



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 10:23 pm BST

PDB ID : 3QU8
Title : Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with the inhibitor 4-(4-Nitrobenzyl)pyridine.
Authors : Shah, M.B.; Pascual, J.; Stout, C.D.; Halpert, J.R.
Deposited on : 2011-02-23
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

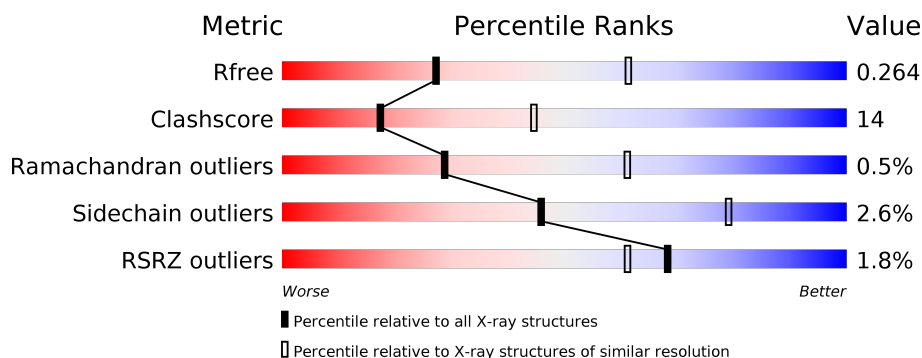
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	A	476	<div> <div></div> <div>76%18% . .</div> </div>
1	B	476	<div> <div>%</div> <div>77%17% . .</div> </div>
1	C	476	<div> <div></div> <div>76%19% . .</div> </div>
1	D	476	<div> <div>%</div> <div>76%20% . .</div> </div>
1	E	476	<div> <div>%</div> <div>73%22% . .</div> </div>
1	F	476	<div> <div>7%</div> <div>71%22% . 5%</div> </div>

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	CM5	D	604	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22964 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 Cytochrome P450 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3732	2416	641	658	17			
1	B	459	Total	C	N	O	S	0	0	0
			3713	2403	639	655	16			
1	C	462	Total	C	N	O	S	0	0	0
			3724	2408	642	658	16			
1	D	458	Total	C	N	O	S	0	0	0
			3693	2389	635	653	16			
1	E	459	Total	C	N	O	S	0	0	0
			3717	2406	640	655	16			
1	F	453	Total	C	N	O	S	0	0	0
			3649	2359	625	649	16			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813

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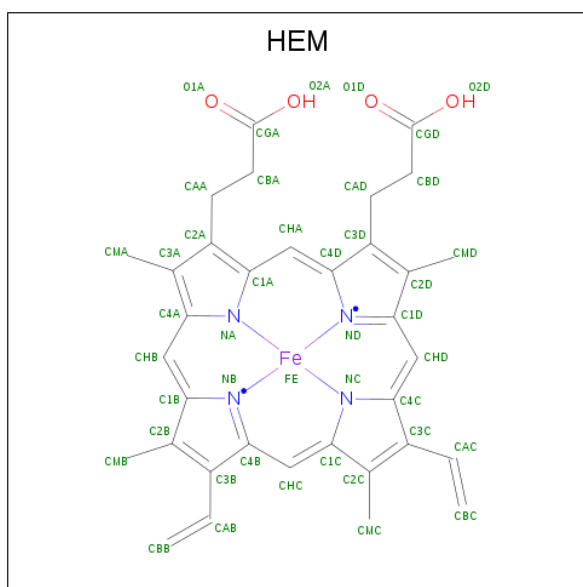
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813
C	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
C	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
C	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
C	26	SER	THR	ENGINEERED MUTATION	UNP P20813
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
C	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
C	492	HIS	-	EXPRESSION TAG	UNP P20813
C	493	HIS	-	EXPRESSION TAG	UNP P20813
C	494	HIS	-	EXPRESSION TAG	UNP P20813
C	495	HIS	-	EXPRESSION TAG	UNP P20813
D	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
D	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
D	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
D	26	SER	THR	ENGINEERED MUTATION	UNP P20813
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
D	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
D	492	HIS	-	EXPRESSION TAG	UNP P20813
D	493	HIS	-	EXPRESSION TAG	UNP P20813
D	494	HIS	-	EXPRESSION TAG	UNP P20813

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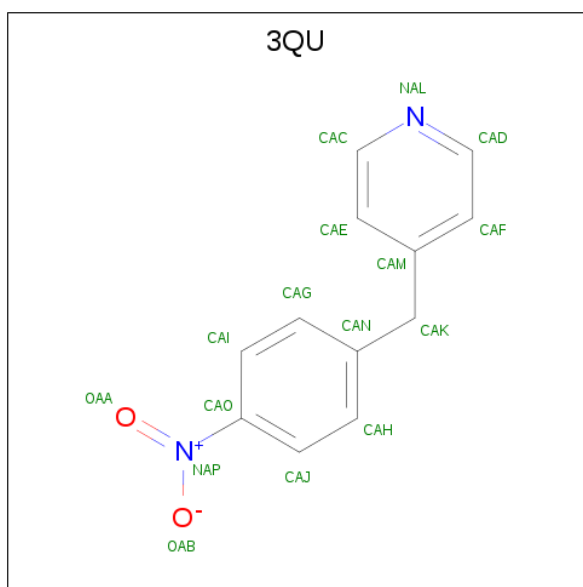
Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	EXPRESSION TAG	UNP P20813
E	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
E	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
E	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
E	26	SER	THR	ENGINEERED MUTATION	UNP P20813
E	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
E	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
E	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
E	492	HIS	-	EXPRESSION TAG	UNP P20813
E	493	HIS	-	EXPRESSION TAG	UNP P20813
E	494	HIS	-	EXPRESSION TAG	UNP P20813
E	495	HIS	-	EXPRESSION TAG	UNP P20813
F	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
F	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
F	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
F	26	SER	THR	ENGINEERED MUTATION	UNP P20813
F	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
F	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
F	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
F	492	HIS	-	EXPRESSION TAG	UNP P20813
F	493	HIS	-	EXPRESSION TAG	UNP P20813
F	494	HIS	-	EXPRESSION TAG	UNP P20813
F	495	HIS	-	EXPRESSION TAG	UNP P20813

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



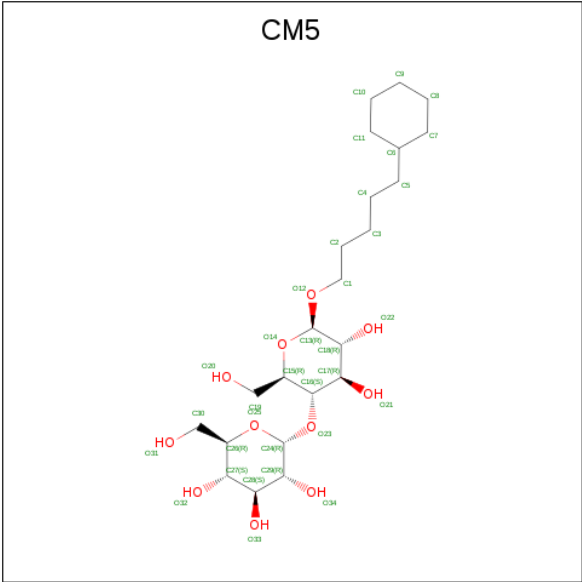
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 4-(4-nitrobenzyl)pyridine (three-letter code: 3QU) (formula: $C_{12}H_{10}N_2O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			7	6	1		
3	B	1	Total	C	N	0	0
			16	12	2		
3	C	1	Total	C	N	0	0
			7	6	1		
3	D	1	Total	C	N	0	0
			13	12	1		
3	E	1	Total	C	N	0	0
			13	12	1		

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: C₂₃H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			34	23	11		
4	B	1	Total	C	O	0	0
			34	23	11		
4	B	1	Total	C	O	0	0
			34	23	11		
4	C	1	Total	C	O	0	0
			34	23	11		
4	D	1	Total	C	O	0	0
			34	23	11		
4	D	1	Total	C	O	0	0
			34	23	11		
4	E	1	Total	C	O	0	0
			34	23	11		
4	F	1	Total	C	O	0	0
			34	23	11		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	23	Total	O	0	0
			23	23		
5	C	29	Total	O	0	0
			29	29		
5	D	38	Total	O	0	0
			38	38		

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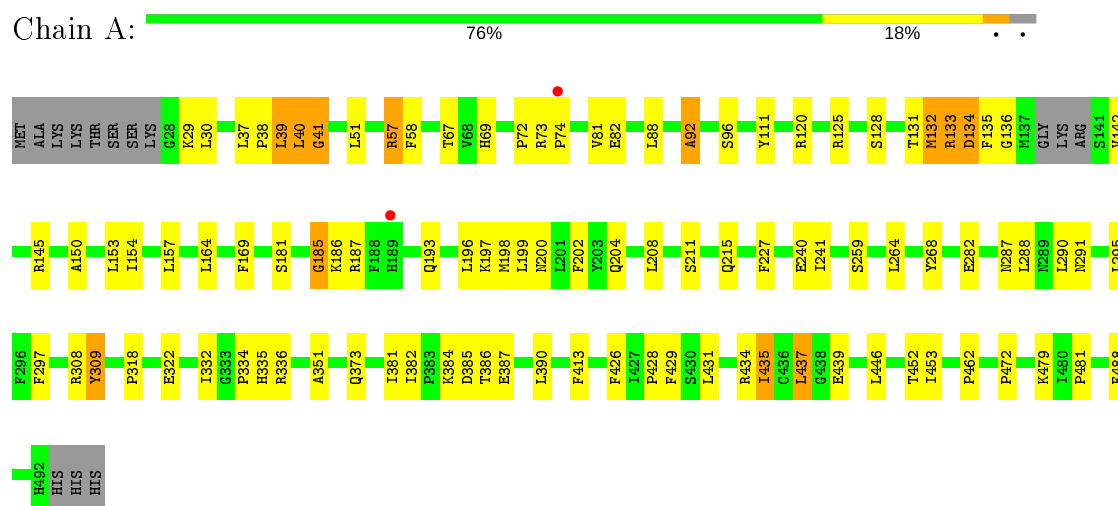
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	23	Total 23	O 23	0	0
5	F	12	Total 12	O 12	0	0

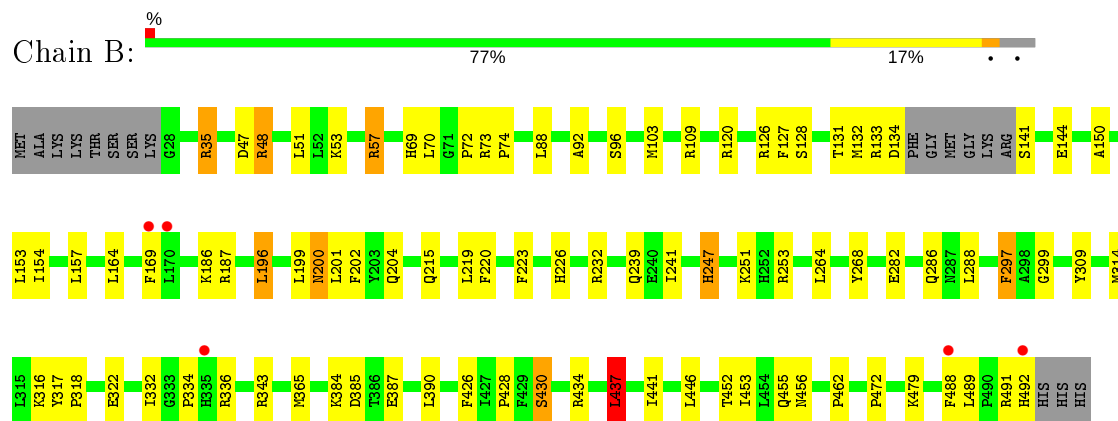
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

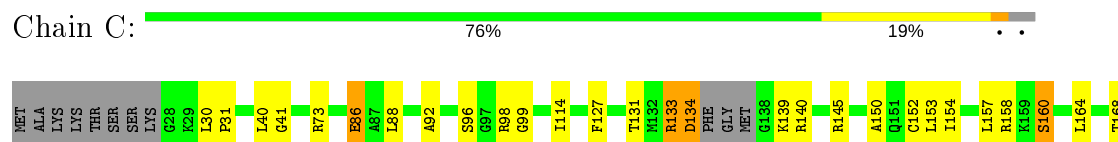
• Molecule 1: Cytochrome P450 2B6



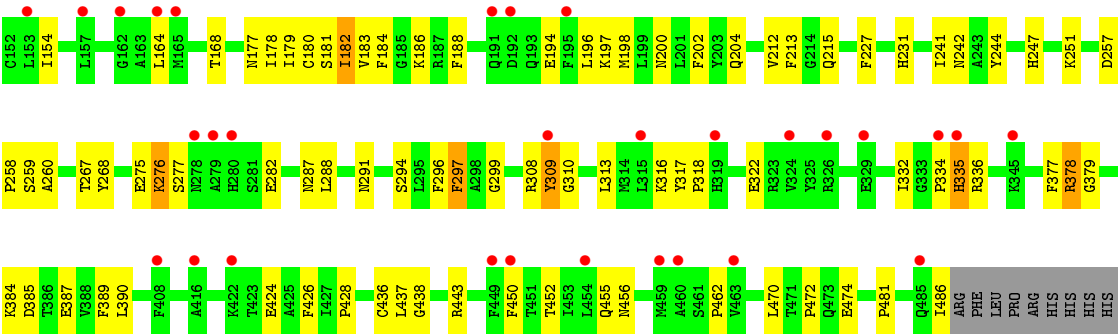
• Molecule 1: Cytochrome P450 2B6



• Molecule 1: Cytochrome P450 2B6







4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	101.88Å 101.88Å 299.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.51 – 2.80 50.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.51-2.80) 88.9 (50.22-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.218 , 0.259 0.226 , 0.264	Depositor DCC
R_{free} test set	3810 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l 0.149 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22964	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: HEM, CM5, 3QU

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	0.84	0/3833	0.75	1/5185 (0.0%)
1	B	0.83	0/3813	0.78	4/5158 (0.1%)
1	C	0.90	2/3822 (0.1%)	0.76	1/5167 (0.0%)
1	D	0.83	0/3791	0.78	2/5129 (0.0%)
1	E	0.82	0/3817	0.75	0/5162
1	F	0.95	1/3745 (0.0%)	0.78	0/5067
All	All	0.86	3/22821 (0.0%)	0.77	8/30868 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	450	PHE	CE2-CZ	5.42	1.47	1.37
1	C	152	CYS	CB-SG	-5.35	1.73	1.81
1	C	86	GLU	CG-CD	5.07	1.59	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	474	GLU	CB-CA-C	-5.88	98.64	110.40
1	A	185	GLY	N-CA-C	5.46	126.76	113.10
1	C	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	103	MET	CG-SD-CE	-5.40	91.57	100.20

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	3732	0	3712	103	0
1	B	3713	0	3702	93	0
1	C	3724	0	3711	83	0
1	D	3693	0	3682	97	0
1	E	3717	0	3713	117	0
1	F	3649	0	3635	100	0
2	A	43	0	30	10	0
2	B	43	0	30	4	0
2	C	43	0	30	9	0
2	D	43	0	30	12	0
2	E	43	0	30	9	0
2	F	43	0	30	18	0
3	A	7	0	4	0	0
3	B	16	0	10	0	0
3	C	7	0	4	0	0
3	D	13	0	10	0	0
3	E	13	0	10	1	0
4	A	34	0	35	1	0
4	B	68	0	77	34	0
4	C	34	0	40	5	0
4	D	68	0	78	12	0
4	E	34	0	40	3	0
4	F	34	0	38	5	0
5	A	25	0	0	1	0
5	B	23	0	0	12	0
5	C	29	0	0	2	0
5	D	38	0	0	5	0
5	E	23	0	0	5	0
5	F	12	0	0	5	0
All	All	22964	0	22681	629	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 14.

The worst 5 of 629 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:608:CM5:C16	4:B:608:CM5:O23	1.64	1.42
4:B:608:CM5:H17	4:B:608:CM5:C24	1.61	1.28
1:A:381:ILE:HG21	1:B:239:GLN:CG	1.65	1.25
1:A:136:GLY:HA2	1:A:142:VAL:CG2	1.65	1.24
1:B:232:ARG:HH12	4:B:602:CM5:C19	1.48	1.24

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	A	458/476 (96%)	436 (95%)	18 (4%)	4 (1%)	17	46
1	B	455/476 (96%)	431 (95%)	21 (5%)	3 (1%)	22	53
1	C	456/476 (96%)	424 (93%)	30 (7%)	2 (0%)	34	66
1	D	454/476 (95%)	424 (93%)	28 (6%)	2 (0%)	34	66
1	E	455/476 (96%)	433 (95%)	22 (5%)	0	100	100
1	F	449/476 (94%)	417 (93%)	29 (6%)	3 (1%)	22	53
All	All	2727/2856 (96%)	2565 (94%)	148 (5%)	14 (0%)	29	61

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	430	SER
1	F	276	LYS
1	F	378	ARG
1	B	430	SER
1	C	190	TYR

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	404/418 (97%)	392 (97%)	12 (3%)	41	75
1	B	403/418 (96%)	391 (97%)	12 (3%)	41	75
1	C	402/418 (96%)	393 (98%)	9 (2%)	52	83
1	D	400/418 (96%)	394 (98%)	6 (2%)	65	89
1	E	404/418 (97%)	390 (96%)	14 (4%)	36	70
1	F	396/418 (95%)	387 (98%)	9 (2%)	50	82
All	All	2409/2508 (96%)	2347 (97%)	62 (3%)	46	79

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	187	ARG
1	D	189	HIS
1	F	186	LYS
1	C	309	TYR
1	D	196	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	231	HIS
1	E	286	GLN
1	C	285	HIS
1	B	455	GLN
1	E	226	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

19 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	$\# Z > 2$
4	CM5	B	608	-	36,36,36	3.20	15 (41%)	49,49,49	5.85	26 (53%)
2	HEM	F	500	1	27,50,50	2.19	5 (18%)	17,82,82	1.38	1 (5%)
4	CM5	F	606	-	36,36,36	3.06	13 (36%)	49,49,49	4.26	25 (51%)
4	CM5	B	602	-	36,36,36	2.89	9 (25%)	49,49,49	4.81	23 (46%)
3	3QU	A	501	2	7,7,17	0.26	0	8,8,22	1.24	0
3	3QU	E	501	2	14,14,17	0.78	0	17,17,22	0.91	1 (5%)
4	CM5	E	605	-	36,36,36	3.51	14 (38%)	49,49,49	3.18	23 (46%)
2	HEM	C	500	1,3	27,50,50	2.79	10 (37%)	17,82,82	1.86	4 (23%)
3	3QU	D	501	2	14,14,17	0.32	0	17,17,22	0.88	0
2	HEM	E	500	1,3	27,50,50	2.19	5 (18%)	17,82,82	1.39	1 (5%)
2	HEM	B	500	1,3	27,50,50	2.15	8 (29%)	17,82,82	2.67	6 (35%)
3	3QU	B	501	2	16,17,17	0.69	1 (6%)	20,22,22	1.79	5 (25%)
2	HEM	A	500	1,3	27,50,50	2.19	5 (18%)	17,82,82	1.38	1 (5%)
4	CM5	D	604	-	36,36,36	4.17	16 (44%)	49,49,49	6.24	24 (48%)
3	3QU	C	501	2	7,7,17	0.26	0	8,8,22	1.23	0
4	CM5	A	601	-	36,36,36	4.23	16 (44%)	49,49,49	5.36	26 (53%)
2	HEM	D	500	1,3	27,50,50	2.19	5 (18%)	17,82,82	1.40	1 (5%)
4	CM5	D	607	-	36,36,36	3.58	13 (36%)	49,49,49	4.87	26 (53%)
4	CM5	C	603	-	36,36,36	3.39	13 (36%)	49,49,49	5.31	22 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CM5	B	608	-	-	11/17/65/65	0/3/3/3
2	HEM	F	500	1	-	2/6/54/54	-
4	CM5	F	606	-	-	5/17/65/65	0/3/3/3
4	CM5	B	602	-	-	9/17/65/65	0/3/3/3
3	3QU	A	501	2	-	-	0/1/1/2
2	HEM	A	500	1,3	-	2/6/54/54	-
4	CM5	E	605	-	-	9/17/65/65	0/3/3/3
2	HEM	C	500	1,3	-	2/6/54/54	-
3	3QU	D	501	2	-	0/4/4/8	0/2/2/2
2	HEM	E	500	1,3	-	0/6/54/54	-
2	HEM	B	500	1,3	-	0/6/54/54	-
3	3QU	B	501	2	-	0/6/8/8	0/2/2/2
3	3QU	E	501	2	-	0/4/4/8	0/2/2/2
4	CM5	D	604	-	1/1/11/11	9/17/65/65	0/3/3/3
3	3QU	C	501	2	-	-	0/1/1/2
4	CM5	A	601	-	-	11/17/65/65	0/3/3/3
2	HEM	D	500	1,3	-	0/6/54/54	-
4	CM5	D	607	-	-	13/17/65/65	0/3/3/3
4	CM5	C	603	-	-	11/17/65/65	0/3/3/3

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	CM5	O21-C17	-13.58	1.11	1.43
4	C	603	CM5	O23-C24	-13.41	1.04	1.41
4	D	604	CM5	C29-C28	-11.25	1.23	1.52
4	E	605	CM5	O23-C24	-11.11	1.10	1.41
4	D	604	CM5	O25-C26	-10.83	1.18	1.44

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	604	CM5	O23-C16-C17	18.91	157.57	107.28
4	C	603	CM5	O33-C28-C27	-17.60	69.67	110.35
4	B	608	CM5	O14-C15-C19	-17.31	63.38	106.44
4	F	606	CM5	O12-C13-C18	-17.22	81.43	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	CM5	O33-C28-C29	-17.03	70.97	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	CM5	C16

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	CM5	C18-C13-O12-C1
4	B	602	CM5	O14-C13-O12-C1
2	A	500	HEM	C1A-C2A-CAA-CBA
2	A	500	HEM	C3A-C2A-CAA-CBA
4	A	601	CM5	C2-C1-O12-C13

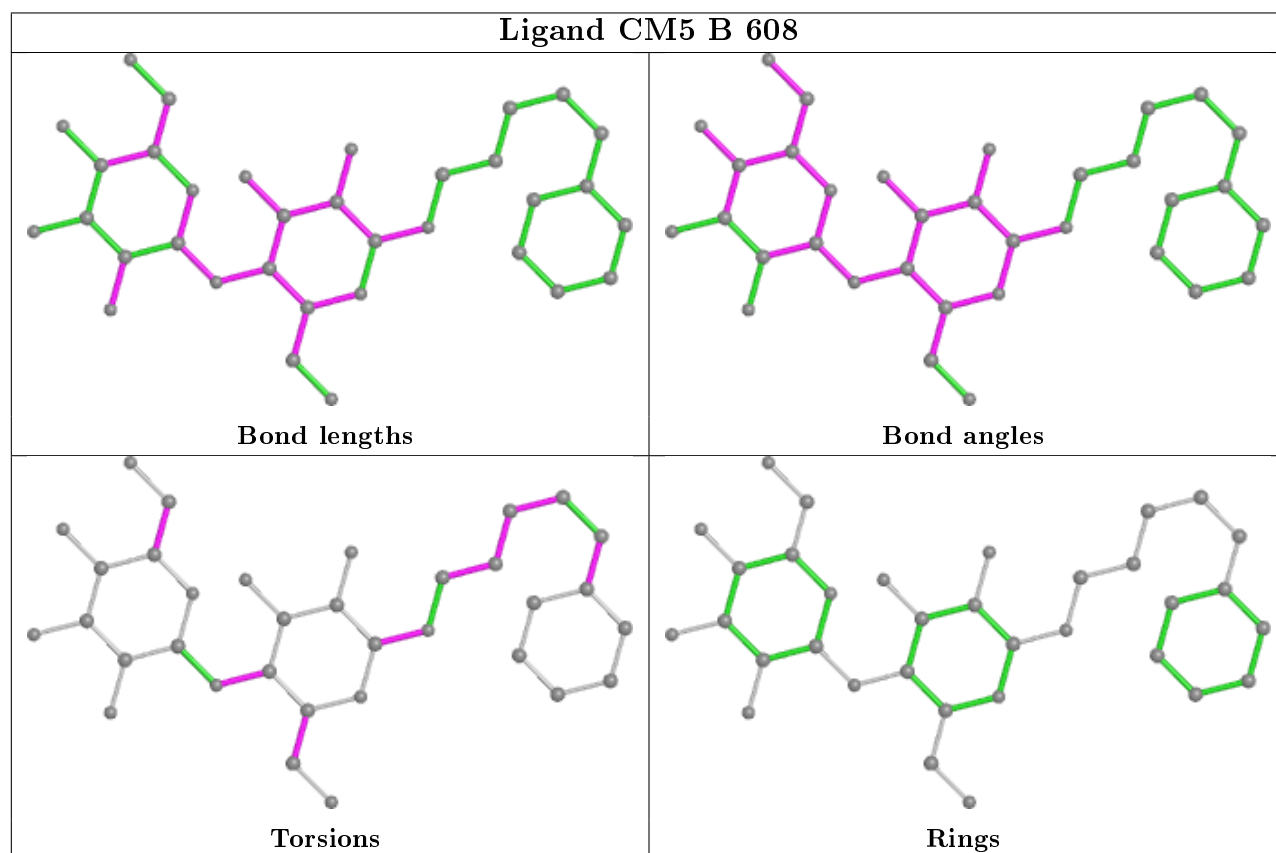
There are no ring outliers.

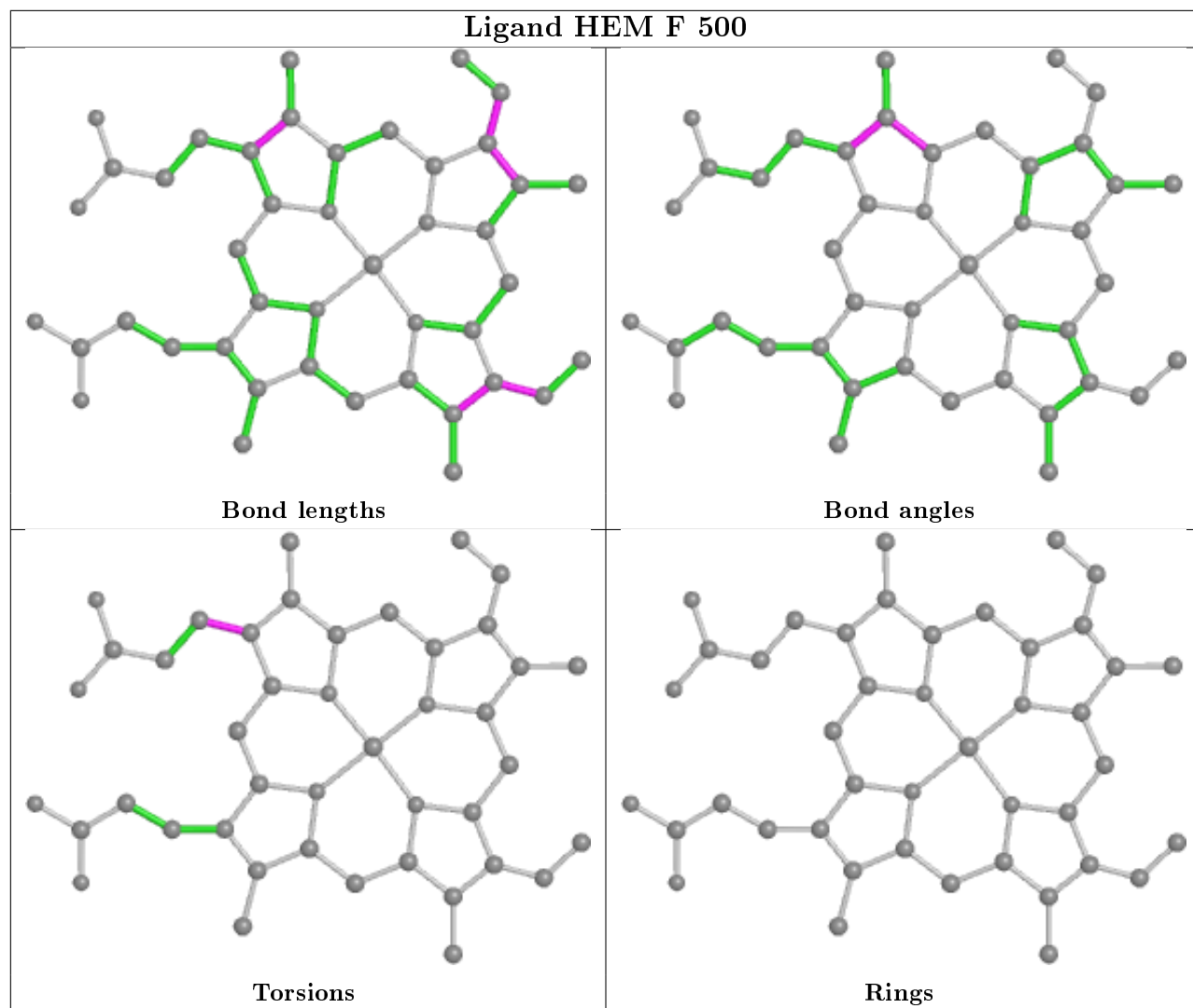
15 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	608	CM5	20	0
2	F	500	HEM	18	0
4	F	606	CM5	5	0
4	B	602	CM5	14	0
3	E	501	3QU	1	0
4	E	605	CM5	3	0
2	C	500	HEM	9	0
2	E	500	HEM	9	0
2	B	500	HEM	4	0
2	A	500	HEM	10	0
4	D	604	CM5	4	0
4	A	601	CM5	1	0
2	D	500	HEM	12	0
4	D	607	CM5	8	0
4	C	603	CM5	5	0

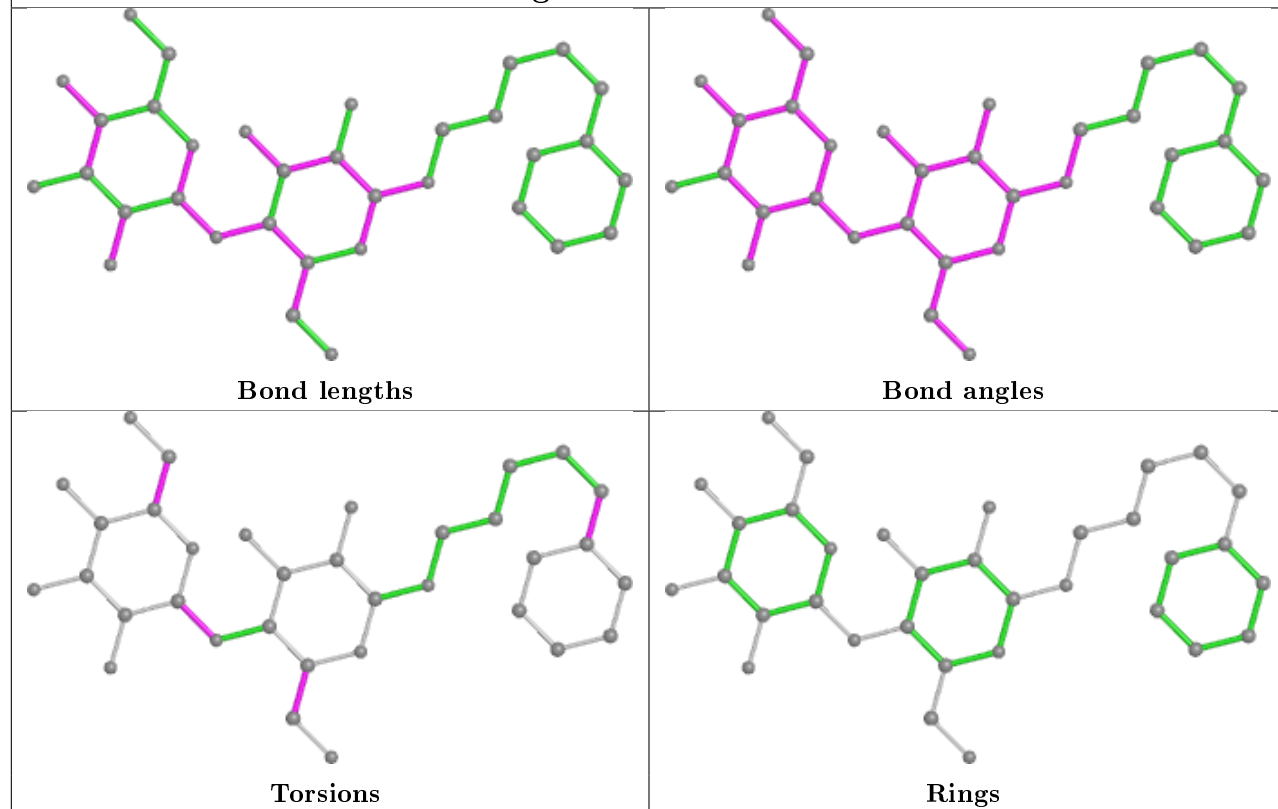
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

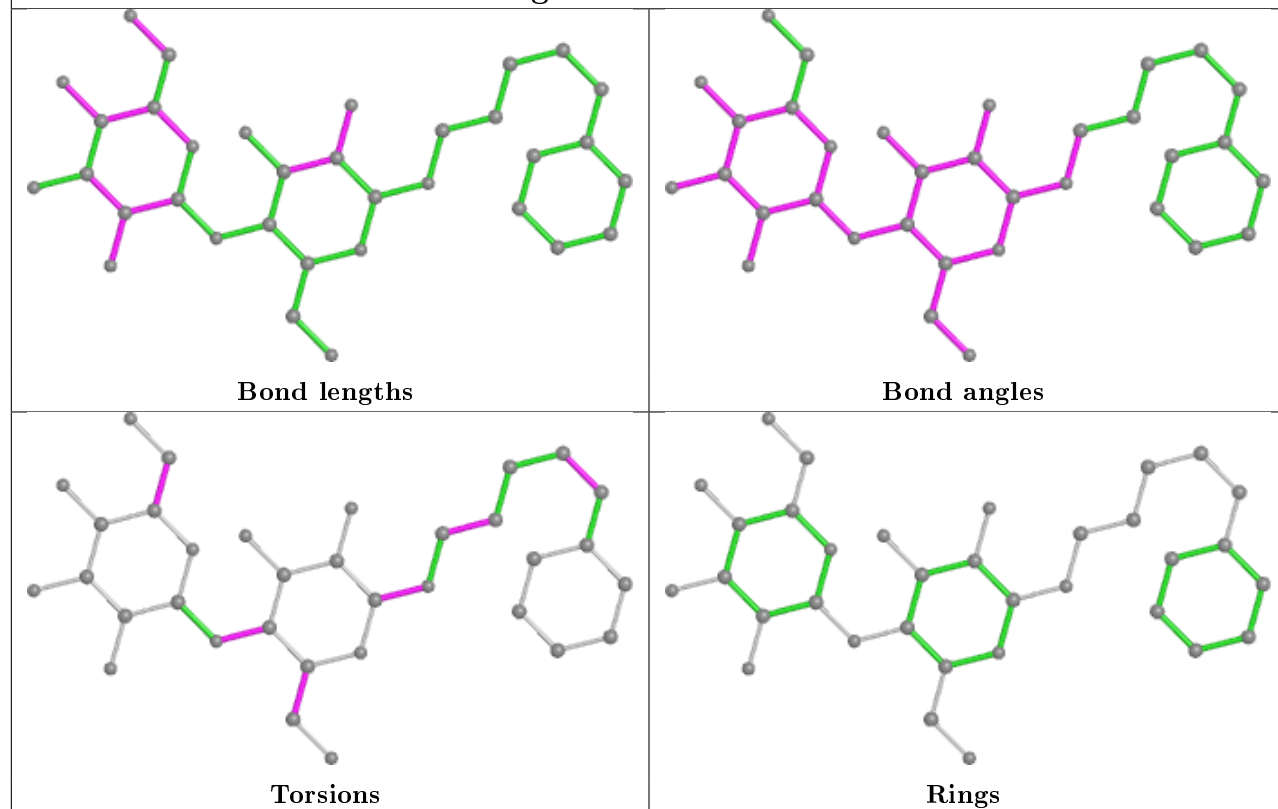


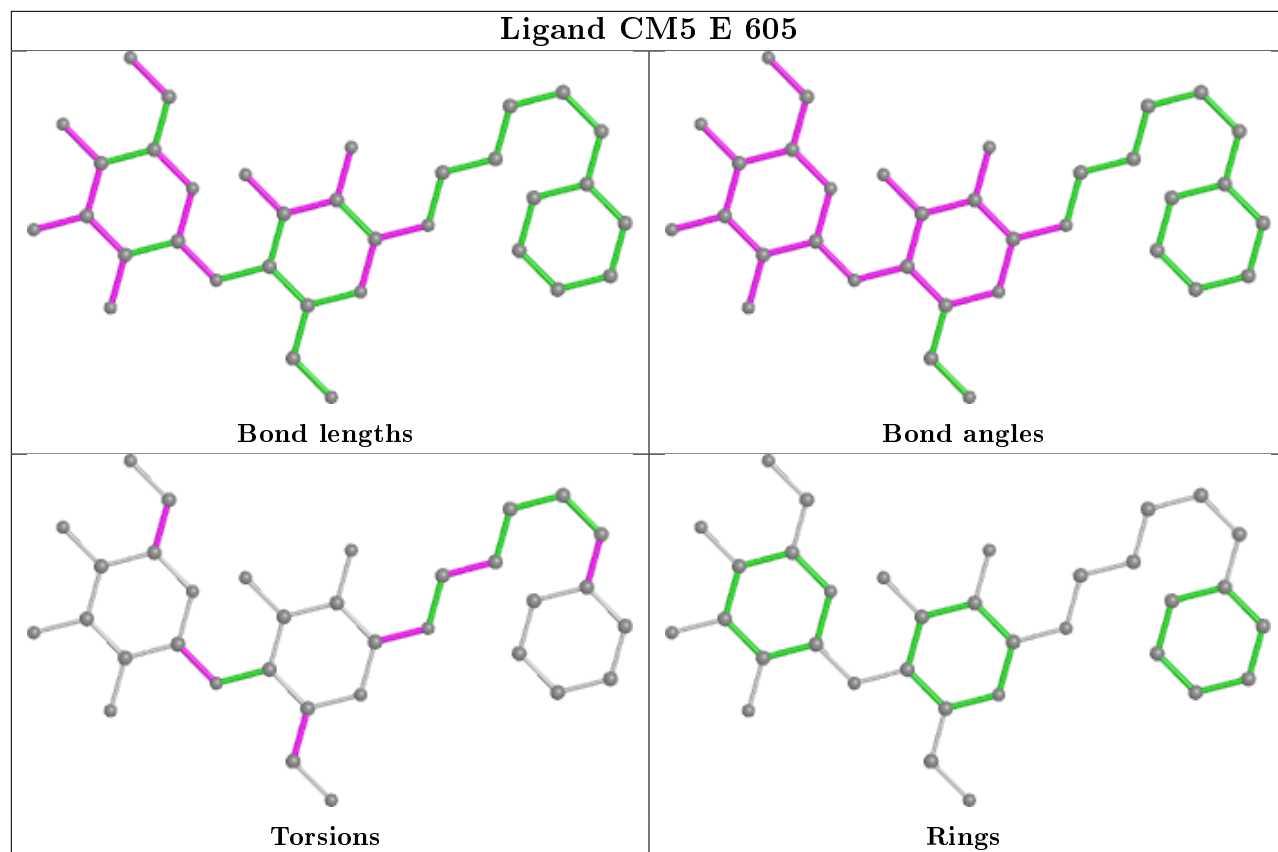


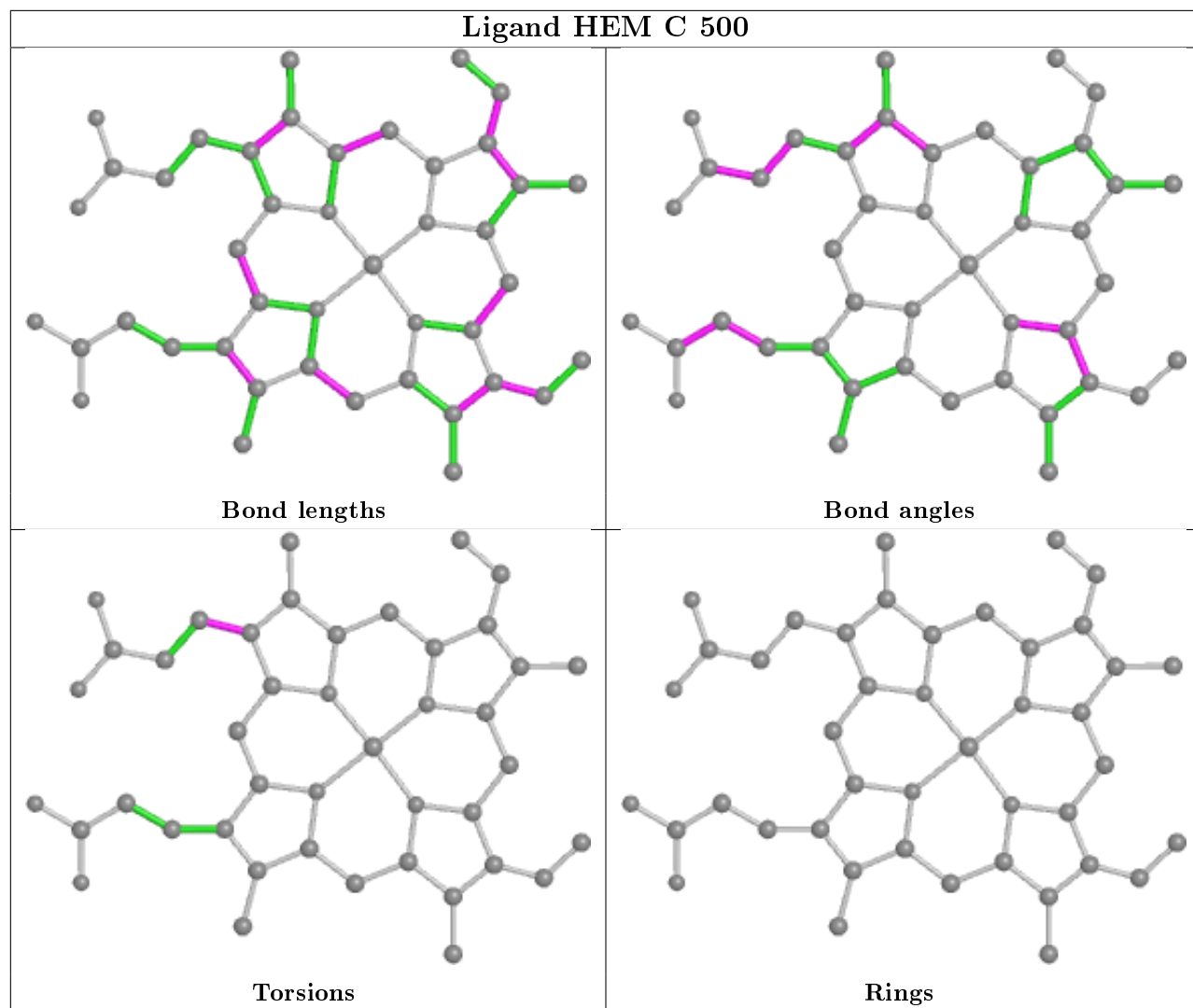
Ligand CM5 F 606

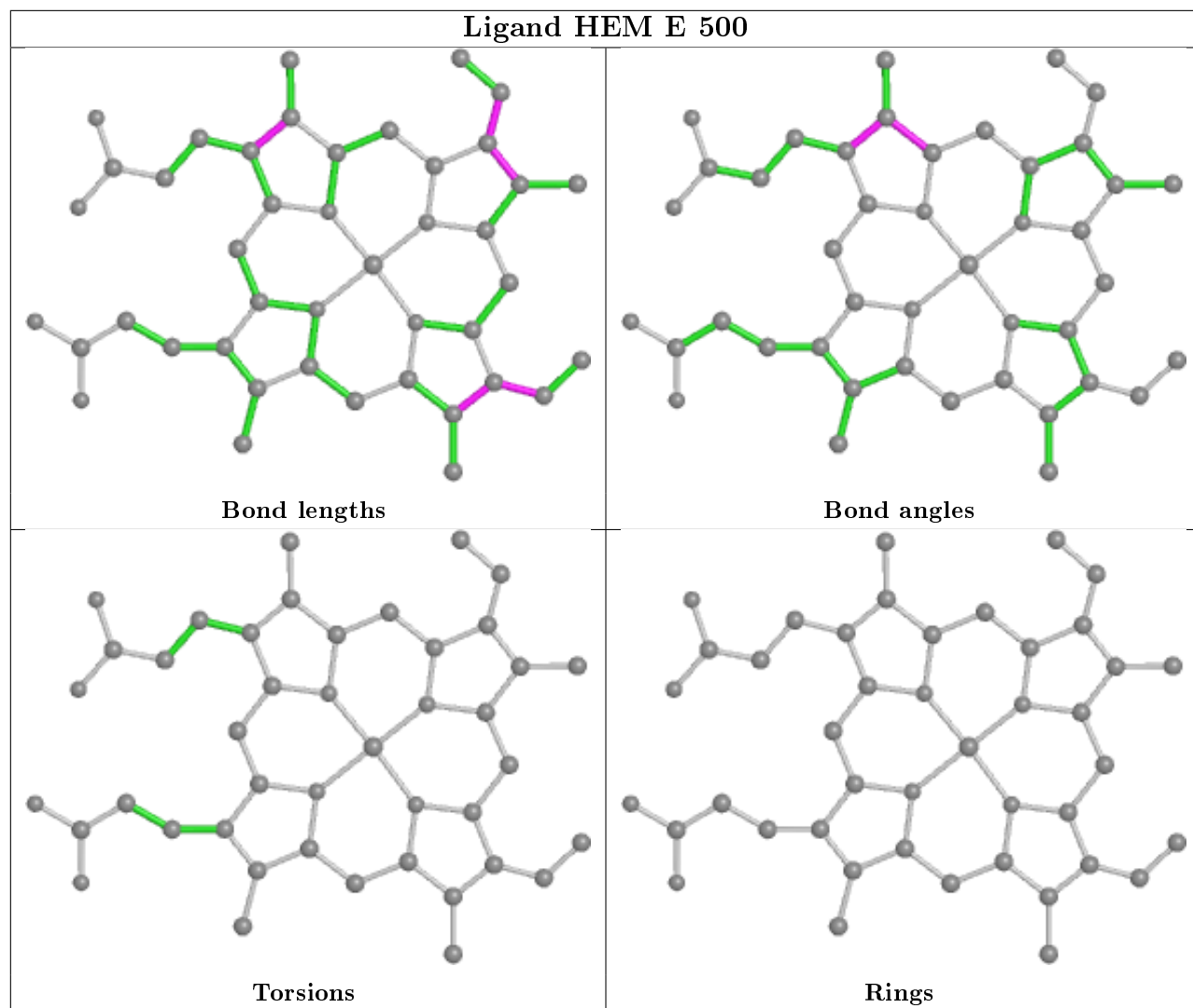


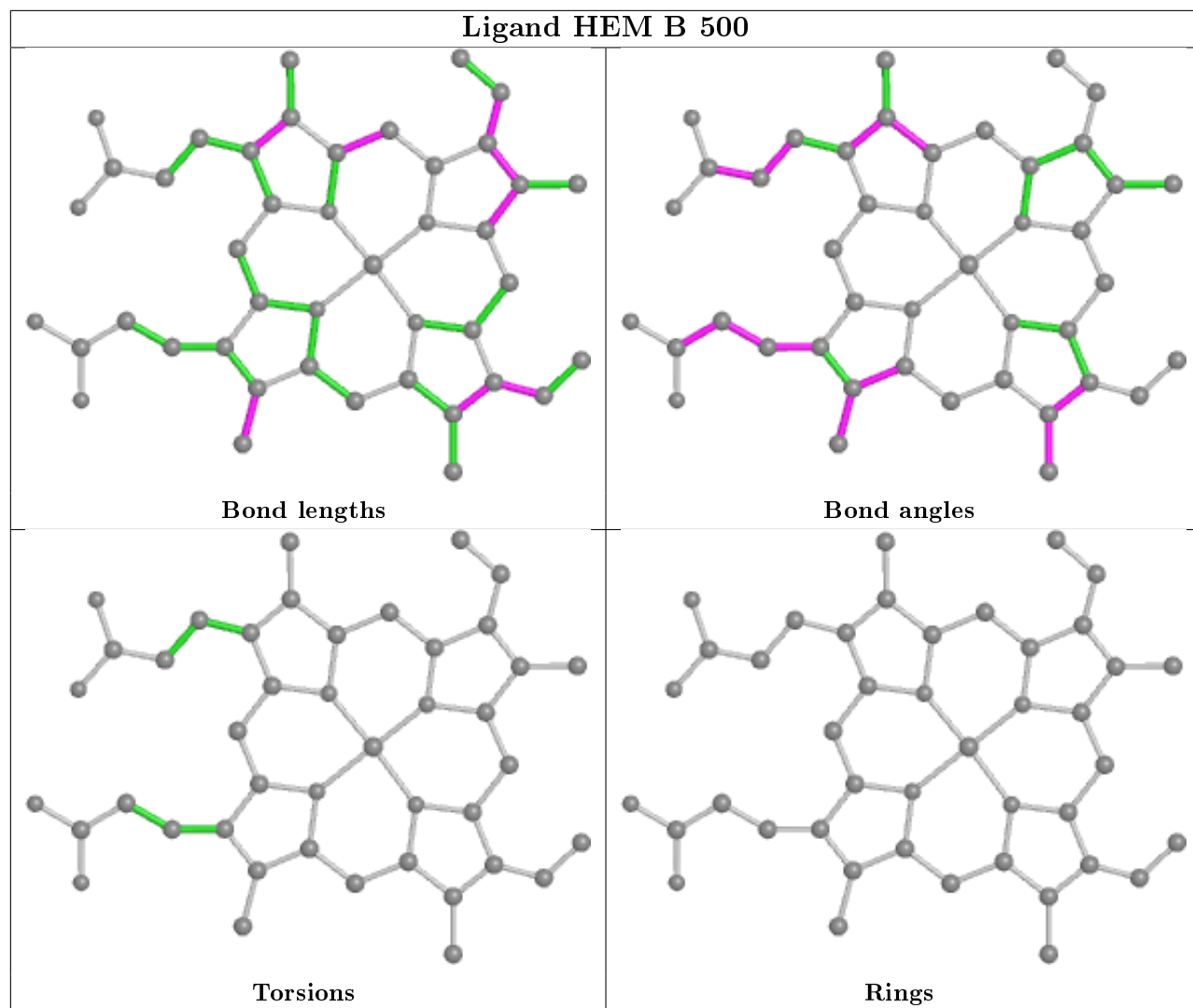
Ligand CM5 B 602

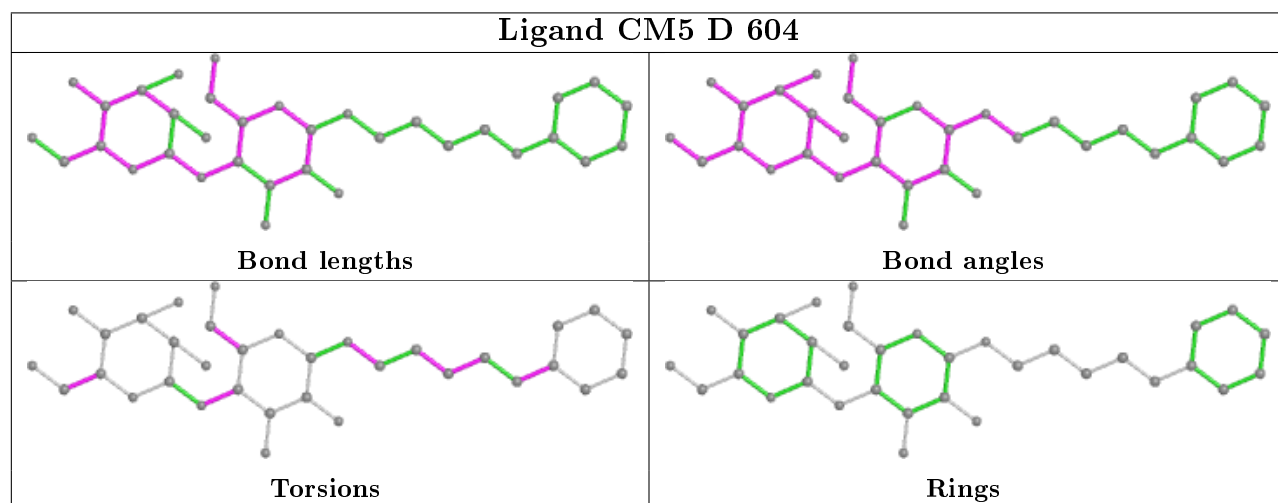
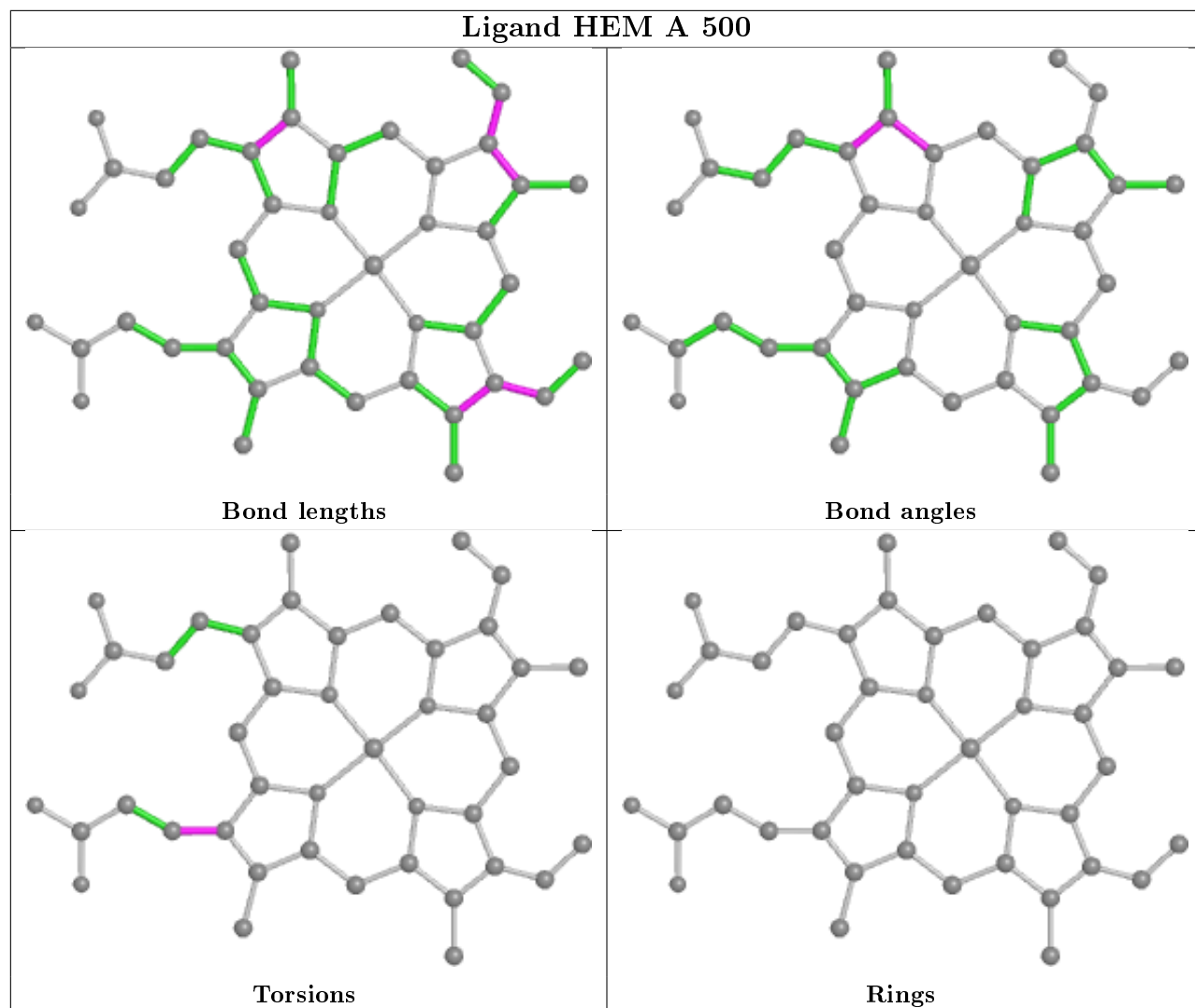


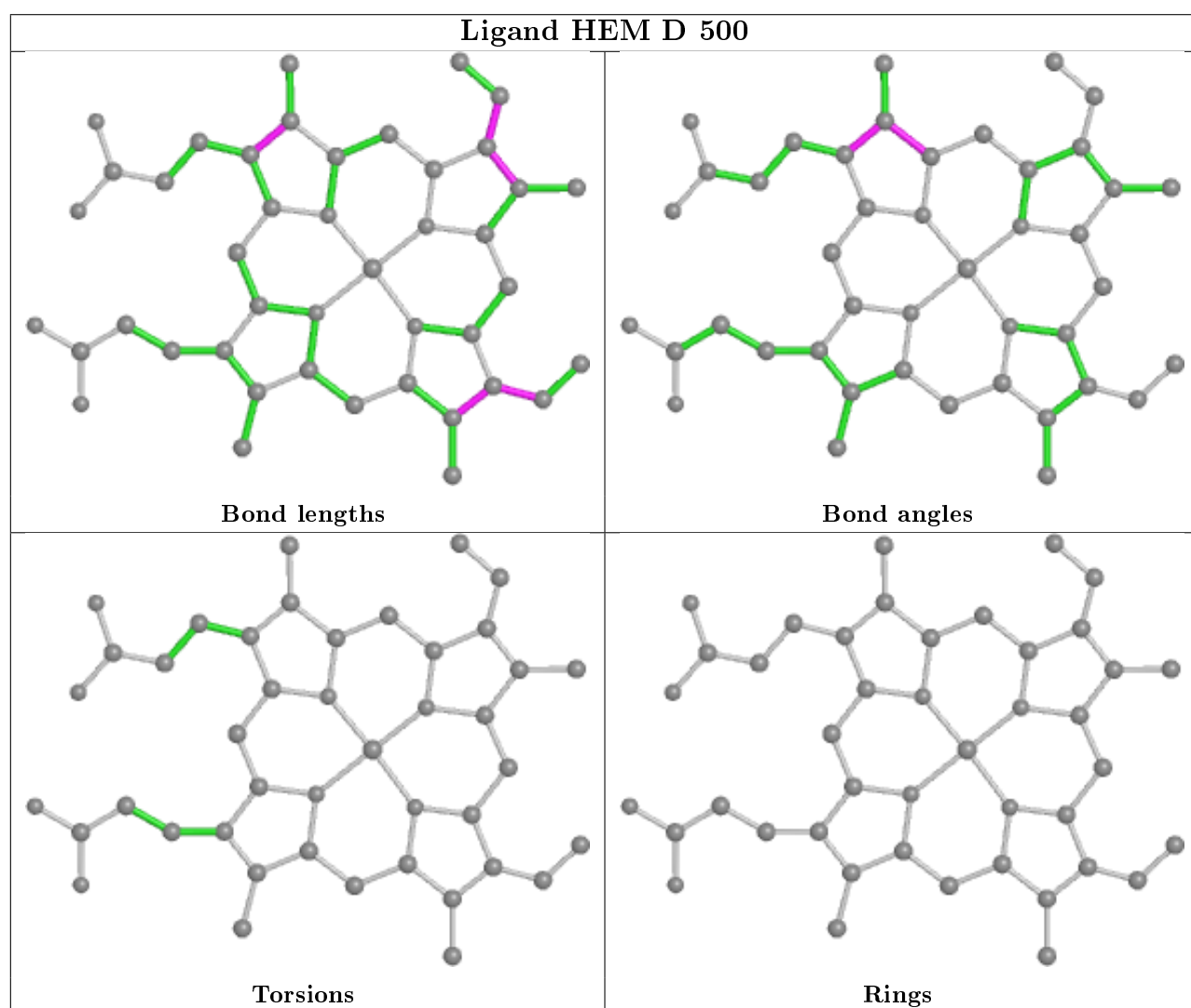
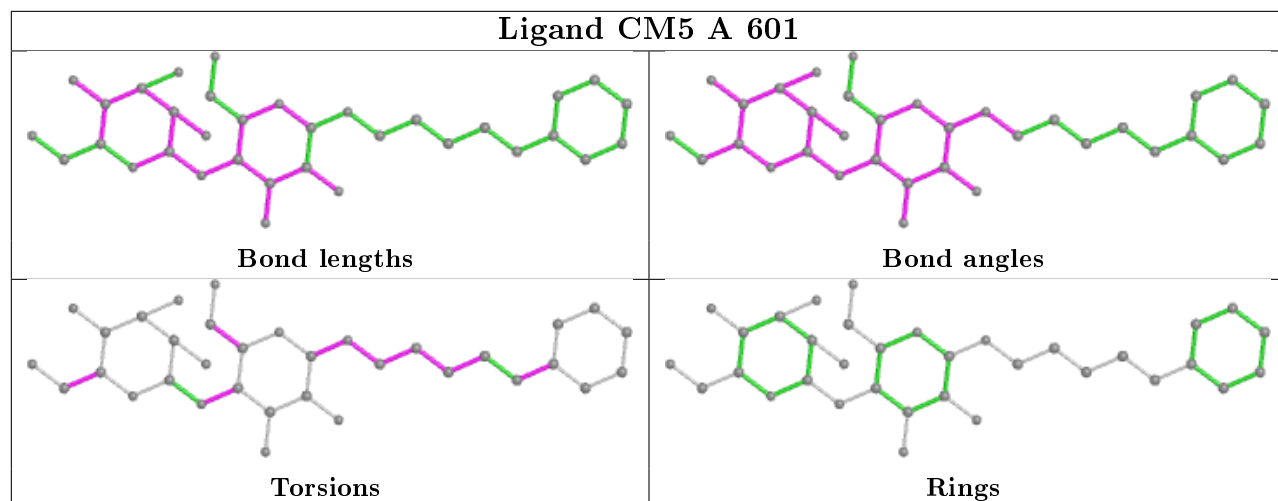


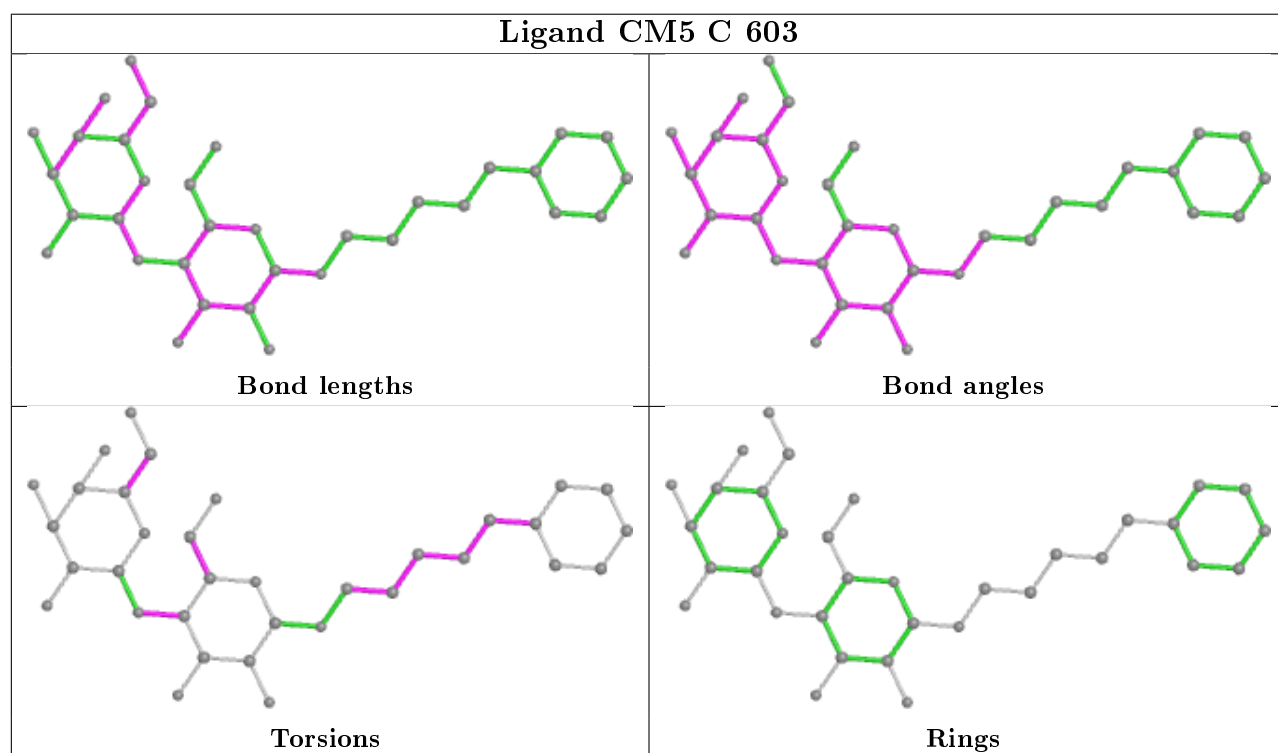
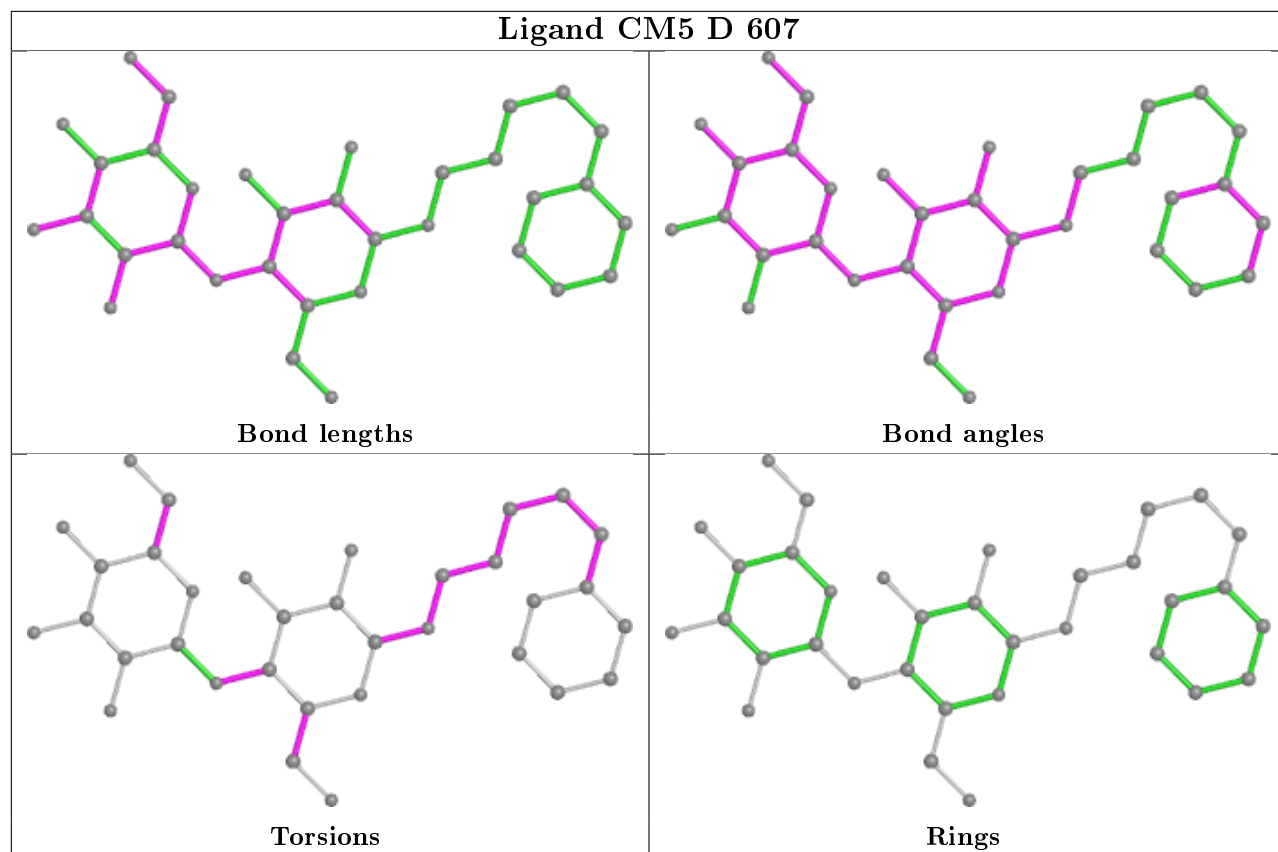












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/476 (97%)	0.09	2 (0%) 92 91	26, 51, 74, 82	0
1	B	459/476 (96%)	0.12	5 (1%) 80 75	28, 51, 74, 82	0
1	C	462/476 (97%)	0.14	2 (0%) 92 91	24, 50, 74, 79	0
1	D	458/476 (96%)	0.07	4 (0%) 84 80	24, 51, 74, 82	0
1	E	459/476 (96%)	0.01	6 (1%) 77 72	26, 51, 74, 87	0
1	F	453/476 (95%)	0.39	31 (6%) 17 10	24, 51, 74, 79	0
All	All	2753/2856 (96%)	0.14	50 (1%) 68 61	24, 51, 74, 87	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	463	VAL	5.7
1	F	153	LEU	4.3
1	F	450	PHE	3.6
1	F	459	MET	3.5
1	F	280	HIS	3.5

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 carbohydrates in this entry.

6.4 Ligands ⓘ

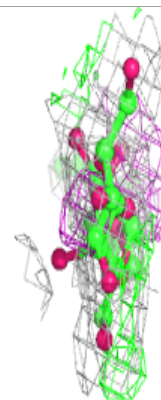
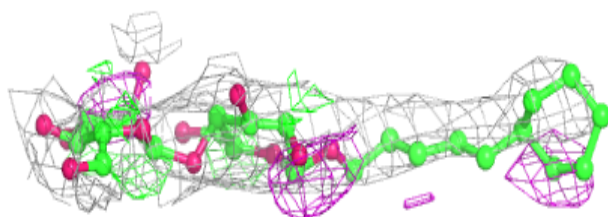
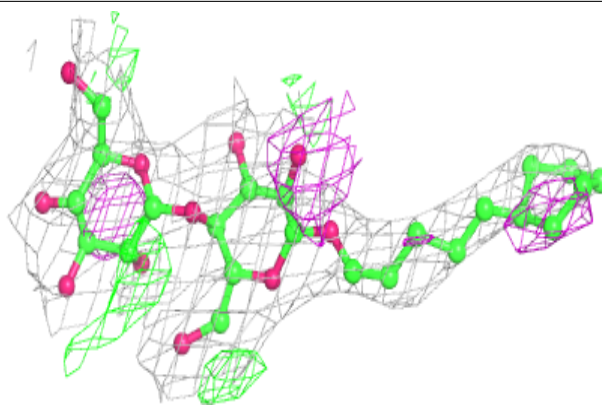
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CM5	F	606	34/34	0.69	0.37	45,62,74,76	0
4	CM5	B	602	34/34	0.69	0.32	61,72,84,85	0
4	CM5	B	608	34/34	0.74	0.26	46,84,100,100	0
4	CM5	D	607	34/34	0.75	0.25	72,97,101,103	0
4	CM5	C	603	34/34	0.76	0.30	54,63,70,71	0
4	CM5	E	605	34/34	0.77	0.28	66,73,91,92	0
4	CM5	A	601	34/34	0.87	0.26	53,60,73,74	0
4	CM5	D	604	34/34	0.88	0.21	58,67,77,79	0
3	3QU	B	501	16/16	0.89	0.41	47,51,60,66	0
3	3QU	D	501	13/16	0.90	0.30	47,49,54,54	0
3	3QU	A	501	7/16	0.90	0.30	47,50,51,52	0
3	3QU	C	501	7/16	0.94	0.26	47,50,51,52	0
2	HEM	F	500	43/43	0.95	0.22	53,65,66,67	0
3	3QU	E	501	13/16	0.95	0.27	55,57,60,63	0
2	HEM	D	500	43/43	0.96	0.22	23,33,38,39	0
2	HEM	A	500	43/43	0.97	0.23	25,31,39,43	0
2	HEM	E	500	43/43	0.97	0.20	17,28,36,40	0
2	HEM	C	500	43/43	0.98	0.16	21,27,36,46	0
2	HEM	B	500	43/43	0.98	0.19	15,20,29,31	0

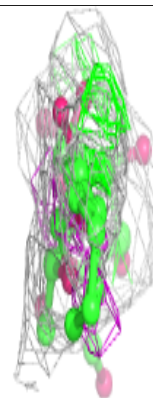
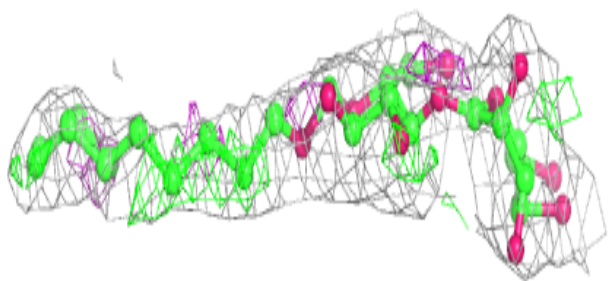
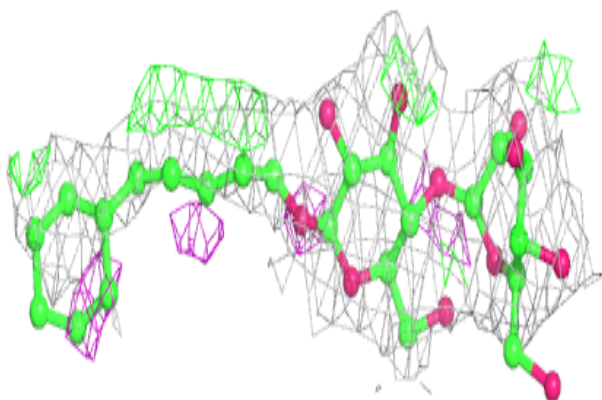
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 F 606:

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

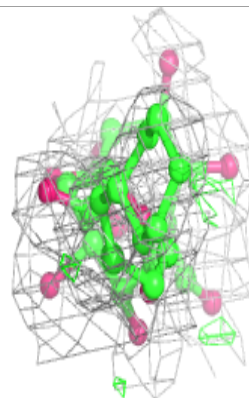
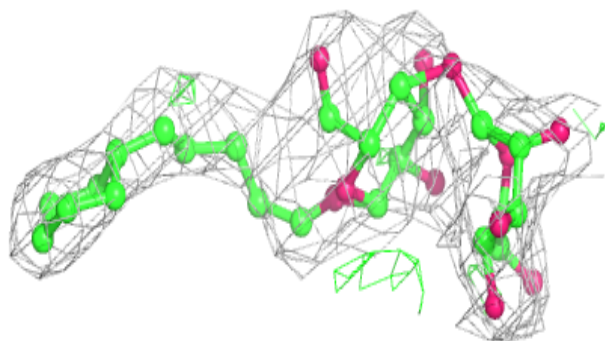
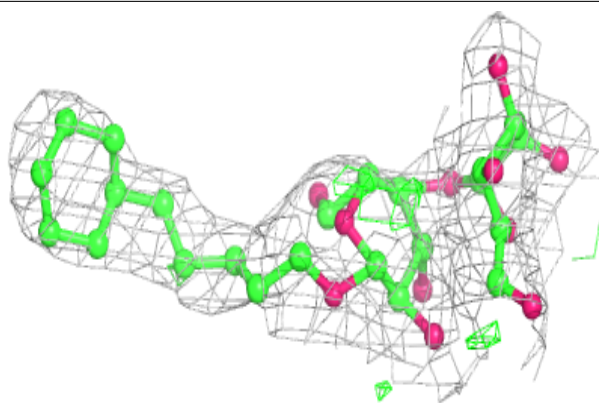
**Electron density around CM5 B 602:**

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

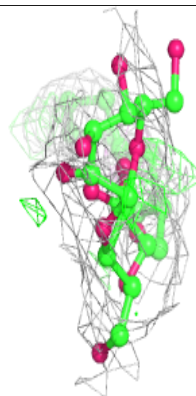
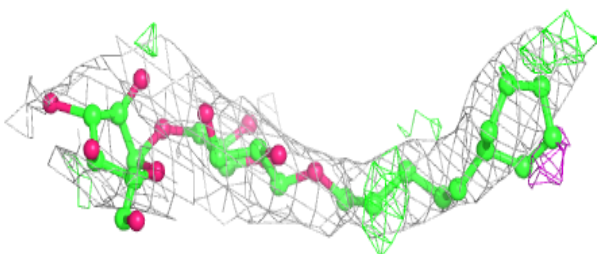
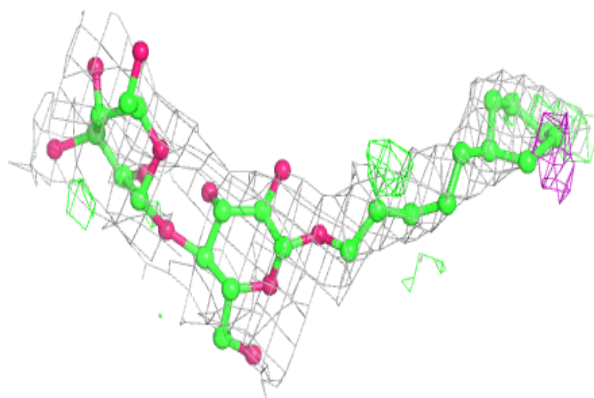


Electron density around CM5 B 608:

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

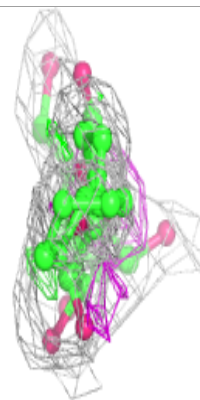
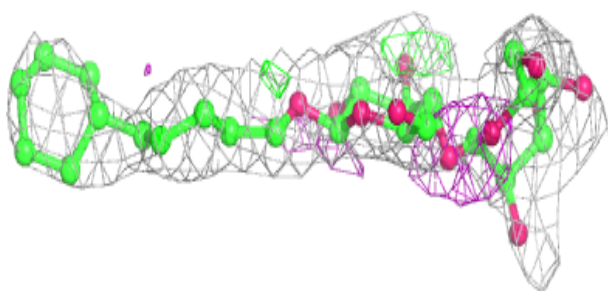
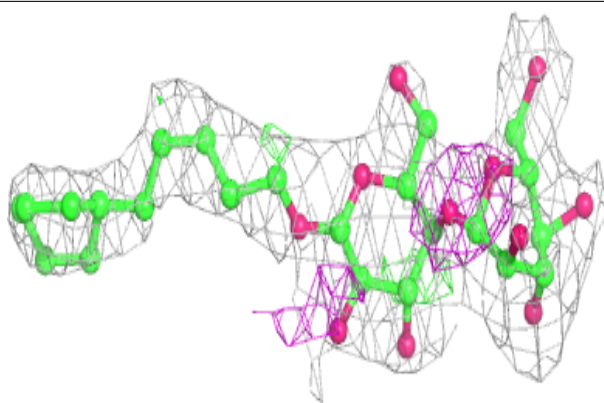
**Electron density around CM5 D 607:**

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

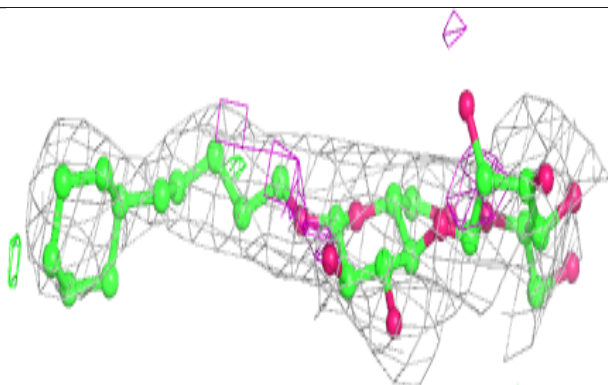
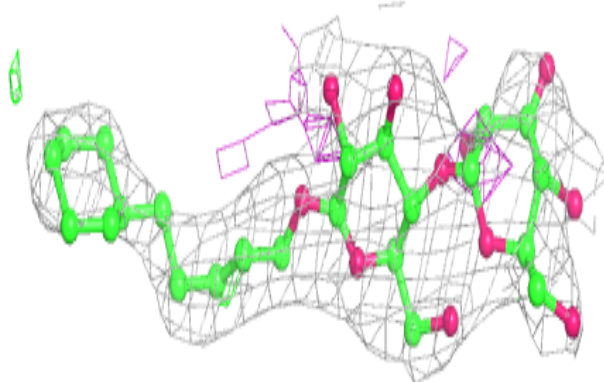


Electron density around CM5 C 603:

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

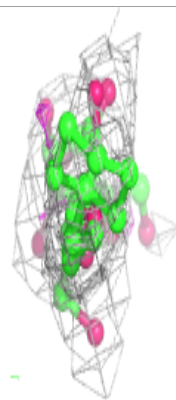
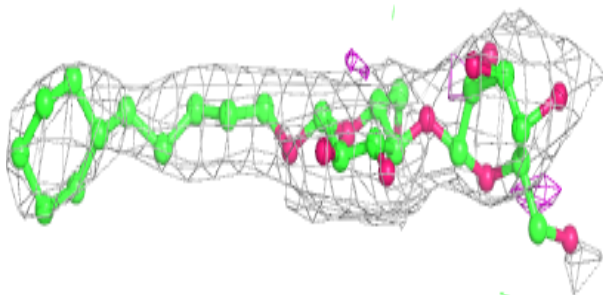
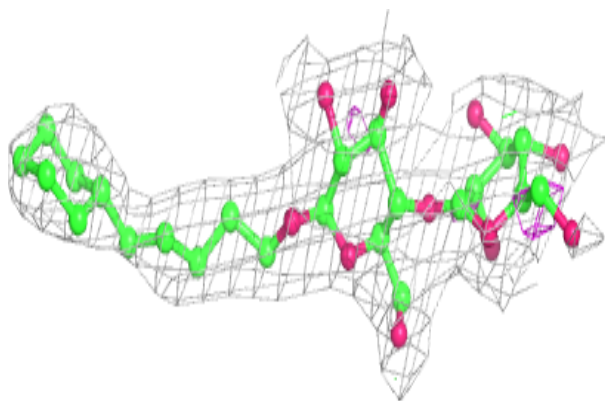
**Electron density around CM5 E 605:**

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

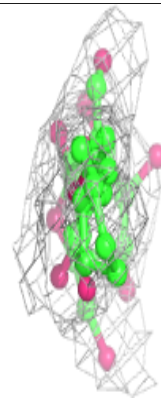
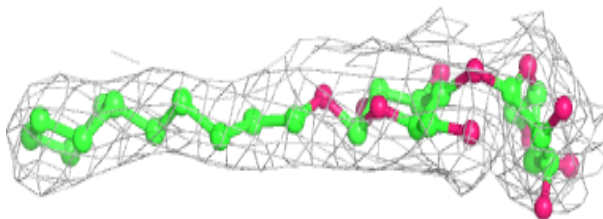
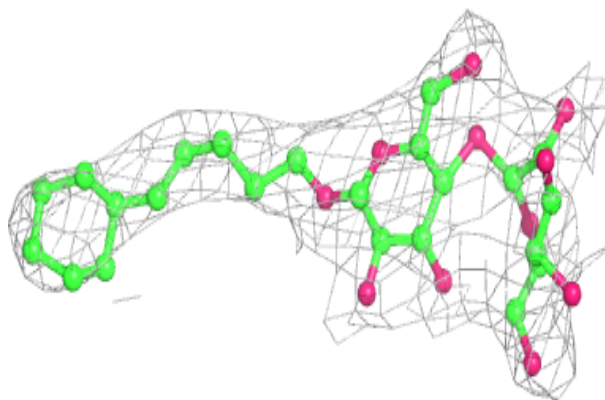


Electron density around CM5 A 601:

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

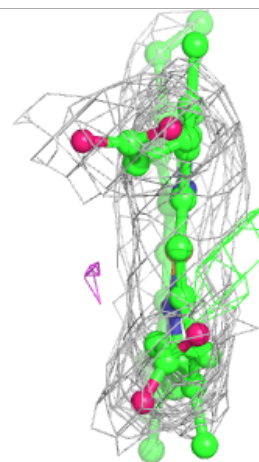
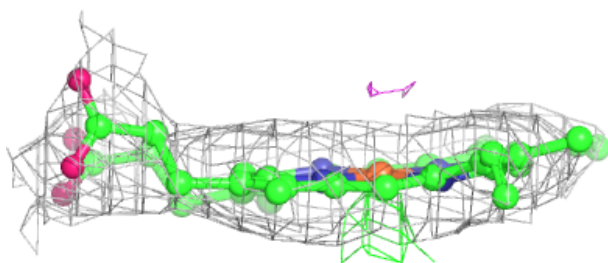
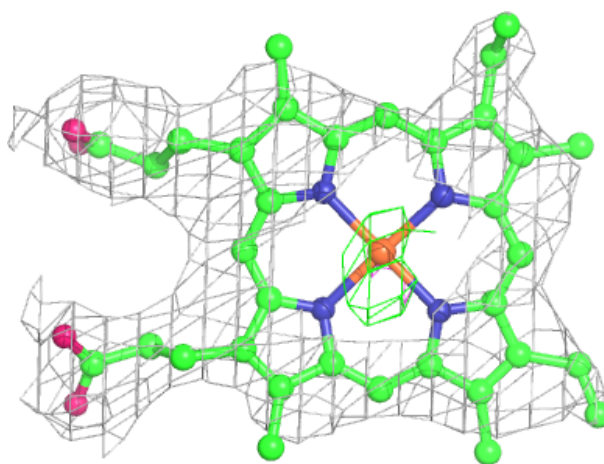
**Electron density around CM5 D 604:**

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



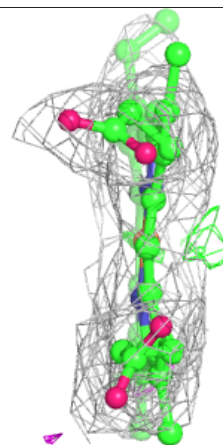
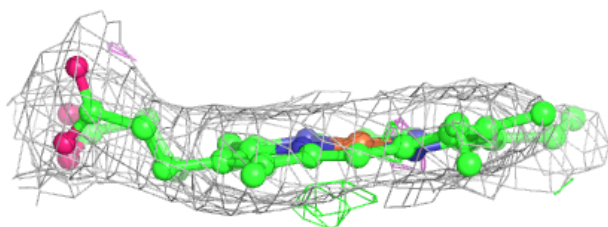
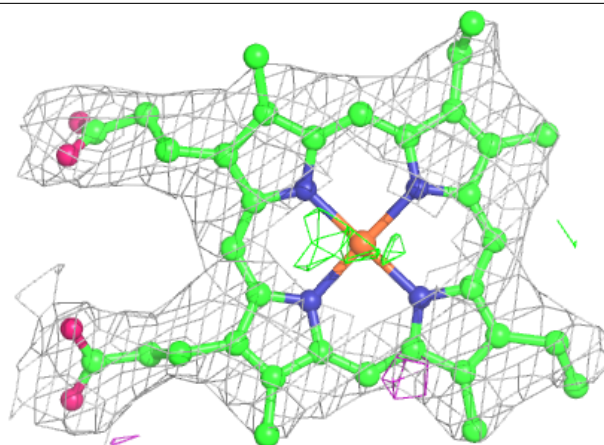
Electron density around HEM F 500:

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



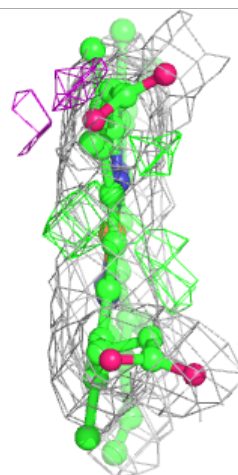
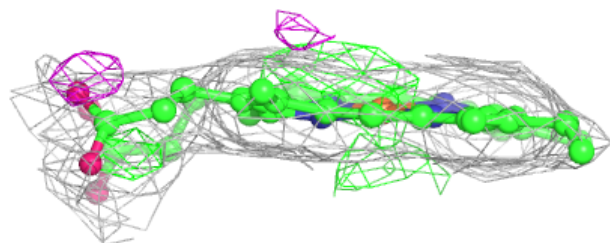
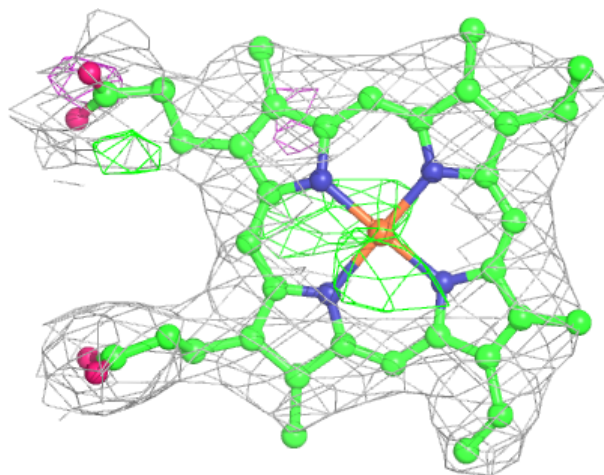
Electron density around HEM D 500:

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



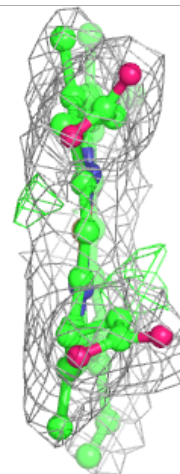
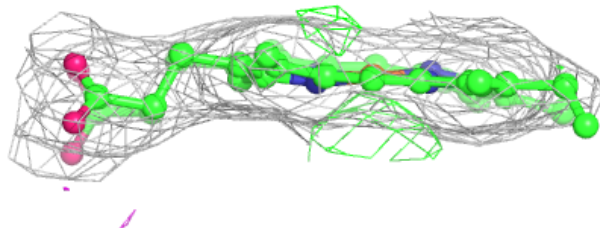
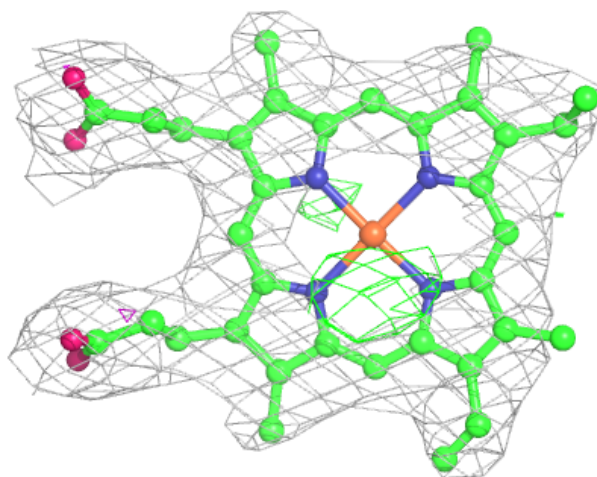
Electron density around HEM A 500:

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



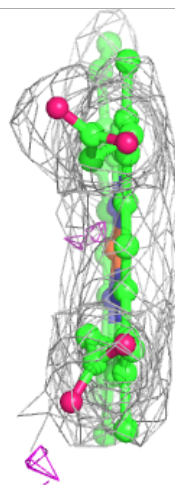
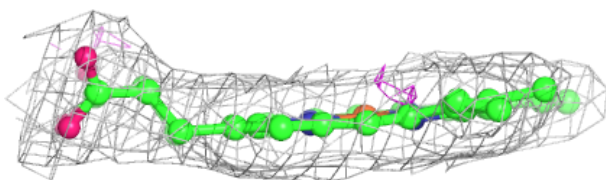
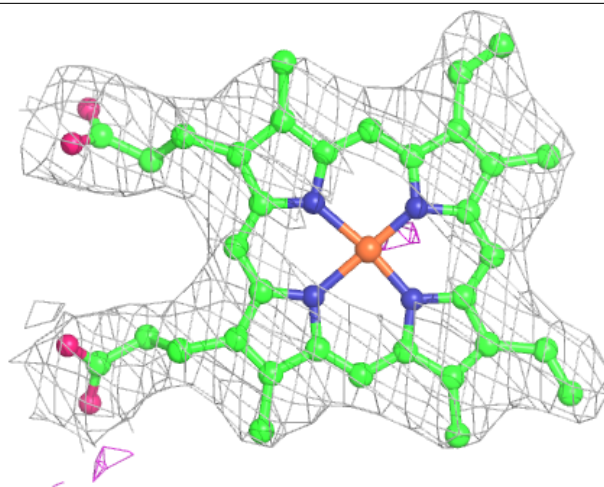
Electron density around HEM E 500:

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



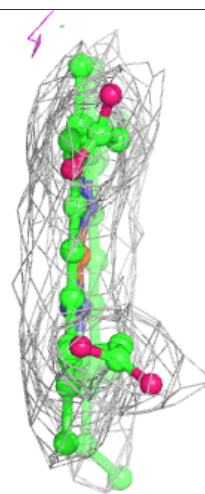
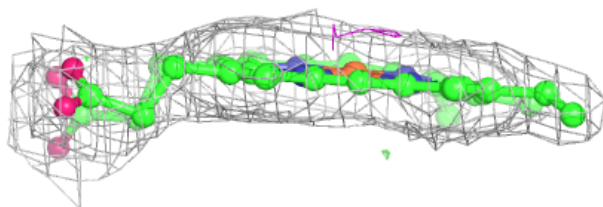
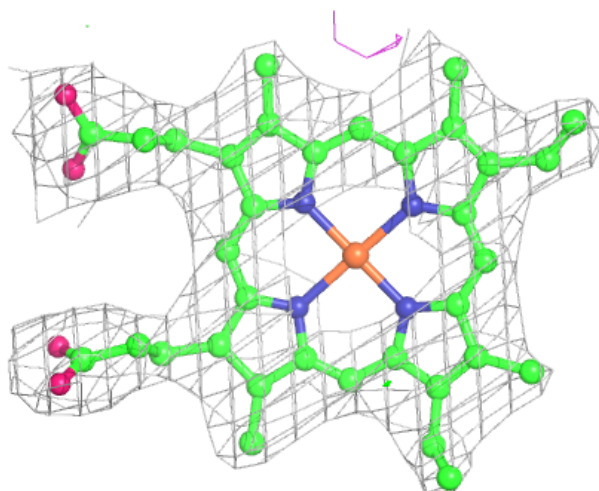
Electron density around HEM C 500:

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



Electron density around HEM B 500:

$2mF_o-DF_c$ (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.