	0
4	M	2555	0	2452	50	0
5	C	172	0	120	16	0
6	L	132	0	144	24	0
6	M	131	0	140	10	0
7	L	65	0	74	6	0
7	M	61	0	63	5	0
8	M	1	0	0	0	0
9	M	48	0	64	3	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
All	All	9871	0	9659	183	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 9.

The worst 5 of 183 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)
3:L:168:HIS:NE2	6:L:1274:BCB:HMC2	1.85	0.92
3:L:177:VAL:HG13	6:L:1274:BCB:HMB3	1.59	0.84
3:L:121:PHE:CE2	3:L:125:ILE:HD11	2.17	0.80
5:C:1334:HEC:HBB3	5:C:1334:HEC:HMB1	1.66	0.76
6:L:1274:BCB:CBB	6:L:1274:BCB:HMB1	2.15	0.75

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%)	304 (92%)	26 (8%)	0	100	100
2	H	239/258 (93%)	221 (92%)	17 (7%)	1 (0%)	34	72
3	L	275/274 (100%)	255 (93%)	18 (6%)	2 (1%)	22	60
4	M	321/324 (99%)	303 (94%)	16 (5%)	2 (1%)	25	64
All	All	1165/1192 (98%)	1083 (93%)	77 (7%)	5 (0%)	34	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE
2	H	153	ARG
4	M	193	ASN
3	L	31	VAL
3	L	133	VAL

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	281/282 (100%)	276 (98%)	5 (2%)	59	85
2	H	200/212 (94%)	196 (98%)	4 (2%)	55	83
3	L	221/219 (101%)	215 (97%)	6 (3%)	44	77
4	M	249/250 (100%)	242 (97%)	7 (3%)	43	77
All	All	951/963 (99%)	929 (98%)	22 (2%)	52	80

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

Mol	Chain	Res	Type
3	L	272	TRP
4	M	194	PHE
4	M	160	CYS
4	M	203	SER
2	H	45	GLU

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

Mol	Chain	Res	Type
2	H	72	HIS
2	H	220	ASN
4	M	257	ASN
4	M	108	HIS
1	C	310	GLN

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	0.80	0	8,9,11	2.86	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
2	FME	H	1	2	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	1	FME	CA-N-CN	-7.14	111.84	122.82
2	H	1	FME	O1-CN-N	-2.38	119.16	125.32
2	H	1	FME	CE-SD-CG	2.15	111.43	100.32

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	C-CA-CB-CG
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	1333	1	32,50,50	2.34	5 (15%)	30,82,82	2.05	7 (23%)
5	HEC	C	1336	1	32,50,50	2.32	6 (18%)	30,82,82	1.32	3 (10%)
6	BCB	M	1325	4	63,74,74	2.88	14 (22%)	72,115,115	2.89	26 (36%)
7	BPB	M	1326	-	45,66,70	2.02	8 (17%)	43,96,101	1.94	12 (27%)
6	BCB	M	1324	-	62,73,74	2.81	16 (25%)	70,113,115	2.89	20 (28%)
9	MQ7	M	1328	-	49,49,49	1.41	2 (4%)	61,63,63	1.32	8 (13%)
5	HEC	C	1334	1	32,50,50	2.27	5 (15%)	30,82,82	1.58	6 (20%)
7	BPB	L	1276	-	49,70,70	1.97	9 (18%)	48,101,101	1.89	12 (25%)
6	BCB	L	1274	3	63,74,74	2.82	13 (20%)	72,115,115	2.67	21 (29%)
6	BCB	L	1275	3	63,74,74	2.71	15 (23%)	72,115,115	2.75	19 (26%)
5	HEC	C	1335	1	32,50,50	2.33	5 (15%)	30,82,82	1.62	5 (16%)

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	1333	1	-	2/10/54/54	-
5	HEC	C	1336	1	-	3/10/54/54	-
6	BCB	M	1325	4	3/3/21/26	16/37/137/137	-
7	BPB	M	1326	-	-	14/33/101/105	0/5/6/6
6	BCB	M	1324	-	3/3/20/26	12/36/136/137	-
9	MQ7	M	1328	-	-	3/41/61/61	0/2/2/2
5	HEC	C	1334	1	-	5/10/54/54	-
7	BPB	L	1276	-	-	12/37/105/105	0/5/6/6
6	BCB	L	1274	3	3/3/21/26	7/37/137/137	-
6	BCB	L	1275	3	3/3/21/26	10/37/137/137	-
5	HEC	C	1335	1	-	2/10/54/54	-

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1325	BCB	CHC-C1C	16.73	1.48	1.33
6	L	1274	BCB	CHC-C1C	16.64	1.48	1.33
6	M	1324	BCB	CHC-C1C	15.95	1.48	1.33
6	L	1275	BCB	CHC-C1C	15.18	1.47	1.33
9	M	1328	MQ7	C3-C2	7.65	1.48	1.35

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1324	BCB	C1C-NC-C4C	-15.28	99.71	106.68
6	M	1325	BCB	C1C-NC-C4C	-15.28	99.71	106.68
6	L	1275	BCB	C1C-NC-C4C	-14.96	99.85	106.68
6	L	1274	BCB	C1C-NC-C4C	-13.70	100.43	106.68
7	L	1276	BPB	O2D-CGD-CBD	8.65	120.45	110.95

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1274	BCB	NC
6	L	1274	BCB	NA
6	L	1274	BCB	ND
6	L	1275	BCB	NC
6	L	1275	BCB	NA

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1336	HEC	C3D-CAD-CBD-CGD
6	L	1274	BCB	C2C-C3C-CAC-CBC
6	L	1274	BCB	C4C-C3C-CAC-CBC
6	L	1275	BCB	C2C-C3C-CAC-CBC
6	L	1275	BCB	C4C-C3C-CAC-CBC

There are no ring outliers.

11 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1333	HEC	2	0
5	C	1336	HEC	3	0
6	M	1325	BCB	7	0
7	M	1326	BPB	5	0

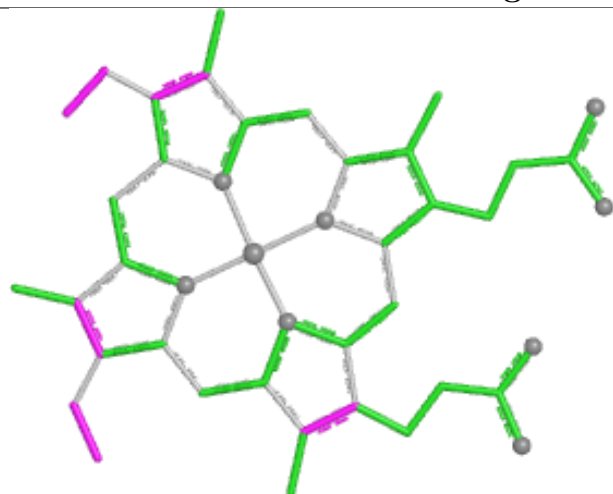
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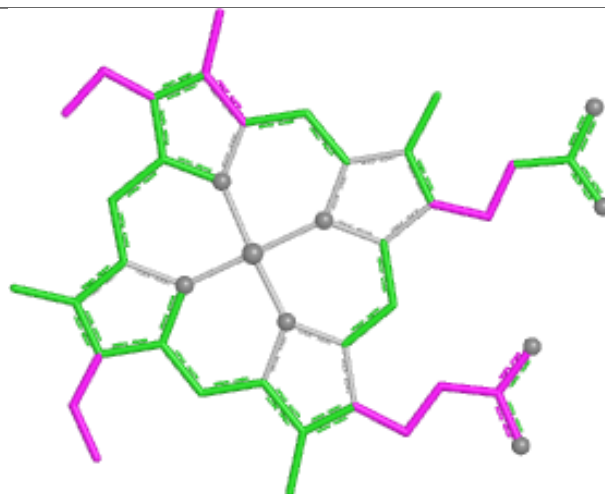
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1324	BCB	3	0
9	M	1328	MQ7	3	0
5	C	1334	HEC	9	0
7	L	1276	BPB	6	0
6	L	1274	BCB	13	0
6	L	1275	BCB	11	0
5	C	1335	HEC	2	0

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

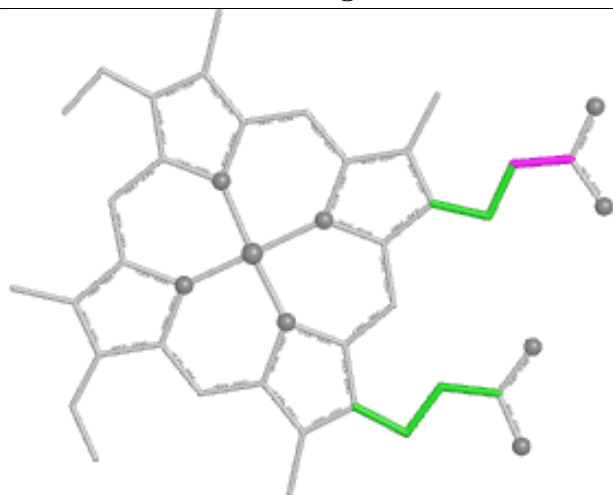
Ligand HEC C 1333



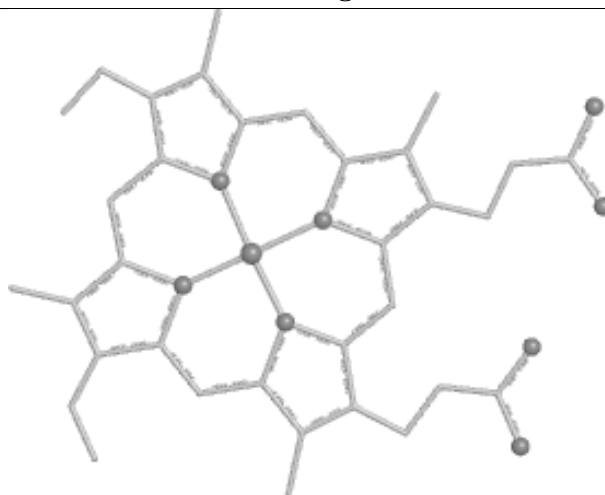
Bond lengths



Bond angles

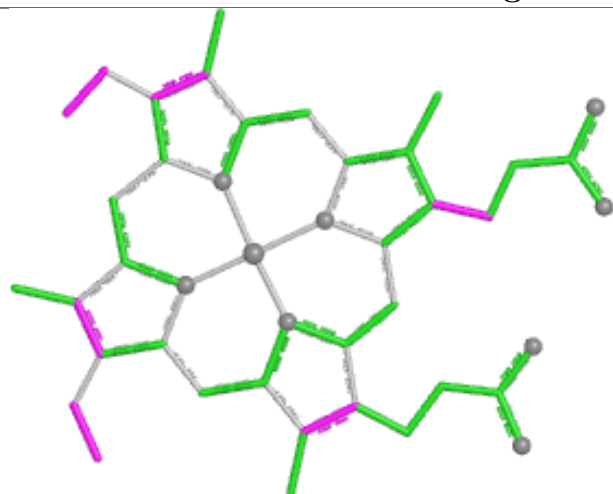


Torsions

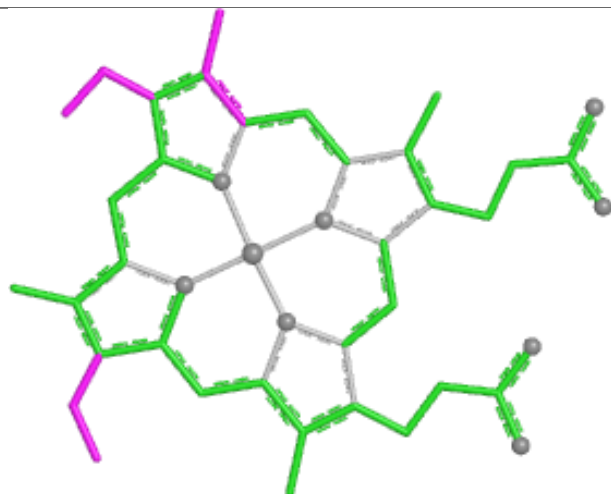


Rings

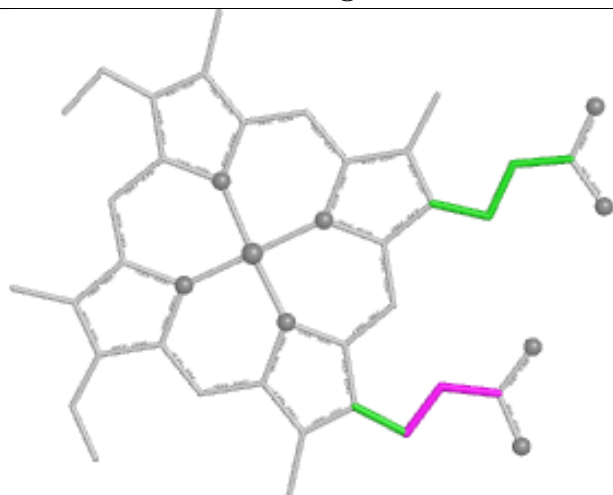
Ligand HEC C 1336



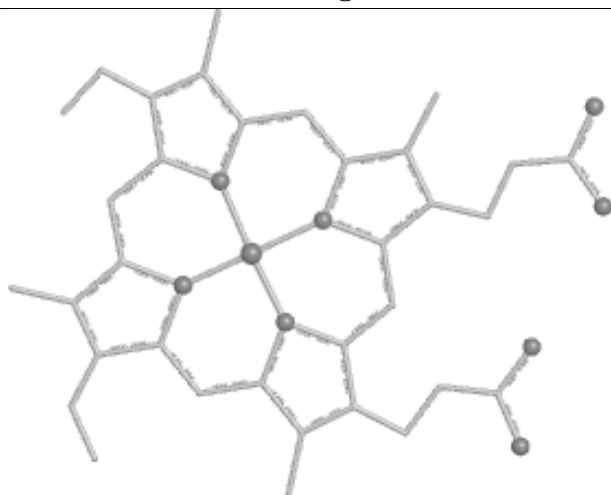
Bond lengths



Bond angles

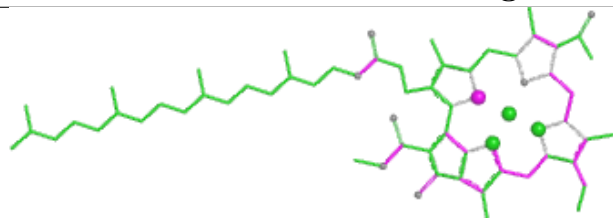


Torsions

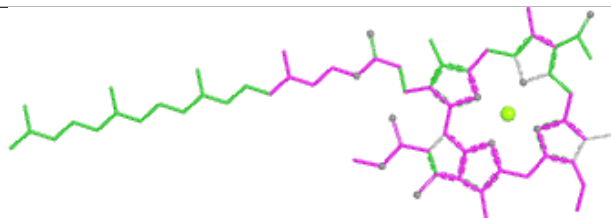


Rings

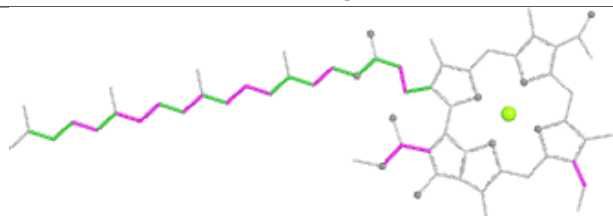
Ligand BCB M 1325



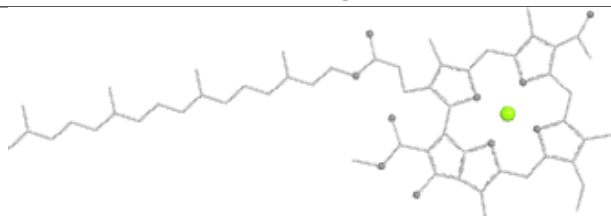
Bond lengths



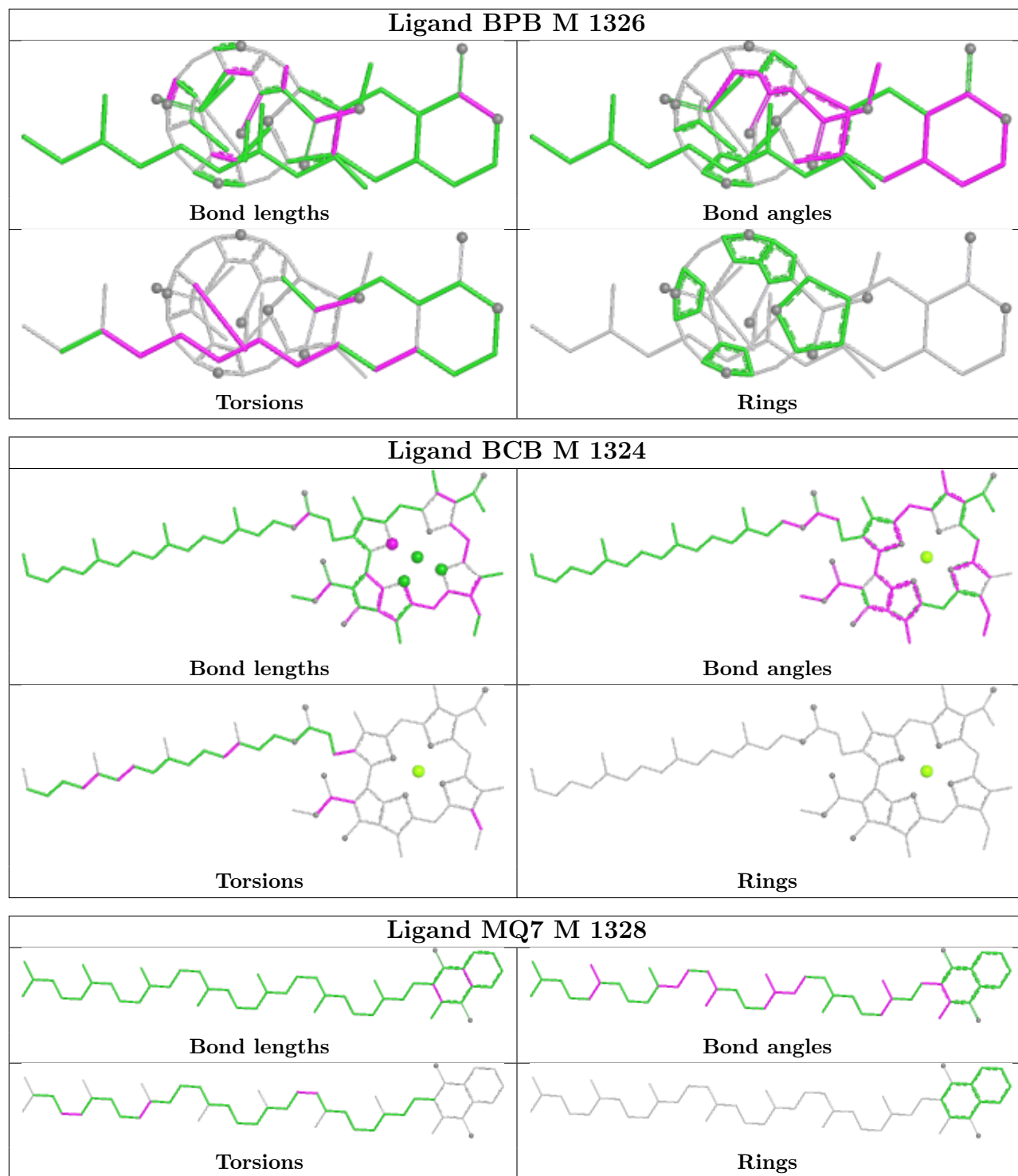
Bond angles



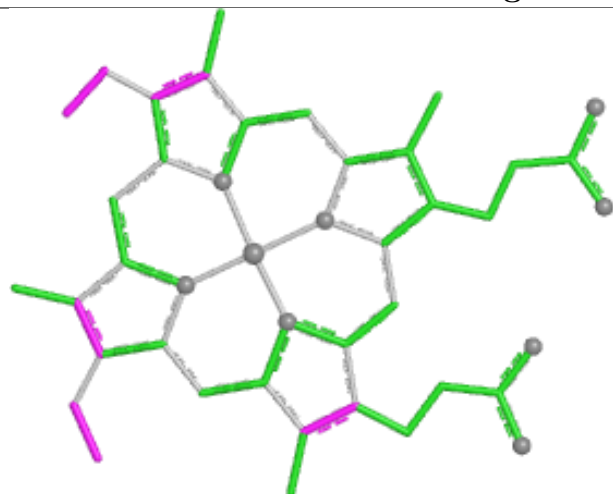
Torsions



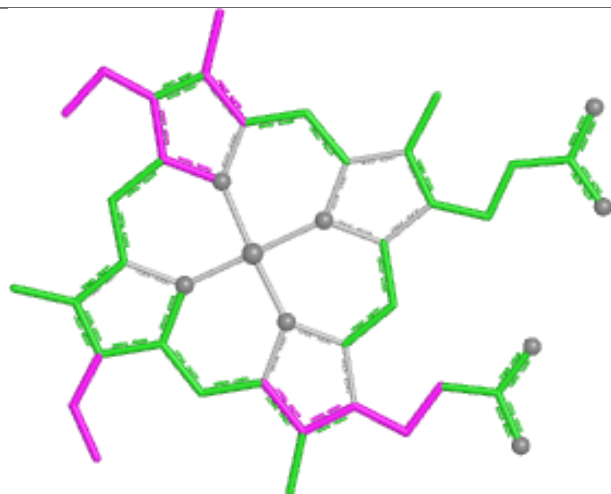
Rings



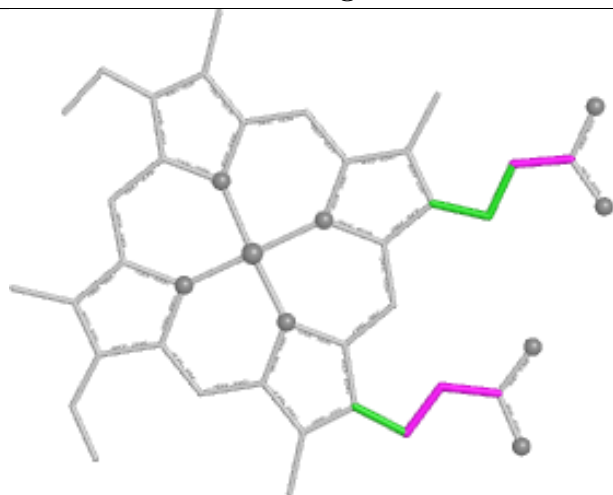
Ligand HEC C 1334



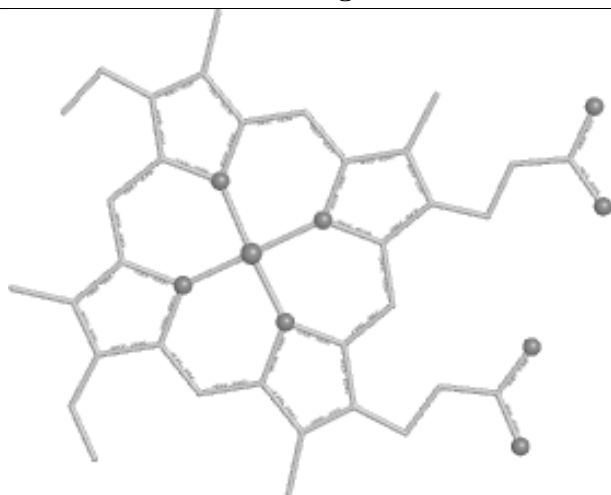
Bond lengths



Bond angles

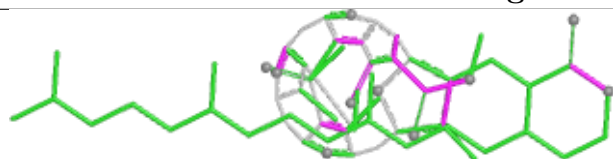


Torsions

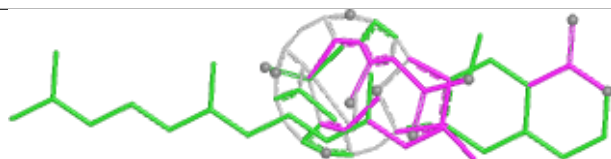


Rings

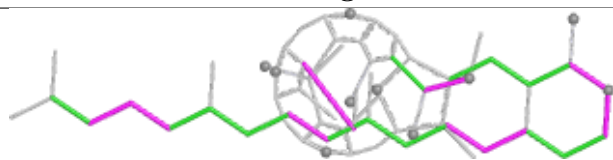
Ligand BPB L 1276



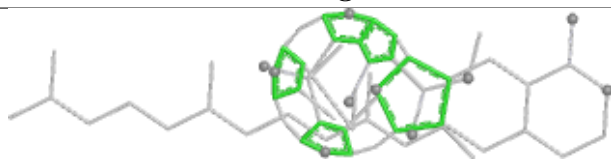
Bond lengths



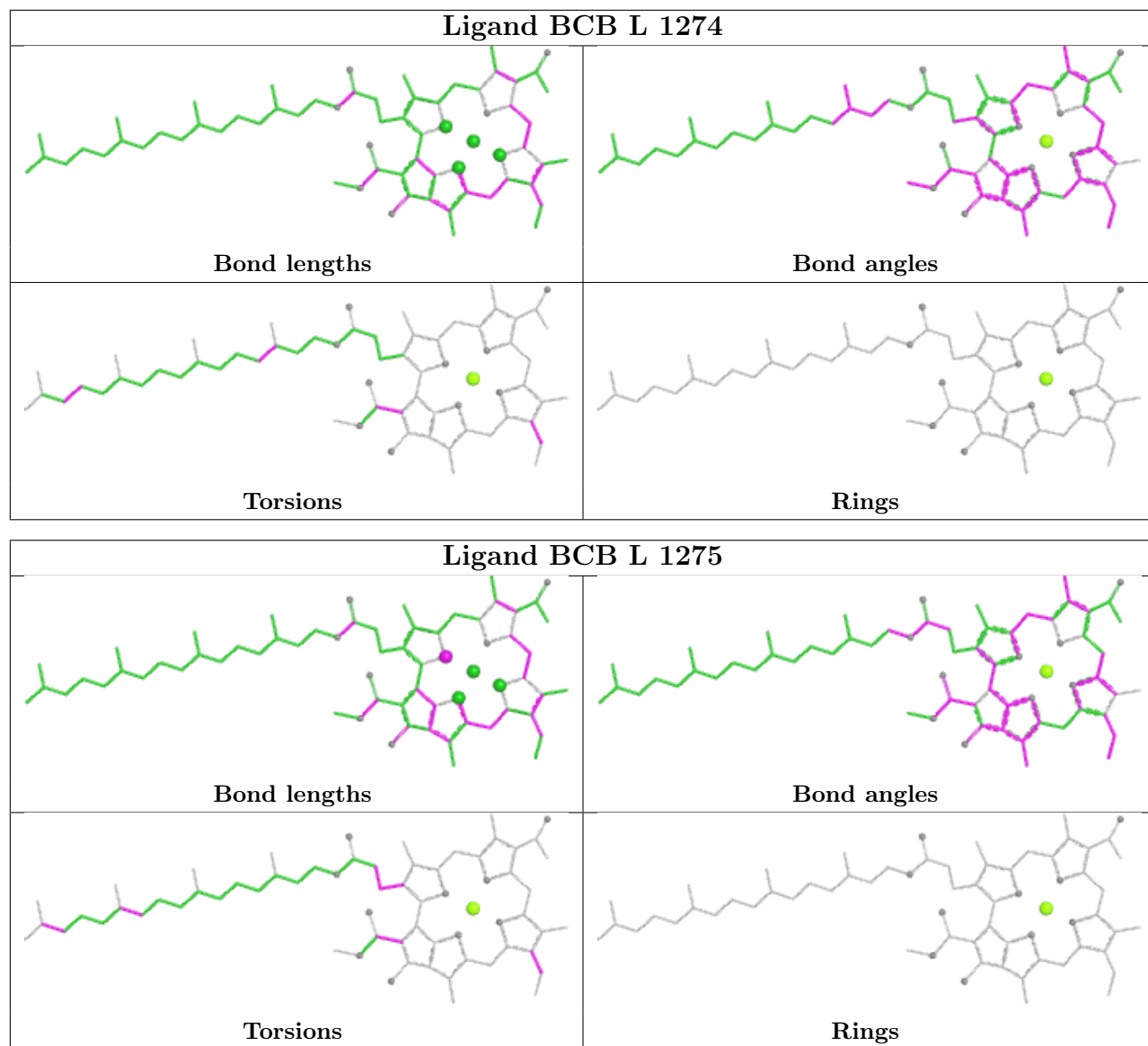
Bond angles

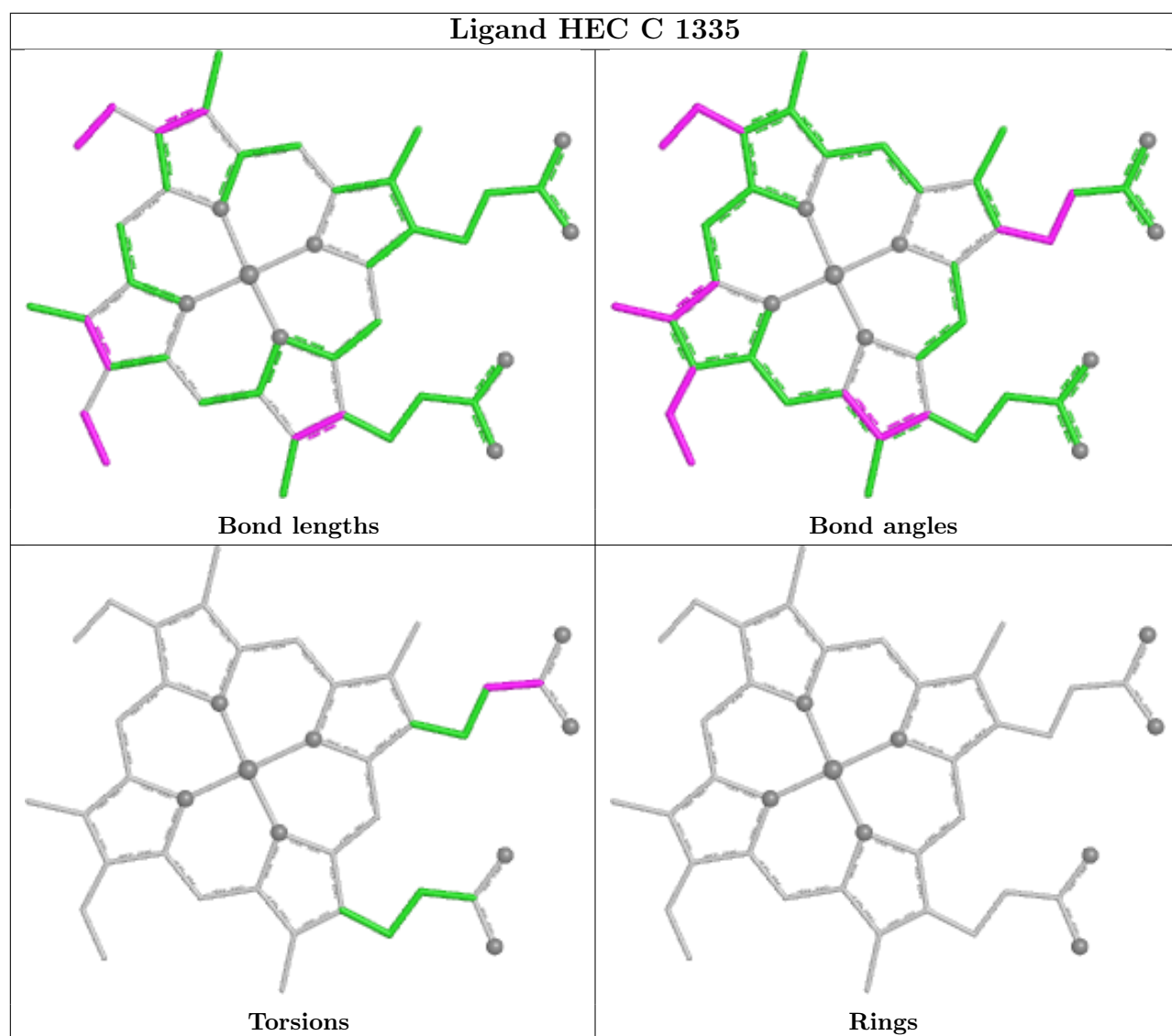


Torsions



Rings





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%)	-0.25	1 (0%) 94 84	18, 31, 45, 51	1 (0%)
2	H	242/258 (93%)	0.11	9 (3%) 41 17	29, 40, 65, 68	8 (3%)
3	L	273/274 (99%)	-0.26	1 (0%) 92 79	16, 28, 49, 57	2 (0%)
4	M	323/324 (99%)	-0.38	1 (0%) 94 84	16, 26, 41, 44	2 (0%)
All	All	1170/1192 (98%)	-0.21	12 (1%) 82 59	16, 32, 51, 68	13 (1%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	93	THR	3.8
2	H	85	THR	3.8
2	H	83	PRO	3.2
2	H	9	HIS	2.9
3	L	13	GLY	2.9

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	0.73	0.35	67,67,68,68	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

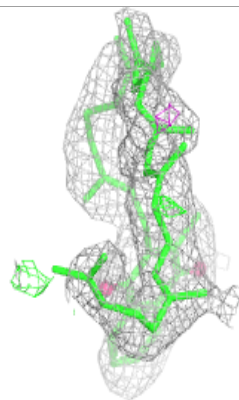
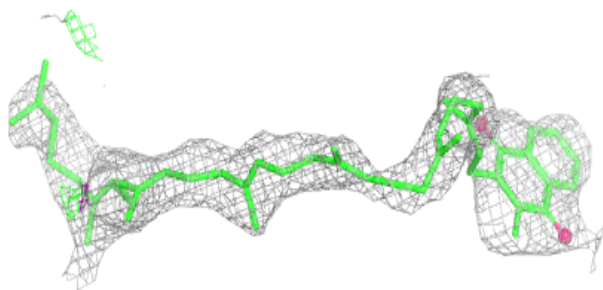
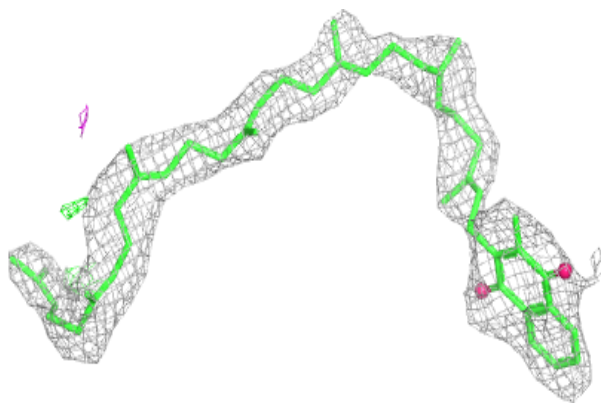
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MQ7	M	1328	48/48	0.87	0.26	39,41,47,48	0
6	BCB	M	1324	65/66	0.89	0.23	18,20,48,49	0
7	BPB	M	1326	61/65	0.90	0.25	19,24,44,45	0
7	BPB	L	1276	65/65	0.91	0.21	23,28,33,35	0
6	BCB	L	1275	66/66	0.92	0.19	18,21,28,28	0
6	BCB	M	1325	66/66	0.93	0.20	15,18,26,27	0
5	HEC	C	1334	43/43	0.93	0.23	27,29,34,36	0
5	HEC	C	1336	43/43	0.94	0.19	25,28,33,34	0
6	BCB	L	1274	66/66	0.94	0.18	10,12,20,21	0
5	HEC	C	1333	43/43	0.95	0.16	25,32,33,34	0
5	HEC	C	1335	43/43	0.96	0.16	20,21,23,24	0
8	FE2	M	1327	1/1	0.99	0.10	24,24,24,24	0

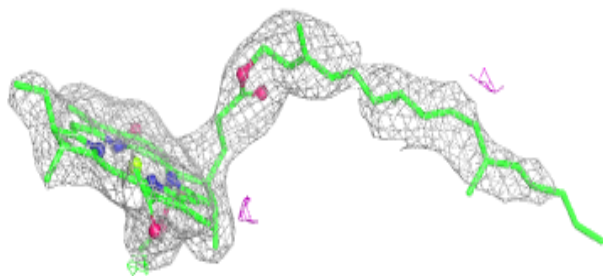
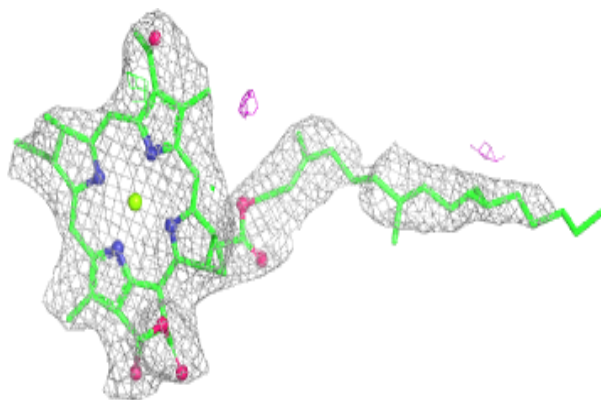
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MQ7 M 1328:

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

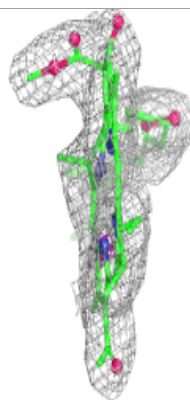
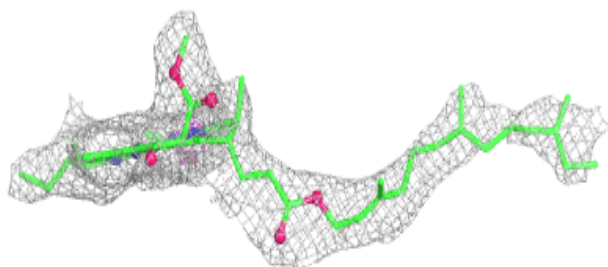
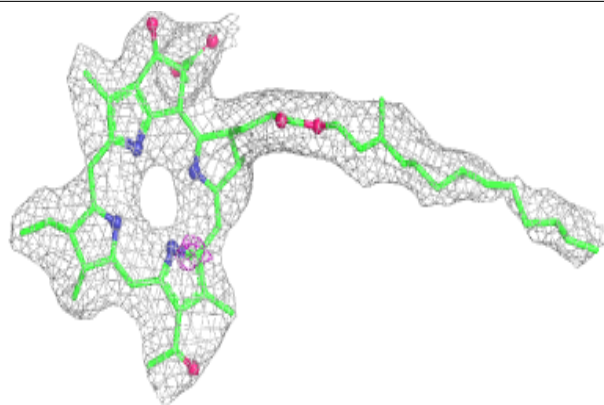
**Electron density around BCB M 1324:**

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

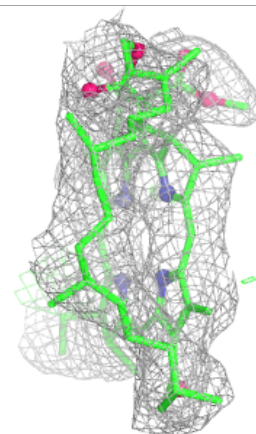
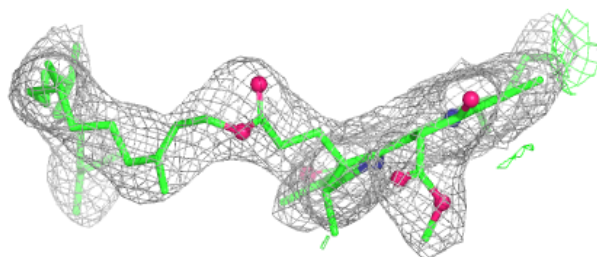
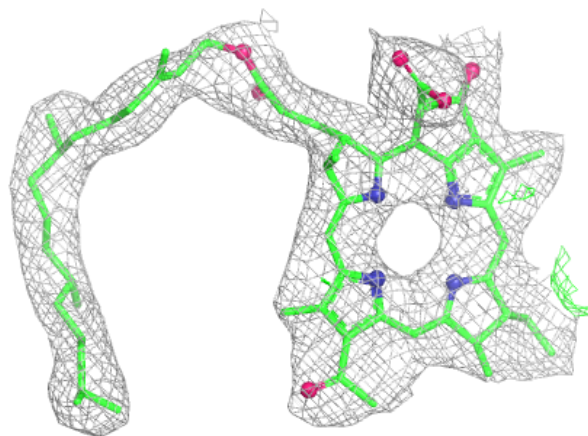


Electron density around BPB M 1326:

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

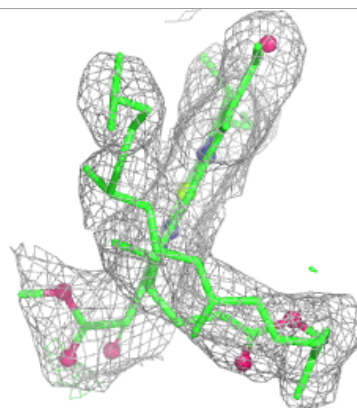
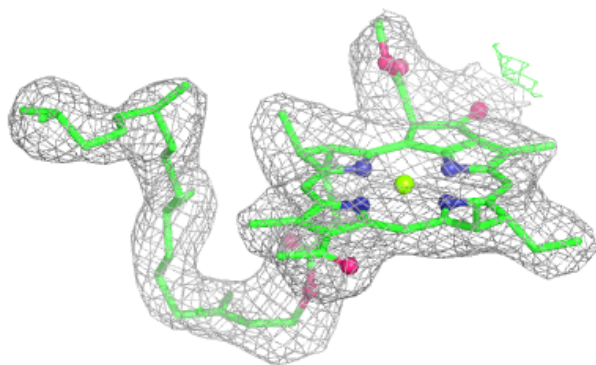
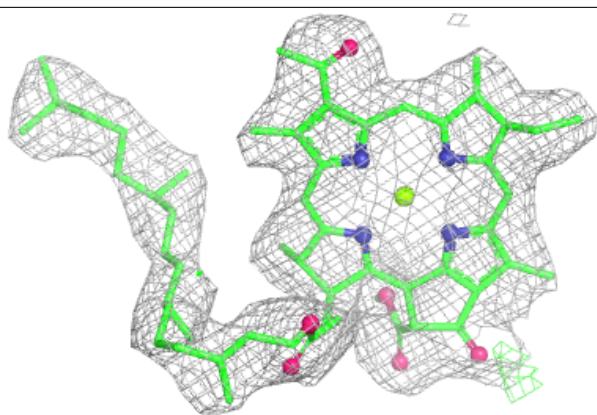
**Electron density around BPB L 1276:**

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and green (positive)

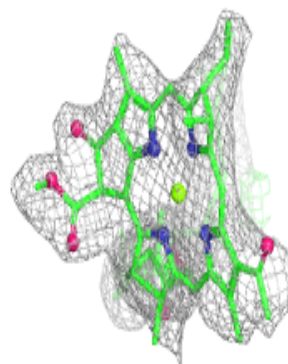
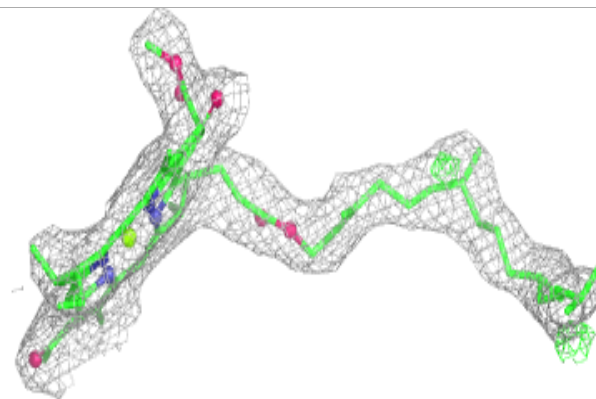
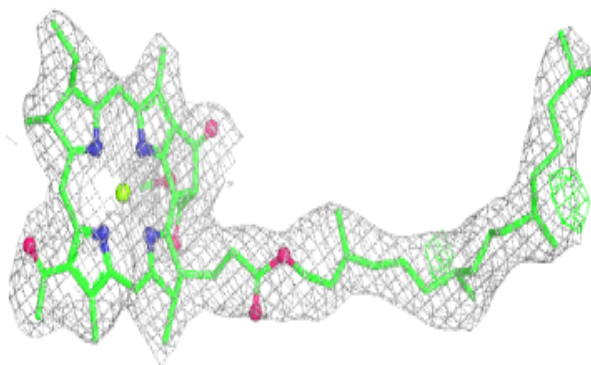


Electron density around BCB L 1275:

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and green (positive)

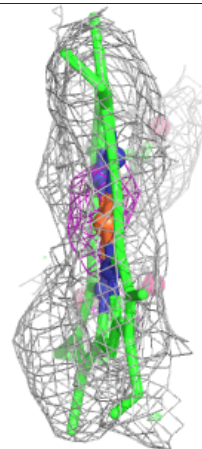
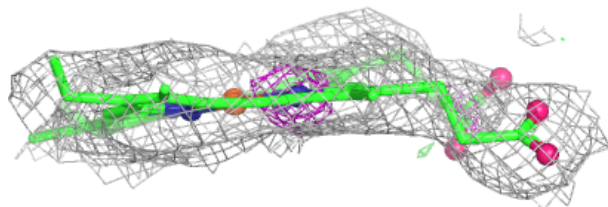
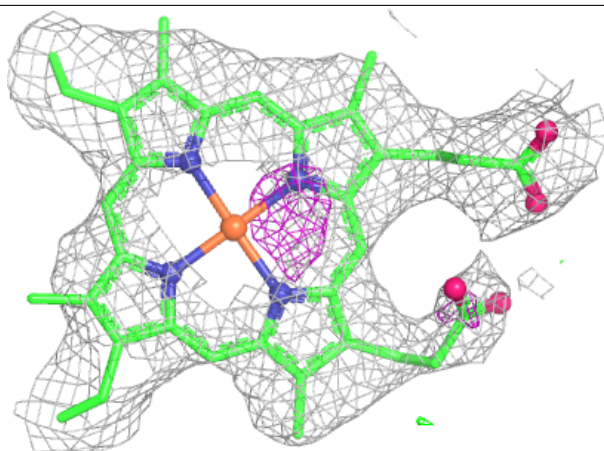
**Electron density around BCB M 1325:**

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and green (positive)



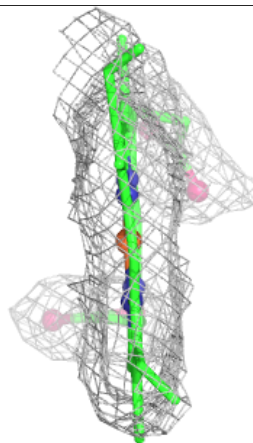
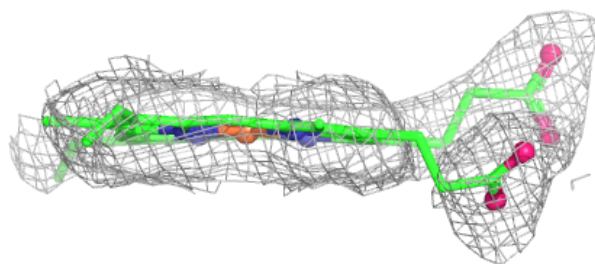
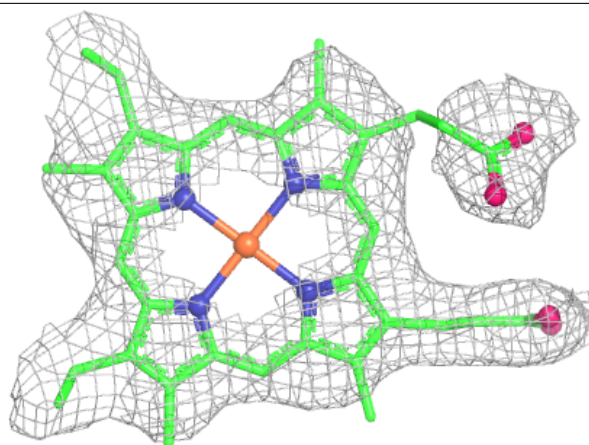
Electron density around HEC C 1334:

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and green (positive)

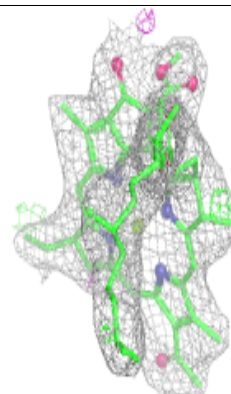
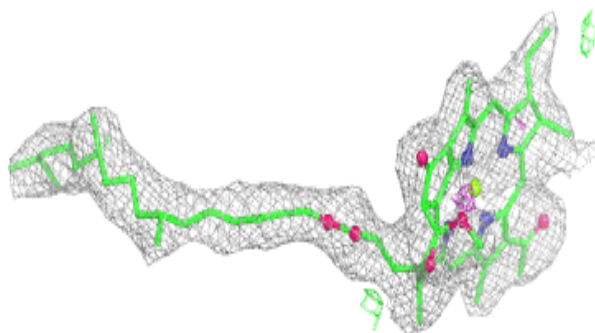
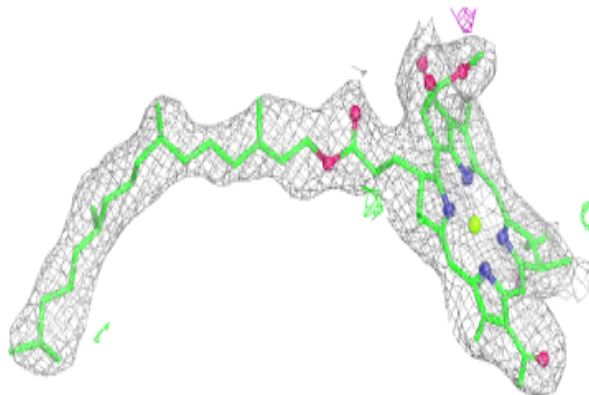


Electron density around HEC C 1336:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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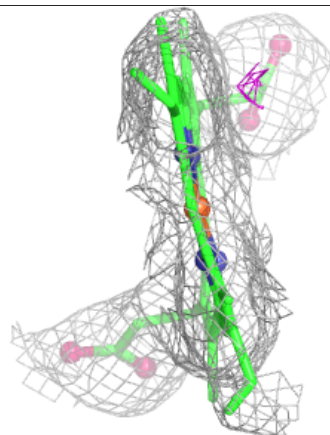
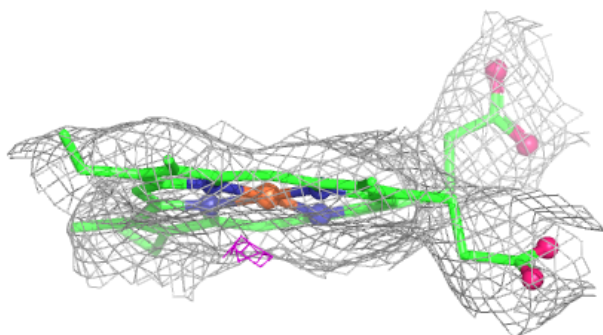
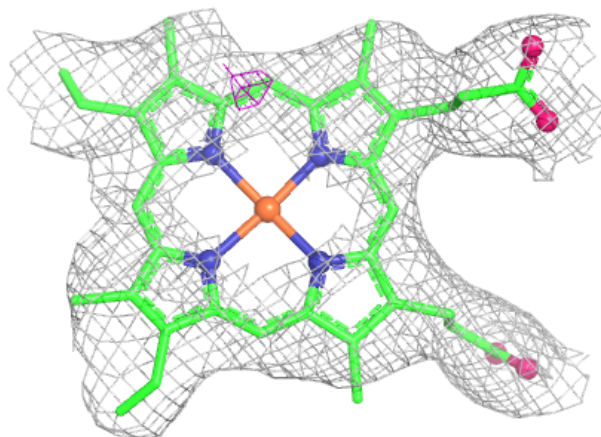
**Electron density around BCB L 1274:**

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and green (positive)



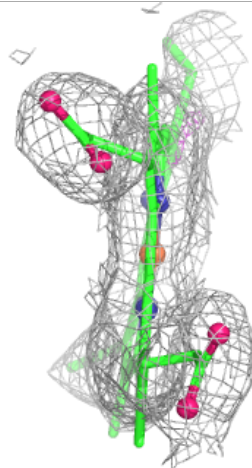
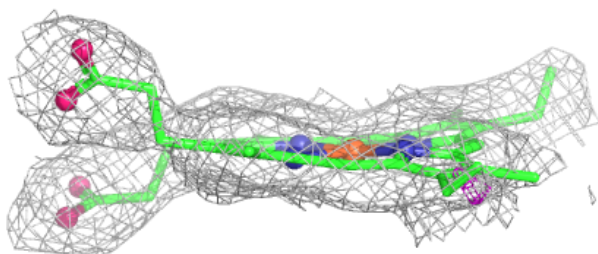
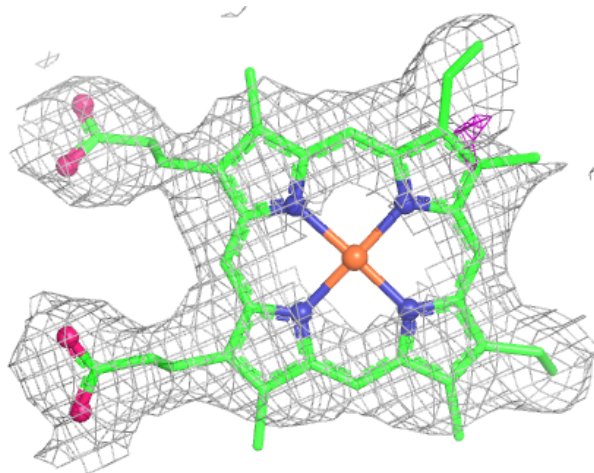
Electron density around HEC C 1333:

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



Electron density around HEC C 1335:

$2mF_o-DF_c$ (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.