



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2022 – 12:08 PM EDT

PDB ID : 6UX0
Title : Isavuconazole bound complex of Acanthamoeba castellanii CYP51
Authors : Sharma, V.; Podust, L.M.
Deposited on : 2019-11-06
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4.02b-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

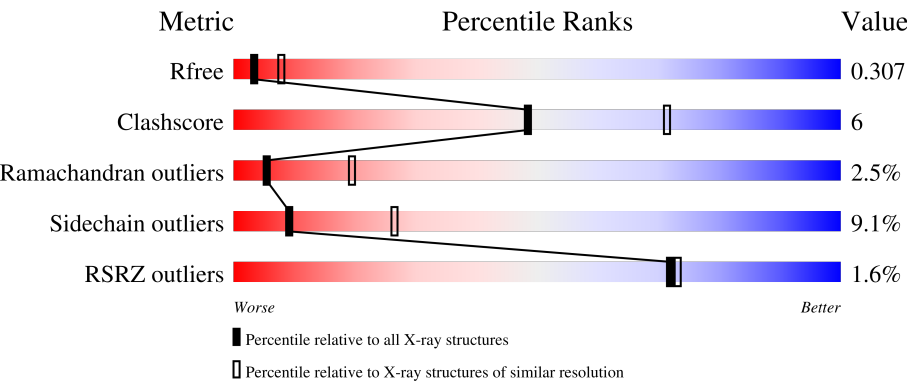
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 $\leq 5\%$. 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	460	<div><div>0%</div><div>66%21%•10%</div></div>
1	B	460	<div><div>75%13%•10%</div></div>
1	C	460	<div><div>2%67%20%•10%</div></div>
1	D	460	<div><div>3%66%23%•10%</div></div>
1	E	460	<div><div>2%72%16%•10%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	460	<div><div></div><div>69%</div><div>19%</div><div>• 10%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19999 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	413	Total	C	N	O	S	0	0	0
			3253	2099	540	596	18			
1	B	414	Total	C	N	O	S	0	0	0
			3262	2103	544	597	18			
1	C	414	Total	C	N	O	S	0	0	0
			3256	2103	541	594	18			
1	D	414	Total	C	N	O	S	0	0	0
			3268	2113	544	593	18			
1	E	413	Total	C	N	O	S	0	0	0
			3255	2101	542	594	18			
1	F	413	Total	C	N	O	S	0	0	0
			3258	2101	543	596	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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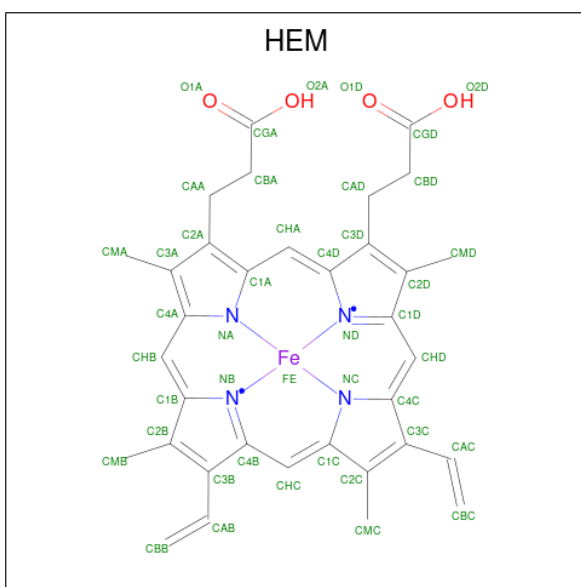
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ALA	-	expression tag	UNP L8GJB3
B	35	LYS	-	expression tag	UNP L8GJB3
B	36	LYS	-	expression tag	UNP L8GJB3
B	37	THR	-	expression tag	UNP L8GJB3
B	38	SER	-	expression tag	UNP L8GJB3
B	39	SER	-	expression tag	UNP L8GJB3
B	40	LYS	-	expression tag	UNP L8GJB3
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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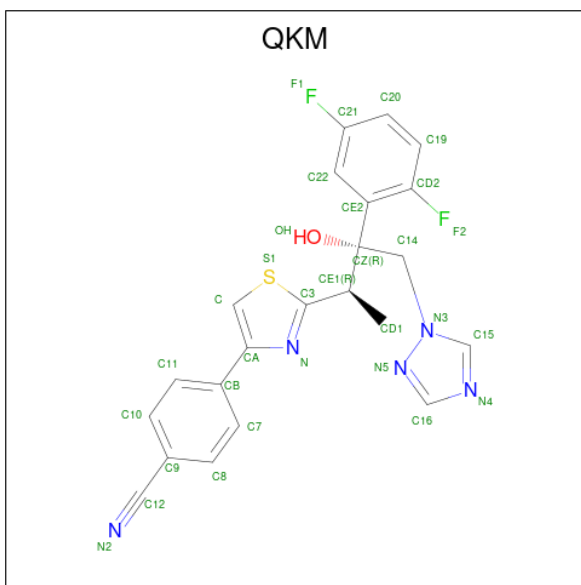
Chain	Residue	Modelled	Actual	Comment	Reference
D	488	HIS	-	expression tag	UNP L8GJB3
D	489	HIS	-	expression tag	UNP L8GJB3
D	490	HIS	-	expression tag	UNP L8GJB3
D	491	HIS	-	expression tag	UNP L8GJB3
D	492	HIS	-	expression tag	UNP L8GJB3
E	33	MET	-	expression tag	UNP L8GJB3
E	34	ALA	-	expression tag	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: $C_{34}H_{32}FeN_4O_4$).



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-{2-[(2R,3R)-3-(2,5-difluorophenyl)-3-hydroxy-4-(1H-1,2,4-triazol-1-yl)butan-2-yl]-1,3-thiazol-4-yl}benzonitrile (three-letter code: QKM) (formula: C₂₂H₁₇F₂N₅OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			31	22	2	5	1	1	0
3	B	1	Total	C	F	N	O	S	
			31	22	2	5	1	1	0
3	C	1	Total	C	F	N	O	S	
			31	22	2	5	1	1	0
3	D	1	Total	C	F	N	O	S	
			31	22	2	5	1	1	0
3	E	1	Total	C	F	N	O	S	
			31	22	2	5	1	1	0
3	F	1	Total	C	F	N	O	S	
			31	22	2	5	1	1	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe		
			1	1	0	0
4	F	1	Total	Fe		
			1	1	0	0

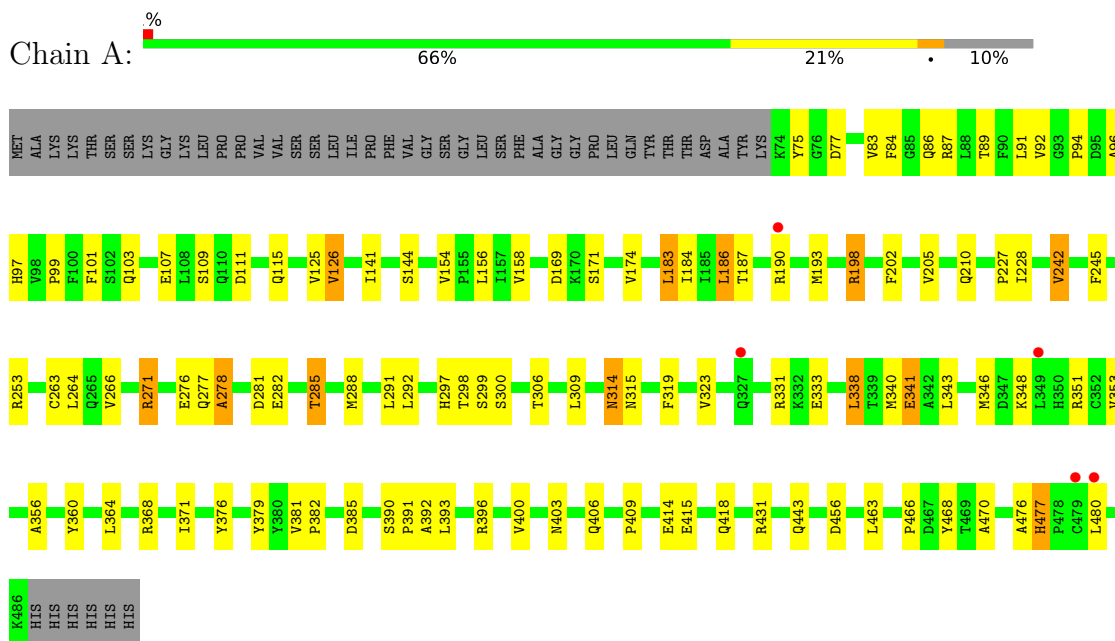
- Molecule 5 is water.

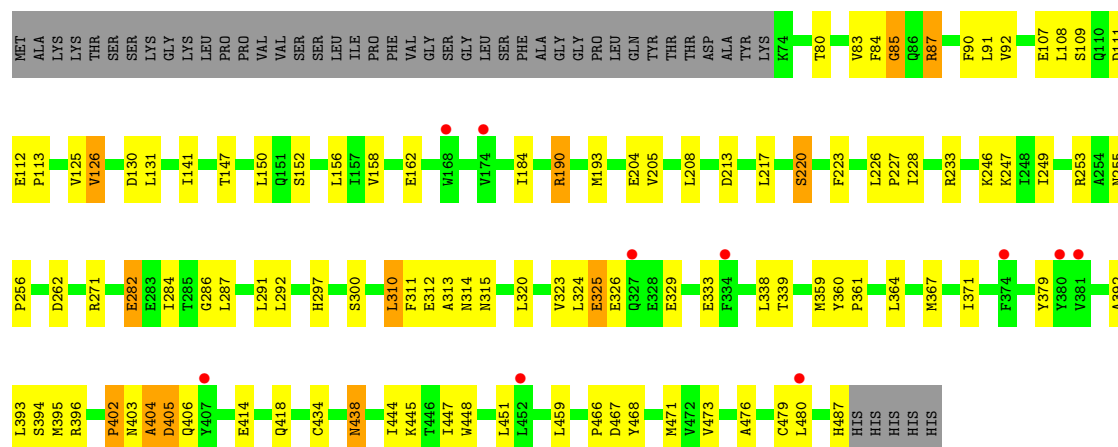
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	O		
			1	1	0	0

3 Residue-property plots [i](#)

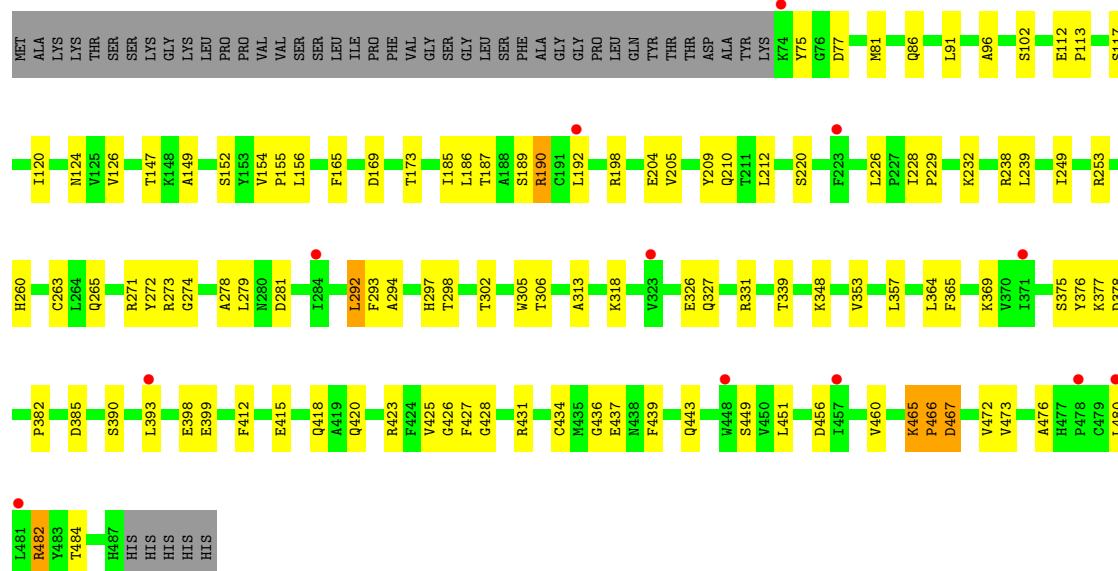
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Obtusifoliol 14alphademethylase

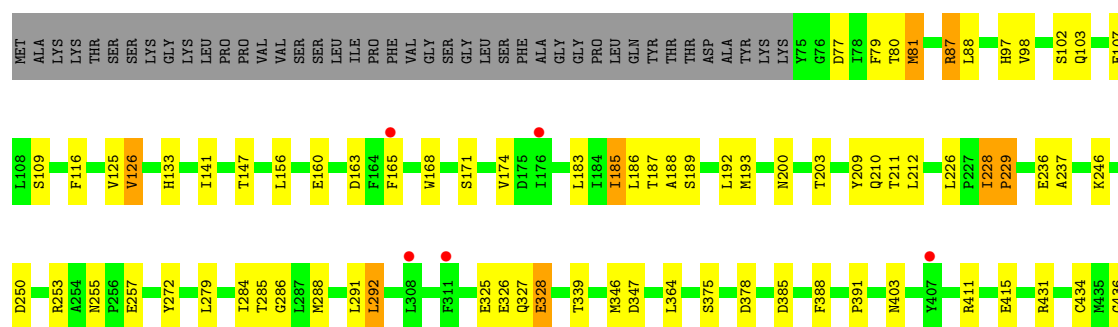
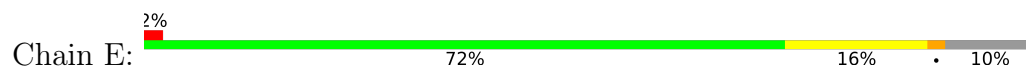


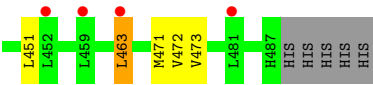


• Molecule 1: Obtusifoliol 14alphademethylase

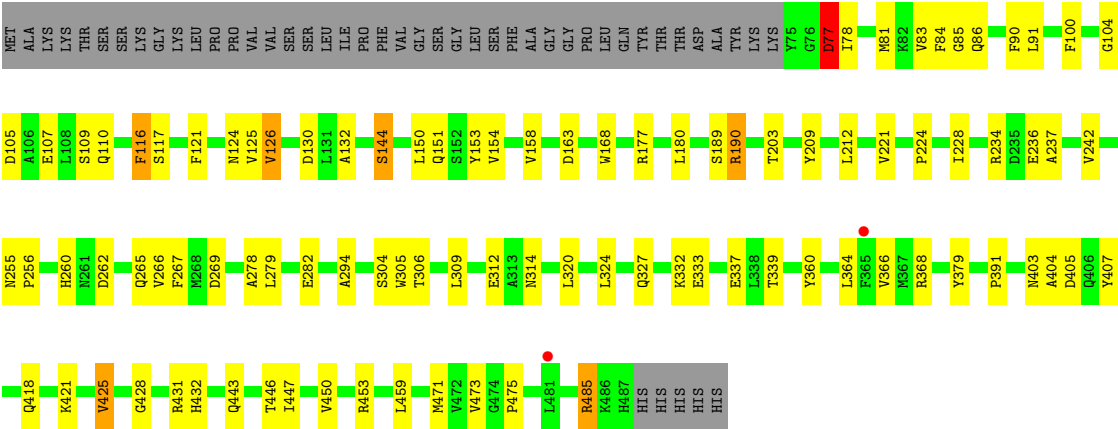


• Molecule 1: Obtusifoliol 14alphademethylase





● Molecule 1: Obtusifoliol 14alphademethylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.45Å 99.06Å 108.71Å 92.61° 96.20° 120.09°	Depositor
Resolution (Å)	107.35 – 2.93 107.35 – 2.93	Depositor EDS
% Data completeness (in resolution range)	94.0 (107.35-2.93) 94.0 (107.35-2.93)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.308 0.217 , 0.307	Depositor DCC
R_{free} test set	3621 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19999	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

5.1 Standard geometry

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

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	0.59	0/3333	0.81	1/4525 (0.0%)
1	B	0.59	0/3342	0.79	2/4536 (0.0%)
1	C	0.61	0/3337	0.78	0/4530
1	D	0.59	0/3348	0.78	1/4541 (0.0%)
1	E	0.58	0/3334	0.75	0/4522
1	F	0.59	0/3338	0.79	1/4529 (0.0%)
All	All	0.59	0/20032	0.78	5/27183 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	190	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	368	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	431	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	368	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	368	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	ALA	Peptide
1	B	476	ALA	Peptide
1	F	81	MET	Peptide

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	3253	0	3136	44	0
1	B	3262	0	3142	26	0
1	C	3256	0	3132	39	0
1	D	3268	0	3174	49	0
1	E	3255	0	3158	31	0
1	F	3258	0	3146	37	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
2	E	43	0	30	3	0
2	F	43	0	30	2	0
3	A	31	0	0	0	0
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	2	0
3	E	31	0	0	0	0
3	F	31	0	0	1	0
4	B	1	0	0	0	0
4	F	1	0	0	0	0
5	E	1	0	0	0	0
All	All	19999	0	19068	235	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 6.

All (235) 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:364:LEU:HD21	1:D:473:VAL:HG21	1.57	0.87
1:A:309:LEU:HD23	1:A:463:LEU:HD11	1.64	0.79
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.71	0.71
1:C:312:GLU:HA	1:C:459:LEU:HD22	1.74	0.70
1:D:190:ARG:HG2	1:D:198:ARG:HG2	1.76	0.68
1:B:242:VAL:HA	1:B:285:THR:HG21	1.76	0.68
1:A:125:VAL:HG12	1:A:126:VAL:HG23	1.76	0.67
1:C:249:ILE:HD11	1:C:284:ILE:HG21	1.77	0.66
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.78	0.65
1:E:160:GLU:HB2	1:E:187:THR:HG22	1.80	0.64
1:E:125:VAL:HG11	1:E:286:GLY:HA3	1.79	0.64
1:F:83:VAL:O	1:F:85:GLY:N	2.31	0.64
1:C:393:LEU:O	1:C:395:MET:N	2.32	0.63
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.80	0.63
1:B:284:ILE:O	1:B:288:MET:HG2	1.99	0.62
1:C:467:ASP:HB2	1:C:476:ALA:HB2	1.81	0.62
1:A:96:ALA:O	1:A:99:PRO:HD2	2.00	0.62
1:A:414:GLU:OE1	1:A:414:GLU:N	2.33	0.61
1:D:460:VAL:HG11	1:D:480:LEU:HD12	1.82	0.61
1:D:156:LEU:HD22	1:D:190:ARG:HD3	1.83	0.61
1:B:219:ILE:HD12	1:B:219:ILE:H	1.66	0.61
1:A:183:LEU:O	1:A:183:LEU:HD12	2.02	0.60
1:D:425:VAL:O	1:D:428:GLY:N	2.35	0.59
1:D:117:SER:HA	1:D:120:ILE:HD12	1.84	0.59
1:F:368:ARG:NH2	2:F:501:HEM:O2A	2.27	0.59
1:C:125:VAL:HG12	1:C:126:VAL:HG23	1.83	0.59
1:D:165:PHE:CD1	1:D:451:LEU:HD21	2.38	0.58
1:C:404:ALA:O	1:C:406:GLN:N	2.36	0.58
1:A:89:THR:HG21	1:A:381:VAL:HG22	1.86	0.58
1:E:160:GLU:CB	1:E:187:THR:HG22	2.34	0.58
1:A:109:SER:HB2	1:A:371:ILE:HD11	1.86	0.57
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.87	0.56
1:D:212:LEU:HD21	1:D:238:ARG:HB2	1.86	0.55
1:B:209:TYR:HA	1:B:212:LEU:HD12	1.89	0.55
1:A:187:THR:OG1	1:A:443:GLN:NE2	2.41	0.54
1:E:364:LEU:HD21	1:E:473:VAL:HG21	1.89	0.54
1:E:125:VAL:HG12	1:E:126:VAL:HG23	1.90	0.53
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.91	0.53
1:C:109:SER:HB2	1:C:371:ILE:HD11	1.90	0.53
1:D:228:ILE:HB	1:D:229:PRO:CD	2.38	0.53
1:D:293:PHE:CE2	1:D:297:HIS:CE1	2.97	0.53
1:F:320:LEU:HG	1:F:324:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LEU:O	1:E:228:ILE:N	2.40	0.53
1:E:168:TRP:CH2	1:E:174:VAL:HG21	2.44	0.53
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.90	0.52
1:F:443:GLN:O	1:F:447:ILE:HG13	2.09	0.52
1:E:165:PHE:CD1	1:E:451:LEU:HD21	2.44	0.52
1:B:94:PRO:O	1:B:98:VAL:HG23	2.09	0.52
1:B:367:MET:O	1:B:368:ARG:NH1	2.43	0.52
1:C:156:LEU:HD23	1:C:190:ARG:HG3	1.91	0.52
1:A:77:ASP:OD2	1:A:376:TYR:OH	2.23	0.52
1:A:271:ARG:CZ	1:A:278:ALA:HB2	2.40	0.51
1:C:113:PRO:HB3	1:C:367:MET:HB2	1.91	0.51
1:D:187:THR:HG21	1:D:443:GLN:HE22	1.76	0.51
1:F:77:ASP:C	1:F:77:ASP:OD1	2.49	0.51
1:F:180:LEU:HD22	1:F:447:ILE:HG21	1.93	0.51
1:A:103:GLN:HE21	1:A:107:GLU:HB3	1.75	0.51
1:E:327:GLN:OE1	1:E:346:MET:SD	2.69	0.51
1:B:285:THR:O	1:B:288:MET:HB2	2.11	0.50
1:A:309:LEU:HD12	1:A:356:ALA:HB2	1.94	0.50
1:C:83:VAL:O	1:C:85:GLY:N	2.44	0.50
1:D:420:GLN:HB3	1:D:423:ARG:HD2	1.93	0.50
1:A:392:ALA:O	1:A:396:ARG:HG2	2.12	0.50
1:F:294:ALA:HB1	3:F:502:QKM:C16	2.41	0.50
1:C:466:PRO:HB2	1:C:468:TYR:CE1	2.46	0.50
1:B:83:VAL:O	1:B:85:GLY:N	2.45	0.49
1:C:226:LEU:O	1:C:228:ILE:N	2.38	0.49
1:D:185:ILE:HD12	1:D:292:LEU:HD21	1.94	0.49
1:A:338:LEU:HD21	1:A:343:LEU:HD21	1.93	0.49
1:D:91:LEU:HB3	1:D:96:ALA:HB1	1.94	0.49
1:C:323:VAL:O	1:C:326:GLU:N	2.46	0.49
1:E:188:ALA:O	1:E:192:LEU:HD12	2.13	0.49
1:C:320:LEU:HG	1:C:324:LEU:HD12	1.94	0.49
1:B:459:LEU:HA	1:B:481:LEU:HD23	1.94	0.49
1:C:158:VAL:O	1:C:162:GLU:HG3	2.12	0.49
1:C:359:MET:HB3	1:C:360:TYR:CD2	2.48	0.49
1:C:438:ASN:N	1:C:438:ASN:OD1	2.46	0.48
1:D:190:ARG:CG	1:D:198:ARG:HG2	2.43	0.48
1:A:141:ILE:HG23	1:A:291:LEU:HD11	1.94	0.48
1:A:186:LEU:CD1	1:A:202:PHE:CZ	2.96	0.48
1:A:193:MET:HG2	1:A:288:MET:HE2	1.96	0.48
1:B:308:LEU:HD23	1:B:481:LEU:HD21	1.95	0.48
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:O	1:A:299:SER:C	2.51	0.48
1:B:368:ARG:NH2	2:B:501:HEM:O2A	2.43	0.48
1:C:255:ASN:N	1:C:256:PRO:HD3	2.29	0.48
1:D:306:THR:HG21	1:D:353:VAL:HG22	1.96	0.48
1:A:156:LEU:HD23	1:A:190:ARG:HD2	1.95	0.47
1:C:246:LYS:O	1:C:247:LYS:C	2.52	0.47
1:F:446:THR:O	1:F:450:VAL:HG23	2.14	0.47
1:E:411:ARG:O	1:E:415:GLU:HB3	2.14	0.47
1:F:130:ASP:OD1	1:F:132:ALA:HB3	2.15	0.47
1:F:100:PHE:CZ	1:F:366:VAL:HG23	2.49	0.47
1:A:94:PRO:HG3	1:A:400:VAL:HG21	1.97	0.47
1:A:319:PHE:CZ	1:A:409:PRO:HD2	2.50	0.47
1:C:226:LEU:HB3	1:C:228:ILE:HG23	1.96	0.47
1:E:272:TYR:CE1	1:E:279:LEU:HD21	2.50	0.47
1:A:403:ASN:HB3	1:A:406:GLN:HE21	1.80	0.47
1:B:217:LEU:N	1:B:220:SER:OG	2.43	0.47
1:D:260:HIS:HB2	1:D:265:GLN:HE21	1.80	0.47
1:F:209:TYR:HA	1:F:212:LEU:HD12	1.97	0.47
1:E:228:ILE:HB	1:E:229:PRO:HD2	1.97	0.46
1:A:245:PHE:CD2	1:A:285:THR:HG23	2.50	0.46
1:A:306:THR:HG21	1:A:353:VAL:HG22	1.96	0.46
1:E:185:ILE:HD12	1:E:292:LEU:HD21	1.97	0.46
1:D:412:PHE:HA	1:D:415:GLU:HB3	1.97	0.46
1:F:305:TRP:CD1	1:F:360:TYR:HB2	2.50	0.46
1:A:91:LEU:HB3	1:A:96:ALA:HB1	1.96	0.46
1:F:234:ARG:O	1:F:237:ALA:HB3	2.15	0.46
1:C:204:GLU:O	1:C:208:LEU:HD13	2.15	0.46
1:C:444:ILE:HA	1:C:447:ILE:HD12	1.97	0.46
1:A:309:LEU:HD23	1:A:463:LEU:CD1	2.41	0.46
1:B:160:GLU:CB	1:B:187:THR:HG22	2.46	0.46
1:D:298:THR:HG21	3:D:502:QKM:C16	2.46	0.46
1:E:80:THR:HG22	1:E:81:MET:N	2.30	0.46
1:C:90:PHE:O	1:C:91:LEU:HD23	2.16	0.46
1:D:112:GLU:HB2	1:D:113:PRO:CD	2.46	0.46
1:E:226:LEU:O	1:E:228:ILE:HG23	2.16	0.46
1:D:272:TYR:CE1	1:D:279:LEU:HD23	2.51	0.46
1:D:226:LEU:CB	1:D:228:ILE:HG23	2.46	0.45
1:C:282:GLU:O	1:C:286:GLY:N	2.45	0.45
1:E:88:LEU:HD22	1:E:388:PHE:CE1	2.52	0.45
1:E:183:LEU:O	1:E:187:THR:HG23	2.17	0.45
1:F:224:PRO:O	1:F:234:ARG:NH2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:THR:HA	1:C:150:LEU:HD12	1.98	0.45
1:C:217:LEU:O	1:C:220:SER:N	2.50	0.45
1:A:343:LEU:HA	1:A:346:MET:SD	2.57	0.45
1:C:107:GLU:O	1:C:108:LEU:HD23	2.17	0.45
1:F:90:PHE:O	1:F:91:LEU:HD23	2.16	0.45
1:D:149:ALA:O	1:D:152:SER:CB	2.65	0.45
1:F:117:SER:HB2	1:F:121:PHE:CE2	2.52	0.45
1:C:184:ILE:HD12	1:C:300:SER:HA	1.98	0.45
1:D:186:LEU:O	1:D:189:SER:OG	2.32	0.45
1:D:382:PRO:HD2	1:D:385:ASP:OD2	2.17	0.45
1:F:262:ASP:O	1:F:266:VAL:HG23	2.17	0.45
1:D:249:ILE:O	1:D:253:ARG:HG3	2.17	0.45
1:D:327:GLN:NE2	1:D:449:SER:OG	2.48	0.45
1:E:436:GLY:HA3	2:E:501:HEM:C3C	2.52	0.45
1:F:305:TRP:CH2	1:F:475:PRO:HB3	2.52	0.45
1:B:412:PHE:HA	1:B:415:GLU:HB3	1.99	0.44
1:C:444:ILE:O	1:C:445:LYS:C	2.55	0.44
1:D:173:THR:HG23	1:D:482:ARG:HA	2.00	0.44
1:B:125:VAL:HG13	1:B:126:VAL:HG23	2.00	0.44
1:E:141:ILE:HG12	1:E:291:LEU:HD11	2.00	0.44
1:A:277:GLN:O	1:A:278:ALA:HB3	2.18	0.44
1:D:271:ARG:CZ	1:D:278:ALA:HB2	2.48	0.44
1:F:177:ARG:HA	1:F:304:SER:OG	2.17	0.44
1:F:260:HIS:HB2	1:F:265:GLN:HE21	1.83	0.44
1:A:340:MET:O	1:A:341:GLU:C	2.55	0.44
1:C:112:GLU:HB2	1:C:113:PRO:HD3	2.00	0.44
1:F:116:PHE:HB3	1:F:221:VAL:HA	2.00	0.44
1:B:281:ASP:O	1:B:285:THR:OG1	2.31	0.44
1:E:284:ILE:O	1:E:288:MET:HG2	2.17	0.44
1:F:364:LEU:HD21	1:F:473:VAL:HG11	2.00	0.43
1:A:281:ASP:O	1:A:285:THR:OG1	2.35	0.43
1:D:294:ALA:HB1	3:D:502:QKM:C16	2.48	0.43
1:C:325:GLU:O	1:C:329:GLU:HG3	2.18	0.43
1:C:448:TRP:CZ3	1:C:451:LEU:HD13	2.53	0.43
1:F:110:GLN:HE22	1:F:432:HIS:CD2	2.36	0.43
1:F:255:ASN:N	1:F:256:PRO:HD3	2.33	0.43
1:A:263:CYS:O	1:A:266:VAL:N	2.51	0.43
1:D:357:LEU:CD2	1:D:427:PHE:CE2	3.01	0.43
1:F:267:PHE:O	1:F:279:LEU:HD12	2.18	0.43
1:D:190:ARG:HG2	1:D:198:ARG:CG	2.47	0.43
1:D:390:SER:HB3	1:D:393:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:GLU:HA	1:F:459:LEU:HD23	2.00	0.43
1:D:209:TYR:O	1:D:210:GLN:C	2.57	0.43
1:D:209:TYR:O	1:D:212:LEU:N	2.51	0.43
1:A:190:ARG:HB2	1:A:198:ARG:HG2	2.01	0.43
1:A:309:LEU:HD21	1:A:360:TYR:HE2	1.84	0.43
1:E:211:THR:HG21	1:E:237:ALA:HB2	2.01	0.43
1:A:111:ASP:O	1:A:115:GLN:OE1	2.37	0.43
1:B:354:LYS:O	1:B:357:LEU:HB3	2.19	0.43
1:C:141:ILE:HG23	1:C:291:LEU:HD11	2.01	0.43
1:C:434:CYS:HA	2:C:501:HEM:CHA	2.48	0.43
1:A:184:ILE:HD12	1:A:300:SER:HA	2.00	0.42
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	2.01	0.42
1:E:209:TYR:O	1:E:212:LEU:N	2.52	0.42
1:A:83:VAL:O	1:A:84:PHE:C	2.58	0.42
1:D:467:ASP:HB2	1:D:476:ALA:HB2	2.01	0.42
1:D:376:TYR:O	1:D:378:ASP:N	2.53	0.42
1:A:97:HIS:HB3	1:A:101:PHE:HD2	1.85	0.42
1:A:348:LYS:O	1:A:351:ARG:N	2.53	0.42
1:D:439:PHE:CD1	1:D:439:PHE:C	2.93	0.42
1:D:465:LYS:O	1:D:466:PRO:O	2.38	0.42
1:D:364:LEU:CD2	1:D:473:VAL:HG21	2.36	0.42
1:F:327:GLN:HE21	1:F:453:ARG:HE	1.66	0.42
1:D:192:LEU:HD23	1:D:263:CYS:SG	2.59	0.42
1:E:325:GLU:O	1:E:328:GLU:N	2.53	0.42
1:B:184:ILE:CD1	1:B:300:SER:HA	2.50	0.42
1:D:185:ILE:CD1	1:D:292:LEU:HD21	2.49	0.42
1:A:390:SER:HB3	1:A:393:LEU:HB2	2.02	0.41
1:C:80:THR:HG21	1:C:87:ARG:HH21	1.85	0.41
1:D:154:VAL:N	1:D:155:PRO:HD2	2.34	0.41
1:E:165:PHE:CE1	1:E:451:LEU:HD21	2.55	0.41
1:F:168:TRP:O	1:F:485:ARG:NH1	2.53	0.41
1:A:89:THR:HG21	1:A:381:VAL:CG2	2.49	0.41
1:B:466:PRO:HB2	1:B:468:TYR:CE1	2.55	0.41
1:F:242:VAL:HG21	1:F:282:GLU:HG2	2.02	0.41
1:A:466:PRO:HB2	1:A:468:TYR:CE2	2.55	0.41
1:B:391:PRO:HA	1:B:425:VAL:HG23	2.03	0.41
1:F:150:LEU:HA	1:F:153:TYR:HD2	1.86	0.41
1:F:154:VAL:O	1:F:158:VAL:HG23	2.20	0.41
1:F:309:LEU:HB3	1:F:407:TYR:CE1	2.55	0.41
1:B:228:ILE:HD12	1:B:229:PRO:HG2	2.02	0.41
1:D:226:LEU:HB3	1:D:228:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:PHE:CD1	1:E:116:PHE:C	2.92	0.41
1:F:125:VAL:HG12	1:F:126:VAL:HG23	2.01	0.41
1:A:154:VAL:O	1:A:158:VAL:HG23	2.21	0.41
1:C:364:LEU:HD21	1:C:473:VAL:HG11	2.03	0.41
1:C:434:CYS:HA	2:C:501:HEM:C4D	2.56	0.41
1:E:434:CYS:HA	2:E:501:HEM:C4D	2.55	0.41
1:B:192:LEU:C	1:B:288:MET:HE1	2.41	0.41
1:F:78:ILE:HD12	1:F:91:LEU:CD2	2.50	0.41
1:A:242:VAL:HG21	1:A:282:GLU:HG2	2.01	0.41
1:B:118:VAL:HB	1:B:119:PRO:CD	2.51	0.41
1:B:228:ILE:HB	1:B:229:PRO:HD2	2.03	0.41
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.51	0.41
1:D:415:GLU:O	1:D:418:GLN:N	2.54	0.41
1:D:436:GLY:O	1:D:437:GLU:C	2.58	0.41
1:E:80:THR:HG21	1:E:87:ARG:HE	1.85	0.41
1:E:103:GLN:HB3	1:E:107:GLU:HB2	2.03	0.41
1:F:425:VAL:O	1:F:428:GLY:N	2.53	0.41
1:B:137:GLN:HG2	1:B:287:LEU:HD11	2.03	0.41
1:B:217:LEU:H	1:B:220:SER:HG	1.66	0.41
1:C:310:LEU:HD23	1:C:311:PHE:CE1	2.56	0.41
1:A:186:LEU:HD12	1:A:202:PHE:CZ	2.56	0.40
1:F:104:GLY:HA2	1:F:431:ARG:CD	2.51	0.40
1:C:361:PRO:CG	1:C:392:ALA:HA	2.51	0.40
1:D:305:TRP:O	1:D:306:THR:C	2.59	0.40
1:F:305:TRP:O	1:F:306:THR:C	2.59	0.40
1:D:326:GLU:OE2	1:D:348:LYS:N	2.54	0.40
1:D:434:CYS:HA	2:D:501:HEM:CHA	2.52	0.40
1:E:246:LYS:O	1:E:250:ASP:OD1	2.39	0.40
1:E:97:HIS:O	1:E:98:VAL:C	2.60	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	411/460 (89%)	353 (86%)	47 (11%)	11 (3%)	5	18
1	B	412/460 (90%)	355 (86%)	46 (11%)	11 (3%)	5	18
1	C	412/460 (90%)	337 (82%)	64 (16%)	11 (3%)	5	18
1	D	412/460 (90%)	340 (82%)	61 (15%)	11 (3%)	5	18
1	E	411/460 (89%)	358 (87%)	46 (11%)	7 (2%)	9	29
1	F	411/460 (89%)	363 (88%)	37 (9%)	11 (3%)	5	18
All	All	2469/2760 (90%)	2106 (85%)	301 (12%)	62 (2%)	5	19

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	VAL
1	C	394	SER
1	C	404	ALA
1	C	405	ASP
1	D	466	PRO
1	F	84	PHE
1	F	333	GLU
1	A	126	VAL
1	A	333	GLU
1	B	251	GLU
1	B	277	GLN
1	B	333	GLU
1	C	84	PHE
1	C	85	GLY
1	C	313	ALA
1	C	403	ASN
1	D	126	VAL
1	D	273	ARG
1	D	377	LYS
1	D	426	GLY
1	E	257	GLU
1	F	116	PHE
1	F	126	VAL
1	A	314	ASN
1	B	126	VAL
1	B	477	HIS
1	B	479	CYS
1	C	227	PRO
1	C	314	ASN
1	C	402	PRO

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Mol	Chain	Res	Type
1	D	232	LYS
1	D	313	ALA
1	D	467	ASP
1	E	126	VAL
1	A	227	PRO
1	A	278	ALA
1	A	431	ARG
1	A	470	ALA
1	B	220	SER
1	D	102	SER
1	E	391	PRO
1	F	332	LYS
1	F	405	ASP
1	D	77	ASP
1	F	77	ASP
1	F	144	SER
1	F	278	ALA
1	F	404	ALA
1	B	257	GLU
1	E	229	PRO
1	E	403	ASN
1	E	463	LEU
1	E	472	VAL
1	F	425	VAL
1	A	382	PRO
1	A	477	HIS
1	A	323	VAL
1	A	391	PRO
1	B	85	GLY
1	B	218	PRO
1	B	478	PRO
1	D	274	GLY

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	336/397 (85%)	301 (90%)	35 (10%)	7	20
1	B	336/397 (85%)	311 (93%)	25 (7%)	13	36
1	C	334/397 (84%)	297 (89%)	37 (11%)	6	18
1	D	337/397 (85%)	310 (92%)	27 (8%)	12	32
1	E	337/397 (85%)	303 (90%)	34 (10%)	7	22
1	F	337/397 (85%)	312 (93%)	25 (7%)	13	36
All	All	2017/2382 (85%)	1834 (91%)	183 (9%)	9	26

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TYR
1	A	86	GLN
1	A	87	ARG
1	A	92	VAL
1	A	144	SER
1	A	169	ASP
1	A	171	SER
1	A	174	VAL
1	A	183	LEU
1	A	186	LEU
1	A	198	ARG
1	A	205	VAL
1	A	210	GLN
1	A	228	ILE
1	A	242	VAL
1	A	253	ARG
1	A	264	LEU
1	A	271	ARG
1	A	276	GLU
1	A	285	THR
1	A	292	LEU
1	A	297	HIS
1	A	314	ASN
1	A	315	ASN
1	A	331	ARG
1	A	338	LEU
1	A	341	GLU
1	A	364	LEU
1	A	379	TYR
1	A	385	ASP

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Mol	Chain	Res	Type
1	A	415	GLU
1	A	418	GLN
1	A	456	ASP
1	A	477	HIS
1	A	480	LEU
1	B	75	TYR
1	B	79	PHE
1	B	87	ARG
1	B	88	LEU
1	B	109	SER
1	B	111	ASP
1	B	117	SER
1	B	125	VAL
1	B	147	THR
1	B	171	SER
1	B	193	MET
1	B	203	THR
1	B	220	SER
1	B	228	ILE
1	B	236	GLU
1	B	255	ASN
1	B	262	ASP
1	B	280	ASN
1	B	285	THR
1	B	292	LEU
1	B	297	HIS
1	B	337	GLU
1	B	339	THR
1	B	477	HIS
1	B	482	ARG
1	C	87	ARG
1	C	92	VAL
1	C	111	ASP
1	C	130	ASP
1	C	131	LEU
1	C	152	SER
1	C	190	ARG
1	C	193	MET
1	C	205	VAL
1	C	213	ASP
1	C	220	SER
1	C	223	PHE

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Mol	Chain	Res	Type
1	C	233	ARG
1	C	253	ARG
1	C	262	ASP
1	C	271	ARG
1	C	282	GLU
1	C	287	LEU
1	C	292	LEU
1	C	297	HIS
1	C	310	LEU
1	C	315	ASN
1	C	325	GLU
1	C	333	GLU
1	C	338	LEU
1	C	339	THR
1	C	379	TYR
1	C	396	ARG
1	C	402	PRO
1	C	405	ASP
1	C	414	GLU
1	C	418	GLN
1	C	438	ASN
1	C	471	MET
1	C	479	CYS
1	C	480	LEU
1	C	487	HIS
1	D	75	TYR
1	D	81	MET
1	D	86	GLN
1	D	124	ASN
1	D	147	THR
1	D	169	ASP
1	D	190	ARG
1	D	204	GLU
1	D	205	VAL
1	D	220	SER
1	D	239	LEU
1	D	281	ASP
1	D	292	LEU
1	D	302	THR
1	D	318	LYS
1	D	331	ARG
1	D	339	THR

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Mol	Chain	Res	Type
1	D	365	PHE
1	D	369	LYS
1	D	375	SER
1	D	398	GLU
1	D	399	GLU
1	D	456	ASP
1	D	465	LYS
1	D	472	VAL
1	D	482	ARG
1	D	484	THR
1	E	77	ASP
1	E	79	PHE
1	E	81	MET
1	E	87	ARG
1	E	102	SER
1	E	109	SER
1	E	133	HIS
1	E	147	THR
1	E	156	LEU
1	E	163	ASP
1	E	171	SER
1	E	185	ILE
1	E	186	LEU
1	E	189	SER
1	E	193	MET
1	E	200	ASN
1	E	203	THR
1	E	210	GLN
1	E	228	ILE
1	E	236	GLU
1	E	253	ARG
1	E	255	ASN
1	E	285	THR
1	E	292	LEU
1	E	326	GLU
1	E	328	GLU
1	E	339	THR
1	E	347	ASP
1	E	375	SER
1	E	378	ASP
1	E	385	ASP
1	E	431	ARG

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Mol	Chain	Res	Type
1	E	463	LEU
1	E	471	MET
1	F	77	ASP
1	F	86	GLN
1	F	105	ASP
1	F	107	GLU
1	F	109	SER
1	F	124	ASN
1	F	144	SER
1	F	151	GLN
1	F	163	ASP
1	F	189	SER
1	F	190	ARG
1	F	203	THR
1	F	228	ILE
1	F	236	GLU
1	F	269	ASP
1	F	314	ASN
1	F	337	GLU
1	F	339	THR
1	F	379	TYR
1	F	391	PRO
1	F	403	ASN
1	F	418	GLN
1	F	421	LYS
1	F	471	MET
1	F	485	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	115	GLN
1	A	133	HIS
1	A	265	GLN
1	A	406	GLN
1	A	418	GLN
1	A	443	GLN
1	B	86	GLN
1	B	103	GLN
1	B	135	ASN
1	B	265	GLN

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Mol	Chain	Res	Type
1	B	443	GLN
1	C	135	ASN
1	C	200	ASN
1	C	255	ASN
1	C	265	GLN
1	C	296	GLN
1	C	432	HIS
1	D	135	ASN
1	D	261	ASN
1	D	265	GLN
1	D	297	HIS
1	D	315	ASN
1	D	327	GLN
1	D	403	ASN
1	D	418	GLN
1	D	443	GLN
1	E	103	GLN
1	E	265	GLN
1	E	315	ASN
1	E	327	GLN
1	E	443	GLN
1	F	103	GLN
1	F	265	GLN
1	F	327	GLN
1	F	418	GLN
1	F	432	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	E	501	1,3	41,50,50	1.53	6 (14%)	45,82,82	2.13	18 (40%)
2	HEM	F	501	1,3	41,50,50	1.53	8 (19%)	45,82,82	1.79	13 (28%)
2	HEM	A	501	1,3	41,50,50	1.58	5 (12%)	45,82,82	2.09	16 (35%)
3	QKM	D	502	2	29,34,34	1.31	4 (13%)	39,49,49	1.69	8 (20%)
3	QKM	E	502	2	29,34,34	1.40	3 (10%)	39,49,49	1.60	9 (23%)
3	QKM	F	502	2	29,34,34	1.43	4 (13%)	39,49,49	1.47	5 (12%)
3	QKM	C	502	2	29,34,34	1.50	4 (13%)	39,49,49	1.79	10 (25%)
2	HEM	C	501	1,3	41,50,50	1.42	5 (12%)	45,82,82	2.58	15 (33%)
2	HEM	B	501	1,3	41,50,50	1.57	8 (19%)	45,82,82	1.87	13 (28%)
3	QKM	A	502	2	29,34,34	1.47	3 (10%)	39,49,49	2.02	13 (33%)
2	HEM	D	501	1,3	41,50,50	1.47	6 (14%)	45,82,82	2.19	12 (26%)
3	QKM	B	502	2	29,34,34	1.43	5 (17%)	39,49,49	2.36	17 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	501	1,3	-	2/12/54/54	-
2	HEM	F	501	1,3	-	2/12/54/54	-
2	HEM	A	501	1,3	-	2/12/54/54	-
3	QKM	D	502	2	-	2/24/27/27	0/4/4/4
3	QKM	E	502	2	-	7/24/27/27	0/4/4/4
3	QKM	F	502	2	-	2/24/27/27	0/4/4/4
3	QKM	C	502	2	-	7/24/27/27	0/4/4/4
2	HEM	C	501	1,3	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1,3	-	0/12/54/54	-
3	QKM	A	502	2	-	8/24/27/27	0/4/4/4
2	HEM	D	501	1,3	-	4/12/54/54	-
3	QKM	B	502	2	-	6/24/27/27	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	C1B-NB	-5.49	1.30	1.40
2	D	501	HEM	C1B-NB	-4.77	1.32	1.40
2	A	501	HEM	C1B-NB	-4.57	1.32	1.40
3	E	502	QKM	CA-N	4.40	1.51	1.37
2	B	501	HEM	C1B-NB	-4.40	1.32	1.40
3	F	502	QKM	CA-N	4.37	1.51	1.37
2	F	501	HEM	C1B-NB	-4.06	1.33	1.40
3	C	502	QKM	C15-N3	4.04	1.37	1.33
2	A	501	HEM	C4B-NB	-3.99	1.30	1.38
2	C	501	HEM	C1B-NB	-3.93	1.33	1.40
3	A	502	QKM	C15-N3	3.90	1.37	1.33
3	B	502	QKM	CB-CA	-3.89	1.42	1.48
3	C	502	QKM	CA-N	3.88	1.49	1.37
3	A	502	QKM	CA-N	3.88	1.49	1.37
3	D	502	QKM	CA-N	3.87	1.49	1.37
3	A	502	QKM	CB-CA	-3.71	1.43	1.48
3	B	502	QKM	CA-N	3.61	1.48	1.37
2	F	501	HEM	C4D-ND	-3.58	1.34	1.40
2	C	501	HEM	C4B-NB	-3.56	1.31	1.38
2	B	501	HEM	C4B-NB	-3.42	1.31	1.38
3	F	502	QKM	C15-N3	3.36	1.37	1.33
3	C	502	QKM	CB-CA	-3.33	1.43	1.48
2	A	501	HEM	C4D-ND	-3.25	1.34	1.40
3	C	502	QKM	CZ-CE1	-3.24	1.50	1.56
2	E	501	HEM	C4B-NB	-3.24	1.32	1.38
3	F	502	QKM	CZ-CE1	-3.19	1.51	1.56
2	F	501	HEM	C4B-NB	-3.00	1.32	1.38
2	D	501	HEM	C4B-NB	-2.90	1.32	1.38
3	D	502	QKM	CB-CA	-2.85	1.44	1.48
3	D	502	QKM	C15-N3	2.81	1.36	1.33
2	D	501	HEM	C4D-ND	-2.80	1.35	1.40
2	C	501	HEM	CHB-C1B	2.73	1.42	1.35
2	B	501	HEM	C4D-ND	-2.71	1.35	1.40
2	D	501	HEM	FE-NB	2.68	2.10	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	QKM	CB-CA	-2.67	1.44	1.48
3	B	502	QKM	C15-N3	2.67	1.36	1.33
3	B	502	QKM	CZ-CE1	-2.62	1.52	1.56
2	F	501	HEM	FE-NB	2.60	2.09	1.96
2	E	501	HEM	CHB-C1B	2.60	1.41	1.35
2	C	501	HEM	C4D-ND	-2.58	1.35	1.40
2	A	501	HEM	C4D-C3D	2.56	1.49	1.45
3	E	502	QKM	CZ-CE2	-2.51	1.49	1.53
2	D	501	HEM	C4D-C3D	2.50	1.49	1.45
2	E	501	HEM	FE-NB	2.49	2.09	1.96
2	C	501	HEM	FE-NB	2.47	2.09	1.96
2	A	501	HEM	FE-NB	2.43	2.08	1.96
3	B	502	QKM	CZ-CE2	-2.42	1.49	1.53
2	B	501	HEM	C4D-C3D	2.38	1.49	1.45
2	E	501	HEM	C4D-ND	-2.35	1.36	1.40
2	F	501	HEM	CHB-C1B	2.35	1.41	1.35
2	F	501	HEM	C3D-C2D	-2.35	1.31	1.36
2	B	501	HEM	FE-NB	2.33	2.08	1.96
2	F	501	HEM	C3B-C4B	2.28	1.49	1.44
2	B	501	HEM	C3B-C4B	2.27	1.49	1.44
2	B	501	HEM	O1D-CGD	2.11	1.29	1.22
2	D	501	HEM	CHB-C1B	2.09	1.40	1.35
2	F	501	HEM	C1D-ND	-2.08	1.34	1.38
2	B	501	HEM	CHB-C1B	2.07	1.40	1.35
3	D	502	QKM	CZ-CE1	-2.06	1.52	1.56
2	E	501	HEM	C1D-ND	-2.03	1.34	1.38
3	F	502	QKM	CB-CA	-2.02	1.45	1.48

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CBA-CAA-C2A	-6.85	100.93	112.62
2	C	501	HEM	CAD-C3D-C4D	6.37	135.80	124.66
2	D	501	HEM	CAD-C3D-C4D	6.36	135.77	124.66
3	B	502	QKM	C-CA-CB	-6.26	120.73	129.44
2	D	501	HEM	C1B-NB-C4B	5.63	110.89	105.07
2	C	501	HEM	C4B-C3B-C2B	-5.26	102.94	107.11
2	E	501	HEM	C1B-NB-C4B	5.05	110.29	105.07
2	C	501	HEM	CHD-C1D-ND	4.83	129.68	124.43
3	A	502	QKM	OH-CZ-CE1	-4.82	100.64	110.59
2	B	501	HEM	C1B-NB-C4B	4.75	109.98	105.07
2	A	501	HEM	C1B-NB-C4B	4.64	109.87	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C1B-NB-C4B	4.56	109.78	105.07
2	D	501	HEM	CAD-C3D-C2D	-4.55	119.40	127.88
2	F	501	HEM	CHD-C1D-ND	4.54	129.37	124.43
2	C	501	HEM	CAD-C3D-C2D	-4.35	119.78	127.88
3	D	502	QKM	C7-CB-CA	-4.30	114.50	121.28
3	D	502	QKM	C8-C9-C12	-4.29	112.84	119.99
2	F	501	HEM	C1B-NB-C4B	4.27	109.48	105.07
3	A	502	QKM	C7-CB-CA	-4.08	114.84	121.28
2	E	501	HEM	C4B-C3B-C2B	-4.08	103.88	107.11
3	B	502	QKM	C20-C21-C22	-4.06	118.01	123.29
2	D	501	HEM	CHD-C1D-ND	4.06	128.84	124.43
2	A	501	HEM	CBD-CAD-C3D	4.05	123.89	112.63
2	F	501	HEM	C4B-C3B-C2B	-3.84	104.06	107.11
3	B	502	QKM	F1-C21-C22	3.78	123.65	118.25
2	D	501	HEM	CHC-C4B-NB	3.78	128.53	124.43
2	E	501	HEM	CHD-C1D-ND	3.77	128.52	124.43
2	C	501	HEM	CBD-CAD-C3D	3.76	123.08	112.63
3	F	502	QKM	C-CA-CB	-3.72	124.27	129.44
3	A	502	QKM	CE2-C22-C21	3.70	122.66	117.56
2	C	501	HEM	C4B-CHC-C1C	3.69	127.42	122.56
2	E	501	HEM	CHA-C4D-ND	3.56	128.78	124.38
2	E	501	HEM	C4A-C3A-C2A	3.55	109.47	107.00
2	E	501	HEM	CHC-C4B-NB	3.53	128.27	124.43
2	A	501	HEM	CHD-C1D-C2D	-3.53	119.47	124.98
3	A	502	QKM	CE2-CZ-CE1	3.52	115.90	110.74
2	D	501	HEM	CHD-C1D-C2D	-3.52	119.49	124.98
2	D	501	HEM	C4B-C3B-C2B	-3.50	104.34	107.11
2	B	501	HEM	CHC-C4B-NB	3.48	128.22	124.43
3	C	502	QKM	CE2-C22-C21	3.47	122.33	117.56
3	E	502	QKM	CB-CA-N	-3.46	114.97	120.78
2	A	501	HEM	C4B-C3B-C2B	-3.44	104.39	107.11
3	F	502	QKM	CE2-C22-C21	3.41	122.25	117.56
3	C	502	QKM	C7-CB-CA	-3.40	115.91	121.28
3	C	502	QKM	C7-C8-C9	-3.40	115.96	120.35
2	F	501	HEM	CHC-C4B-NB	3.40	128.12	124.43
2	B	501	HEM	C4B-C3B-C2B	-3.39	104.42	107.11
2	B	501	HEM	CHD-C1D-ND	3.38	128.10	124.43
3	B	502	QKM	CE2-C22-C21	3.37	122.20	117.56
2	A	501	HEM	C4B-CHC-C1C	3.36	126.99	122.56
3	D	502	QKM	C10-C9-C12	3.35	125.58	119.99
3	B	502	QKM	CE2-CZ-CE1	3.31	115.58	110.74
3	A	502	QKM	C10-C9-C8	3.30	124.92	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	QKM	CB-CA-N	-3.30	115.24	120.78
2	E	501	HEM	CHA-C4D-C3D	-3.29	119.15	125.33
2	C	501	HEM	CHC-C4B-NB	3.28	128.00	124.43
2	A	501	HEM	O2D-CGD-O1D	-3.28	115.13	123.30
2	B	501	HEM	C4B-CHC-C1C	3.28	126.88	122.56
2	E	501	HEM	O2A-CGA-CBA	3.23	124.41	114.03
3	C	502	QKM	OH-CZ-CE1	-3.21	103.97	110.59
3	C	502	QKM	CD1-CE1-C3	-3.19	104.24	108.59
3	D	502	QKM	OH-CZ-CE1	-3.10	104.20	110.59
3	C	502	QKM	C10-C11-CB	-3.10	116.67	121.13
2	A	501	HEM	CHC-C4B-NB	3.09	127.79	124.43
2	F	501	HEM	CHD-C1D-C2D	-3.08	120.16	124.98
3	B	502	QKM	C8-C9-C12	-3.08	114.86	119.99
2	B	501	HEM	CBD-CAD-C3D	3.04	121.09	112.63
2	A	501	HEM	CHD-C1D-ND	3.03	127.72	124.43
2	A	501	HEM	CAD-C3D-C4D	2.99	129.88	124.66
3	F	502	QKM	CD1-CE1-CZ	-2.98	106.01	111.57
2	F	501	HEM	CAD-CBD-CGD	-2.97	107.21	113.60
2	D	501	HEM	CBD-CAD-C3D	2.97	120.88	112.63
3	B	502	QKM	CD1-CE1-CZ	-2.97	106.03	111.57
2	C	501	HEM	C3B-C2B-C1B	2.97	108.69	106.49
3	B	502	QKM	CZ-CE2-CD2	-2.95	119.06	123.07
2	D	501	HEM	C4B-CHC-C1C	2.94	126.44	122.56
3	A	502	QKM	C8-C9-C12	-2.91	115.13	119.99
3	F	502	QKM	CZ-CE1-C3	2.91	117.88	112.77
2	B	501	HEM	CAD-C3D-C4D	2.90	129.73	124.66
2	A	501	HEM	CHB-C1B-NB	2.89	127.96	124.38
3	B	502	QKM	F2-CD2-CE2	2.88	122.45	118.98
3	E	502	QKM	C14-CZ-CE1	-2.87	104.36	110.08
3	B	502	QKM	CZ-CE1-C3	2.86	117.80	112.77
3	E	502	QKM	OH-CZ-CE2	-2.85	103.08	107.11
3	B	502	QKM	OH-CZ-CE1	-2.84	104.74	110.59
2	A	501	HEM	CBA-CAA-C2A	-2.83	107.78	112.62
2	E	501	HEM	C4B-CHC-C1C	2.83	126.29	122.56
3	B	502	QKM	C19-CD2-CE2	-2.83	119.49	123.44
2	C	501	HEM	CAD-CBD-CGD	-2.82	107.52	113.60
2	B	501	HEM	CMD-C2D-C1D	2.81	129.32	125.04
2	C	501	HEM	CMA-C3A-C4A	-2.80	124.16	128.46
2	C	501	HEM	CHD-C1D-C2D	-2.78	120.63	124.98
2	A	501	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
3	A	502	QKM	C7-C8-C9	-2.76	116.79	120.35
2	B	501	HEM	CHD-C1D-C2D	-2.71	120.74	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	CHA-C4D-ND	2.71	127.73	124.38
3	E	502	QKM	F2-CD2-C19	-2.70	112.58	118.59
3	A	502	QKM	C11-CB-C7	2.70	122.96	117.59
2	D	501	HEM	CAD-CBD-CGD	-2.61	107.98	113.60
2	E	501	HEM	CAD-CBD-CGD	-2.61	107.98	113.60
2	B	501	HEM	CHA-C4D-C3D	-2.59	120.47	125.33
2	A	501	HEM	CAD-CBD-CGD	-2.57	108.07	113.60
3	C	502	QKM	C10-C9-C8	2.56	123.59	118.96
3	B	502	QKM	C22-CE2-CZ	2.56	122.54	118.61
3	E	502	QKM	F2-CD2-CE2	2.55	122.05	118.98
2	E	501	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
2	F	501	HEM	C4B-CHC-C1C	2.54	125.91	122.56
2	A	501	HEM	C2D-C1D-ND	2.44	112.81	109.88
2	B	501	HEM	CHA-C4D-ND	2.41	127.36	124.38
2	A	501	HEM	CMD-C2D-C1D	2.41	128.72	125.04
2	E	501	HEM	CMD-C2D-C1D	2.40	128.70	125.04
3	E	502	QKM	CZ-CE2-CD2	2.39	126.32	123.07
2	E	501	HEM	CAD-C3D-C4D	2.39	128.84	124.66
3	B	502	QKM	C11-CB-C7	2.38	122.34	117.59
3	F	502	QKM	OH-CZ-C14	2.38	111.88	108.24
2	E	501	HEM	O2A-CGA-O1A	-2.38	117.38	123.30
2	B	501	HEM	O2A-CGA-O1A	-2.37	117.38	123.30
2	E	501	HEM	CMA-C3A-C4A	-2.35	124.84	128.46
3	D	502	QKM	C11-CB-CA	2.30	124.92	121.28
3	E	502	QKM	N4-C15-N3	-2.30	109.46	112.24
2	E	501	HEM	CBA-CAA-C2A	-2.29	108.72	112.62
3	E	502	QKM	CE2-CZ-CE1	2.26	114.06	110.74
3	C	502	QKM	C11-CB-C7	2.26	122.10	117.59
3	D	502	QKM	CD1-CE1-C3	-2.26	105.51	108.59
3	A	502	QKM	F1-C21-C20	2.26	122.38	118.54
3	D	502	QKM	OH-CZ-C14	2.23	111.66	108.24
2	F	501	HEM	O2A-CGA-CBA	2.23	121.19	114.03
3	C	502	QKM	C22-CE2-CZ	2.22	122.01	118.61
3	B	502	QKM	N4-C15-N3	-2.21	109.57	112.24
2	B	501	HEM	O2A-CGA-CBA	2.20	121.11	114.03
3	E	502	QKM	C10-C9-C8	2.20	122.94	118.96
3	A	502	QKM	OH-CZ-CE2	2.18	110.20	107.11
2	C	501	HEM	CMC-C2C-C3C	2.17	128.75	124.68
3	C	502	QKM	OH-CZ-CE2	2.15	110.16	107.11
2	D	501	HEM	CAA-CBA-CGA	-2.13	107.78	113.76
2	F	501	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
3	A	502	QKM	C11-C10-C9	-2.12	117.61	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	CAD-C3D-C4D	2.11	128.35	124.66
2	E	501	HEM	O2D-CGD-CBD	2.10	120.77	114.03
2	C	501	HEM	CHC-C4B-C3B	-2.09	121.38	124.57
2	A	501	HEM	CHA-C4D-C3D	-2.08	121.42	125.33
2	F	501	HEM	CAA-CBA-CGA	-2.08	107.93	113.76
2	E	501	HEM	CAA-CBA-CGA	2.07	119.57	113.76
3	B	502	QKM	C20-C19-CD2	2.06	121.53	119.05
3	B	502	QKM	C10-C9-C8	2.05	122.67	118.96
2	D	501	HEM	CHB-C1B-NB	2.05	126.91	124.38
2	F	501	HEM	CMC-C2C-C3C	2.04	128.50	124.68
3	A	502	QKM	C10-C11-CB	-2.04	118.20	121.13
3	D	502	QKM	CE2-C22-C21	2.03	120.36	117.56

There are no chirality outliers.

All (48) 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	C2D-C3D-CAD-CBD
2	D	501	HEM	C4D-C3D-CAD-CBD
3	A	502	QKM	N-CA-CB-C7
3	A	502	QKM	N-CA-CB-C11
3	A	502	QKM	C-CA-CB-C7
3	A	502	QKM	CD2-CE2-CZ-CE1
3	A	502	QKM	CZ-C14-N3-C15
3	B	502	QKM	N-CA-CB-C7
3	B	502	QKM	N-CA-CB-C11
3	B	502	QKM	C-CA-CB-C7
3	B	502	QKM	C-CA-CB-C11
3	B	502	QKM	CZ-C14-N3-C15
3	C	502	QKM	CD2-CE2-CZ-CE1
3	C	502	QKM	CZ-C14-N3-C15
3	D	502	QKM	CZ-C14-N3-C15
3	E	502	QKM	N-CA-CB-C7
3	E	502	QKM	N-CA-CB-C11
3	E	502	QKM	C-CA-CB-C7
3	E	502	QKM	C-CA-CB-C11
3	E	502	QKM	CZ-C14-N3-C15
3	F	502	QKM	CZ-C14-N3-C15
3	A	502	QKM	C-CA-CB-C11
3	C	502	QKM	N-CA-CB-C7

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Mol	Chain	Res	Type	Atoms
3	A	502	QKM	CZ-C14-N3-N5
3	F	502	QKM	CZ-C14-N3-N5
2	C	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	F	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O2D
3	C	502	QKM	N-CA-CB-C11
3	D	502	QKM	N-CA-CB-C7
2	C	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAA-CBA-CGA-O1A
3	B	502	QKM	CZ-C14-N3-N5
3	C	502	QKM	CZ-C14-N3-N5
3	E	502	QKM	CZ-C14-N3-N5
2	E	501	HEM	CAA-CBA-CGA-O2A
3	E	502	QKM	N3-C14-CZ-CE2
3	C	502	QKM	N-C3-CE1-CD1
3	C	502	QKM	C-CA-CB-C7
3	A	502	QKM	C22-CE2-CZ-CE1

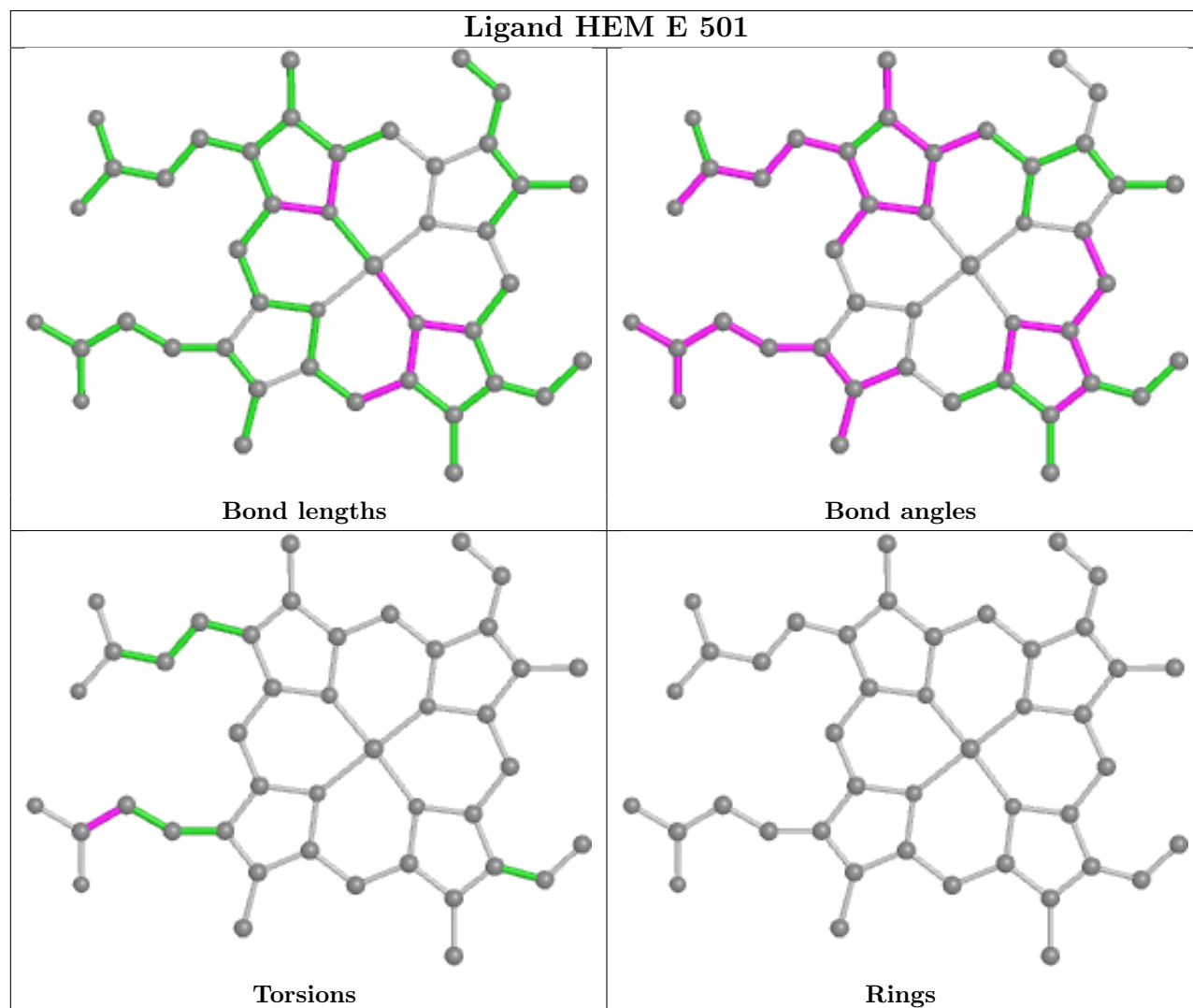
There are no ring outliers.

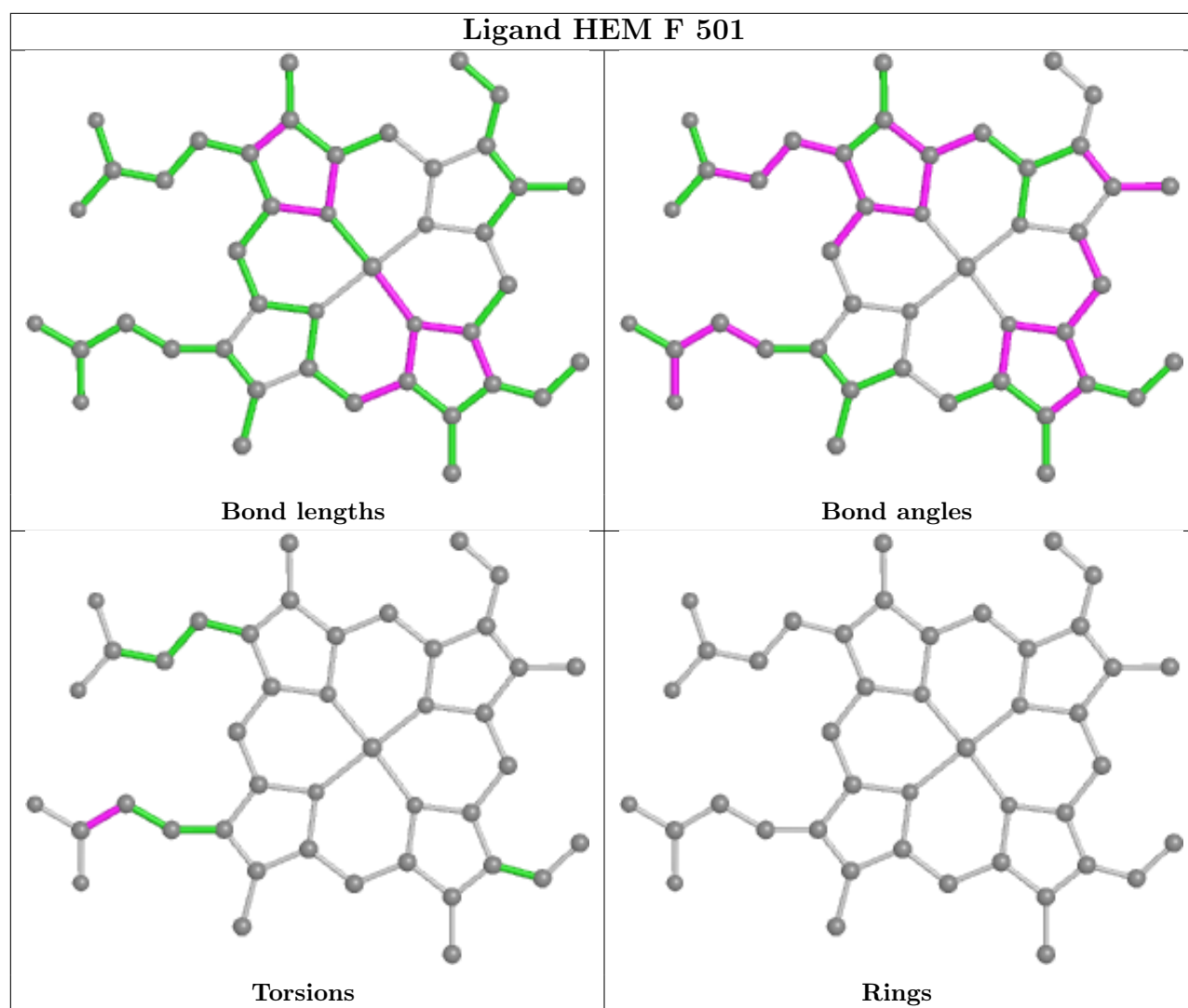
8 monomers are involved in 19 short contacts:

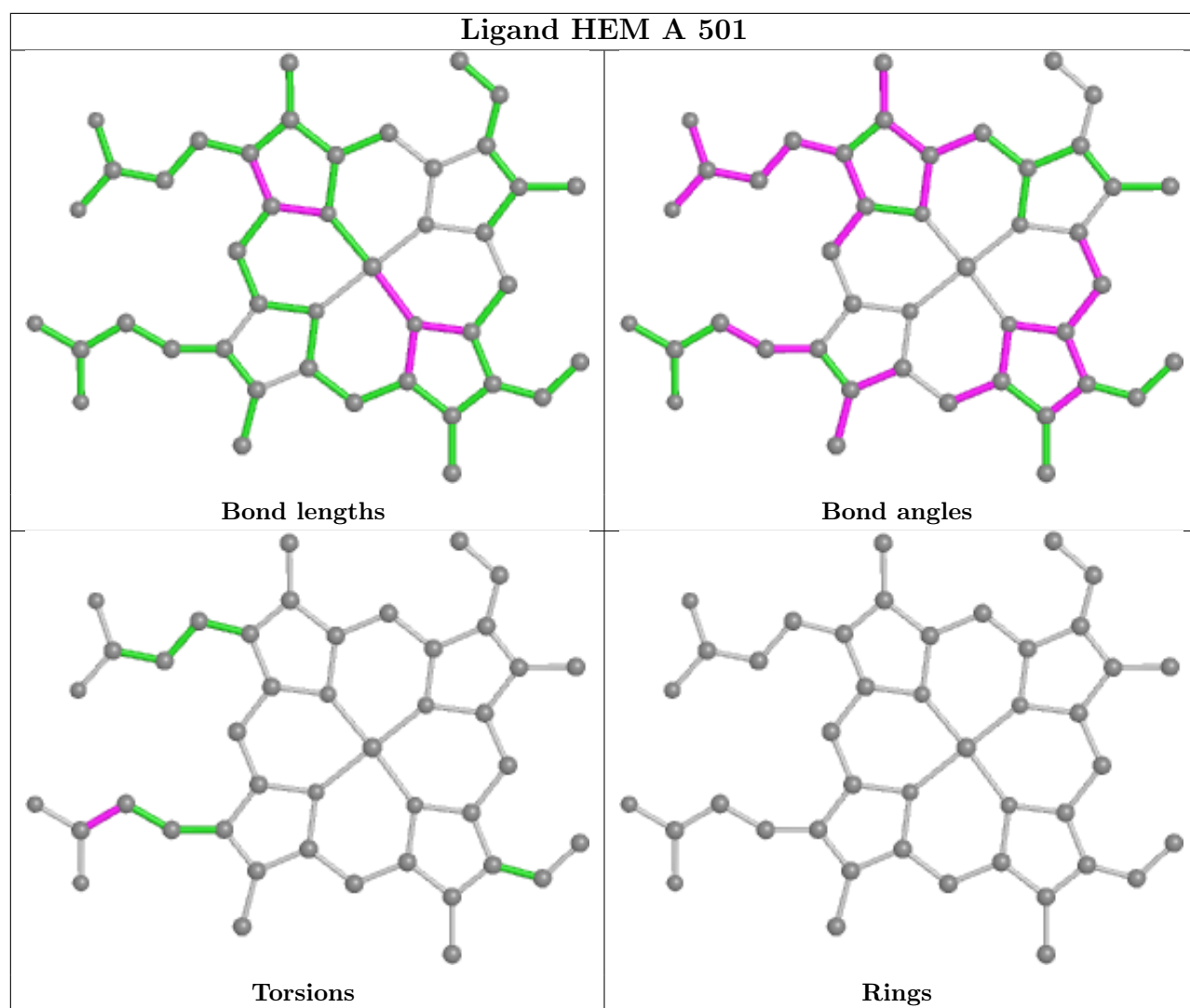
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	HEM	3	0
2	F	501	HEM	2	0
2	A	501	HEM	1	0
3	D	502	QKM	2	0
3	F	502	QKM	1	0
2	C	501	HEM	5	0
2	B	501	HEM	2	0
2	D	501	HEM	3	0

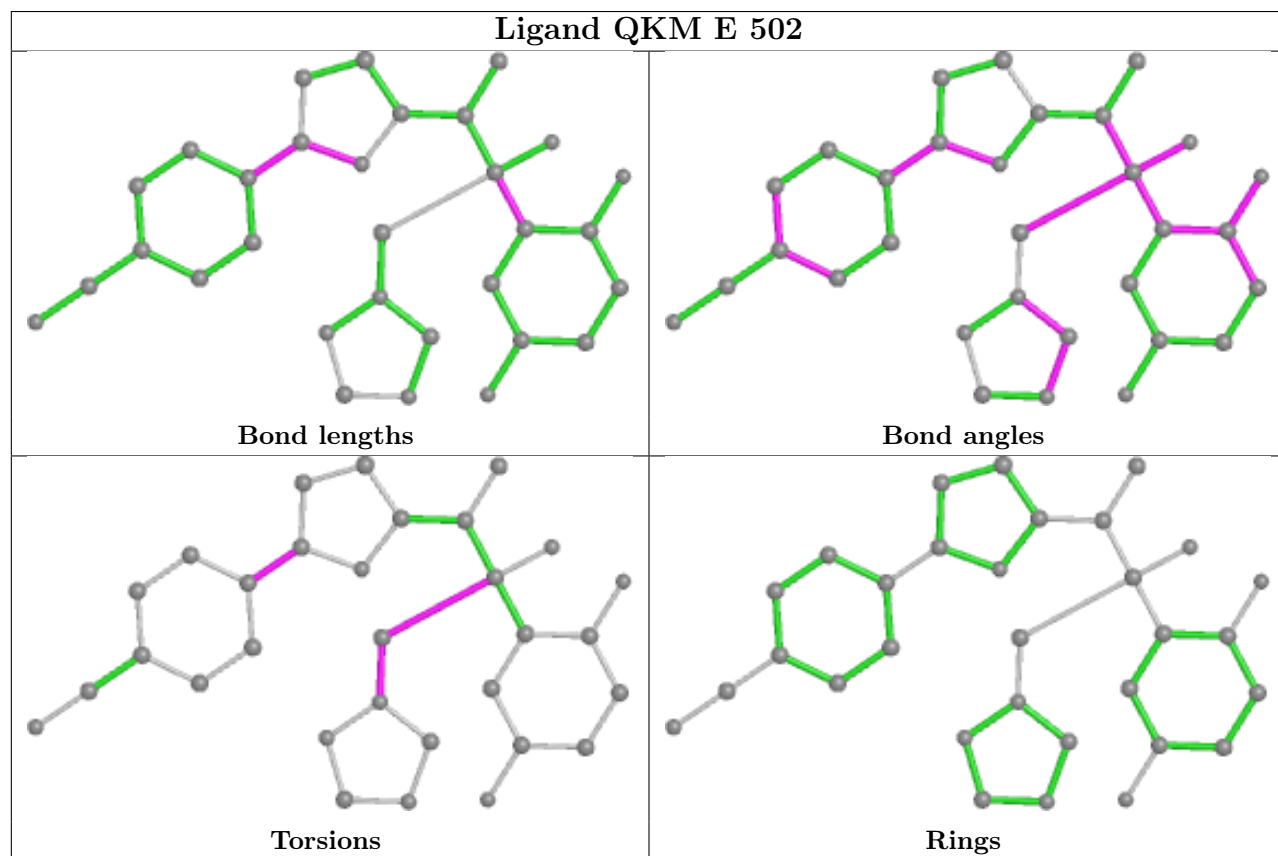
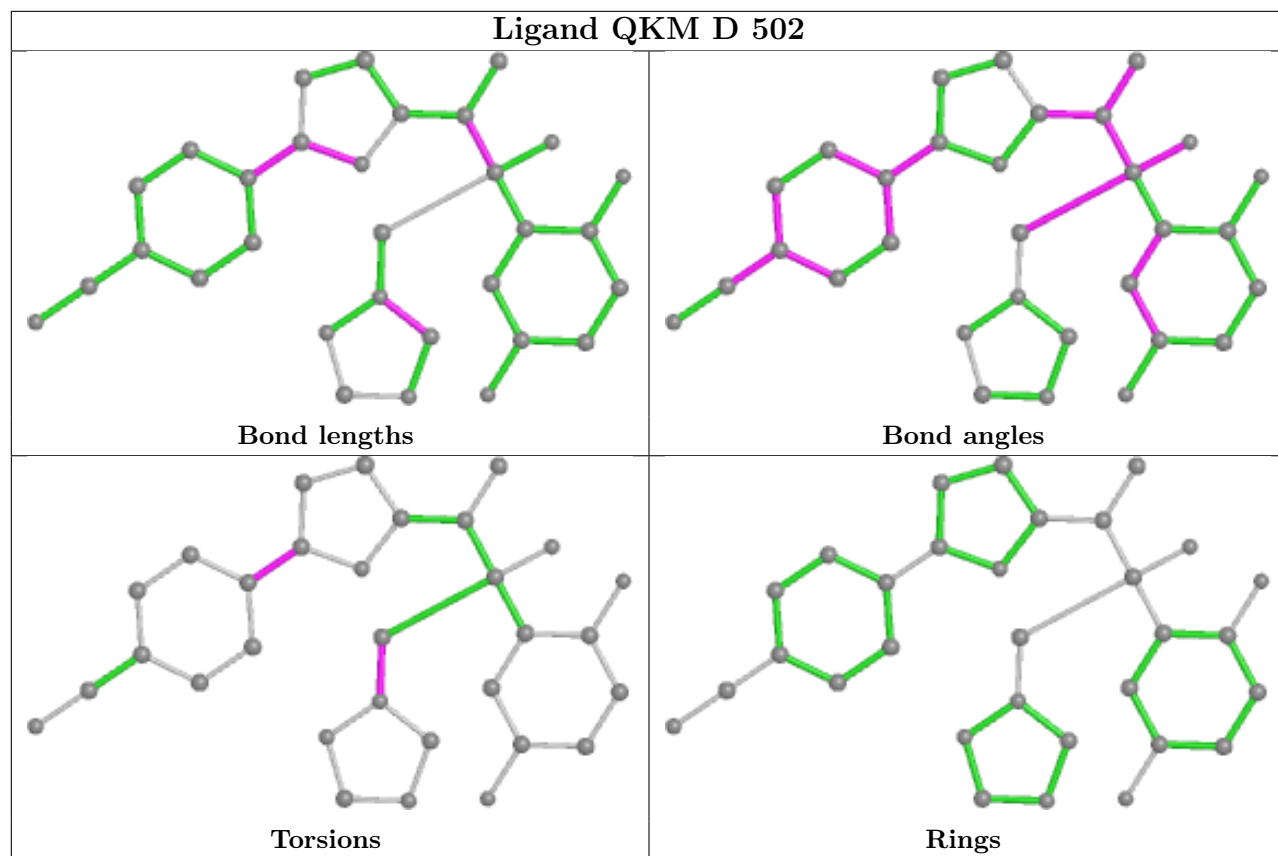
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

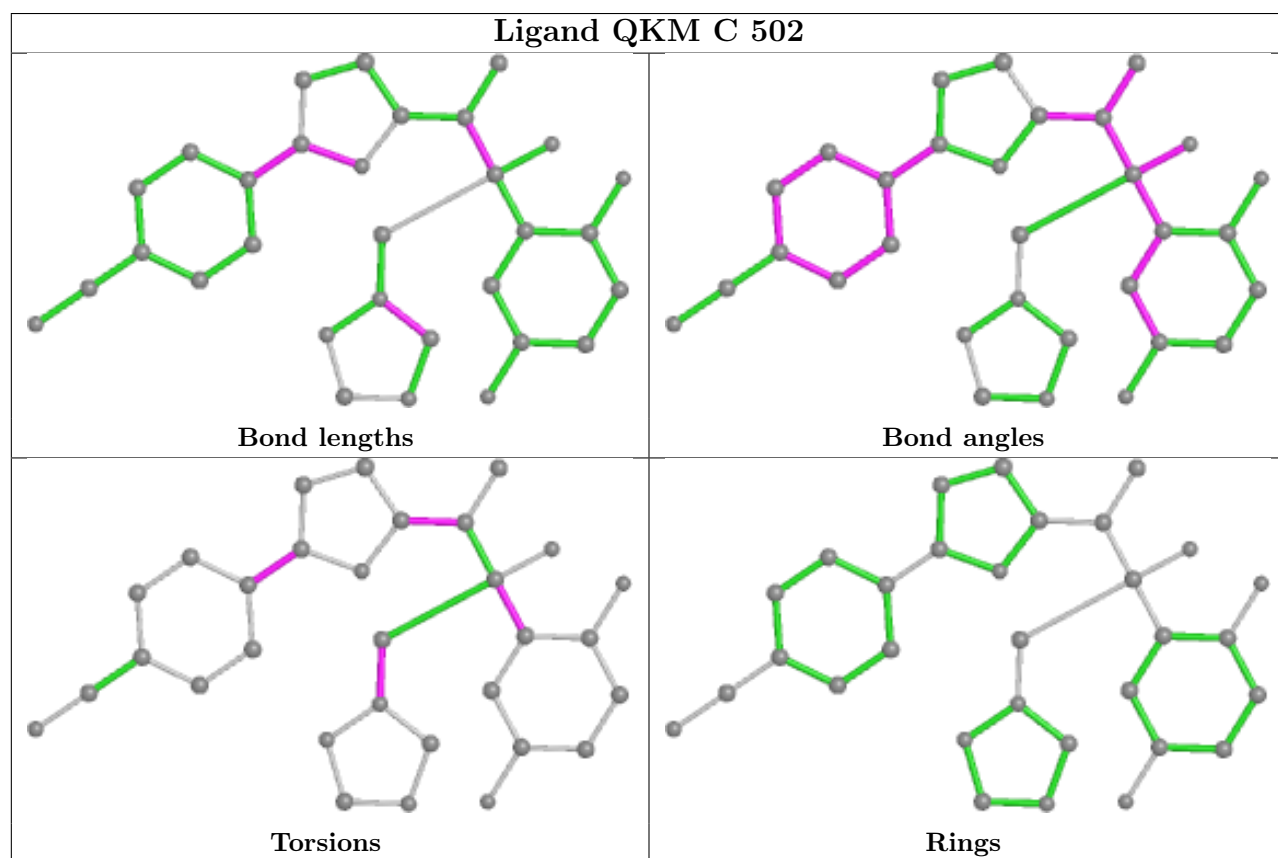
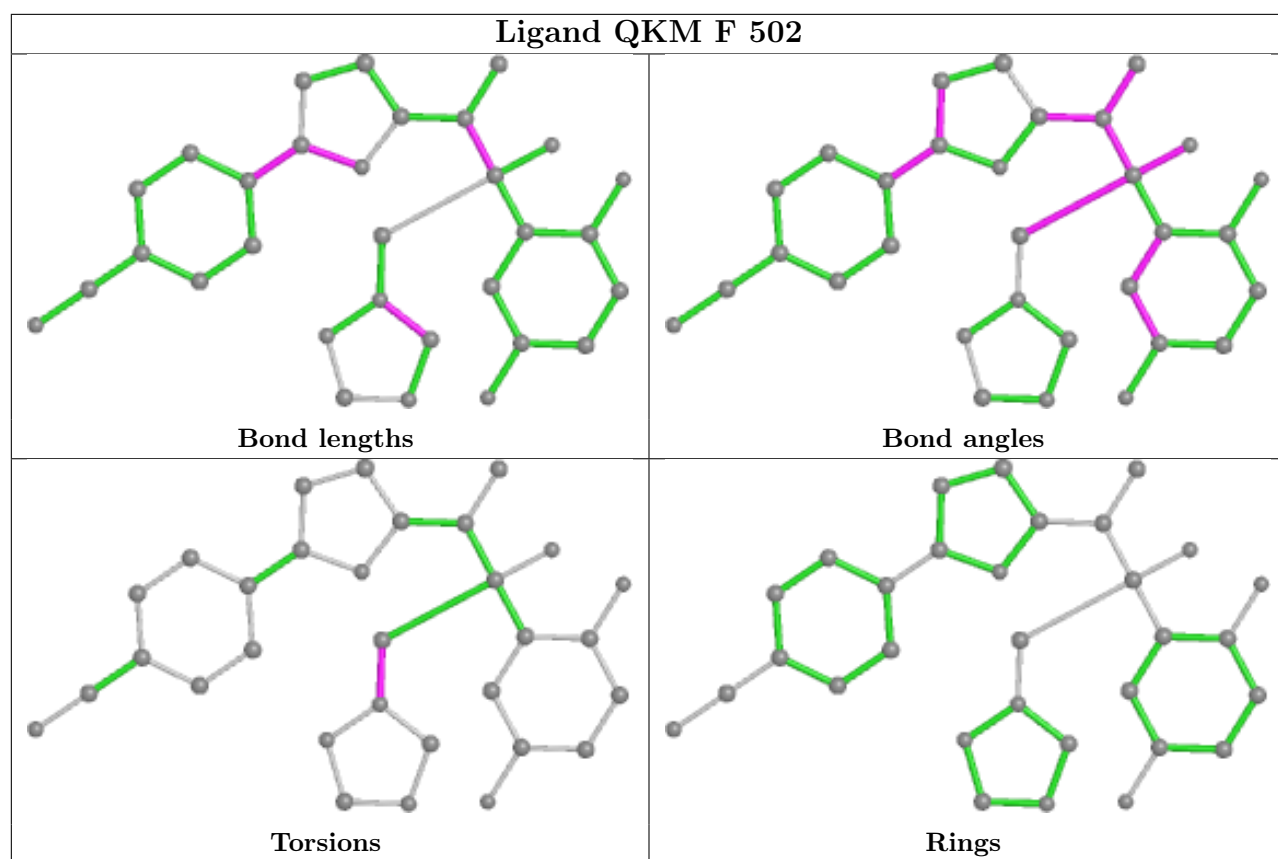
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

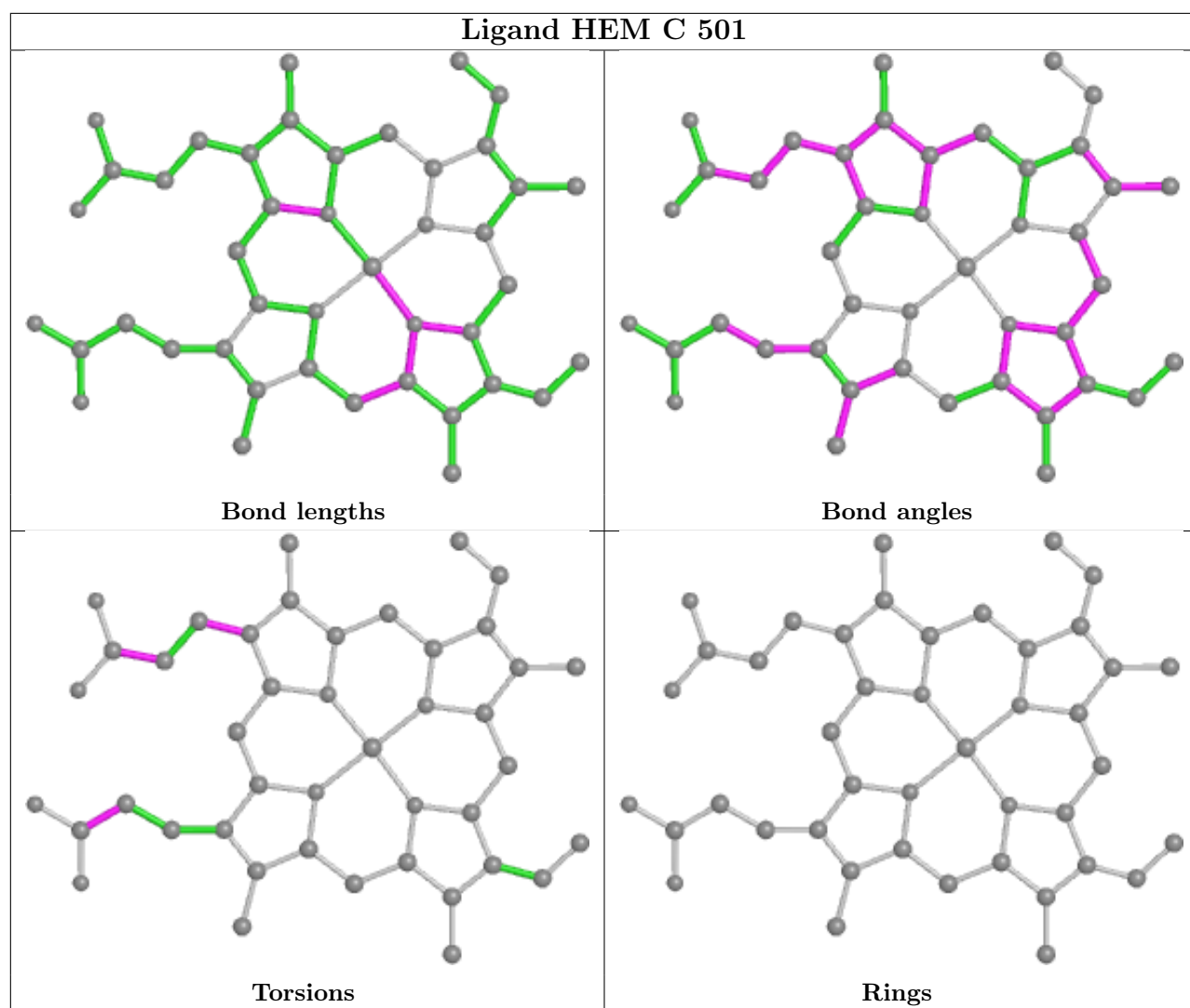


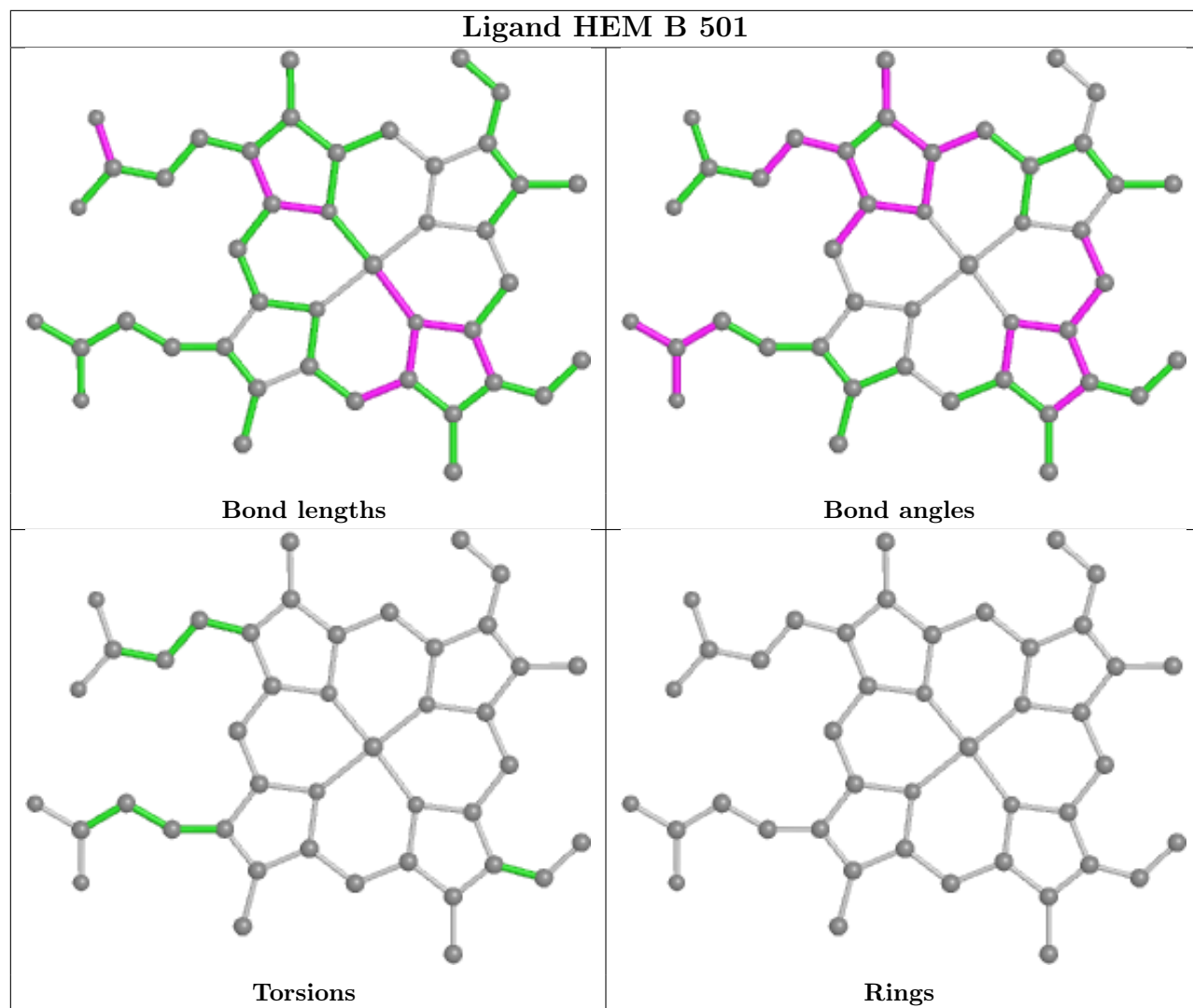


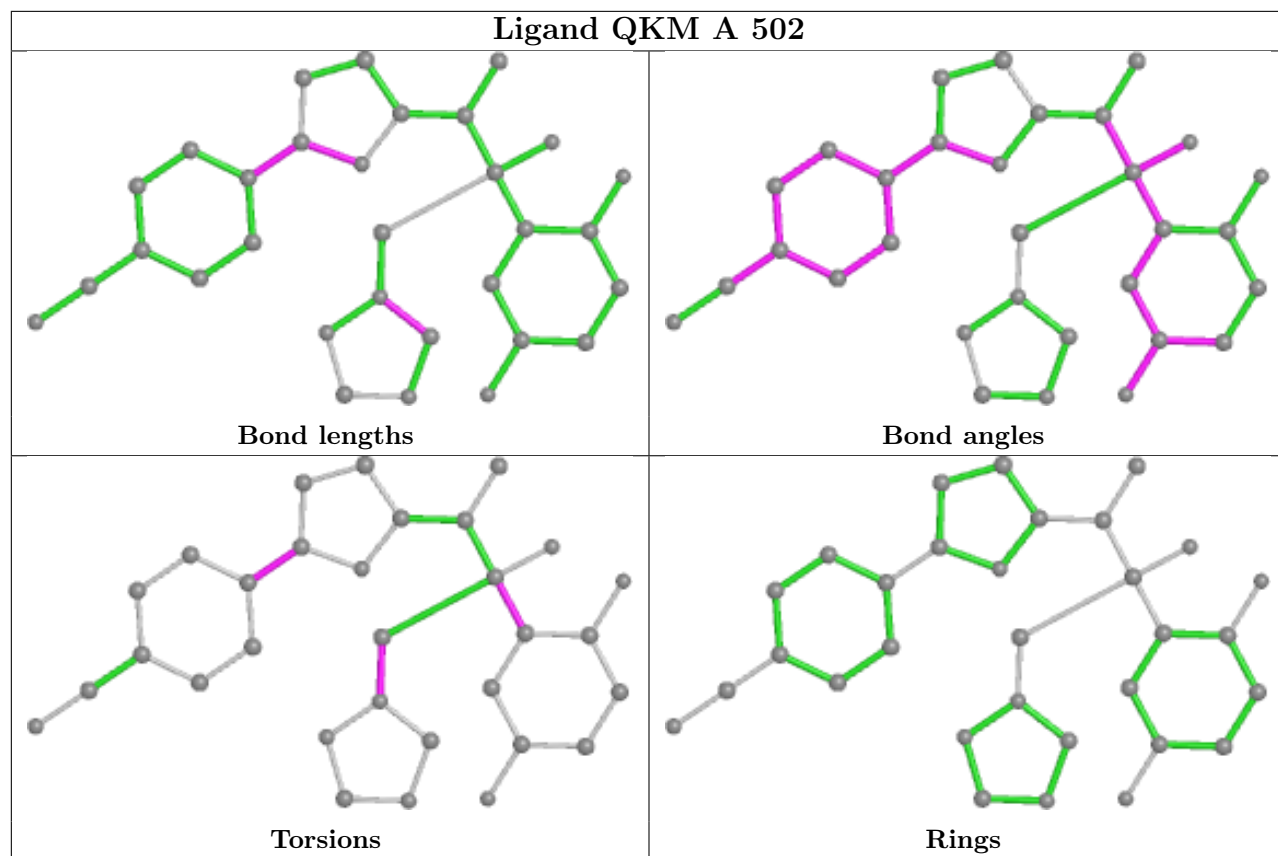


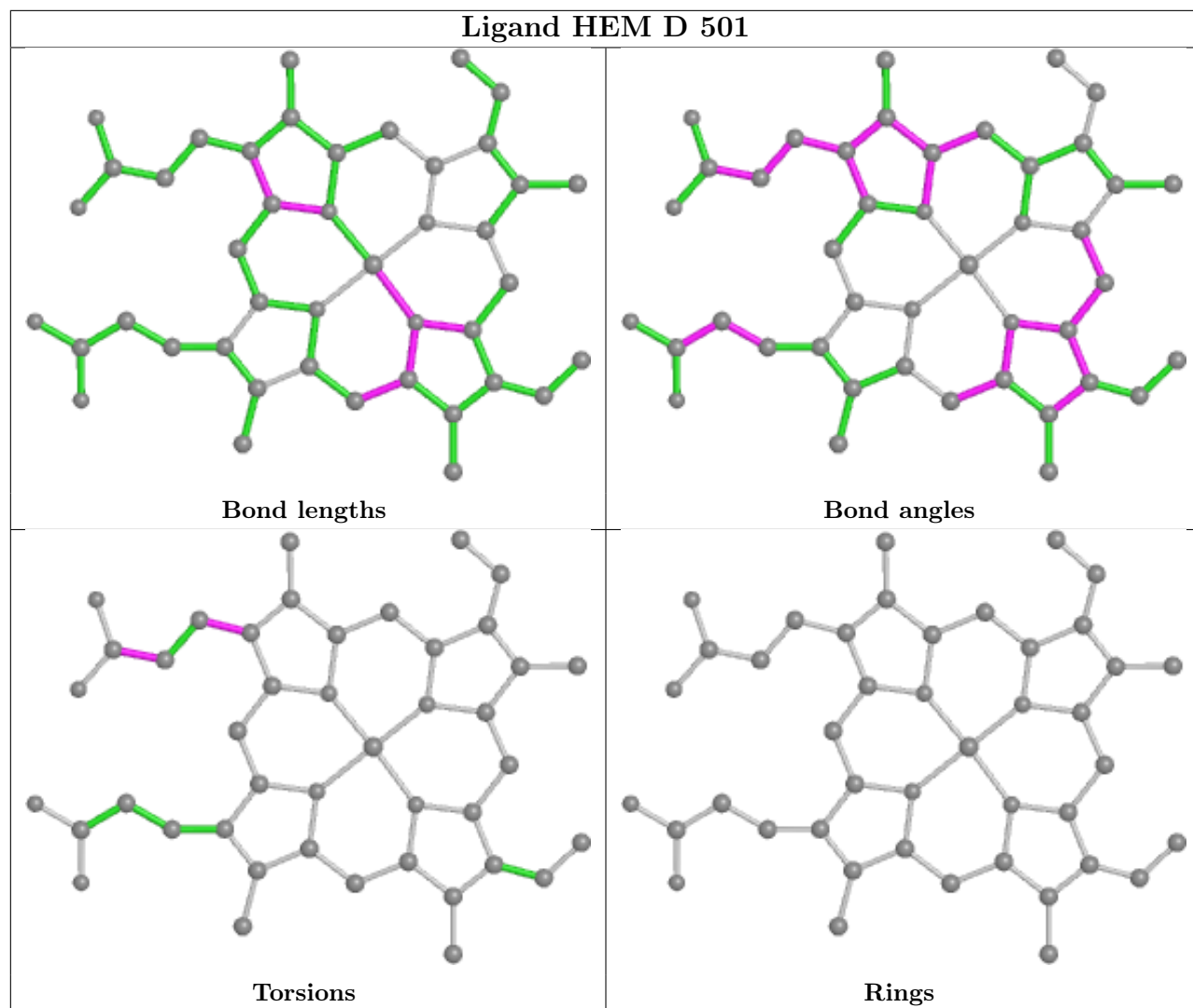


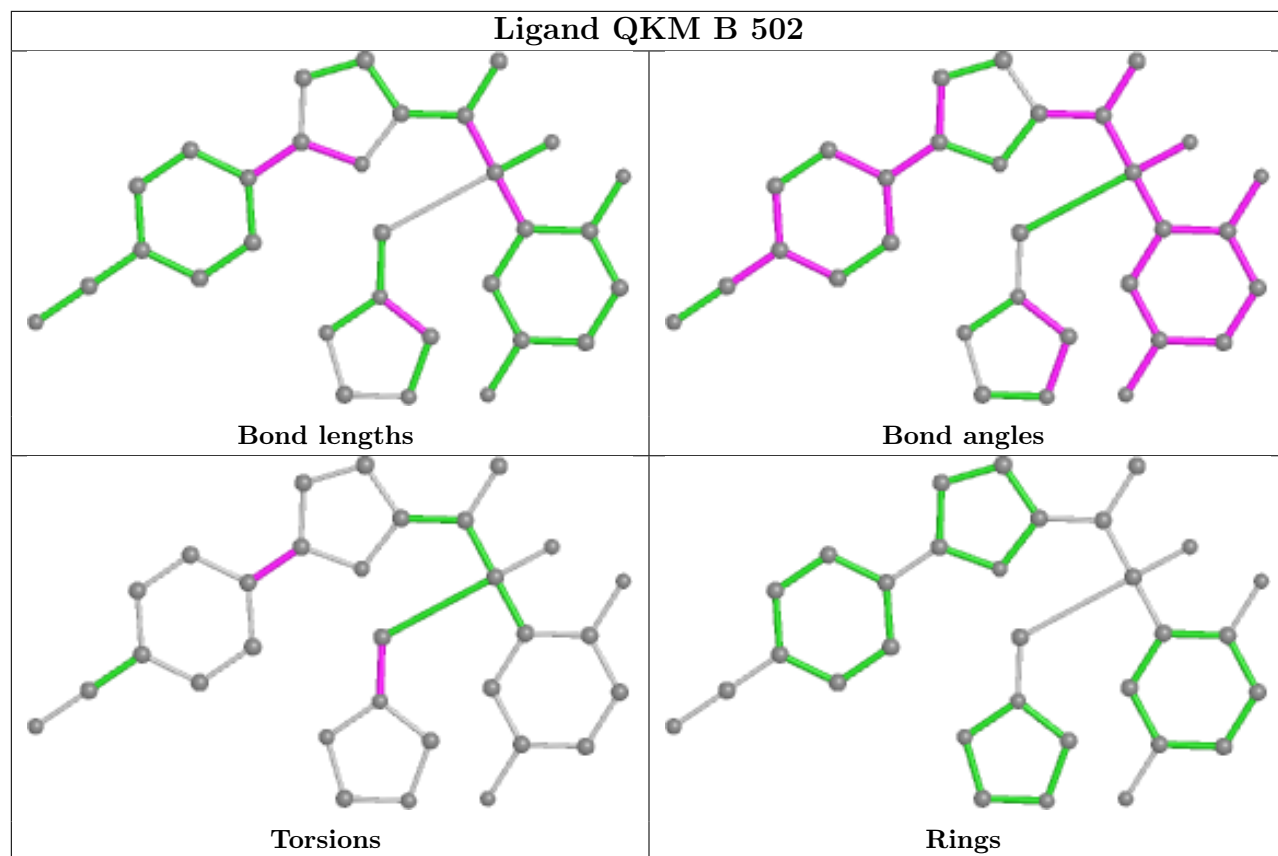












5.7 Other polymers [i](#)

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 ⓘ

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	413/460 (89%)	-0.10	5 (1%) 79 80	57, 90, 132, 155	0
1	B	414/460 (90%)	-0.08	2 (0%) 91 91	58, 96, 132, 163	0
1	C	414/460 (90%)	0.03	10 (2%) 59 59	59, 100, 145, 175	0
1	D	414/460 (90%)	0.09	12 (2%) 51 51	66, 106, 145, 200	0
1	E	413/460 (89%)	-0.04	9 (2%) 62 63	63, 106, 155, 176	0
1	F	413/460 (89%)	-0.06	2 (0%) 91 91	56, 93, 129, 172	0
All	All	2481/2760 (89%)	-0.03	40 (1%) 72 73	56, 98, 142, 200	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	LYS	7.3
1	C	174	VAL	5.1
1	C	168	TRP	4.2
1	E	308	LEU	4.0
1	C	380	TYR	4.0
1	B	223	PHE	3.9
1	C	452	LEU	3.8
1	A	349	LEU	3.4
1	E	407	TYR	3.1
1	E	165	PHE	3.0
1	C	381	VAL	3.0
1	C	327	GLN	2.9
1	A	327	GLN	2.9
1	D	323	VAL	2.8
1	A	480	LEU	2.6
1	A	190	ARG	2.6
1	E	311	PHE	2.5
1	C	374	PHE	2.5
1	C	407	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	481	LEU	2.3
1	B	334	PHE	2.3
1	E	459	LEU	2.3
1	E	463	LEU	2.2
1	A	479	CYS	2.2
1	C	334	PHE	2.2
1	D	448	TRP	2.2
1	E	176	ILE	2.2
1	D	393	LEU	2.2
1	D	480	LEU	2.2
1	E	481	LEU	2.2
1	D	371	ILE	2.2
1	E	452	LEU	2.1
1	D	192	LEU	2.1
1	D	284	ILE	2.1
1	D	457	ILE	2.1
1	F	365	PHE	2.1
1	D	478	PRO	2.1
1	D	481	LEU	2.1
1	D	223	PHE	2.0
1	C	480	LEU	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.

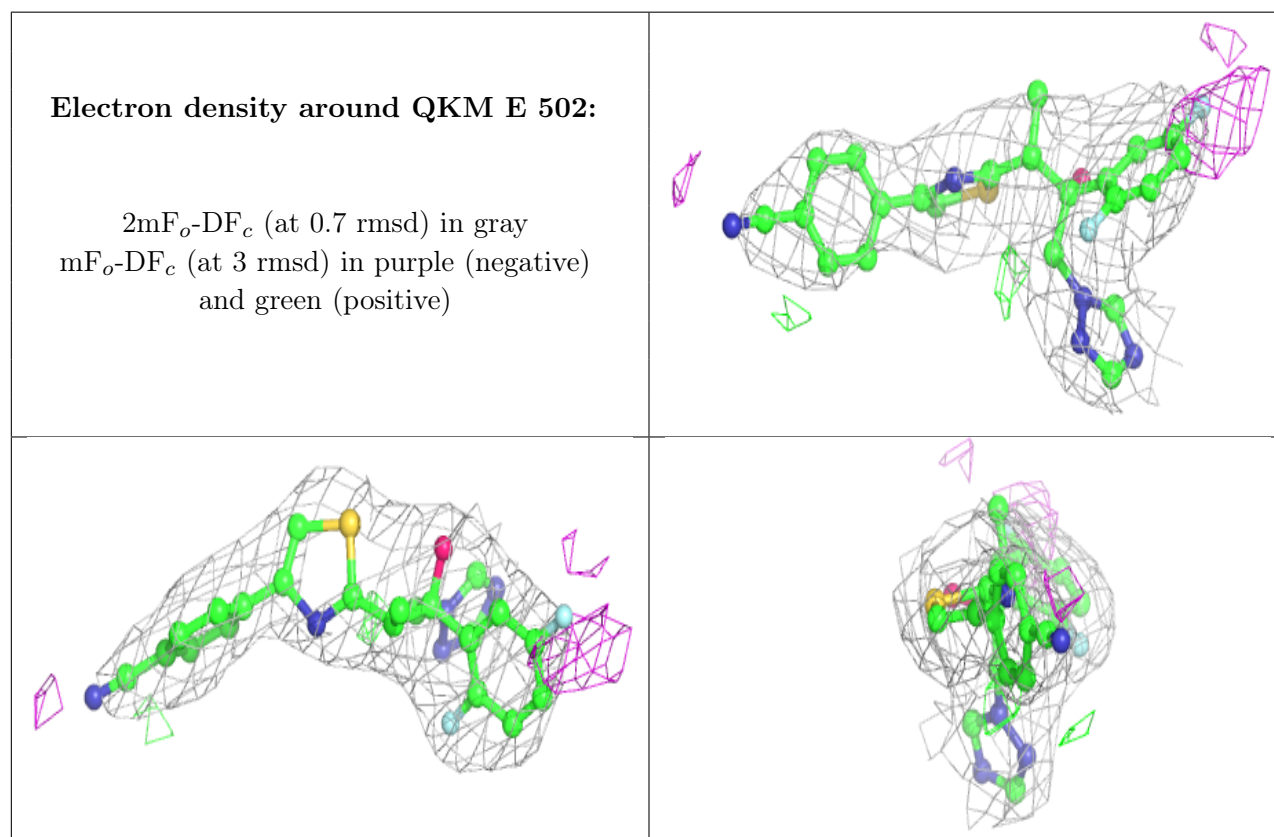
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QKM	E	502	31/31	0.95	0.25	61,88,101,109	0
3	QKM	B	502	31/31	0.97	0.27	60,70,115,126	0

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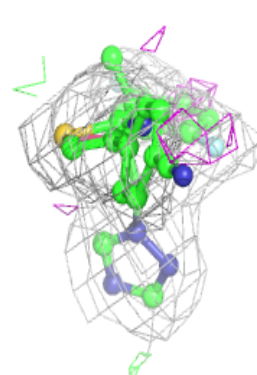
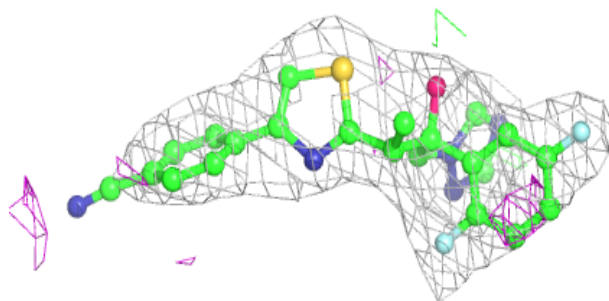
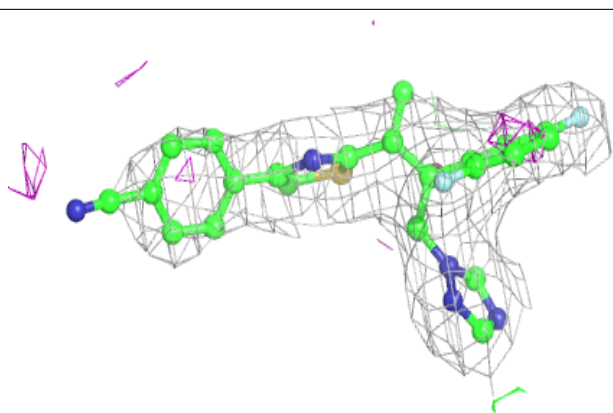
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QKM	D	502	31/31	0.97	0.22	75,83,95,106	0
3	QKM	A	502	31/31	0.97	0.21	57,71,86,116	0
3	QKM	F	502	31/31	0.97	0.23	46,64,91,108	0
2	HEM	C	501	43/43	0.98	0.22	56,64,79,99	0
3	QKM	C	502	31/31	0.98	0.24	64,74,103,112	0
2	HEM	E	501	43/43	0.98	0.23	60,68,84,99	0
2	HEM	F	501	43/43	0.98	0.22	37,66,82,88	0
2	HEM	B	501	43/43	0.98	0.19	46,62,76,83	0
4	FE	B	503	1/1	0.98	0.24	76,76,76,76	0
4	FE	F	503	1/1	0.98	0.23	80,80,80,80	0
2	HEM	A	501	43/43	0.99	0.21	57,64,85,100	0
2	HEM	D	501	43/43	0.99	0.21	52,62,86,103	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.

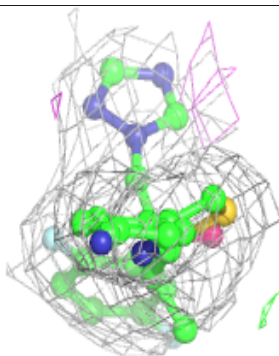
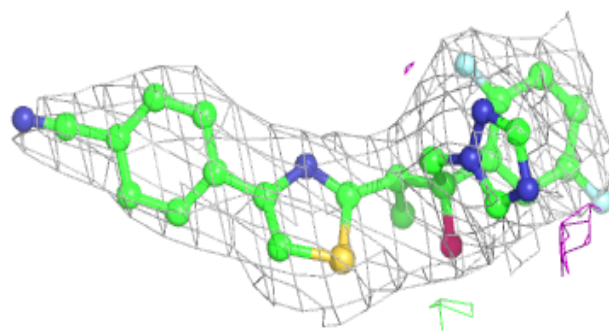
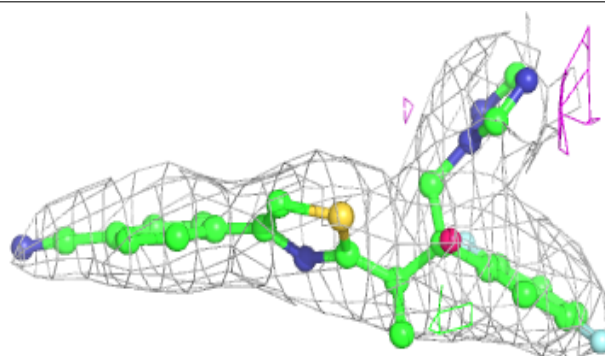


Electron density around QKM B 502:

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

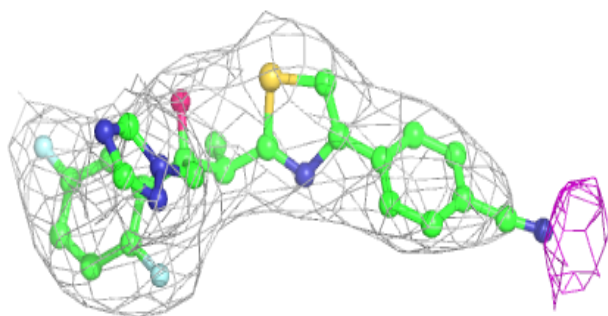
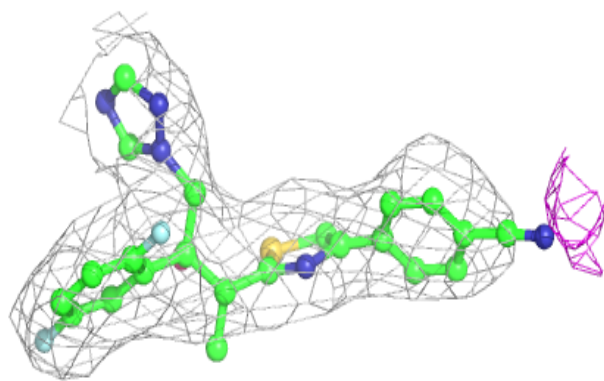
**Electron density around QKM D 502:**

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

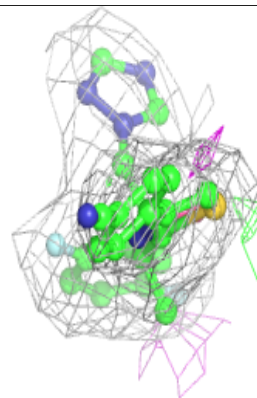
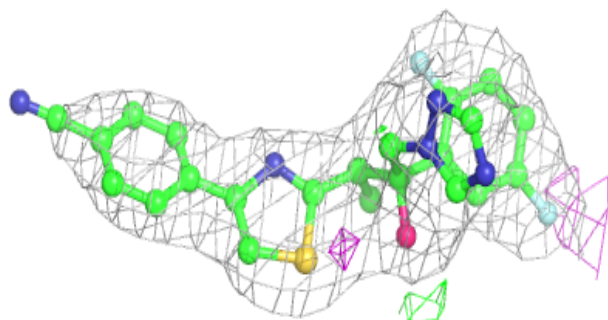
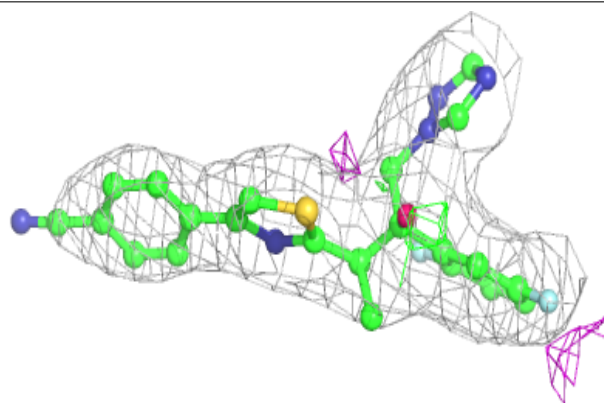


Electron density around QKM A 502:

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

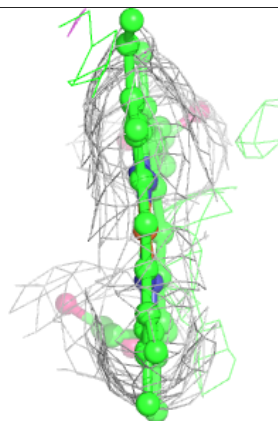
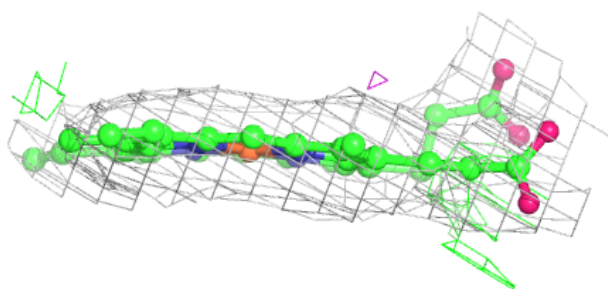
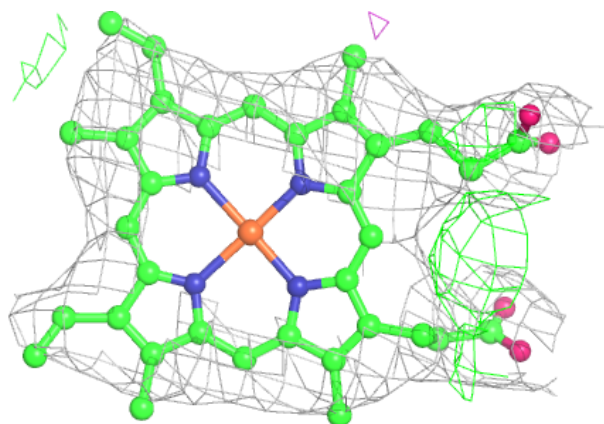
**Electron density around QKM F 502:**

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

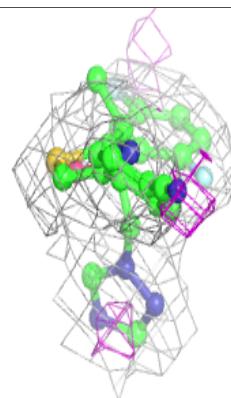
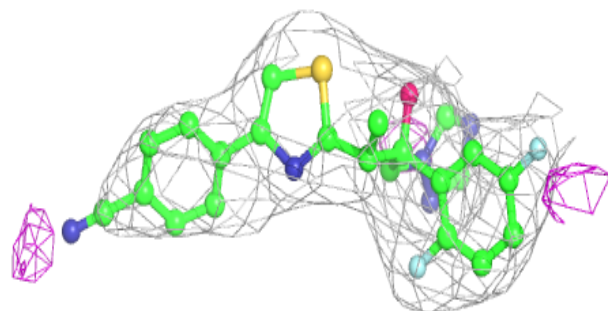
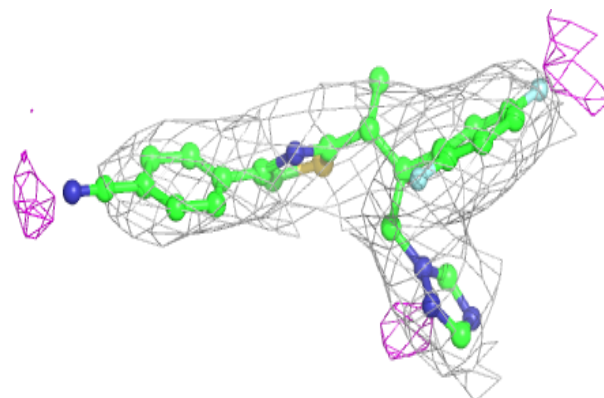


Electron density around HEM C 501:

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

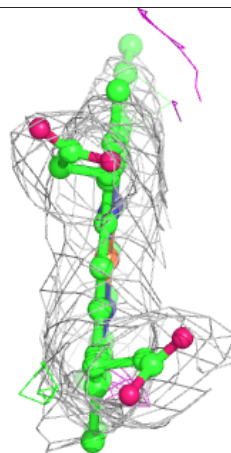
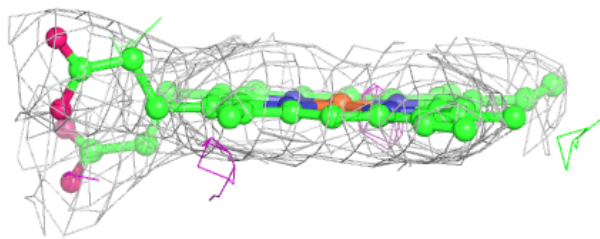
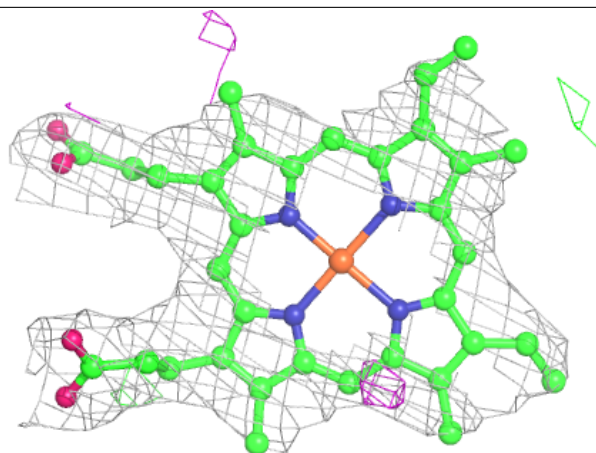
**Electron density around QKM C 502:**

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



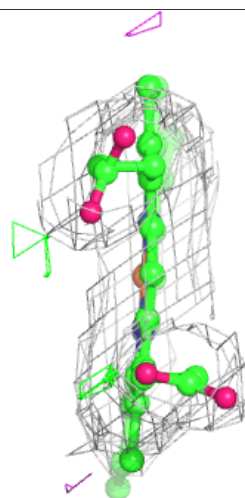
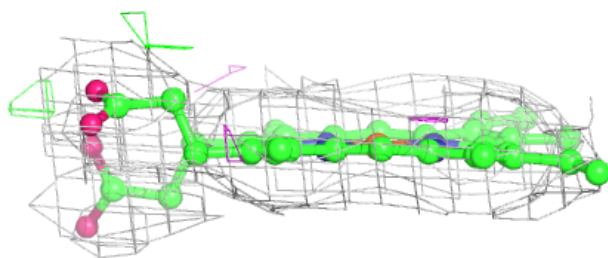
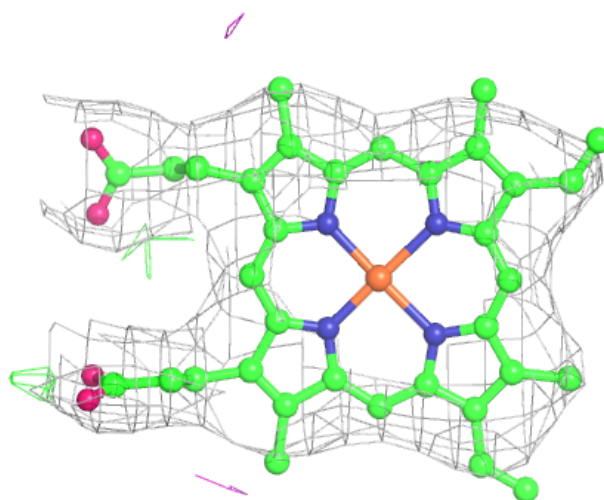
Electron density around HEM E 501:

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



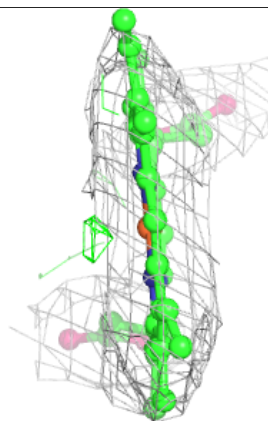
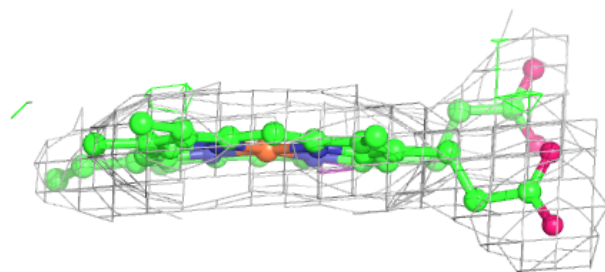
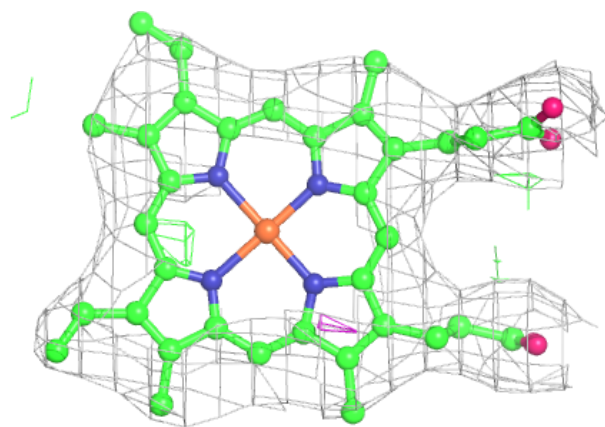
Electron density around HEM F 501:

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



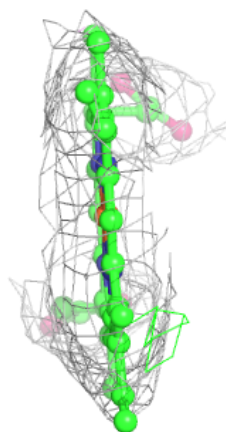
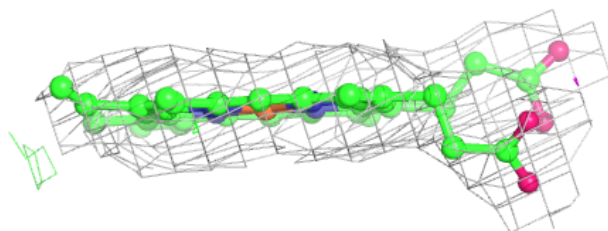
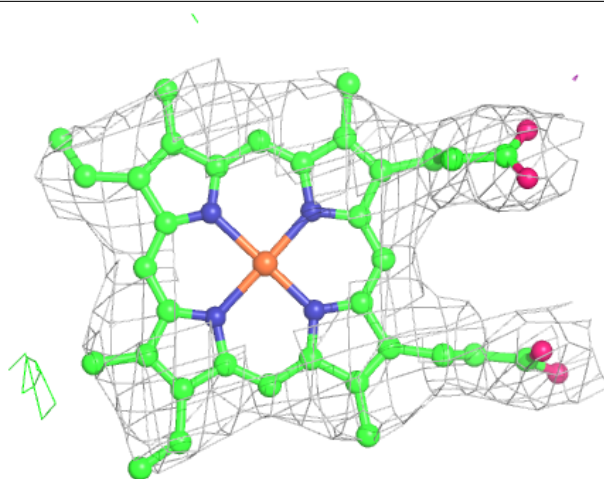
Electron density around HEM B 501:

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



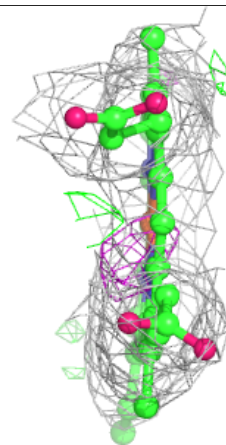
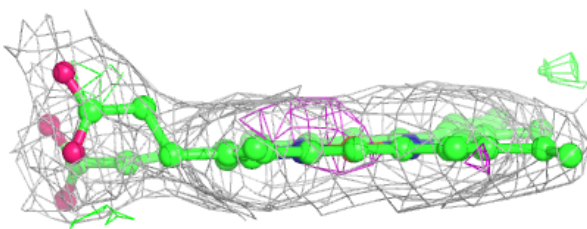
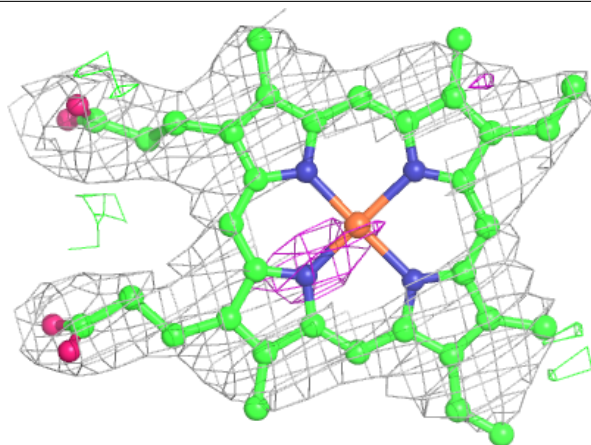
Electron density around HEM A 501:

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



Electron density around HEM D 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 [i](#)

There are no such residues in this entry.