



wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 04:41 PM UTC

PDB ID : 3QU8 / pdb_00003qu8
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 types of validation reports are described at

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

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

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

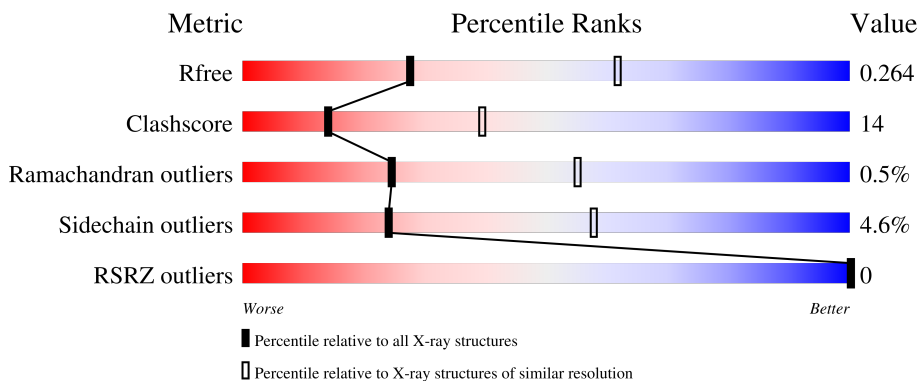
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	 74% 20% . .
1	B	476	 74% 20% . .
1	C	476	 73% 21% . .
1	D	476	 72% 21% . .
1	E	476	 70% 24% . .

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Mol	Chain	Length	Quality of chain
1	F	476	 68% 24% 5%

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

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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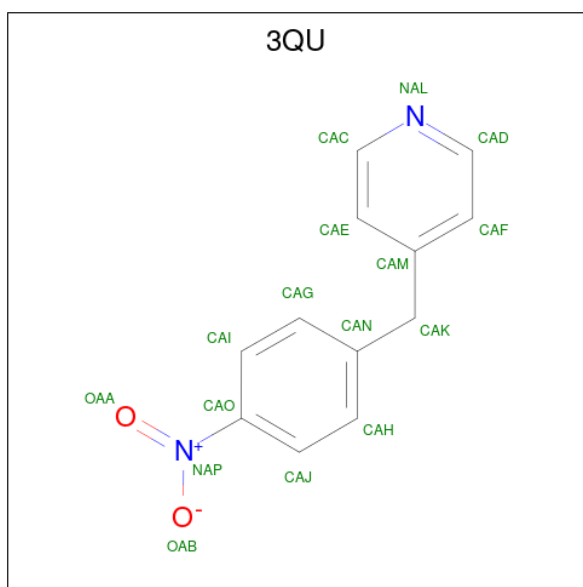
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	LYS	HIS	engineered mutation	UNP P20813
B	24	THR	PRO	engineered mutation	UNP P20813
B	25	SER	ASN	engineered mutation	UNP P20813
B	26	SER	THR	engineered mutation	UNP P20813
B	27	LYS	HIS	engineered mutation	UNP P20813
B	28	GLY	ASP	engineered mutation	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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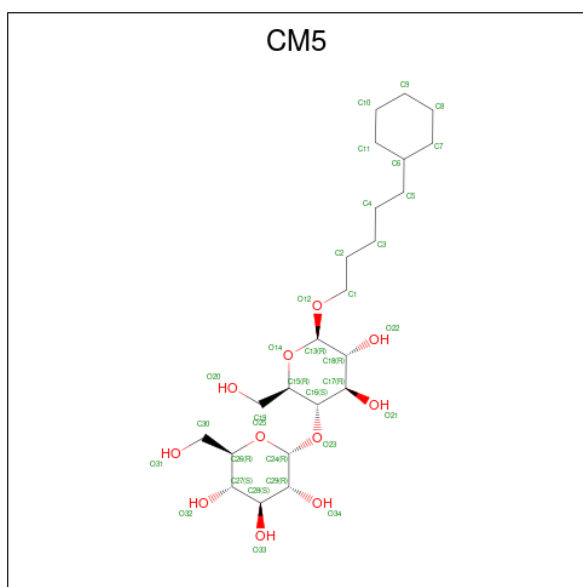
Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	expression tag	UNP P20813
E	2	ALA	GLU	engineered mutation	UNP P20813
E	22	LYS	ARG	engineered mutation	UNP P20813
E	23	LYS	HIS	engineered mutation	UNP P20813
E	24	THR	PRO	engineered mutation	UNP P20813
E	25	SER	ASN	engineered mutation	UNP P20813
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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (CCD ID: CM5) (formula: C₂₃H₄₂O₁₁).



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

- Molecule 5 is water.

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

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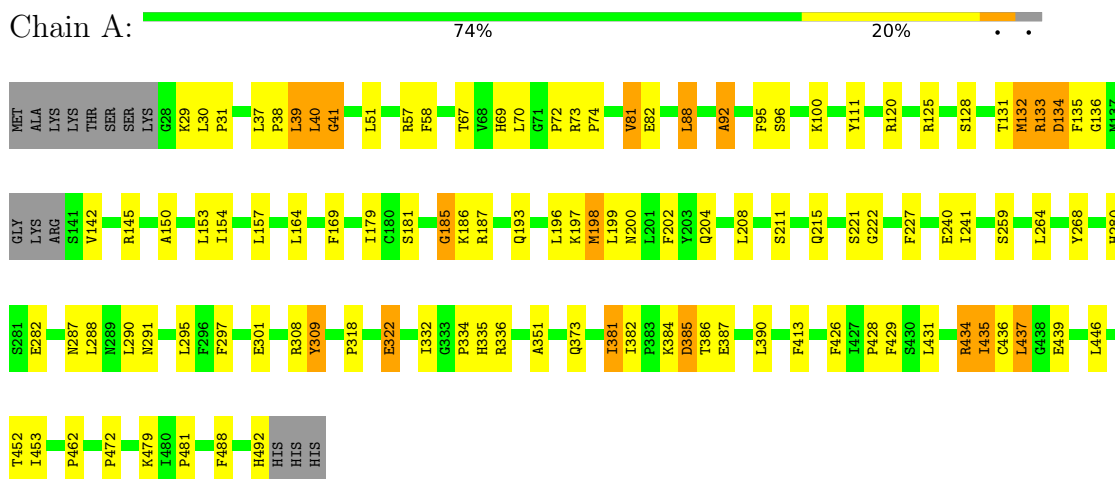
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	23	Total 23	O 23	0	0
5	F	12	Total 12	O 12	0	0

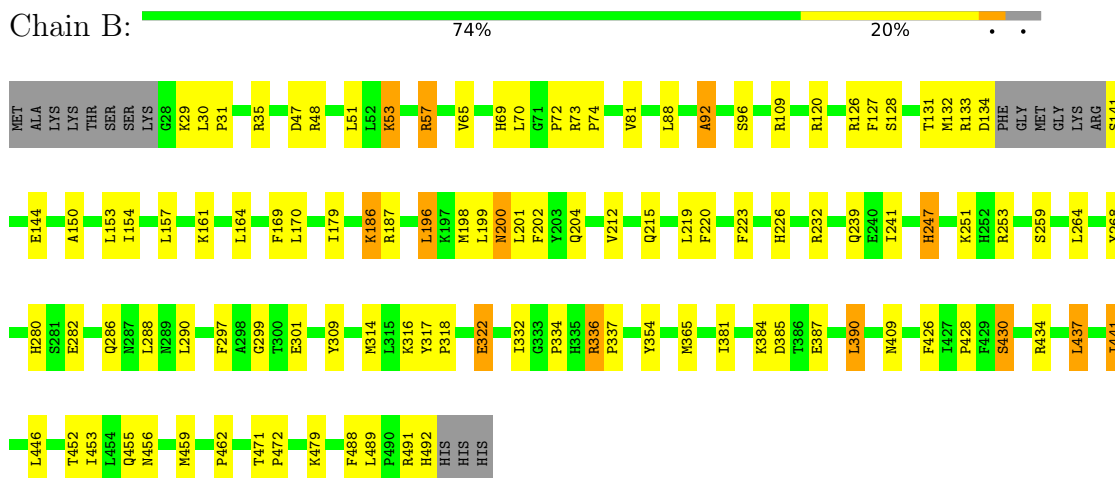
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Cytochrome P450 2B6

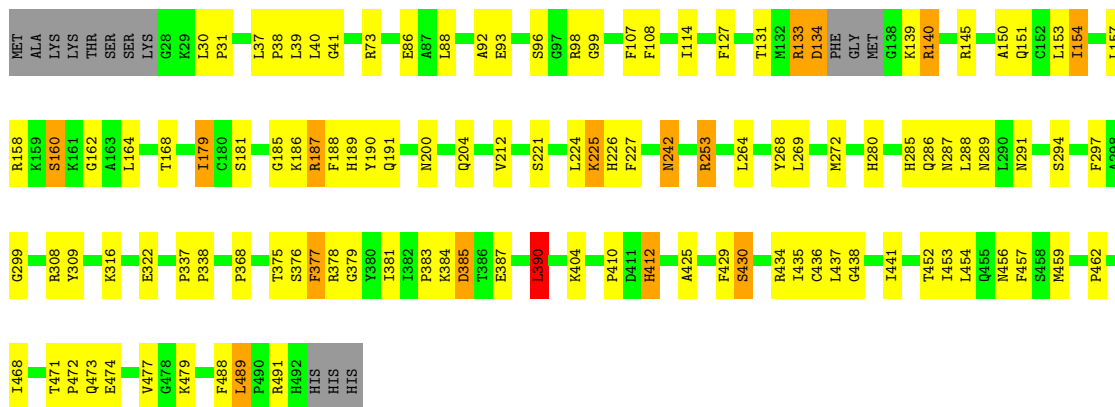


- Molecule 1: Cytochrome P450 2B6

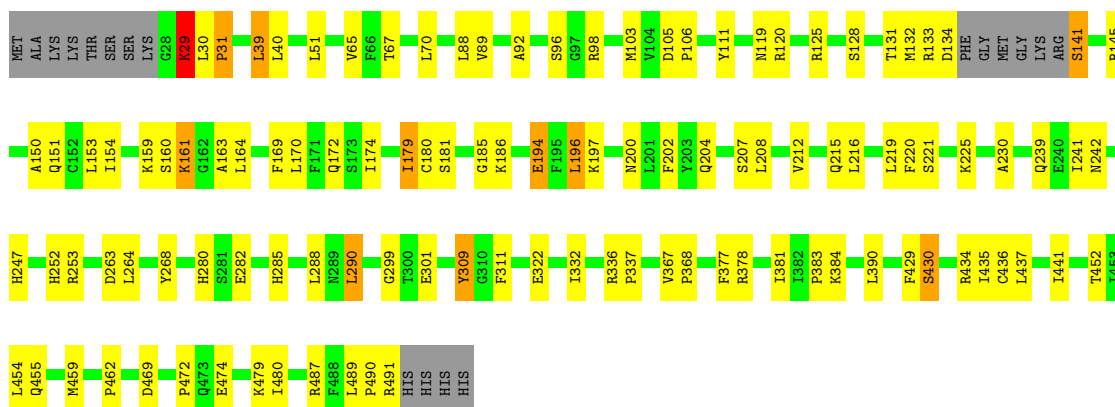


- Molecule 1: Cytochrome P450 2B6

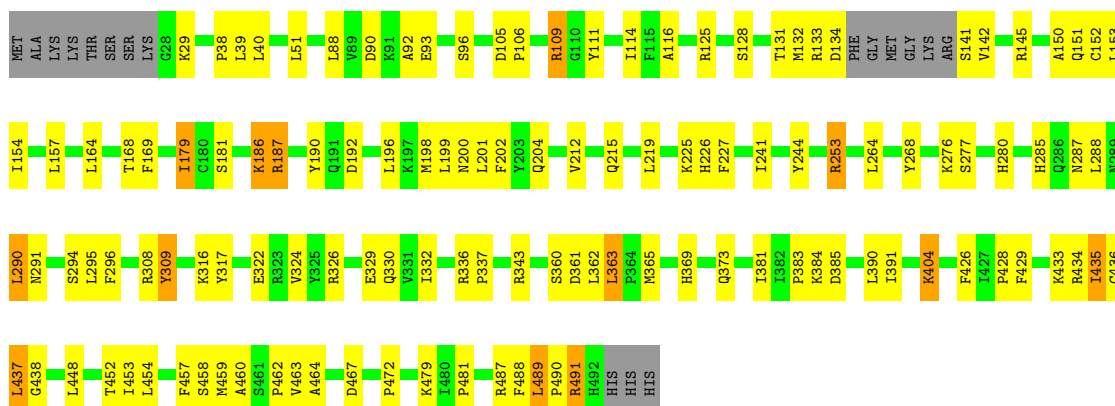




• Molecule 1: Cytochrome P450 2B6



• Molecule 1: Cytochrome P450 2B6



• Molecule 1: Cytochrome P450 2B6



MET	ALA	LYS	LYS	THR	SER	LYS	G29	P38	L39	D47	R48	R49	G50	L51	V68	R73	M77	V81	E82	E86	A87	L88	V88	D90	K91	A92	E93	A94	F95	R98	G99	M103	I114	M119	R120	R125	R126	F127	S128	T131	M132	R133	D134	PHE	GLY	
MET	GLY	LYS	ARG	S141	R145	E148	E149	A150	Q151	I164	L164	T168	F169	L170	M177	I178	I179	C180	S181	I182	V183	F184	G185	K186	E194	F195	L196	K197	M198	L199	N200	L201	F202	Y203	Q204	V212	F213	G214	Q215	F227	A230	H231	I241	N242	H247	K251
D257	P258	S259	A260	T267	Y268	E275	K276	S277	E282	N287	L288	N289	L290	N291	T292	L293	S294	L295	F296	F297	A298	G299	E301	T302	L307	R308	Y309	G310	L313	K316	Y317	P318	E322	I332	R336	F377	R378	G379	Y380	I381	K384	D385	T386	E387	V388	
F389	L390	N409	E424	A425	F426	I427	P428	C436	L437	G438	I441	A442	R443	T462	Q455	N456	M459	P462	L470	T471	P472	G473	E474	V477	P481	I486	ARG	PHE	LEU	PRO	ARG	HIS	HIS	HIS	HIS	ARG	PHE	LEU	PRO	ARG	HIS	HIS	HIS	HIS		

4 Data and refinement statistics i

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 50.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.51-2.80) 88.9 (50.51-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.81Å)	Xtrriage
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	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.043 for -h,-k,l 0.149 for h,-h-k,-l 0.048 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22964	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CM5, HEM, 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	1.06	2/3833 (0.1%)	1.06	6/5185 (0.1%)
1	B	1.05	2/3813 (0.1%)	1.08	10/5158 (0.2%)
1	C	1.11	4/3822 (0.1%)	1.06	9/5167 (0.2%)
1	D	1.05	4/3791 (0.1%)	1.09	10/5129 (0.2%)
1	E	1.02	1/3817 (0.0%)	1.05	9/5162 (0.2%)
1	F	1.11	2/3745 (0.1%)	1.11	12/5067 (0.2%)
All	All	1.07	15/22821 (0.1%)	1.07	56/30868 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ALA	CA-CB	-6.19	1.43	1.53
1	E	90	ASP	N-CA	6.09	1.54	1.46
1	F	183	VAL	CA-CB	-5.83	1.48	1.55
1	C	93	GLU	CA-C	5.68	1.60	1.52
1	D	89	VAL	C-O	-5.67	1.17	1.24

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	40	LEU	N-CA-C	-9.21	103.15	114.75
1	F	183	VAL	CB-CA-C	-7.98	103.86	111.44
1	A	185	GLY	N-CA-C	7.70	126.76	114.90
1	D	480	ILE	CA-C-N	7.32	124.93	119.66
1	D	480	ILE	C-N-CA	7.32	124.93	119.66

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	107	0
1	B	3713	0	3702	97	0
1	C	3724	0	3711	87	0
1	D	3693	0	3682	100	0
1	E	3717	0	3713	123	0
1	F	3649	0	3635	103	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	652	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 652 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:O23	4:B:608:CM5:C16	1.64	1.42
1:D:454:LEU:CD2	1:D:459:MET:HE1	1.60	1.29
4:B:608:CM5:C24	4:B:608:CM5:H17	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

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%)	14	41
1	B	455/476 (96%)	431 (95%)	21 (5%)	3 (1%)	18	47
1	C	456/476 (96%)	424 (93%)	30 (7%)	2 (0%)	30	60
1	D	454/476 (95%)	424 (93%)	28 (6%)	2 (0%)	30	60
1	E	455/476 (96%)	433 (95%)	22 (5%)	0	100	100
1	F	449/476 (94%)	417 (93%)	29 (6%)	3 (1%)	18	47
All	All	2727/2856 (96%)	2565 (94%)	148 (5%)	14 (0%)	24	55

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/418 (97%)	386 (96%)	18 (4%)	24	58
1	B	403/418 (96%)	380 (94%)	23 (6%)	18	49
1	C	402/418 (96%)	382 (95%)	20 (5%)	22	54
1	D	400/418 (96%)	385 (96%)	15 (4%)	29	64
1	E	404/418 (97%)	383 (95%)	21 (5%)	21	53
1	F	396/418 (95%)	381 (96%)	15 (4%)	29	64
All	All	2409/2508 (96%)	2297 (95%)	112 (5%)	24	58

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	404	LYS
1	F	441	ILE
1	D	309	TYR
1	F	381	ILE
1	F	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	233	GLN
1	E	286	GLN
1	D	485	GLN
1	E	357	GLN
1	B	172	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	3QU	B	501	2	17,17,17	0.81	1 (5%)	20,22,22	1.75	7 (35%)
2	HEM	C	500	1,3	50,50,50	2.52	22 (44%)	67,82,82	2.25	23 (34%)
2	HEM	D	500	1,3	50,50,50	1.91	7 (14%)	67,82,82	1.31	4 (5%)
4	CM5	F	606	-	36,36,36	3.00	13 (36%)	49,49,49	4.34	25 (51%)
4	CM5	C	603	-	36,36,36	3.34	13 (36%)	49,49,49	5.38	22 (44%)
2	HEM	F	500	1	50,50,50	1.91	9 (18%)	67,82,82	1.30	5 (7%)
3	3QU	C	501	2	7,7,17	0.29	0	8,8,22	1.29	0
4	CM5	E	605	-	36,36,36	3.44	14 (38%)	49,49,49	3.20	23 (46%)
4	CM5	B	602	-	36,36,36	2.84	9 (25%)	49,49,49	4.88	23 (46%)
2	HEM	B	500	1,3	50,50,50	1.88	12 (24%)	67,82,82	1.70	15 (22%)
3	3QU	D	501	2	14,14,17	0.33	0	17,17,22	0.90	0
4	CM5	D	607	-	36,36,36	3.53	13 (36%)	49,49,49	4.99	26 (53%)
3	3QU	E	501	2	14,14,17	0.86	0	17,17,22	0.95	1 (5%)
2	HEM	E	500	1,3	50,50,50	1.91	8 (16%)	67,82,82	1.31	5 (7%)
2	HEM	A	500	1,3	50,50,50	1.91	9 (18%)	67,82,82	1.32	5 (7%)
3	3QU	A	501	2	7,7,17	0.28	0	8,8,22	1.31	0
4	CM5	A	601	-	36,36,36	4.12	16 (44%)	49,49,49	5.41	26 (53%)
4	CM5	B	608	-	36,36,36	3.16	15 (41%)	49,49,49	5.96	27 (55%)
4	CM5	D	604	-	36,36,36	4.12	16 (44%)	49,49,49	6.30	24 (48%)

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	3QU	B	501	2	-	0/6/8/8	0/2/2/2
2	HEM	C	500	1,3	-	6/14/54/54	-
2	HEM	D	500	1,3	-	7/14/54/54	-
4	CM5	F	606	-	-	5/17/65/65	0/3/3/3
4	CM5	C	603	-	-	11/17/65/65	0/3/3/3
2	HEM	F	500	1	-	6/14/54/54	-
3	3QU	C	501	2	-	-	0/1/1/2
4	CM5	E	605	-	-	9/17/65/65	0/3/3/3
4	CM5	B	602	-	-	9/17/65/65	0/3/3/3
2	HEM	B	500	1,3	-	6/14/54/54	-
3	3QU	D	501	2	-	0/4/4/8	0/2/2/2
4	CM5	D	607	-	-	13/17/65/65	0/3/3/3
3	3QU	E	501	2	-	0/4/4/8	0/2/2/2
2	HEM	E	500	1,3	-	2/14/54/54	-
2	HEM	A	500	1,3	-	4/14/54/54	-
3	3QU	A	501	2	-	-	0/1/1/2
4	CM5	A	601	-	-	11/17/65/65	0/3/3/3
4	CM5	B	608	-	-	11/17/65/65	0/3/3/3
4	CM5	D	604	-	1/1/11/11	9/17/65/65	0/3/3/3

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	CM5	O23-C24	-13.40	1.04	1.41
4	A	601	CM5	O21-C17	-12.91	1.11	1.43
4	E	605	CM5	O23-C24	-11.11	1.10	1.41
4	D	604	CM5	C29-C28	-11.05	1.23	1.52
4	D	604	CM5	O25-C26	-10.77	1.18	1.44

The worst 5 of 261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	604	CM5	O23-C16-C17	19.80	157.57	107.23
4	F	606	CM5	O12-C13-C18	-17.68	81.43	108.27
4	B	608	CM5	O14-C15-C19	-17.38	63.38	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	CM5	O33-C28-C27	-17.27	69.67	110.38
4	B	608	CM5	O14-C13-O12	-16.72	70.54	110.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	CM5	C16

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C1A-C2A-CAA-CBA
2	A	500	HEM	C3A-C2A-CAA-CBA
2	D	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	F	500	HEM	C2C-C3C-CAC-CBC

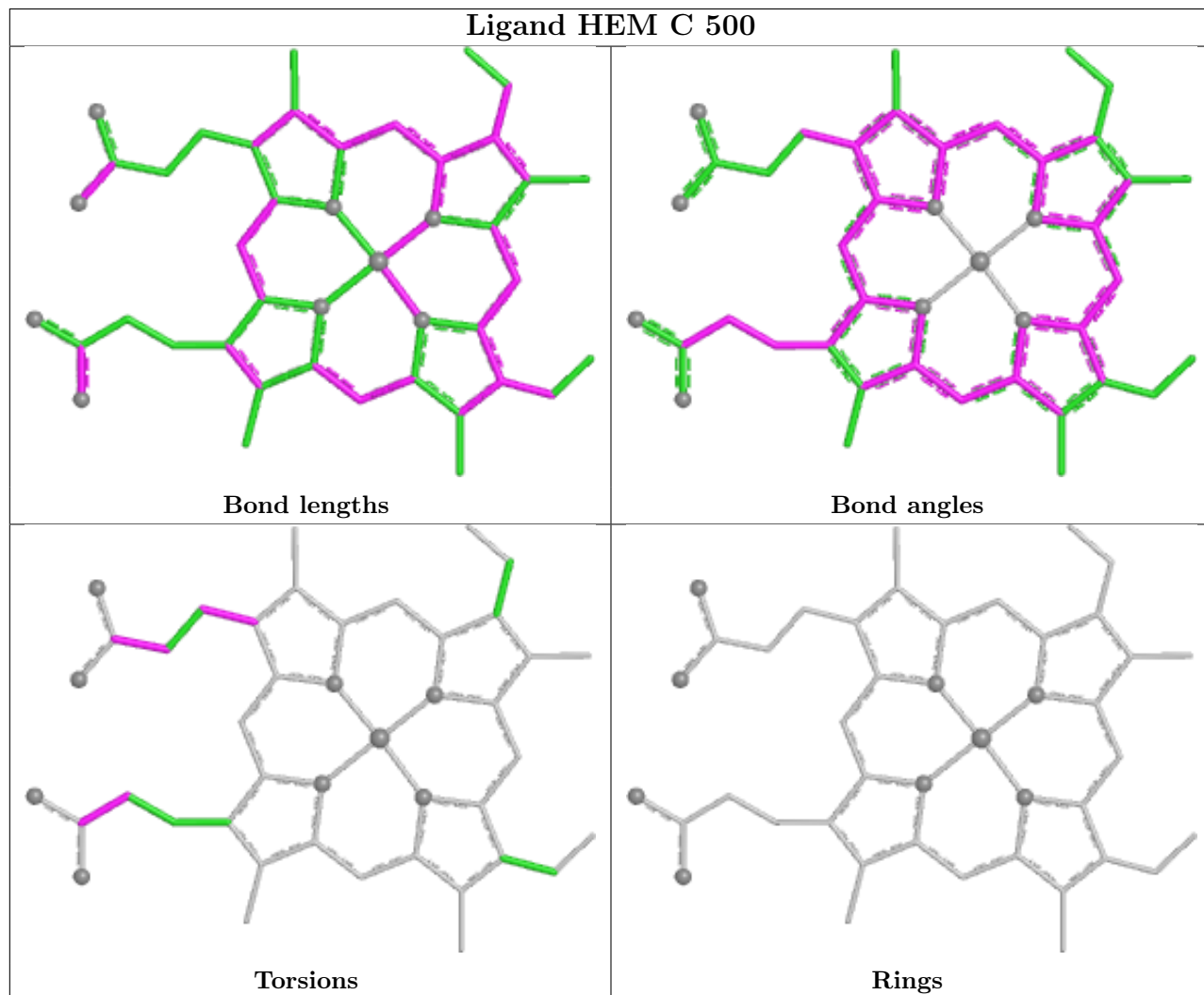
There are no ring outliers.

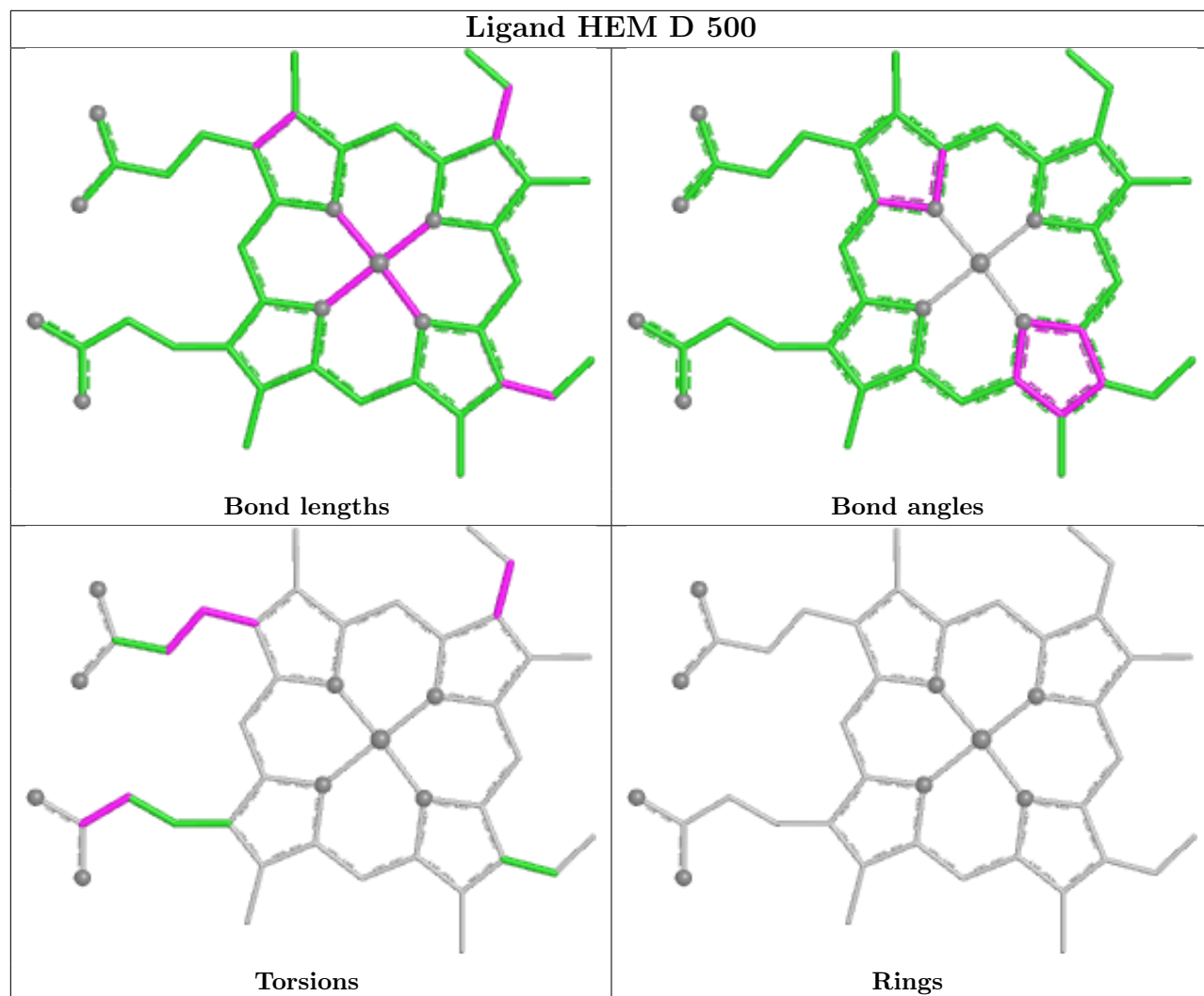
15 monomers are involved in 122 short contacts:

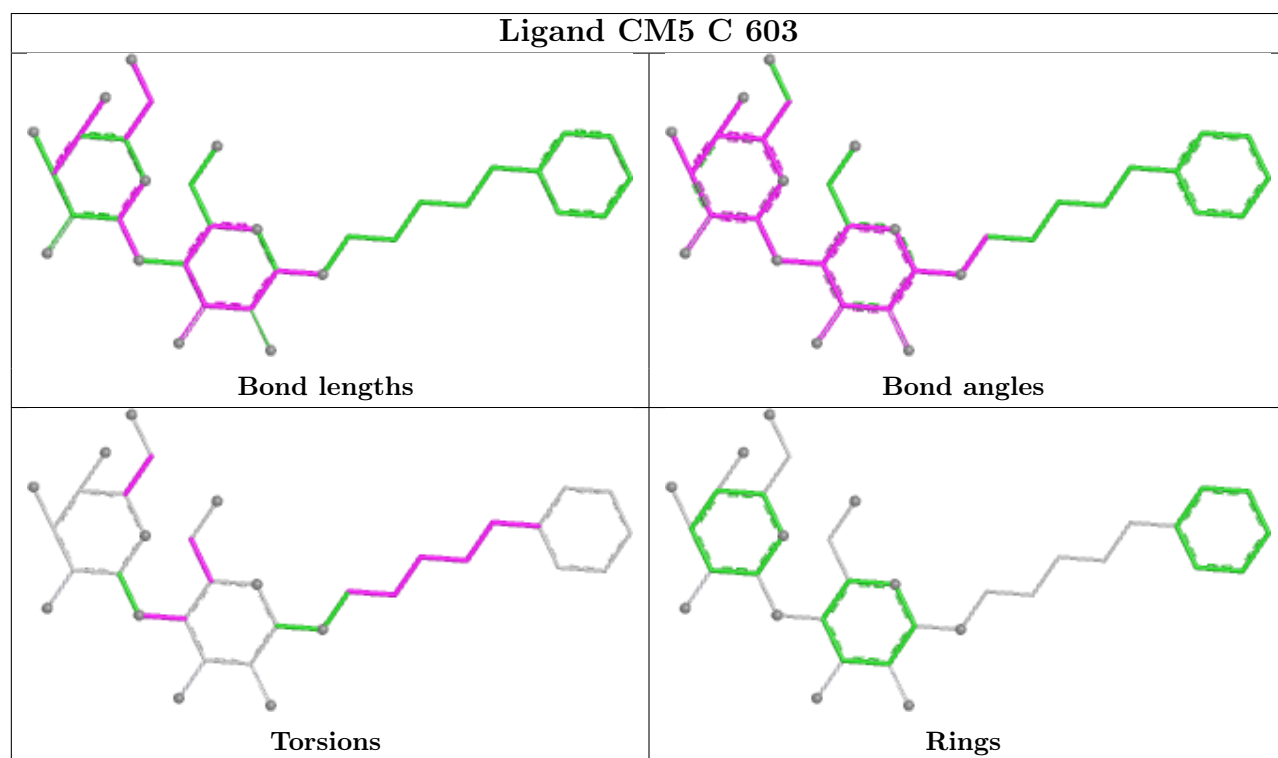
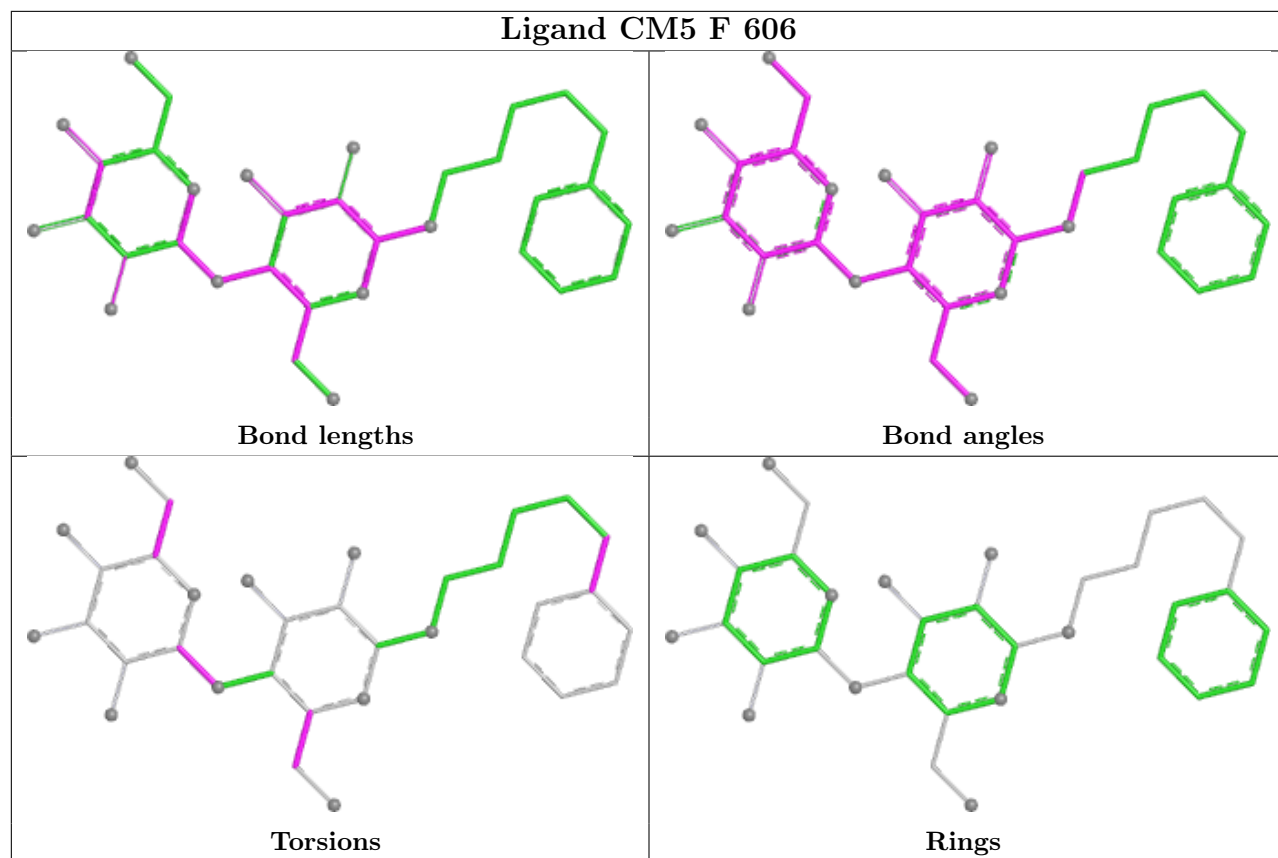
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	HEM	9	0
2	D	500	HEM	12	0
4	F	606	CM5	5	0
4	C	603	CM5	5	0
2	F	500	HEM	18	0
4	E	605	CM5	3	0
4	B	602	CM5	14	0
2	B	500	HEM	4	0
4	D	607	CM5	8	0
3	E	501	3QU	1	0
2	E	500	HEM	9	0
2	A	500	HEM	10	0
4	A	601	CM5	1	0
4	B	608	CM5	20	0
4	D	604	CM5	4	0

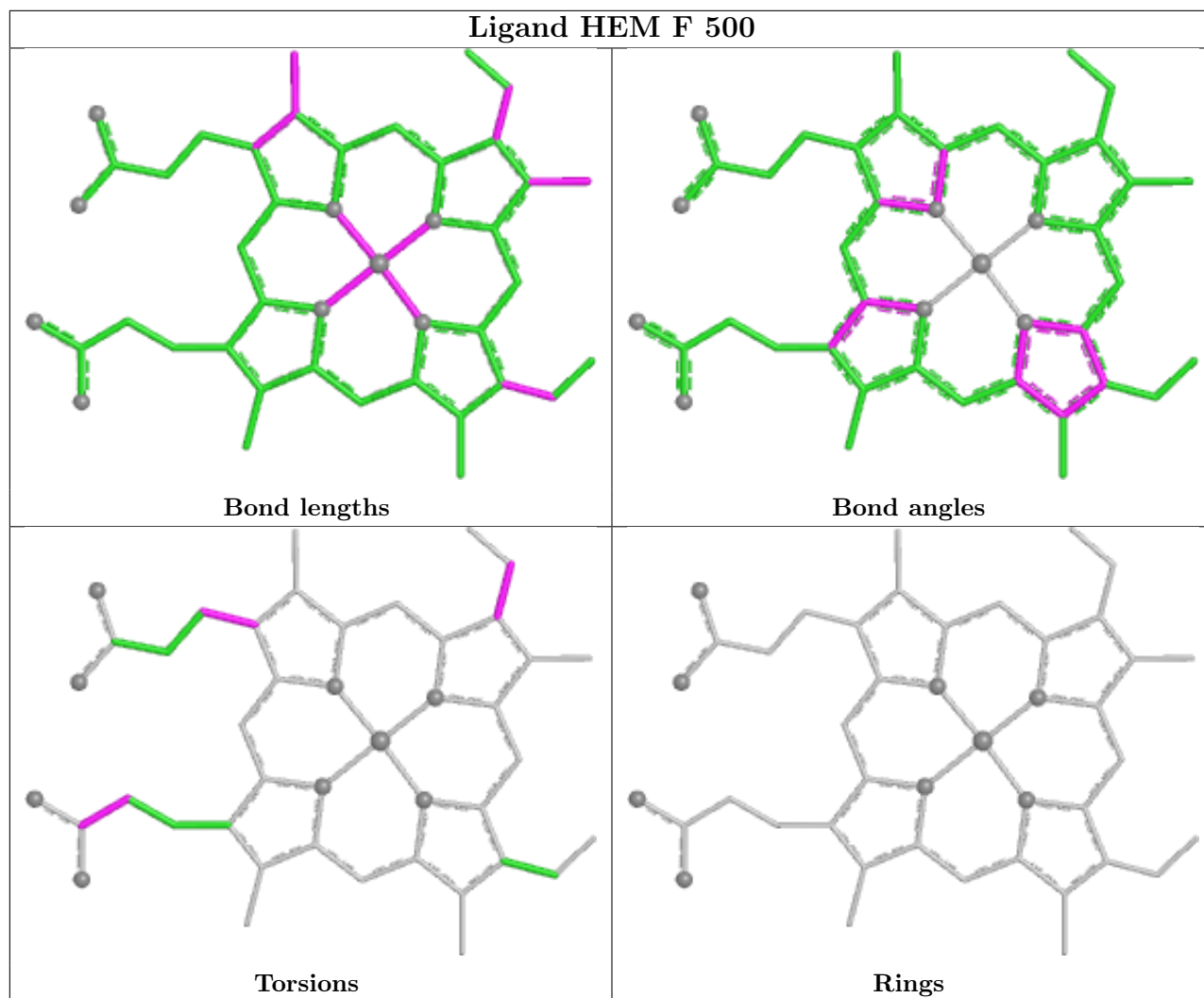
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

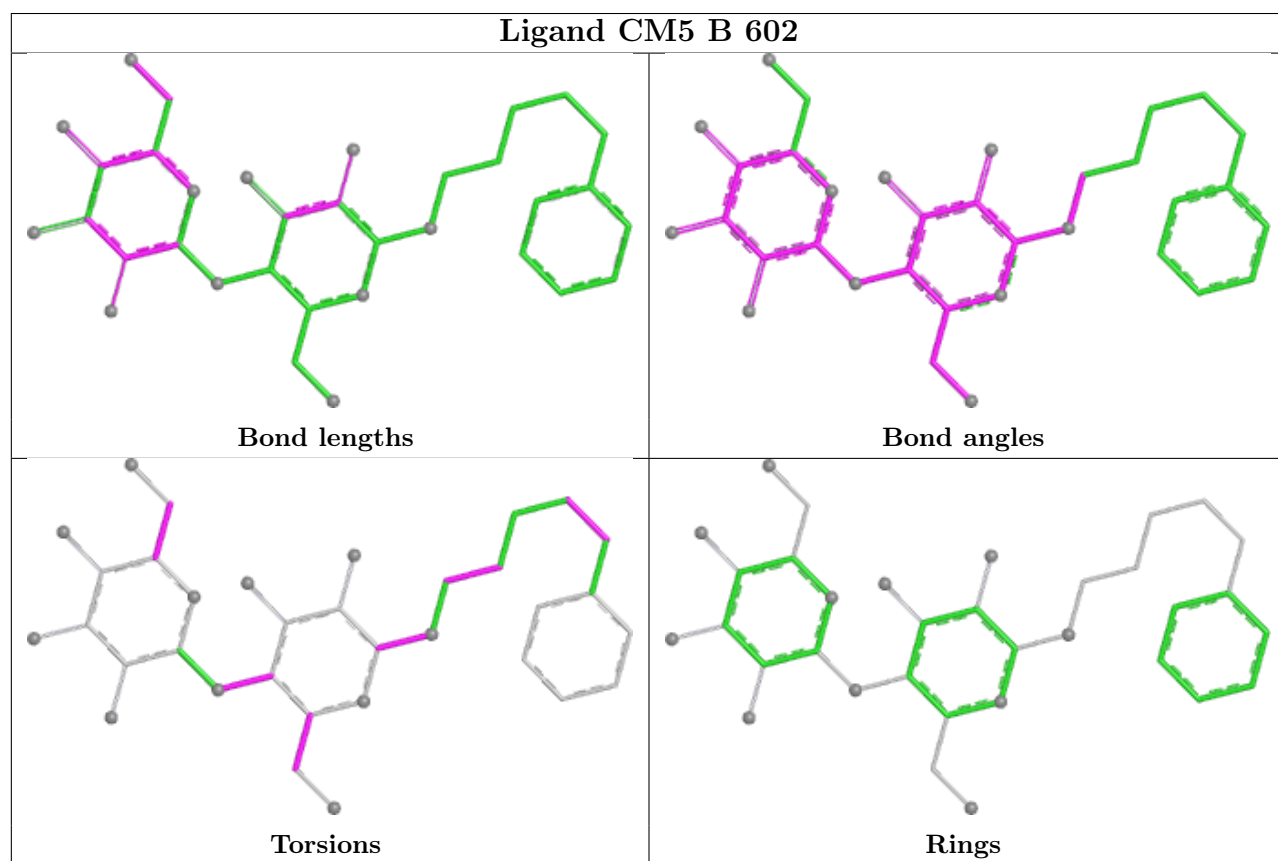
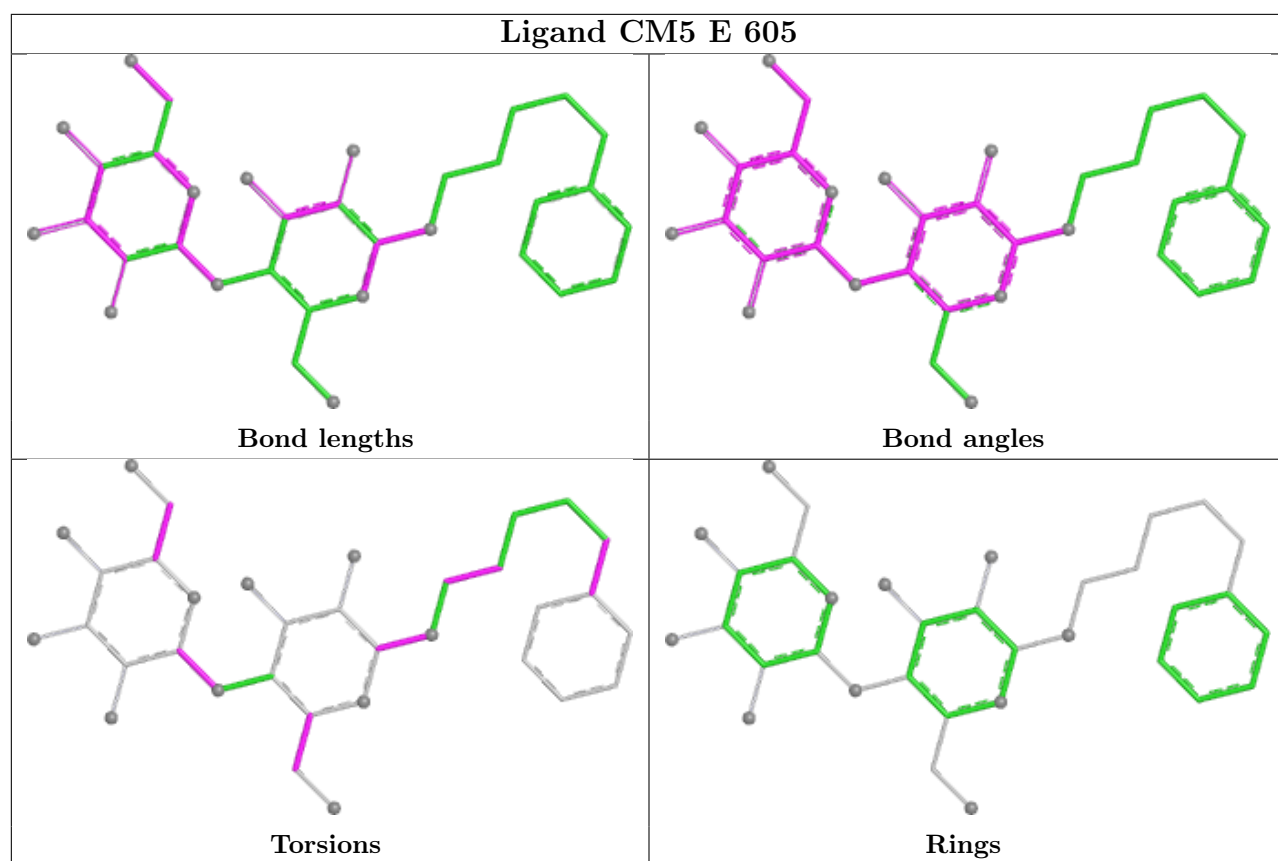
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

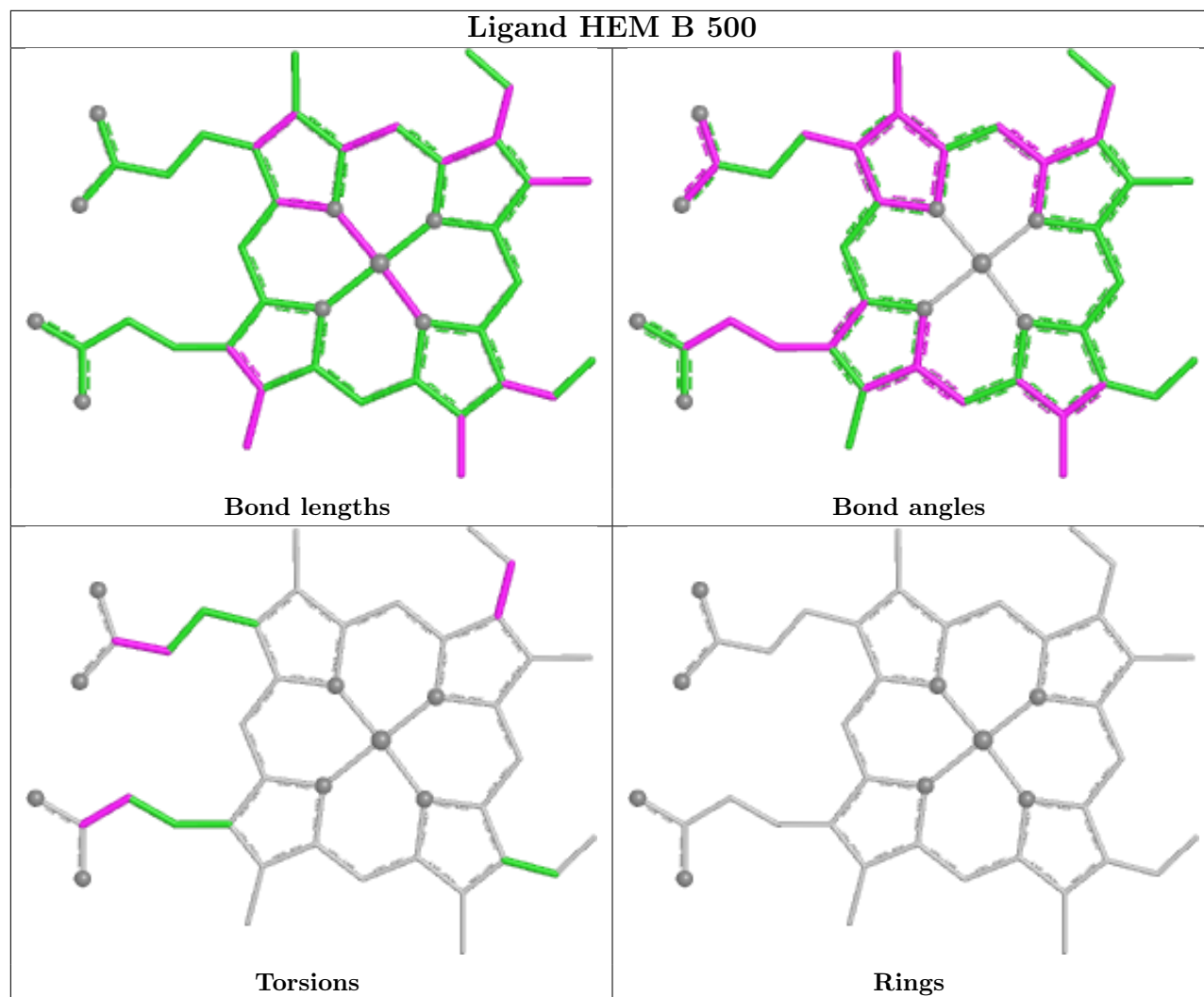


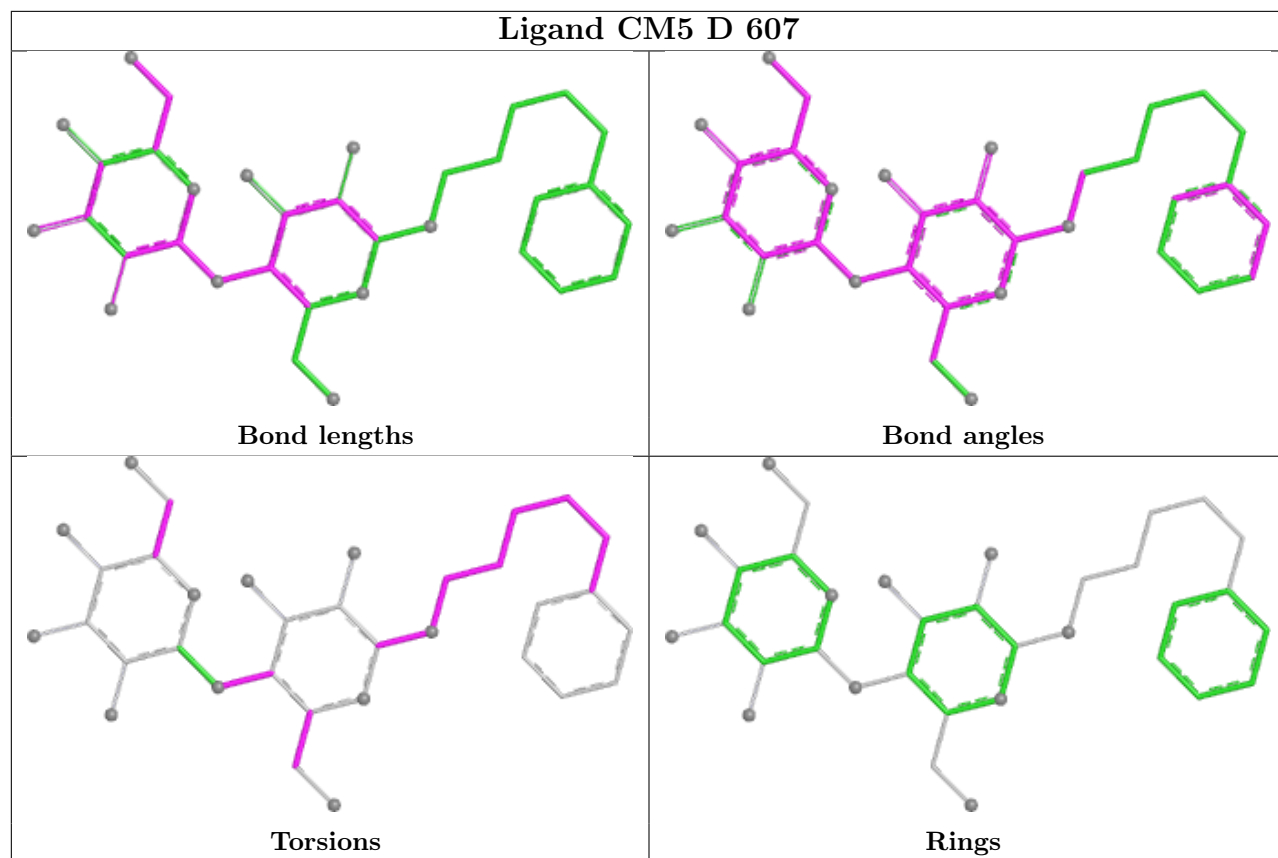


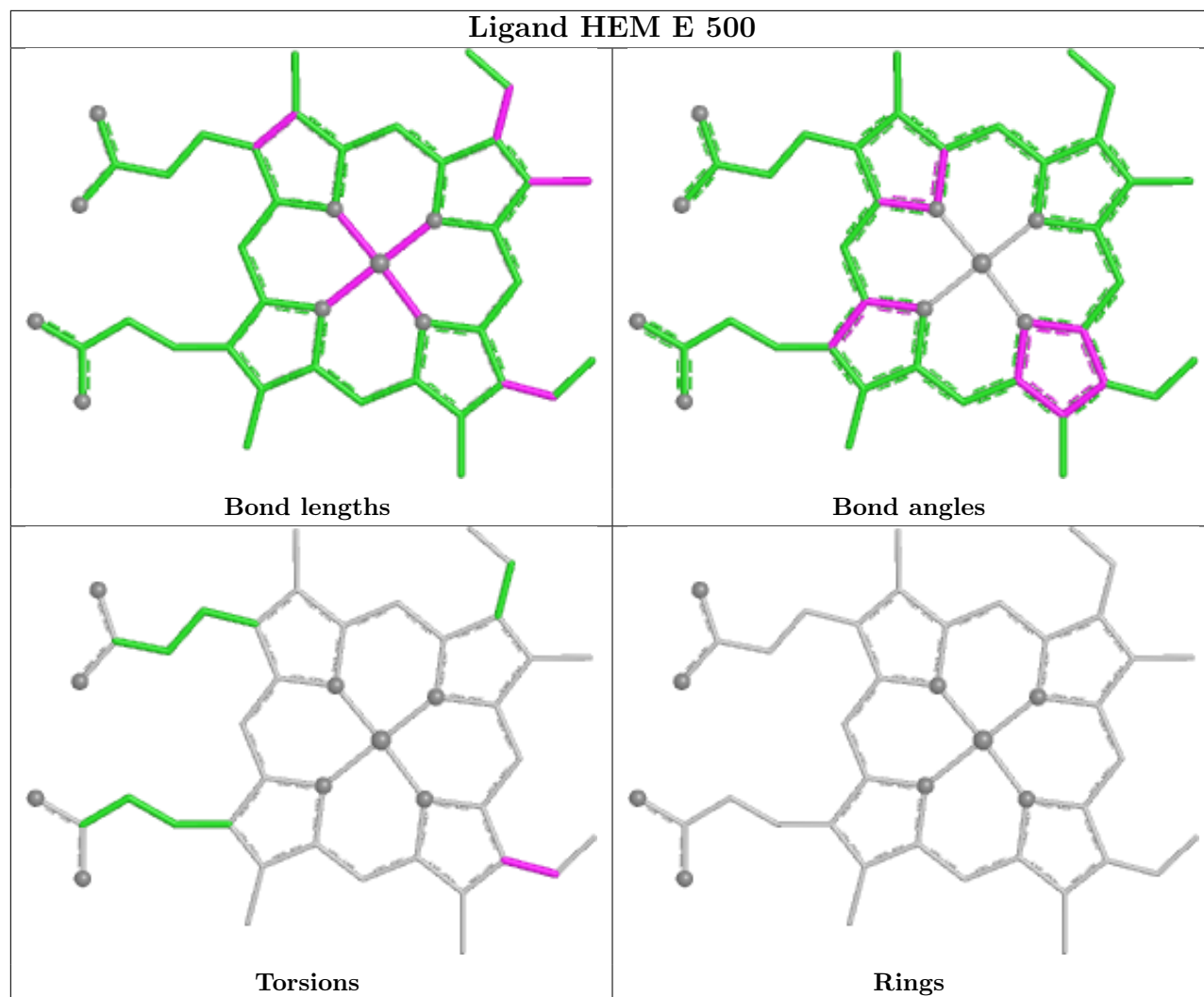


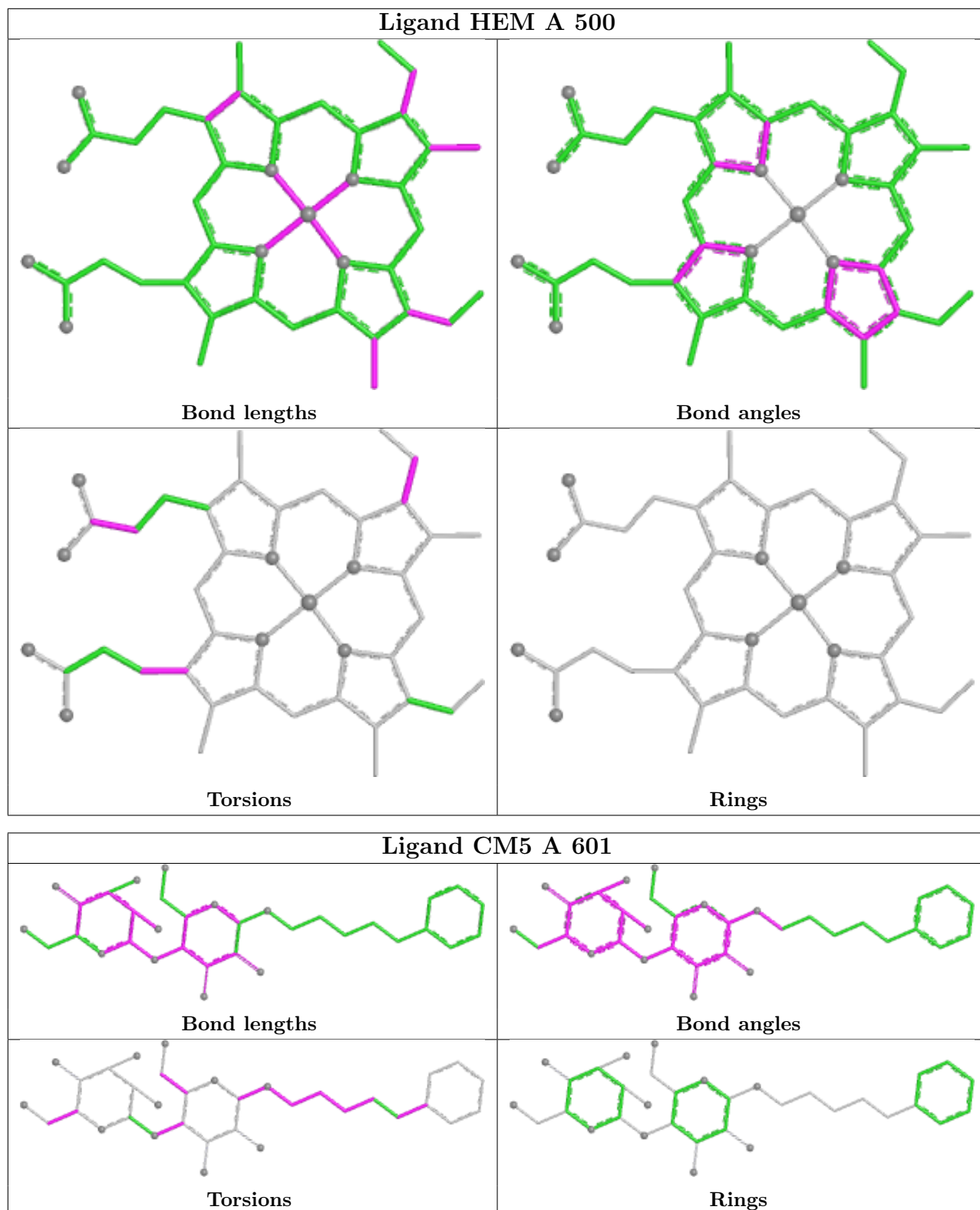


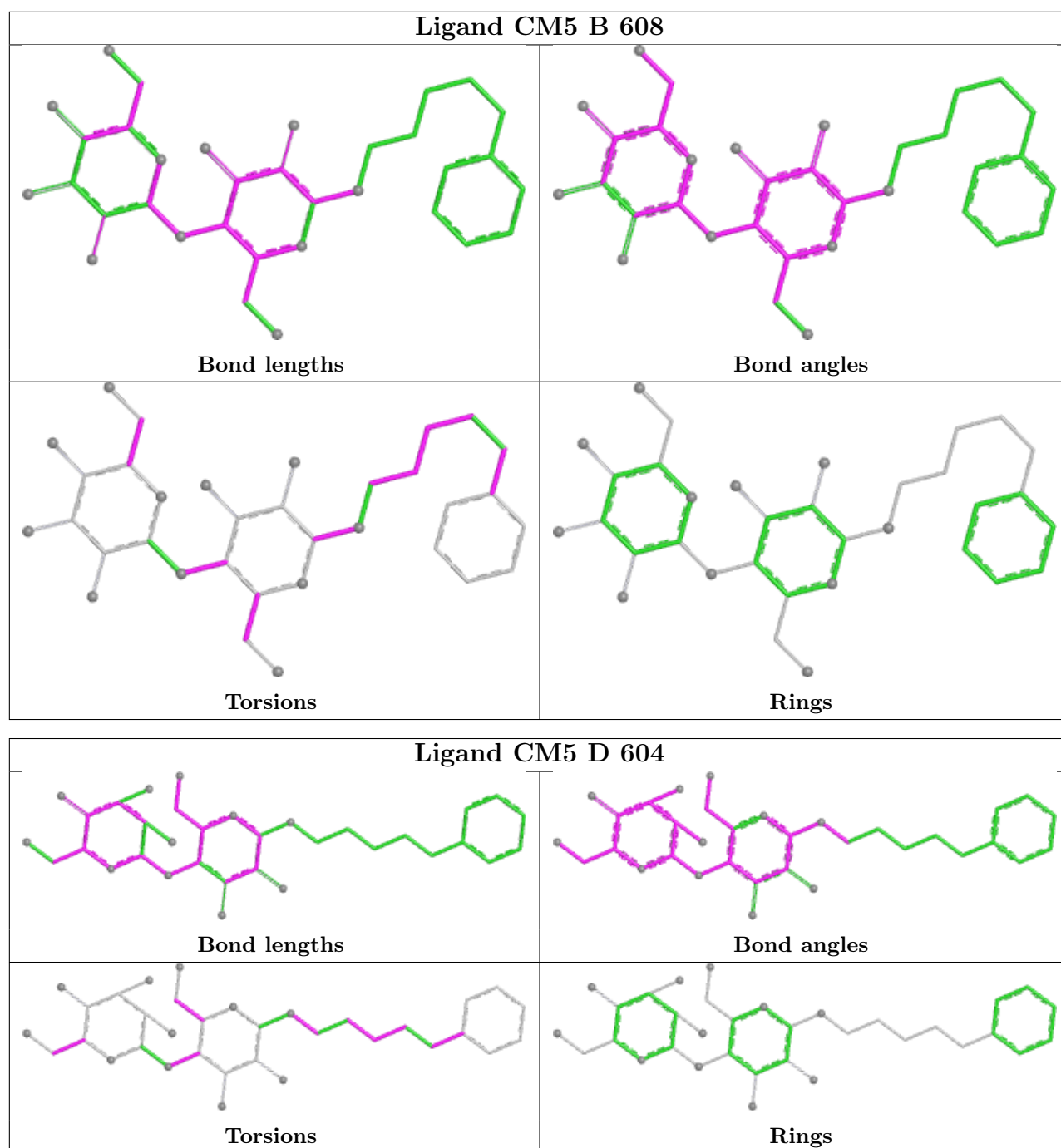












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/476 (97%)	-1.55	0 100 100	26, 51, 74, 82	0
1	B	459/476 (96%)	-1.55	0 100 100	28, 51, 74, 82	0
1	C	462/476 (97%)	-1.56	0 100 100	24, 50, 74, 79	0
1	D	458/476 (96%)	-1.56	0 100 100	24, 51, 74, 82	0
1	E	459/476 (96%)	-1.58	0 100 100	26, 51, 74, 87	0
1	F	453/476 (95%)	-1.44	0 100 100	24, 51, 74, 79	0
All	All	2753/2856 (96%)	-1.54	0 100 100	24, 51, 74, 87	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

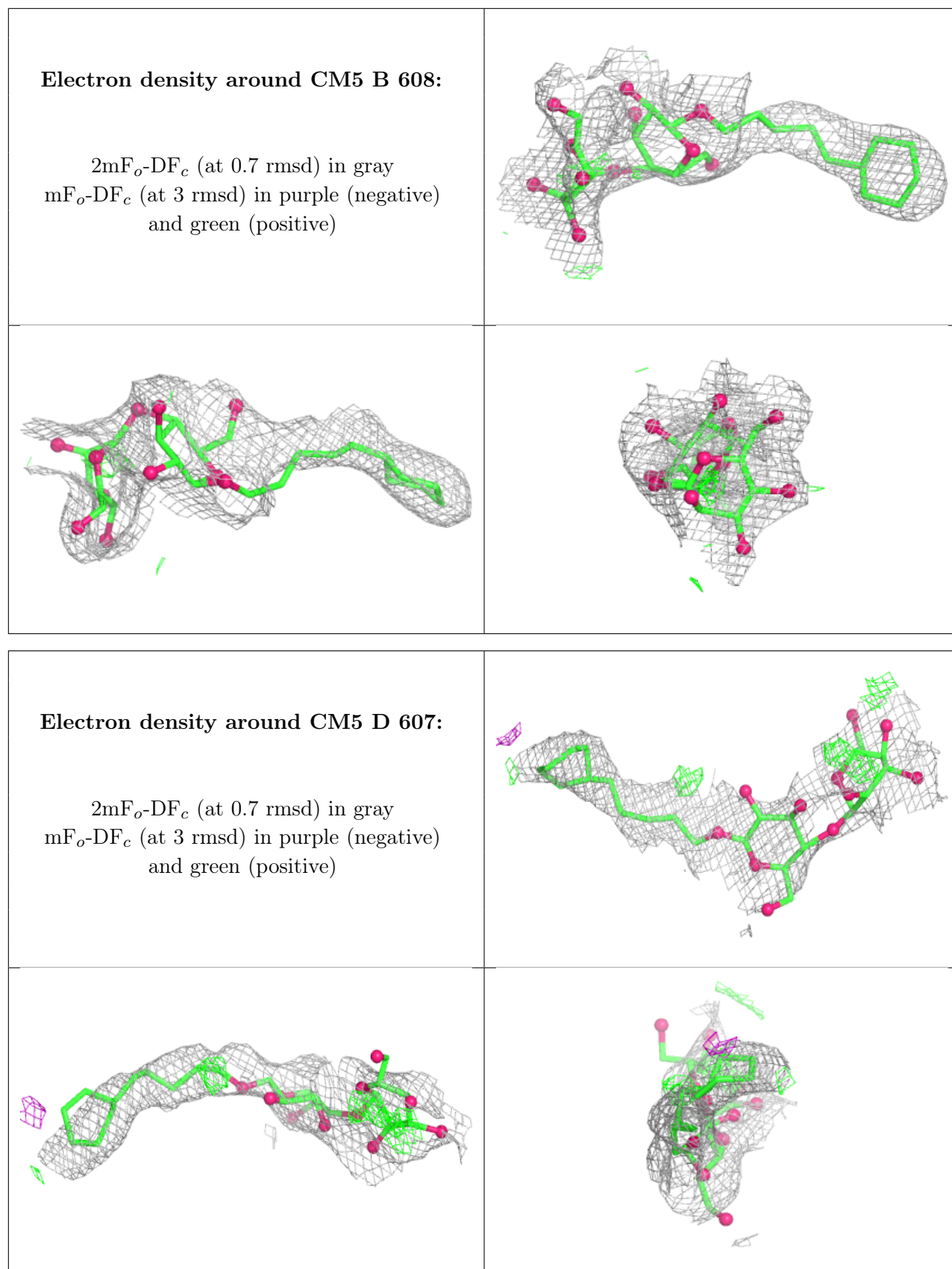
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CM5	B	608	34/34	0.98	0.05	46,84,100,100	0

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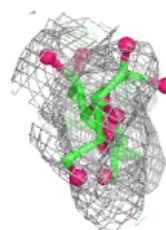
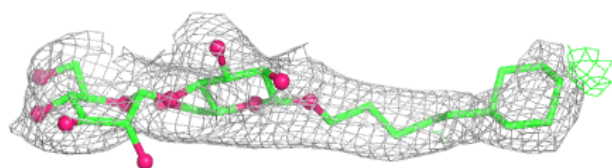
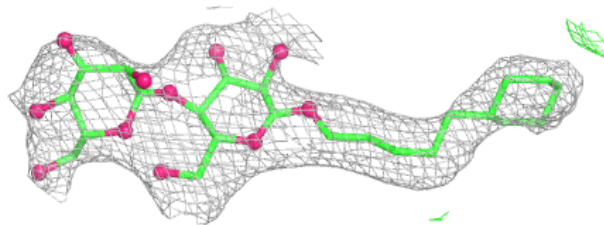
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CM5	D	607	34/34	0.98	0.07	72,97,101,103	0
4	CM5	E	605	34/34	0.98	0.04	66,73,91,92	0
3	3QU	C	501	7/16	0.99	0.06	47,50,51,52	0
3	3QU	E	501	13/16	0.99	0.04	55,57,60,63	0
4	CM5	A	601	34/34	0.99	0.04	53,60,73,74	0
4	CM5	B	602	34/34	0.99	0.04	61,72,84,85	0
2	HEM	F	500	43/43	0.99	0.04	53,65,66,67	0
4	CM5	C	603	34/34	0.99	0.05	54,63,70,71	0
4	CM5	D	604	34/34	0.99	0.04	58,67,77,79	0
3	3QU	A	501	7/16	0.99	0.05	47,50,51,52	0
3	3QU	B	501	16/16	0.99	0.04	47,51,60,66	0
4	CM5	F	606	34/34	0.99	0.06	45,62,74,76	0
2	HEM	C	500	43/43	1.00	0.03	21,27,36,46	0
2	HEM	D	500	43/43	1.00	0.03	23,33,38,39	0
3	3QU	D	501	13/16	1.00	0.04	47,49,54,54	0
2	HEM	E	500	43/43	1.00	0.02	17,28,36,40	0
2	HEM	A	500	43/43	1.00	0.03	25,31,39,43	0
2	HEM	B	500	43/43	1.00	0.02	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.

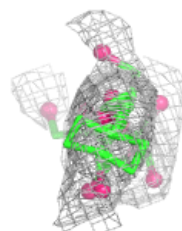
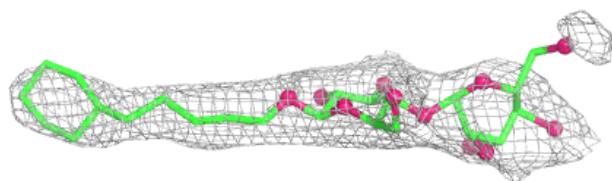
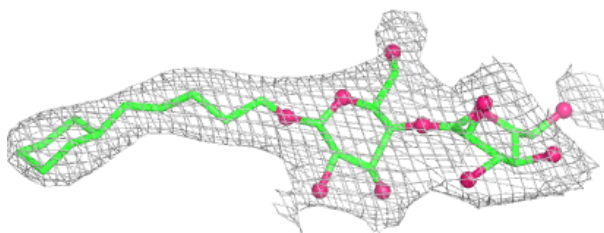


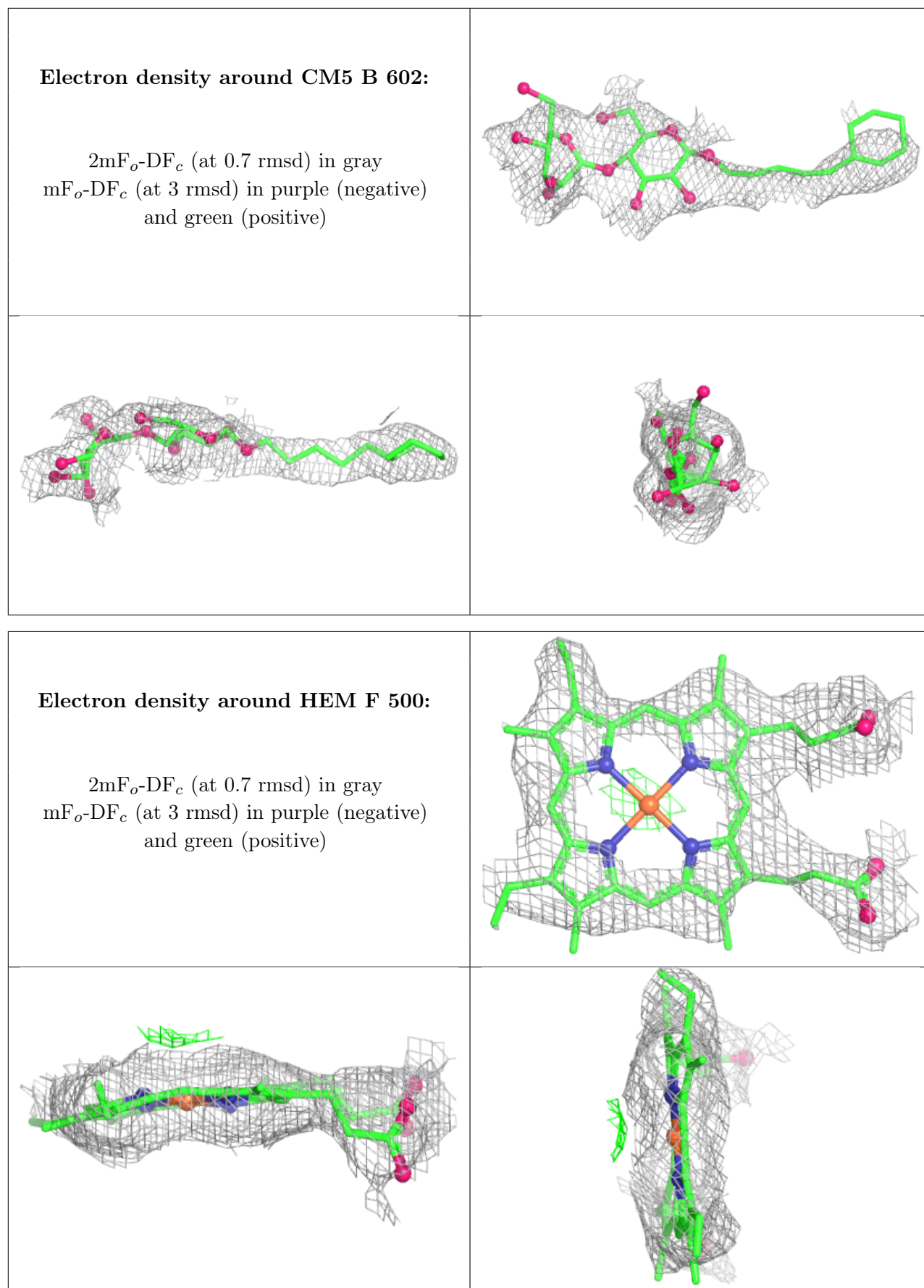
Electron density around CM5 E 605:

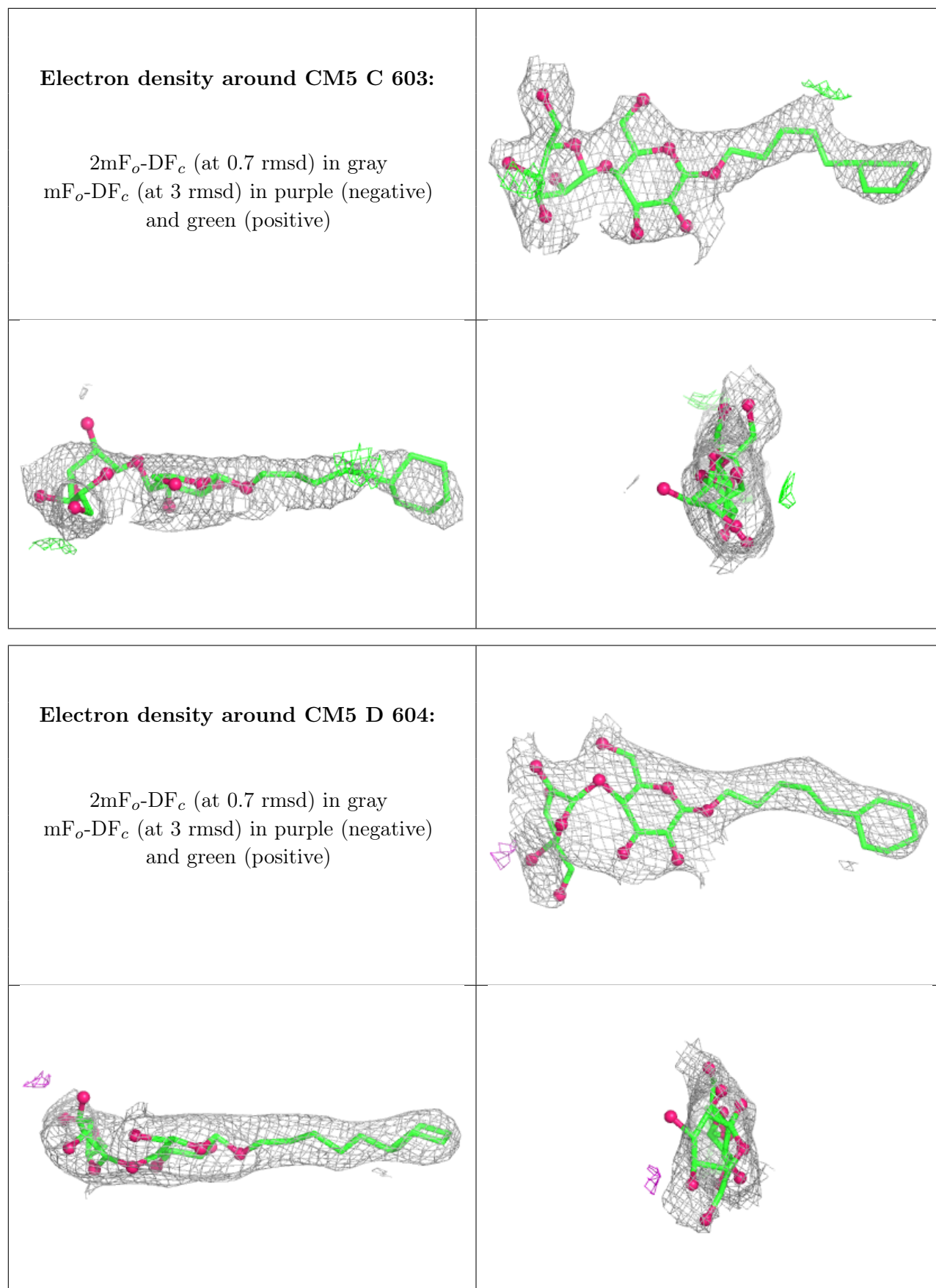
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CM5 A 601:**

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

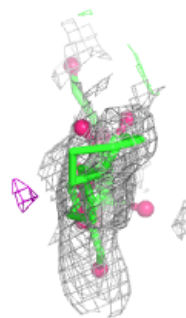
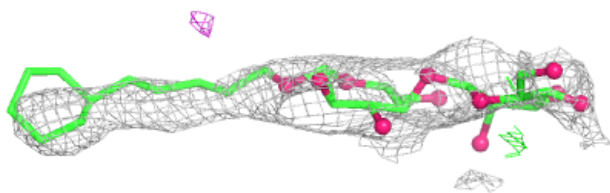
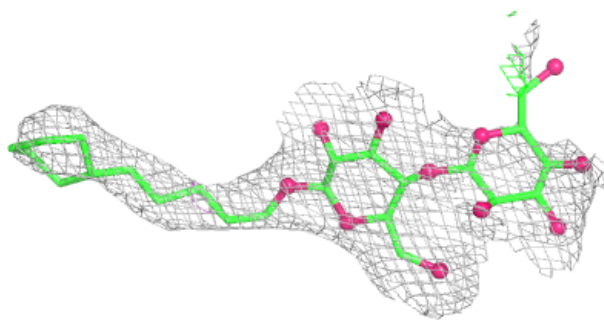






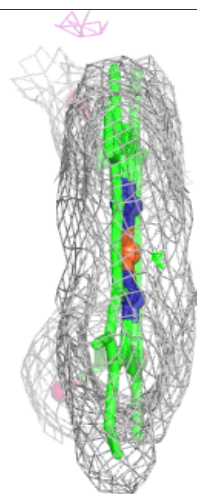
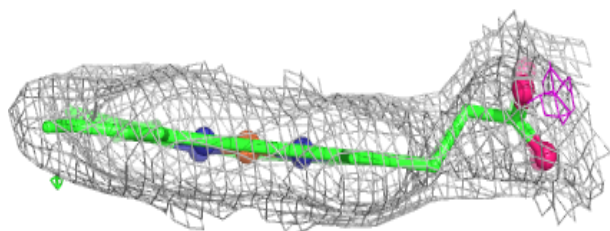
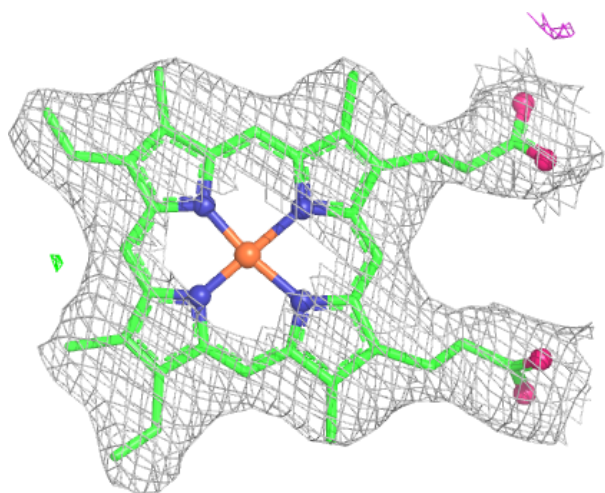
Electron density around CM5 F 606:

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



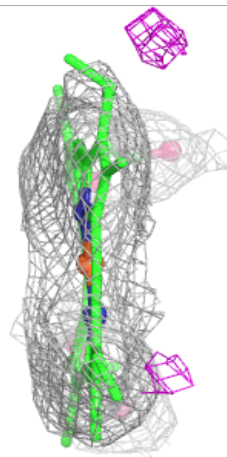
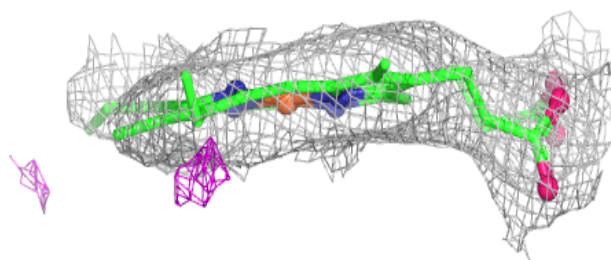
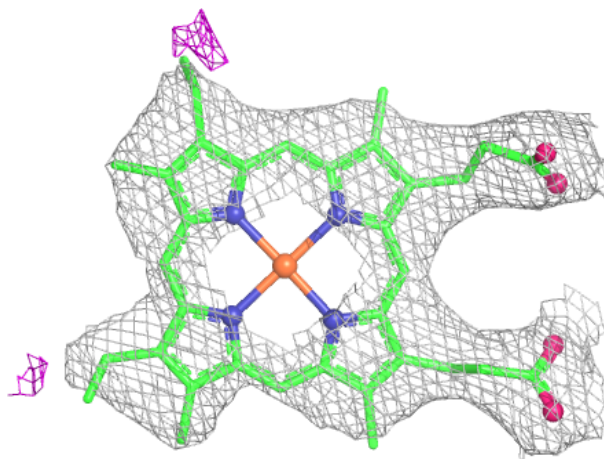
Electron density around HEM C 500:

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



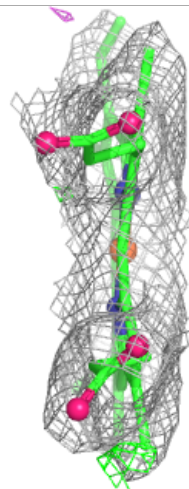
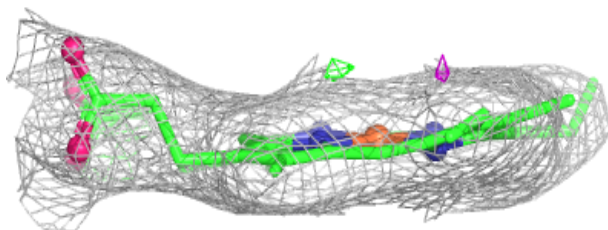
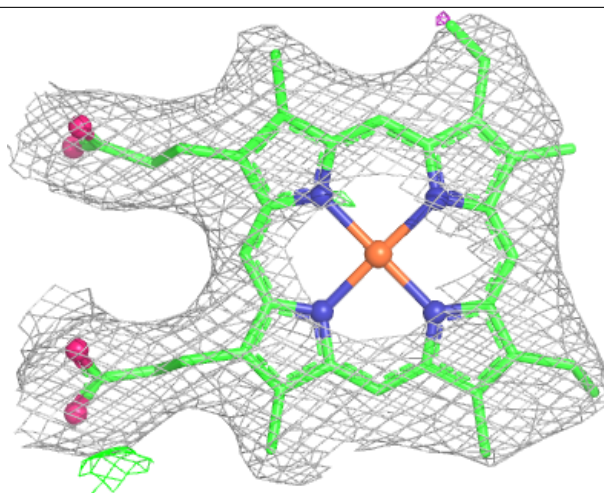
Electron density around HEM D 500:

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



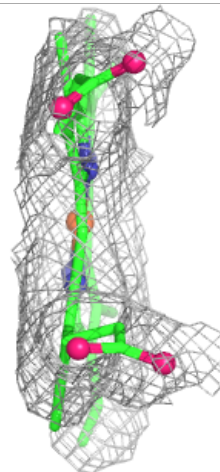
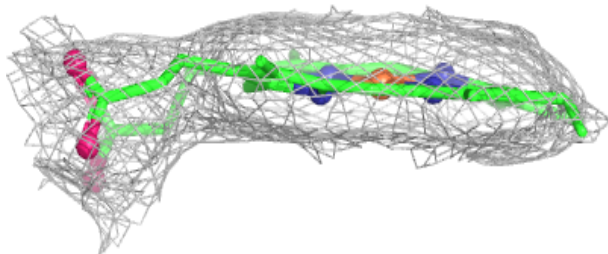
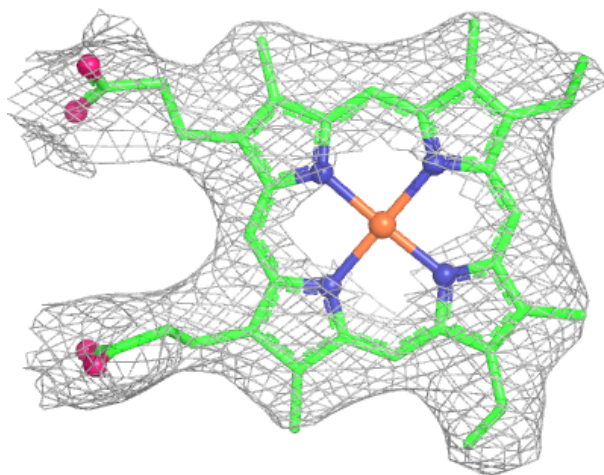
Electron density around HEM E 500:

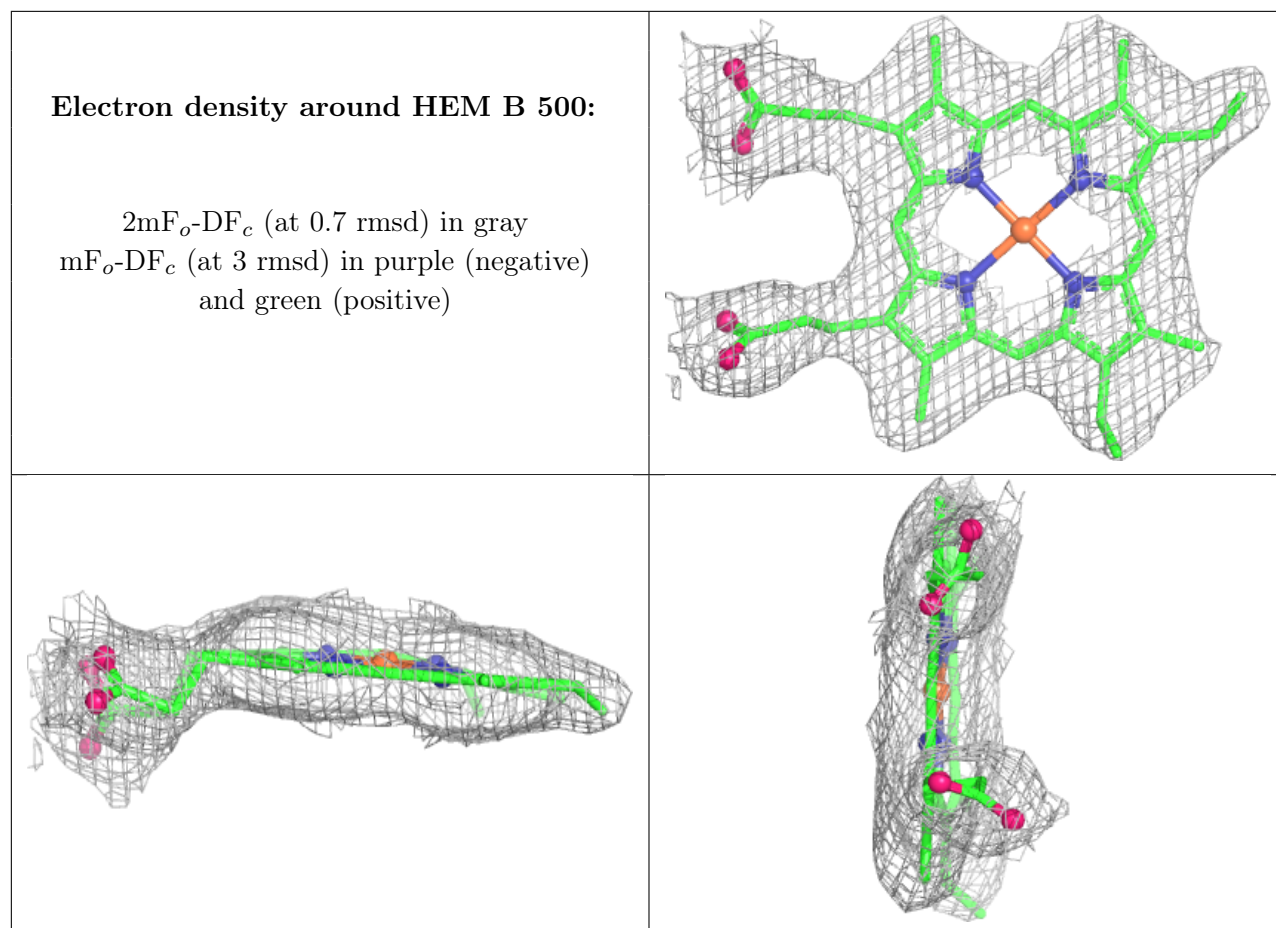
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.