



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:35 AM UTC

PDB ID : 6RR5 / pdb_00006rr5
Title : Structure of 50% reduced KpDyP
Authors : Pfanzagl, V.; Beale, J.; Hofbauer, S.
Deposited on : 2019-05-17
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

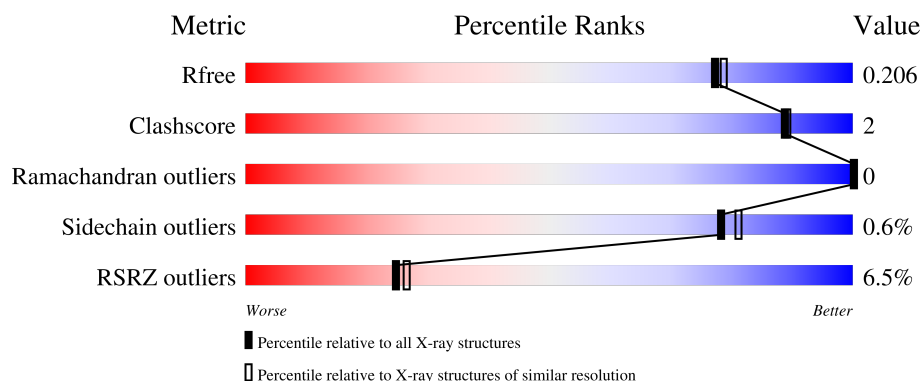
1 Overall quality at a glance

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	303	6% 89% 10% .
1	B	303	7% 91% 7% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10547 atoms, of which 4882 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.

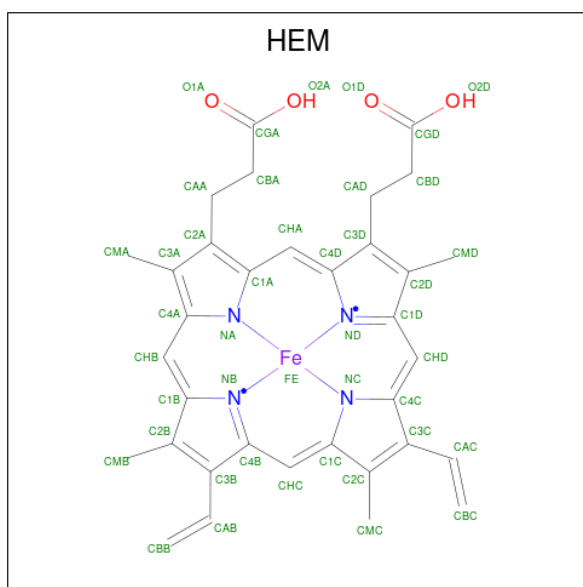
- Molecule 1 is a protein called Iron-dependent peroxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	H	N	O	S	0	12	0
			4826	1529	2388	436	463	10			
1	B	298	Total	C	H	N	O	S	0	5	0
			4657	1483	2302	416	448	8			

There are 8 discrepancies between the modelled and reference sequences:

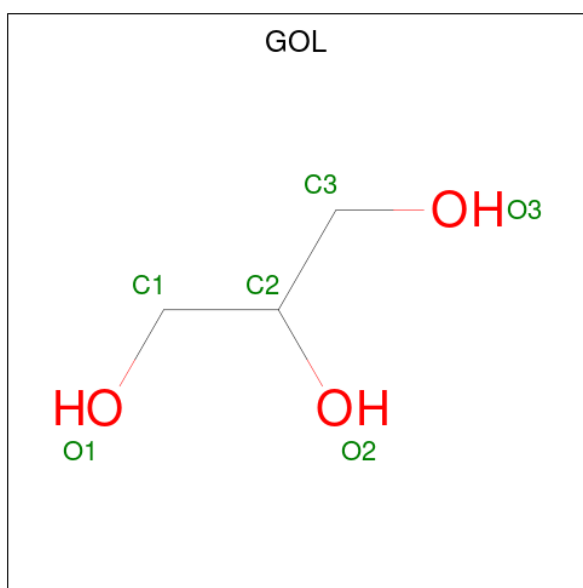
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP A0A0W8ATM9
A	-1	LEU	-	expression tag	UNP A0A0W8ATM9
A	0	GLY	-	expression tag	UNP A0A0W8ATM9
A	300	GLY	-	expression tag	UNP A0A0W8ATM9
B	-2	PRO	-	expression tag	UNP A0A0W8ATM9
B	-1	LEU	-	expression tag	UNP A0A0W8ATM9
B	0	GLY	-	expression tag	UNP A0A0W8ATM9
B	300	GLY	-	expression tag	UNP A0A0W8ATM9

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 146	C 68	Fe 2	H 60	N 8	O 8	0	1
2	B	1	Total 146	C 68	Fe 2	H 60	N 8	O 8	0	1

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	1
			42	9	24	9		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

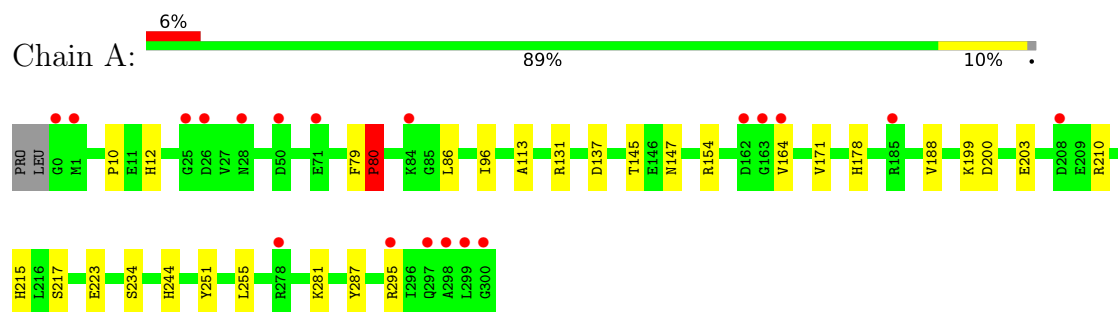
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	337	Total	O	0	0
			337	337		
5	B	307	Total	O	0	0
			307	307		

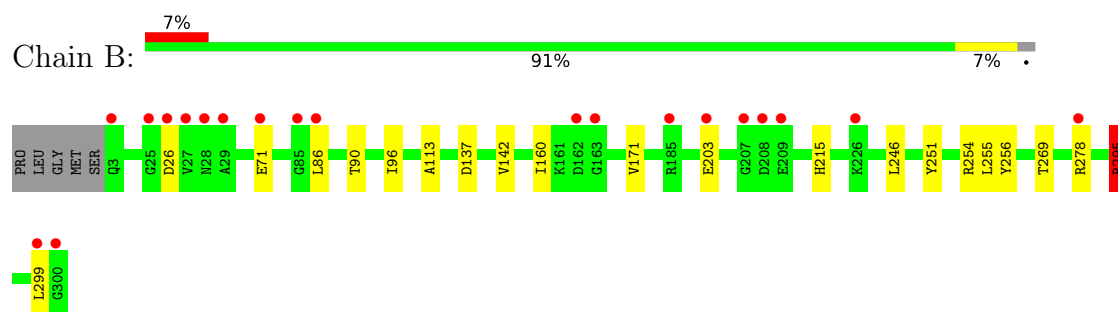
3 Residue-property plots [i](#)

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: Iron-dependent peroxidase



- Molecule 1: Iron-dependent peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.89Å 76.65Å 76.58Å 90.00° 108.01° 90.00°	Depositor
Resolution (Å)	47.67 – 1.90 47.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.67-1.90) 98.6 (47.67-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.184 , 0.201 (Not available) , 0.206	Depositor DCC
R_{free} test set	986 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10547	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.32	22/2501 (0.9%)	1.34	21/3376 (0.6%)
1	B	1.04	10/2402 (0.4%)	1.16	12/3245 (0.4%)
All	All	1.19	32/4903 (0.7%)	1.26	33/6621 (0.5%)

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	3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	PRO	N-CA	18.16	1.68	1.47
1	A	80	PRO	C-N	-17.77	1.07	1.33
1	A	215	HIS	CE1-NE2	-12.14	1.20	1.32
1	B	254[A]	ARG	C-N	-11.49	1.18	1.33
1	B	254[B]	ARG	C-N	-11.49	1.18	1.33
1	A	188	VAL	C-N	10.84	1.49	1.33
1	A	210	ARG	C-N	10.52	1.47	1.33
1	B	215	HIS	CE1-NE2	-9.32	1.23	1.32
1	A	79	PHE	C-N	8.99	1.44	1.33
1	B	256	TYR	C-O	-8.39	1.13	1.24
1	A	178	HIS	CE1-NE2	-7.58	1.25	1.32
1	A	203	GLU	C-O	-7.07	1.15	1.23
1	A	200[A]	ASP	C-N	-7.06	1.22	1.33
1	A	200[B]	ASP	C-N	-7.06	1.22	1.33
1	A	154	ARG	C-O	-6.99	1.16	1.24
1	A	86	LEU	C-O	-6.76	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	LEU	C-O	-6.65	1.16	1.24
1	B	142	VAL	C-O	-6.56	1.17	1.24
1	A	217	SER	C-O	-6.41	1.16	1.24
1	A	147	ASN	C-N	6.40	1.48	1.33
1	A	178	HIS	ND1-CE1	-6.17	1.26	1.32
1	B	160	ILE	C-O	-5.93	1.17	1.24
1	A	10	PRO	C-O	-5.78	1.16	1.23
1	A	215	HIS	C-O	-5.53	1.17	1.24
1	A	244	HIS	CE1-NE2	-5.41	1.27	1.32
1	B	278	ARG	C-O	-5.36	1.17	1.24
1	A	199	LYS	C-O	-5.35	1.18	1.23
1	B	269	THR	C-O	-5.29	1.18	1.24
1	A	178	HIS	CG-ND1	-5.25	1.32	1.38
1	A	223	GLU	C-O	-5.19	1.18	1.24
1	B	90	THR	C-O	-5.13	1.17	1.23
1	A	131	ARG	C-O	-5.04	1.17	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	PHE	CA-C-N	14.27	134.15	120.03
1	A	79	PHE	C-N-CA	14.27	134.15	120.03
1	A	188	VAL	O-C-N	-13.40	111.84	120.42
1	A	80	PRO	CB-CA-C	10.09	124.17	110.95
1	A	80	PRO	O-C-N	8.65	133.55	123.00
1	A	210	ARG	O-C-N	-7.75	112.24	121.39
1	A	199	LYS	CA-C-O	-7.30	113.23	120.89
1	A	80	PRO	CA-N-CD	-7.08	102.09	112.00
1	A	147	ASN	O-C-N	-6.96	113.63	121.43
1	A	210	ARG	CA-C-N	6.83	126.81	119.78
1	A	210	ARG	C-N-CA	6.83	126.81	119.78
1	B	295	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	B	26	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	79	PHE	O-C-N	-6.18	115.93	121.31
1	B	299	LEU	CA-C-O	-6.09	114.63	120.90
1	A	154	ARG	CA-C-O	-5.86	114.33	120.55
1	B	255[A]	LEU	CA-C-N	5.86	132.73	121.54
1	B	255[A]	LEU	C-N-CA	5.86	132.73	121.54
1	B	255[B]	LEU	CA-C-N	5.86	132.73	121.54
1	B	255[B]	LEU	C-N-CA	5.86	132.73	121.54
1	B	269	THR	CA-C-O	-5.77	114.95	120.90
1	A	145	THR	CA-CB-OG1	-5.72	101.01	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	VAL	N-CA-CB	5.64	114.85	110.45
1	B	295	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	B	86	LEU	CA-C-O	-5.53	114.66	120.63
1	A	164	VAL	CA-C-O	-5.52	115.21	120.95
1	B	137	ASP	N-CA-C	-5.28	103.56	110.53
1	A	137	ASP	N-CA-C	-5.17	103.57	110.55
1	A	178	HIS	ND1-CE1-NE2	-5.16	103.24	108.40
1	B	203	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	188	VAL	CA-C-N	5.04	125.32	119.47
1	A	188	VAL	C-N-CA	5.04	125.32	119.47
1	A	80	PRO	N-CA-C	-5.03	103.86	111.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	HIS	Mainchain
1	A	295[A]	ARG	Mainchain
1	A	295[B]	ARG	Mainchain

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	2438	2388	2368	8	0
1	B	2355	2302	2288	4	0
2	A	86	60	60	3	0
2	B	86	60	60	4	0
3	A	36	48	48	2	0
3	B	18	24	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	337	0	0	1	0
5	B	307	0	0	0	0
All	All	5665	4882	4848	19	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 2.

All (19) 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:80:PRO:CA	1:A:80:PRO:N	1.68	1.40
1:A:80:PRO:N	1:A:80:PRO:C	2.54	0.65
2:B:401[A]:HEM:HBC2	2:B:401[A]:HEM:HMC2	1.85	0.58
2:B:401[B]:HEM:HBC2	2:B:401[B]:HEM:HMC2	1.85	0.58
1:B:295:ARG:HH21	1:B:295:ARG:HG3	1.71	0.56
1:A:234:SER:N	3:A:402[B]:GOL:H12	2.21	0.55
1:B:171:VAL:HG22	1:B:251:TYR:CE1	2.48	0.49
1:A:96:ILE:HD13	1:A:113:ALA:HB1	1.98	0.45
2:B:401[A]:HEM:CMB	2:B:401[A]:HEM:HBB2	2.48	0.44
2:B:401[B]:HEM:HBB2	2:B:401[B]:HEM:CMB	2.48	0.44
1:A:234:SER:H	3:A:402[B]:GOL:H12	1.83	0.44
1:B:96:ILE:HD13	1:B:113:ALA:HB1	2.00	0.43
1:A:255:LEU:HD11	1:A:287:TYR:CD1	2.55	0.42
1:A:171:VAL:HG22	1:A:251:TYR:CE1	2.55	0.41
1:A:281[A]:LYS:NZ	5:A:505:HOH:O	2.52	0.41
1:B:171:VAL:HG22	1:B:251:TYR:CD1	2.56	0.40
2:A:401[A]:HEM:HBB2	2:A:401[A]:HEM:CMB	2.52	0.40
2:A:401[B]:HEM:HBB2	2:A:401[B]:HEM:CMB	2.52	0.40
2:A:401[B]:HEM:HMC1	2:A:401[B]:HEM:HBC2	2.03	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	311/303 (103%)	307 (99%)	4 (1%)	0	100	100
1	B	300/303 (99%)	293 (98%)	7 (2%)	0	100	100
All	All	611/606 (101%)	600 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/244 (104%)	253 (100%)	1 (0%)	84	87
1	B	244/244 (100%)	242 (99%)	2 (1%)	73	75
All	All	498/488 (102%)	495 (99%)	3 (1%)	78	81

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	PRO
1	B	71	GLU
1	B	295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	257	ASN
1	B	260	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
3	GOL	A	402[A]	-	5,5,5	0.30	0	5,5,5	0.50	0
3	GOL	A	403	-	5,5,5	0.04	0	5,5,5	0.08	0
2	HEM	B	401[A]	5,1	50,50,50	2.11	17 (34%)	67,82,82	1.80	13 (19%)
3	GOL	B	404	-	5,5,5	0.09	0	5,5,5	0.28	0
3	GOL	B	403	-	5,5,5	0.06	0	5,5,5	0.19	0
3	GOL	A	402[C]	-	5,5,5	0.36	0	5,5,5	1.33	1 (20%)
2	HEM	A	401[B]	5,1	50,50,50	2.01	16 (32%)	67,82,82	1.67	14 (20%)
3	GOL	A	404	-	5,5,5	0.22	0	5,5,5	0.49	0
3	GOL	A	402[B]	-	5,5,5	0.28	0	5,5,5	1.03	0
3	GOL	B	402	-	5,5,5	0.30	0	5,5,5	0.42	0
3	GOL	A	405	-	5,5,5	0.10	0	5,5,5	0.27	0
2	HEM	B	401[B]	5,1	50,50,50	2.11	17 (34%)	67,82,82	1.80	13 (19%)
2	HEM	A	401[A]	5,1	50,50,50	2.01	16 (32%)	67,82,82	1.67	14 (20%)

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	GOL	A	402[A]	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
2	HEM	B	401[A]	5,1	-	4/14/54/54	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	A	402[C]	-	-	0/4/4/4	-
2	HEM	A	401[B]	5,1	-	4/14/54/54	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	A	402[B]	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-
2	HEM	B	401[B]	5,1	-	4/14/54/54	-
2	HEM	A	401[A]	5,1	-	4/14/54/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[A]	HEM	FE-NB	6.23	2.14	1.94
2	B	401[B]	HEM	FE-NB	6.23	2.14	1.94
2	A	401[A]	HEM	FE-NB	5.36	2.11	1.94
2	A	401[B]	HEM	FE-NB	5.36	2.11	1.94
2	B	401[A]	HEM	FE-NC	5.16	2.12	1.95
2	B	401[B]	HEM	FE-NC	5.16	2.12	1.95
2	A	401[B]	HEM	C1B-NB	-4.77	1.32	1.40
2	A	401[A]	HEM	C1B-NB	-4.74	1.32	1.40
2	B	401[A]	HEM	C1B-NB	-4.55	1.32	1.40
2	B	401[B]	HEM	C1B-NB	-4.55	1.32	1.40
2	A	401[A]	HEM	FE-NC	4.53	2.10	1.95
2	A	401[B]	HEM	FE-NC	4.53	2.10	1.95
2	A	401[B]	HEM	C4B-NB	-4.36	1.30	1.38
2	A	401[A]	HEM	C4B-NB	-4.35	1.30	1.38
2	B	401[A]	HEM	C4B-NB	-3.90	1.31	1.38
2	B	401[B]	HEM	C4B-NB	-3.90	1.31	1.38
2	A	401[A]	HEM	C4D-ND	-3.90	1.33	1.40
2	A	401[B]	HEM	C4D-ND	-3.90	1.33	1.40
2	B	401[A]	HEM	C4D-ND	-3.88	1.33	1.40
2	B	401[B]	HEM	C4D-ND	-3.88	1.33	1.40
2	B	401[A]	HEM	C4C-NC	-3.50	1.33	1.39
2	B	401[B]	HEM	C4C-NC	-3.50	1.33	1.39
2	A	401[A]	HEM	C1D-C2D	3.26	1.51	1.44
2	A	401[B]	HEM	C1D-C2D	3.26	1.51	1.44
2	A	401[A]	HEM	FE-NA	3.20	2.05	1.95
2	A	401[B]	HEM	FE-NA	3.20	2.05	1.95
2	A	401[A]	HEM	C1C-NC	-3.18	1.33	1.39
2	A	401[B]	HEM	C1C-NC	-3.18	1.33	1.39
2	A	401[A]	HEM	C4C-NC	-3.10	1.33	1.39
2	A	401[B]	HEM	C4C-NC	-3.09	1.33	1.39
2	B	401[A]	HEM	C1D-ND	-3.04	1.32	1.38
2	B	401[B]	HEM	C1D-ND	-3.04	1.32	1.38
2	B	401[A]	HEM	C1D-C2D	2.95	1.50	1.44
2	B	401[B]	HEM	C1D-C2D	2.95	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[A]	HEM	C1A-NA	-2.91	1.34	1.39
2	B	401[B]	HEM	C1A-NA	-2.91	1.34	1.39
2	B	401[A]	HEM	C4A-NA	-2.83	1.34	1.39
2	B	401[B]	HEM	C4A-NA	-2.83	1.34	1.39
2	A	401[A]	HEM	C4A-NA	-2.71	1.34	1.39
2	A	401[B]	HEM	C4A-NA	-2.71	1.34	1.39
2	B	401[A]	HEM	FE-NA	2.71	2.04	1.95
2	B	401[B]	HEM	FE-NA	2.71	2.04	1.95
2	A	401[A]	HEM	O2D-CGD	-2.59	1.22	1.30
2	A	401[B]	HEM	O2D-CGD	-2.59	1.22	1.30
2	B	401[A]	HEM	O2A-CGA	-2.55	1.22	1.30
2	B	401[B]	HEM	O2A-CGA	-2.55	1.22	1.30
2	B	401[A]	HEM	C1C-C2C	-2.42	1.40	1.45
2	B	401[B]	HEM	C1C-C2C	-2.42	1.40	1.45
2	A	401[A]	HEM	C1A-NA	-2.42	1.35	1.39
2	A	401[B]	HEM	C1A-NA	-2.42	1.35	1.39
2	B	401[A]	HEM	C3B-C4B	2.41	1.49	1.44
2	B	401[B]	HEM	C3B-C4B	2.41	1.49	1.44
2	A	401[A]	HEM	C1D-ND	-2.41	1.34	1.38
2	A	401[B]	HEM	C1D-ND	-2.41	1.34	1.38
2	B	401[A]	HEM	C1C-NC	-2.40	1.35	1.39
2	B	401[B]	HEM	C1C-NC	-2.40	1.35	1.39
2	B	401[A]	HEM	C4D-C3D	2.31	1.49	1.45
2	B	401[B]	HEM	C4D-C3D	2.31	1.49	1.45
2	A	401[A]	HEM	C4D-C3D	2.30	1.48	1.45
2	A	401[B]	HEM	C4D-C3D	2.30	1.48	1.45
2	B	401[A]	HEM	O2D-CGD	-2.30	1.23	1.30
2	B	401[B]	HEM	O2D-CGD	-2.30	1.23	1.30
2	A	401[B]	HEM	C3B-C4B	2.20	1.49	1.44
2	A	401[A]	HEM	C3B-C4B	2.15	1.49	1.44
2	A	401[A]	HEM	O2A-CGA	-2.12	1.23	1.30
2	A	401[B]	HEM	O2A-CGA	-2.12	1.23	1.30

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[A]	HEM	C3B-C4B-NB	-5.59	105.45	109.47
2	B	401[B]	HEM	C3B-C4B-NB	-5.59	105.45	109.47
2	B	401[A]	HEM	C1B-NB-C4B	5.12	111.27	105.21
2	B	401[B]	HEM	C1B-NB-C4B	5.12	111.27	105.21
2	A	401[B]	HEM	C1B-NB-C4B	4.78	110.87	105.21
2	A	401[A]	HEM	C1B-NB-C4B	4.78	110.86	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	HEM	CHC-C4B-NB	4.59	129.36	124.42
2	A	401[A]	HEM	CHC-C4B-NB	4.52	129.29	124.42
2	B	401[A]	HEM	O2A-CGA-CBA	4.48	128.15	114.00
2	B	401[B]	HEM	O2A-CGA-CBA	4.48	128.15	114.00
2	B	401[A]	HEM	CHC-C4B-NB	4.10	128.84	124.42
2	B	401[B]	HEM	CHC-C4B-NB	4.10	128.84	124.42
2	B	401[A]	HEM	CHB-C1B-NB	3.85	129.13	124.37
2	B	401[B]	HEM	CHB-C1B-NB	3.85	129.13	124.37
2	A	401[A]	HEM	O2A-CGA-O1A	-3.66	113.93	123.33
2	A	401[B]	HEM	O2A-CGA-O1A	-3.66	113.93	123.33
2	B	401[A]	HEM	CAA-CBA-CGA	-3.63	104.04	113.67
2	B	401[B]	HEM	CAA-CBA-CGA	-3.63	104.04	113.67
2	A	401[A]	HEM	CHB-C1B-NB	3.55	128.75	124.37
2	A	401[B]	HEM	CHB-C1B-NB	3.52	128.72	124.37
2	A	401[A]	HEM	C4C-NC-C1C	3.02	110.74	105.82
2	A	401[B]	HEM	C4C-NC-C1C	2.99	110.70	105.82
2	B	401[A]	HEM	C4C-NC-C1C	2.99	110.70	105.82
2	B	401[B]	HEM	C4C-NC-C1C	2.99	110.70	105.82
2	B	401[A]	HEM	CHD-C4C-NC	2.95	127.67	124.45
2	B	401[B]	HEM	CHD-C4C-NC	2.95	127.67	124.45
2	B	401[A]	HEM	CMD-C2D-C1D	2.76	129.34	125.03
2	B	401[B]	HEM	CMD-C2D-C1D	2.76	129.34	125.03
2	A	401[B]	HEM	C3B-C4B-NB	-2.73	107.51	109.47
2	A	401[A]	HEM	C3B-C4B-NB	-2.66	107.56	109.47
3	A	402[C]	GOL	C3-C2-C1	2.64	121.49	111.80
2	B	401[A]	HEM	O1A-CGA-CBA	-2.63	114.75	123.09
2	B	401[B]	HEM	O1A-CGA-CBA	-2.63	114.75	123.09
2	A	401[A]	HEM	CAA-CBA-CGA	-2.61	106.75	113.67
2	A	401[B]	HEM	CAA-CBA-CGA	-2.61	106.75	113.67
2	B	401[A]	HEM	O2A-CGA-O1A	-2.58	116.70	123.33
2	B	401[B]	HEM	O2A-CGA-O1A	-2.58	116.70	123.33
2	A	401[A]	HEM	CHD-C4C-NC	2.46	127.14	124.45
2	A	401[B]	HEM	CHD-C4C-NC	2.43	127.10	124.45
2	A	401[A]	HEM	O2D-CGD-CBD	2.41	121.62	114.00
2	A	401[B]	HEM	O2D-CGD-CBD	2.41	121.62	114.00
2	A	401[A]	HEM	CBA-CAA-C2A	2.41	119.19	112.53
2	A	401[B]	HEM	CBA-CAA-C2A	2.41	119.19	112.53
2	A	401[B]	HEM	CMA-C3A-C4A	2.37	129.02	125.42
2	A	401[A]	HEM	CMA-C3A-C4A	2.34	128.99	125.42
2	B	401[A]	HEM	CHB-C1B-C2B	-2.29	120.43	126.95
2	B	401[B]	HEM	CHB-C1B-C2B	-2.29	120.43	126.95
2	A	401[A]	HEM	CMD-C2D-C1D	2.27	128.59	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	HEM	CMD-C2D-C1D	2.27	128.59	125.03
2	A	401[A]	HEM	CHA-C4D-C3D	-2.26	121.06	125.23
2	A	401[B]	HEM	CHA-C4D-C3D	-2.26	121.06	125.23
2	A	401[A]	HEM	CHB-C1B-C2B	-2.20	120.70	126.95
2	A	401[B]	HEM	CHB-C1B-C2B	-2.20	120.70	126.95
2	B	401[A]	HEM	C1D-C2D-C3D	-2.03	104.84	106.98
2	B	401[B]	HEM	C1D-C2D-C3D	-2.03	104.84	106.98

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-C3
3	A	404	GOL	O2-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3
2	B	401[A]	HEM	CAD-CBD-CGD-O1D
2	B	401[B]	HEM	CAD-CBD-CGD-O1D
2	B	401[A]	HEM	CAD-CBD-CGD-O2D
2	B	401[B]	HEM	CAD-CBD-CGD-O2D
2	A	401[A]	HEM	CAA-CBA-CGA-O1A
2	A	401[B]	HEM	CAA-CBA-CGA-O1A
2	B	401[A]	HEM	CAA-CBA-CGA-O1A
2	B	401[B]	HEM	CAA-CBA-CGA-O1A
2	B	401[A]	HEM	CAA-CBA-CGA-O2A
2	B	401[B]	HEM	CAA-CBA-CGA-O2A
2	A	401[A]	HEM	CAD-CBD-CGD-O1D
2	A	401[B]	HEM	CAD-CBD-CGD-O1D
2	A	401[A]	HEM	CAA-CBA-CGA-O2A
2	A	401[B]	HEM	CAA-CBA-CGA-O2A
2	A	401[A]	HEM	CAD-CBD-CGD-O2D
2	A	401[B]	HEM	CAD-CBD-CGD-O2D
3	B	402	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

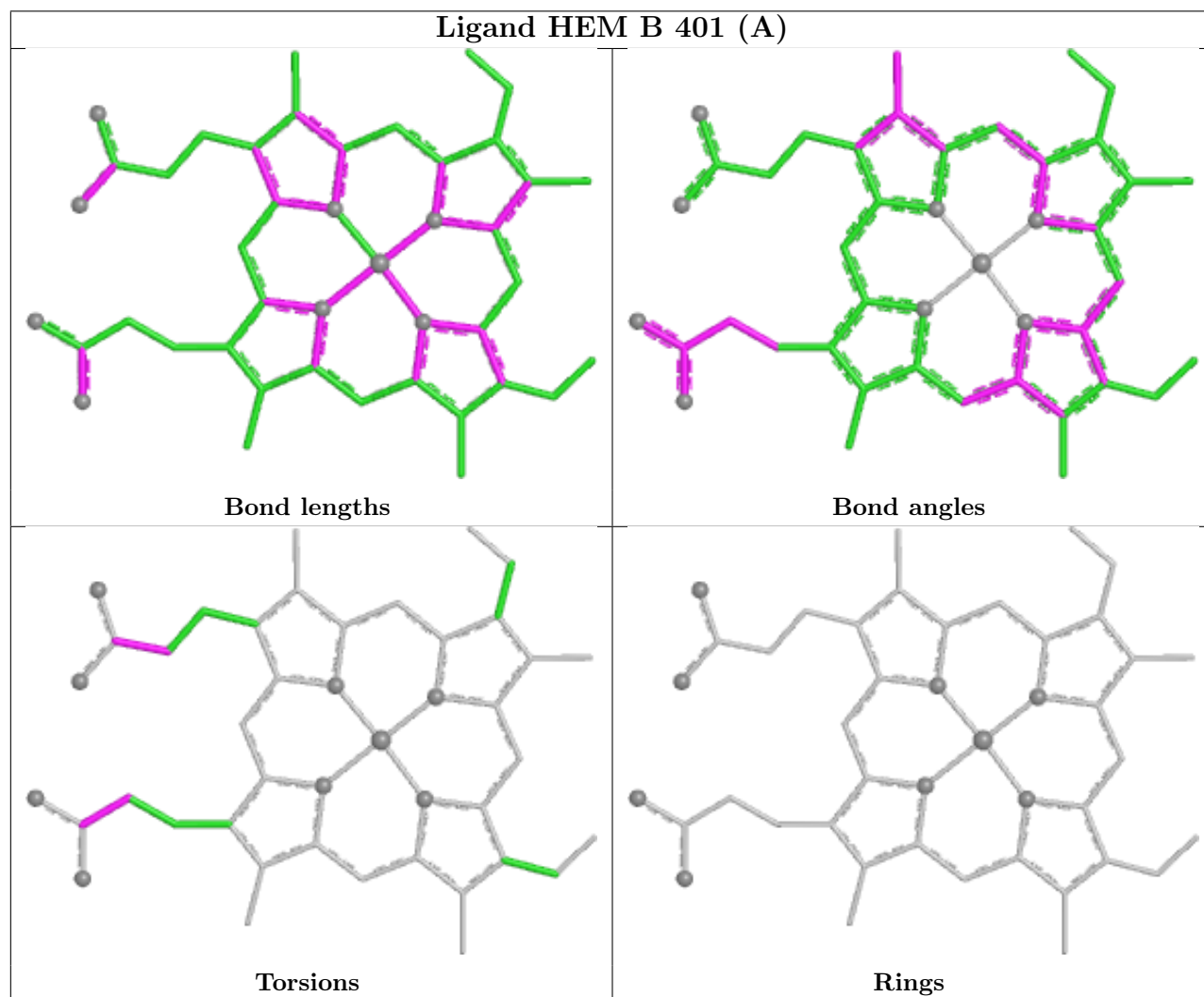
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[A]	HEM	2	0
2	A	401[B]	HEM	2	0

Continued on next page...

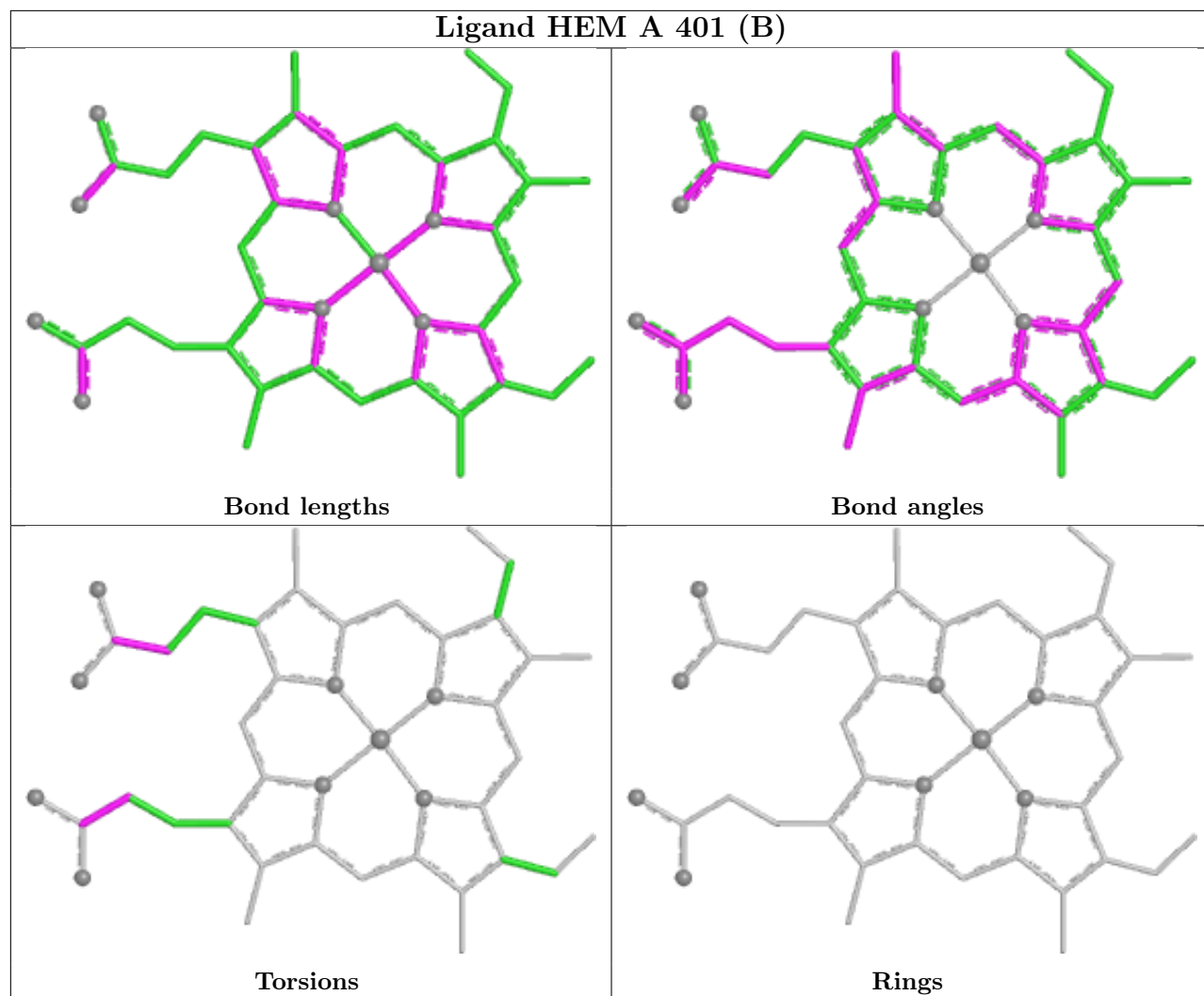
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[B]	GOL	2	0
2	B	401[B]	HEM	2	0
2	A	401[A]	HEM	1	0

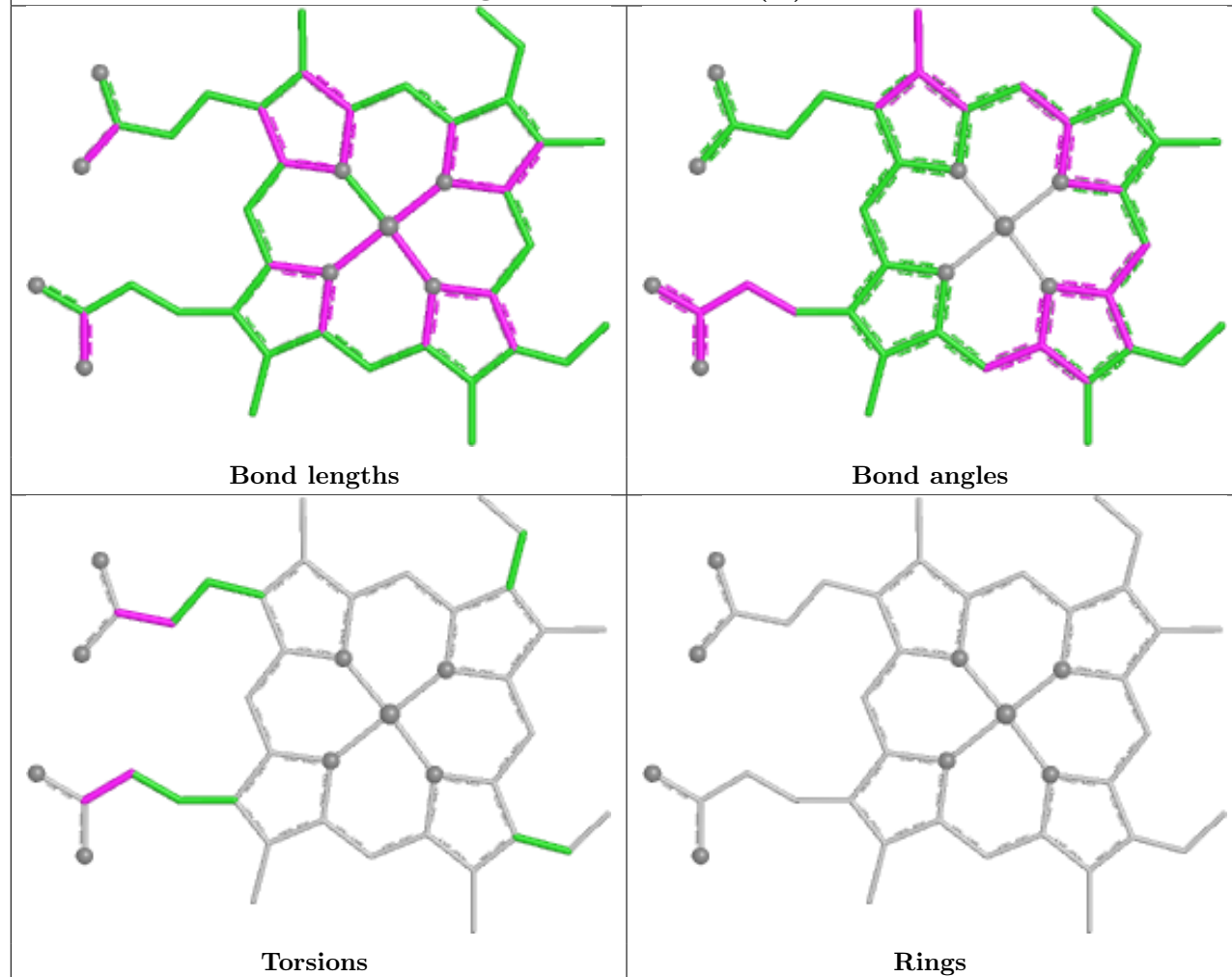
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

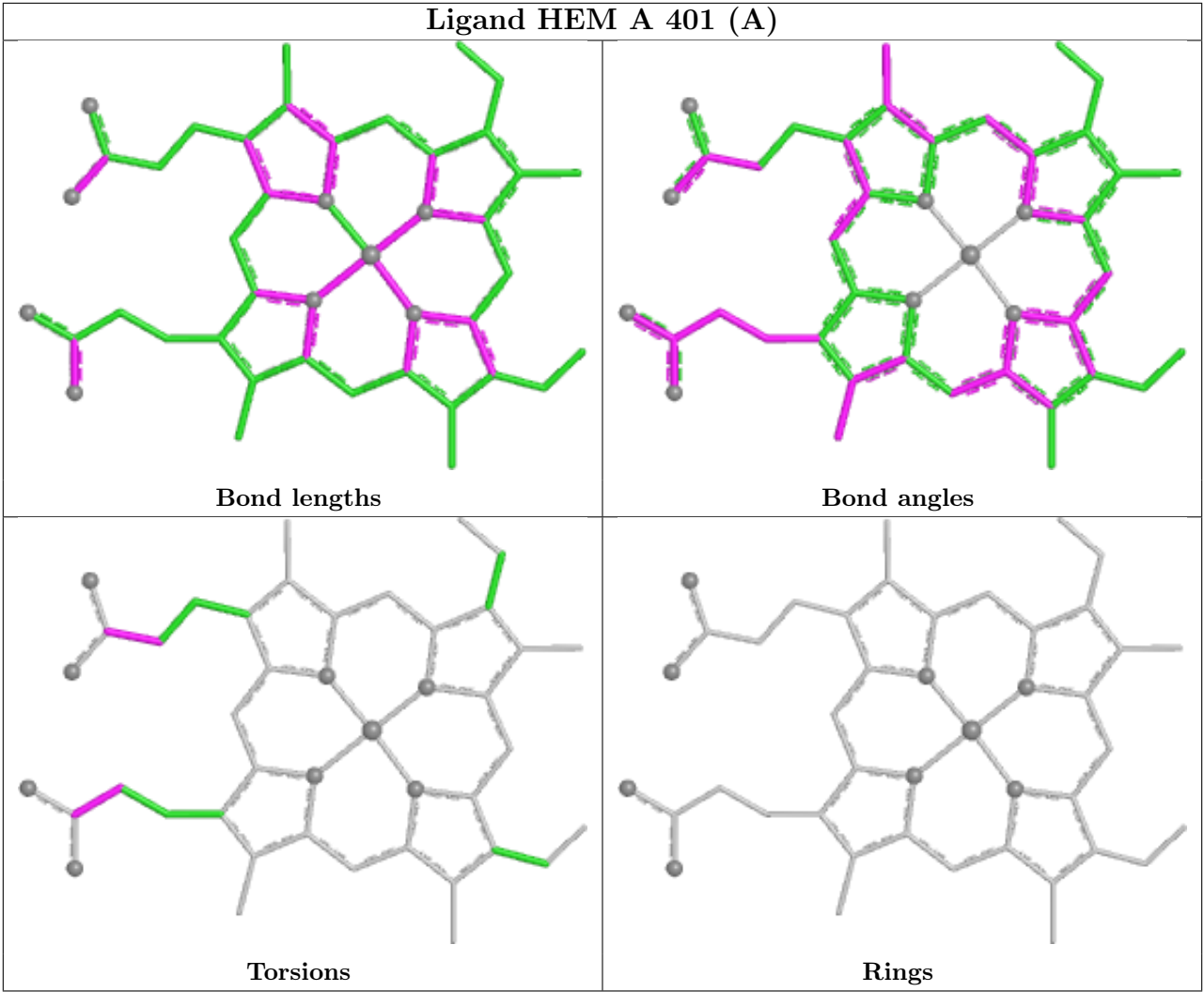


Ligand HEM A 401 (B)



Ligand HEM B 401 (B)





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	254[A]:ARG	C	255[A]:LEU	N	1.18

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	254[B]:ARG	C	255[B]:LEU	N	1.16
1	A	80:PRO	C	81[B]:VAL	N	1.07
1	A	80:PRO	C	81[A]:VAL	N	1.07

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	301/303 (99%)	0.22	19 (6%) 26 27	2, 7, 29, 47	11 (3%)
1	B	298/303 (98%)	0.29	20 (6%) 24 25	2, 8, 31, 58	4 (1%)
All	All	599/606 (98%)	0.25	39 (6%) 25 26	2, 8, 30, 58	15 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	GLY	7.1
1	B	299	LEU	4.8
1	A	300	GLY	4.7
1	A	0	GLY	4.5
1	A	298	ALA	4.2
1	A	25	GLY	3.8
1	B	26	ASP	3.5
1	B	28	ASN	3.5
1	A	297	GLN	3.3
1	B	27	VAL	3.1
1	A	208[A]	ASP	2.9
1	A	295[A]	ARG	2.9
1	B	185	ARG	2.9
1	A	299	LEU	2.7
1	B	278	ARG	2.7
1	A	28	ASN	2.7
1	B	209	GLU	2.7
1	A	50	ASP	2.6
1	A	26	ASP	2.6
1	B	85	GLY	2.6
1	B	3	GLN	2.6
1	A	162	ASP	2.6
1	B	25	GLY	2.5
1	A	71	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	71	GLU	2.5
1	A	84	LYS	2.5
1	A	1	MET	2.4
1	B	208	ASP	2.4
1	B	29	ALA	2.4
1	A	164	VAL	2.4
1	A	163	GLY	2.4
1	A	185	ARG	2.3
1	B	162	ASP	2.2
1	B	203	GLU	2.2
1	B	86	LEU	2.2
1	B	163	GLY	2.1
1	B	207	GLY	2.1
1	B	226	LYS	2.1
1	A	278[A]	ARG	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(Å ²)	Q<0.9
3	GOL	B	403	6/6	0.67	0.23	43,44,45,45	0
3	GOL	A	402[B]	6/6	0.74	0.20	15,16,18,18	14
3	GOL	A	402[C]	6/6	0.74	0.20	19,20,24,24	14
3	GOL	A	402[A]	6/6	0.74	0.20	19,20,24,24	14
3	GOL	B	404	6/6	0.76	0.21	21,21,21,21	0
3	GOL	A	405	6/6	0.79	0.18	21,21,21,21	0
3	GOL	B	402	6/6	0.81	0.20	21,30,33,33	0
3	GOL	A	403	6/6	0.82	0.18	23,28,31,31	0

Continued on next page...

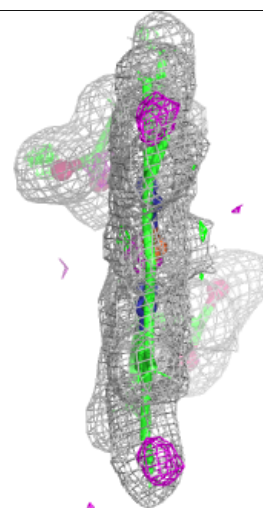
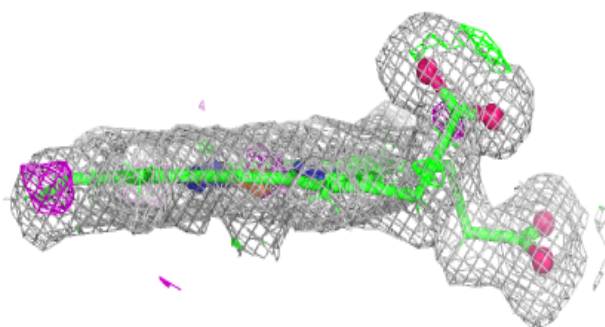
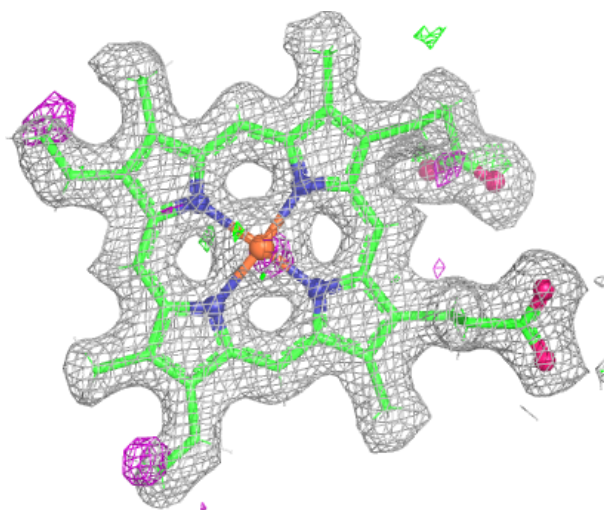
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	404	6/6	0.88	0.15	25,30,32,32	0
4	MG	A	406	1/1	0.91	0.07	20,20,20,20	0
4	MG	B	405	1/1	0.94	0.06	20,20,20,20	0
2	HEM	B	401[B]	43/43	0.97	0.06	3,3,4,6	73
2	HEM	A	401[A]	43/43	0.97	0.06	3,3,4,6	73
2	HEM	A	401[B]	43/43	0.97	0.06	3,3,4,6	73
2	HEM	B	401[A]	43/43	0.97	0.06	3,3,4,6	73

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.

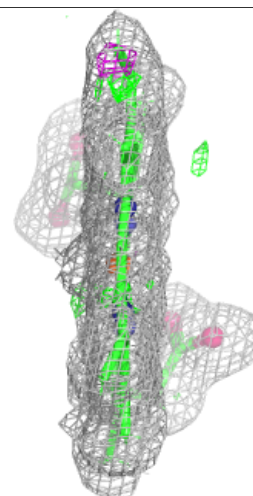
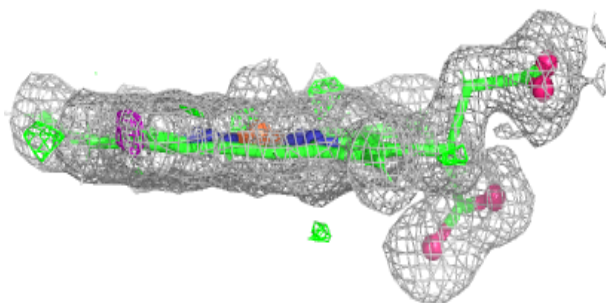
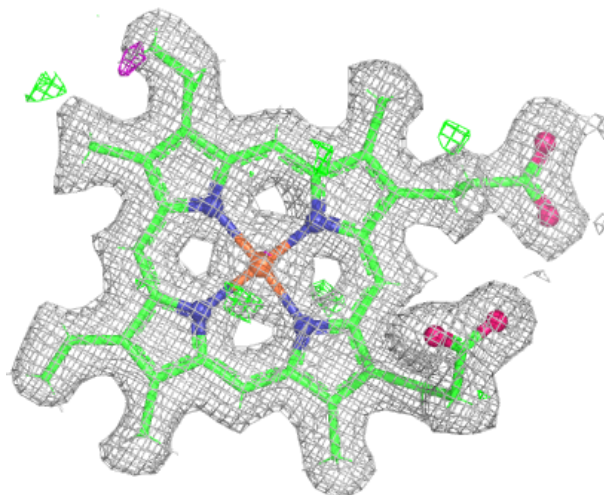
Electron density around HEM B 401 (B):

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



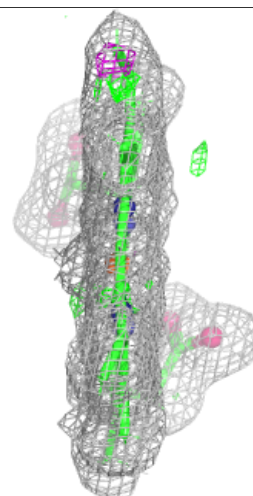
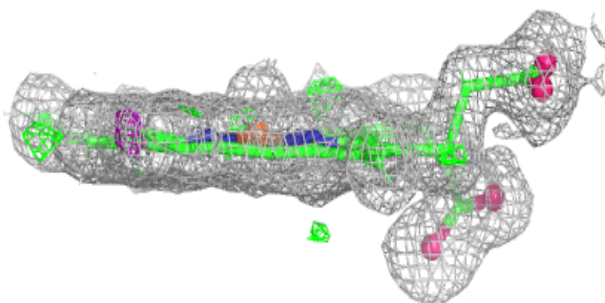
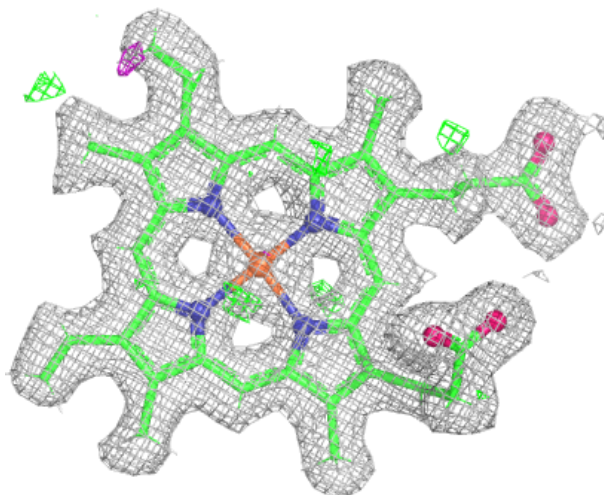
Electron density around HEM A 401 (A):

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



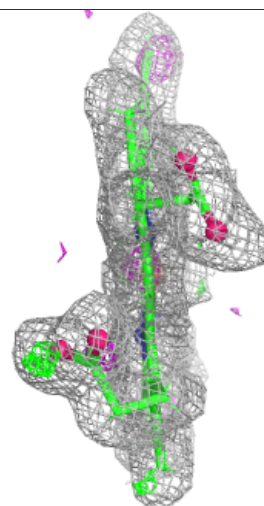
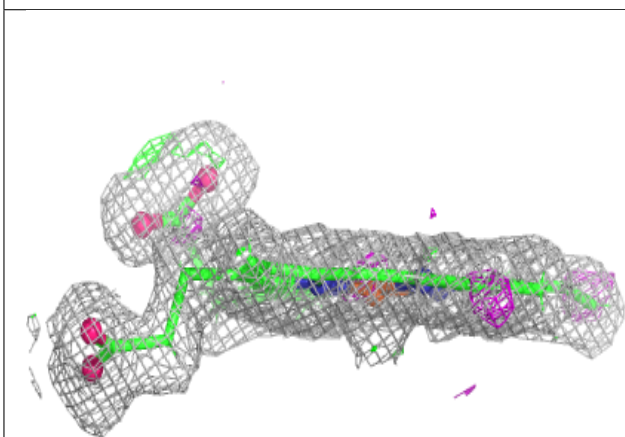
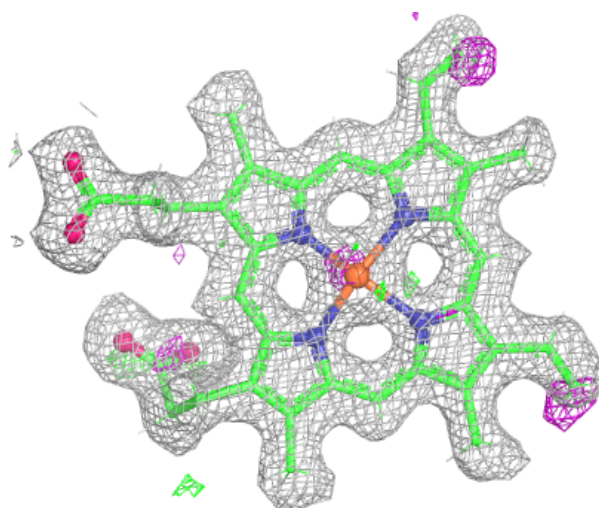
Electron density around HEM A 401 (B):

$2mF_o-DF_c$ (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 (A):

$2mF_o-DF_c$ (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.