



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:08 PM UTC

PDB ID : 6RR4 / pdb_00006rr4
Title : Structure of 25% 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

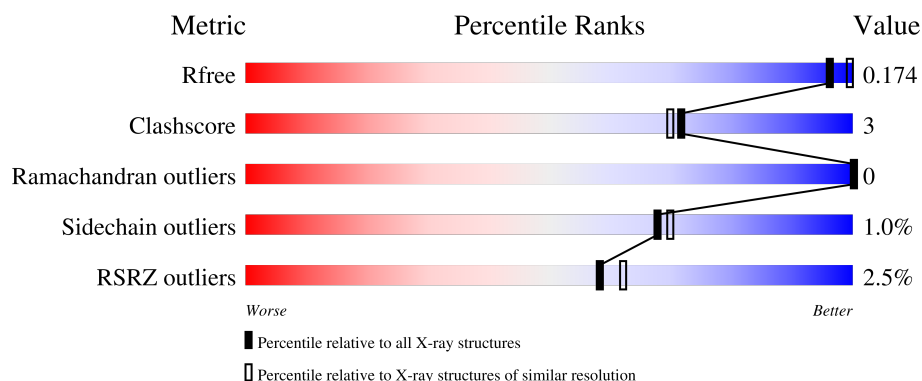
1 Overall quality at a glance

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	 3% 78% 20% ..
1	B	303	 2% 83% 15% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10654 atoms, of which 4935 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	13	0
			4841	1535	2400	434	462	10			
1	B	298	Total	C	H	N	O	S	0	10	0
			4738	1508	2343	422	457	8			

There are 8 discrepancies between the modelled and reference sequences:

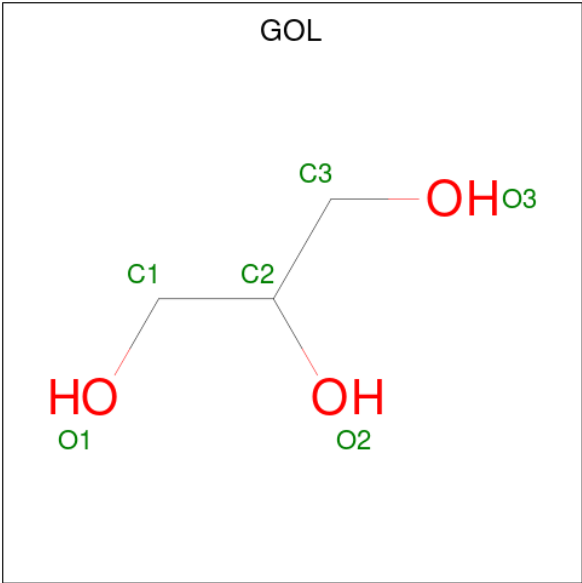
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP A0A0W8ATM9
A	-1	LEU	-	expression tag	UNP A0A0W8ATM9
A	0	GLY	-	expression tag	UNP A0A0W8ATM9
A	300	GLY	-	expression tag	UNP A0A0W8ATM9
B	-2	PRO	-	expression tag	UNP A0A0W8ATM9
B	-1	LEU	-	expression tag	UNP A0A0W8ATM9
B	0	GLY	-	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	C	Fe	H	N	O	0	1
			146	68	2	60	8	8		
2	B	1	Total	C	Fe	H	N	O	0	1
			146	68	2	60	8	8		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	1
			28	6	16	6		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

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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	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		

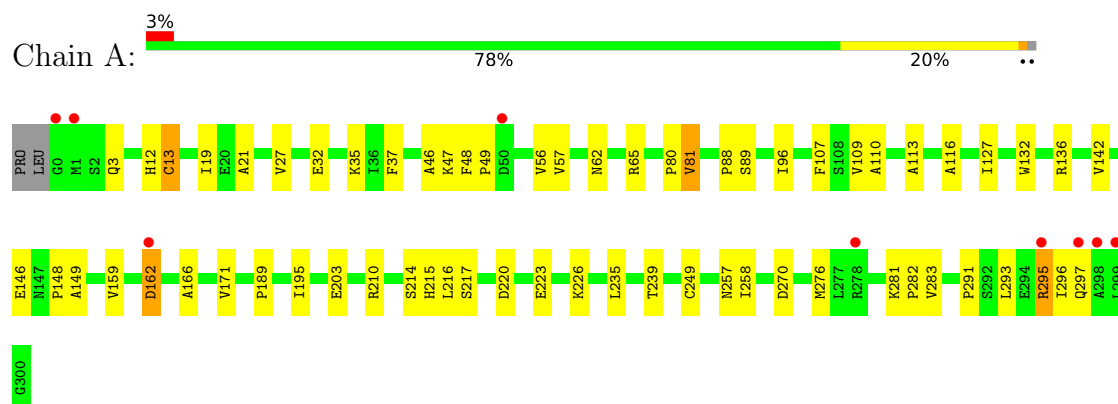
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	336	Total	O	0	0
			336	336		
5	B	319	Total	O	0	0
			319	319		

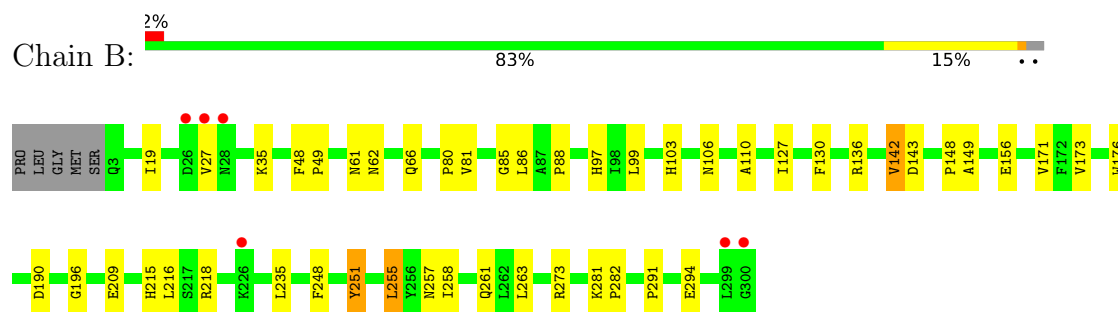
3 Residue-property plots

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: 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)	48.40 – 1.90 48.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.40-1.90) 98.5 (48.40-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.169 , 0.181 0.167 , 0.174	Depositor DCC
R_{free} test set	982 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10654	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 6.86% 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: HEM, GOL, MG

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	1.68	49/2504 (2.0%)	1.34	11/3381 (0.3%)
1	B	1.62	35/2442 (1.4%)	1.32	3/3299 (0.1%)
All	All	1.65	84/4946 (1.7%)	1.33	14/6680 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	PHE	C-N	13.54	1.51	1.33
1	A	210	ARG	C-N	13.51	1.50	1.33
1	A	281	LYS	C-N	11.97	1.49	1.33
1	B	62	ASN	C-N	-9.81	1.21	1.33
1	A	295[B]	ARG	C-N	-9.49	1.22	1.33
1	A	295[C]	ARG	C-N	-9.49	1.22	1.33
1	A	235	LEU	C-O	-7.91	1.15	1.24
1	A	291	PRO	C-O	-7.39	1.14	1.23
1	A	49	PRO	C-O	-7.15	1.15	1.24
1	B	61	ASN	C-O	-7.12	1.15	1.24
1	A	21	ALA	C-O	-7.00	1.15	1.23
1	A	195	ILE	C-O	-6.84	1.16	1.23
1	B	291	PRO	C-O	-6.83	1.15	1.23
1	B	27	VAL	C-O	-6.75	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	HIS	C-O	-6.71	1.16	1.24
1	B	263	LEU	C-O	-6.68	1.16	1.24
1	A	80	PRO	C-O	-6.62	1.15	1.23
1	B	49	PRO	C-O	-6.62	1.16	1.24
1	A	282	PRO	C-O	-6.52	1.16	1.23
1	A	281	LYS	C-O	-6.39	1.17	1.24
1	A	217	SER	C-O	-6.30	1.16	1.24
1	A	81	VAL	C-O	-6.29	1.17	1.24
1	A	149	ALA	C-O	-6.27	1.16	1.24
1	B	282	PRO	C-O	-6.25	1.17	1.23
1	A	13[A]	CYS	C-N	-6.23	1.24	1.33
1	A	13[B]	CYS	C-N	-6.23	1.24	1.33
1	B	218	ARG	C-O	-6.18	1.16	1.24
1	B	130	PHE	C-O	-6.08	1.16	1.23
1	A	283	VAL	C-O	-6.02	1.17	1.24
1	B	88	PRO	C-O	-6.00	1.16	1.23
1	B	149	ALA	C-O	-5.89	1.16	1.24
1	A	215	HIS	CE1-NE2	-5.88	1.26	1.32
1	B	80	PRO	C-O	-5.88	1.15	1.23
1	A	239	THR	C-O	-5.88	1.16	1.23
1	B	173	VAL	C-O	-5.85	1.18	1.24
1	A	148	PRO	C-O	-5.83	1.15	1.23
1	A	46	ALA	C-O	-5.81	1.17	1.24
1	A	132	TRP	C-O	-5.74	1.16	1.23
1	B	258	ILE	C-O	-5.74	1.17	1.24
1	A	223	GLU	C-O	-5.73	1.17	1.24
1	A	110	ALA	C-O	-5.69	1.17	1.24
1	A	249	CYS	C-O	-5.69	1.17	1.23
1	A	88	PRO	C-O	-5.65	1.16	1.23
1	A	19	ILE	C-O	-5.64	1.18	1.24
1	B	261	GLN	C-O	-5.63	1.17	1.24
1	B	257	ASN	C-O	-5.62	1.17	1.24
1	B	110	ALA	C-O	-5.61	1.17	1.24
1	A	116	ALA	C-O	-5.58	1.17	1.24
1	A	214	SER	C-O	-5.57	1.17	1.23
1	A	127	ILE	C-O	-5.56	1.18	1.24
1	A	107	PHE	C-O	-5.54	1.17	1.24
1	B	66	GLN	C-O	-5.50	1.17	1.24
1	A	270	ASP	C-O	-5.50	1.16	1.24
1	B	251	TYR	C-O	-5.47	1.17	1.24
1	B	19	ILE	C-O	-5.46	1.18	1.24
1	B	156	GLU	C-O	-5.45	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	HIS	C-O	-5.45	1.17	1.24
1	A	216	LEU	C-O	-5.39	1.17	1.24
1	A	65	ARG	C-O	-5.37	1.17	1.24
1	A	109	VAL	C-O	-5.37	1.17	1.24
1	B	106	ASN	C-O	-5.34	1.18	1.24
1	B	235	LEU	C-O	-5.32	1.18	1.24
1	B	148	PRO	C-O	-5.30	1.16	1.23
1	A	189	PRO	C-O	-5.29	1.17	1.24
1	A	159	VAL	C-O	-5.29	1.18	1.24
1	A	3	GLN	C-N	-5.27	1.21	1.33
1	A	27	VAL	C-O	-5.25	1.17	1.24
1	A	257	ASN	C-O	-5.25	1.18	1.24
1	A	89	SER	C-O	-5.24	1.18	1.24
1	A	56	VAL	C-O	-5.22	1.18	1.24
1	B	248	PHE	C-O	-5.21	1.17	1.24
1	B	97	HIS	C-O	-5.21	1.18	1.24
1	B	196	GLY	C-O	-5.18	1.17	1.24
1	B	190	ASP	CG-OD2	-5.18	1.15	1.25
1	A	220	ASP	CG-OD1	-5.13	1.15	1.25
1	A	146	GLU	C-O	-5.12	1.17	1.24
1	A	62	ASN	C-O	-5.10	1.18	1.24
1	A	258	ILE	C-O	-5.10	1.18	1.24
1	B	216	LEU	C-O	-5.09	1.18	1.24
1	B	281	LYS	C-O	-5.09	1.18	1.24
1	B	127	ILE	C-O	-5.08	1.18	1.24
1	B	103	HIS	CE1-NE2	-5.08	1.27	1.32
1	A	203	GLU	C-O	-5.06	1.17	1.23
1	B	35	LYS	C-O	-5.05	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLN	O-C-N	7.07	132.19	123.21
1	A	281	LYS	CA-C-N	7.05	127.60	119.99
1	A	281	LYS	C-N-CA	7.05	127.60	119.99
1	B	48	PHE	O-C-N	-6.72	114.92	121.17
1	A	281	LYS	O-C-N	-6.63	117.17	121.88
1	A	3	GLN	CA-C-O	-6.16	114.02	120.54
1	B	142	VAL	CA-C-O	-6.11	114.04	121.13
1	A	297	GLN	CB-CG-CD	5.99	122.79	112.60
1	A	210	ARG	O-C-N	-5.77	114.58	121.39
1	A	297	GLN	CB-CA-C	5.70	121.75	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ASN	CA-C-O	-5.43	115.11	120.82
1	A	12	HIS	CA-C-O	-5.39	114.20	120.56
1	A	81	VAL	N-CA-CB	-5.23	104.83	110.53
1	A	162	ASP	CA-CB-CG	-5.16	107.44	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296[B]	ILE	Mainchain
1	B	255[B]	LEU	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	2441	2400	2380	11	0
1	B	2395	2343	2324	17	0
2	A	86	60	60	3	0
2	B	86	60	60	5	0
3	A	36	48	48	0	0
3	B	18	24	24	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	336	0	0	0	0
5	B	319	0	0	0	0
All	All	5719	4935	4896	33	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 3.

All (33) 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:B:81[B]:VAL:HG11	1:B:85:GLY:HA2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81[B]:VAL:CG1	1:B:85:GLY:HA2	2.24	0.68
1:B:81[B]:VAL:CG1	1:B:85:GLY:N	2.60	0.64
1:A:47:LYS:HD3	1:A:48:PHE:CE2	2.36	0.61
1:B:294:GLU:N	1:B:294:GLU:OE1	2.35	0.60
2:B:401[B]:HEM:HMC2	2:B:401[B]:HEM:HBC2	1.84	0.60
1:B:81[B]:VAL:CG1	1:B:85:GLY:CA	2.83	0.56
1:B:99:LEU:O	1:B:99:LEU:HD12	2.06	0.54
1:A:295[C]:ARG:HH11	1:A:295[C]:ARG:HG2	1.73	0.54
1:B:81[B]:VAL:HG11	1:B:85:GLY:CA	2.36	0.54
1:B:81[B]:VAL:HG12	1:B:85:GLY:N	2.23	0.53
1:B:143[B]:ASP:OD1	3:B:402:GOL:O3	2.26	0.52
1:A:295[C]:ARG:C	1:A:295[C]:ARG:HD2	2.37	0.50
1:A:32:GLU:OE1	1:A:35:LYS:HE3	2.12	0.49
1:A:96[A]:ILE:HD13	1:A:113:ALA:HB1	1.94	0.48
1:B:255[A]:LEU:HD23	1:B:255[A]:LEU:C	2.39	0.47
1:A:13[A]:CYS:O	1:A:13[A]:CYS:SG	2.72	0.47
1:B:99:LEU:HD12	1:B:99:LEU:C	2.41	0.46
1:B:255[A]:LEU:HD23	1:B:255[A]:LEU:O	2.16	0.45
1:A:37:PHE:HD2	1:A:57[B]:VAL:CG2	2.29	0.45
1:B:171:VAL:HG22	1:B:251:TYR:CE2	2.52	0.45
1:B:143[B]:ASP:OD2	2:B:401[B]:HEM:C4A	2.70	0.45
1:B:136:ARG:HA	1:B:142:VAL:HA	1.99	0.45
1:A:295[C]:ARG:HG2	1:A:295[C]:ARG:NH1	2.32	0.44
2:A:401[A]:HEM:HBC2	2:A:401[A]:HEM:HMC2	1.99	0.44
2:B:401[A]:HEM:HMC2	2:B:401[A]:HEM:HBC2	1.99	0.44
1:B:86:LEU:HD11	1:B:273:ARG:CZ	2.50	0.42
1:A:162:ASP:HA	1:A:166:ALA:HB2	2.02	0.42
2:B:401[B]:HEM:CMB	2:B:401[B]:HEM:HBB2	2.50	0.42
1:A:276:MET:HE1	2:A:401[B]:HEM:C4B	2.54	0.41
1:A:136:ARG:HA	1:A:142:VAL:HA	2.02	0.41
1:B:176:TRP:CD2	2:B:401[B]:HEM:HBB1	2.55	0.41
2:A:401[B]:HEM:CMB	2:A:401[B]:HEM:HBB2	2.52	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	312/303 (103%)	306 (98%)	6 (2%)	0	100	100
1	B	305/303 (101%)	299 (98%)	6 (2%)	0	100	100
All	All	617/606 (102%)	605 (98%)	12 (2%)	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	255/244 (104%)	251 (98%)	4 (2%)	55	54
1	B	249/244 (102%)	248 (100%)	1 (0%)	84	87
All	All	504/488 (103%)	499 (99%)	5 (1%)	68	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	171	VAL
1	A	226	LYS
1	A	293	LEU
1	B	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	66	GLN
1	B	260	GLN
1	B	297	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 ⓘ

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	$\# Z > 2$
2	HEM	A	401[A]	1,5	50,50,50	1.24	4 (8%)	67,82,82	1.58	13 (19%)
3	GOL	B	403	-	5,5,5	0.35	0	5,5,5	0.46	0
2	HEM	B	401[B]	1,5	50,50,50	1.94	15 (30%)	67,82,82	2.04	12 (17%)
3	GOL	A	405	-	5,5,5	0.11	0	5,5,5	0.43	0
3	GOL	B	402	-	5,5,5	0.68	0	5,5,5	1.09	0
3	GOL	B	404	-	5,5,5	0.29	0	5,5,5	0.36	0
3	GOL	A	406	-	5,5,5	0.10	0	5,5,5	0.33	0
3	GOL	A	403	-	5,5,5	0.05	0	5,5,5	0.20	0
2	HEM	B	401[A]	1,5	50,50,50	1.20	5 (10%)	67,82,82	1.63	17 (25%)
3	GOL	A	402[B]	-	5,5,5	0.10	0	5,5,5	0.16	0
2	HEM	A	401[B]	1,5	50,50,50	2.39	16 (32%)	67,82,82	1.65	11 (16%)
3	GOL	A	404	-	5,5,5	0.11	0	5,5,5	0.24	0
3	GOL	A	402[A]	-	5,5,5	0.10	0	5,5,5	0.17	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
2	HEM	A	401[A]	1,5	-	4/14/54/54	-
3	GOL	B	403	-	-	2/4/4/4	-
2	HEM	B	401[B]	1,5	-	4/14/54/54	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	B	402	-	-	4/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
2	HEM	B	401[A]	1,5	-	4/14/54/54	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
2	HEM	A	401[B]	1,5	-	4/14/54/54	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	A	402[A]	-	-	0/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	HEM	C4B-NB	-6.19	1.26	1.38
2	A	401[B]	HEM	C1B-NB	-5.96	1.29	1.40
2	A	401[B]	HEM	FE-NB	5.88	2.13	1.94
2	B	401[B]	HEM	FE-NB	5.03	2.10	1.94
2	B	401[B]	HEM	FE-NC	5.00	2.11	1.95
2	A	401[B]	HEM	FE-NC	4.83	2.11	1.95
2	A	401[B]	HEM	C4C-NC	-4.41	1.31	1.39
2	B	401[B]	HEM	C1B-NB	-4.37	1.32	1.40
2	A	401[B]	HEM	C4A-NA	-4.25	1.31	1.39
2	A	401[B]	HEM	C1C-NC	-4.04	1.32	1.39
2	B	401[B]	HEM	C4B-NB	-4.03	1.30	1.38
2	B	401[B]	HEM	C4D-ND	-3.90	1.33	1.40
2	A	401[B]	HEM	C4D-ND	-3.85	1.33	1.40
2	A	401[B]	HEM	C1D-C2D	3.69	1.52	1.44
2	B	401[B]	HEM	C1D-ND	-3.46	1.32	1.38
2	A	401[B]	HEM	O2D-CGD	-3.27	1.20	1.30
2	A	401[B]	HEM	C4D-C3D	3.26	1.50	1.45
2	A	401[B]	HEM	FE-NA	3.16	2.05	1.95
2	A	401[A]	HEM	C3B-C4B	3.13	1.51	1.44
2	A	401[B]	HEM	C3B-C4B	3.06	1.50	1.44
2	B	401[B]	HEM	C1C-NC	-2.98	1.34	1.39
2	B	401[A]	HEM	C3B-C4B	2.92	1.50	1.44
2	A	401[A]	HEM	C3C-C2C	2.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	HEM	C4A-NA	-2.69	1.34	1.39
2	B	401[B]	HEM	FE-NA	2.61	2.03	1.95
2	A	401[B]	HEM	C1A-NA	-2.58	1.34	1.39
2	B	401[A]	HEM	C1D-C2D	2.47	1.49	1.44
2	B	401[B]	HEM	C4C-NC	-2.41	1.35	1.39
2	A	401[B]	HEM	C1D-ND	-2.35	1.34	1.38
2	A	401[B]	HEM	O2A-CGA	-2.27	1.23	1.30
2	A	401[A]	HEM	C1D-C2D	2.20	1.49	1.44
2	B	401[B]	HEM	C1D-C2D	2.11	1.48	1.44
2	B	401[B]	HEM	C3D-C2D	-2.07	1.32	1.36
2	B	401[A]	HEM	C3C-C2C	2.06	1.41	1.37
2	B	401[A]	HEM	C1B-NB	-2.05	1.36	1.40
2	B	401[A]	HEM	CHD-C4C	2.04	1.42	1.38
2	B	401[B]	HEM	C1A-NA	-2.04	1.35	1.39
2	B	401[B]	HEM	O2A-CGA	-2.03	1.24	1.30
2	A	401[A]	HEM	C1B-NB	-2.02	1.36	1.40
2	B	401[B]	HEM	O2D-CGD	-2.01	1.24	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[B]	HEM	CHC-C4B-NB	7.36	132.34	124.42
2	B	401[B]	HEM	C1B-NB-C4B	6.54	112.95	105.21
2	A	401[B]	HEM	C1B-NB-C4B	6.07	112.39	105.21
2	B	401[B]	HEM	C3B-C4B-NB	-4.58	106.18	109.47
2	B	401[B]	HEM	CHB-C1B-NB	4.48	129.91	124.37
2	A	401[A]	HEM	C3B-C4B-NB	4.37	112.60	109.47
2	A	401[B]	HEM	CHC-C4B-NB	4.07	128.80	124.42
2	B	401[B]	HEM	CHD-C4C-NC	4.05	128.87	124.45
2	B	401[A]	HEM	C3B-C4B-NB	3.78	112.18	109.47
2	B	401[B]	HEM	CHD-C1D-ND	3.48	128.17	124.42
2	A	401[A]	HEM	C2B-C1B-NB	3.47	113.83	109.84
2	B	401[B]	HEM	C4C-NC-C1C	3.40	111.37	105.82
2	A	401[B]	HEM	C4C-NC-C1C	3.36	111.31	105.82
2	B	401[A]	HEM	C2B-C1B-NB	3.26	113.59	109.84
2	A	401[B]	HEM	C3B-C2B-C1B	-3.20	104.01	106.41
2	A	401[A]	HEM	O2A-CGA-O1A	-3.13	115.29	123.33
2	A	401[B]	HEM	C3B-C4B-NB	-3.12	107.23	109.47
2	B	401[B]	HEM	CHA-C4D-ND	3.10	128.20	124.37
2	B	401[B]	HEM	CAD-C3D-C4D	3.09	130.08	124.70
2	B	401[A]	HEM	C2A-C1A-NA	3.04	113.52	110.15
2	A	401[A]	HEM	C4B-C3B-C2B	-2.88	104.64	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[A]	HEM	C2D-C1D-ND	2.81	113.16	109.90
2	A	401[B]	HEM	CHD-C4C-NC	2.77	127.47	124.45
2	B	401[A]	HEM	O2D-CGD-CBD	2.75	122.68	114.00
2	B	401[A]	HEM	C4B-C3B-C2B	-2.73	104.77	107.28
2	A	401[A]	HEM	C2D-C1D-ND	2.70	113.03	109.90
2	B	401[A]	HEM	C1D-C2D-C3D	-2.69	104.15	106.98
2	A	401[B]	HEM	CHB-C1B-NB	2.66	127.66	124.37
2	B	401[A]	HEM	O2A-CGA-CBA	2.62	122.28	114.00
2	A	401[A]	HEM	CAA-CBA-CGA	-2.56	106.88	113.67
2	A	401[A]	HEM	C2A-C1A-NA	2.55	112.98	110.15
2	B	401[B]	HEM	CHD-C1D-C2D	-2.47	121.13	125.03
2	B	401[A]	HEM	C4A-NA-C1A	-2.46	101.81	105.82
2	B	401[A]	HEM	CAA-CBA-CGA	-2.44	107.18	113.67
2	A	401[A]	HEM	C1D-C2D-C3D	-2.37	104.48	106.98
2	B	401[A]	HEM	C3D-C4D-ND	2.37	112.77	110.17
2	A	401[A]	HEM	CHB-C1B-C2B	-2.35	120.28	126.95
2	B	401[A]	HEM	CMD-C2D-C1D	2.33	128.67	125.03
2	A	401[B]	HEM	C1D-C2D-C3D	-2.33	104.53	106.98
2	A	401[B]	HEM	CHA-C4D-ND	2.31	127.23	124.37
2	B	401[A]	HEM	CHB-C1B-C2B	-2.29	120.43	126.95
2	B	401[B]	HEM	CMD-C2D-C1D	2.25	128.55	125.03
2	A	401[B]	HEM	CMA-C3A-C4A	2.24	128.83	125.42
2	B	401[B]	HEM	CHA-C4D-C3D	-2.21	121.15	125.23
2	A	401[B]	HEM	CHA-C4D-C3D	-2.19	121.19	125.23
2	A	401[A]	HEM	O2D-CGD-O1D	-2.18	117.72	123.33
2	A	401[A]	HEM	CHC-C4B-C3B	-2.18	120.73	125.07
2	B	401[A]	HEM	CHD-C1D-C2D	-2.15	121.64	125.03
2	A	401[A]	HEM	C3D-C4D-ND	2.13	112.51	110.17
2	A	401[A]	HEM	CMD-C2D-C1D	2.13	128.36	125.03
2	B	401[A]	HEM	CHC-C4B-C3B	-2.06	120.95	125.07
2	B	401[A]	HEM	CBD-CAD-C3D	-2.06	106.83	112.53
2	B	401[A]	HEM	CHC-C4B-NB	2.05	126.63	124.42

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	C1-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3
3	A	405	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	402	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
2	B	401[A]	HEM	CAD-CBD-CGD-O1D
2	A	401[A]	HEM	CAA-CBA-CGA-O1A
2	A	401[A]	HEM	CAD-CBD-CGD-O2D
2	B	401[A]	HEM	CAD-CBD-CGD-O2D
3	B	403	GOL	O2-C2-C3-O3
2	A	401[B]	HEM	CAD-CBD-CGD-O1D
2	A	401[A]	HEM	CAD-CBD-CGD-O1D
2	A	401[B]	HEM	CAD-CBD-CGD-O2D
2	B	401[B]	HEM	CAD-CBD-CGD-O2D
2	B	401[B]	HEM	CAD-CBD-CGD-O1D
2	A	401[A]	HEM	CAA-CBA-CGA-O2A
2	B	401[A]	HEM	CAA-CBA-CGA-O1A
2	B	401[A]	HEM	CAA-CBA-CGA-O2A
2	B	401[B]	HEM	CAA-CBA-CGA-O2A
2	B	401[B]	HEM	CAA-CBA-CGA-O1A
2	A	401[B]	HEM	CAA-CBA-CGA-O2A
2	A	401[B]	HEM	CAA-CBA-CGA-O1A

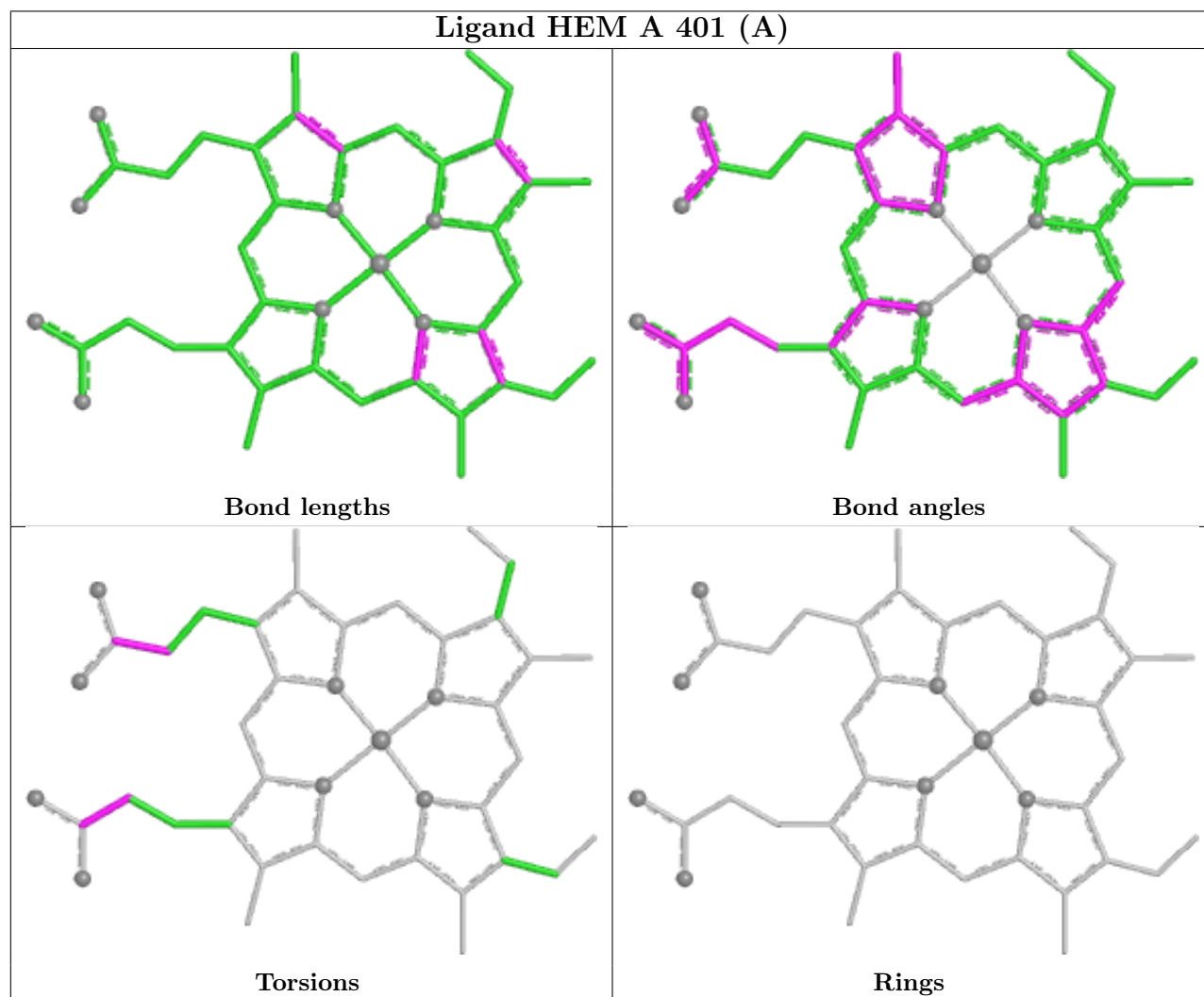
There are no ring outliers.

5 monomers are involved in 9 short contacts:

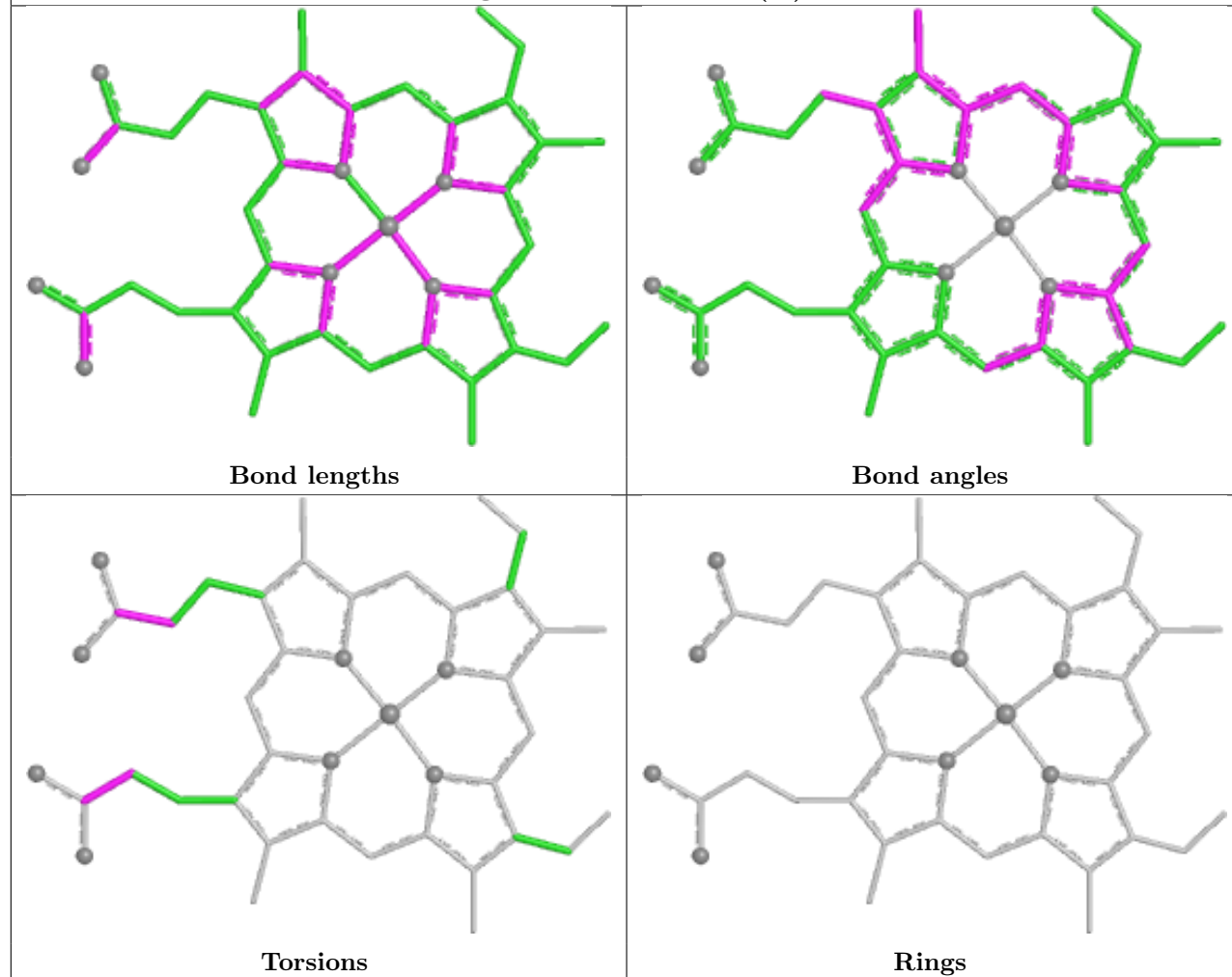
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[A]	HEM	1	0
2	B	401[B]	HEM	4	0
3	B	402	GOL	1	0
2	B	401[A]	HEM	1	0
2	A	401[B]	HEM	2	0

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

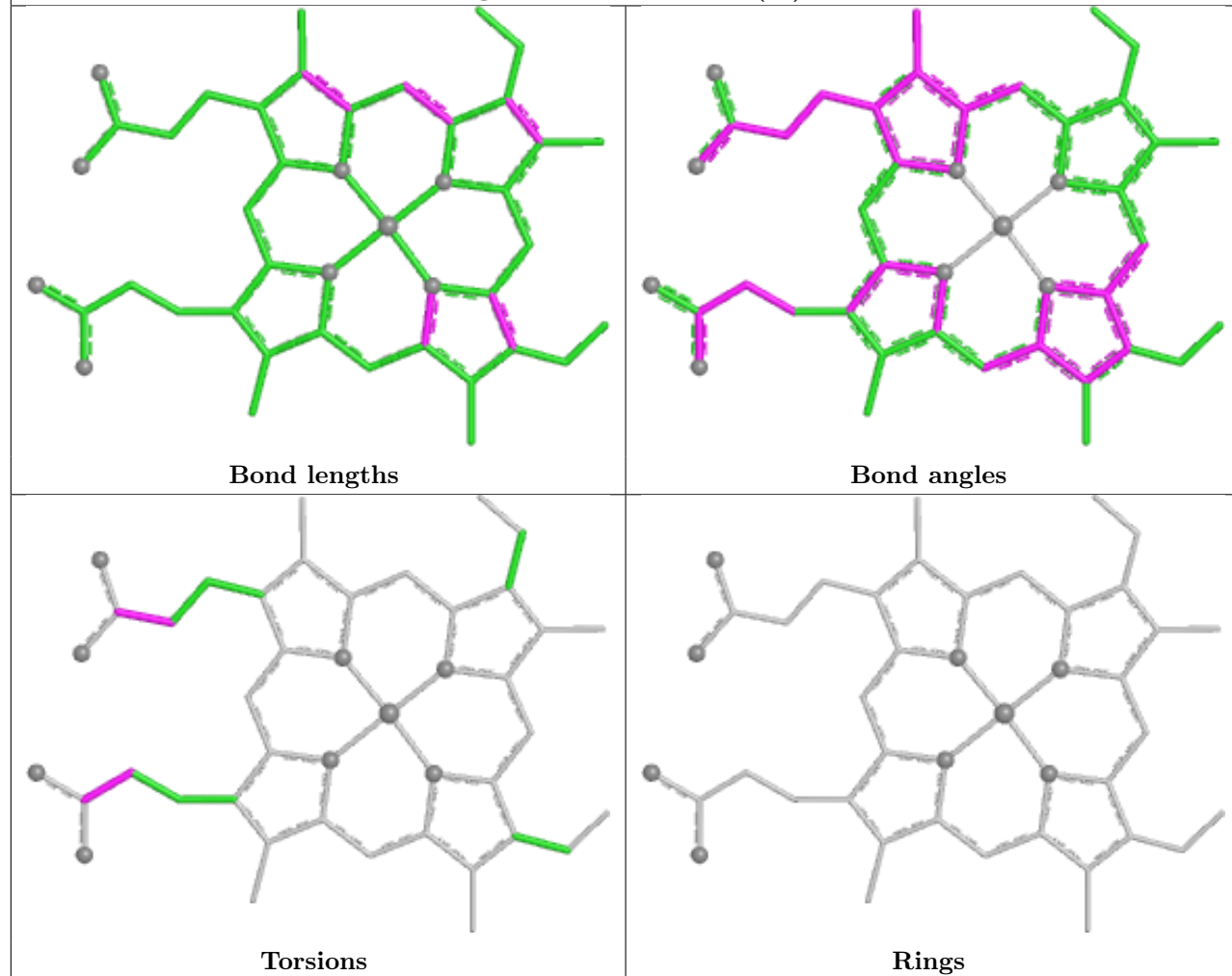
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

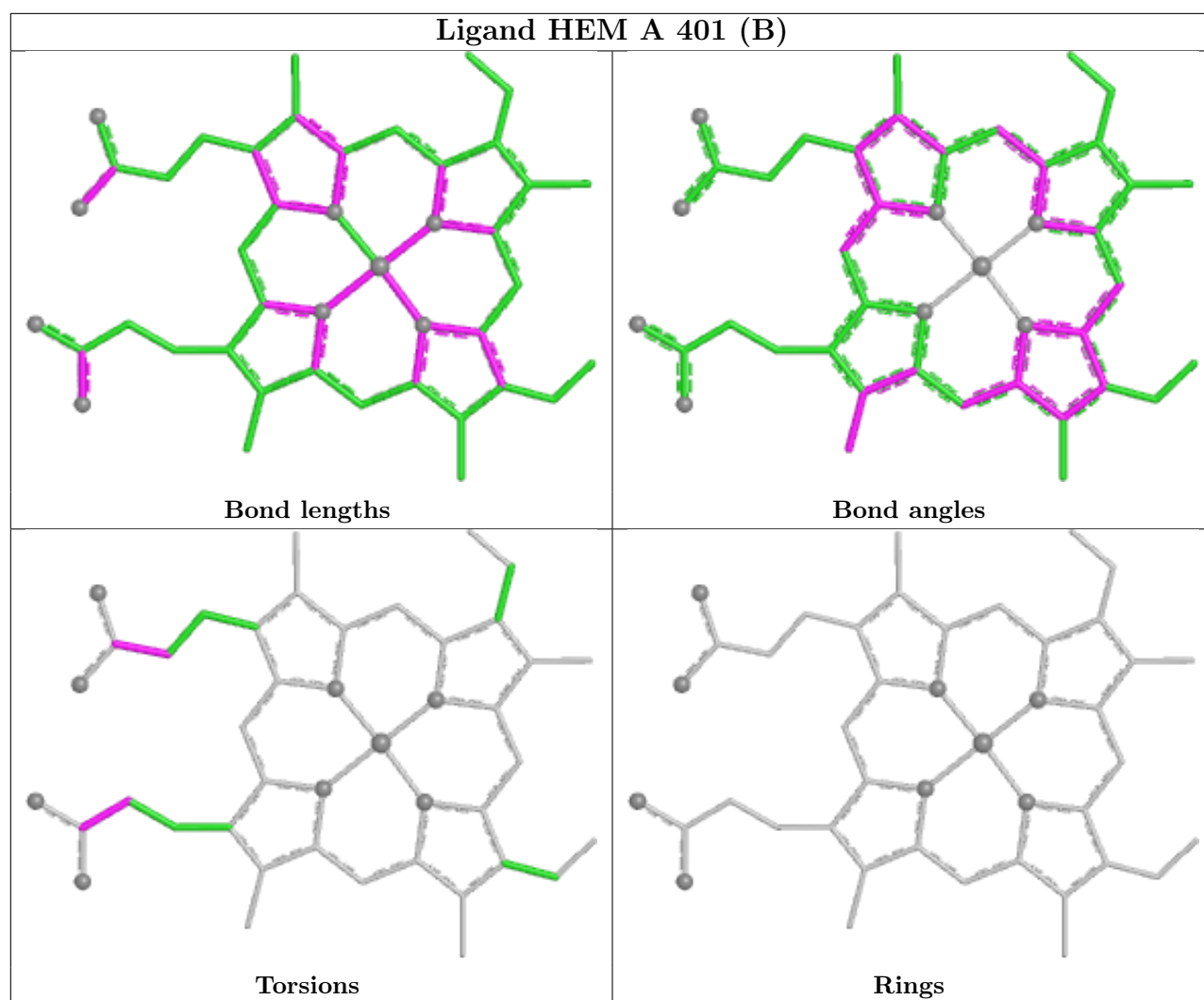


Ligand HEM B 401 (B)



Ligand HEM B 401 (A)





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	301/303 (99%)	-0.13	9 (2%) 52 56	2, 7, 29, 47	12 (3%)
1	B	298/303 (98%)	-0.12	6 (2%) 65 69	2, 9, 31, 63	9 (3%)
All	All	599/606 (98%)	-0.13	15 (2%) 58 62	2, 8, 30, 63	21 (3%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295[B]	ARG	5.5
1	B	300	GLY	5.4
1	A	0	GLY	5.1
1	A	298	ALA	3.4
1	A	297	GLN	3.2
1	B	299	LEU	2.6
1	B	28	ASN	2.4
1	B	226	LYS	2.3
1	B	26	ASP	2.3
1	B	27	VAL	2.3
1	A	50	ASP	2.2
1	A	278[A]	ARG	2.1
1	A	299	LEU	2.1
1	A	1	MET	2.1
1	A	162	ASP	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 ⓘ

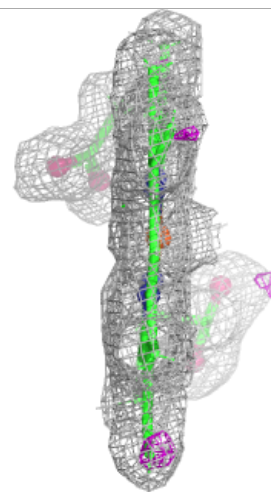
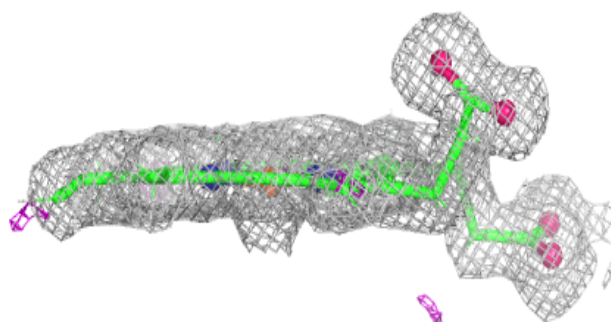
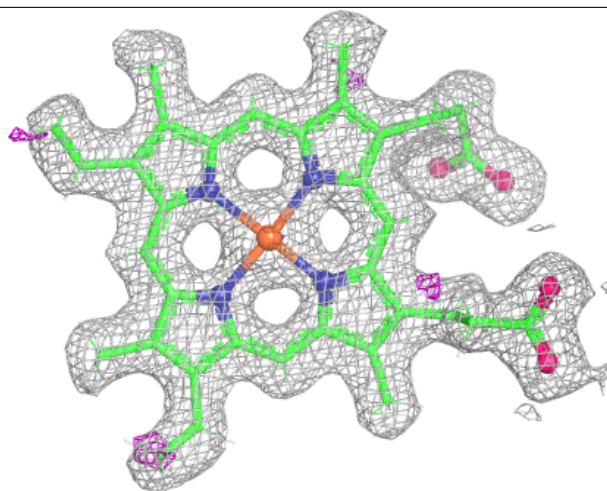
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.72	0.21	42,43,45,45	0
3	GOL	A	405	6/6	0.80	0.15	21,21,21,21	0
3	GOL	B	404	6/6	0.84	0.16	19,19,19,19	0
3	GOL	A	402[A]	6/6	0.86	0.13	19,20,23,23	14
3	GOL	A	402[B]	6/6	0.86	0.13	15,15,17,18	14
3	GOL	A	403	6/6	0.86	0.14	23,28,31,31	0
3	GOL	A	404	6/6	0.88	0.14	24,29,32,32	0
3	GOL	A	406	6/6	0.88	0.15	21,21,21,21	0
3	GOL	B	402	6/6	0.89	0.16	20,29,32,32	0
2	HEM	B	401[B]	43/43	0.96	0.06	3,3,5,6	73
2	HEM	B	401[A]	43/43	0.96	0.06	3,3,5,6	73
4	MG	A	407	1/1	0.96	0.05	20,20,20,20	0
4	MG	B	405	1/1	0.96	0.06	19,19,19,19	0
2	HEM	A	401[B]	43/43	0.98	0.06	3,3,5,6	73
2	HEM	A	401[A]	43/43	0.98	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.

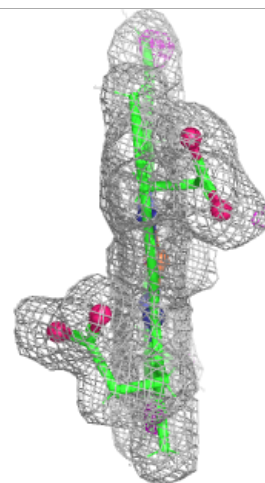
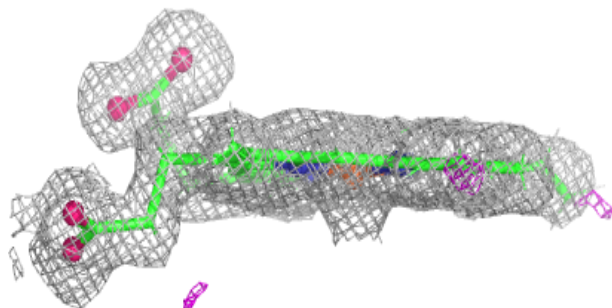
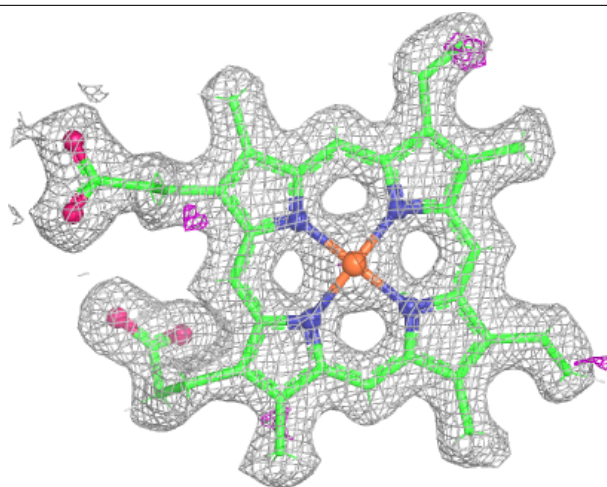
Electron density around HEM B 401 (B):

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



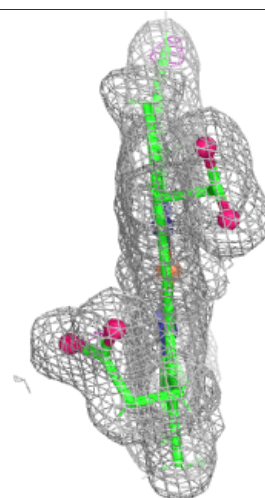
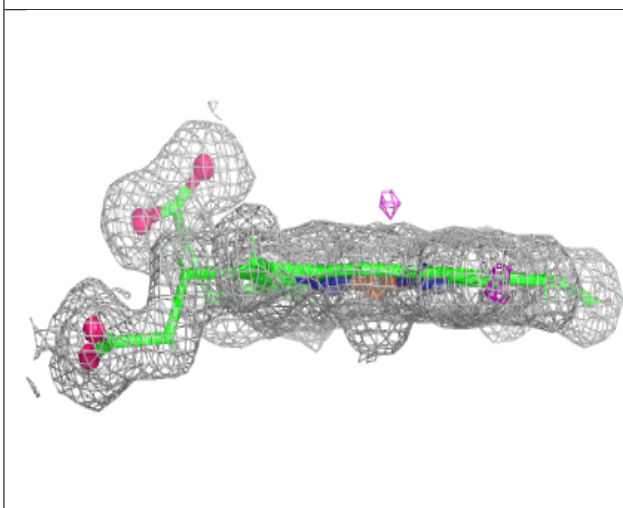
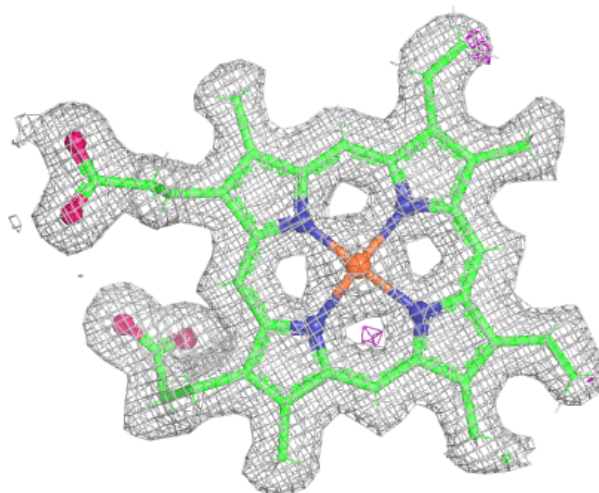
Electron density around HEM B 401 (A):

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



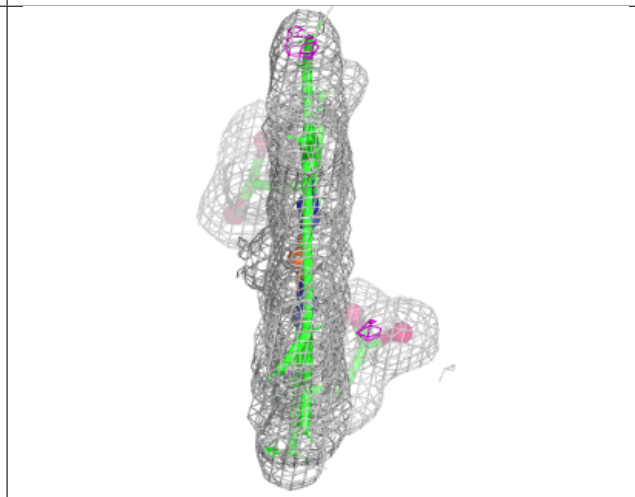
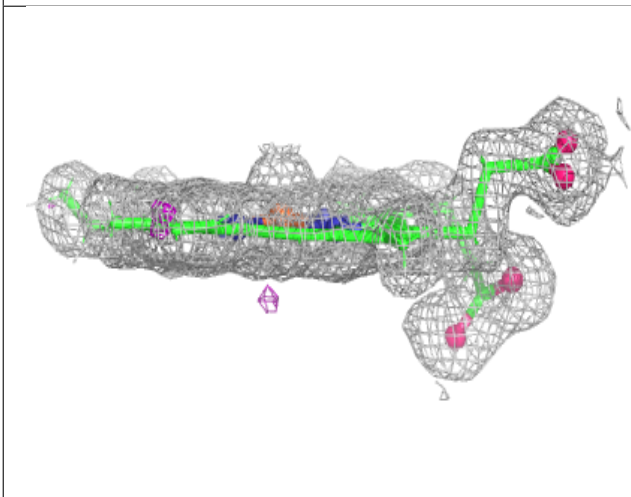
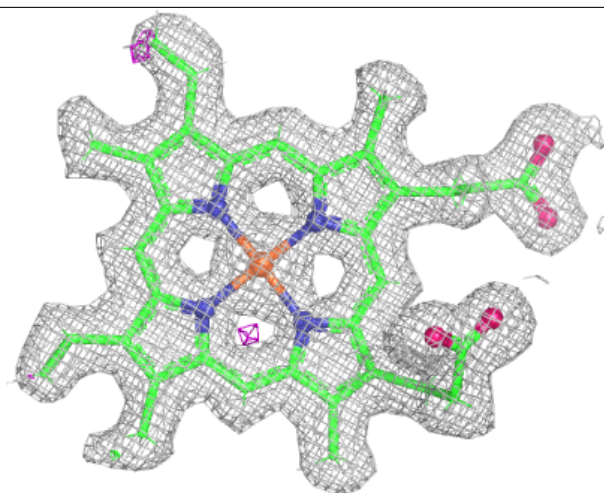
Electron density around HEM A 401 (B):

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.