Full wwPDB X-ray Structure Validation Report (i)

Jun 30, 2022 – 12:08 PM EDT

PDB ID	:	6UW2
Title	:	Clotrimazole bound complex of Acanthamoeba castellanii CYP51
Authors	:	Sharma, V.; Podust, L.M.
Deposited on	:	2019-11-04
Resolution	:	2.92 Å(reported)

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

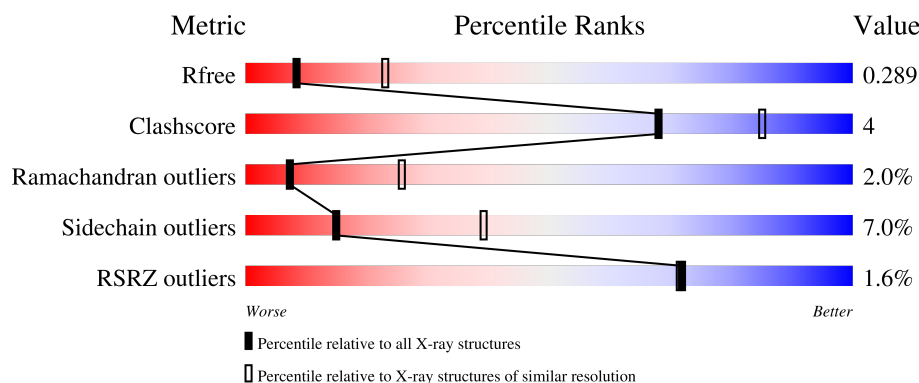|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.92 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.289
Clashscore		4
Ramachandran outliers		2.0%
Sidechain outliers		7.0%
RSRZ outliers		1.6%

Worse   *Better*

█ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	460	80% 16% • •
1	B	460	85% 11% • •
1	C	460	3% 81% 14% • •
1	D	460	2% 82% 13% • •
1	E	460	2% 85% 11% • •

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Mol	Chain	Length	Quality of chain
1	F	460	3% 85% 11%

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
4	GAI	C	503	-	X	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 21601 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 Obtusifoliol 14alphademethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3543	2291	591	643	18			
1	B	447	Total	C	N	O	S	0	0	0
			3528	2282	580	648	18			
1	C	446	Total	C	N	O	S	0	0	0
			3460	2239	577	627	17			
1	D	447	Total	C	N	O	S	0	0	0
			3531	2287	586	640	18			
1	E	448	Total	C	N	O	S	0	0	0
			3545	2295	591	641	18			
1	F	448	Total	C	N	O	S	0	0	0
			3528	2284	586	640	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP L8GJB3
A	34	ALA	-	expression tag	UNP L8GJB3
A	35	LYS	-	expression tag	UNP L8GJB3
A	36	LYS	-	expression tag	UNP L8GJB3
A	37	THR	-	expression tag	UNP L8GJB3
A	38	SER	-	expression tag	UNP L8GJB3
A	39	SER	-	expression tag	UNP L8GJB3
A	40	LYS	-	expression tag	UNP L8GJB3
A	41	GLY	-	expression tag	UNP L8GJB3
A	42	LYS	-	expression tag	UNP L8GJB3
A	487	HIS	-	expression tag	UNP L8GJB3
A	488	HIS	-	expression tag	UNP L8GJB3
A	489	HIS	-	expression tag	UNP L8GJB3
A	490	HIS	-	expression tag	UNP L8GJB3
A	491	HIS	-	expression tag	UNP L8GJB3
A	492	HIS	-	expression tag	UNP L8GJB3
B	33	MET	-	expression tag	UNP L8GJB3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ALA	-	expression tag	UNP L8GJB3
B	35	LYS	-	expression tag	UNP L8GJB3
B	36	LYS	-	expression tag	UNP L8GJB3
B	37	THR	-	expression tag	UNP L8GJB3
B	38	SER	-	expression tag	UNP L8GJB3
B	39	SER	-	expression tag	UNP L8GJB3
B	40	LYS	-	expression tag	UNP L8GJB3
B	41	GLY	-	expression tag	UNP L8GJB3
B	42	LYS	-	expression tag	UNP L8GJB3
B	487	HIS	-	expression tag	UNP L8GJB3
B	488	HIS	-	expression tag	UNP L8GJB3
B	489	HIS	-	expression tag	UNP L8GJB3
B	490	HIS	-	expression tag	UNP L8GJB3
B	491	HIS	-	expression tag	UNP L8GJB3
B	492	HIS	-	expression tag	UNP L8GJB3
C	33	MET	-	expression tag	UNP L8GJB3
C	34	ALA	-	expression tag	UNP L8GJB3
C	35	LYS	-	expression tag	UNP L8GJB3
C	36	LYS	-	expression tag	UNP L8GJB3
C	37	THR	-	expression tag	UNP L8GJB3
C	38	SER	-	expression tag	UNP L8GJB3
C	39	SER	-	expression tag	UNP L8GJB3
C	40	LYS	-	expression tag	UNP L8GJB3
C	41	GLY	-	expression tag	UNP L8GJB3
C	42	LYS	-	expression tag	UNP L8GJB3
C	487	HIS	-	expression tag	UNP L8GJB3
C	488	HIS	-	expression tag	UNP L8GJB3
C	489	HIS	-	expression tag	UNP L8GJB3
C	490	HIS	-	expression tag	UNP L8GJB3
C	491	HIS	-	expression tag	UNP L8GJB3
C	492	HIS	-	expression tag	UNP L8GJB3
D	33	MET	-	expression tag	UNP L8GJB3
D	34	ALA	-	expression tag	UNP L8GJB3
D	35	LYS	-	expression tag	UNP L8GJB3
D	36	LYS	-	expression tag	UNP L8GJB3
D	37	THR	-	expression tag	UNP L8GJB3
D	38	SER	-	expression tag	UNP L8GJB3
D	39	SER	-	expression tag	UNP L8GJB3
D	40	LYS	-	expression tag	UNP L8GJB3
D	41	GLY	-	expression tag	UNP L8GJB3
D	42	LYS	-	expression tag	UNP L8GJB3
D	487	HIS	-	expression tag	UNP L8GJB3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	488	HIS	-	expression tag	UNP L8GJB3
D	489	HIS	-	expression tag	UNP L8GJB3
D	490	HIS	-	expression tag	UNP L8GJB3
D	491	HIS	-	expression tag	UNP L8GJB3
D	492	HIS	-	expression tag	UNP L8GJB3
E	33	MET	-	expression tag	UNP L8GJB3
E	34	ALA	-	expression tag	UNP L8GJB3
E	35	LYS	-	expression tag	UNP L8GJB3
E	36	LYS	-	expression tag	UNP L8GJB3
E	37	THR	-	expression tag	UNP L8GJB3
E	38	SER	-	expression tag	UNP L8GJB3
E	39	SER	-	expression tag	UNP L8GJB3
E	40	LYS	-	expression tag	UNP L8GJB3
E	41	GLY	-	expression tag	UNP L8GJB3
E	42	LYS	-	expression tag	UNP L8GJB3
E	487	HIS	-	expression tag	UNP L8GJB3
E	488	HIS	-	expression tag	UNP L8GJB3
E	489	HIS	-	expression tag	UNP L8GJB3
E	490	HIS	-	expression tag	UNP L8GJB3
E	491	HIS	-	expression tag	UNP L8GJB3
E	492	HIS	-	expression tag	UNP L8GJB3
F	33	MET	-	expression tag	UNP L8GJB3
F	34	ALA	-	expression tag	UNP L8GJB3
F	35	LYS	-	expression tag	UNP L8GJB3
F	36	LYS	-	expression tag	UNP L8GJB3
F	37	THR	-	expression tag	UNP L8GJB3
F	38	SER	-	expression tag	UNP L8GJB3
F	39	SER	-	expression tag	UNP L8GJB3
F	40	LYS	-	expression tag	UNP L8GJB3
F	41	GLY	-	expression tag	UNP L8GJB3
F	42	LYS	-	expression tag	UNP L8GJB3
F	487	HIS	-	expression tag	UNP L8GJB3
F	488	HIS	-	expression tag	UNP L8GJB3
F	489	HIS	-	expression tag	UNP L8GJB3
F	490	HIS	-	expression tag	UNP L8GJB3
F	491	HIS	-	expression tag	UNP L8GJB3
F	492	HIS	-	expression tag	UNP L8GJB3

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
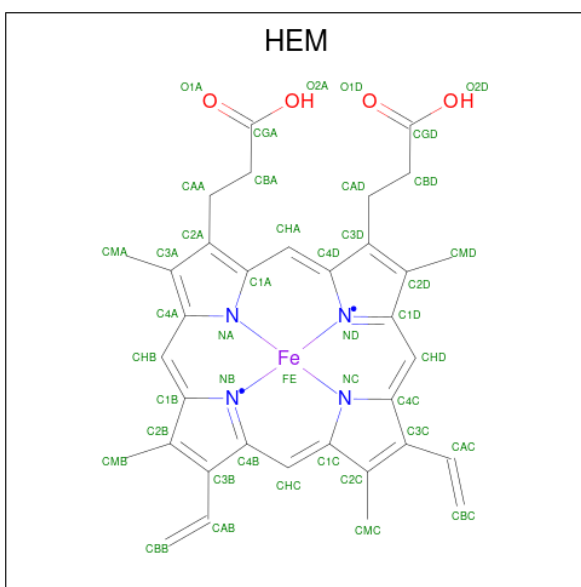
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-[(2-CHLOROPHENYL)(DIPHENYL)METHYL]-1H-IMIDAZOLE (three-letter code: CL6) (formula: $C_{22}H_{17}ClN_2$) (labeled as "Ligand of Interest" by depositor).
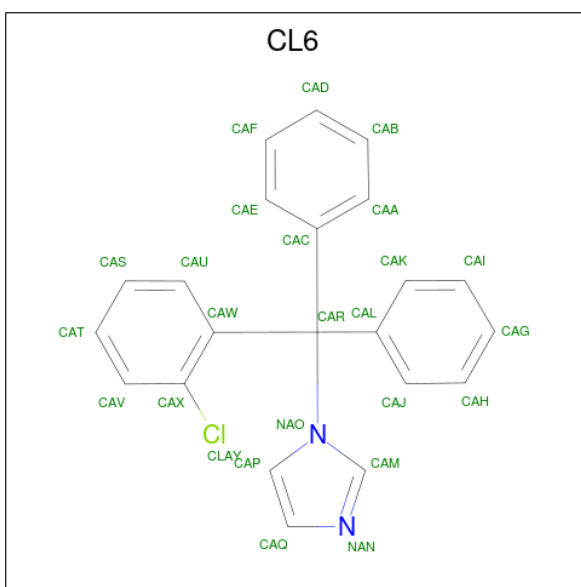
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	E	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	F	1	Total	C	Cl	N	0	0
			25	22	1	2		

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).
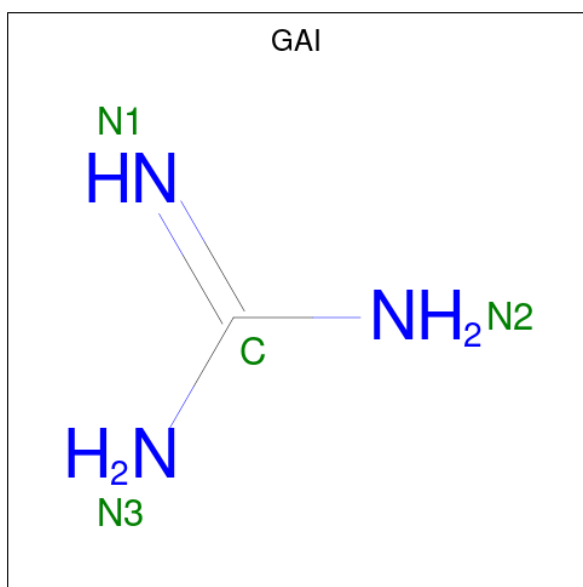
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 4	C 1	N 3	0	0
4	C	1	Total 4	C 1	N 3	0	0
4	F	1	Total 4	C 1	N 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	10	Total 10	O 10	0	0
5	C	12	Total 12	O 12	0	0
5	D	9	Total 9	O 9	0	0
5	E	4	Total 4	O 4	0	0
5	F	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
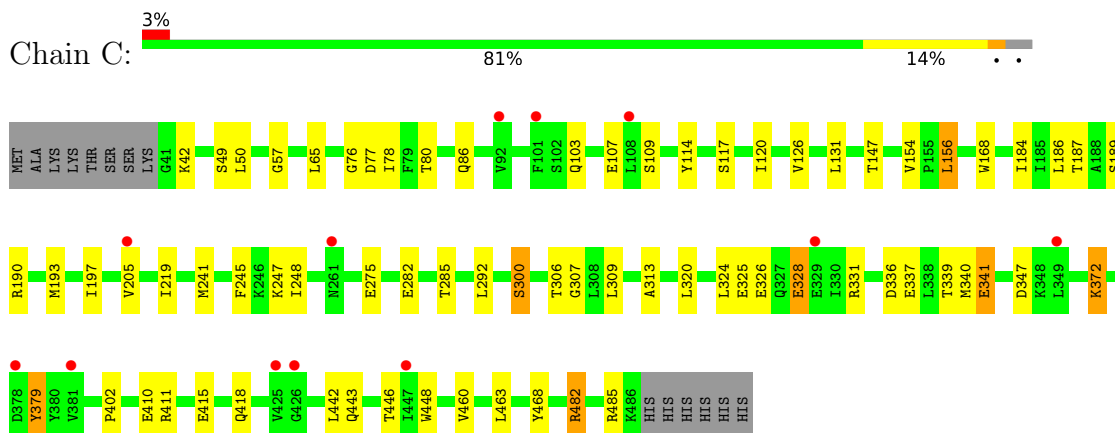
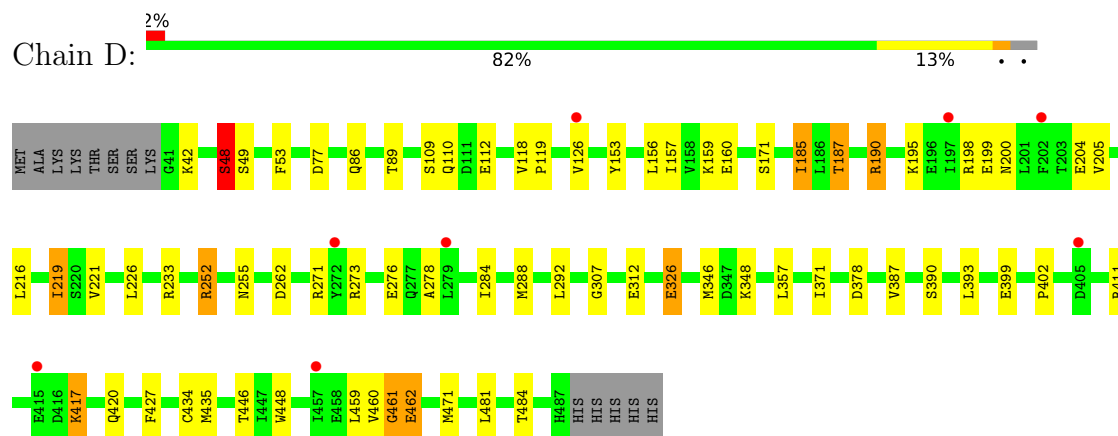• Molecule 1: Obtusifoliol 14alphademethylase

Chain A:

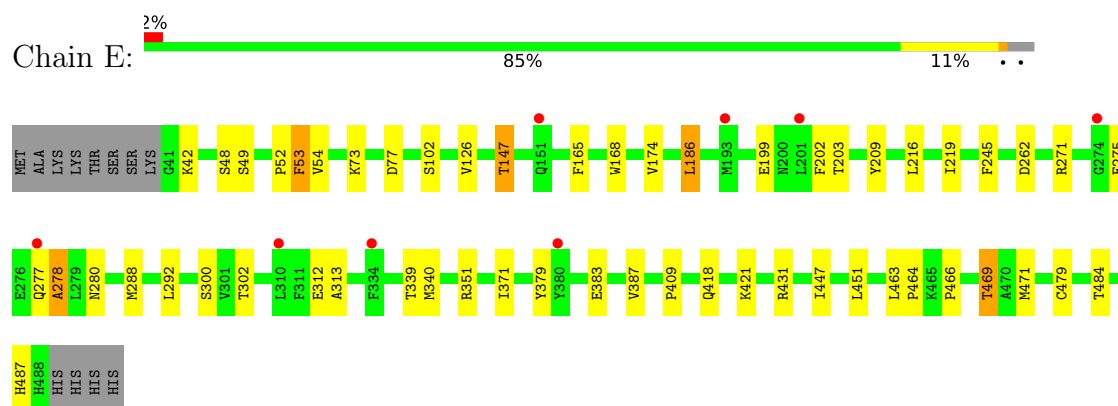• Molecule 1: Obtusifoliol 14alphademethylase

Chain B:

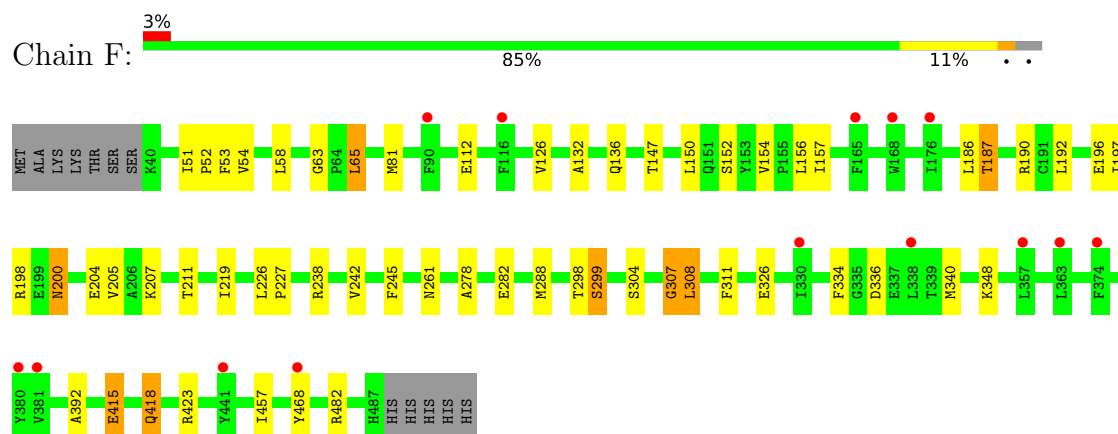• Molecule 1: Obtusifoliol 14alphademethylase

Chain C:

• Molecule 1: Obtusifoliol 14alphademethylase

Chain D:

2%

82% 13%

MET ALA LYS THR SER SER LYS G41 K42 S49 F53 D77 Q86 T89 S109 Q110 D111 E112 V118 P119 V126 Y153 L156 I157 V158 K159 E160 S171 I185 L186 T187 R190 K195 E196 I197 R198 E199 N200 L201 F202 T203 E204 V205

L216 I219 S220 V221 L226 R233 R252 N255 D262 R271 Y272 R273 E276 Q277 A278 L279 I284 M288 L292 G307 E312 E326 M346 D347 K348 L357 I371 D378 V387 S390 L393 E399 P402 D405 R411

E415 D416 K417 Q420 F427 C434 M435 T446 I447 W448 I457 E458 L459 V460 G461 E462 M471 L481 T484 H487 HIS HIS HIS HIS

• Molecule 1: Obtusifoliol 14alphademethylase

Chain E:

2%

85% 11%

MET ALA LYS LYS THR SER SER LYS G41 K42 S48 S49 P52 F53 V54 K73 D77 S102 V126 T147 Q151 F165 W168 V174 L186 M193 E199 N200 L201 F202 T203 Y209 L216 I219 F245 D262 R271 G274 E275

E276 Q277 A278 L279 N280 M288 L292 S300 V301 T302 L310 F311 E312 A313 F334 T339 M340 R351 I371 Y379 Y380 E383 V387 P409 Q418 K421 R431 I447 L451 L463 P464 K465 P466 T469 A470 M471 C479 T484

H487 H488 HIS HIS HIS

• Molecule 1: Obtusifoliol 14alphademethylase

Chain F:

3%

85% 11%

MET ALA LYS THR SER SER K40 I51 P52 F53 V54 L58 G63 P64 L65 M81 F90 E112 F116 V126 A132 Q136 T147 L150 Q151 S152 Y153 V154 P155 L156 I157 F165 W168 I176 L186 T187 R190 C191 L192 E196 I197

R198 E199 N200 E204 V205 A206 K207 T211 I219 L226 P227 R238 V242 F245 N261 A278 E282 M288 T298 S299 S304 G307 L308 F311 E326 I330 F334 G335 D336 E337 L338 T339 M340 K348 L357 L363 F374

Y380 V381 A392 E415 Q418 R423 Y441 I457 Y468 R482 H487 HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.98Å 177.22Å 181.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.13 – 2.92 126.81 – 2.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (127.13-2.92) 100.0 (126.81-2.92)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.209 , 0.290 0.212 , 0.289	Depositor DCC
R_{free} test set	4043 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21601	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CL6, GAI

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	A	0.55	0/3631	0.75	0/4922
1	B	0.52	0/3615	0.74	0/4900
1	C	0.55	0/3548	0.75	0/4822
1	D	0.52	0/3619	0.73	0/4903
1	E	0.52	0/3633	0.72	0/4922
1	F	0.55	0/3615	0.72	0/4900
All	All	0.53	0/21661	0.74	0/29369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	3543	0	3469	27	0
1	B	3528	0	3458	18	0
1	C	3460	0	3332	22	0
1	D	3531	0	3480	24	0
1	E	3545	0	3498	19	0
1	F	3528	0	3469	22	0
2	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	25	0	17	1	0
3	B	25	0	17	4	0
3	C	25	0	17	3	0
3	D	25	0	17	4	0
3	E	25	0	17	3	0
3	F	25	0	17	2	0
4	B	4	0	4	0	0
4	C	4	0	5	0	0
4	F	4	0	4	0	0
5	A	4	0	0	0	0
5	B	10	0	0	0	0
5	C	12	0	0	0	0
5	D	9	0	0	0	0
5	E	4	0	0	0	0
5	F	7	0	0	0	0
All	All	21601	0	21001	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ILE:HD11	1:D:226:LEU:HD22	1.72	0.70
1:A:297:HIS:CD2	1:A:472:VAL:HG22	2.27	0.70
1:B:125:VAL:HG12	1:B:126:VAL:HG23	1.79	0.65
1:A:412:PHE:HA	1:A:415:GLU:HB3	1.81	0.63
1:A:183:LEU:O	1:A:187:THR:HG23	2.00	0.60
1:A:200:ASN:HD22	1:A:200:ASN:N	2.00	0.60
1:A:403:ASN:HB3	1:A:406:GLN:HG3	1.84	0.59
1:D:252:ARG:NH2	1:D:262:ASP:OD2	2.37	0.58
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.84	0.58
1:B:186:LEU:HD12	1:B:202:PHE:CE1	2.39	0.57
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.86	0.57
1:D:109:SER:HB3	1:D:371:ILE:HD11	1.86	0.56
1:F:65:LEU:HD11	1:F:392:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:CL6:CAM	3:B:502:CL6:HAU	2.35	0.56
1:D:157:ILE:HG22	1:D:446:THR:HG21	1.88	0.56
1:D:271:ARG:HD2	1:D:278:ALA:HB2	1.87	0.56
1:F:190:ARG:HE	1:F:198:ARG:HG2	1.72	0.55
1:A:150:LEU:O	1:A:154:VAL:HG23	2.07	0.54
1:B:218:PRO:O	1:B:221:VAL:HG12	2.08	0.54
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.89	0.54
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.89	0.54
1:C:187:THR:OG1	1:C:443:GLN:NE2	2.41	0.53
3:E:502:CL6:HAU	3:E:502:CL6:CAM	2.39	0.53
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.91	0.52
1:E:165:PHE:CD1	1:E:451:LEU:HD21	2.45	0.52
1:A:190:ARG:NH2	1:A:261:ASN:O	2.43	0.52
1:C:184:ILE:HD12	1:C:300:SER:HA	1.91	0.52
3:C:502:CL6:HAU	3:C:502:CL6:CAM	2.39	0.52
2:E:501:HEM:HBC2	2:E:501:HEM:HMC1	1.92	0.52
1:D:460:VAL:O	1:D:461:GLY:O	2.28	0.52
1:F:154:VAL:HG21	1:F:340:MET:HB2	1.91	0.51
1:F:226:LEU:HD12	1:F:227:PRO:CD	2.39	0.51
1:E:147:THR:HG22	1:E:340:MET:HE1	1.91	0.51
1:C:402:PRO:O	1:C:411:ARG:NH2	2.44	0.50
1:F:226:LEU:HD12	1:F:227:PRO:HD2	1.94	0.50
1:F:52:PRO:O	1:F:54:VAL:N	2.44	0.50
1:A:197:ILE:HD11	1:A:248:ILE:HG13	1.93	0.50
1:C:117:SER:HA	1:C:120:ILE:HD12	1.93	0.50
1:F:415:GLU:HG3	1:F:423:ARG:HH21	1.76	0.50
1:E:271:ARG:CG	1:E:278:ALA:HB2	2.41	0.50
1:B:412:PHE:HA	1:B:415:GLU:HB3	1.94	0.50
1:C:156:LEU:HG	1:C:190:ARG:HD2	1.94	0.49
3:B:502:CL6:HAK	3:B:502:CL6:CAE	2.43	0.49
1:F:150:LEU:O	1:F:154:VAL:HG23	2.13	0.49
1:C:309:LEU:HD23	1:C:463:LEU:HD11	1.93	0.49
1:F:311:PHE:CE2	1:F:457:ILE:HB	2.48	0.49
1:D:160:GLU:HB3	1:D:187:THR:HG22	1.94	0.49
1:D:307:GLY:HA3	1:D:448:TRP:CZ2	2.48	0.48
1:F:156:LEU:HD23	1:F:190:ARG:HG2	1.94	0.48
1:E:271:ARG:HG3	1:E:278:ALA:HB2	1.94	0.48
1:F:196:GLU:O	1:F:200:ASN:ND2	2.47	0.48
1:C:442:LEU:O	1:C:446:THR:OG1	2.31	0.48
1:B:47:VAL:HA	1:B:75:TYR:CE2	2.48	0.48
1:C:168:TRP:O	1:C:485:ARG:NH2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLU:OE2	1:F:348:LYS:N	2.47	0.48
1:B:305:TRP:O	1:B:306:THR:C	2.52	0.48
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.95	0.48
1:D:284:ILE:O	1:D:288:MET:HG2	2.13	0.47
1:A:297:HIS:NE2	1:A:472:VAL:HG22	2.29	0.47
1:A:343:LEU:HD13	1:A:442:LEU:HD23	1.96	0.47
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.94	0.47
1:F:65:LEU:HD12	1:F:468:TYR:CE1	2.49	0.47
1:A:485:ARG:HG3	1:A:486:LYS:N	2.29	0.47
1:B:244:MET:O	1:B:248:ILE:HD12	2.15	0.47
1:E:186:LEU:CD1	1:E:202:PHE:CZ	2.98	0.47
3:A:502:CL6:CAE	3:A:502:CL6:HAK	2.43	0.47
3:B:502:CL6:CAL	3:B:502:CL6:CLAY	3.00	0.47
1:C:154:VAL:HG11	1:C:339:THR:HA	1.97	0.47
1:C:411:ARG:O	1:C:415:GLU:N	2.45	0.47
2:C:501:HEM:CBD	2:C:501:HEM:HHA	2.46	0.46
1:E:186:LEU:HD13	1:E:202:PHE:CZ	2.50	0.46
3:D:502:CL6:CAE	3:D:502:CL6:HAK	2.45	0.46
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.98	0.46
1:C:328:GLU:HA	1:C:331:ARG:HB2	1.98	0.46
2:F:501:HEM:HMC1	2:F:501:HEM:HBC2	1.98	0.46
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.97	0.46
1:C:76:GLY:O	1:C:78:ILE:N	2.49	0.46
1:D:216:LEU:O	1:D:471:MET:HG2	2.15	0.46
1:B:193:MET:HB3	1:B:197:ILE:HD12	1.98	0.46
1:E:147:THR:HG22	1:E:340:MET:CE	2.45	0.46
1:B:405:ASP:N	1:B:405:ASP:OD1	2.48	0.45
1:E:245:PHE:CE2	1:E:288:MET:HG3	2.52	0.45
1:A:255:ASN:O	1:A:258:VAL:HG12	2.17	0.45
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.47	0.45
1:E:52:PRO:O	1:E:54:VAL:N	2.50	0.45
1:F:238:ARG:O	1:F:242:VAL:HG23	2.16	0.45
1:A:69:THR:HG22	1:A:73:LYS:HE2	1.99	0.45
1:A:218:PRO:O	1:A:221:VAL:HG22	2.18	0.44
1:C:460:VAL:HG21	1:C:482:ARG:NH1	2.33	0.44
1:D:200:ASN:HD22	1:D:200:ASN:N	2.15	0.44
1:D:459:LEU:HA	1:D:481:LEU:HD23	1.99	0.44
1:E:168:TRP:CH2	1:E:174:VAL:HG21	2.52	0.44
1:C:114:TYR:CZ	3:C:502:CL6:HAT	2.53	0.44
1:D:185:ILE:HD12	1:D:292:LEU:HD22	2.00	0.44
1:D:357:LEU:CD2	1:D:427:PHE:CE2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:SER:HB3	1:E:469:THR:HB	1.99	0.44
1:D:390:SER:HB3	1:D:393:LEU:HB3	1.99	0.44
1:F:192:LEU:HB3	1:F:288:MET:HE1	2.00	0.44
1:F:132:ALA:O	1:F:136:GLN:NE2	2.50	0.44
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.99	0.44
1:A:467:ASP:OD2	1:A:470:ALA:HB2	2.19	0.43
1:D:434:CYS:HA	2:D:501:HEM:C4D	2.53	0.43
3:D:502:CL6:CLAY	3:D:502:CL6:CAL	3.03	0.43
1:F:197:ILE:CG2	1:F:205:VAL:HG21	2.49	0.43
1:C:107:GLU:HA	1:C:372:LYS:HB2	2.00	0.43
1:C:197:ILE:HG12	1:C:248:ILE:HD13	1.99	0.43
1:B:228:ILE:O	1:B:229:PRO:C	2.56	0.43
1:C:307:GLY:HA3	1:C:448:TRP:CZ2	2.54	0.43
1:B:209:TYR:CD2	1:B:209:TYR:C	2.92	0.43
1:B:463:LEU:HD12	1:B:464:PRO:HD2	1.99	0.43
1:D:89:THR:O	1:D:387:VAL:HA	2.19	0.43
1:E:216:LEU:O	1:E:471:MET:HG2	2.19	0.43
1:A:63:GLY:N	1:A:64:PRO:HD3	2.34	0.42
1:B:361:PRO:HA	1:B:362:PRO:HD3	1.87	0.42
1:E:351:ARG:HB3	1:E:409:PRO:O	2.19	0.42
1:E:42:LYS:O	1:E:379:TYR:HA	2.19	0.42
3:E:502:CL6:CAM	3:E:502:CL6:CAU	2.95	0.42
1:B:114:TYR:CZ	3:B:502:CL6:HAT	2.54	0.42
1:B:434:CYS:HA	2:B:501:HEM:C4D	2.53	0.42
3:C:502:CL6:CAM	3:C:502:CL6:CAU	2.97	0.42
1:A:468:TYR:HA	1:A:473:VAL:HG13	2.01	0.42
1:C:339:THR:O	1:C:341:GLU:N	2.53	0.42
1:A:160:GLU:HB3	1:A:187:THR:HG22	2.00	0.42
1:D:326:GLU:OE2	1:D:348:LYS:N	2.53	0.42
1:A:330:ILE:HD13	1:A:346:MET:HG2	2.01	0.42
1:F:192:LEU:HB3	1:F:288:MET:CE	2.50	0.42
1:A:209:TYR:CD1	1:A:209:TYR:C	2.93	0.42
1:E:102:SER:O	1:E:431:ARG:NH1	2.53	0.42
1:C:65:LEU:HD23	1:C:468:TYR:CE2	2.55	0.41
1:A:63:GLY:N	1:A:64:PRO:CD	2.83	0.41
1:A:118:VAL:N	1:A:119:PRO:HD2	2.35	0.41
1:F:157:ILE:HA	1:F:187:THR:HG22	2.01	0.41
1:F:307:GLY:O	1:F:308:LEU:C	2.58	0.41
1:D:190:ARG:HG2	1:D:198:ARG:HG2	2.03	0.41
3:E:502:CL6:CAE	3:E:502:CL6:HAK	2.50	0.41
1:F:245:PHE:CE2	1:F:288:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:TYR:O	1:D:156:LEU:N	2.52	0.41
1:B:327:GLN:O	1:B:331:ARG:HB2	2.20	0.41
3:D:502:CL6:HAU	3:D:502:CL6:CAM	2.51	0.41
3:F:502:CL6:CAJ	3:F:502:CL6:HAP	2.51	0.41
1:A:305:TRP:HB3	1:A:356:ALA:HB1	2.02	0.41
1:D:402:PRO:O	1:D:411:ARG:NH1	2.50	0.41
1:A:77:ASP:OD2	1:A:376:TYR:OH	2.37	0.41
1:A:307:GLY:HA3	1:A:448:TRP:CZ2	2.56	0.41
1:C:42:LYS:O	1:C:379:TYR:HA	2.21	0.41
1:E:463:LEU:HD12	1:E:464:PRO:HD2	2.02	0.41
1:B:197:ILE:HD11	1:B:248:ILE:HD13	2.03	0.41
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.51	0.41
1:D:195:LYS:O	1:D:199:GLU:N	2.45	0.41
2:D:501:HEM:C4D	3:D:502:CL6:HAM	2.56	0.41
3:F:502:CL6:HAK	3:F:502:CL6:CAE	2.51	0.41
1:C:245:PHE:CD2	1:C:285:THR:HG23	2.55	0.40
1:A:319:PHE:O	1:A:323:VAL:HG23	2.22	0.40
1:E:275:GLU:C	1:E:277:GLN:H	2.25	0.40
1:F:298:THR:O	1:F:299:SER:C	2.59	0.40
1:B:434:CYS:HA	2:B:501:HEM:CHA	2.51	0.40
1:C:324:LEU:HD23	1:C:324:LEU:O	2.21	0.40
1:E:209:TYR:CD1	1:E:209:TYR:C	2.94	0.40
1:A:129:ALA:O	1:A:134:ARG:NH1	2.54	0.40
1:D:118:VAL:HB	1:D:119:PRO:HD3	2.03	0.40
1:E:277:GLN:O	1:E:278:ALA:HB3	2.20	0.40
2:F:501:HEM:HHA	2:F:501:HEM:CBD	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/460 (97%)	412 (92%)	24 (5%)	11 (2%)	5	20
1	B	445/460 (97%)	414 (93%)	27 (6%)	4 (1%)	17	46
1	C	444/460 (96%)	385 (87%)	46 (10%)	13 (3%)	4	17
1	D	445/460 (97%)	405 (91%)	30 (7%)	10 (2%)	6	23
1	E	446/460 (97%)	410 (92%)	28 (6%)	8 (2%)	8	28
1	F	446/460 (97%)	396 (89%)	42 (9%)	8 (2%)	8	28
All	All	2673/2760 (97%)	2422 (91%)	197 (7%)	54 (2%)	7	26

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	57	GLY
1	A	277	GLN
1	B	126	VAL
1	C	49	SER
1	C	77	ASP
1	D	49	SER
1	D	461	GLY
1	E	53	PHE
1	E	487	HIS
1	F	53	PHE
1	A	77	ASP
1	C	103	GLN
1	C	313	ALA
1	C	340	MET
1	C	341	GLU
1	D	53	PHE
1	D	462	GLU
1	E	48	SER
1	E	49	SER
1	E	77	ASP
1	E	278	ALA
1	E	313	ALA
1	F	308	LEU
1	F	334	PHE
1	A	126	VAL
1	B	53	PHE
1	B	377	LYS
1	C	126	VAL
1	C	306	THR

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Mol	Chain	Res	Type
1	C	328	GLU
1	C	336	ASP
1	D	126	VAL
1	E	126	VAL
1	F	126	VAL
1	F	418	GLN
1	A	41	GLY
1	A	42	LYS
1	A	49	SER
1	A	278	ALA
1	B	63	GLY
1	C	57	GLY
1	D	48	SER
1	F	278	ALA
1	C	275	GLU
1	C	337	GLU
1	D	77	ASP
1	D	276	GLU
1	D	346	MET
1	D	417	LYS
1	F	63	GLY
1	A	62	GLY
1	F	307	GLY
1	A	258	VAL

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	A	368/397 (93%)	339 (92%)	29 (8%)	12	33
1	B	370/397 (93%)	345 (93%)	25 (7%)	16	40
1	C	352/397 (89%)	326 (93%)	26 (7%)	13	36
1	D	370/397 (93%)	343 (93%)	27 (7%)	14	37
1	E	372/397 (94%)	348 (94%)	24 (6%)	17	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	368/397 (93%)	346 (94%)	22 (6%)	19	47
All	All	2200/2382 (92%)	2047 (93%)	153 (7%)	15	39

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	59	SER
1	A	73	LYS
1	A	115	GLN
1	A	130	ASP
1	A	133	HIS
1	A	152	SER
1	A	156	LEU
1	A	187	THR
1	A	190	ARG
1	A	195	LYS
1	A	200	ASN
1	A	203	THR
1	A	219	ILE
1	A	232	LYS
1	A	233	ARG
1	A	271	ARG
1	A	285	THR
1	A	292	LEU
1	A	301	VAL
1	A	302	THR
1	A	328	GLU
1	A	366	VAL
1	A	378	ASP
1	A	418	GLN
1	A	425	VAL
1	A	443	GLN
1	A	482	ARG
1	A	484	THR
1	B	111	ASP
1	B	112	GLU
1	B	139	LYS
1	B	151	GLN
1	B	152	SER
1	B	182	GLU
1	B	190	ARG

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Mol	Chain	Res	Type
1	B	207	LYS
1	B	219	ILE
1	B	253	ARG
1	B	259	LYS
1	B	271	ARG
1	B	292	LEU
1	B	302	THR
1	B	318	LYS
1	B	325	GLU
1	B	331	ARG
1	B	336	ASP
1	B	337	GLU
1	B	405	ASP
1	B	416	ASP
1	B	418	GLN
1	B	472	VAL
1	B	479	CYS
1	B	484	THR
1	C	50	LEU
1	C	80	THR
1	C	86	GLN
1	C	109	SER
1	C	131	LEU
1	C	147	THR
1	C	156	LEU
1	C	186	LEU
1	C	189	SER
1	C	193	MET
1	C	205	VAL
1	C	219	ILE
1	C	241	MET
1	C	247	LYS
1	C	282	GLU
1	C	292	LEU
1	C	300	SER
1	C	320	LEU
1	C	325	GLU
1	C	326	GLU
1	C	347	ASP
1	C	372	LYS
1	C	379	TYR
1	C	410	GLU

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Mol	Chain	Res	Type
1	C	418	GLN
1	C	482	ARG
1	D	42	LYS
1	D	48	SER
1	D	86	GLN
1	D	110	GLN
1	D	112	GLU
1	D	159	LYS
1	D	171	SER
1	D	185	ILE
1	D	187	THR
1	D	190	ARG
1	D	204	GLU
1	D	205	VAL
1	D	219	ILE
1	D	221	VAL
1	D	233	ARG
1	D	252	ARG
1	D	255	ASN
1	D	273	ARG
1	D	312	GLU
1	D	326	GLU
1	D	378	ASP
1	D	399	GLU
1	D	417	LYS
1	D	420	GLN
1	D	435	MET
1	D	462	GLU
1	D	484	THR
1	E	53	PHE
1	E	73	LYS
1	E	147	THR
1	E	186	LEU
1	E	199	GLU
1	E	203	THR
1	E	219	ILE
1	E	262	ASP
1	E	280	ASN
1	E	292	LEU
1	E	300	SER
1	E	302	THR
1	E	312	GLU

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Mol	Chain	Res	Type
1	E	339	THR
1	E	371	ILE
1	E	383	GLU
1	E	387	VAL
1	E	418	GLN
1	E	421	LYS
1	E	447	ILE
1	E	466	PRO
1	E	469	THR
1	E	479	CYS
1	E	484	THR
1	F	51	ILE
1	F	58	LEU
1	F	65	LEU
1	F	81	MET
1	F	112	GLU
1	F	147	THR
1	F	152	SER
1	F	186	LEU
1	F	187	THR
1	F	200	ASN
1	F	204	GLU
1	F	207	LYS
1	F	211	THR
1	F	219	ILE
1	F	261	ASN
1	F	282	GLU
1	F	299	SER
1	F	304	SER
1	F	336	ASP
1	F	415	GLU
1	F	418	GLN
1	F	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	200	ASN
1	A	255	ASN
1	A	315	ASN
1	A	327	GLN

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Mol	Chain	Res	Type
1	A	350	HIS
1	A	408	ASN
1	A	418	GLN
1	A	487	HIS
1	B	210	GLN
1	B	261	ASN
1	B	315	ASN
1	B	327	GLN
1	C	103	GLN
1	C	265	GLN
1	C	315	ASN
1	C	327	GLN
1	C	418	GLN
1	C	443	GLN
1	D	103	GLN
1	D	124	ASN
1	D	135	ASN
1	D	200	ASN
1	D	297	HIS
1	D	315	ASN
1	E	103	GLN
1	E	115	GLN
1	E	124	ASN
1	E	135	ASN
1	E	315	ASN
1	E	327	GLN
1	E	432	HIS
1	E	443	GLN
1	F	103	GLN
1	F	115	GLN
1	F	124	ASN
1	F	135	ASN
1	F	200	ASN
1	F	261	ASN
1	F	265	GLN
1	F	314	ASN
1	F	327	GLN
1	F	418	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands are 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	$\#\|Z\| > 2$
3	CL6	C	502	2	26,28,28	1.98	4 (15%)	35,39,39	2.32	8 (22%)
3	CL6	D	502	2	26,28,28	1.78	3 (11%)	35,39,39	2.16	6 (17%)
2	HEM	F	501	1,3	41,50,50	1.39	6 (14%)	45,82,82	2.03	13 (28%)
3	CL6	B	502	2	26,28,28	2.17	3 (11%)	35,39,39	2.10	6 (17%)
3	CL6	F	502	2	26,28,28	1.88	3 (11%)	35,39,39	2.45	5 (14%)
2	HEM	E	501	1,3	41,50,50	1.40	5 (12%)	45,82,82	1.88	14 (31%)
2	HEM	A	501	1,3	41,50,50	1.40	7 (17%)	45,82,82	1.92	13 (28%)
2	HEM	C	501	1,3	41,50,50	1.43	4 (9%)	45,82,82	2.19	15 (33%)
3	CL6	A	502	2	26,28,28	1.75	4 (15%)	35,39,39	2.10	8 (22%)
4	GAI	C	503	-	3,3,3	3.59	3 (100%)	3,3,3	0.91	0
4	GAI	F	503	-	3,3,3	0.68	0	3,3,3	1.33	0
2	HEM	B	501	1,3	41,50,50	1.45	6 (14%)	45,82,82	1.98	13 (28%)
2	HEM	D	501	1,3	41,50,50	1.43	8 (19%)	45,82,82	2.20	16 (35%)
3	CL6	E	502	2	26,28,28	1.93	3 (11%)	35,39,39	2.44	7 (20%)
4	GAI	B	503	-	3,3,3	3.09	1 (33%)	3,3,3	1.61	1 (33%)

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
3	CL6	C	502	2	-	0/18/24/24	0/4/4/4
3	CL6	D	502	2	-	0/18/24/24	0/4/4/4
2	HEM	F	501	1,3	-	4/12/54/54	-
3	CL6	B	502	2	-	0/18/24/24	0/4/4/4
3	CL6	F	502	2	-	0/18/24/24	0/4/4/4
2	HEM	E	501	1,3	-	6/12/54/54	-
2	HEM	A	501	1,3	-	5/12/54/54	-
2	HEM	C	501	1,3	-	6/12/54/54	-
3	CL6	A	502	2	-	0/18/24/24	0/4/4/4
2	HEM	B	501	1,3	-	0/12/54/54	-
2	HEM	D	501	1,3	-	8/12/54/54	-
3	CL6	E	502	2	-	0/18/24/24	0/4/4/4

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	CL6	CAP-NAO	-7.74	1.32	1.38
3	F	502	CL6	CAX-CAW	7.52	1.51	1.39
3	E	502	CL6	CAP-NAO	-6.98	1.33	1.38
3	B	502	CL6	CAX-CAW	6.87	1.50	1.39
3	A	502	CL6	CAX-CAW	6.66	1.50	1.39
3	C	502	CL6	CAX-CAW	6.66	1.50	1.39
3	D	502	CL6	CAX-CAW	6.49	1.50	1.39
3	C	502	CL6	CAP-NAO	-5.80	1.34	1.38
3	E	502	CL6	CAX-CAW	5.54	1.48	1.39
4	B	503	GAI	C-N3	-5.09	1.27	1.36
4	C	503	GAI	C-N3	-4.95	1.27	1.36
2	C	501	HEM	C1B-NB	-4.83	1.32	1.40
2	E	501	HEM	C1B-NB	-4.60	1.32	1.40
3	F	502	CL6	CAP-NAO	-4.46	1.35	1.38
3	D	502	CL6	CAP-NAO	-4.06	1.35	1.38
2	F	501	HEM	C1B-NB	-3.99	1.33	1.40
2	B	501	HEM	C1B-NB	-3.99	1.33	1.40
2	A	501	HEM	C1B-NB	-3.91	1.33	1.40
2	D	501	HEM	C1B-NB	-3.64	1.34	1.40
2	C	501	HEM	C4B-NB	-3.53	1.31	1.38
3	A	502	CL6	CAP-NAO	-3.20	1.36	1.38
2	D	501	HEM	C4B-NB	-3.16	1.32	1.38
2	A	501	HEM	C4B-NB	-3.11	1.32	1.38
2	B	501	HEM	C4D-ND	-3.11	1.34	1.40
2	F	501	HEM	C4B-NB	-3.04	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C4B-NB	-2.94	1.32	1.38
2	B	501	HEM	FE-NB	2.89	2.11	1.96
4	C	503	GAI	C-N1	2.80	1.36	1.30
3	C	502	CL6	CAX-CLAY	2.80	1.80	1.73
2	E	501	HEM	C4B-NB	-2.75	1.33	1.38
2	B	501	HEM	CHB-C1B	2.70	1.41	1.35
2	A	501	HEM	FE-NB	2.67	2.10	1.96
2	D	501	HEM	FE-NB	2.65	2.10	1.96
2	A	501	HEM	C4D-ND	-2.62	1.35	1.40
2	D	501	HEM	C1D-ND	-2.52	1.33	1.38
4	C	503	GAI	C-N2	-2.51	1.31	1.36
2	F	501	HEM	FE-NB	2.50	2.09	1.96
3	F	502	CL6	CAX-CLAY	2.47	1.79	1.73
2	D	501	HEM	CHB-C1B	2.44	1.41	1.35
2	E	501	HEM	FE-NB	2.41	2.08	1.96
2	F	501	HEM	CHB-C1B	2.39	1.41	1.35
2	E	501	HEM	C3B-C4B	2.38	1.49	1.44
2	D	501	HEM	C4D-ND	-2.38	1.36	1.40
2	B	501	HEM	C4D-C3D	2.37	1.49	1.45
2	D	501	HEM	C3B-C4B	2.35	1.49	1.44
3	A	502	CL6	CAX-CLAY	2.26	1.79	1.73
2	D	501	HEM	C4D-C3D	2.25	1.48	1.45
3	B	502	CL6	CAX-CLAY	2.24	1.79	1.73
2	A	501	HEM	C3B-C4B	2.20	1.49	1.44
2	F	501	HEM	C1D-ND	-2.18	1.34	1.38
2	C	501	HEM	FE-NB	2.17	2.07	1.96
2	A	501	HEM	CHB-C1B	2.14	1.40	1.35
2	E	501	HEM	C4D-ND	-2.14	1.36	1.40
2	A	501	HEM	C1D-C2D	2.14	1.48	1.44
3	D	502	CL6	CAX-CLAY	2.13	1.78	1.73
3	C	502	CL6	CAA-CAC	2.09	1.42	1.39
3	E	502	CL6	CAX-CLAY	2.07	1.78	1.73
2	C	501	HEM	CHB-C1B	2.05	1.40	1.35
2	F	501	HEM	C4D-ND	-2.04	1.36	1.40
3	A	502	CL6	CAR-NAO	2.00	1.54	1.51

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	CL6	CAM-NAO-CAR	-8.89	119.33	126.71
3	F	502	CL6	CAM-NAO-CAR	-8.87	119.35	126.71
3	D	502	CL6	CAM-NAO-CAR	-8.09	120.00	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	CL6	CAM-NAO-CAR	-7.55	120.45	126.71
3	C	502	CL6	CAM-NAO-CAR	-7.47	120.51	126.71
3	A	502	CL6	CAM-NAO-CAR	-7.23	120.71	126.71
3	C	502	CL6	CAL-CAR-CAW	-7.18	102.44	112.00
2	D	501	HEM	CAD-C3D-C4D	6.64	136.27	124.66
3	F	502	CL6	CAL-CAR-CAW	-6.39	103.48	112.00
3	E	502	CL6	CAP-NAO-CAM	6.16	112.16	108.25
3	F	502	CL6	CAP-NAO-CAM	5.97	112.04	108.25
2	C	501	HEM	CAD-C3D-C4D	5.63	134.49	124.66
3	E	502	CL6	CAL-CAR-CAW	-5.60	104.54	112.00
2	F	501	HEM	CAD-C3D-C4D	5.57	134.39	124.66
3	B	502	CL6	CAP-NAO-CAM	5.38	111.67	108.25
3	B	502	CL6	CAL-CAR-CAW	-5.37	104.84	112.00
2	C	501	HEM	C1B-NB-C4B	5.05	110.29	105.07
2	B	501	HEM	CHD-C1D-ND	4.99	129.85	124.43
3	A	502	CL6	CAL-CAR-CAW	-4.98	105.37	112.00
2	C	501	HEM	CHD-C1D-ND	4.76	129.61	124.43
3	F	502	CL6	CAW-CAR-NAO	4.76	113.37	106.11
2	A	501	HEM	C1B-NB-C4B	4.73	109.96	105.07
2	E	501	HEM	C1B-NB-C4B	4.72	109.95	105.07
3	C	502	CL6	CAP-NAO-CAM	4.67	111.21	108.25
2	D	501	HEM	C1B-NB-C4B	4.59	109.81	105.07
2	D	501	HEM	CAD-C3D-C2D	-4.57	119.36	127.88
2	F	501	HEM	C1B-NB-C4B	4.38	109.60	105.07
3	D	502	CL6	CAU-CAW-CAR	4.27	124.13	121.05
2	B	501	HEM	C1B-NB-C4B	4.20	109.41	105.07
2	C	501	HEM	C4B-C3B-C2B	-4.10	103.86	107.11
3	D	502	CL6	CAP-NAO-CAM	4.07	110.83	108.25
2	B	501	HEM	CHC-C4B-NB	4.06	128.84	124.43
3	A	502	CL6	CAP-NAO-CAR	3.92	129.58	124.95
2	C	501	HEM	CHC-C4B-NB	3.88	128.65	124.43
2	E	501	HEM	C4B-C3B-C2B	-3.87	104.04	107.11
3	A	502	CL6	CAC-CAR-CAW	3.86	117.14	112.00
3	D	502	CL6	CAL-CAR-CAW	-3.85	106.87	112.00
2	B	501	HEM	CHD-C1D-C2D	-3.84	118.97	124.98
2	F	501	HEM	CHC-C4B-NB	3.79	128.54	124.43
2	E	501	HEM	CAD-C3D-C4D	3.78	131.27	124.66
2	C	501	HEM	CAD-C3D-C2D	-3.77	120.86	127.88
2	A	501	HEM	CAD-CBD-CGD	-3.71	105.63	113.60
2	D	501	HEM	CHD-C1D-ND	3.64	128.39	124.43
2	F	501	HEM	CAD-C3D-C2D	-3.63	121.11	127.88
2	B	501	HEM	C4B-C3B-C2B	-3.57	104.28	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	CL6	CAP-NAO-CAR	3.56	129.16	124.95
3	E	502	CL6	CAU-CAW-CAR	3.55	123.61	121.05
3	C	502	CL6	CAW-CAR-NAO	3.55	111.52	106.11
2	A	501	HEM	CHA-C4D-C3D	-3.46	118.83	125.33
2	D	501	HEM	CMA-C3A-C4A	-3.41	123.23	128.46
2	F	501	HEM	CBD-CAD-C3D	3.35	121.94	112.63
2	A	501	HEM	CBD-CAD-C3D	3.27	121.71	112.63
2	A	501	HEM	CHC-C4B-NB	3.23	127.94	124.43
2	D	501	HEM	CHC-C4B-NB	3.23	127.94	124.43
2	E	501	HEM	CHC-C4B-NB	3.22	127.93	124.43
2	A	501	HEM	CHA-C4D-ND	3.22	128.36	124.38
2	A	501	HEM	CAD-C3D-C4D	3.15	130.17	124.66
3	B	502	CL6	CAW-CAR-NAO	3.13	110.88	106.11
2	B	501	HEM	C2C-C3C-C4C	-3.09	104.74	106.90
3	F	502	CL6	CAP-NAO-CAR	3.07	128.58	124.95
2	D	501	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
2	B	501	HEM	C4B-CHC-C1C	3.06	126.59	122.56
3	E	502	CL6	CAP-NAO-CAR	3.01	128.51	124.95
2	A	501	HEM	CHD-C1D-ND	2.99	127.68	124.43
2	E	501	HEM	CHD-C1D-ND	2.98	127.66	124.43
2	B	501	HEM	CBD-CAD-C3D	2.93	120.75	112.63
2	A	501	HEM	CMD-C2D-C1D	2.91	129.47	125.04
2	F	501	HEM	C4B-C3B-C2B	-2.89	104.82	107.11
2	F	501	HEM	CHD-C1D-ND	2.89	127.57	124.43
2	D	501	HEM	CBA-CAA-C2A	2.87	117.51	112.62
3	E	502	CL6	CAR-CAW-CAX	-2.86	120.84	122.65
2	F	501	HEM	CHA-C4D-ND	2.82	127.86	124.38
3	C	502	CL6	CAP-NAO-CAR	2.80	128.26	124.95
3	D	502	CL6	CAW-CAR-NAO	2.80	110.38	106.11
2	E	501	HEM	C4B-CHC-C1C	2.74	126.17	122.56
2	F	501	HEM	CMD-C2D-C1D	2.73	129.20	125.04
2	D	501	HEM	CBD-CAD-C3D	2.70	120.13	112.63
2	C	501	HEM	CHD-C1D-C2D	-2.64	120.85	124.98
2	C	501	HEM	CHA-C4D-ND	2.64	127.65	124.38
2	F	501	HEM	CHA-C4D-C3D	-2.64	120.37	125.33
2	B	501	HEM	CAD-C3D-C4D	2.64	129.27	124.66
2	D	501	HEM	CMD-C2D-C1D	2.63	129.05	125.04
3	E	502	CL6	CAC-CAR-CAW	2.58	115.44	112.00
2	A	501	HEM	CHD-C1D-C2D	-2.54	121.01	124.98
2	B	501	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
2	C	501	HEM	O2A-CGA-CBA	2.53	122.16	114.03
2	C	501	HEM	O2A-CGA-O1A	-2.53	117.00	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	CAD-CBD-CGD	-2.52	108.17	113.60
2	C	501	HEM	CBD-CAD-C3D	2.47	119.48	112.63
2	E	501	HEM	CAD-CBD-CGD	-2.45	108.33	113.60
2	A	501	HEM	CHB-C1B-NB	2.45	127.41	124.38
3	B	502	CL6	CAP-NAO-CAR	2.44	127.83	124.95
3	A	502	CL6	CAF-CAE-CAC	2.44	123.32	120.76
2	E	501	HEM	CBD-CAD-C3D	2.43	119.36	112.63
2	D	501	HEM	C4B-CHC-C1C	2.40	125.73	122.56
2	A	501	HEM	C4B-CHC-C1C	2.39	125.71	122.56
2	E	501	HEM	CHD-C1D-C2D	-2.39	121.25	124.98
4	B	503	GAI	N3-C-N2	2.39	121.81	116.13
2	E	501	HEM	O2A-CGA-CBA	2.38	121.69	114.03
2	A	501	HEM	C3D-C4D-ND	2.38	112.82	110.17
2	C	501	HEM	CHB-C1B-NB	2.35	127.28	124.38
3	B	502	CL6	CAU-CAW-CAR	2.34	122.74	121.05
2	D	501	HEM	CHB-C1B-NB	2.32	127.25	124.38
3	A	502	CL6	CAU-CAW-CAX	-2.31	114.03	116.62
2	F	501	HEM	CHB-C1B-NB	2.30	127.22	124.38
3	A	502	CL6	CAP-NAO-CAM	2.29	109.70	108.25
3	C	502	CL6	CAK-CAL-CAR	2.27	125.53	120.94
3	C	502	CL6	CAA-CAC-CAR	2.26	125.52	120.94
2	E	501	HEM	CMD-C2D-C1D	2.20	128.40	125.04
2	D	501	HEM	C2C-C3C-C4C	-2.18	105.38	106.90
2	F	501	HEM	CMA-C3A-C4A	-2.14	125.18	128.46
2	E	501	HEM	CAD-C3D-C2D	-2.14	123.90	127.88
2	C	501	HEM	C3B-C2B-C1B	2.13	108.06	106.49
2	D	501	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
2	E	501	HEM	CAA-CBA-CGA	-2.12	107.83	113.76
2	D	501	HEM	CMA-C3A-C2A	2.12	128.93	124.94
2	B	501	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
2	E	501	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
2	C	501	HEM	CHA-C4D-C3D	-2.09	121.40	125.33
2	B	501	HEM	CMC-C2C-C3C	2.09	128.58	124.68
2	C	501	HEM	C4B-CHC-C1C	2.08	125.30	122.56
3	A	502	CL6	CAA-CAC-CAR	2.07	125.12	120.94
2	D	501	HEM	CAD-CBD-CGD	-2.05	109.19	113.60
2	B	501	HEM	CHC-C4B-C3B	-2.02	121.47	124.57
3	C	502	CL6	CAW-CAX-CLAY	2.00	123.98	121.68

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2D-C3D-CAD-CBD
2	C	501	HEM	C4D-C3D-CAD-CBD
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C2D-C3D-CAD-CBD
2	D	501	HEM	C4D-C3D-CAD-CBD
2	F	501	HEM	C2D-C3D-CAD-CBD
2	F	501	HEM	C4D-C3D-CAD-CBD
2	E	501	HEM	C2D-C3D-CAD-CBD
2	E	501	HEM	C4D-C3D-CAD-CBD
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
2	F	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	C2D-C3D-CAD-CBD
2	D	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O1D
2	E	501	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAD-CBD-CGD-O1D
2	E	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	CL6	3	0
3	D	502	CL6	4	0
2	F	501	HEM	3	0
3	B	502	CL6	4	0
3	F	502	CL6	2	0
2	E	501	HEM	2	0
2	A	501	HEM	3	0
2	C	501	HEM	4	0
3	A	502	CL6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	4	0
2	D	501	HEM	4	0
3	E	502	CL6	3	0

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

Ligand CL6 C 502
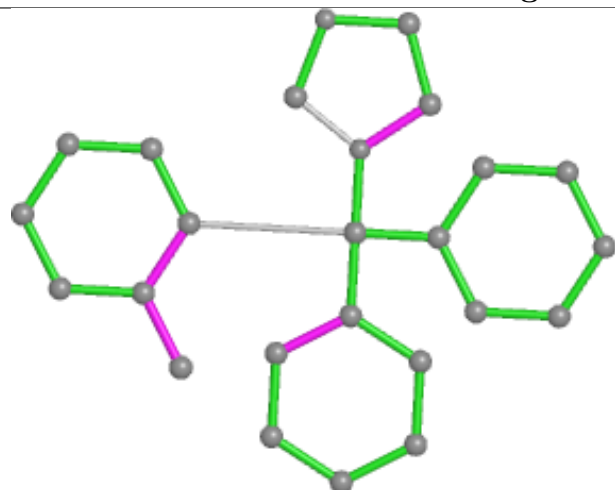
Bond lengths
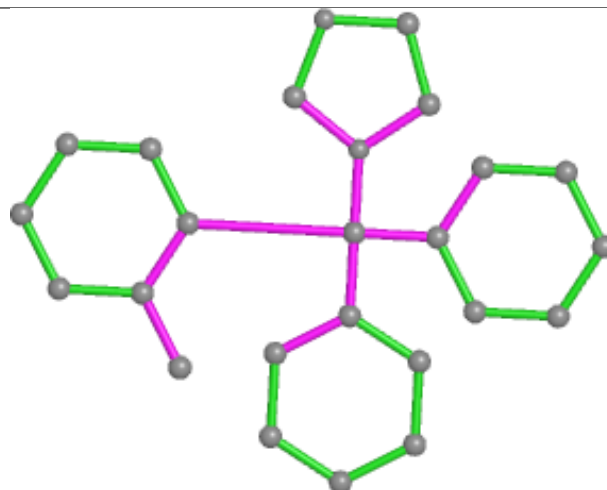
Bond angles
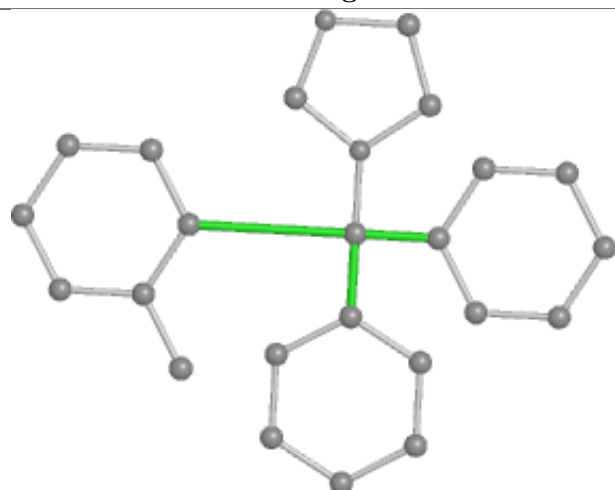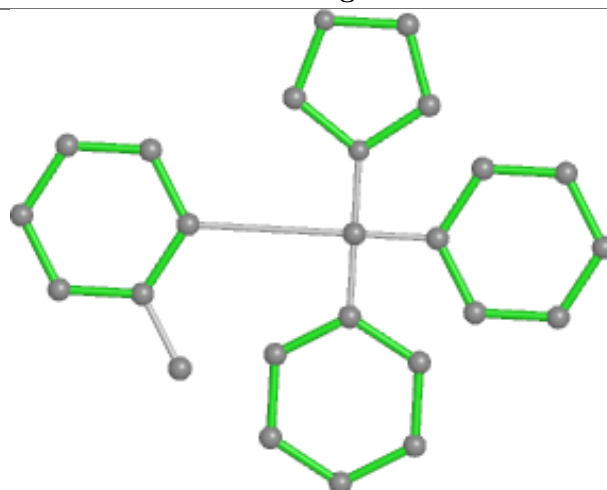
Torsions

Rings

Ligand CL6 D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM F 501
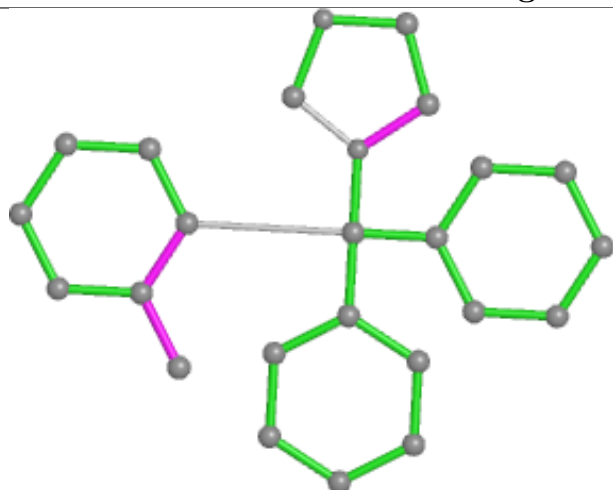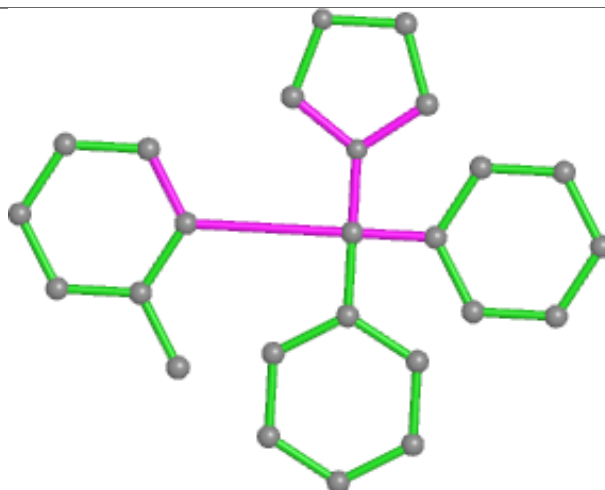
Bond lengths
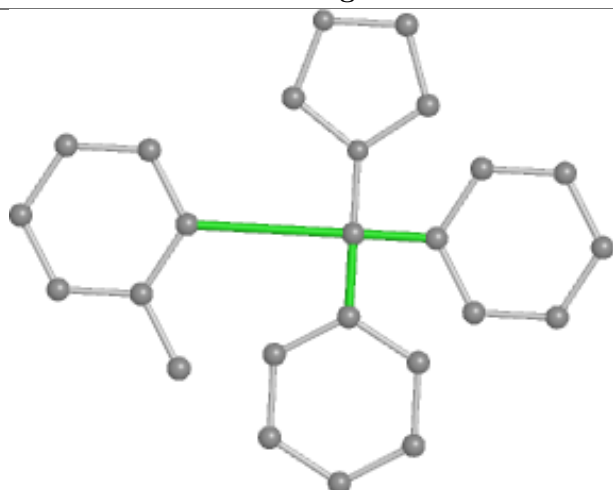
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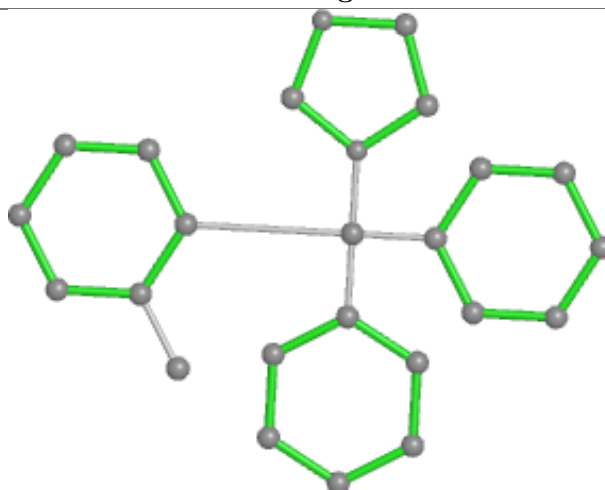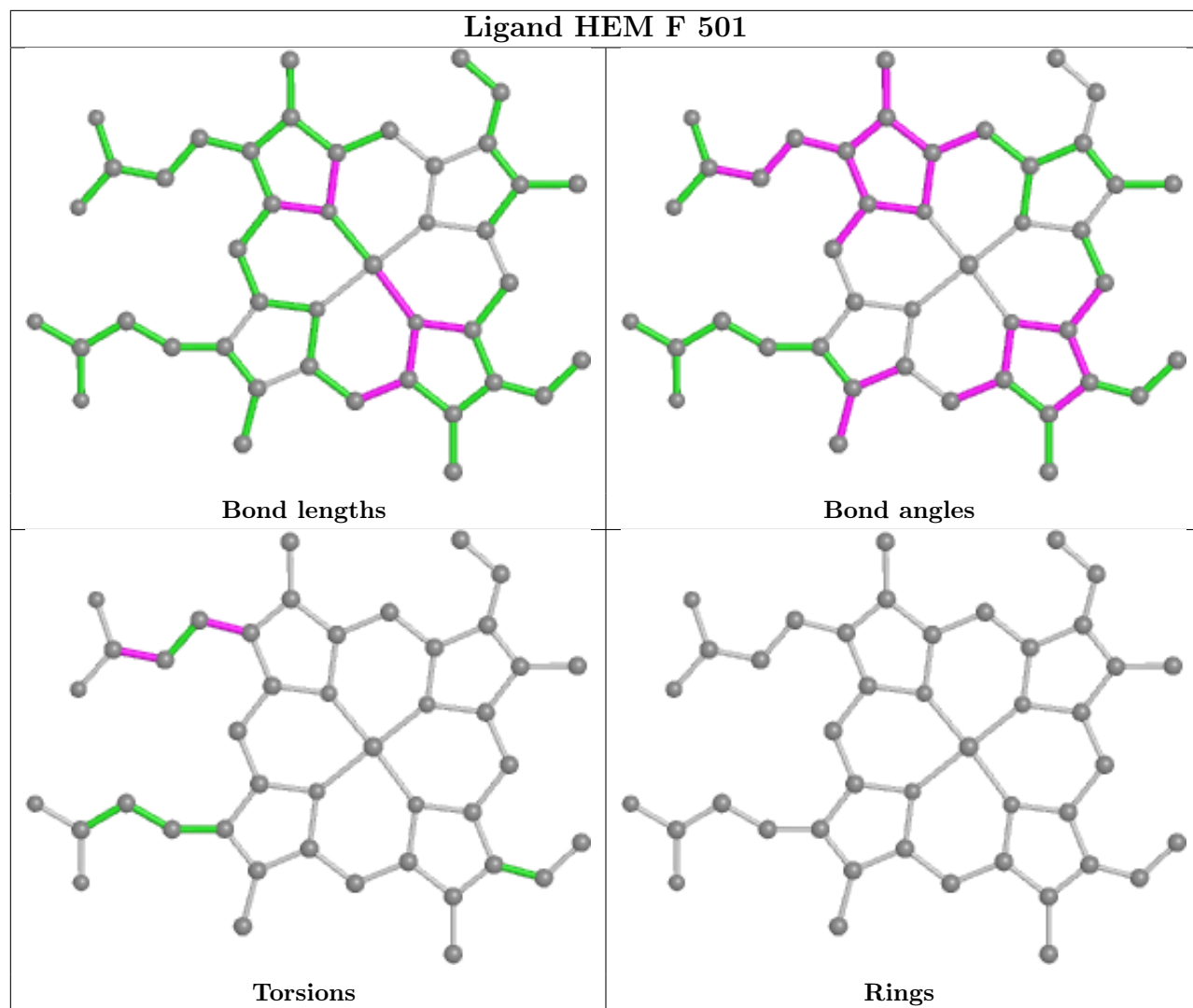
Torsions

Rings
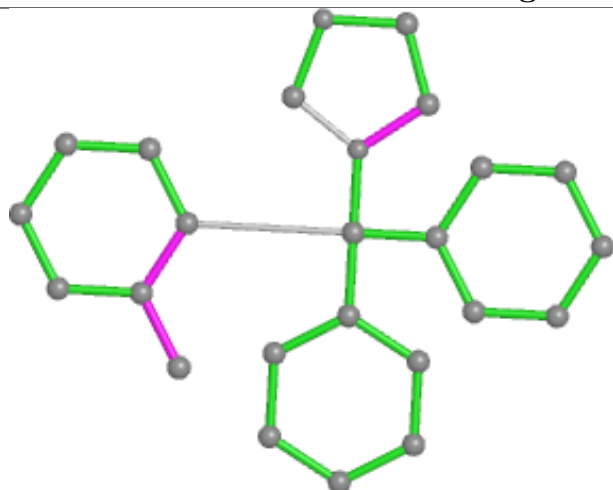
Ligand CL6 B 502

Bond lengths
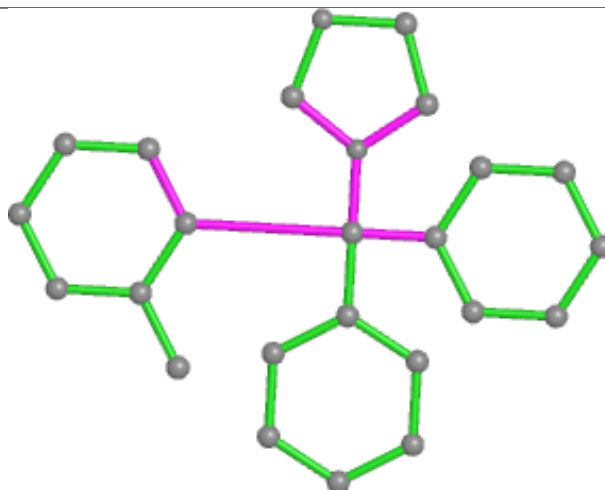
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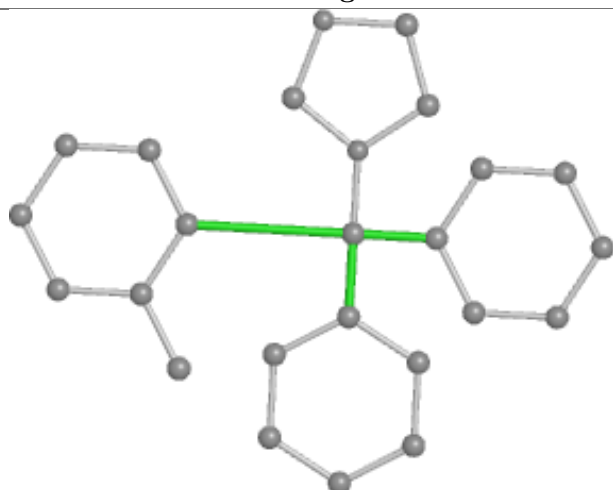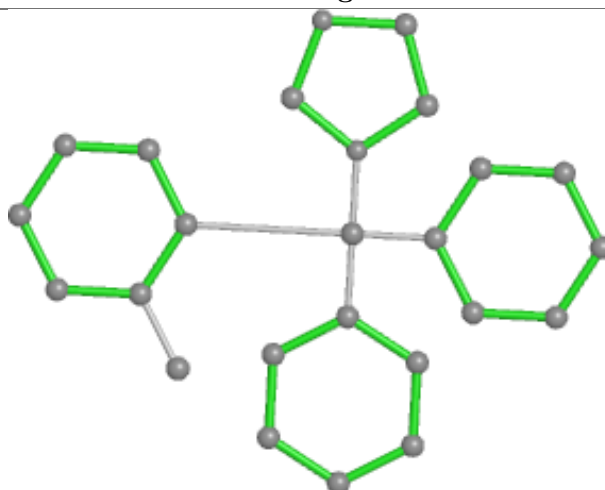
Torsions

Rings

Ligand CL6 F 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 501

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report
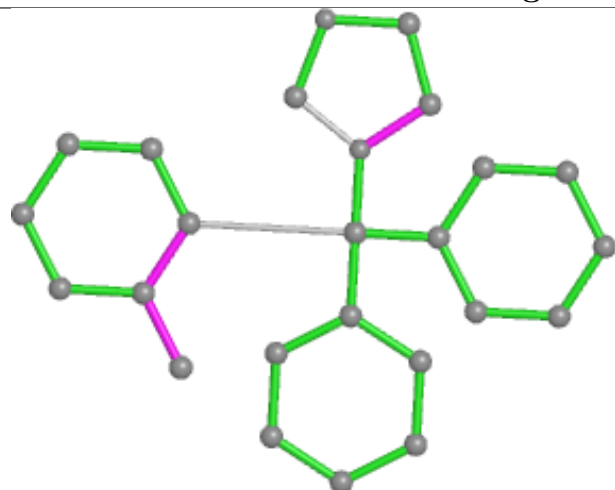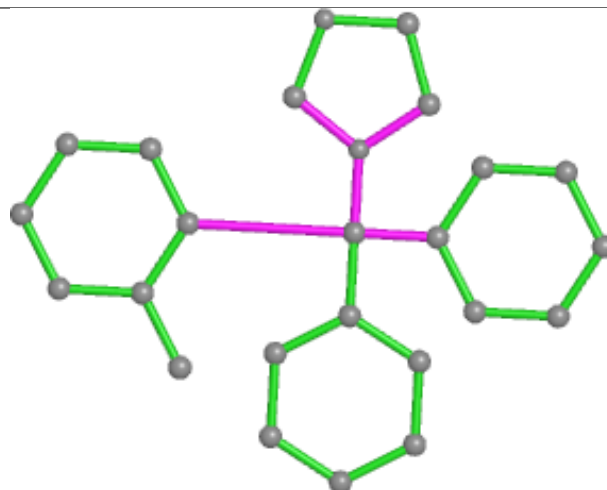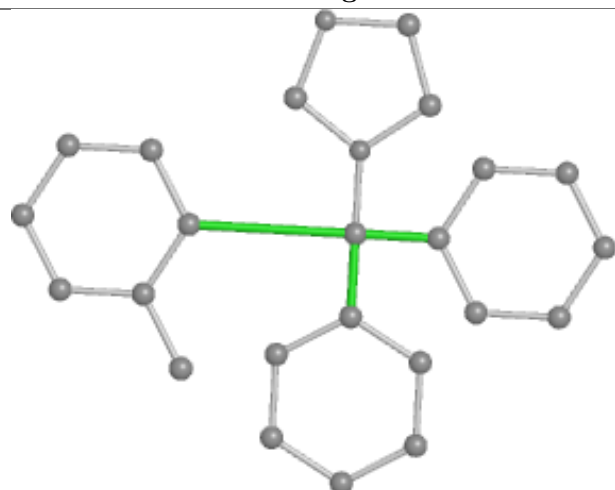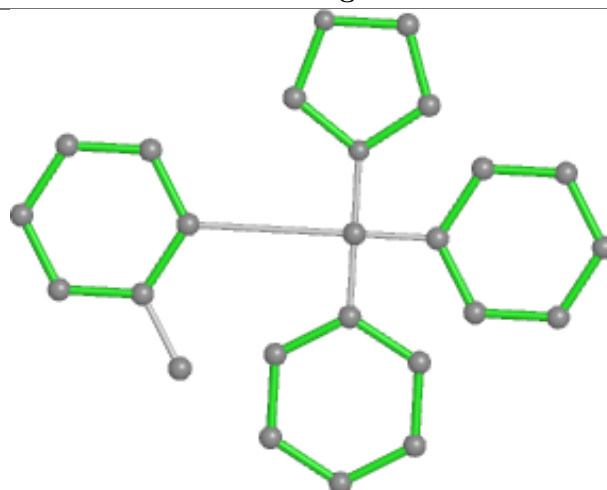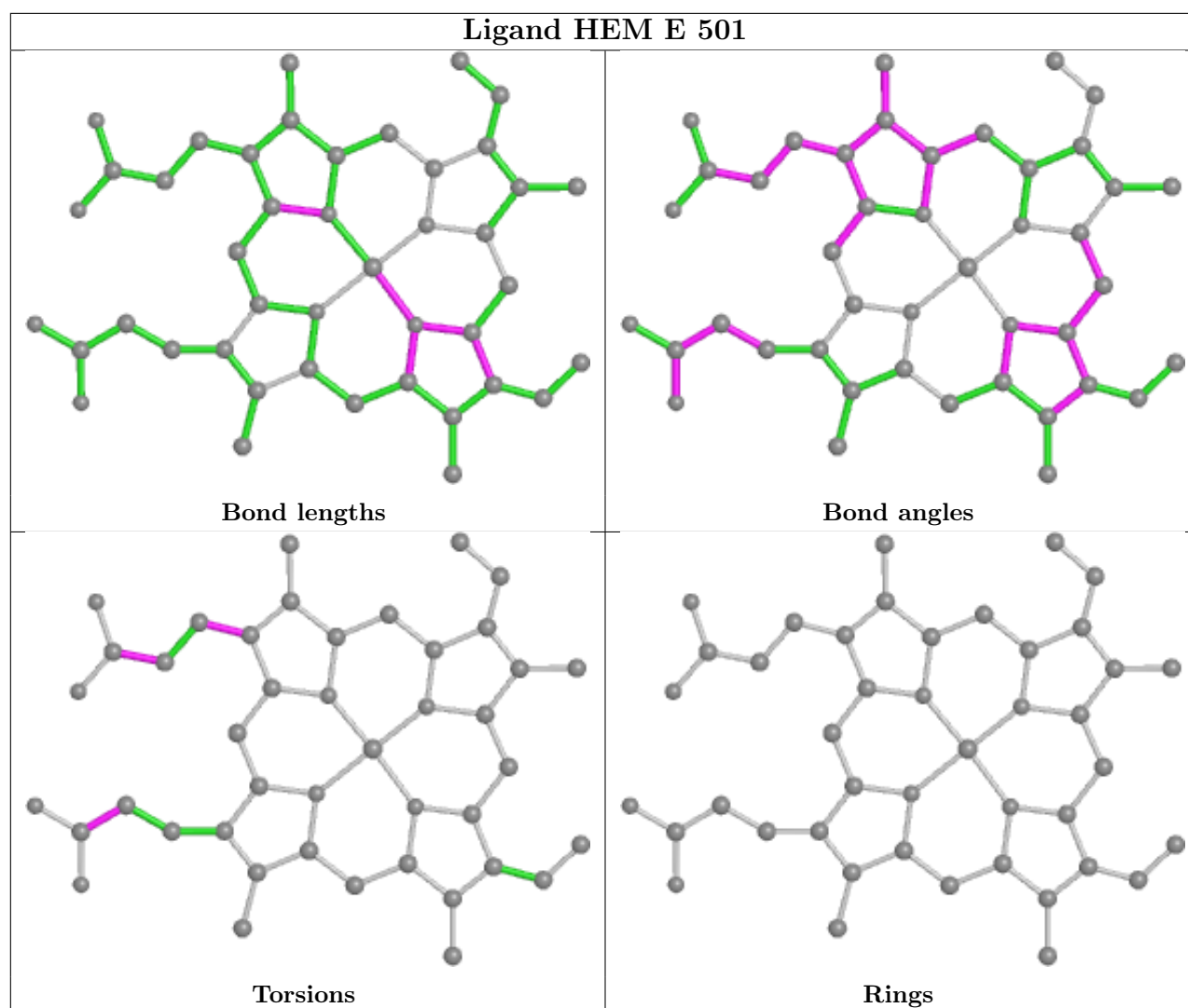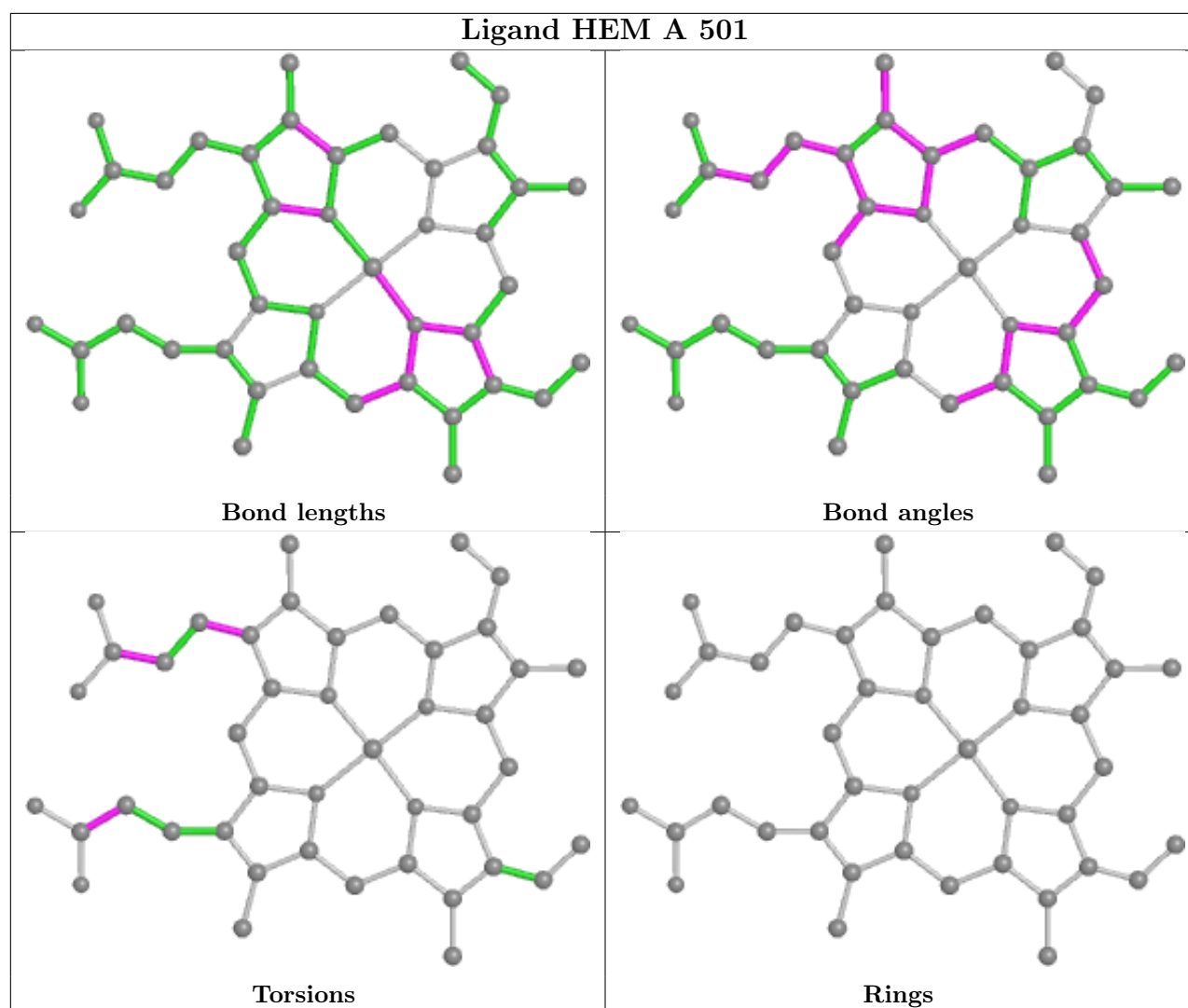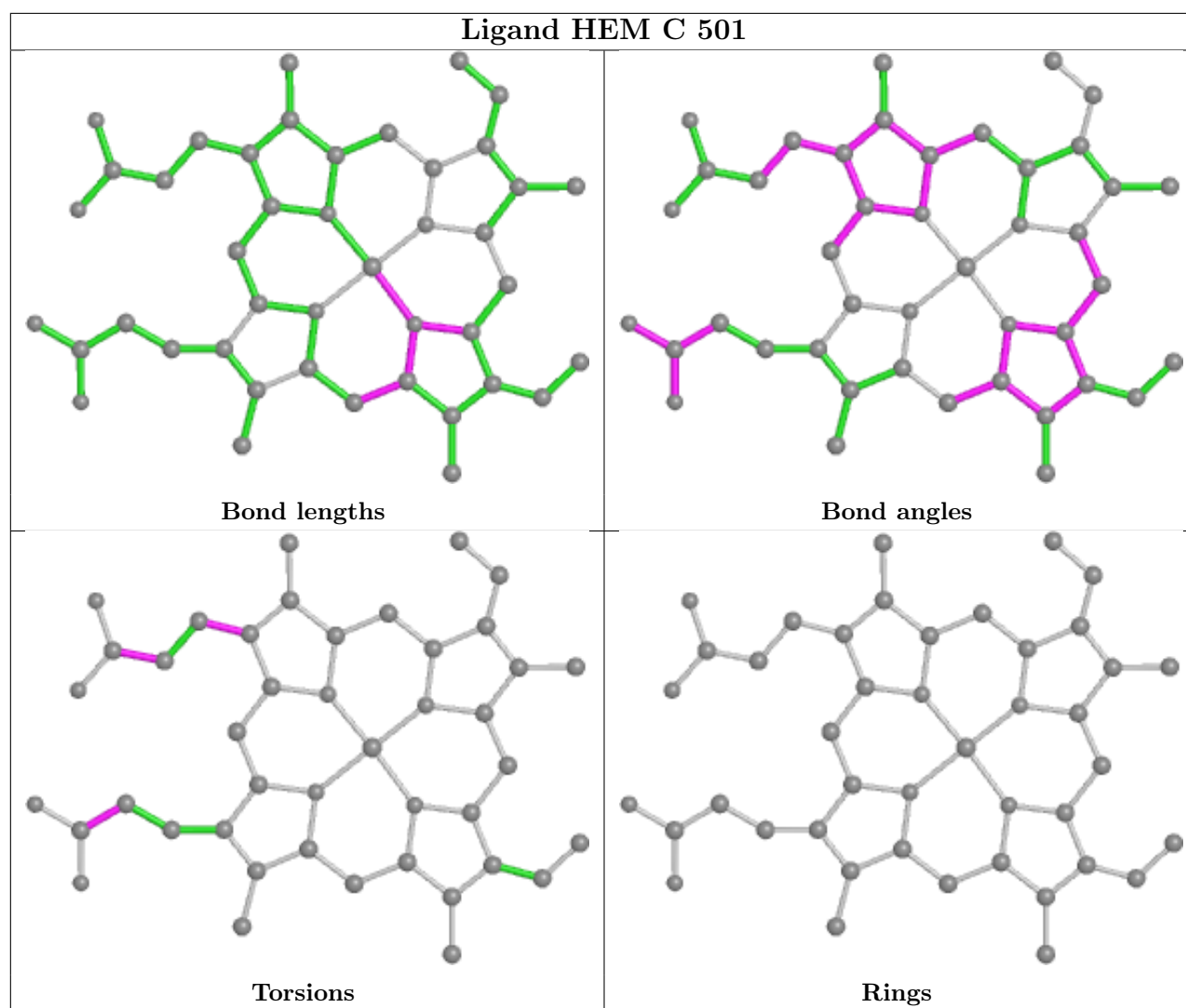
Ligand CL6 A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand CL6 E 502
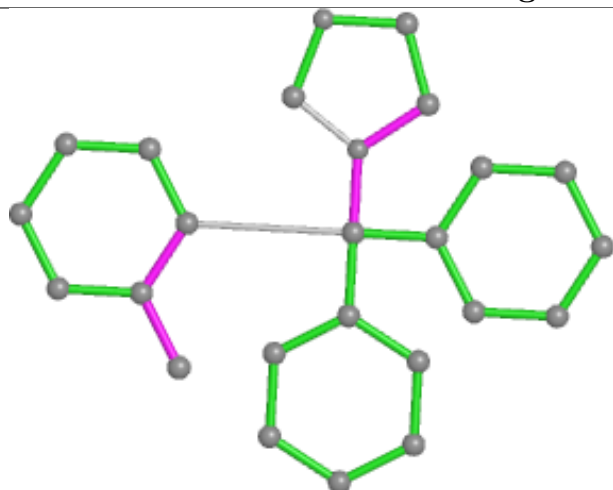
Bond lengths
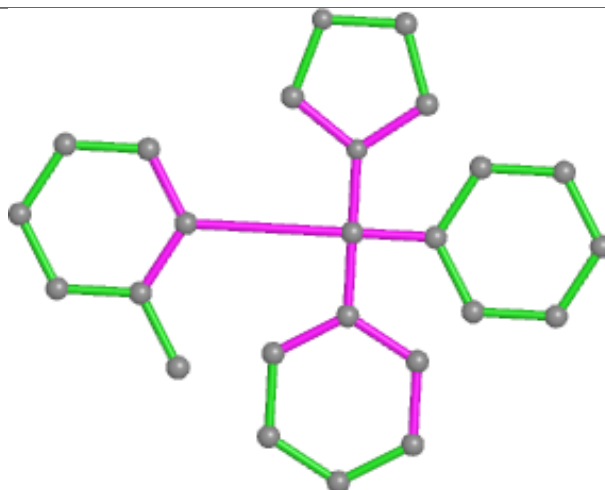
Bond angles
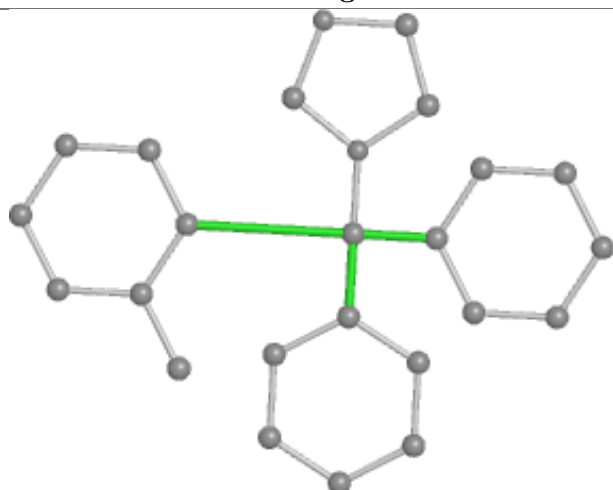
Torsions
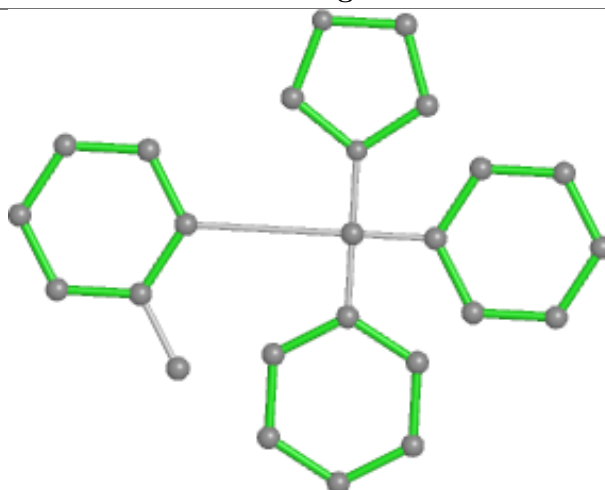
Rings
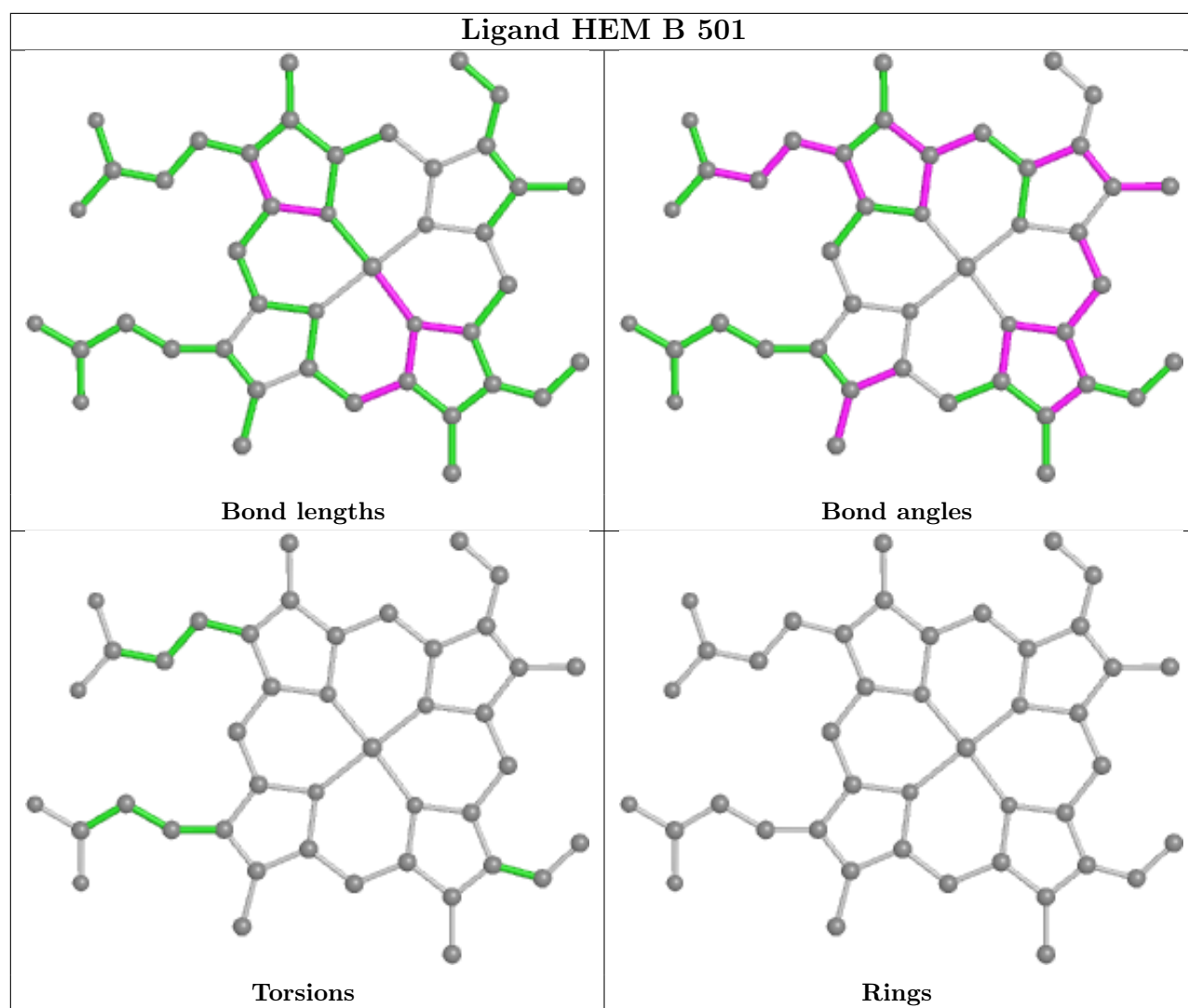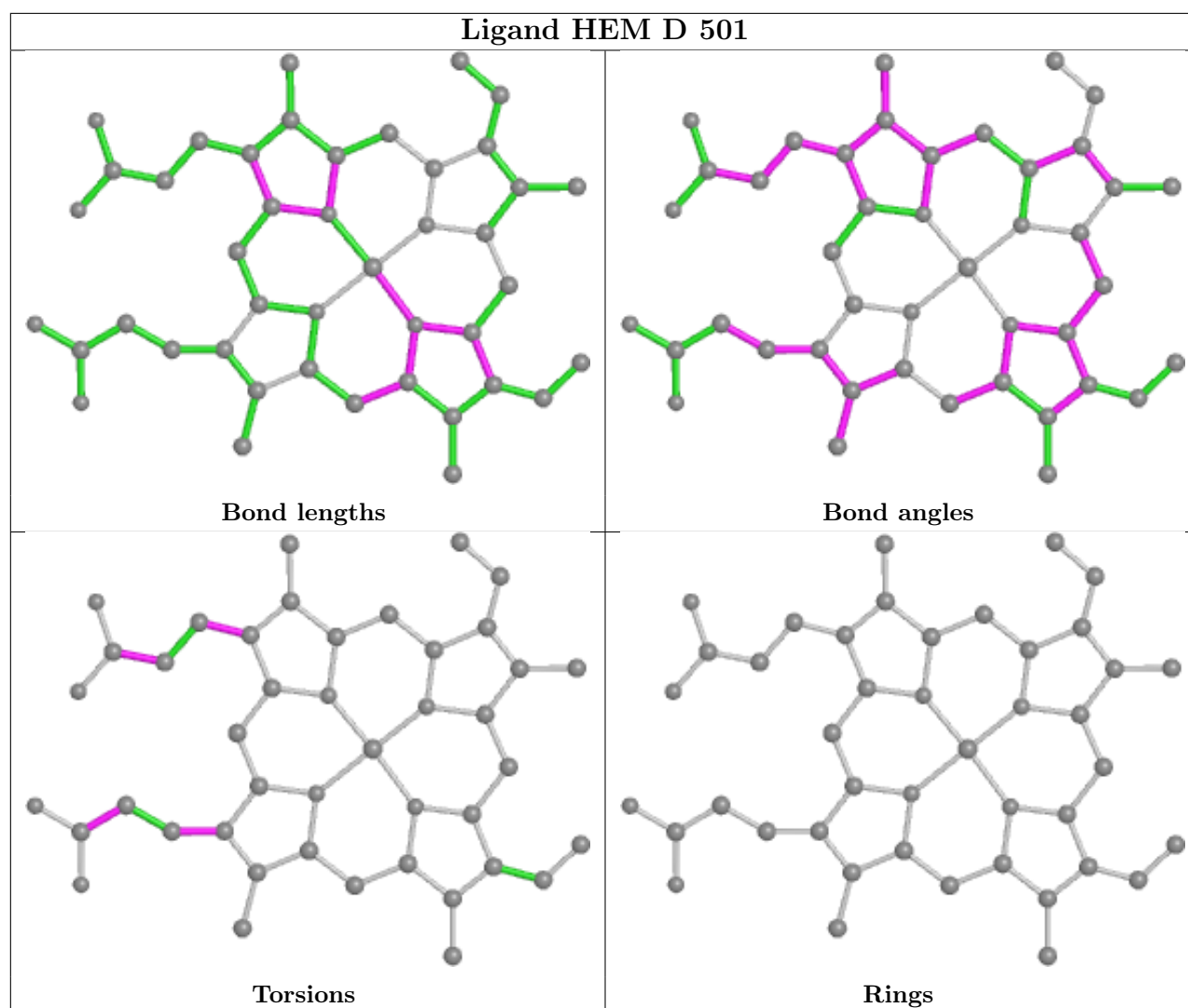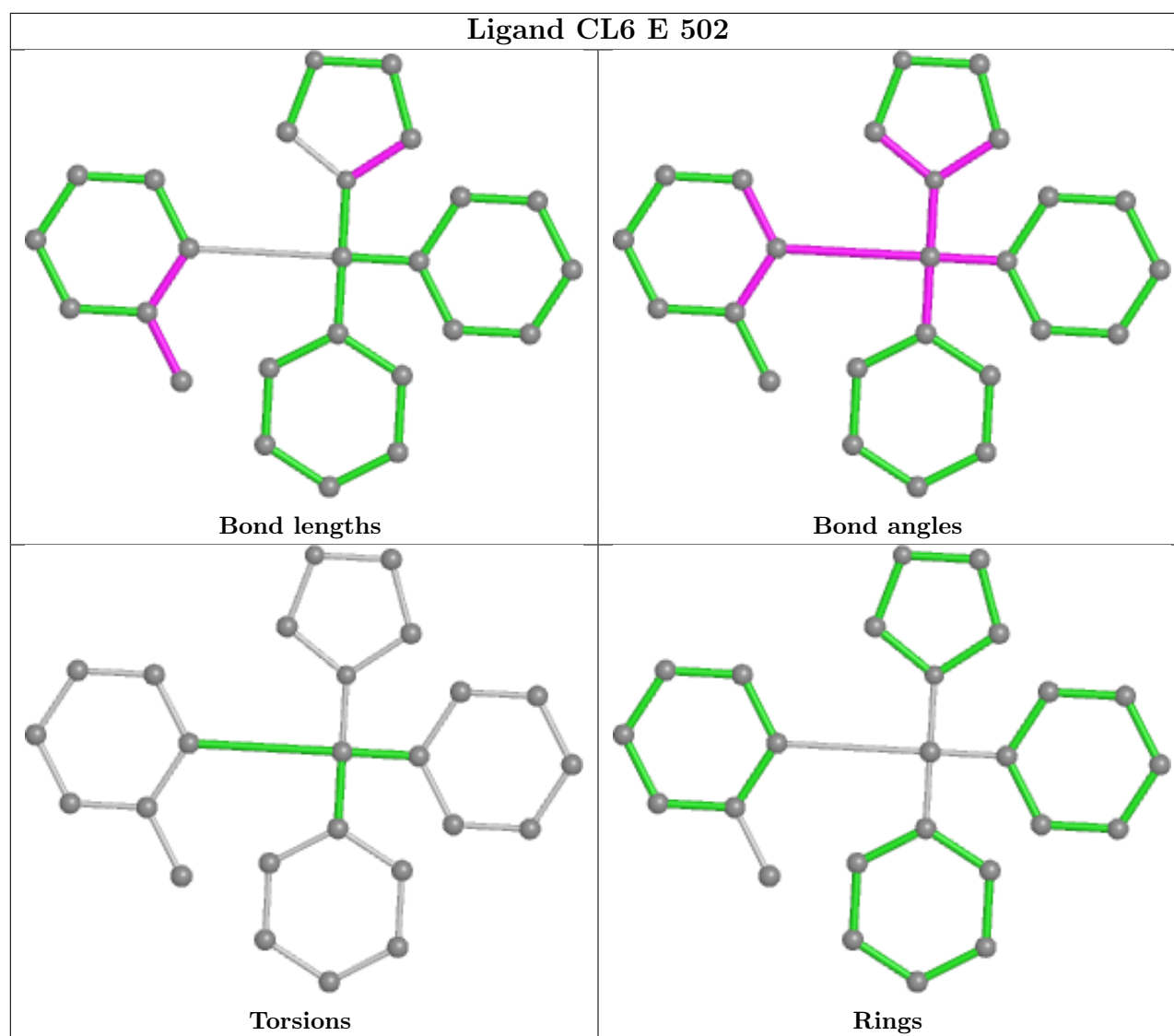
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	449/460 (97%)	0.29	1 (0%)	95	95	48, 71, 97, 133	0
1	B	447/460 (97%)	0.20	1 (0%)	95	95	46, 66, 90, 126	0
1	C	446/460 (96%)	0.34	12 (2%)	54	51	53, 84, 116, 148	0
1	D	447/460 (97%)	0.28	8 (1%)	68	67	53, 82, 114, 151	0
1	E	448/460 (97%)	0.41	8 (1%)	68	67	59, 83, 113, 142	0
1	F	448/460 (97%)	0.45	14 (3%)	49	45	60, 86, 114, 136	0
All	All	2685/2760 (97%)	0.33	44 (1%)	72	71	46, 78, 112, 151	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	GLU	4.2
1	F	380	TYR	4.1
1	F	381	VAL	3.8
1	D	457	ILE	3.8
1	F	338	LEU	3.7
1	A	488	HIS	3.3
1	D	197	ILE	3.0
1	F	330	ILE	2.9
1	C	108	LEU	2.7
1	C	349	LEU	2.7
1	D	405	ASP	2.7
1	E	274	GLY	2.7
1	C	426	GLY	2.6
1	C	101	PHE	2.6
1	F	165	PHE	2.6
1	D	279	LEU	2.6
1	E	193	MET	2.5
1	D	126	VAL	2.5
1	F	90	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	447	ILE	2.4
1	C	425	VAL	2.4
1	E	334	PHE	2.4
1	F	374	PHE	2.3
1	C	261	ASN	2.3
1	F	357	LEU	2.3
1	F	116	PHE	2.3
1	F	168	TRP	2.2
1	E	310	LEU	2.2
1	F	363	LEU	2.2
1	C	329	GLU	2.2
1	E	380	TYR	2.2
1	C	378	ASP	2.2
1	E	151	GLN	2.2
1	E	277	GLN	2.1
1	C	381	VAL	2.1
1	F	468	TYR	2.1
1	B	415	GLU	2.1
1	E	201	LEU	2.1
1	F	441	TYR	2.1
1	D	202	PHE	2.1
1	C	205	VAL	2.1
1	D	272	TYR	2.0
1	F	176	ILE	2.0
1	C	92	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(Å^2)	Q<0.9
4	GAI	F	503	4/4	0.85	0.28	57,62,65,66	0
4	GAI	C	503	4/4	0.95	0.25	35,36,37,38	0
4	GAI	B	503	4/4	0.96	0.20	60,62,62,65	0
3	CL6	A	502	25/25	0.97	0.31	57,68,74,84	0
3	CL6	C	502	25/25	0.98	0.24	60,67,87,89	0
3	CL6	D	502	25/25	0.98	0.31	68,73,76,76	0
3	CL6	E	502	25/25	0.98	0.33	68,74,80,83	0
3	CL6	F	502	25/25	0.98	0.29	62,72,88,94	0
2	HEM	C	501	43/43	0.98	0.26	49,56,79,87	0
2	HEM	D	501	43/43	0.98	0.26	45,56,63,72	0
2	HEM	B	501	43/43	0.98	0.24	46,56,60,72	0
3	CL6	B	502	25/25	0.99	0.27	46,56,64,75	0
2	HEM	E	501	43/43	0.99	0.26	57,61,73,94	0
2	HEM	F	501	43/43	0.99	0.30	68,74,83,90	0
2	HEM	A	501	43/43	0.99	0.24	42,47,66,72	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.
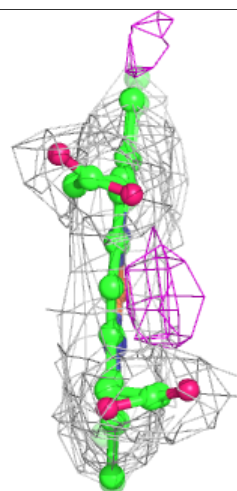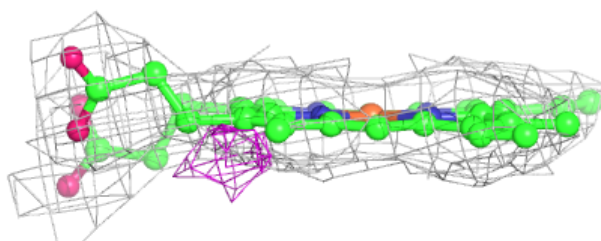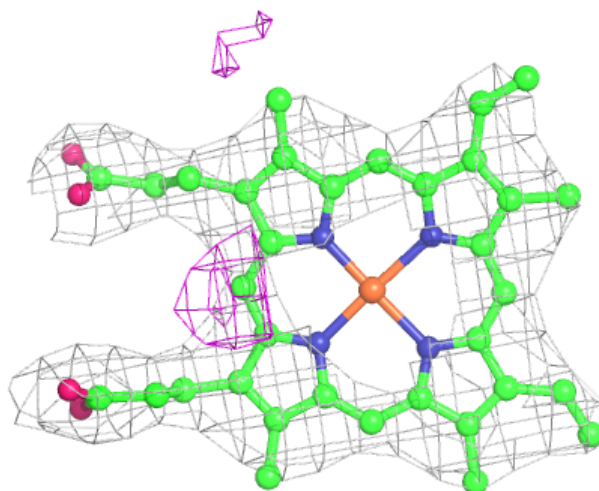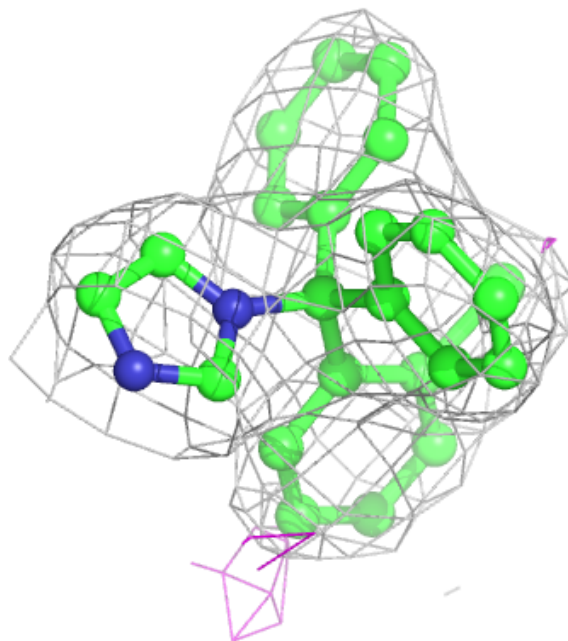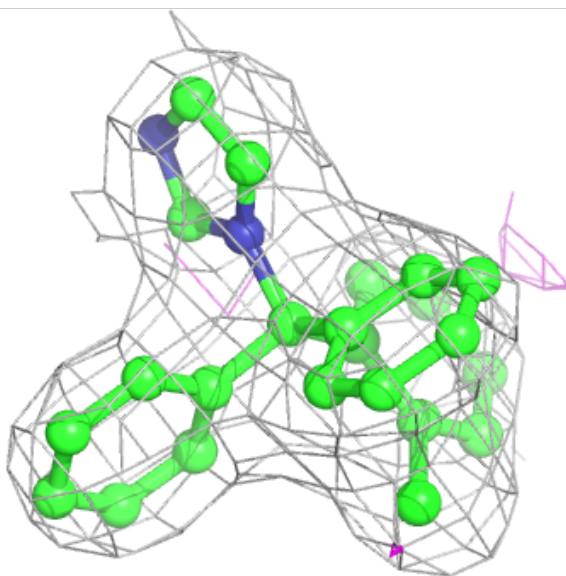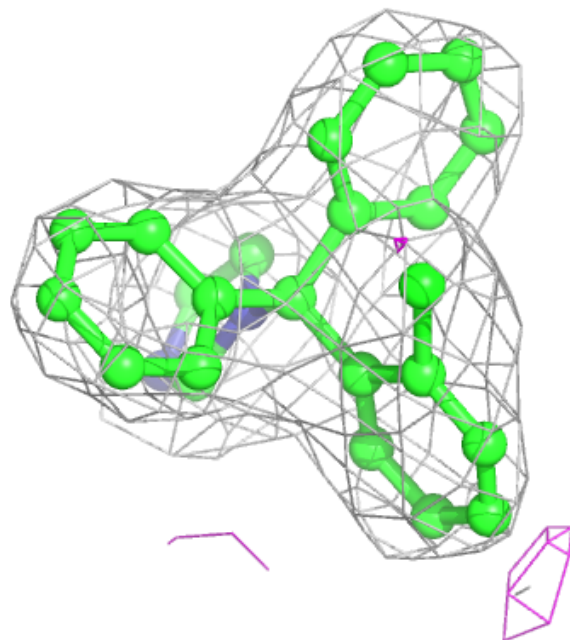
Electron density around CL6 A 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
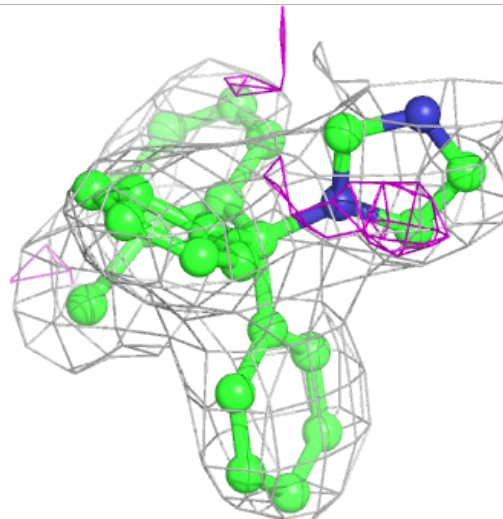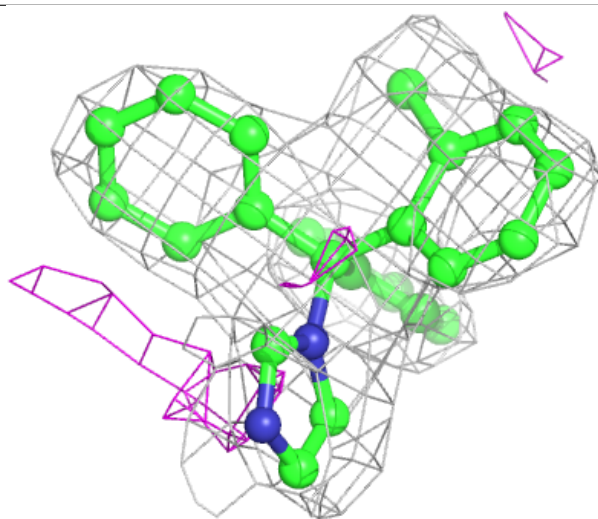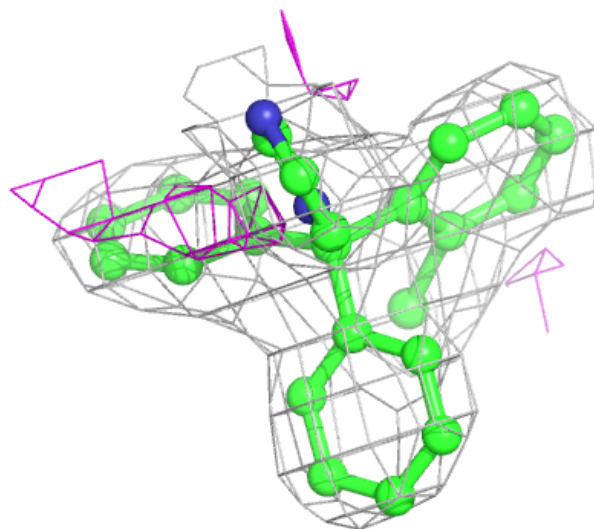
Electron density around CL6 C 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
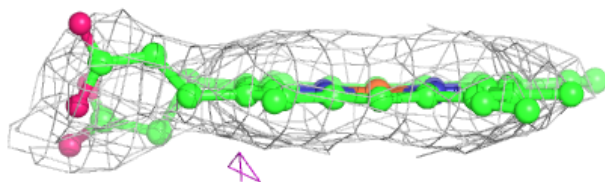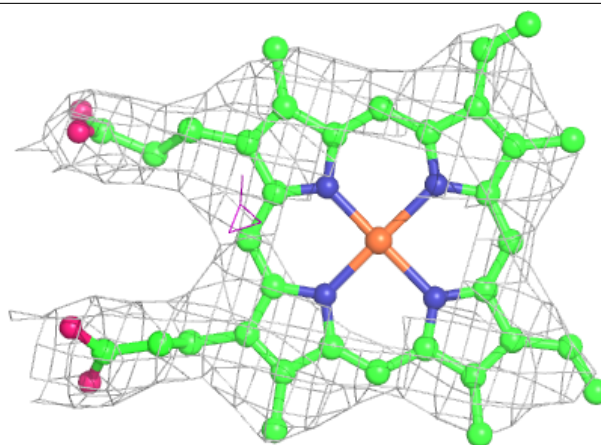and green (positive)
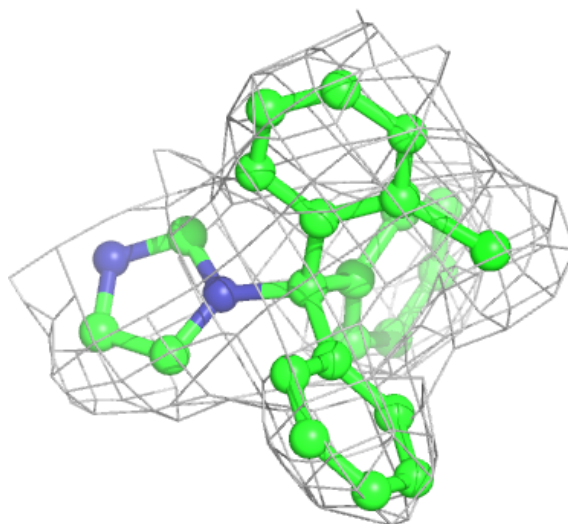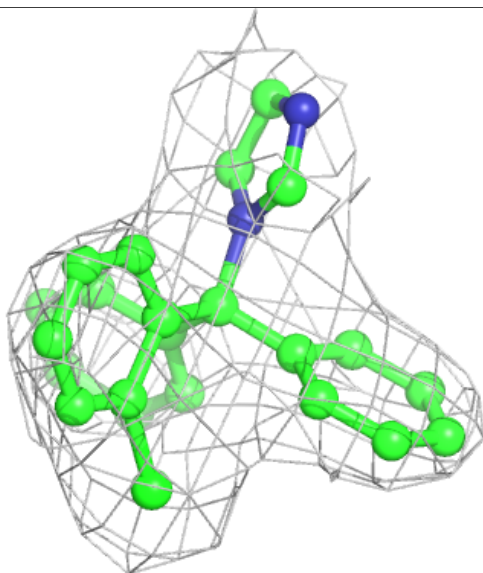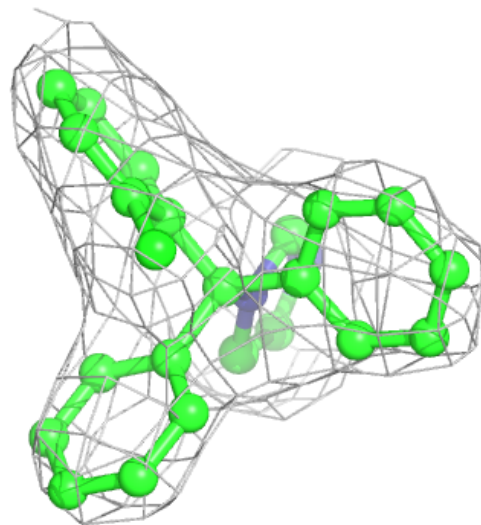
Electron density around CL6 D 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
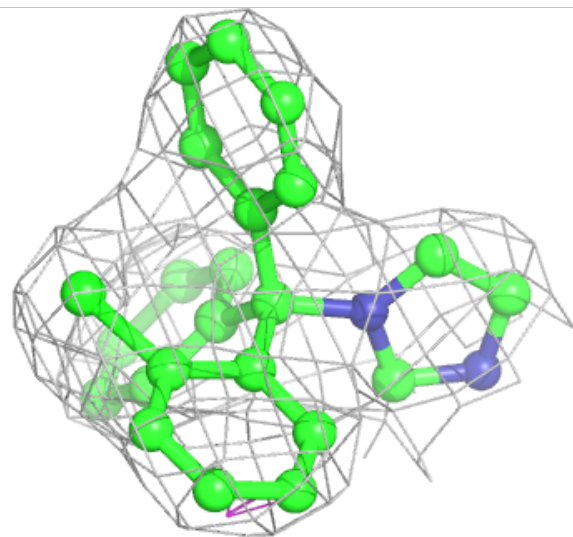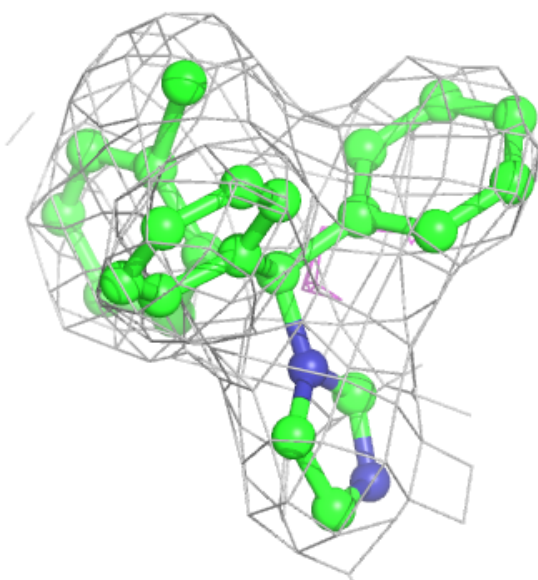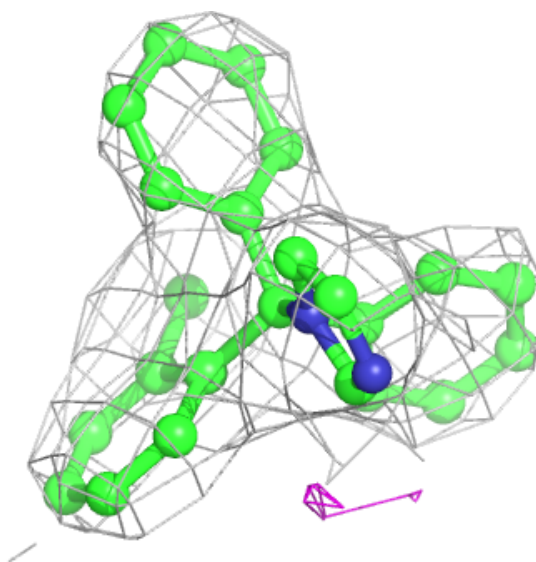
Electron density around CL6 E 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
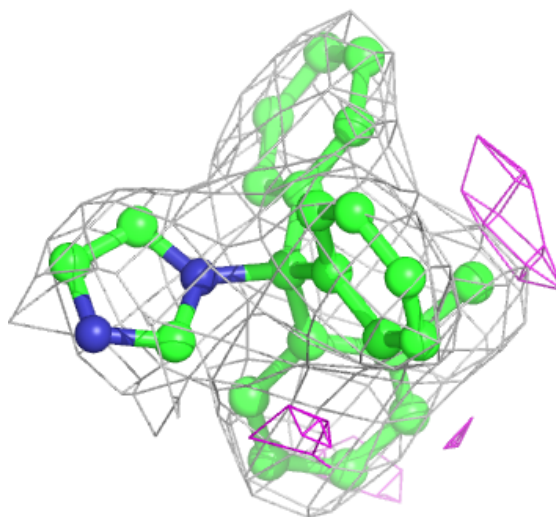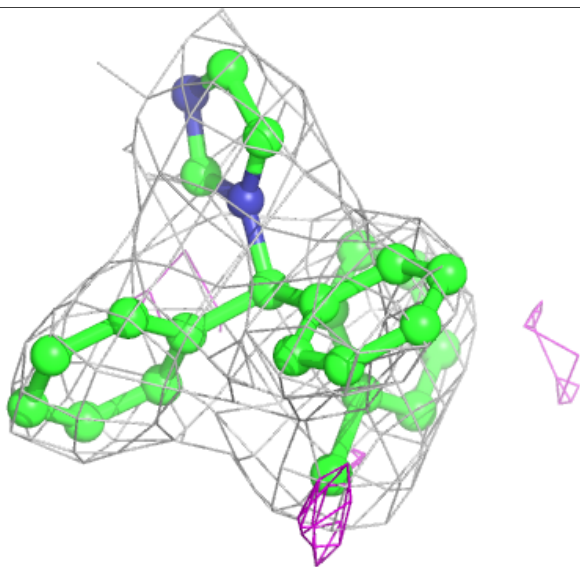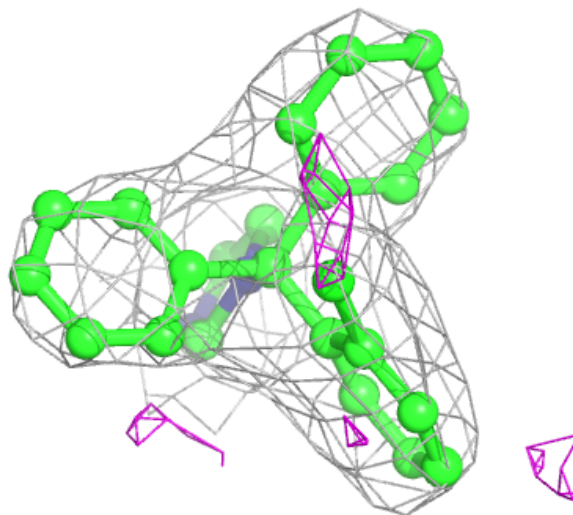
Electron density around CL6 F 502:

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mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
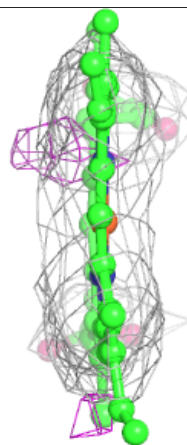and green (positive)
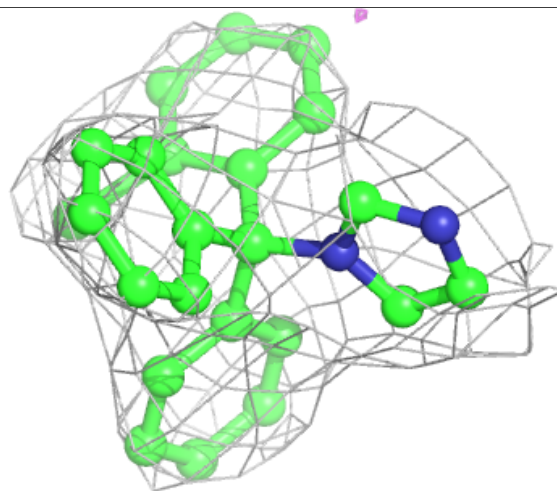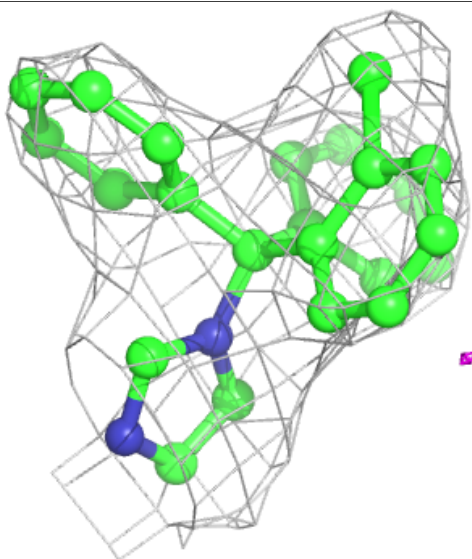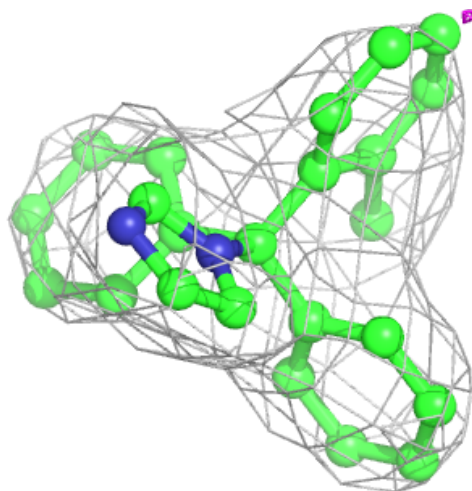
Electron density around HEM C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
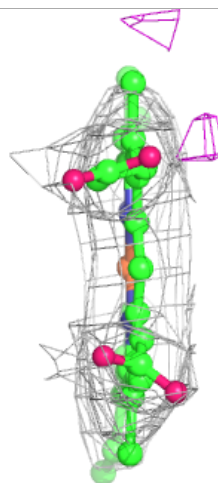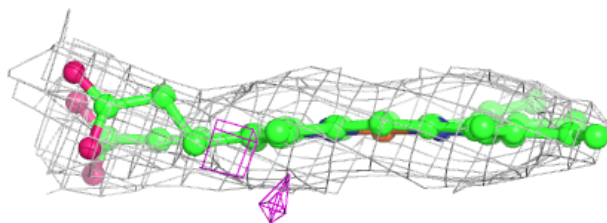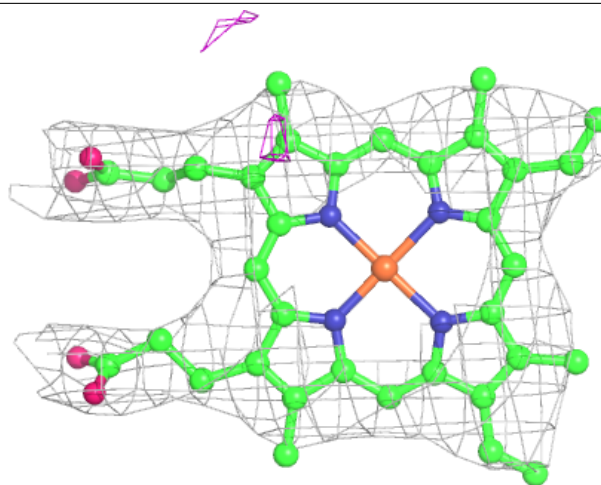
Electron density around HEM D 501:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
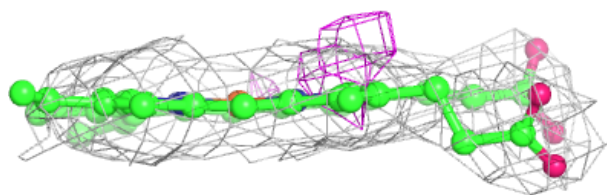and green (positive)
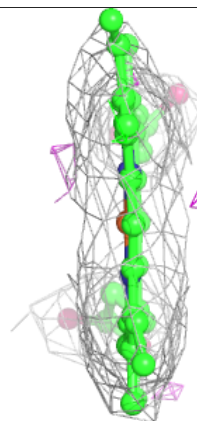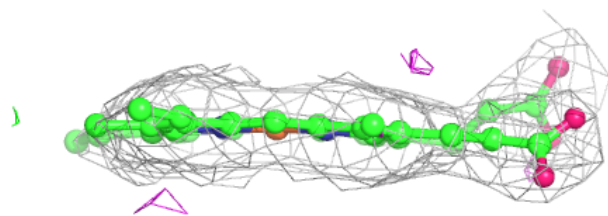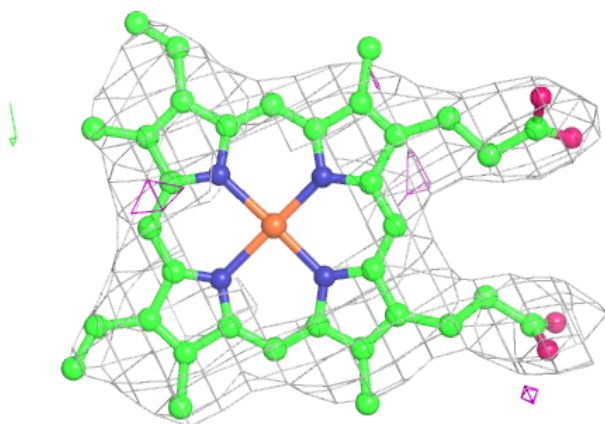
Electron density around HEM B 501:

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

Electron density around CL6 B 502:

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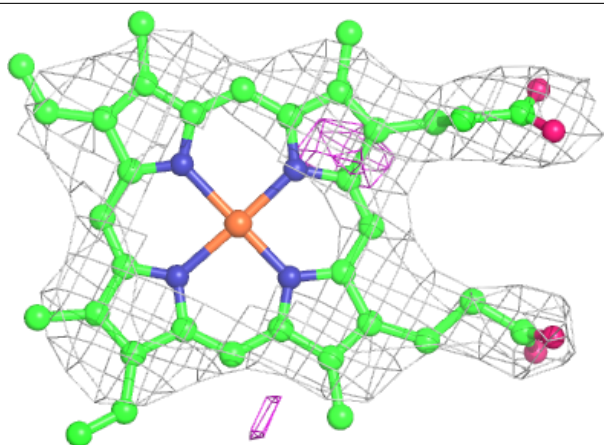and green (positive)
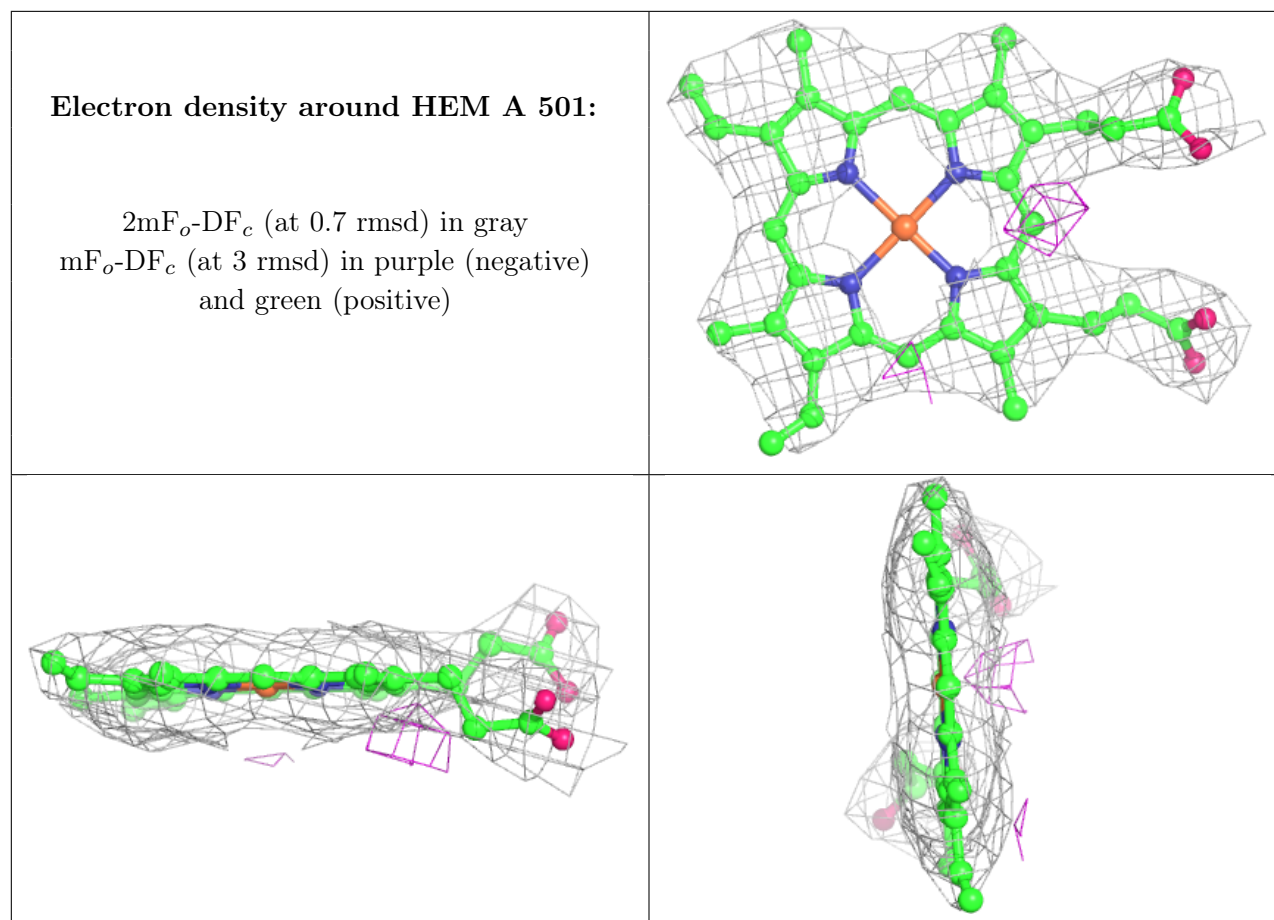
Electron density around HEM E 501:

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

Electron density around HEM F 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 HEM A 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.