



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:53 AM UTC

PDB ID : 3ZSN / pdb_00003zsn
Title : Structure of the mixed-function P450 MycG F286A mutant in complex with mycinamicin IV
Authors : Li, S.; Kells, P.M.; Rutaganira, F.U.; Anzai, Y.; Kato, F.; Sherman, D.H.; Podust, L.M.
Deposited on : 2011-06-29
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

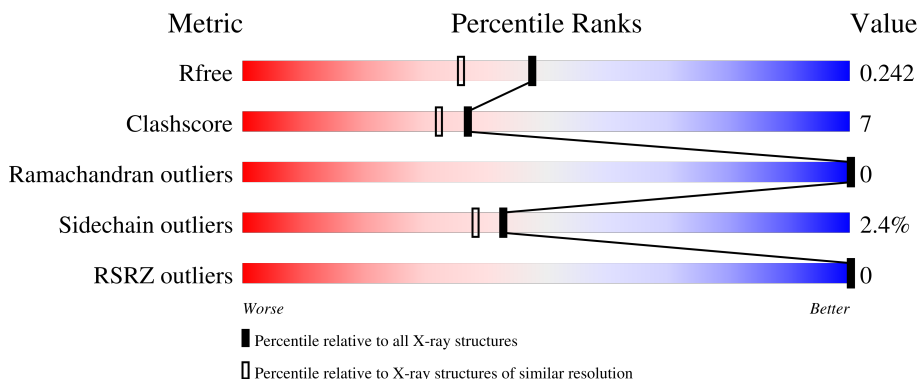
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	417	
1	B	417	
1	C	417	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10761 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 P-450-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	5	0
			3113	1949	570	582	12			
1	B	393	Total	C	N	O	S	0	7	0
			3141	1966	579	585	11			
1	C	393	Total	C	N	O	S	0	6	0
			3132	1962	579	580	11			

There are 63 discrepancies between the modelled and reference sequences:

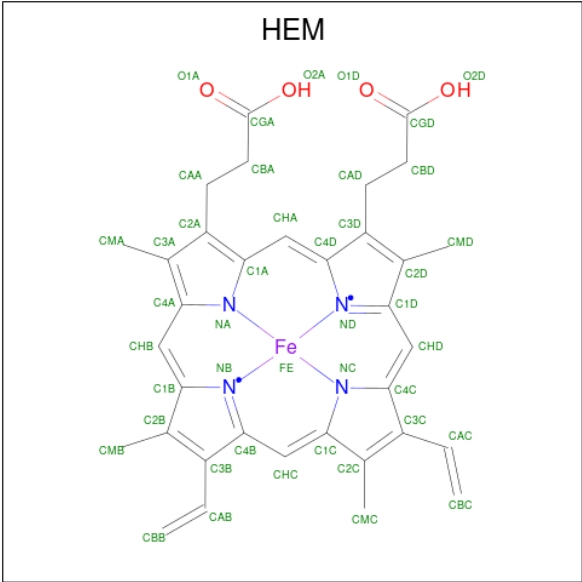
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q59523
A	-18	GLY	-	expression tag	UNP Q59523
A	-17	SER	-	expression tag	UNP Q59523
A	-16	SER	-	expression tag	UNP Q59523
A	-15	HIS	-	expression tag	UNP Q59523
A	-14	HIS	-	expression tag	UNP Q59523
A	-13	HIS	-	expression tag	UNP Q59523
A	-12	HIS	-	expression tag	UNP Q59523
A	-11	HIS	-	expression tag	UNP Q59523
A	-10	HIS	-	expression tag	UNP Q59523
A	-9	SER	-	expression tag	UNP Q59523
A	-8	SER	-	expression tag	UNP Q59523
A	-7	GLY	-	expression tag	UNP Q59523
A	-6	LEU	-	expression tag	UNP Q59523
A	-5	VAL	-	expression tag	UNP Q59523
A	-4	PRO	-	expression tag	UNP Q59523
A	-3	ARG	-	expression tag	UNP Q59523
A	-2	GLY	-	expression tag	UNP Q59523
A	-1	SER	-	expression tag	UNP Q59523
A	0	HIS	-	expression tag	UNP Q59523
A	286	ALA	PHE	engineered mutation	UNP Q59523
B	-19	MET	-	expression tag	UNP Q59523
B	-18	GLY	-	expression tag	UNP Q59523

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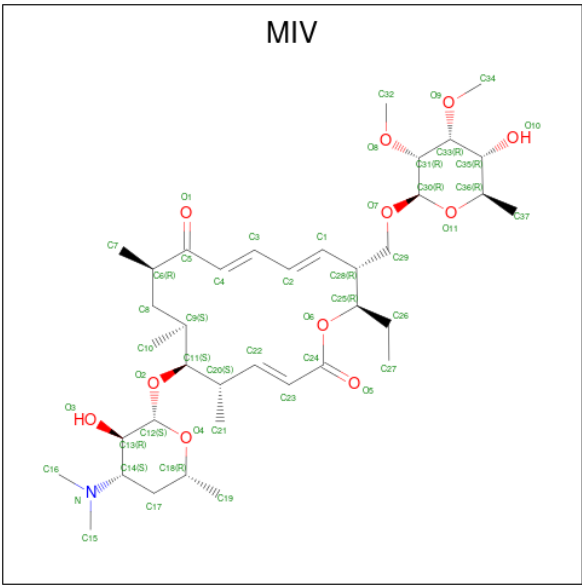
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q59523
B	-16	SER	-	expression tag	UNP Q59523
B	-15	HIS	-	expression tag	UNP Q59523
B	-14	HIS	-	expression tag	UNP Q59523
B	-13	HIS	-	expression tag	UNP Q59523
B	-12	HIS	-	expression tag	UNP Q59523
B	-11	HIS	-	expression tag	UNP Q59523
B	-10	HIS	-	expression tag	UNP Q59523
B	-9	SER	-	expression tag	UNP Q59523
B	-8	SER	-	expression tag	UNP Q59523
B	-7	GLY	-	expression tag	UNP Q59523
B	-6	LEU	-	expression tag	UNP Q59523
B	-5	VAL	-	expression tag	UNP Q59523
B	-4	PRO	-	expression tag	UNP Q59523
B	-3	ARG	-	expression tag	UNP Q59523
B	-2	GLY	-	expression tag	UNP Q59523
B	-1	SER	-	expression tag	UNP Q59523
B	0	HIS	-	expression tag	UNP Q59523
B	286	ALA	PHE	engineered mutation	UNP Q59523
C	-19	MET	-	expression tag	UNP Q59523
C	-18	GLY	-	expression tag	UNP Q59523
C	-17	SER	-	expression tag	UNP Q59523
C	-16	SER	-	expression tag	UNP Q59523
C	-15	HIS	-	expression tag	UNP Q59523
C	-14	HIS	-	expression tag	UNP Q59523
C	-13	HIS	-	expression tag	UNP Q59523
C	-12	HIS	-	expression tag	UNP Q59523
C	-11	HIS	-	expression tag	UNP Q59523
C	-10	HIS	-	expression tag	UNP Q59523
C	-9	SER	-	expression tag	UNP Q59523
C	-8	SER	-	expression tag	UNP Q59523
C	-7	GLY	-	expression tag	UNP Q59523
C	-6	LEU	-	expression tag	UNP Q59523
C	-5	VAL	-	expression tag	UNP Q59523
C	-4	PRO	-	expression tag	UNP Q59523
C	-3	ARG	-	expression tag	UNP Q59523
C	-2	GLY	-	expression tag	UNP Q59523
C	-1	SER	-	expression tag	UNP Q59523
C	0	HIS	-	expression tag	UNP Q59523
C	286	ALA	PHE	engineered mutation	UNP Q59523

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



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

- Molecule 3 is MYCINAMICIN IV (CCD ID: MIV) (formula: C₃₇H₆₁NO₁₁).



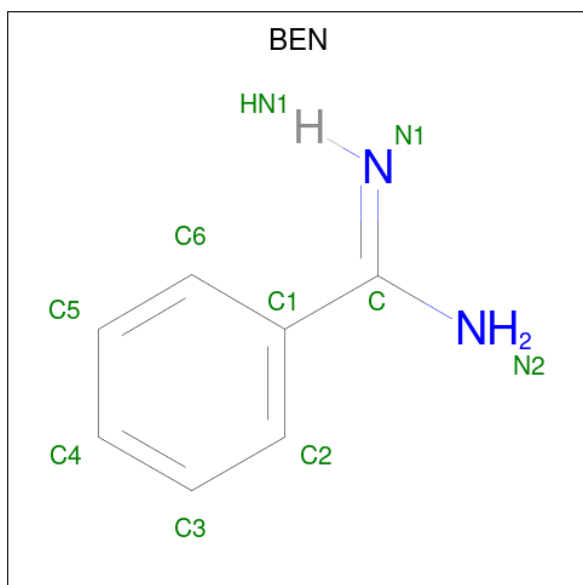
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			49	37	1	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			49	37	1	11		
3	C	1	Total	C	N	O	0	0
			49	37	1	11		

- Molecule 4 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	B	1	Total	C	N	0	0
			9	7	2		
4	B	1	Total	C	N	0	0
			9	7	2		
4	C	1	Total	C	N	0	0
			9	7	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

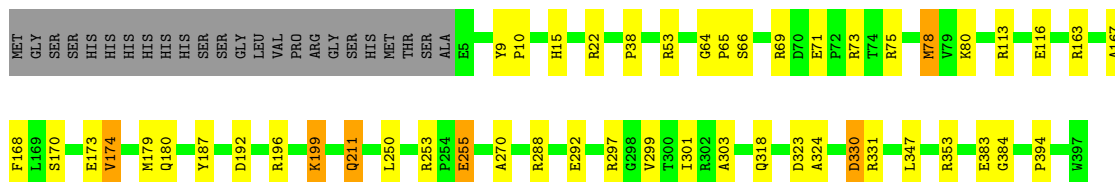
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	338	Total	O	0	0
			338	338		
6	B	340	Total	O	0	0
			340	340		
6	C	343	Total	O	0	0
			343	343		

3 Residue-property plots

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

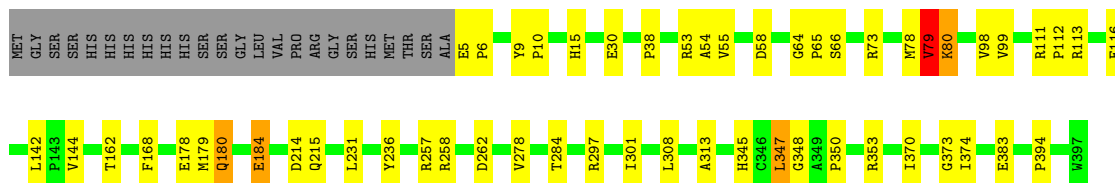
• Molecule 1: P-450-LIKE PROTEIN

Chain A: 



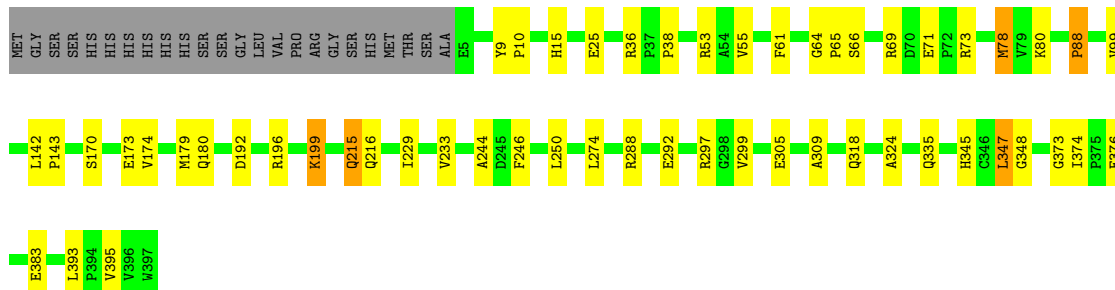
• Molecule 1: P-450-LIKE PROTEIN

Chain B: 



• Molecule 1: P-450-LIKE PROTEIN

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	58.21Å 100.94Å 440.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	220.42 – 1.90 220.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.6 (220.42-1.90) 88.4 (220.42-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.245 0.183 , 0.242	Depositor DCC
R_{free} test set	4576 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.478 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10761	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: HEM, BEN, MIV, GOL

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	1.24	2/3177 (0.1%)	1.13	6/4322 (0.1%)
1	B	1.26	6/3205 (0.2%)	1.13	7/4358 (0.2%)
1	C	1.24	3/3196 (0.1%)	1.12	5/4347 (0.1%)
All	All	1.25	11/9578 (0.1%)	1.12	18/13027 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	GLY	N-CA	8.50	1.52	1.45
1	B	301	ILE	CA-CB	-7.25	1.45	1.54
1	A	64	GLY	N-CA	6.74	1.50	1.45
1	B	64	GLY	N-CA	6.61	1.50	1.45
1	B	278	VAL	CA-CB	5.78	1.61	1.54
1	B	79	VAL	CA-CB	5.52	1.60	1.53
1	A	301	ILE	CA-CB	-5.38	1.47	1.54
1	B	64	GLY	CA-C	5.18	1.55	1.51
1	C	309	ALA	CA-CB	5.11	1.59	1.53
1	C	244	ALA	CA-CB	5.09	1.61	1.53
1	B	313	ALA	C-O	5.06	1.30	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	LEU	CA-C-N	-7.27	112.21	119.56
1	B	142	LEU	C-N-CA	-7.27	112.21	119.56
1	C	305	GLU	CA-C-N	6.36	126.86	119.99
1	C	305	GLU	C-N-CA	6.36	126.86	119.99
1	A	199	LYS	N-CA-C	-6.30	105.75	113.50
1	C	199	LYS	N-CA-C	-6.06	106.01	113.41
1	C	88	PRO	N-CA-C	-5.92	104.79	110.47
1	B	55	VAL	N-CA-C	5.69	116.34	110.36
1	B	30	GLU	CA-C-N	-5.63	114.01	119.87
1	B	30	GLU	C-N-CA	-5.63	114.01	119.87
1	B	297	ARG	CA-CB-CG	-5.44	103.22	114.10
1	A	288	ARG	N-CA-C	-5.36	101.44	109.95
1	A	174	VAL	N-CA-C	-5.35	100.65	108.99
1	A	253	ARG	CA-C-N	5.31	124.76	119.24
1	A	253	ARG	C-N-CA	5.31	124.76	119.24
1	C	55	VAL	N-CA-C	5.27	115.48	110.42
1	B	231	LEU	N-CA-C	5.17	116.92	111.28
1	A	270	ALA	N-CA-C	-5.10	105.90	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	214	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	3086	47	0
1	B	3141	0	3125	36	0
1	C	3132	0	3124	50	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	4	0
3	A	49	0	61	4	0
3	B	49	0	61	3	0
3	C	49	0	61	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	7	0	0
4	B	18	0	14	0	0
4	C	9	0	7	0	0
5	A	18	0	23	1	0
5	B	12	0	16	1	0
5	C	12	0	16	0	0
6	A	338	0	0	8	0
6	B	340	0	0	6	0
6	C	343	0	0	7	0
All	All	10761	0	9691	139	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 7.

All (139) 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:A:78:MET:HE2	1:A:80:LYS:CE	1.60	1.30
1:C:78:MET:HE2	1:C:80:LYS:NZ	1.64	1.12
1:C:78:MET:HE2	1:C:80:LYS:CE	1.82	1.10
1:A:78:MET:HE2	1:A:80:LYS:HE3	1.11	1.04
1:C:233[B]:VAL:HG11	3:C:460:MIV:C2	1.88	1.03
1:C:78:MET:CE	1:C:80:LYS:NZ	2.28	0.97
1:C:78:MET:CE	1:C:80:LYS:HZ2	1.77	0.96
1:C:192:ASP:HB2	6:C:2216:HOH:O	1.69	0.93
1:C:78:MET:HE2	1:C:80:LYS:HE3	1.52	0.92
1:C:347[A]:LEU:C	1:C:347[A]:LEU:HD23	1.95	0.91
1:A:78:MET:HE2	1:A:80:LYS:NZ	1.86	0.89
1:B:347[A]:LEU:C	1:B:347[A]:LEU:HD23	2.00	0.87
1:C:233[B]:VAL:CG1	3:C:460:MIV:C2	2.53	0.86
1:B:179:MET:HE1	3:B:460:MIV:H13	1.60	0.84
1:A:78:MET:CE	1:A:80:LYS:NZ	2.43	0.80
1:A:78:MET:CE	1:A:80:LYS:CE	2.54	0.79
1:A:174:VAL:CG2	1:A:179[B]:MET:HG3	2.14	0.78
1:A:78:MET:CE	1:A:80:LYS:HE3	2.05	0.75
1:C:179:MET:HE3	6:C:2209:HOH:O	1.89	0.72
1:A:53:ARG:HD3	6:A:2080:HOH:O	1.90	0.71
1:A:394:PRO:HB3	6:A:2162:HOH:O	1.92	0.70
1:C:78:MET:HE2	1:C:80:LYS:HZ2	1.37	0.69
1:B:15:HIS:HE1	1:B:383:GLU:OE2	1.76	0.68
1:B:215:GLN:HB2	6:B:2224:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG21	1:A:179[B]:MET:HG3	1.77	0.66
1:A:15:HIS:HE1	1:A:383:GLU:OE2	1.78	0.66
1:A:196:ARG:HA	1:A:199:LYS:HE2	1.78	0.66
1:C:25:GLU:OE1	6:C:2044:HOH:O	2.13	0.66
1:B:179:MET:SD	3:B:460:MIV:H82C	2.37	0.65
1:C:347[A]:LEU:C	1:C:347[A]:LEU:CD2	2.71	0.64
1:C:215:GLN:HE21	1:C:215:GLN:HA	1.63	0.64
1:C:233[B]:VAL:CG1	3:C:460:MIV:H2	2.26	0.64
1:C:196:ARG:HA	1:C:199:LYS:HE2	1.78	0.63
1:C:15:HIS:HE1	1:C:383:GLU:OE2	1.82	0.63
1:A:170:SER:HA	3:A:460:MIV:H212	1.79	0.63
1:A:174:VAL:HG23	1:A:179[B]:MET:HG3	1.80	0.62
2:A:450:HEM:HBC2	2:A:450:HEM:HMC1	1.80	0.62
1:A:53:ARG:CD	6:A:2080:HOH:O	2.46	0.61
1:B:215:GLN:CB	6:B:2224:HOH:O	2.49	0.60
1:A:192:ASP:O	1:A:196:ARG:HG2	2.02	0.60
1:C:9:TYR:CG	1:C:10:PRO:HA	2.39	0.58
1:A:347:LEU:C	1:A:347:LEU:HD23	2.28	0.58
1:B:9:TYR:CG	1:B:10:PRO:HA	2.39	0.58
1:A:78:MET:CE	1:A:80:LYS:HZ2	2.17	0.58
1:B:345[A]:HIS:HE1	6:B:2316:HOH:O	1.87	0.57
1:C:36:ARG:HD3	6:C:2080:HOH:O	2.03	0.57
1:B:98:VAL:HG11	1:B:347[A]:LEU:HD11	1.85	0.57
1:C:345[A]:HIS:HE1	6:C:2321:HOH:O	1.87	0.57
1:B:38:PRO:HD2	1:B:73:ARG:O	2.05	0.56
1:A:255:GLU:OE1	1:C:292:GLU:HB2	2.05	0.56
1:A:353:ARG:HD2	6:A:2315:HOH:O	2.04	0.56
2:B:450:HEM:HBC2	2:B:450:HEM:HMC2	1.88	0.56
1:A:318:GLN:NE2	1:A:324:ALA:H	2.03	0.55
1:A:69:ARG:O	1:A:78:MET:HE1	2.05	0.55
5:B:1400:GOL:H31	6:B:2208:HOH:O	2.06	0.55
1:B:394:PRO:HB3	6:B:2183:HOH:O	2.07	0.54
1:B:180:GLN:O	1:B:184:GLU:HG3	2.08	0.54
1:A:22:ARG:HH22	1:C:335:GLN:NE2	2.06	0.53
1:A:113:ARG:NH2	6:A:2148:HOH:O	2.38	0.53
1:A:179[B]:MET:HE1	3:A:460:MIV:H13	1.91	0.53
1:A:113:ARG:HD2	1:A:116:GLU:OE1	2.09	0.53
1:C:318:GLN:NE2	1:C:324:ALA:H	2.06	0.53
1:A:179[A]:MET:SD	3:A:460:MIV:H82C	2.50	0.52
1:C:99:VAL:HG12	1:C:347[B]:LEU:HD11	1.91	0.52
1:B:78:MET:HB3	1:B:80:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLN:HE22	1:A:324:ALA:H	1.57	0.51
5:A:1399:GOL:H31	6:A:2191:HOH:O	2.11	0.50
1:C:179:MET:CE	6:C:2209:HOH:O	2.55	0.50
1:C:347[A]:LEU:HD23	1:C:347[A]:LEU:O	2.11	0.50
2:C:450:HEM:HMC2	2:C:450:HEM:HBC2	1.93	0.50
1:B:99:VAL:HG12	1:B:347[B]:LEU:HD11	1.94	0.50
1:B:373:GLY:O	1:B:374:ILE:HG23	2.11	0.50
1:A:167:ALA:O	1:A:179[B]:MET:HG2	2.12	0.50
1:C:142:LEU:HB3	1:C:143:PRO:HD3	1.93	0.50
1:C:170:SER:HA	3:C:460:MIV:H212	1.93	0.49
1:C:318:GLN:HE22	1:C:324:ALA:H	1.59	0.49
1:A:9:TYR:CG	1:A:10:PRO:HA	2.48	0.49
1:C:233[B]:VAL:HG11	3:C:460:MIV:C3	2.40	0.49
1:A:347:LEU:HD23	1:A:347:LEU:O	2.14	0.48
1:C:71:GLU:HB2	1:C:78:MET:HE3	1.94	0.48
1:C:179:MET:SD	3:C:460:MIV:H82C	2.54	0.47
6:A:2033:HOH:O	1:C:53[B]:ARG:NH2	2.47	0.47
1:A:163:ARG:CZ	1:B:178:GLU:HG2	2.45	0.47
1:B:9:TYR:CD1	1:B:10:PRO:HA	2.49	0.47
1:C:9:TYR:CD1	1:C:10:PRO:HA	2.50	0.46
1:B:5:GLU:HG2	1:B:5:GLU:O	2.14	0.46
1:B:111:ARG:HB3	1:B:112:PRO:HD3	1.97	0.46
1:B:257:ARG:NH2	1:B:370:ILE:O	2.45	0.46
1:C:348:GLY:HA3	2:C:450:HEM:C3C	2.50	0.46
1:A:15:HIS:CE1	1:A:383:GLU:OE2	2.65	0.45
1:A:196:ARG:O	1:A:199:LYS:HG2	2.16	0.45
1:B:347[A]:LEU:HD23	1:B:347[A]:LEU:O	2.15	0.45
1:A:211:GLN:HE21	1:A:211:GLN:HB3	1.56	0.45
1:A:323:ASP:HA	1:C:88:PRO:HB2	1.99	0.45
1:C:215:GLN:O	1:C:215:GLN:HG3	2.17	0.45
1:B:113:ARG:HD2	1:B:116:GLU:OE1	2.16	0.44
1:C:78:MET:CE	1:C:80:LYS:HZ1	2.24	0.44
1:B:113:ARG:HD2	1:B:113:ARG:HA	1.77	0.44
1:B:353:ARG:HD2	6:B:2319:HOH:O	2.16	0.44
1:C:174:VAL:O	3:C:460:MIV:H161	2.18	0.44
1:C:69:ARG:O	1:C:78:MET:HE1	2.18	0.44
1:B:347[A]:LEU:C	1:B:347[A]:LEU:CD2	2.79	0.43
1:C:216:GLN:O	6:C:2225:HOH:O	2.21	0.43
1:A:65:PRO:O	1:A:66:SER:C	2.61	0.43
1:A:187:TYR:OH	6:A:2200:HOH:O	2.19	0.43
2:C:450:HEM:HBC2	2:C:450:HEM:CMC	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLU:N	1:B:6:PRO:HD2	2.34	0.43
1:A:71:GLU:CG	1:A:78:MET:HE3	2.48	0.43
3:A:460:MIV:O10	3:A:460:MIV:H342	2.18	0.43
1:C:373:GLY:O	1:C:374:ILE:HG23	2.19	0.42
1:C:393:LEU:O	1:C:395:VAL:HG13	2.19	0.42
1:B:15:HIS:CE1	1:B:383:GLU:OE2	2.65	0.42
1:A:75:ARG:HD2	1:A:384:GLY:O	2.20	0.42
1:B:144:VAL:HG11	1:B:162:THR:HG23	2.02	0.42
1:A:330[A]:ASP:O	1:A:331:ARG:C	2.62	0.42
2:B:450:HEM:HBC2	2:B:450:HEM:CMC	2.48	0.42
1:A:297:ARG:HD3	1:A:297:ARG:HA	1.87	0.42
1:B:348:GLY:HA3	2:B:450:HEM:C3C	2.55	0.42
1:C:192:ASP:OD1	1:C:192:ASP:C	2.62	0.42
2:A:450:HEM:HBC2	2:A:450:HEM:CMC	2.49	0.41
1:C:61:PHE:HB3	1:C:288:ARG:HB3	2.02	0.41
1:A:330[B]:ASP:O	1:A:330[B]:ASP:OD1	2.37	0.41
1:C:65:PRO:O	1:C:66:SER:C	2.63	0.41
1:C:297:ARG:HA	1:C:297:ARG:HD3	1.92	0.41
1:B:236:TYR:CD1	1:B:236:TYR:C	2.98	0.41
1:A:38:PRO:HD2	1:A:73:ARG:O	2.20	0.41
1:A:71:GLU:OE1	1:A:78:MET:HE3	2.20	0.41
1:B:79:VAL:HG11	3:B:460:MIV:H22	2.02	0.41
1:A:168:PHE:N	1:A:168:PHE:CD1	2.88	0.41
1:C:229:ILE:O	1:C:233[B]:VAL:HG23	2.21	0.41
1:B:284:THR:OG1	1:B:308:LEU:HB3	2.20	0.41
1:C:38:PRO:HD2	1:C:73:ARG:O	2.21	0.41
1:A:292:GLU:HA	1:A:303:ALA:HB2	2.02	0.41
1:B:65:PRO:O	1:B:66:SER:C	2.63	0.41
1:B:258:ARG:NH1	1:B:262:ASP:OD2	2.53	0.41
2:C:450:HEM:HMB2	2:C:450:HEM:HBB2	2.04	0.40
1:B:54:ALA:O	1:B:58:ASP:HB2	2.21	0.40
1:B:168:PHE:N	1:B:168:PHE:CD1	2.89	0.40
1:C:246:PHE:CE1	1:C:274:LEU:HB3	2.56	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	396/417 (95%)	381 (96%)	15 (4%)	0	100	100
1	B	398/417 (95%)	390 (98%)	8 (2%)	0	100	100
1	C	397/417 (95%)	389 (98%)	8 (2%)	0	100	100
All	All	1191/1251 (95%)	1160 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	326/345 (94%)	317 (97%)	9 (3%)	38	32
1	B	330/345 (96%)	322 (98%)	8 (2%)	43	38
1	C	329/345 (95%)	320 (97%)	9 (3%)	39	34
All	All	985/1035 (95%)	959 (97%)	26 (3%)	43	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	173	GLU
1	A	180	GLN
1	A	211	GLN
1	A	250	LEU

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Mol	Chain	Res	Type
1	A	255	GLU
1	A	299	VAL
1	A	330[A]	ASP
1	A	330[B]	ASP
1	B	53	ARG
1	B	79	VAL
1	B	80	LYS
1	B	180	GLN
1	B	184	GLU
1	B	347[A]	LEU
1	B	347[B]	LEU
1	B	350	PRO
1	C	78	MET
1	C	173	GLU
1	C	180	GLN
1	C	215	GLN
1	C	250	LEU
1	C	299	VAL
1	C	347[A]	LEU
1	C	347[B]	LEU
1	C	376	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	124	GLN
1	A	130	GLN
1	A	211	GLN
1	A	318	GLN
1	A	320	GLN
1	B	15	HIS
1	B	130	GLN
1	B	259	GLN
1	B	318	GLN
1	B	320	GLN
1	C	15	HIS
1	C	215	GLN
1	C	318	GLN
1	C	320	GLN
1	C	335	GLN
1	C	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	MIV	B	460	-	51,51,51	1.18	2 (3%)	64,71,71	1.47	12 (18%)
5	GOL	C	1399	-	5,5,5	0.81	0	5,5,5	1.72	1 (20%)
2	HEM	B	450	1,6	50,50,50	1.64	9 (18%)	67,82,82	1.29	7 (10%)
2	HEM	C	450	1	50,50,50	1.77	7 (14%)	67,82,82	1.52	9 (13%)
5	GOL	A	1399	-	5,5,5	0.65	0	5,5,5	3.15	1 (20%)
5	GOL	B	1400	-	5,5,5	0.69	0	5,5,5	2.99	1 (20%)
4	BEN	B	1398	-	9,9,9	0.58	0	7,11,11	0.95	1 (14%)
2	HEM	A	450	1,6	50,50,50	1.89	9 (18%)	67,82,82	1.41	8 (11%)
5	GOL	A	1400	-	5,5,5	1.02	0	5,5,5	1.66	1 (20%)
3	MIV	C	460	-	51,51,51	1.22	4 (7%)	64,71,71	1.73	15 (23%)
3	MIV	A	460	-	51,51,51	1.16	3 (5%)	64,71,71	1.61	14 (21%)
4	BEN	B	1399	-	9,9,9	1.52	1 (11%)	7,11,11	0.87	0
4	BEN	C	1398	-	9,9,9	1.00	0	7,11,11	2.73	4 (57%)
5	GOL	B	1401	-	5,5,5	0.62	0	5,5,5	1.37	0
5	GOL	C	1400	-	5,5,5	0.49	0	5,5,5	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	1401	-	5,5,5	0.70	0	5,5,5	1.25	1 (20%)
4	BEN	A	1398	-	9,9,9	0.58	0	7,11,11	0.96	0

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	MIV	B	460	-	-	8/55/91/91	0/2/3/3
5	GOL	C	1399	-	-	2/4/4/4	-
2	HEM	B	450	1,6	-	0/14/54/54	-
2	HEM	C	450	1	-	0/14/54/54	-
5	GOL	A	1399	-	-	3/4/4/4	-
5	GOL	B	1400	-	-	2/4/4/4	-
4	BEN	B	1398	-	-	2/4/4/4	0/1/1/1
2	HEM	A	450	1,6	-	0/14/54/54	-
5	GOL	A	1400	-	-	3/4/4/4	-
3	MIV	C	460	-	-	11/55/91/91	0/2/3/3
3	MIV	A	460	-	-	9/55/91/91	0/2/3/3
4	BEN	B	1399	-	-	4/4/4/4	0/1/1/1
4	BEN	C	1398	-	-	1/4/4/4	0/1/1/1
5	GOL	B	1401	-	-	2/4/4/4	-
5	GOL	C	1400	-	-	0/4/4/4	-
5	GOL	A	1401	-	-	4/4/4/4	-
4	BEN	A	1398	-	-	2/4/4/4	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	HEM	C3D-C2D	6.91	1.51	1.36
2	A	450	HEM	FE-ND	6.53	2.15	1.94
2	B	450	HEM	C3D-C2D	5.85	1.49	1.36
2	C	450	HEM	C3D-C2D	5.82	1.49	1.36
3	B	460	MIV	O6-C24	5.59	1.46	1.34
3	A	460	MIV	O6-C24	5.37	1.45	1.34
3	C	460	MIV	O6-C24	5.29	1.45	1.34
2	C	450	HEM	FE-ND	4.69	2.09	1.94
2	C	450	HEM	CMA-C3A	4.05	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	HEM	FE-ND	3.82	2.06	1.94
2	A	450	HEM	CMA-C3A	3.49	1.57	1.50
2	C	450	HEM	CAC-C3C	3.37	1.56	1.47
2	A	450	HEM	FE-NB	3.26	2.05	1.94
2	C	450	HEM	FE-NA	3.24	2.05	1.95
2	B	450	HEM	FE-NB	3.15	2.04	1.94
2	B	450	HEM	CAC-C3C	3.03	1.55	1.47
2	A	450	HEM	CAC-C3C	2.94	1.55	1.47
2	B	450	HEM	CMA-C3A	2.91	1.56	1.50
2	C	450	HEM	FE-NB	2.79	2.03	1.94
2	A	450	HEM	CAB-C3B	2.78	1.54	1.47
2	C	450	HEM	CAB-C3B	2.72	1.54	1.47
4	B	1399	BEN	C1-C	2.64	1.52	1.47
2	A	450	HEM	CMB-C2B	2.53	1.55	1.50
3	A	460	MIV	O7-C30	2.50	1.44	1.40
3	C	460	MIV	O9-C33	2.48	1.48	1.42
2	B	450	HEM	CAB-C3B	2.44	1.53	1.47
2	A	450	HEM	C4D-ND	-2.33	1.36	1.40
2	B	450	HEM	FE-NA	2.31	2.02	1.95
3	C	460	MIV	C31-C33	2.30	1.57	1.52
2	B	450	HEM	CMC-C2C	2.14	1.55	1.50
3	C	460	MIV	O7-C30	2.13	1.43	1.40
3	B	460	MIV	O9-C33	2.10	1.47	1.42
2	A	450	HEM	CMC-C2C	2.06	1.55	1.50
3	A	460	MIV	C31-C33	2.04	1.56	1.52
2	B	450	HEM	C3C-C4C	-2.02	1.42	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1399	GOL	C3-C2-C1	-6.58	87.67	111.80
5	B	1400	GOL	C3-C2-C1	-6.55	87.76	111.80
2	A	450	HEM	C4D-ND-C1D	5.14	111.30	105.21
3	C	460	MIV	O9-C33-C31	4.77	119.96	108.93
2	C	450	HEM	CHD-C4C-NC	4.71	129.59	124.45
4	C	1398	BEN	C5-C6-C1	4.66	124.95	120.36
3	A	460	MIV	O8-C31-C33	4.25	118.77	108.93
3	C	460	MIV	O8-C31-C33	4.24	118.74	108.93
2	B	450	HEM	CHD-C4C-NC	4.18	129.00	124.45
2	A	450	HEM	C1D-C2D-C3D	-4.02	102.75	106.98
4	C	1398	BEN	C3-C2-C1	-3.85	116.58	120.36
3	C	460	MIV	C34-O9-C33	3.84	124.34	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	450	HEM	C4D-ND-C1D	3.79	109.70	105.21
3	A	460	MIV	C30-O11-C36	3.74	120.01	113.63
5	C	1399	GOL	O2-C2-C3	3.70	124.48	109.18
3	A	460	MIV	O7-C30-C31	3.56	115.05	108.31
2	C	450	HEM	CAC-C3C-C4C	-3.53	116.40	124.82
2	C	450	HEM	C4C-C3C-C2C	3.52	109.86	106.81
3	C	460	MIV	C20-C22-C23	-3.41	117.27	126.30
3	C	460	MIV	O6-C25-C26	3.36	112.24	106.90
3	B	460	MIV	C20-C22-C23	-3.34	117.46	126.30
3	C	460	MIV	C30-O11-C36	3.34	119.33	113.63
3	A	460	MIV	O6-C24-O5	-3.34	118.00	123.34
2	B	450	HEM	C1D-C2D-C3D	-3.30	103.51	106.98
3	B	460	MIV	C21-C20-C22	-3.27	102.52	109.91
5	A	1400	GOL	O2-C2-C3	3.14	122.19	109.18
2	C	450	HEM	C1D-C2D-C3D	-3.08	103.75	106.98
3	A	460	MIV	C20-C22-C23	-3.01	118.35	126.30
2	A	450	HEM	CHD-C4C-NC	2.97	127.69	124.45
3	B	460	MIV	O8-C31-C33	2.97	115.81	108.93
3	C	460	MIV	O6-C24-C23	2.95	117.82	111.39
3	B	460	MIV	C30-O11-C36	2.93	118.64	113.63
2	B	450	HEM	CAC-C3C-C4C	-2.87	117.97	124.82
3	C	460	MIV	C18-C17-C14	-2.80	105.68	110.46
2	B	450	HEM	C4D-ND-C1D	2.78	108.50	105.21
3	A	460	MIV	C2-C3-C4	-2.78	118.08	124.65
2	A	450	HEM	CBD-CAD-C3D	-2.77	104.86	112.53
3	C	460	MIV	O6-C24-O5	-2.77	118.90	123.34
4	C	1398	BEN	C4-C5-C6	-2.75	116.84	120.24
3	B	460	MIV	O6-C24-C23	2.74	117.34	111.39
3	B	460	MIV	C35-C33-C31	-2.72	105.60	111.72
3	A	460	MIV	C21-C20-C22	-2.66	103.89	109.91
5	A	1401	GOL	C3-C2-C1	-2.65	102.07	111.80
3	C	460	MIV	C21-C20-C22	-2.61	104.01	109.91
3	A	460	MIV	O6-C25-C26	2.59	111.02	106.90
2	A	450	HEM	C4B-C3B-C2B	2.55	109.63	107.28
3	A	460	MIV	O1-C5-C6	-2.54	117.08	121.40
3	C	460	MIV	O1-C5-C6	-2.48	117.18	121.40
3	C	460	MIV	C2-C3-C4	-2.48	118.79	124.65
3	A	460	MIV	C30-C31-C33	-2.43	106.00	110.74
4	C	1398	BEN	C4-C3-C2	2.38	123.17	120.24
3	B	460	MIV	O1-C5-C6	-2.37	117.36	121.40
3	B	460	MIV	C12-C13-C14	2.36	112.92	109.15
2	C	450	HEM	CAD-C3D-C4D	2.35	128.79	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	MIV	C28-C1-C2	-2.34	119.91	125.40
3	B	460	MIV	C10-C9-C8	2.32	114.20	110.68
3	B	460	MIV	O6-C24-O5	-2.24	119.75	123.34
2	C	450	HEM	C2A-C1A-NA	-2.23	107.68	110.15
3	C	460	MIV	C28-C1-C2	-2.22	120.18	125.40
3	A	460	MIV	O3-C13-C14	2.22	113.93	109.87
3	C	460	MIV	O3-C13-C14	2.20	113.89	109.87
2	A	450	HEM	CHC-C4B-NB	2.17	126.75	124.42
2	A	450	HEM	CAC-C3C-C4C	-2.16	119.66	124.82
2	B	450	HEM	CBD-CAD-C3D	-2.13	106.64	112.53
3	A	460	MIV	O9-C33-C31	2.13	113.86	108.93
3	A	460	MIV	O6-C24-C23	2.11	115.99	111.39
2	A	450	HEM	CHB-C4A-NA	2.09	127.65	123.86
3	B	460	MIV	C30-C31-C33	-2.07	106.72	110.74
4	B	1398	BEN	C6-C1-C2	2.06	121.18	118.57
2	B	450	HEM	O2D-CGD-O1D	-2.05	118.06	123.33
2	C	450	HEM	CBC-CAC-C3C	-2.05	117.29	127.53
3	B	460	MIV	C2-C3-C4	-2.05	119.81	124.65
2	B	450	HEM	C4C-C3C-C2C	2.03	108.58	106.81
2	C	450	HEM	O2D-CGD-O1D	-2.03	118.12	123.33
3	C	460	MIV	O2-C11-C20	-2.01	106.89	110.93

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	460	MIV	O6-C25-C26-C27
3	A	460	MIV	C28-C25-C26-C27
3	B	460	MIV	O6-C25-C26-C27
3	B	460	MIV	C28-C25-C26-C27
3	C	460	MIV	O6-C25-C26-C27
3	C	460	MIV	C28-C25-C26-C27
5	A	1401	GOL	O1-C1-C2-C3
5	A	1401	GOL	C1-C2-C3-O3
5	A	1401	GOL	O2-C2-C3-O3
5	B	1401	GOL	O1-C1-C2-O2
5	B	1401	GOL	O1-C1-C2-C3
3	C	460	MIV	C30-C31-O8-C32
3	C	460	MIV	C35-C33-O9-C34
3	A	460	MIV	C1-C2-C3-C4
3	C	460	MIV	C33-C31-O8-C32
3	A	460	MIV	C31-C30-O7-C29

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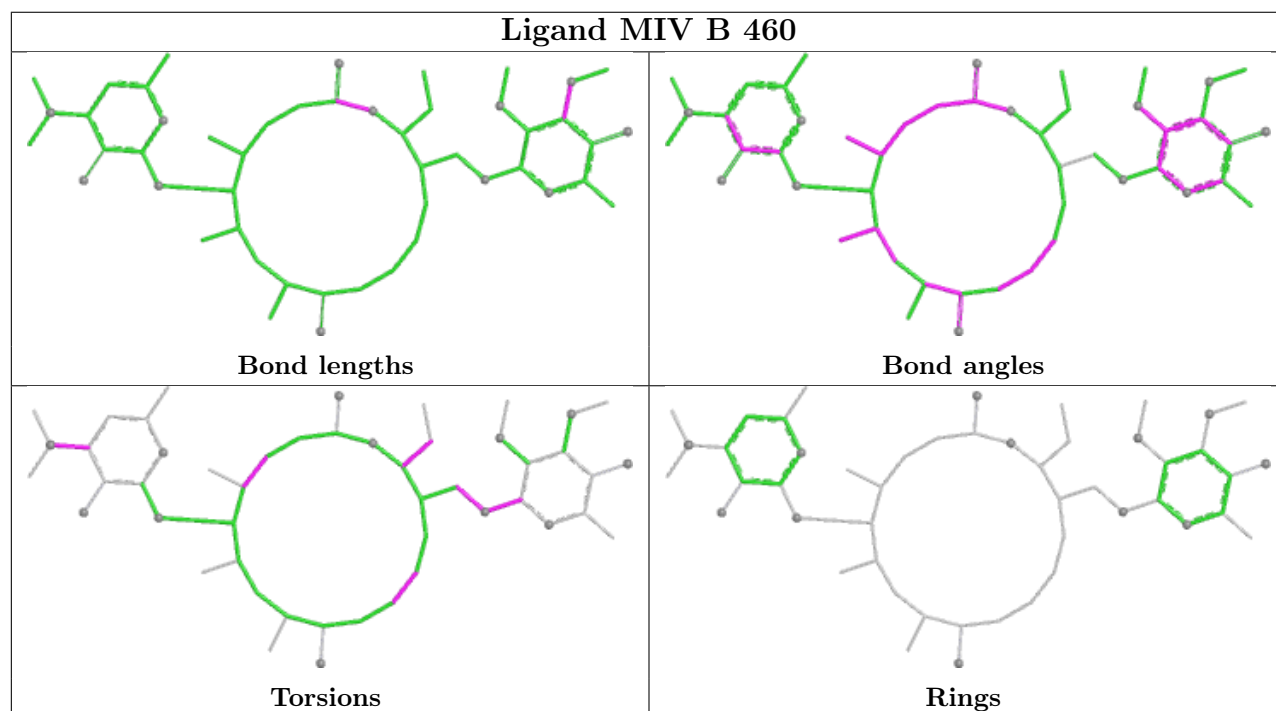
Mol	Chain	Res	Type	Atoms
3	B	460	MIV	C31-C30-O7-C29
3	C	460	MIV	C31-C30-O7-C29
5	A	1399	GOL	C1-C2-C3-O3
5	A	1400	GOL	C1-C2-C3-O3
5	C	1399	GOL	C1-C2-C3-O3
3	A	460	MIV	O11-C30-O7-C29
3	C	460	MIV	O11-C30-O7-C29
5	A	1400	GOL	O2-C2-C3-O3
5	B	1400	GOL	O1-C1-C2-O2
5	C	1399	GOL	O2-C2-C3-O3
3	B	460	MIV	O11-C30-O7-C29
3	A	460	MIV	C30-C31-O8-C32
3	C	460	MIV	C1-C2-C3-C4
5	A	1401	GOL	O1-C1-C2-O2
3	B	460	MIV	C1-C2-C3-C4
3	A	460	MIV	C33-C31-O8-C32
5	A	1399	GOL	O2-C2-C3-O3
5	B	1400	GOL	O1-C1-C2-C3
3	B	460	MIV	C17-C14-N-C15
5	A	1399	GOL	O1-C1-C2-O2
3	A	460	MIV	C28-C29-O7-C30
3	B	460	MIV	C28-C29-O7-C30
3	C	460	MIV	C28-C29-O7-C30
3	C	460	MIV	C26-C25-C28-C29
3	B	460	MIV	C11-C20-C22-C23
4	A	1398	BEN	N2-C-C1-C2
4	B	1398	BEN	N2-C-C1-C2
4	B	1399	BEN	N2-C-C1-C2
4	B	1399	BEN	N2-C-C1-C6
3	A	460	MIV	C35-C33-O9-C34
5	A	1400	GOL	O1-C1-C2-C3
3	C	460	MIV	C4-C5-C6-C8
4	A	1398	BEN	N2-C-C1-C6
4	B	1398	BEN	N2-C-C1-C6
4	B	1399	BEN	N1-C-C1-C2
4	B	1399	BEN	N1-C-C1-C6
4	C	1398	BEN	N1-C-C1-C6

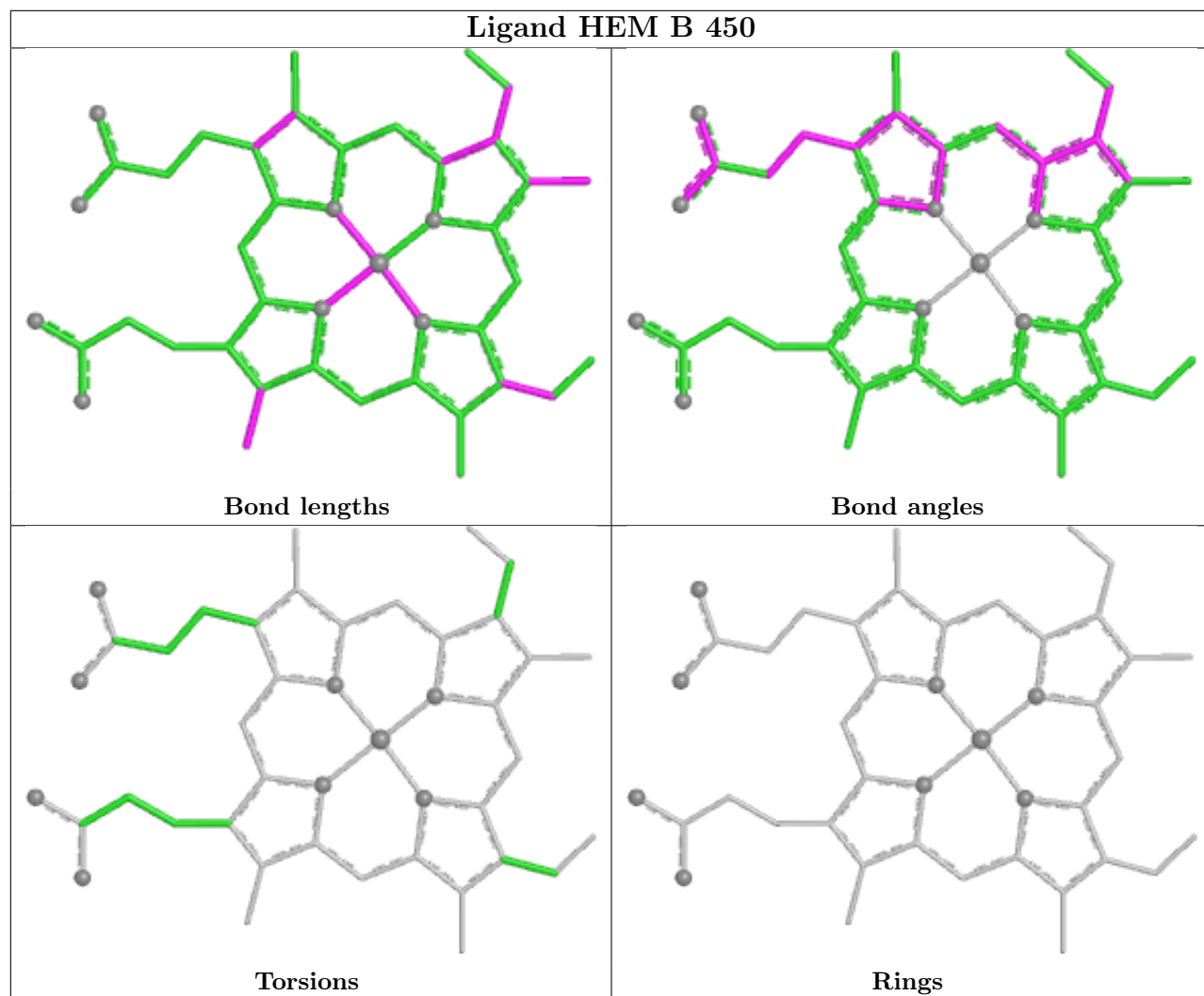
There are no ring outliers.

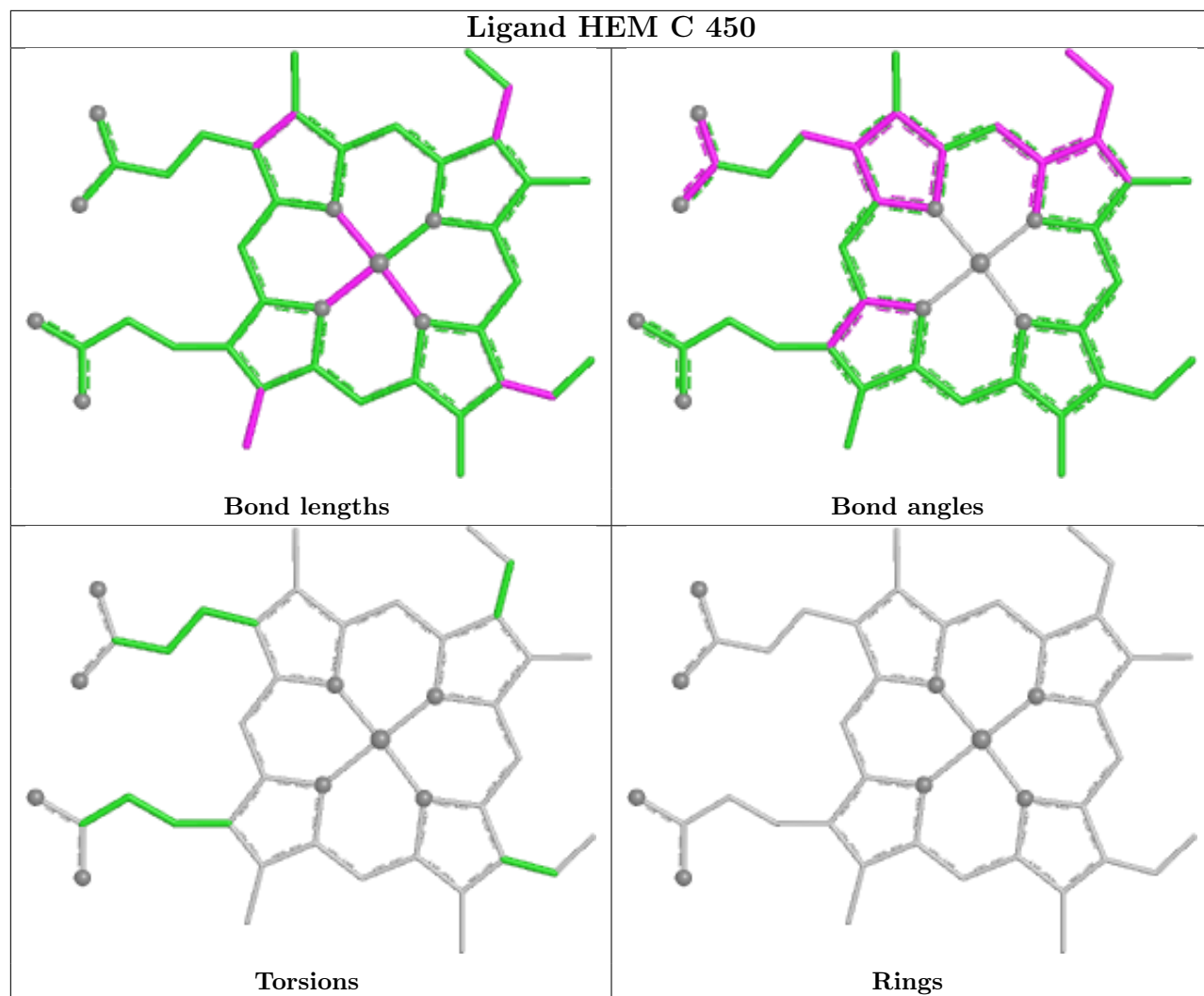
8 monomers are involved in 25 short contacts:

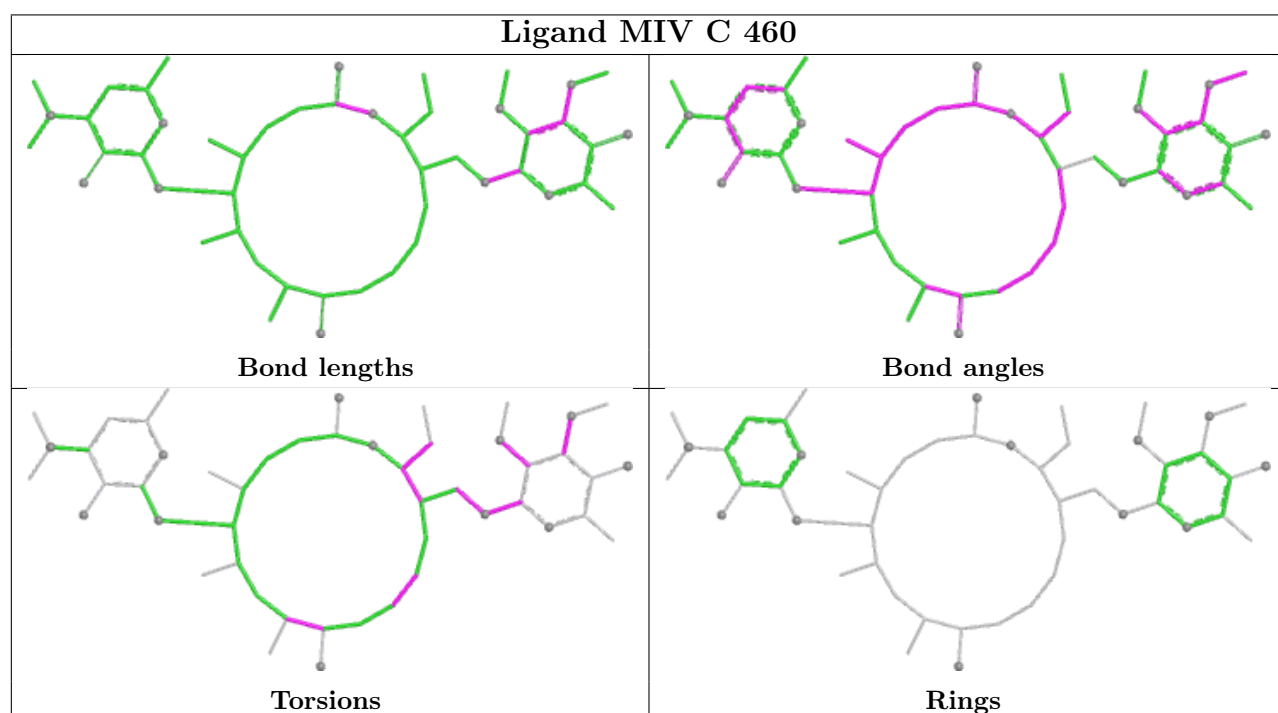
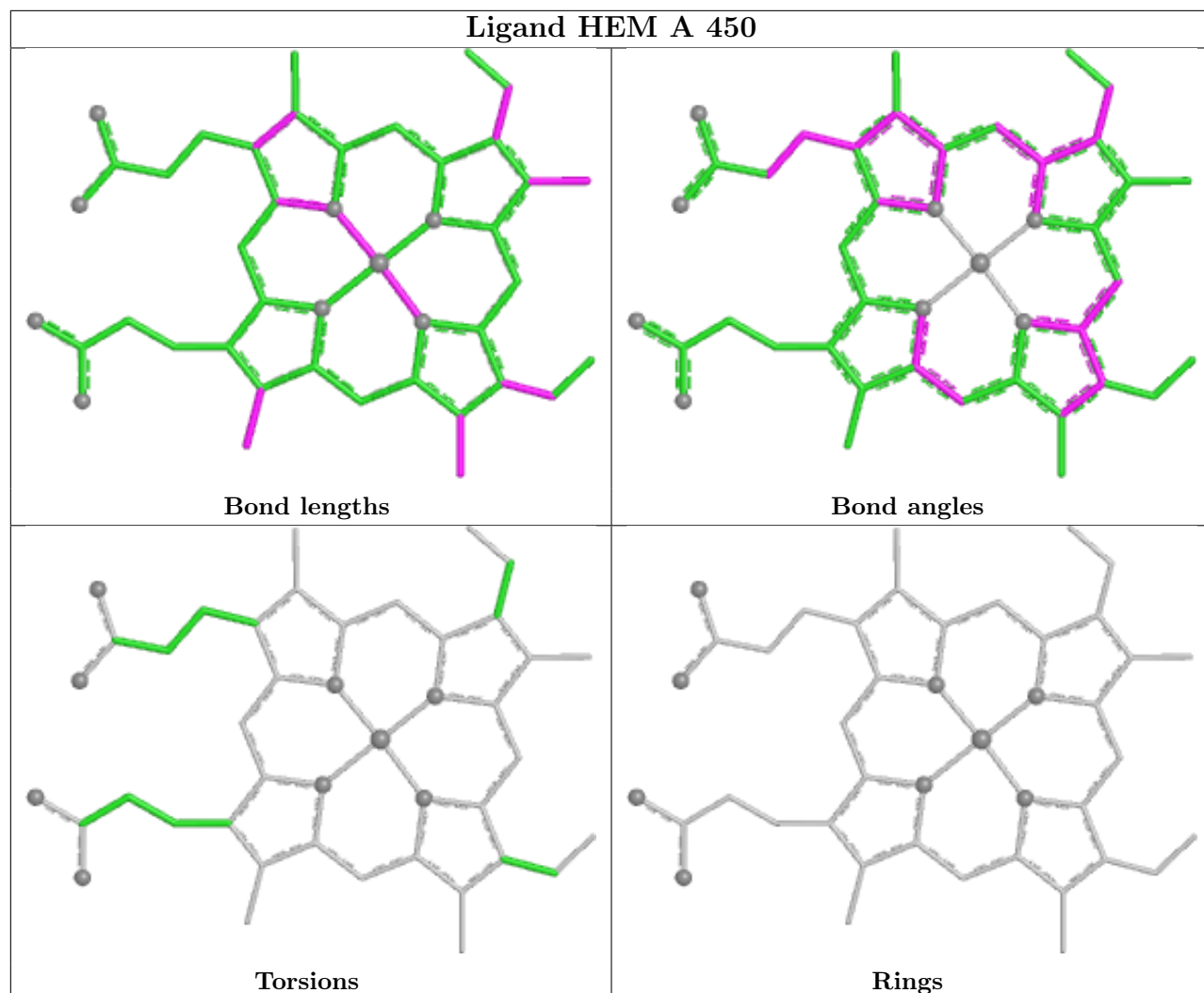
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	460	MIV	3	0
2	B	450	HEM	3	0
2	C	450	HEM	4	0
5	A	1399	GOL	1	0
5	B	1400	GOL	1	0
2	A	450	HEM	2	0
3	C	460	MIV	7	0
3	A	460	MIV	4	0

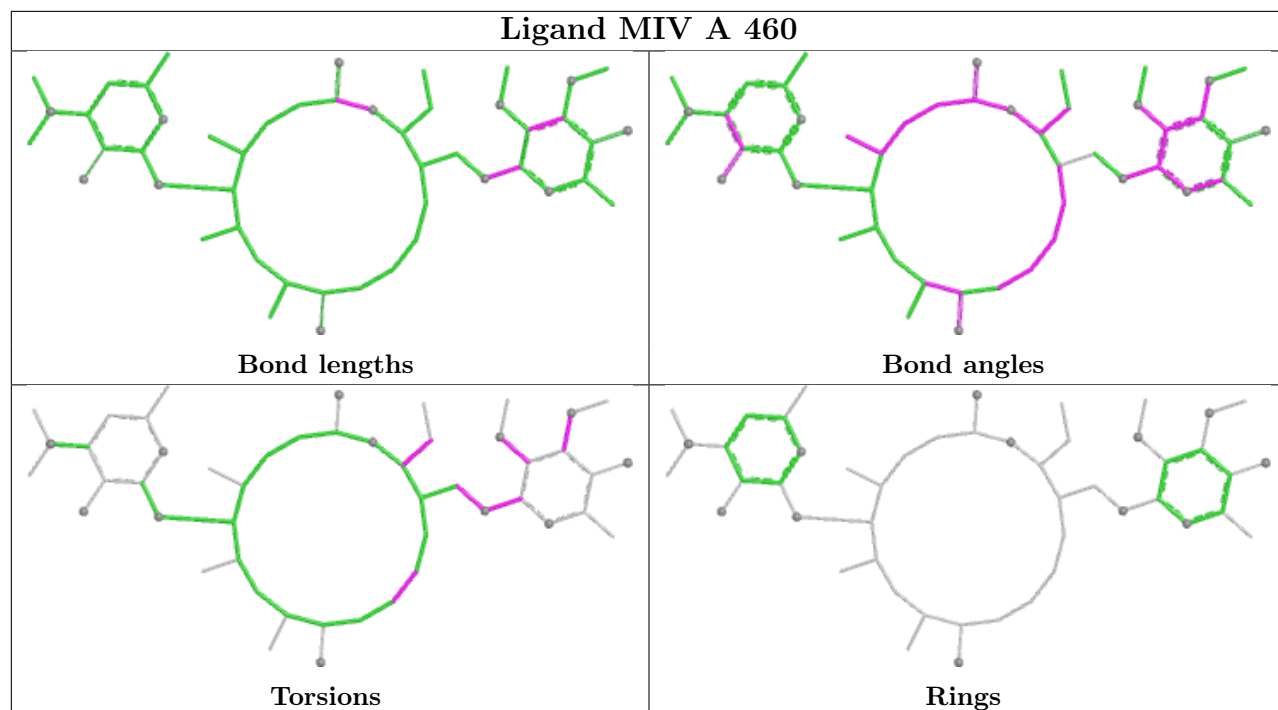
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	393/417 (94%)	-1.34	0 100 100	7, 21, 40, 48	5 (1%)
1	B	393/417 (94%)	-1.32	0 100 100	7, 21, 40, 51	7 (1%)
1	C	393/417 (94%)	-1.32	0 100 100	7, 21, 40, 52	6 (1%)
All	All	1179/1251 (94%)	-1.33	0 100 100	7, 21, 40, 52	18 (1%)

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.

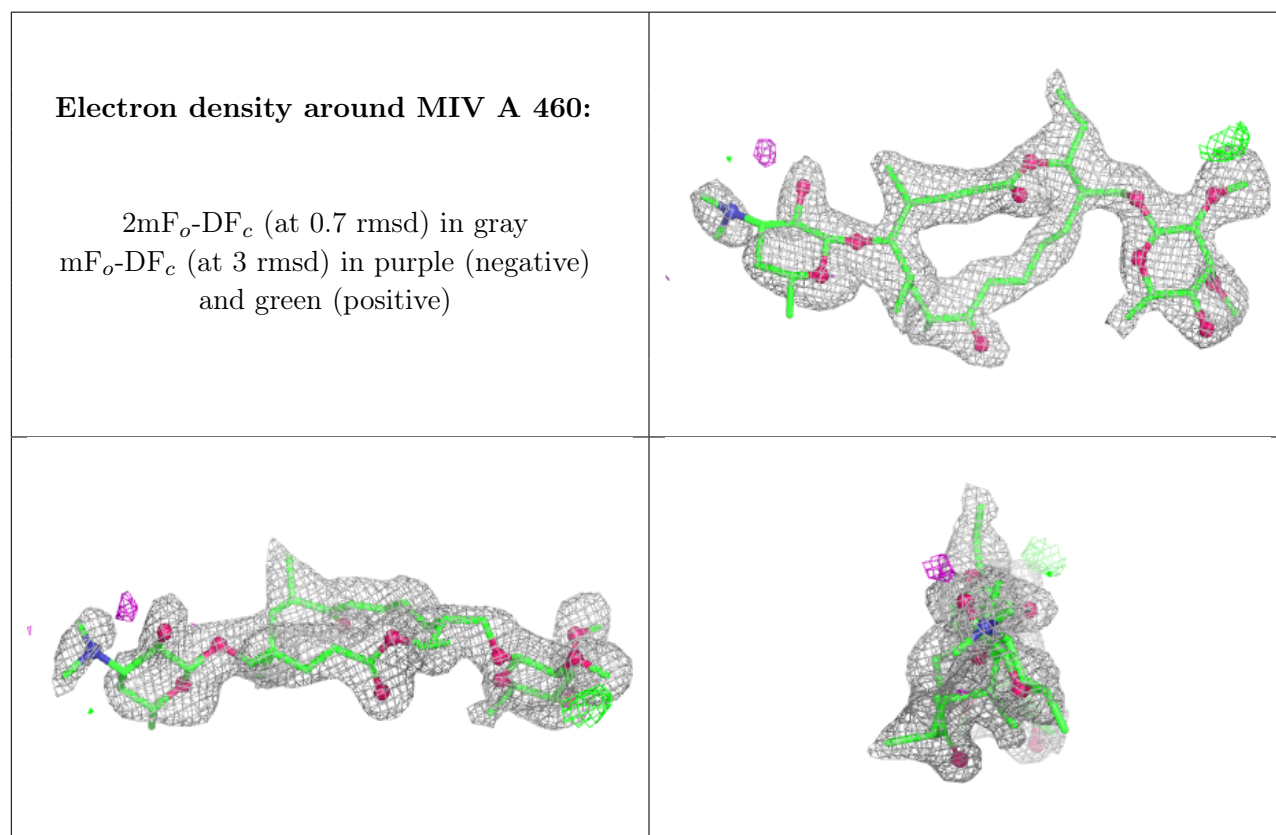
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MIV	A	460	49/49	0.98	0.05	34,41,54,55	0
3	MIV	B	460	49/49	0.98	0.05	33,41,53,54	0
3	MIV	C	460	49/49	0.98	0.05	33,41,51,51	0
4	BEN	B	1399	9/9	0.98	0.07	42,43,44,46	0
5	GOL	C	1400	6/6	0.98	0.04	19,22,24,25	0

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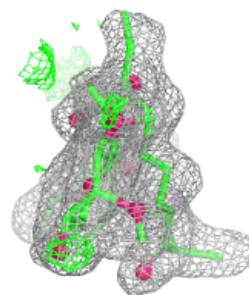
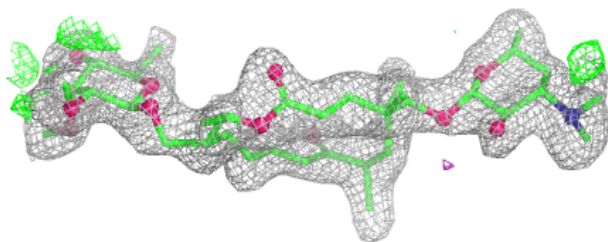
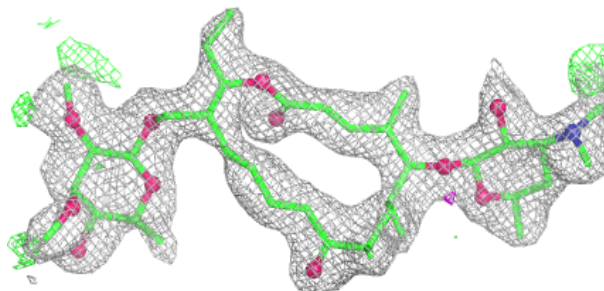
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BEN	A	1398	9/9	0.99	0.04	34,36,38,38	9
4	BEN	C	1398	9/9	0.99	0.06	34,35,36,36	9
5	GOL	A	1399	6/6	0.99	0.03	20,23,23,27	0
5	GOL	A	1400	6/6	0.99	0.04	11,21,22,22	0
5	GOL	A	1401	6/6	0.99	0.05	22,33,35,38	0
5	GOL	B	1400	6/6	0.99	0.04	18,23,26,26	0
5	GOL	B	1401	6/6	0.99	0.04	19,32,35,38	0
5	GOL	C	1399	6/6	0.99	0.04	15,20,21,21	0
4	BEN	B	1398	9/9	0.99	0.04	34,36,37,38	9
2	HEM	C	450	43/43	1.00	0.03	7,12,15,22	0
2	HEM	A	450	43/43	1.00	0.02	7,12,15,20	0
2	HEM	B	450	43/43	1.00	0.02	9,12,16,21	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.

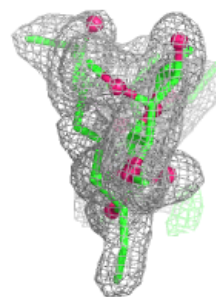
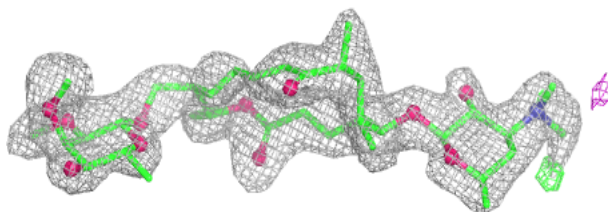
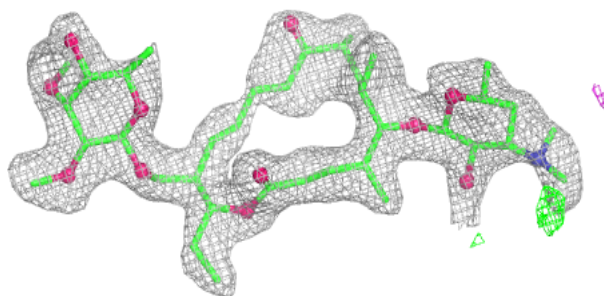


Electron density around MIV B 460:

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

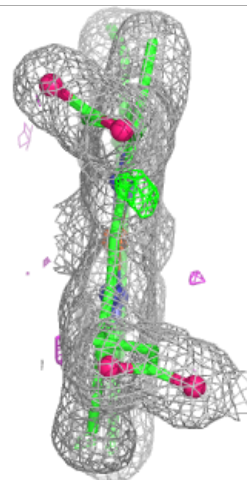
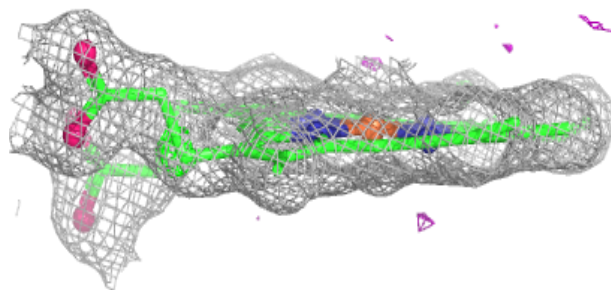
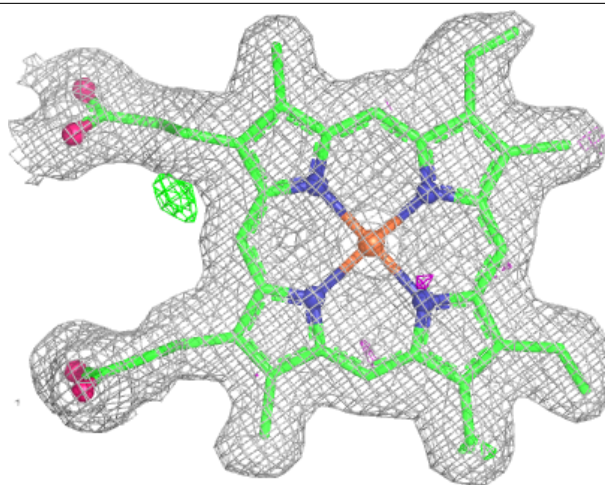
**Electron density around MIV C 460:**

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



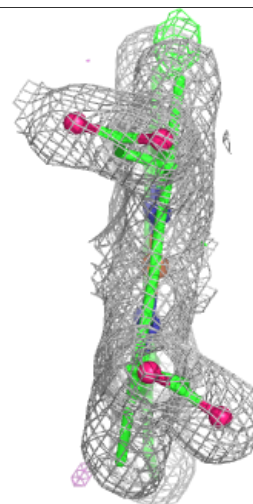
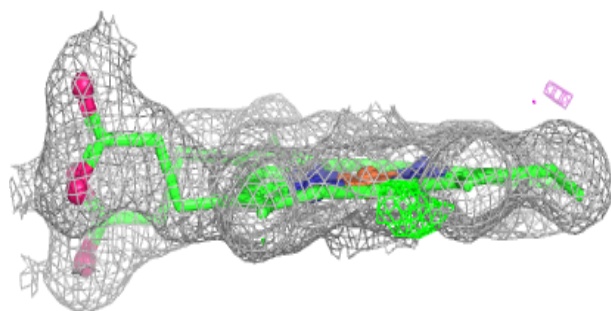
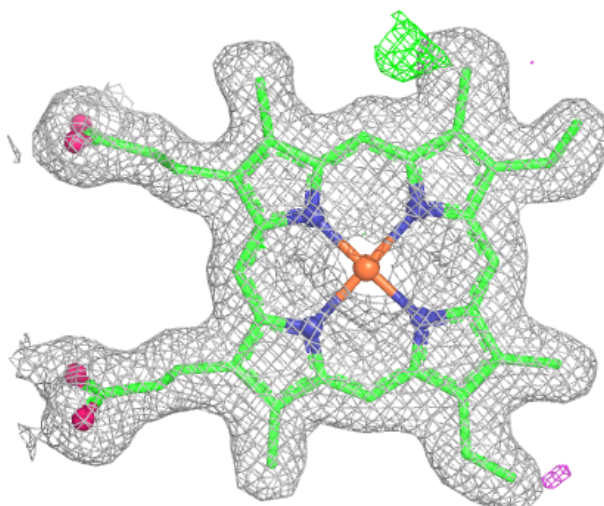
Electron density around HEM C 450:

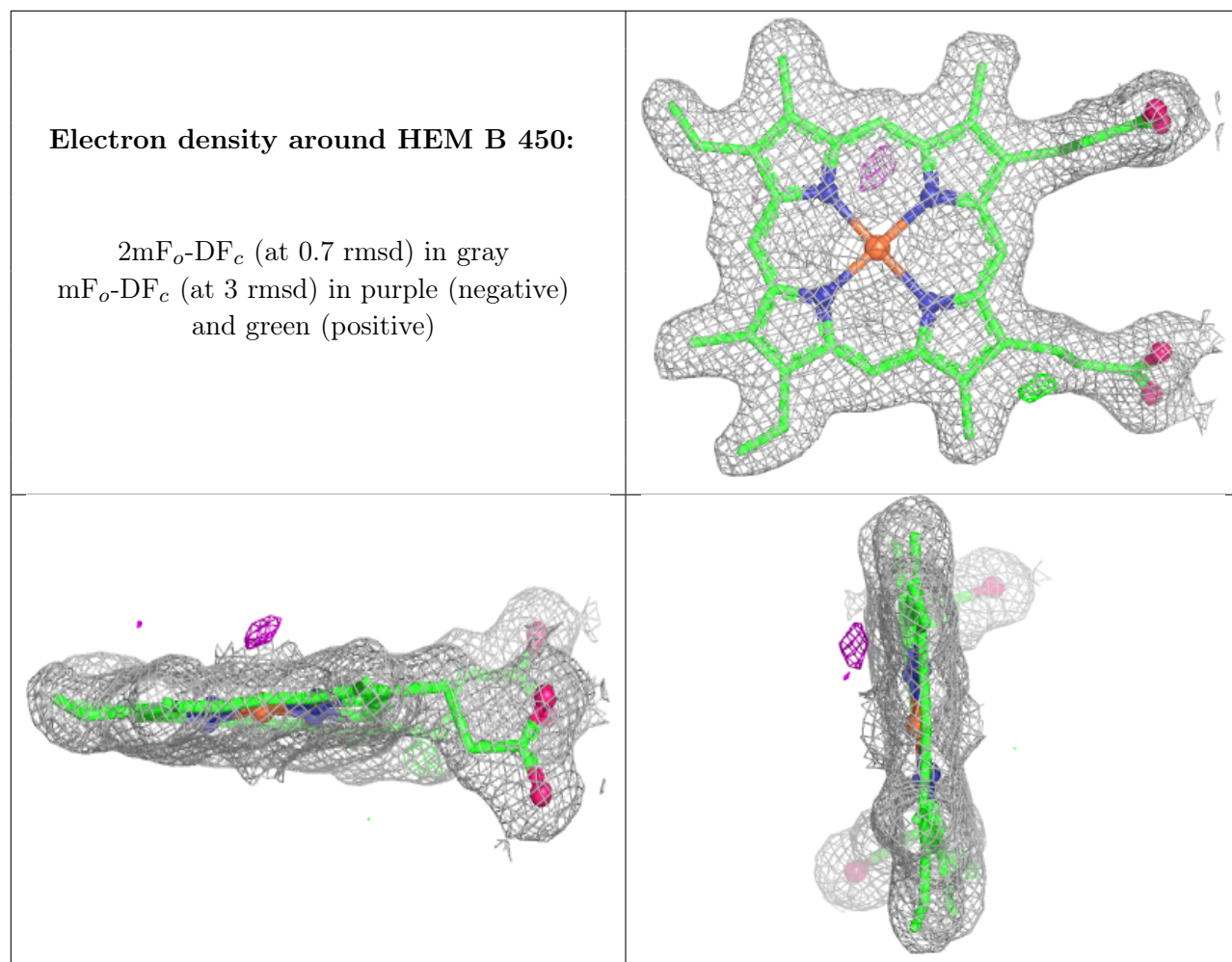
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 450:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.