



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 PM UTC

PDB ID : 7ABW / pdb_00007abw
Title : Crystal structure of siderophore reductase FoxB
Authors : Josts, I.; Tidow, H.
Deposited on : 2020-09-09
Resolution : 3.35 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

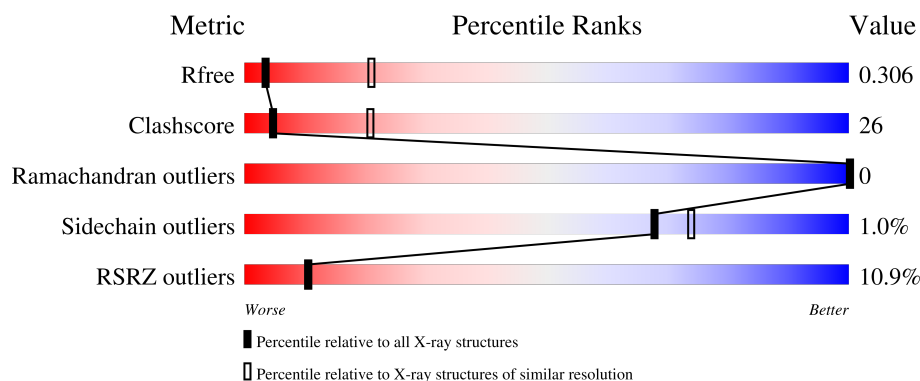
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

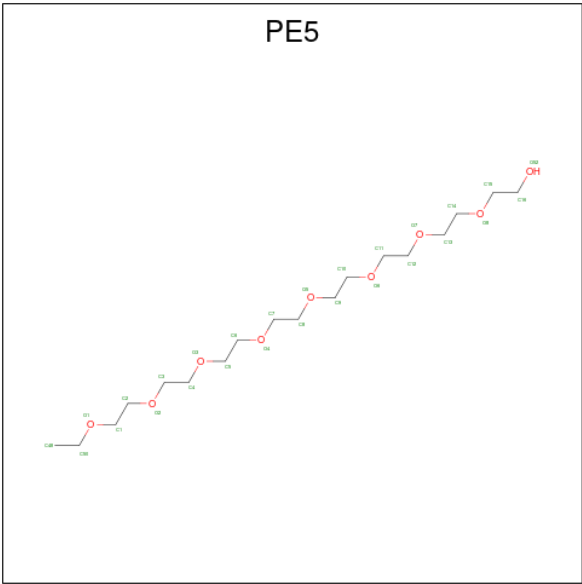
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	382	7% 55% 37% 6%
1	B	382	13% 58% 34% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

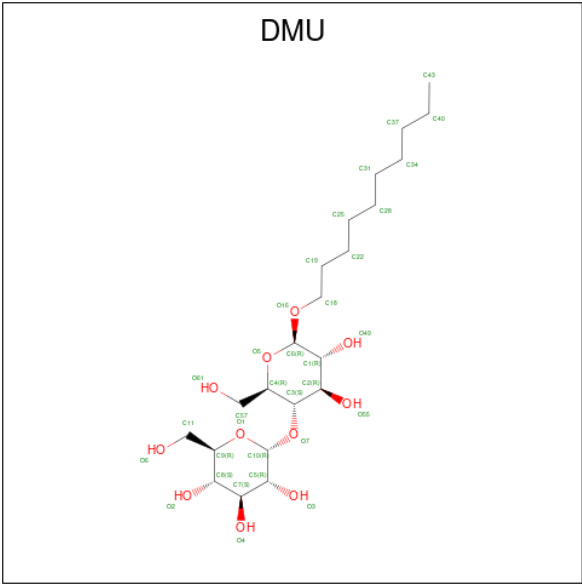
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	A	402	-	-	X	-
2	HEM	B	401	-	-	X	-

- Molecule 3 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: $C_{18}H_{38}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	11	6		

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	11	1		

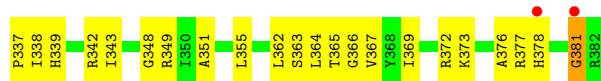
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			12	11	1		
4	B	1	Total	C	O	0	0
			12	11	1		
4	B	1	Total	C	O	0	0
			12	11	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	1	Total	Zn	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	237.06Å 114.32Å 64.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 3.35 46.36 – 3.35	Depositor EDS
% Data completeness (in resolution range)	59.3 (46.36-3.35) 59.3 (46.36-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.265 , 0.299 0.263 , 0.306	Depositor DCC
R_{free} test set	767 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6047	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: PE5, ZN, HEM, DMU

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	0.83	4/2959 (0.1%)	1.15	11/4029 (0.3%)
1	B	0.83	3/3009 (0.1%)	1.26	19/4096 (0.5%)
All	All	0.83	7/5968 (0.1%)	1.21	30/8125 (0.4%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	TYR	C-N	11.57	1.50	1.33
1	A	111	GLU	C-O	-6.99	1.16	1.23
1	A	74	TYR	C-O	-6.93	1.15	1.23
1	B	129	VAL	C-O	-6.47	1.19	1.24
1	A	75	MET	C-O	-5.99	1.16	1.23
1	B	130	PRO	C-O	-5.76	1.17	1.24
1	A	129	VAL	CA-CB	5.16	1.57	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	GLY	N-CA-C	-15.80	87.86	110.46
1	B	83	HIS	CB-CA-C	14.54	138.81	110.17
1	A	110	GLY	N-CA-C	-12.93	82.53	113.18
1	A	147	LEU	N-CA-C	-10.62	99.78	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	TYR	CA-C-N	10.40	131.53	119.47
1	B	336	TYR	C-N-CA	10.40	131.53	119.47
1	B	381	GLY	CA-C-N	8.50	137.00	121.70
1	B	381	GLY	C-N-CA	8.50	137.00	121.70
1	A	372	ARG	CD-NE-CZ	8.12	135.76	124.40
1	B	83	HIS	N-CA-C	-7.88	92.40	109.81
1	B	298	HIS	CA-CB-CG	7.30	121.10	113.80
1	A	372	ARG	NE-CZ-NH1	-7.13	114.37	121.50
1	A	296	GLY	CA-C-O	-7.10	117.33	122.23
1	B	335	GLN	O-C-N	6.88	129.52	122.09
1	B	83	HIS	CA-C-N	6.74	128.27	119.84
1	B	83	HIS	C-N-CA	6.74	128.27	119.84
1	B	91	PRO	CB-CA-C	-6.62	102.92	111.46
1	B	296	GLY	CA-C-O	-6.24	117.92	122.23
1	A	375	ARG	CG-CD-NE	6.23	125.71	112.00
1	A	138	ASN	N-CA-C	-6.12	98.42	108.76
1	B	131	TRP	CA-C-O	-5.96	114.54	120.80
1	A	110	GLY	CA-C-N	5.93	132.29	122.33
1	A	110	GLY	C-N-CA	5.93	132.29	122.33
1	B	89	THR	CB-CA-C	-5.86	99.59	109.72
1	B	100	HIS	CA-C-N	5.38	127.93	120.29
1	B	100	HIS	C-N-CA	5.38	127.93	120.29
1	A	138	ASN	CB-CA-C	-5.36	100.01	109.70
1	A	144	ASN	N-CA-C	-5.32	106.49	112.87
1	B	220	ASN	CA-C-N	-5.20	117.06	122.89
1	B	220	ASN	C-N-CA	-5.20	117.06	122.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	372	ARG	Sidechain

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	2863	0	2800	141	0
1	B	2911	0	2845	144	0
2	A	86	0	60	35	0
2	B	86	0	60	42	0
3	A	17	0	21	0	0
4	A	45	0	63	1	0
4	B	36	0	63	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	6047	0	5912	307	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 26.

All (307) 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:24:GLY:CA	2:A:402:HEM:HBB2	1.57	1.33
1:B:378:HIS:O	1:B:381:GLY:O	1.66	1.13
1:B:147:LEU:HD12	1:B:220:ASN:HD22	1.13	1.11
1:A:24:GLY:HA2	2:A:402:HEM:HBB2	1.13	1.10
1:A:150:MET:O	2:A:402:HEM:HBC1	1.53	1.09
1:A:24:GLY:HA3	2:A:402:HEM:HBB2	1.41	1.01
1:A:24:GLY:CA	2:A:402:HEM:CBB	2.45	0.94
1:B:147:LEU:HD12	1:B:220:ASN:ND2	1.82	0.93
2:B:401:HEM:HBC2	2:B:401:HEM:HHH	1.50	0.93
2:A:401:HEM:HBC2	2:A:401:HEM:HMC2	1.48	0.93
1:B:24:GLY:HA2	2:B:402:HEM:CBB	2.00	0.92
1:B:236:ILE:HD11	1:B:328:GLY:O	1.72	0.88
1:B:275:ILE:HG21	1:B:295:PHE:HD2	1.41	0.85
1:B:154:ALA:HB2	2:B:402:HEM:CBC	2.05	0.85
1:B:45:TYR:HD2	1:B:83:HIS:CE1	1.94	0.84
1:B:154:ALA:HB2	2:B:402:HEM:HBC1	1.59	0.83
2:A:401:HEM:HBC2	2:A:401:HEM:CMC	2.08	0.82
1:A:24:GLY:HA3	2:A:402:HEM:CBB	2.05	0.82
1:B:44:PHE:HD2	1:B:116:ARG:HH21	1.25	0.81
1:A:12:VAL:HG11	1:A:160:ASP:HB2	1.61	0.80
2:A:402:HEM:HBC2	2:A:402:HEM:CMC	2.12	0.80
2:A:402:HEM:HBC2	2:A:402:HEM:HMC1	1.63	0.80
1:A:16:THR:HG22	1:A:20:LEU:HB2	1.62	0.79
1:B:336:TYR:HB3	1:B:337:PRO:HD3	1.64	0.79
1:B:121:CYS:HB3	1:B:127:ASN:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLY:HA2	1:B:369:ILE:HG12	1.64	0.78
1:B:30:LEU:HD21	1:B:133:LEU:HA	1.65	0.78
1:A:24:GLY:HA2	2:A:402:HEM:CBB	2.07	0.77
1:A:150:MET:O	2:A:402:HEM:CBC	2.32	0.77
1:B:241:TYR:HE2	1:B:287:GLU:OE2	1.67	0.77
1:B:13:GLY:O	2:B:401:HEM:CBC	2.32	0.77
1:B:362:LEU:CD2	2:B:401:HEM:CBB	2.63	0.76
1:A:195:PHE:CZ	1:A:199:ARG:HD2	2.20	0.76
1:A:219:LEU:HD21	1:A:336:TYR:HD2	1.50	0.76
1:B:73:TRP:CD1	1:B:90:VAL:HG12	2.22	0.74
1:B:362:LEU:HD23	2:B:401:HEM:HBB2	1.68	0.74
1:A:2:ARG:HB3	1:A:3:PRO:HD3	1.68	0.74
1:B:86:LEU:C	1:B:86:LEU:HD23	2.13	0.73
1:A:20:LEU:HD11	1:A:157:TRP:CE3	2.24	0.72
1:B:362:LEU:HD21	2:B:401:HEM:CBB	2.20	0.71
1:B:40:LEU:HB3	1:B:125:PRO:HB3	1.72	0.71
1:B:135:PHE:CD1	1:B:139:LEU:HA	2.25	0.71
1:A:198:HIS:HD1	1:A:365:THR:HG23	1.56	0.71
1:B:362:LEU:CD2	2:B:401:HEM:HBB2	2.21	0.70
2:B:402:HEM:CBB	2:B:402:HEM:HMB2	2.18	0.70
1:B:45:TYR:CD2	1:B:83:HIS:HE1	2.10	0.70
1:A:150:MET:C	2:A:402:HEM:HBC1	2.16	0.70
1:B:362:LEU:HD23	2:B:401:HEM:CBB	2.22	0.70
1:B:45:TYR:HD2	1:B:83:HIS:HE1	1.40	0.69
1:B:89:THR:HG21	1:B:103:PHE:HE2	1.57	0.69
1:B:219:LEU:HD12	1:B:339:HIS:ND1	2.07	0.69
1:A:279:ILE:HG12	1:A:295:PHE:CE1	2.28	0.69
1:A:89:THR:HG21	1:A:103:PHE:CE2	2.27	0.69
2:A:401:HEM:HBD1	2:A:401:HEM:HHA	1.74	0.69
1:B:45:TYR:CD2	1:B:83:HIS:CE1	2.80	0.69
2:B:401:HEM:HBC2	2:B:401:HEM:CHD	2.14	0.69
1:B:373:LYS:HD3	1:B:377:ARG:NH1	2.07	0.68
1:B:86:LEU:HD23	1:B:86:LEU:O	1.93	0.68
2:A:401:HEM:HHA	2:A:401:HEM:HBA2	1.76	0.68
1:B:236:ILE:CD1	1:B:328:GLY:O	2.41	0.68
1:B:152:GLY:HA2	1:B:155:MET:HG2	1.74	0.68
1:B:20:LEU:HD21	1:B:157:TRP:CG	2.29	0.67
1:B:275:ILE:HG21	1:B:295:PHE:CD2	2.26	0.67
1:B:13:GLY:O	2:B:401:HEM:HBC2	1.94	0.67
1:B:91:PRO:HB3	1:B:96:ALA:HB3	1.77	0.67
1:B:135:PHE:HD1	1:B:139:LEU:HA	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HD23	1:B:92:ARG:NH1	2.09	0.66
1:A:359:ILE:HG21	2:A:402:HEM:HBB1	1.77	0.66
1:A:152:GLY:HA2	1:A:155:MET:HE3	1.78	0.66
1:A:1:MET:HE2	1:A:4:VAL:HG11	1.77	0.65
1:B:373:LYS:O	1:B:377:ARG:HG3	1.97	0.64
1:B:362:LEU:HD21	2:B:401:HEM:HBB1	1.77	0.64
1:A:89:THR:HG21	1:A:103:PHE:HE2	1.62	0.64
1:A:344:ALA:HB3	1:A:348:GLY:HA3	1.80	0.64
1:A:205:LEU:HD23	2:A:401:HEM:CBB	2.27	0.64
1:B:20:LEU:HD21	1:B:157:TRP:CD2	2.33	0.64
1:A:10:ARG:NH2	2:A:401:HEM:O1A	2.31	0.63
1:B:10:ARG:HG2	2:B:401:HEM:CGD	2.28	0.63
1:B:241:TYR:CE2	1:B:287:GLU:OE2	2.50	0.63
1:A:60:VAL:CG2	1:A:75:MET:HE1	2.29	0.63
1:A:239:SER:HB2	1:A:242:GLU:H	1.63	0.63
1:A:287:GLU:HG3	1:A:288:TYR:CD2	2.34	0.62
2:B:401:HEM:HHD	2:B:401:HEM:CBC	2.24	0.62
1:B:89:THR:OG1	1:B:101:ASP:O	2.17	0.62
1:B:55:SER:OG	1:B:260:ASP:OD1	2.17	0.61
1:A:106:ASP:OD1	1:A:107:PRO:HD2	1.99	0.61
1:A:198:HIS:ND1	1:A:365:THR:HG23	2.15	0.61
1:B:71:LEU:CD2	1:B:92:ARG:NH1	2.64	0.61
1:A:137:HIS:CB	2:A:402:HEM:HMD3	2.29	0.60
1:A:20:LEU:HD11	1:A:157:TRP:CD2	2.35	0.60
1:A:283:TYR:CZ	1:A:285:SER:OG	2.54	0.60
1:A:191:TYR:HB2	1:A:372:ARG:HE	1.66	0.60
1:A:137:HIS:HB3	2:A:402:HEM:HMD3	1.83	0.59
1:B:60:VAL:HG21	1:B:259:TYR:CG	2.37	0.59
1:A:289:ASN:OD1	1:A:311:GLY:HA3	2.02	0.59
1:B:197:LEU:HD23	1:B:365:THR:HG21	1.84	0.59
1:A:120:ALA:HB3	1:A:127:ASN:OD1	2.01	0.59
1:A:53:ARG:HB3	1:A:80:ALA:HB2	1.84	0.59
1:B:334:LEU:HD22	1:B:343:ILE:HD11	1.85	0.59
1:A:157:TRP:HH2	2:A:402:HEM:HAB	1.67	0.59
1:B:252:LEU:HD13	1:B:288:TYR:HA	1.83	0.58
2:B:401:HEM:HMD1	2:B:401:HEM:HBD1	1.85	0.58
1:A:245:GLY:HA2	1:A:288:TYR:CE1	2.38	0.58
1:A:284:TYR:HB2	1:A:291:PHE:CE1	2.39	0.58
1:A:41:ASN:ND2	1:A:126:ALA:HA	2.18	0.58
1:A:121:CYS:O	1:A:123:PHE:CD1	2.57	0.57
2:B:402:HEM:HBC2	2:B:402:HEM:CMC	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TRP:HE1	1:A:209:LEU:HD23	1.68	0.57
1:B:216:SER:HB3	2:B:402:HEM:CBC	2.34	0.57
1:A:234:SER:OG	1:A:235:PRO:HD2	2.05	0.57
1:B:133:LEU:HD21	2:B:402:HEM:O1D	2.03	0.57
1:A:75:MET:HA	1:A:86:LEU:O	2.05	0.57
1:B:129:VAL:HB	1:B:130:PRO:HD3	1.86	0.57
1:B:137:HIS:ND1	2:B:402:HEM:HMD2	2.20	0.57
1:A:165:ALA:O	1:A:169:LEU:HB2	2.05	0.57
1:B:1:MET:O	1:B:1:MET:HG2	2.04	0.56
1:B:6:VAL:HG22	1:B:167:LEU:HD11	1.86	0.56
1:A:146:GLY:HA2	1:A:149:LEU:HB3	1.87	0.56
1:B:144:ASN:HB3	1:B:148:TYR:CD1	2.39	0.56
1:A:206:TRP:HE1	2:A:401:HEM:HMB3	1.70	0.56
1:B:16:THR:HB	1:B:20:LEU:HD13	1.88	0.56
1:B:73:TRP:CD1	1:B:88:ALA:O	2.59	0.56
1:A:206:TRP:NE1	2:A:401:HEM:HMB3	2.21	0.56
1:A:305:SER:HB3	1:A:321:VAL:HA	1.88	0.56
2:A:402:HEM:CMC	2:A:402:HEM:CBC	2.84	0.56
1:A:324:GLN:HA	1:A:330:ARG:HH21	1.71	0.55
1:A:66:ARG:HB2	1:A:66:ARG:NH2	2.21	0.55
1:A:134:GLU:HG3	1:A:137:HIS:HE1	1.71	0.55
1:A:157:TRP:CH2	2:A:402:HEM:HAB	2.41	0.55
1:B:100:HIS:HB3	1:B:115:LYS:HB2	1.88	0.55
1:B:236:ILE:CG1	1:B:328:GLY:O	2.54	0.55
1:B:313:ASP:HB3	1:B:315:ARG:HG2	1.88	0.55
1:B:244:ARG:HD2	1:B:247:LEU:HD12	1.88	0.55
1:B:363:SER:O	1:B:367:VAL:HG23	2.07	0.55
2:B:402:HEM:CBC	2:B:402:HEM:CMC	2.84	0.55
1:B:313:ASP:OD2	1:B:315:ARG:HD3	2.06	0.55
1:B:245:GLY:HA2	1:B:288:TYR:CE2	2.42	0.55
1:B:24:GLY:HA2	2:B:402:HEM:HBB1	1.84	0.55
1:A:219:LEU:HD21	1:A:336:TYR:CD2	2.38	0.54
1:B:210:ALA:HB3	1:B:211:PRO:HD3	1.90	0.54
1:A:189:ASN:HB2	1:A:192:ARG:H	1.72	0.54
1:A:67:TYR:OH	1:A:115:LYS:HD3	2.08	0.54
1:A:134:GLU:HG3	1:A:137:HIS:CE1	2.42	0.54
1:A:37:ASP:OD2	1:A:116:ARG:NH2	2.41	0.54
1:B:21:PHE:CE1	1:B:364:LEU:HD11	2.43	0.54
1:B:339:HIS:NE2	2:B:402:HEM:C1B	2.68	0.54
1:A:189:ASN:HB2	1:A:192:ARG:CB	2.37	0.54
1:A:304:LYS:O	1:A:322:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:O	1:A:41:ASN:N	2.42	0.53
1:A:142:PRO:HD2	1:A:145:TRP:HE3	1.73	0.53
1:A:362:LEU:HD21	2:A:401:HEM:HBB2	1.90	0.53
1:A:334:LEU:C	1:A:337:PRO:HD2	2.34	0.53
1:B:245:GLY:HA2	1:B:288:TYR:CZ	2.44	0.53
1:A:240:VAL:HG21	1:A:308:PHE:CG	2.44	0.52
1:B:13:GLY:CA	2:B:401:HEM:HBC2	2.38	0.52
1:B:13:GLY:O	2:B:401:HEM:HBC1	2.10	0.52
1:B:24:GLY:HA2	2:B:402:HEM:HBB2	1.87	0.52
2:A:402:HEM:HMC1	2:A:402:HEM:CBC	2.34	0.52
1:B:161:CYS:HA	1:B:206:TRP:CE3	2.45	0.52
1:A:239:SER:OG	1:A:242:GLU:OE1	2.26	0.52
1:B:216:SER:HB3	2:B:402:HEM:HBC2	1.91	0.52
1:A:143:GLY:C	1:A:145:TRP:N	2.67	0.52
1:B:89:THR:OG1	1:B:89:THR:O	2.28	0.51
2:B:402:HEM:HMB2	2:B:402:HEM:HBB2	1.91	0.51
1:A:44:PHE:O	1:A:84:PRO:HD2	2.09	0.51
1:B:133:LEU:O	1:B:137:HIS:HB2	2.10	0.51
1:B:70:GLN:C	1:B:92:ARG:HG3	2.35	0.51
1:A:203:LEU:O	1:A:207:LEU:HD13	2.11	0.51
1:B:373:LYS:HD3	1:B:377:ARG:HH11	1.73	0.51
1:A:71:LEU:O	1:A:89:THR:HA	2.12	0.50
1:B:72:VAL:HG22	1:B:89:THR:HG22	1.93	0.50
1:A:150:MET:HE3	2:A:402:HEM:CBC	2.41	0.50
1:A:157:TRP:CZ2	1:A:359:ILE:HD13	2.47	0.50
1:B:291:PHE:O	1:B:308:PHE:HA	2.12	0.50
1:A:367:VAL:O	1:A:370:TRP:HB3	2.11	0.50
1:A:10:ARG:NE	2:A:401:HEM:O1A	2.44	0.50
1:A:230:VAL:HG22	4:A:404:DMU:H10	1.94	0.50
1:A:111:GLU:HA	1:A:111:GLU:OE1	2.12	0.50
1:A:67:TYR:OH	1:A:112:GLU:OE1	2.21	0.49
1:A:208:LEU:O	1:A:211:PRO:HD2	2.12	0.49
1:A:275:ILE:HD12	1:A:307:LEU:HD11	1.94	0.49
1:B:334:LEU:O	1:B:338:ILE:HG13	2.13	0.49
1:B:76:GLU:HG2	1:B:86:LEU:HB3	1.95	0.49
1:B:121:CYS:SG	1:B:124:GLN:HB2	2.53	0.49
1:B:106:ASP:HB3	1:B:109:SER:OG	2.12	0.49
1:B:2:ARG:NH1	1:B:167:LEU:O	2.46	0.49
1:B:208:LEU:O	1:B:211:PRO:HD2	2.13	0.49
1:A:245:GLY:HA2	1:A:288:TYR:CZ	2.48	0.49
1:A:364:LEU:O	1:A:367:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLY:HA3	1:B:108:VAL:HG21	1.95	0.48
1:B:372:ARG:NH2	1:B:376:ALA:HB2	2.27	0.48
1:B:10:ARG:CG	2:B:401:HEM:CGD	2.91	0.48
1:A:128:LEU:O	1:A:132:VAL:HG23	2.14	0.48
1:B:131:TRP:O	1:B:134:GLU:N	2.45	0.48
1:A:75:MET:HB2	1:A:87:LEU:HG	1.96	0.48
1:B:302:MET:HE1	1:B:334:LEU:HD21	1.96	0.48
1:A:143:GLY:C	1:A:145:TRP:H	2.22	0.48
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.74	0.47
1:A:20:LEU:HD21	1:A:157:TRP:CE2	2.49	0.47
2:B:401:HEM:HMD1	2:B:401:HEM:CBD	2.44	0.47
1:B:334:LEU:HD22	1:B:343:ILE:CD1	2.45	0.47
1:A:33:HIS:NE2	2:A:402:HEM:O2A	2.48	0.47
1:A:141:LEU:HB3	1:A:142:PRO:CD	2.44	0.47
1:A:240:VAL:HG21	1:A:308:PHE:CD2	2.50	0.47
1:B:8:LEU:CD2	1:B:163:VAL:HG21	2.45	0.47
2:B:402:HEM:HBD2	2:B:402:HEM:HHA	1.97	0.47
1:B:169:LEU:HA	1:B:203:LEU:HD22	1.97	0.47
1:A:113:VAL:HG22	1:A:113:VAL:O	2.15	0.47
1:B:25:LEU:HA	1:B:25:LEU:HD12	1.71	0.47
1:B:82:GLY:C	1:B:83:HIS:O	2.54	0.47
1:B:270:ALA:HB2	1:B:295:PHE:CZ	2.50	0.47
2:B:401:HEM:CBD	2:B:401:HEM:CMD	2.93	0.47
1:B:71:LEU:O	1:B:90:VAL:N	2.40	0.47
1:B:302:MET:HG3	1:B:302:MET:O	2.14	0.47
1:B:342:ARG:HG3	1:B:349:ARG:HD2	1.97	0.47
1:B:206:TRP:CZ2	2:B:401:HEM:C3B	3.03	0.46
1:B:7:LEU:HD13	1:B:7:LEU:HA	1.80	0.46
1:A:151:GLY:O	1:A:154:ALA:HB3	2.15	0.46
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.61	0.46
1:A:120:ALA:O	1:A:127:ASN:HB3	2.15	0.46
2:A:401:HEM:HMC2	2:A:401:HEM:CBC	2.34	0.46
1:B:71:LEU:HD23	1:B:92:ARG:CZ	2.45	0.46
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.77	0.46
1:B:139:LEU:O	1:B:140:THR:OG1	2.27	0.46
1:A:106:ASP:HB3	1:A:109:SER:O	2.16	0.46
1:A:231:SER:HA	1:A:234:SER:O	2.16	0.46
1:A:263:PHE:CE1	1:A:279:ILE:HD12	2.50	0.46
1:A:10:ARG:CZ	2:A:401:HEM:O1A	2.64	0.45
1:A:12:VAL:CG1	1:A:160:ASP:HB2	2.40	0.45
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:PRO:HG3	1:B:98:VAL:CG1	2.46	0.45
1:B:206:TRP:CZ2	2:B:401:HEM:C4B	3.04	0.45
1:A:284:TYR:CE2	1:A:286:PHE:HD1	2.35	0.45
1:B:118:TRP:CD1	1:B:118:TRP:O	2.70	0.45
1:B:364:LEU:O	1:B:365:THR:C	2.59	0.45
1:A:109:SER:O	1:A:109:SER:OG	2.35	0.45
1:B:99:GLU:O	1:B:117:LEU:HD13	2.17	0.45
1:A:313:ASP:OD2	1:A:315:ARG:NH2	2.48	0.44
1:B:118:TRP:O	1:B:118:TRP:CG	2.70	0.44
1:B:226:PHE:CE1	1:B:230:VAL:HG21	2.52	0.44
1:B:302:MET:CE	1:B:334:LEU:HD21	2.47	0.44
1:B:348:GLY:O	1:B:351:ALA:HB3	2.17	0.44
1:A:210:ALA:HB3	1:A:211:PRO:HD3	2.00	0.44
1:B:169:LEU:HG	1:B:170:PRO:HD2	2.00	0.44
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.80	0.44
1:A:205:LEU:HD21	1:A:362:LEU:HD21	1.98	0.44
1:A:33:HIS:CD2	2:A:402:HEM:O2A	2.71	0.43
1:A:103:PHE:HE1	1:A:115:LYS:HD2	1.83	0.43
1:B:91:PRO:HG3	1:B:98:VAL:HG11	2.00	0.43
1:B:137:HIS:CD2	1:B:138:ASN:OD1	2.71	0.43
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.77	0.43
1:B:70:GLN:CA	1:B:92:ARG:HG3	2.48	0.43
1:B:121:CYS:CB	1:B:127:ASN:HD22	2.31	0.43
1:B:137:HIS:CE1	2:B:402:HEM:HMD2	2.53	0.43
1:A:244:ARG:HD2	1:A:247:LEU:HD12	2.00	0.43
1:A:324:GLN:CA	1:A:330:ARG:HH21	2.31	0.43
1:B:118:TRP:CD2	1:B:130:PRO:HB3	2.53	0.43
1:A:109:SER:O	1:A:111:GLU:N	2.52	0.43
1:B:281:GLU:HB3	1:B:306:TRP:CH2	2.53	0.43
1:A:222:PRO:HG2	1:A:223:SER:H	1.84	0.43
2:B:401:HEM:HBB2	2:B:401:HEM:CHC	2.48	0.43
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.82	0.43
1:A:189:ASN:HB2	1:A:192:ARG:HB2	2.00	0.42
1:A:195:PHE:CE2	1:A:199:ARG:HD2	2.54	0.42
1:B:28:SER:O	1:B:31:ALA:HB3	2.19	0.42
1:B:13:GLY:C	2:B:401:HEM:HBC2	2.43	0.42
1:A:3:PRO:HB3	1:B:276:ALA:HB3	2.01	0.42
1:A:155:MET:HE2	1:A:221:LEU:CD1	2.50	0.42
1:B:362:LEU:CD2	2:B:401:HEM:HBB1	2.42	0.42
1:B:18:LEU:H	1:B:18:LEU:HD23	1.84	0.42
1:B:56:PRO:O	1:B:60:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:CB	1:A:167:LEU:HD12	2.49	0.42
1:B:234:SER:OG	1:B:235:PRO:HD2	2.19	0.42
2:B:401:HEM:HHB	2:B:401:HEM:HBA1	2.01	0.42
1:A:129:VAL:HB	1:A:130:PRO:HD3	2.00	0.42
1:A:361:GLY:O	1:A:365:THR:HG22	2.20	0.42
1:B:240:VAL:O	1:B:244:ARG:HB2	2.20	0.42
1:A:141:LEU:HB3	1:A:142:PRO:HD2	2.02	0.42
1:A:220:ASN:OD1	2:A:402:HEM:HAC	2.20	0.42
1:A:342:ARG:HE	1:A:349:ARG:HD2	1.85	0.42
1:A:346:LEU:N	1:A:347:PRO:CD	2.83	0.42
1:A:75:MET:HB3	1:A:75:MET:HE2	1.60	0.42
1:A:279:ILE:HG12	1:A:295:PHE:CD1	2.55	0.42
1:A:372:ARG:HA	1:A:375:ARG:HD3	2.02	0.42
2:B:401:HEM:CBB	2:B:401:HEM:HHC	2.50	0.42
1:A:158:PHE:CE2	1:A:214:LEU:HD13	2.55	0.41
1:A:270:ALA:HB2	1:A:295:PHE:CE2	2.55	0.41
1:B:208:LEU:HD13	1:B:355:LEU:HD21	2.01	0.41
1:A:41:ASN:ND2	1:A:125:PRO:O	2.53	0.41
2:B:401:HEM:CBB	2:B:401:HEM:CHC	2.98	0.41
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.77	0.41
1:A:310:HIS:CD2	1:A:315:ARG:NH2	2.89	0.41
1:B:19:PHE:HB3	1:B:153:VAL:HG11	2.03	0.41
1:B:373:LYS:HG2	1:B:377:ARG:HE	1.86	0.41
1:A:3:PRO:HB3	1:B:276:ALA:CB	2.51	0.41
1:A:283:TYR:OH	1:A:285:SER:OG	2.33	0.41
1:B:50:GLY:C	1:B:108:VAL:HG21	2.46	0.41
1:B:129:VAL:N	1:B:130:PRO:CD	2.83	0.41
1:A:144:ASN:HB3	1:A:148:TYR:CE2	2.56	0.41
1:A:295:PHE:O	1:A:304:LYS:HA	2.21	0.41
1:B:86:LEU:C	1:B:86:LEU:CD2	2.85	0.40
1:B:282:LEU:HD23	1:B:293:ALA:HA	2.01	0.40
1:A:2:ARG:CB	1:A:3:PRO:HD3	2.46	0.40
1:A:362:LEU:CD2	2:A:401:HEM:HBB2	2.52	0.40
1:A:32:PHE:O	1:A:36:ILE:HG13	2.21	0.40
1:B:203:LEU:O	1:B:207:LEU:HG	2.21	0.40
1:A:161:CYS:HA	1:A:206:TRP:CZ3	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	356/382 (93%)	332 (93%)	24 (7%)	0	100	100
1	B	361/382 (94%)	346 (96%)	15 (4%)	0	100	100
All	All	717/764 (94%)	678 (95%)	39 (5%)	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	285/303 (94%)	283 (99%)	2 (1%)	76	77
1	B	289/303 (95%)	285 (99%)	4 (1%)	59	69
All	All	574/606 (95%)	568 (99%)	6 (1%)	68	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	140	THR
1	B	87	LEU
1	B	90	VAL
1	B	98	VAL
1	B	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	41	ASN
1	A	83	HIS
1	A	137	HIS
1	B	34	HIS
1	B	83	HIS
1	B	127	ASN
1	B	194	ASN
1	B	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
4	DMU	B	403	-	11,11,34	0.63	0	10,10,45	0.70	0
3	PE5	A	403	-	16,16,26	0.51	0	15,15,25	0.38	0
2	HEM	B	401	1	50,50,50	3.20	30 (60%)	67,82,82	2.83	26 (38%)
2	HEM	A	401	1	50,50,50	2.77	22 (44%)	67,82,82	2.34	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMU	B	404	-	11,11,34	0.56	0	10,10,45	0.79	0
2	HEM	B	402	1	50,50,50	3.08	30 (60%)	67,82,82	2.42	28 (41%)
4	DMU	A	405	-	34,34,34	1.14	2 (5%)	45,45,45	1.92	16 (35%)
4	DMU	A	404	-	11,11,34	0.48	0	10,10,45	0.71	0
2	HEM	A	402	1	50,50,50	3.44	27 (54%)	67,82,82	2.48	20 (29%)
4	DMU	B	405	-	11,11,34	0.73	0	10,10,45	0.42	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
4	DMU	B	403	-	-	6/9/9/59	-
3	PE5	A	403	-	-	7/14/14/24	-
2	HEM	B	401	1	-	5/14/54/54	-
2	HEM	A	401	1	-	6/14/54/54	-
4	DMU	B	404	-	-	7/9/9/59	-
2	HEM	B	402	1	-	6/14/54/54	-
4	DMU	A	405	-	-	6/19/59/59	0/2/2/2
4	DMU	A	404	-	-	5/9/9/59	-
2	HEM	A	402	1	-	6/14/54/54	-
4	DMU	B	405	-	-	5/9/9/59	-

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	HEM	FE-NB	9.67	2.24	1.94
2	B	401	HEM	C4D-ND	-7.88	1.26	1.40
2	A	402	HEM	C4D-ND	-7.62	1.27	1.40
2	B	401	HEM	FE-NB	6.98	2.16	1.94
2	A	402	HEM	C1D-ND	-6.88	1.25	1.38
2	A	402	HEM	C1B-NB	-6.56	1.28	1.40
2	A	402	HEM	C1C-C2C	-6.20	1.33	1.45
2	A	401	HEM	FE-NB	6.19	2.13	1.94
2	A	402	HEM	C4B-NB	-5.94	1.27	1.38
2	A	402	HEM	C4C-NC	-5.92	1.28	1.39
2	B	401	HEM	C1D-ND	-5.78	1.27	1.38
2	B	402	HEM	C1B-NB	-5.76	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	FE-NC	5.74	2.14	1.95
2	A	401	HEM	C4D-ND	-5.71	1.30	1.40
2	B	401	HEM	C1B-NB	-5.64	1.30	1.40
2	A	401	HEM	C1B-NB	-5.54	1.30	1.40
2	A	402	HEM	FE-NC	5.44	2.13	1.95
2	B	402	HEM	C4A-NA	-5.33	1.29	1.39
2	B	401	HEM	C4C-NC	-5.30	1.29	1.39
2	B	402	HEM	C1C-C2C	-5.25	1.34	1.45
2	B	402	HEM	C1A-C2A	-5.25	1.34	1.44
2	A	401	HEM	C4C-NC	-5.24	1.29	1.39
2	B	401	HEM	C4B-NB	-5.17	1.28	1.38
2	A	401	HEM	C1D-ND	-5.11	1.28	1.38
2	A	401	HEM	FE-ND	-4.99	1.79	1.94
2	B	402	HEM	C4D-ND	-4.93	1.31	1.40
2	B	402	HEM	C4B-NB	-4.91	1.29	1.38
2	B	402	HEM	C1D-ND	-4.72	1.29	1.38
2	B	402	HEM	C1A-NA	-4.61	1.30	1.39
2	B	402	HEM	C4A-C3A	-4.59	1.32	1.43
2	B	402	HEM	FE-ND	-4.57	1.80	1.94
2	B	402	HEM	C3B-C2B	-4.50	1.28	1.37
2	B	401	HEM	C1A-NA	-4.43	1.31	1.39
2	A	401	HEM	C3C-C4C	-4.41	1.38	1.46
2	B	401	HEM	C1C-NC	-4.40	1.31	1.39
2	A	402	HEM	C1C-NC	-4.38	1.31	1.39
2	A	401	HEM	C1C-C2C	-4.37	1.36	1.45
2	B	402	HEM	C3C-C4C	-4.36	1.38	1.46
2	A	402	HEM	C4A-NA	-4.06	1.32	1.39
2	B	401	HEM	C1C-C2C	-4.01	1.37	1.45
2	A	402	HEM	C1A-NA	-3.98	1.32	1.39
2	A	401	HEM	O2D-CGD	-3.97	1.17	1.30
2	B	402	HEM	C4C-NC	-3.94	1.32	1.39
2	A	402	HEM	C3C-C4C	-3.94	1.39	1.46
2	B	402	HEM	C2A-C3A	-3.92	1.28	1.38
2	A	401	HEM	C4B-NB	-3.87	1.31	1.38
2	A	401	HEM	C3D-C2D	-3.86	1.28	1.36
2	A	402	HEM	O2A-CGA	-3.75	1.18	1.30
2	A	401	HEM	C4A-NA	-3.73	1.32	1.39
2	B	401	HEM	C3B-C2B	-3.70	1.29	1.37
2	B	402	HEM	O2A-CGA	-3.70	1.18	1.30
2	B	401	HEM	C3C-C4C	-3.65	1.39	1.46
2	B	402	HEM	C1C-NC	-3.64	1.32	1.39
2	B	402	HEM	CAB-C3B	-3.58	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEM	O2D-CGD	-3.56	1.19	1.30
2	B	401	HEM	C4D-C3D	-3.51	1.39	1.45
2	B	401	HEM	C1B-C2B	-3.44	1.37	1.44
2	A	402	HEM	O2D-CGD	-3.43	1.19	1.30
2	B	402	HEM	CMA-C3A	-3.38	1.43	1.50
2	A	401	HEM	C1C-NC	-3.37	1.33	1.39
2	A	402	HEM	C1A-C2A	-3.31	1.38	1.44
2	B	401	HEM	O2D-CGD	-3.22	1.20	1.30
2	B	402	HEM	CHA-C1A	-3.20	1.32	1.39
2	A	401	HEM	CHD-C4C	-3.19	1.32	1.38
2	B	401	HEM	O2A-CGA	-3.15	1.20	1.30
2	B	401	HEM	C1A-C2A	-3.14	1.38	1.44
2	B	401	HEM	C4A-NA	-3.06	1.33	1.39
2	A	402	HEM	C3B-C2B	-3.02	1.31	1.37
2	B	401	HEM	CAB-C3B	-3.01	1.39	1.47
2	A	401	HEM	O2A-CGA	-3.00	1.20	1.30
2	A	402	HEM	C3D-C2D	-2.98	1.30	1.36
2	B	402	HEM	CAC-C3C	-2.98	1.39	1.47
2	B	401	HEM	CHA-C1A	-2.96	1.32	1.39
2	A	402	HEM	CAC-C3C	-2.96	1.39	1.47
2	A	402	HEM	C2A-C3A	-2.95	1.31	1.38
2	A	402	HEM	C1B-C2B	-2.91	1.38	1.44
2	A	401	HEM	C4A-C3A	-2.90	1.36	1.43
2	A	402	HEM	FE-NA	2.89	2.04	1.95
2	B	401	HEM	C4A-C3A	-2.86	1.36	1.43
2	B	401	HEM	C3D-C2D	-2.82	1.30	1.36
2	A	401	HEM	C1A-NA	-2.79	1.34	1.39
2	A	402	HEM	C4A-C3A	-2.75	1.36	1.43
2	B	401	HEM	C2A-C3A	-2.74	1.31	1.38
2	A	401	HEM	FE-NC	2.67	2.04	1.95
2	B	401	HEM	FE-ND	-2.64	1.86	1.94
2	B	401	HEM	FE-NA	2.61	2.03	1.95
2	B	402	HEM	CHB-C4A	-2.53	1.33	1.39
2	A	402	HEM	CMD-C2D	-2.51	1.45	1.50
2	B	402	HEM	C1B-C2B	-2.37	1.39	1.44
2	B	401	HEM	CBA-CGA	-2.33	1.45	1.50
2	B	402	HEM	C3B-C4B	-2.30	1.40	1.44
4	A	405	DMU	O4-C7	2.28	1.48	1.43
2	B	402	HEM	FE-NB	2.28	2.01	1.94
2	A	401	HEM	C2A-C3A	-2.27	1.33	1.38
2	A	402	HEM	C4D-C3D	-2.25	1.41	1.45
2	B	402	HEM	C3D-C2D	-2.25	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C1B-C2B	-2.25	1.40	1.44
2	A	401	HEM	CHD-C1D	-2.23	1.34	1.39
4	A	405	DMU	O1-C10	2.22	1.47	1.41
2	B	402	HEM	C3C-C2C	-2.15	1.32	1.37
2	B	401	HEM	CMD-C2D	-2.12	1.46	1.50
2	A	402	HEM	CMA-C3A	-2.11	1.46	1.50
2	B	401	HEM	CHB-C4A	-2.09	1.34	1.39
2	B	401	HEM	CAA-C2A	-2.09	1.46	1.51
2	B	402	HEM	CHC-C1C	-2.08	1.34	1.38
2	A	402	HEM	CAB-C3B	-2.08	1.41	1.47
2	B	401	HEM	CAD-C3D	-2.07	1.46	1.51
2	B	402	HEM	CMD-C2D	-2.05	1.46	1.50
2	A	401	HEM	CHB-C4A	-2.04	1.34	1.39
2	A	402	HEM	CAD-C3D	-2.03	1.46	1.51
2	B	402	HEM	CHD-C1D	-2.01	1.34	1.39

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	C3B-C4B-NB	-9.85	102.39	109.47
2	B	402	HEM	CHC-C4B-NB	8.07	133.11	124.42
2	A	402	HEM	C4D-ND-C1D	7.78	114.42	105.21
2	B	401	HEM	CHA-C4D-ND	7.78	134.00	124.37
2	B	401	HEM	C1B-NB-C4B	6.79	113.25	105.21
2	A	401	HEM	CAD-C3D-C4D	6.53	136.07	124.70
2	A	402	HEM	CHD-C1D-ND	6.00	130.88	124.42
2	A	402	HEM	CHC-C1C-NC	5.78	130.75	124.45
2	B	401	HEM	CHC-C4B-NB	5.74	130.60	124.42
2	B	402	HEM	CHA-C4D-ND	5.56	131.25	124.37
2	A	401	HEM	CHD-C1D-ND	5.46	130.30	124.42
2	A	402	HEM	CHC-C4B-NB	5.36	130.19	124.42
2	A	401	HEM	CAD-C3D-C2D	-5.35	117.85	127.87
2	A	402	HEM	CHA-C4D-ND	5.27	130.89	124.37
2	B	401	HEM	C4D-ND-C1D	5.24	111.42	105.21
2	A	402	HEM	C4C-NC-C1C	5.07	114.08	105.82
2	A	401	HEM	CAA-C2A-C1A	5.04	134.77	124.94
2	A	401	HEM	CHD-C1D-C2D	-4.94	117.23	125.03
2	B	401	HEM	CHB-C1B-NB	4.84	130.35	124.37
2	A	402	HEM	C1B-NB-C4B	4.83	110.93	105.21
2	B	401	HEM	CAA-CBA-CGA	-4.83	100.86	113.67
2	A	402	HEM	C2D-C1D-ND	-4.69	104.48	109.90
2	B	401	HEM	CHA-C4D-C3D	-4.68	116.60	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	HEM	CHD-C4C-NC	4.48	129.34	124.45
2	B	402	HEM	O2D-CGD-O1D	-4.40	112.02	123.33
2	B	401	HEM	C4C-NC-C1C	4.25	112.75	105.82
4	A	405	DMU	C7-C8-C9	4.01	117.50	110.23
2	B	401	HEM	CBB-CAB-C3B	-3.93	107.91	127.53
2	B	402	HEM	CBB-CAB-C3B	-3.90	108.06	127.53
2	B	402	HEM	C4C-C3C-C2C	3.86	110.16	106.81
2	A	401	HEM	C3B-C4B-NB	-3.85	106.70	109.47
2	B	402	HEM	CMB-C2B-C1B	3.84	131.04	125.03
4	A	405	DMU	O5-C6-O16	3.79	119.01	110.04
2	B	402	HEM	CBC-CAC-C3C	-3.78	108.63	127.53
4	A	405	DMU	O16-C6-C1	3.72	113.92	108.27
2	B	402	HEM	CHA-C4D-C3D	-3.70	118.40	125.23
2	A	401	HEM	O2D-CGD-O1D	-3.67	113.90	123.33
4	A	405	DMU	C2-C3-C4	3.65	119.02	110.93
2	A	402	HEM	C4C-C3C-C2C	3.63	109.96	106.81
2	A	402	HEM	C3B-C4B-NB	-3.60	106.88	109.47
2	A	402	HEM	CHD-C4C-C3C	3.59	131.25	125.21
2	A	401	HEM	CHC-C4B-NB	3.58	128.28	124.42
4	A	405	DMU	O3-C5-C10	3.58	118.60	110.08
2	A	401	HEM	CHD-C4C-NC	3.55	128.31	124.45
2	B	402	HEM	C1C-CHC-C4B	-3.54	118.50	126.02
2	A	402	HEM	O2D-CGD-O1D	-3.51	114.31	123.33
2	B	401	HEM	CAD-C3D-C4D	-3.50	118.59	124.70
2	B	402	HEM	C1A-CHA-C4D	-3.50	118.02	126.25
2	A	401	HEM	C1B-NB-C4B	3.48	109.32	105.21
2	B	401	HEM	CAD-C3D-C2D	3.46	134.34	127.87
4	A	405	DMU	C10-C5-C7	3.40	117.16	110.01
2	B	401	HEM	CBA-CAA-C2A	-3.38	103.19	112.53
2	B	401	HEM	C4B-C3B-C2B	3.29	110.31	107.28
2	B	402	HEM	C1B-NB-C4B	3.26	109.07	105.21
2	B	401	HEM	CHD-C1D-ND	3.26	127.93	124.42
2	B	402	HEM	C3B-C4B-NB	-3.18	107.19	109.47
2	B	401	HEM	C2D-C1D-ND	-3.06	106.37	109.90
2	B	402	HEM	CHB-C1B-NB	3.03	128.11	124.37
4	A	405	DMU	C18-O16-C6	2.98	118.78	113.68
2	B	402	HEM	CHA-C1A-NA	2.94	129.19	123.86
2	B	402	HEM	O2D-CGD-CBD	2.92	123.24	114.00
2	A	401	HEM	CHB-C4A-NA	2.92	129.15	123.86
2	B	402	HEM	C4A-CHB-C1B	-2.91	119.41	126.25
2	A	401	HEM	CAA-C2A-C3A	-2.91	120.55	127.07
2	B	402	HEM	C4C-CHD-C1D	-2.89	119.88	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	HEM	C4A-C3A-C2A	2.88	110.11	106.82
2	A	401	HEM	O2A-CGA-O1A	-2.87	115.96	123.33
2	B	402	HEM	CHD-C1D-ND	2.85	127.49	124.42
2	A	401	HEM	CHA-C4D-ND	2.82	127.86	124.37
4	A	405	DMU	C10-O7-C3	-2.82	111.29	117.98
2	B	401	HEM	CMD-C2D-C1D	2.82	129.44	125.03
2	A	402	HEM	O2A-CGA-O1A	-2.81	116.11	123.33
2	A	401	HEM	CBA-CAA-C2A	2.80	120.27	112.53
2	A	402	HEM	C3D-C4D-ND	-2.73	107.18	110.17
2	B	402	HEM	CHC-C4B-C3B	-2.72	119.64	125.07
2	A	401	HEM	CBD-CAD-C3D	2.68	119.94	112.53
2	B	401	HEM	CMB-C2B-C1B	2.67	129.21	125.03
2	A	402	HEM	O2D-CGD-CBD	2.60	122.22	114.00
2	B	402	HEM	CMA-C3A-C4A	-2.56	121.52	125.42
2	A	401	HEM	C1A-CHA-C4D	-2.54	120.28	126.25
4	A	405	DMU	O5-C4-C3	2.51	114.91	109.72
2	A	401	HEM	CBC-CAC-C3C	-2.48	115.14	127.53
2	A	401	HEM	CAD-CBD-CGD	-2.48	107.09	113.67
2	B	401	HEM	CHD-C4C-C3C	2.48	129.39	125.21
2	B	401	HEM	CBC-CAC-C3C	-2.44	115.31	127.53
2	B	401	HEM	O2D-CGD-O1D	-2.44	117.06	123.33
4	A	405	DMU	C1-C2-C3	2.37	115.06	109.68
2	B	402	HEM	CHA-C1A-C2A	-2.37	120.12	125.30
4	A	405	DMU	O49-C1-C2	-2.34	104.86	110.38
2	A	401	HEM	CMD-C2D-C1D	2.34	128.68	125.03
2	A	402	HEM	CMB-C2B-C1B	2.23	128.52	125.03
2	A	401	HEM	C4A-C3A-C2A	2.22	109.36	106.82
2	A	401	HEM	CHB-C4A-C3A	-2.22	120.99	127.43
2	B	402	HEM	C3C-C2C-C1C	-2.22	104.95	107.05
2	B	401	HEM	CAD-CBD-CGD	-2.22	107.78	113.67
2	A	401	HEM	CHB-C1B-NB	2.21	127.10	124.37
2	B	402	HEM	CMB-C2B-C3B	-2.21	123.08	128.43
2	B	402	HEM	CHB-C4A-NA	2.21	127.87	123.86
2	B	401	HEM	C4C-C3C-C2C	2.19	108.71	106.81
2	A	402	HEM	C2A-C1A-NA	-2.19	107.73	110.15
2	A	402	HEM	C4A-NA-C1A	2.18	109.38	105.82
4	A	405	DMU	O49-C1-C6	2.16	115.22	110.08
2	A	401	HEM	C2D-C1D-ND	2.14	112.38	109.90
2	B	401	HEM	CHB-C4A-NA	2.14	127.73	123.86
4	A	405	DMU	C6-C1-C2	2.12	114.46	110.01
2	B	401	HEM	C1A-CHA-C4D	-2.11	121.28	126.25
2	B	401	HEM	CHB-C1B-C2B	-2.09	121.01	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	HEM	CHC-C1C-NC	2.09	126.73	124.45
4	A	405	DMU	C57-C4-C3	-2.07	107.55	113.38
2	B	402	HEM	C4D-ND-C1D	2.07	107.66	105.21
2	A	402	HEM	C3A-C4A-NA	-2.06	106.83	110.14
2	A	401	HEM	O2A-CGA-CBA	2.05	120.48	114.00
4	A	405	DMU	O7-C10-C5	2.05	113.13	108.09
2	A	401	HEM	CMB-C2B-C1B	2.04	128.22	125.03
4	A	405	DMU	O2-C8-C7	-2.04	105.57	110.38
2	A	402	HEM	CAC-C3C-C2C	-2.00	121.92	128.43

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2D-C3D-CAD-CBD
2	A	401	HEM	C4D-C3D-CAD-CBD
2	A	402	HEM	C2B-C3B-CAB-CBB
2	A	402	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	C4D-C3D-CAD-CBD
2	A	401	HEM	C1A-C2A-CAA-CBA
2	A	401	HEM	C2A-CAA-CBA-CGA
3	A	403	PE5	O7-C13-C14-O8
4	A	405	DMU	C1-C6-O16-C18
4	B	403	DMU	O16-C18-C19-C22
4	B	404	DMU	O16-C18-C19-C22
2	A	401	HEM	C3A-C2A-CAA-CBA
4	B	404	DMU	C18-C19-C22-C25
4	A	405	DMU	O5-C6-O16-C18
4	B	403	DMU	C25-C28-C31-C34
4	B	404	DMU	C19-C22-C25-C28
4	B	405	DMU	C25-C28-C31-C34
4	A	404	DMU	C19-C18-O16-C6
4	B	404	DMU	C19-C18-O16-C6
4	B	405	DMU	C19-C18-O16-C6
4	B	403	DMU	C31-C34-C37-C40
4	A	404	DMU	C19-C22-C25-C28
4	B	405	DMU	C22-C25-C28-C31
4	B	403	DMU	C28-C31-C34-C37
4	A	404	DMU	C34-C37-C40-C43
4	A	405	DMU	C19-C18-O16-C6
4	A	405	DMU	C18-C19-C22-C25

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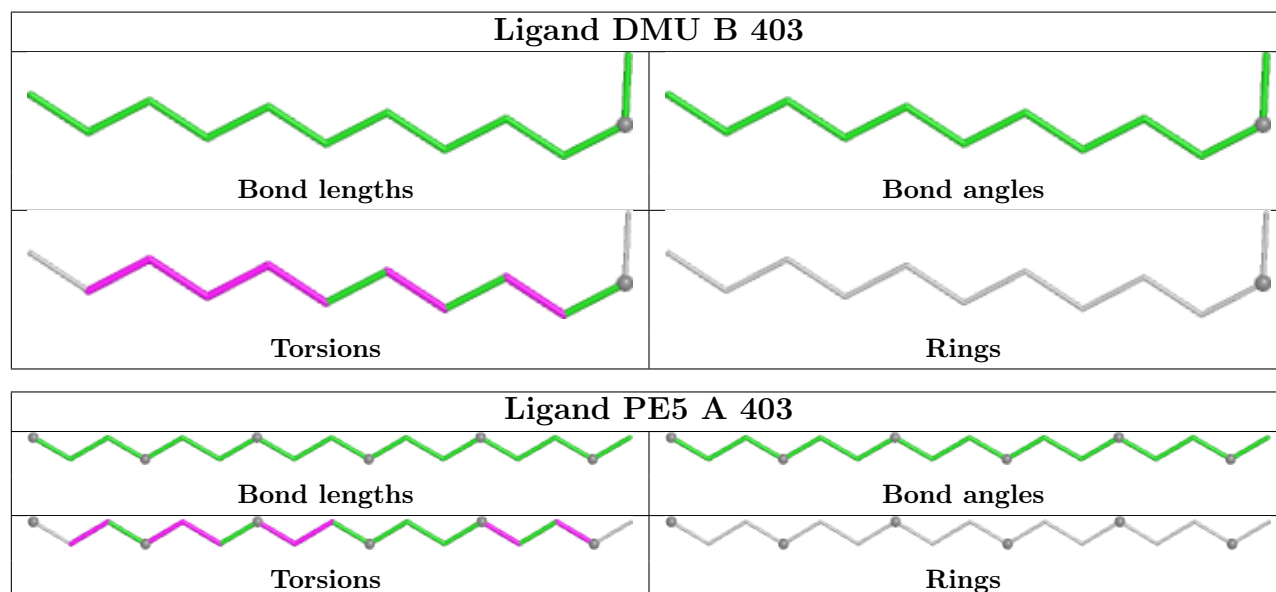
Mol	Chain	Res	Type	Atoms
4	A	404	DMU	C25-C28-C31-C34
4	A	405	DMU	C22-C25-C28-C31
4	B	404	DMU	C25-C28-C31-C34
3	A	403	PE5	C8-C7-O4-C6
3	A	403	PE5	C7-C8-O5-C9
2	B	402	HEM	C2B-C3B-CAB-CBB
4	A	404	DMU	C31-C34-C37-C40
4	B	403	DMU	C19-C22-C25-C28
4	B	405	DMU	C34-C37-C40-C43
4	B	404	DMU	C28-C31-C34-C37
2	B	401	HEM	C2B-C3B-CAB-CBB
2	B	402	HEM	C4B-C3B-CAB-CBB
2	A	401	HEM	C3D-CAD-CBD-CGD
4	B	404	DMU	C31-C34-C37-C40
2	B	402	HEM	CAA-CBA-CGA-O1A
2	A	402	HEM	C3D-CAD-CBD-CGD
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	A	402	HEM	CAD-CBD-CGD-O1D
2	B	402	HEM	CAD-CBD-CGD-O1D
2	B	402	HEM	CAD-CBD-CGD-O2D
3	A	403	PE5	C11-C12-O7-C13
2	B	402	HEM	CAA-CBA-CGA-O2A
2	A	402	HEM	CAD-CBD-CGD-O2D
3	A	403	PE5	C13-C14-O8-C15
4	B	403	DMU	C34-C37-C40-C43
3	A	403	PE5	O6-C11-C12-O7
3	A	403	PE5	O8-C15-C16-O52
4	B	405	DMU	C19-C22-C25-C28
2	A	402	HEM	CAA-CBA-CGA-O2A
4	A	405	DMU	C34-C37-C40-C43

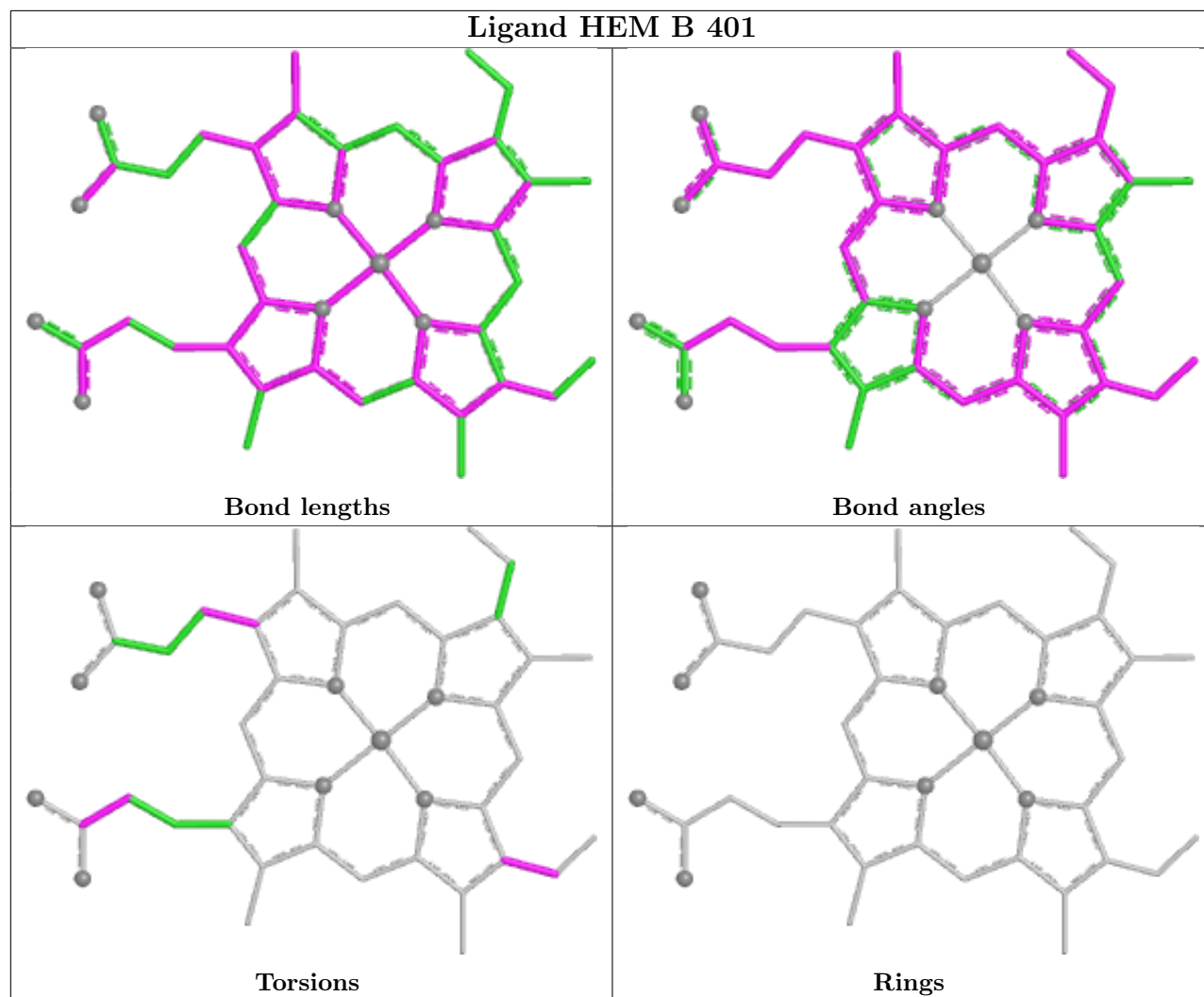
There are no ring outliers.

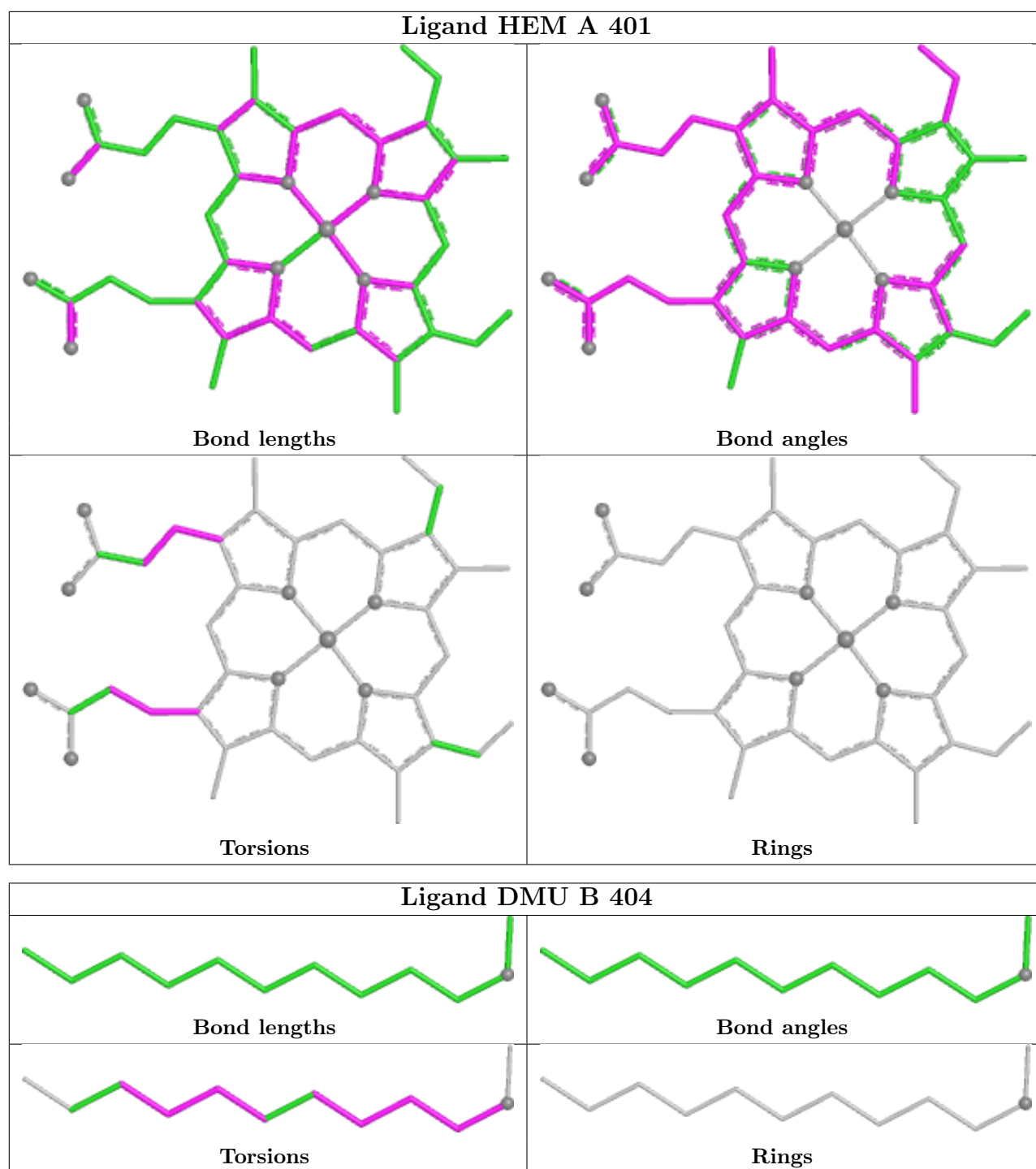
5 monomers are involved in 78 short contacts:

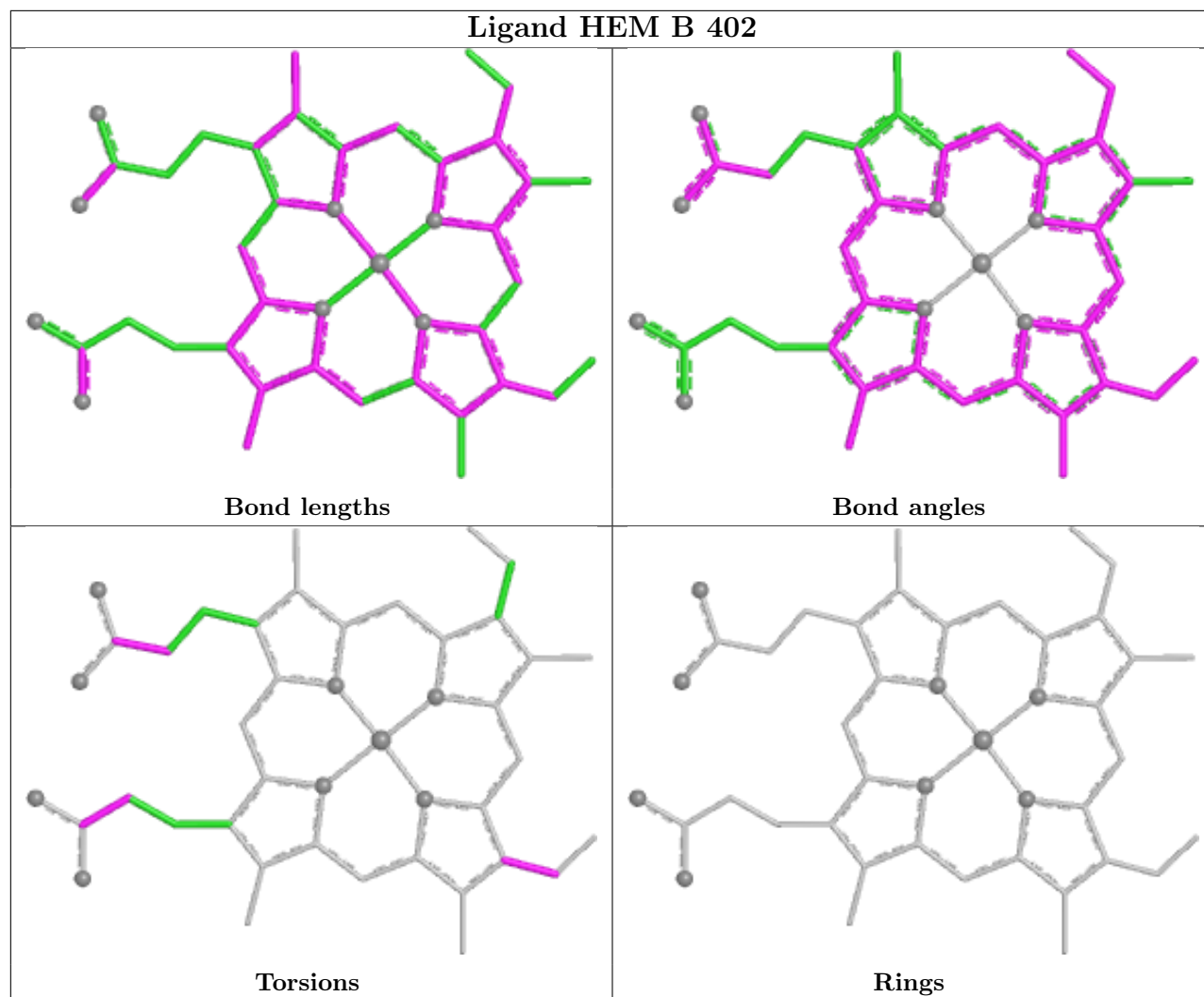
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	26	0
2	A	401	HEM	13	0
2	B	402	HEM	16	0
4	A	404	DMU	1	0
2	A	402	HEM	22	0

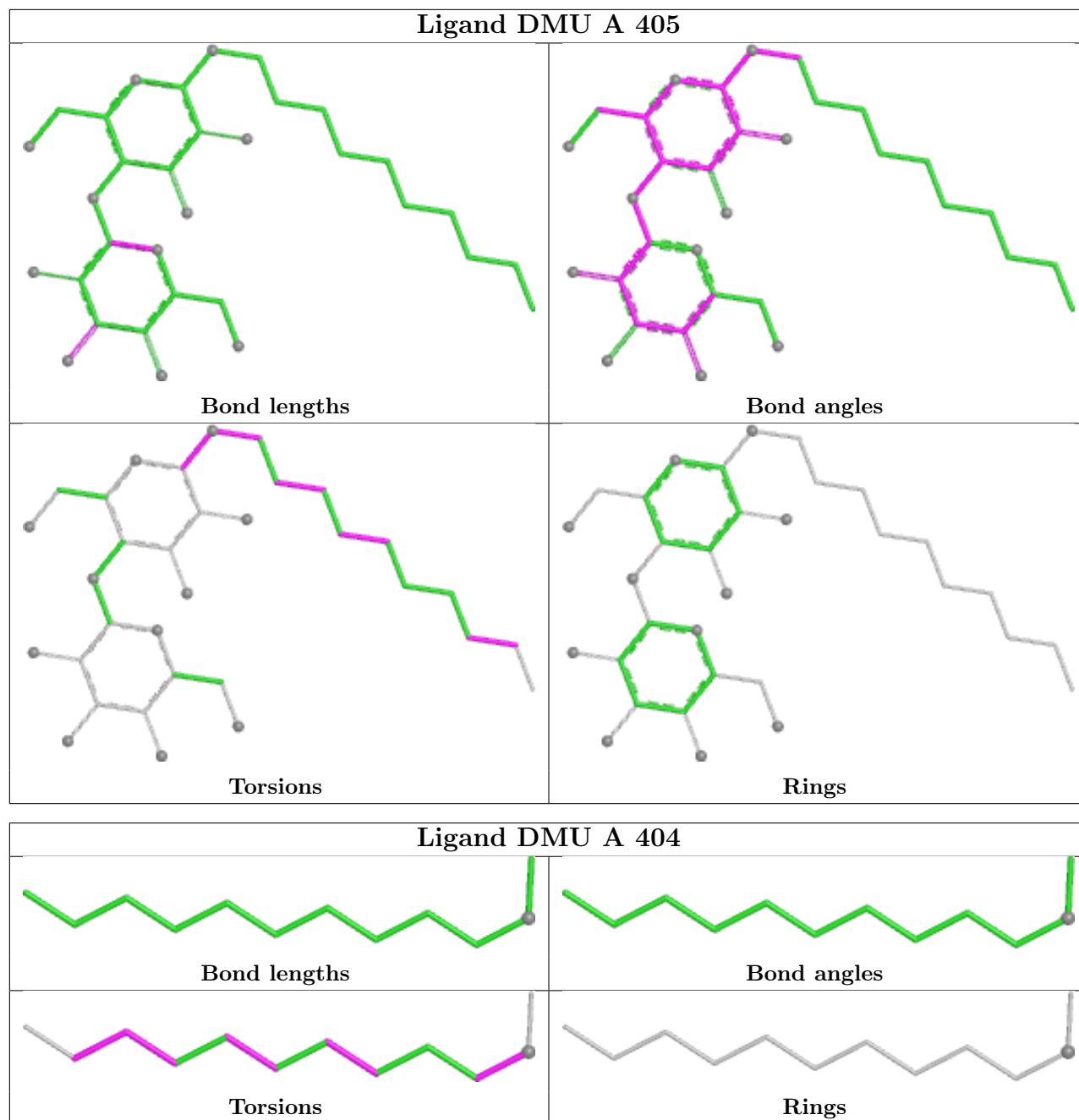
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

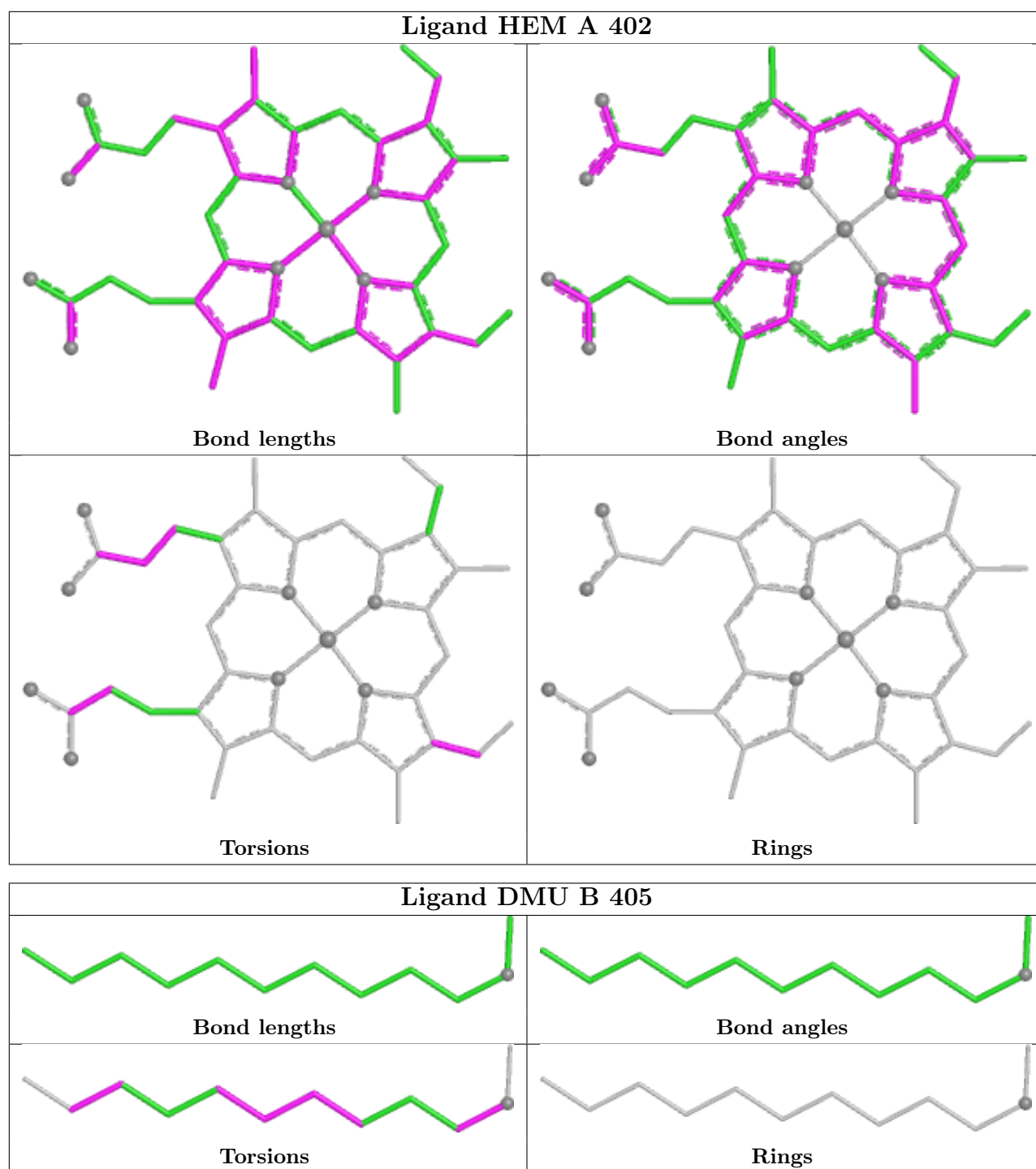












5.7 Other polymers [i](#)

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	360/382 (94%)	0.43	28 (7%) 19 15	6, 21, 64, 98	0
1	B	365/382 (95%)	1.01	51 (13%) 6 7	16, 54, 90, 103	0
All	All	725/764 (94%)	0.72	79 (10%) 10 10	6, 34, 86, 103	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	381	GLY	7.1
1	B	90	VAL	4.7
1	A	2	ARG	4.7
1	A	110	GLY	4.6
1	A	286	PHE	4.5
1	B	303	GLY	4.2
1	B	73	TRP	4.0
1	B	247	LEU	4.0
1	B	196	ASP	3.9
1	B	285	SER	3.9
1	A	124	GLN	3.9
1	B	71	LEU	3.8
1	B	70	GLN	3.7
1	B	92	ARG	3.6
1	B	299	ASP	3.5
1	B	317	LEU	3.5
1	B	286	PHE	3.5
1	A	101	ASP	3.5
1	B	297	ASP	3.4
1	B	117	LEU	3.4
1	A	1	MET	3.4
1	A	120	ALA	3.3
1	B	74	TYR	3.3
1	B	88	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	101	ASP	3.3
1	B	91	PRO	3.2
1	B	7	LEU	3.2
1	B	265	LEU	3.2
1	B	316	LEU	3.2
1	A	3	PRO	3.1
1	B	287	GLU	3.1
1	B	270	ALA	3.0
1	A	8	LEU	3.0
1	A	378	HIS	3.0
1	B	4	VAL	3.0
1	B	283	TYR	2.9
1	B	327	TRP	2.8
1	A	94	ALA	2.8
1	A	168	THR	2.7
1	A	5	LEU	2.7
1	B	118	TRP	2.7
1	A	376	ALA	2.7
1	A	298	HIS	2.6
1	A	90	VAL	2.5
1	B	99	GLU	2.5
1	A	170	PRO	2.5
1	B	323	GLY	2.5
1	B	11	TYR	2.5
1	A	166	TRP	2.5
1	A	239	SER	2.4
1	B	258	ASP	2.4
1	B	302	MET	2.4
1	B	98	VAL	2.4
1	B	48	GLY	2.3
1	A	256	ARG	2.3
1	B	192	ARG	2.3
1	B	378	HIS	2.3
1	B	123	PHE	2.3
1	B	217	VAL	2.3
1	B	111	GLU	2.3
1	A	6	VAL	2.3
1	B	95	GLY	2.3
1	B	152	GLY	2.3
1	A	34	HIS	2.2
1	A	252	LEU	2.2
1	A	39	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	166	TRP	2.2
1	A	4	VAL	2.2
1	B	47	VAL	2.1
1	A	138	ASN	2.1
1	B	55	SER	2.1
1	B	115	LYS	2.1
1	B	6	VAL	2.1
1	A	70	GLN	2.1
1	B	61	GLN	2.1
1	A	73	TRP	2.0
1	B	204	TRP	2.0
1	B	120	ALA	2.0
1	B	233	PHE	2.0

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.

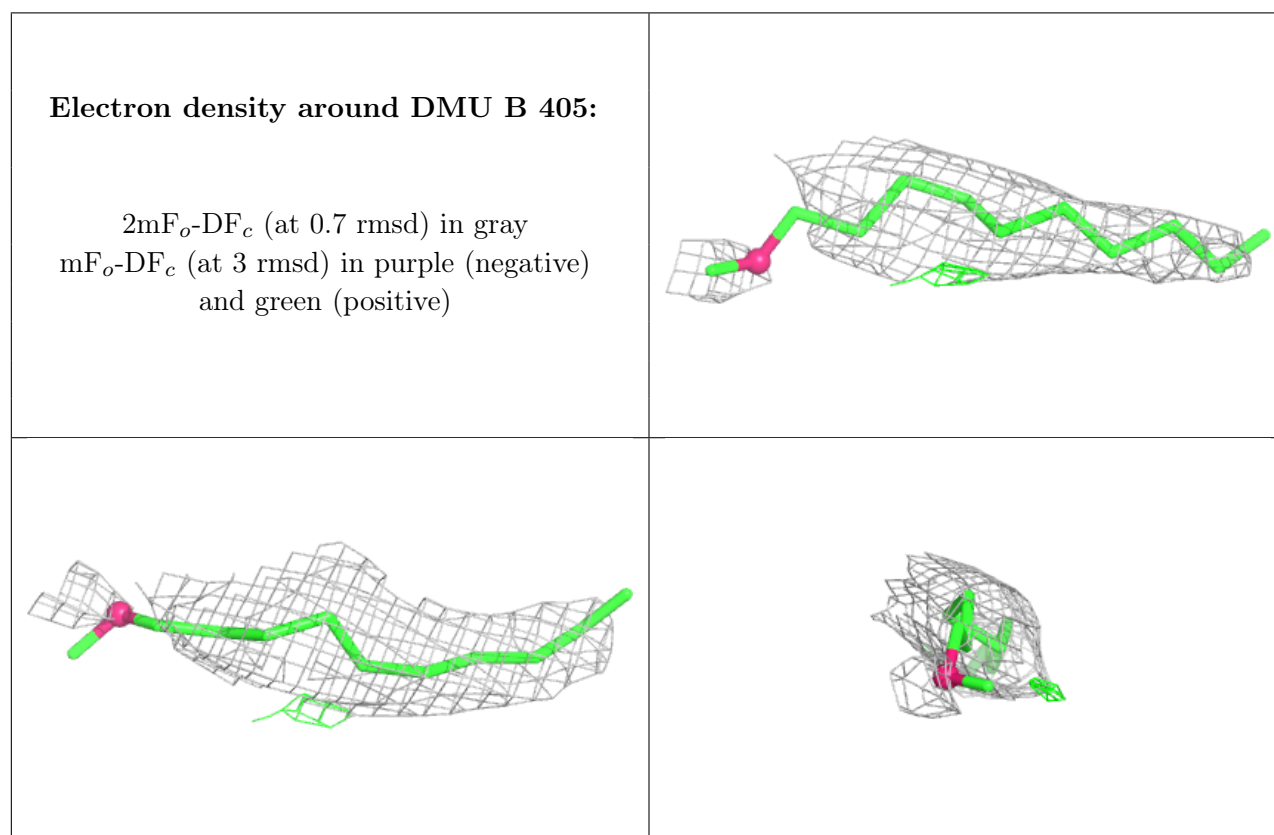
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMU	B	405	12/33	0.71	0.25	27,33,49,49	0
3	PE5	A	403	17/27	0.78	0.21	25,38,46,50	0
4	DMU	A	405	33/33	0.81	0.19	30,54,64,65	0
4	DMU	B	404	12/33	0.86	0.20	12,18,32,32	0
4	DMU	B	403	12/33	0.89	0.19	22,29,34,34	0
2	HEM	A	401	43/43	0.92	0.15	20,32,38,49	0
4	DMU	A	404	12/33	0.92	0.15	12,13,15,17	0
5	ZN	A	406	1/1	0.93	0.11	47,47,47,47	0
5	ZN	A	407	1/1	0.93	0.06	67,67,67,67	0
2	HEM	A	402	43/43	0.95	0.15	8,16,20,23	0

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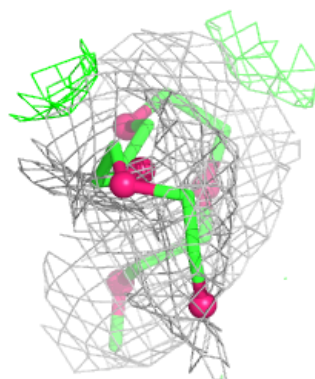
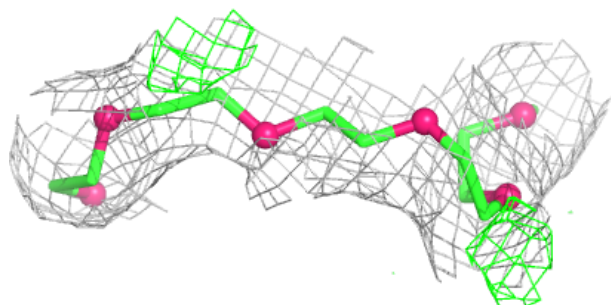
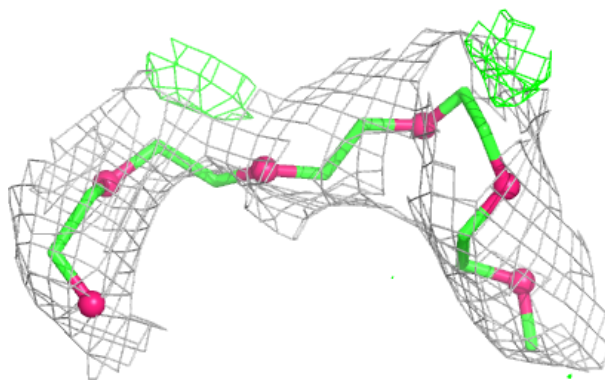
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	401	43/43	0.95	0.12	15,25,33,40	0
2	HEM	B	402	43/43	0.96	0.11	14,23,32,40	0
5	ZN	B	406	1/1	0.97	0.12	61,61,61,61	0

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.

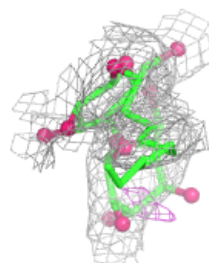
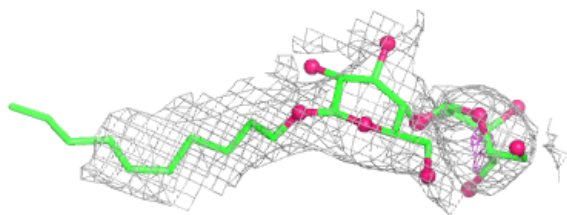
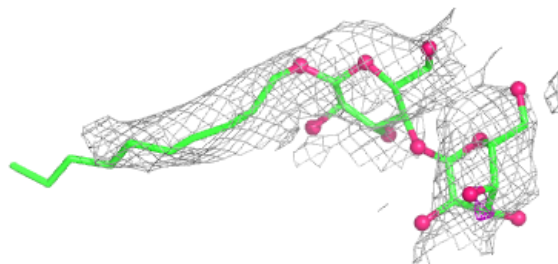


Electron density around PE5 A 403:

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

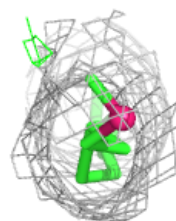
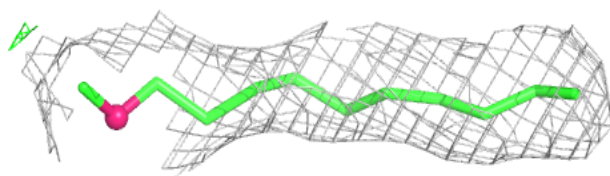
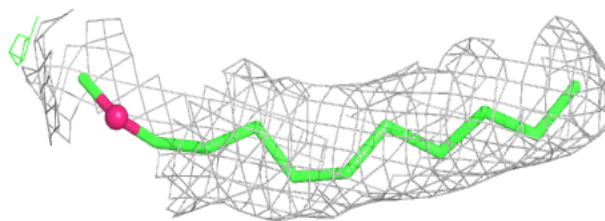
**Electron density around DMU A 405:**

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

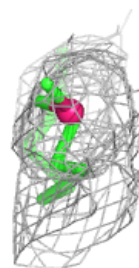
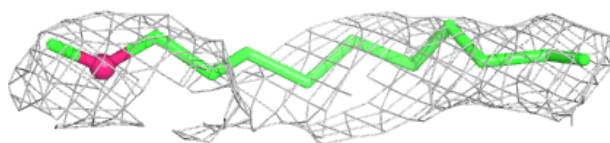
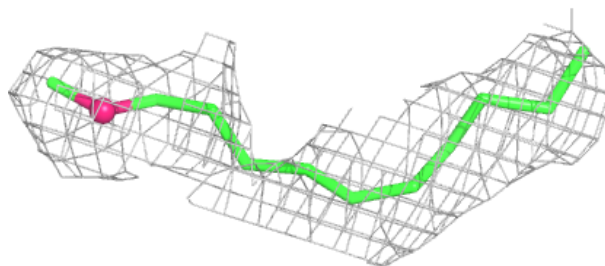


Electron density around DMU B 404:

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

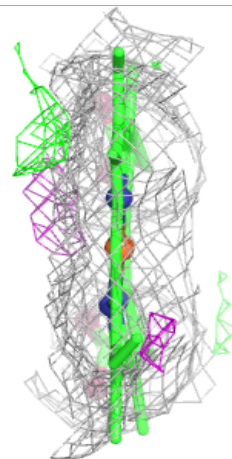
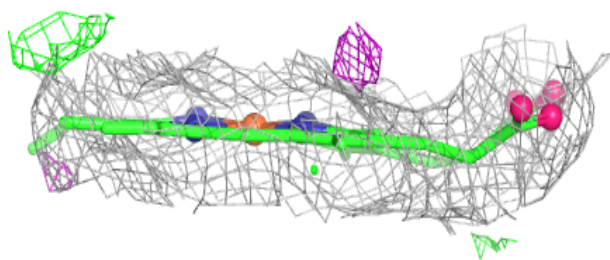
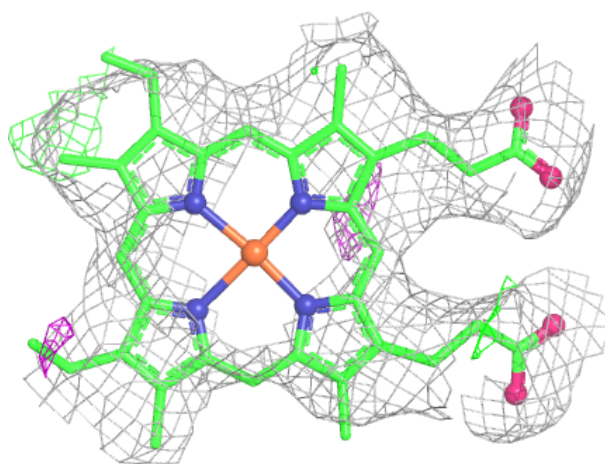
**Electron density around DMU B 403:**

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



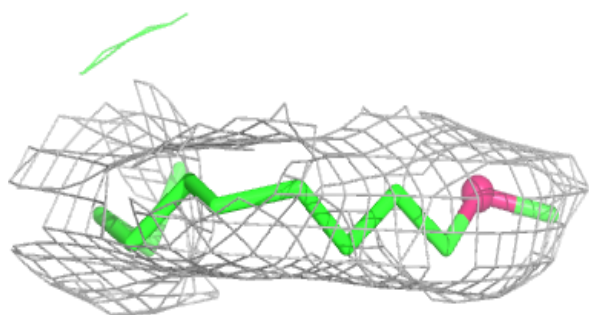
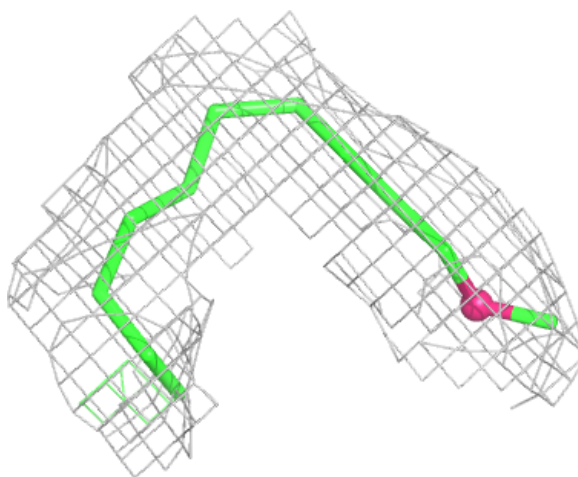
Electron density around HEM A 401:

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



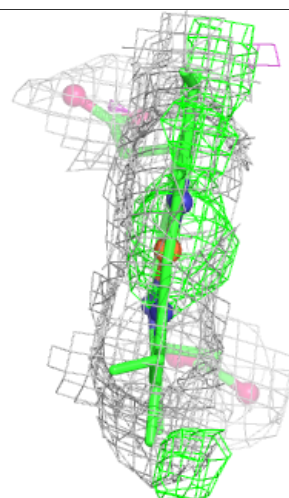
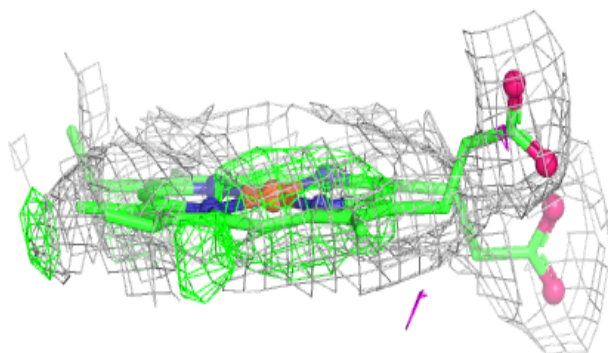
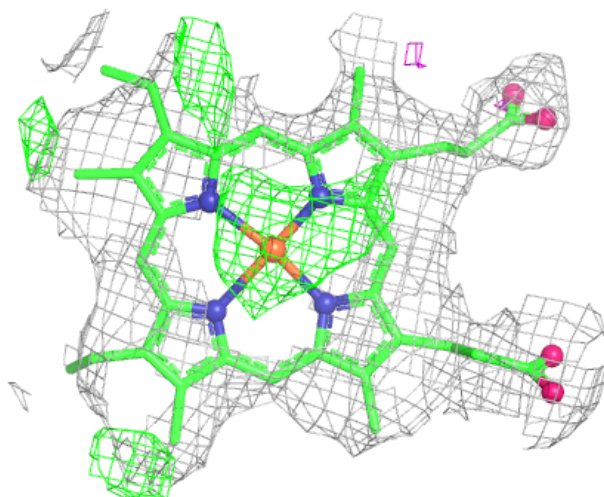
Electron density around DMU A 404:

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



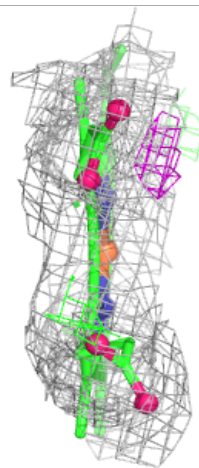
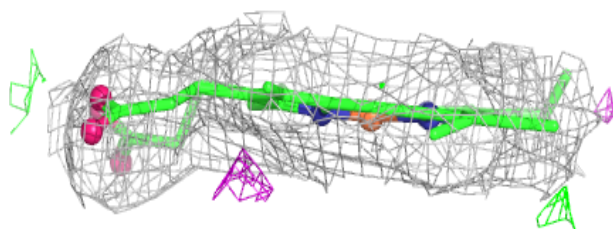
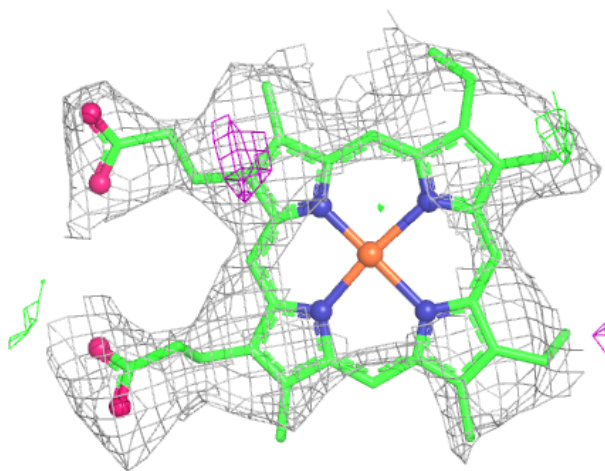
Electron density around HEM A 402:

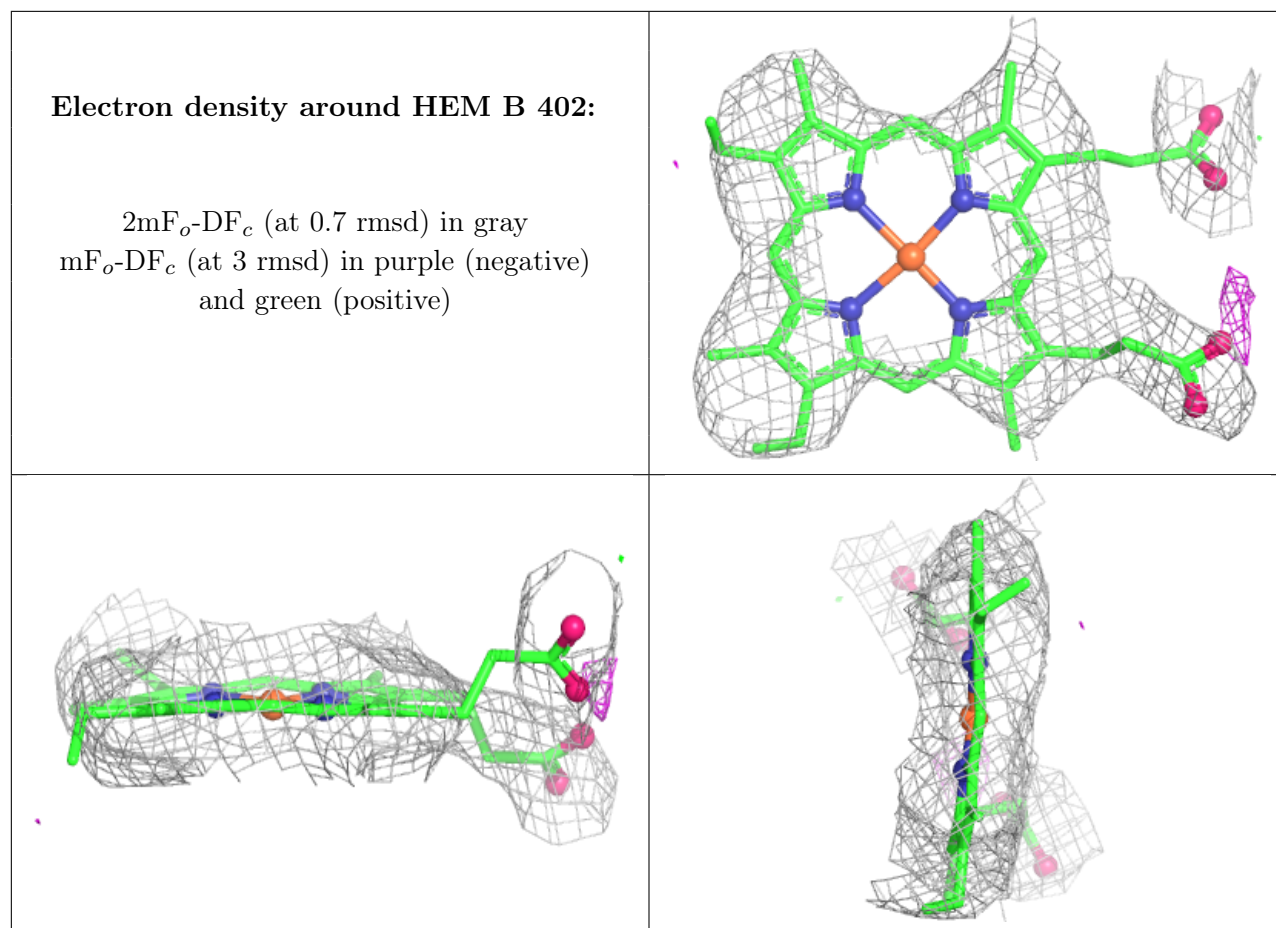
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 401:

$2mF_o-DF_c$ (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.