WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 01:10 pm GMT

PDB ID	:	5FW4
Title	:	Structure of Thermobifida fusca DyP-type Peroxidase and Activity towards Kraft Lignin and Lignin Model Compounds
Authors	:	Rahmanpour, R.; Rea, D.; Jamshidi, S.; Fulop, V.; Bugg, T.D.H.
Deposited on	:	2016-02-11
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
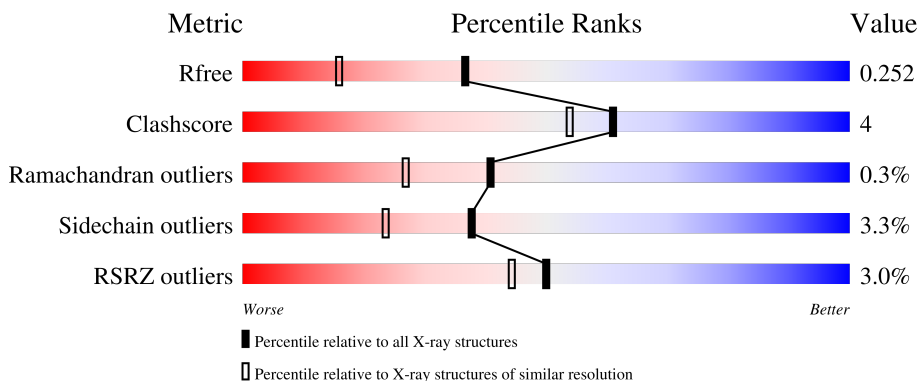
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	430	% 75% 10% · 14%
1	B	430	4% 79% 6% · 14%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6088 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DYE-DECOLORIZING PEROXIDASE TFU_3078.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2793	1726	528	529	10			
1	B	368	Total	C	N	O	S	0	0	0
			2793	1726	528	529	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	LYS	GLU	conflict	UNP Q47KB1
B	13	LYS	GLU	conflict	UNP Q47KB1

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

HEM

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

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

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).
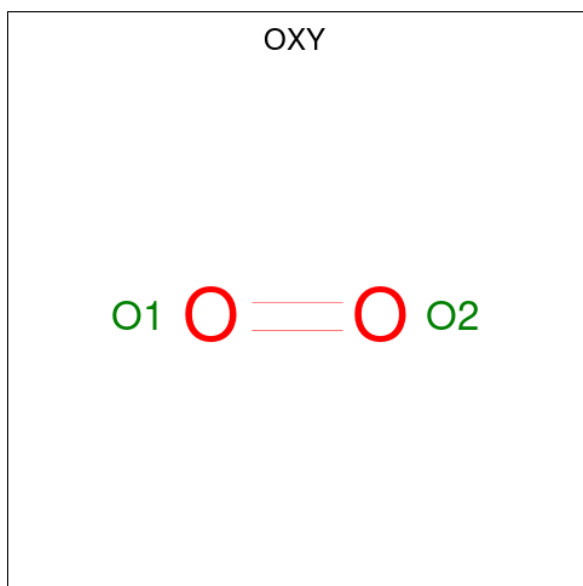
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 2	O 2	0	0
3	B	1	Total 2	O 2	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total 216	O 216	0	0
4	B	196	Total 196	O 196	0	0

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: DYE-DECOLORIZING PEROXIDASE TFU_3078
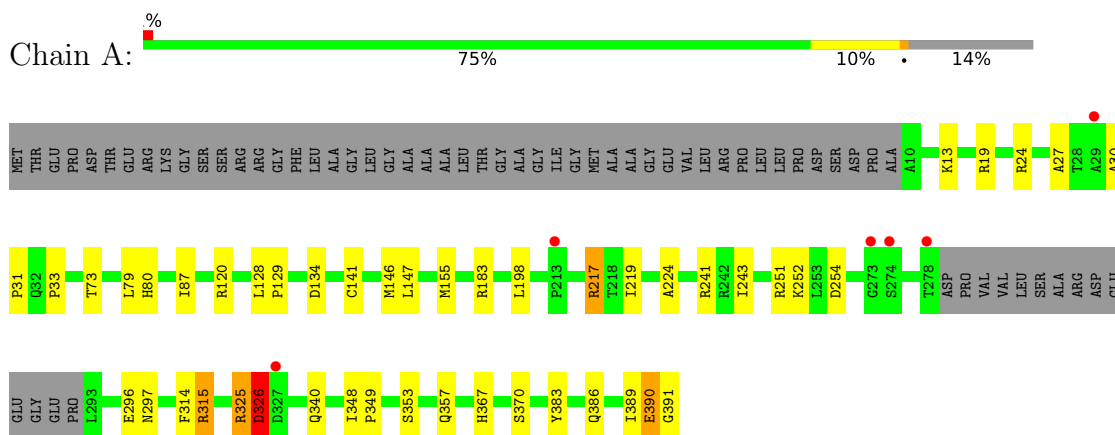
• Molecule 1: DYE-DECOLORIZING PEROXIDASE TFU_3078
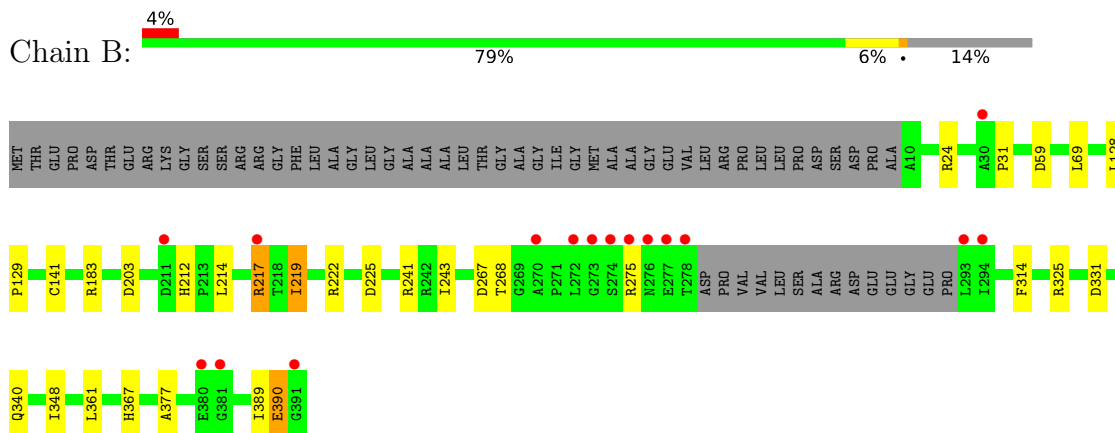
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.36Å 110.21Å 46.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.21 – 1.80 41.21 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.21-1.80) 99.7 (41.21-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.204 , 0.249 0.208 , 0.252	Depositor DCC
R_{free} test set	2805 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.9	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.70	0/2851	0.91	7/3875 (0.2%)
1	B	0.67	0/2851	0.84	3/3875 (0.1%)
All	All	0.69	0/5702	0.87	10/7750 (0.1%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	A	315	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	24	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	24	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	155	MET	CG-SD-CE	5.69	109.30	100.20
1	B	331	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	331	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	134	ASP	CB-CG-OD1	5.07	122.87	118.30
1	B	24	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	326	ASP	O-C-N	-5.01	114.68	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2793	0	2722	30	0
1	B	2793	0	2722	20	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	216	0	0	1	2
4	B	196	0	0	3	1
All	All	6088	0	5504	50	3

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 4.

All (50) 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:141:CYS:HB3	4:B:2096:HOH:O	1.44	1.14
1:A:325:ARG:HG2	1:A:326:ASP:O	1.74	0.86
1:B:129:PRO:HD2	1:B:348:ILE:HD12	1.64	0.77
1:A:128:LEU:HD22	1:A:348:ILE:HD11	1.72	0.71
1:A:386:GLN:NE2	1:A:391:GLY:OXT	2.22	0.68
1:A:219:ILE:HD11	1:A:314:PHE:CB	2.25	0.66
1:A:27:ALA:HB2	1:A:80:HIS:HB3	1.78	0.65
1:A:219:ILE:HD11	1:A:314:PHE:HB3	1.79	0.65
1:A:254:ASP:OD1	1:A:254:ASP:C	2.37	0.62
1:A:129:PRO:HD2	1:A:348:ILE:HD12	1.82	0.60
1:A:146:MET:HG2	1:A:147:LEU:N	2.17	0.58
1:B:241:ARG:HB3	1:B:243:ILE:HD11	1.87	0.57
1:B:275:ARG:NH2	4:B:2174:HOH:O	2.40	0.54
1:A:33:PRO:HG2	1:A:80:HIS:CE1	2.43	0.53
1:A:386:GLN:O	1:A:390:GLU:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:OD1	1:A:254:ASP:O	2.25	0.53
1:A:79:LEU:HD23	1:A:87:ILE:CD1	2.39	0.53
1:A:217:ARG:NH1	1:B:225:ASP:OD2	2.44	0.50
2:A:401:HEM:HBB2	2:A:401:HEM:HMB2	1.94	0.49
1:A:251:ARG:HB3	4:A:2160:HOH:O	2.11	0.49
1:B:390:GLU:HG3	4:B:2018:HOH:O	2.13	0.49
1:A:79:LEU:HD23	1:A:87:ILE:HD12	1.95	0.48
1:A:128:LEU:CD2	1:A:348:ILE:HD11	2.40	0.48
1:B:243:ILE:HD12	1:B:367:HIS:CG	2.48	0.48
1:B:219:ILE:HD11	1:B:314:PHE:HB3	1.96	0.47
1:A:296:GLU:OE1	1:A:296:GLU:N	2.37	0.47
1:A:30:ALA:HA	1:A:31:PRO:C	2.35	0.47
1:B:219:ILE:HD11	1:B:314:PHE:CB	2.45	0.46
1:B:129:PRO:CD	1:B:348:ILE:HD12	2.41	0.46
1:A:241:ARG:HB3	1:A:243:ILE:HD11	1.99	0.45
1:B:203:ASP:OD1	1:B:203:ASP:C	2.55	0.45
1:A:243:ILE:CD1	1:A:367:HIS:ND1	2.80	0.44
1:A:224:ALA:O	1:B:129:PRO:HB3	2.17	0.44
1:B:69:LEU:CD1	1:B:389:ILE:HD11	2.47	0.44
1:B:128:LEU:HD22	1:B:348:ILE:HD11	1.98	0.44
1:A:120:ARG:NH1	1:A:390:GLU:OE2	2.51	0.44
1:B:243:ILE:CD1	1:B:367:HIS:ND1	2.81	0.43
1:B:129:PRO:HD2	1:B:348:ILE:CD1	2.43	0.43
1:A:128:LEU:HD22	1:A:348:ILE:CD1	2.46	0.43
1:B:267:ASP:OD1	1:B:268:THR:N	2.52	0.42
2:A:401:HEM:HBB2	2:A:401:HEM:CMB	2.49	0.42
1:A:353:SER:O	1:A:357:GLN:HB2	2.20	0.41
1:A:219:ILE:HD11	1:A:314:PHE:HB2	2.03	0.41
1:A:141:CYS:HA	1:A:370:SER:O	2.20	0.41
1:A:73:THR:HG21	1:A:383:TYR:HA	2.02	0.41
1:B:214:LEU:HA	1:B:217:ARG:HD3	2.02	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.82	0.41
1:B:31:PRO:CB	1:B:377:ALA:HA	2.50	0.41
1:B:361:LEU:HD21	2:B:401:HEM:C3B	2.56	0.40
1:A:348:ILE:HB	1:A:349:PRO:HD3	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2120:HOH:O	4:B:2120:HOH:O[2_555]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2193:HOH:O	4:A:2193:HOH:O[2_655]	2.11	0.09
4:A:2112:HOH:O	4:A:2112:HOH:O[2_655]	2.15	0.05

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

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	364/430 (85%)	356 (98%)	7 (2%)	1 (0%)	41	27
1	B	364/430 (85%)	355 (98%)	8 (2%)	1 (0%)	41	27
All	All	728/860 (85%)	711 (98%)	15 (2%)	2 (0%)	41	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	GLU
1	B	390	GLU

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	274/318 (86%)	264 (96%)	10 (4%)	35	20
1	B	274/318 (86%)	266 (97%)	8 (3%)	42	29
All	All	548/636 (86%)	530 (97%)	18 (3%)	38	23

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	19	ARG
1	A	183	ARG
1	A	217	ARG
1	A	252	LYS
1	A	297	ASN
1	A	315	ARG
1	A	325	ARG
1	A	340	GLN
1	A	389	ILE
1	B	59	ASP
1	B	183	ARG
1	B	212	HIS
1	B	217	ARG
1	B	219	ILE
1	B	222	ARG
1	B	325	ARG
1	B	340	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	351	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
3	OXY	B	402	-	1,1,1	0.03	0	-		
2	HEM	A	401	3,1	41,50,50	1.25	4 (9%)	45,82,82	1.97	16 (35%)
2	HEM	B	401	1	41,50,50	1.29	5 (12%)	45,82,82	1.96	14 (31%)
3	OXY	A	402	2	1,1,1	0.03	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	3,1	-	4/12/54/54	-
2	HEM	B	401	1	-	4/12/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C1B-NB	-3.87	1.33	1.40
2	B	401	HEM	C1B-NB	-3.41	1.34	1.40
2	B	401	HEM	C4B-NB	-2.96	1.32	1.38
2	B	401	HEM	C4D-ND	-2.43	1.36	1.40
2	A	401	HEM	C4B-NB	-2.41	1.33	1.38
2	A	401	HEM	CHB-C1B	2.38	1.41	1.35
2	B	401	HEM	FE-NB	2.38	2.08	1.96
2	B	401	HEM	C3B-C4B	2.35	1.49	1.44
2	A	401	HEM	FE-NB	2.09	2.07	1.96

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	C1B-NB-C4B	5.59	110.85	105.07
2	B	401	HEM	CHD-C1D-ND	4.96	129.82	124.43
2	A	401	HEM	C1B-NB-C4B	4.61	109.84	105.07
2	A	401	HEM	CHC-C4B-NB	4.36	129.17	124.43
2	B	401	HEM	CHC-C4B-NB	4.16	128.95	124.43
2	A	401	HEM	CMC-C2C-C3C	3.51	131.24	124.68
2	B	401	HEM	CHD-C1D-C2D	-3.46	119.58	124.98
2	A	401	HEM	CHA-C4D-C3D	-3.32	119.10	125.33
2	A	401	HEM	CHA-C4D-ND	3.15	128.28	124.38
2	A	401	HEM	CHD-C1D-ND	2.88	127.56	124.43
2	A	401	HEM	CHD-C1D-C2D	-2.84	120.55	124.98
2	B	401	HEM	CHB-C1B-NB	2.79	127.83	124.38
2	B	401	HEM	C4B-CHC-C1C	2.77	126.22	122.56
2	A	401	HEM	C4B-C3B-C2B	-2.63	105.03	107.11
2	B	401	HEM	CHA-C4D-ND	2.63	127.63	124.38
2	B	401	HEM	CHA-C4D-C3D	-2.59	120.46	125.33
2	A	401	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
2	B	401	HEM	C4A-C3A-C2A	2.51	108.75	107.00
2	B	401	HEM	CAD-C3D-C4D	2.44	128.92	124.66
2	A	401	HEM	CHB-C1B-NB	2.44	127.39	124.38
2	B	401	HEM	CMC-C2C-C3C	2.33	129.04	124.68
2	B	401	HEM	O2A-CGA-CBA	2.29	121.39	114.03
2	A	401	HEM	CAD-C3D-C4D	2.29	128.65	124.66
2	B	401	HEM	O2D-CGD-CBD	2.20	121.09	114.03
2	A	401	HEM	C3D-C4D-ND	2.15	112.56	110.17
2	A	401	HEM	C3C-C4C-NC	-2.15	106.88	110.94
2	A	401	HEM	C4A-C3A-C2A	2.09	108.45	107.00
2	A	401	HEM	C4B-CHC-C1C	2.06	125.28	122.56
2	A	401	HEM	CMD-C2D-C1D	2.01	128.11	125.04
2	B	401	HEM	O2D-CGD-O1D	-2.01	118.29	123.30

There are no chirality outliers.

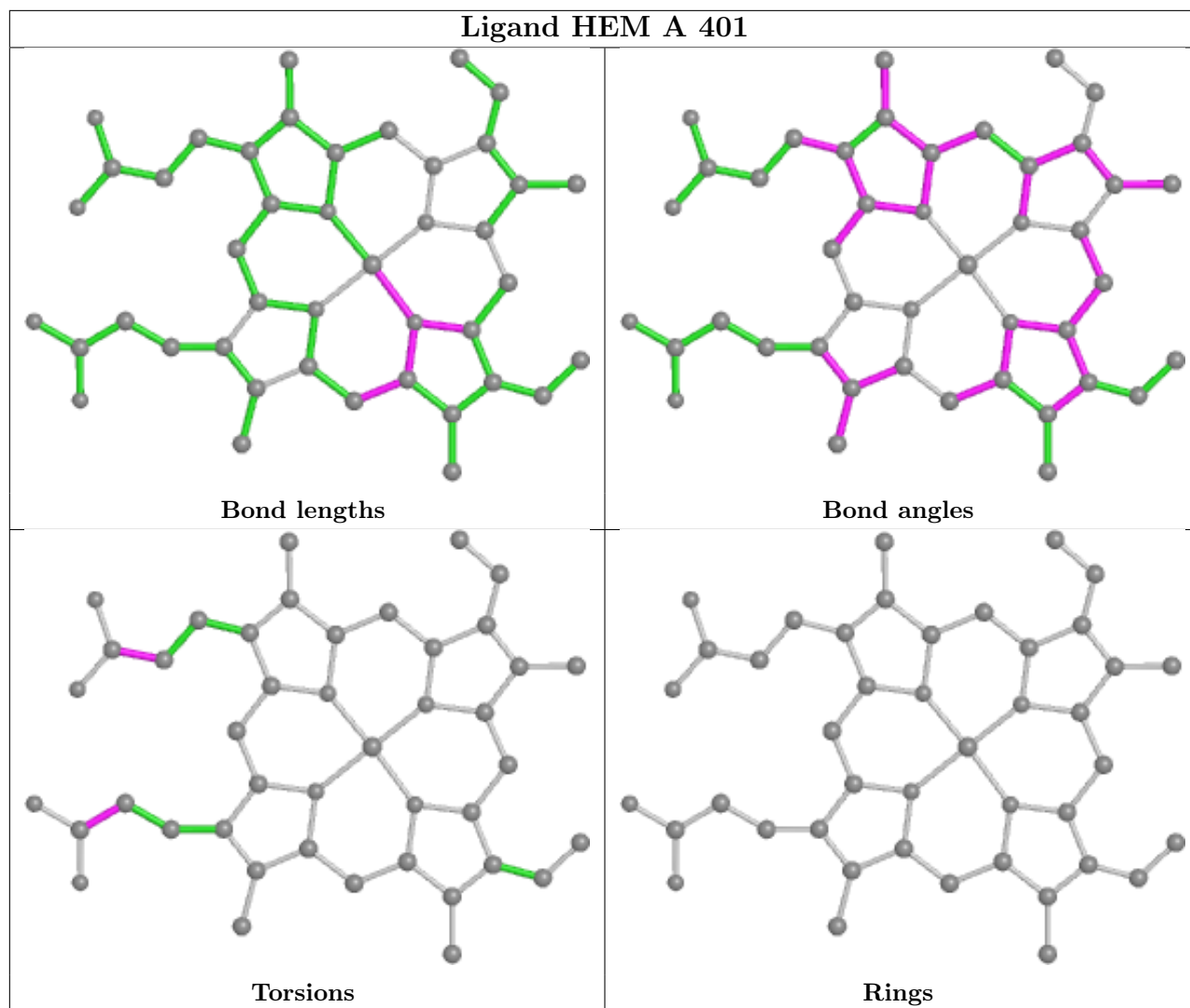All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 401

Bond lengths

Bond angles

Torsions

Rings
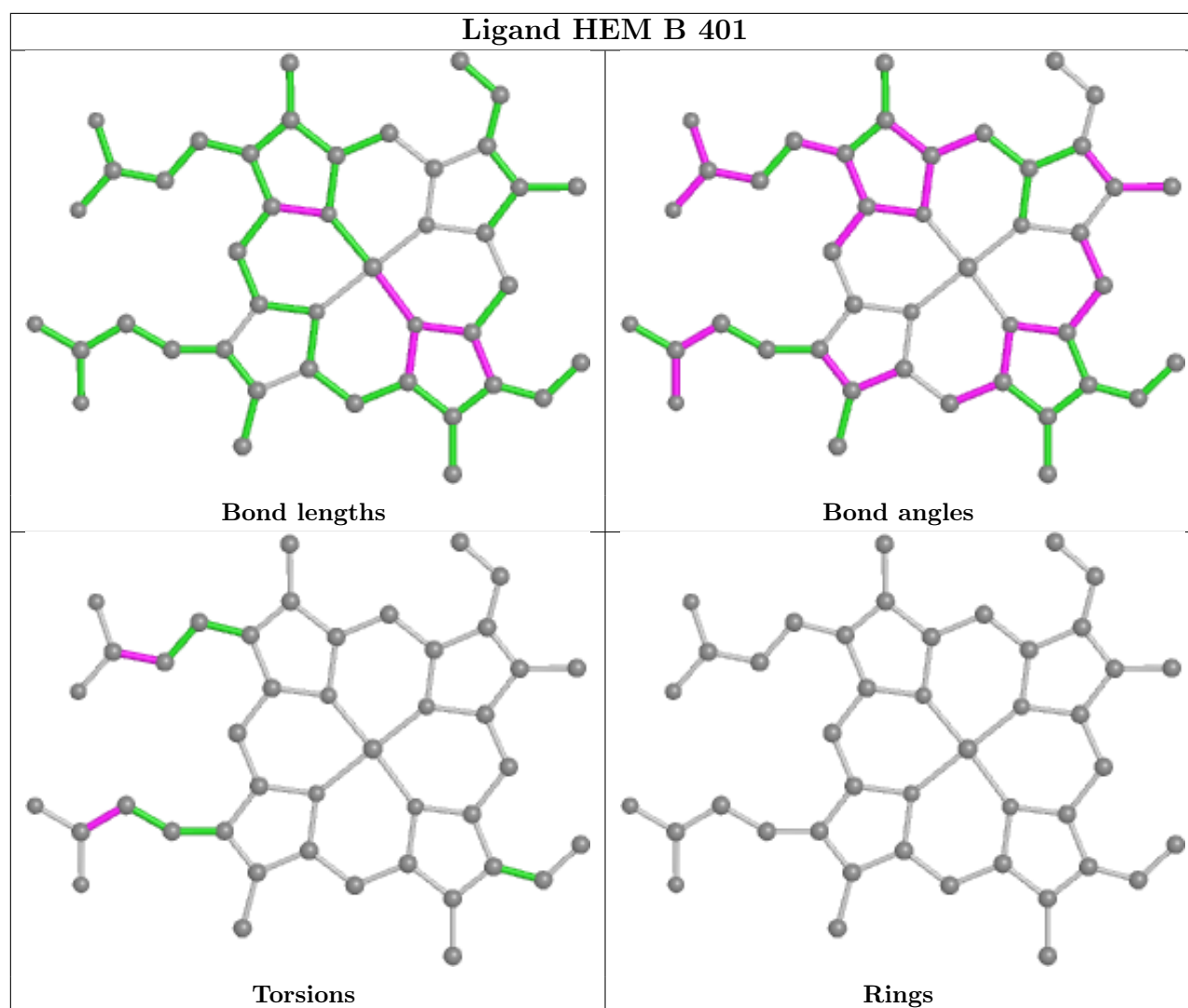
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	368/430 (85%)	0.02	6 (1%)	72	68	15, 29, 48, 67	0
1	B	368/430 (85%)	0.25	16 (4%)	35	29	16, 30, 50, 78	0
All	All	736/860 (85%)	0.13	22 (2%)	50	44	15, 29, 48, 78	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	LEU	5.9
1	B	391	GLY	5.8
1	B	275	ARG	5.3
1	B	278	THR	5.0
1	B	274	SER	4.9
1	A	273	GLY	4.9
1	A	278	THR	4.6
1	B	276	ASN	4.3
1	B	380	GLU	3.6
1	B	381	GLY	3.6
1	B	273	GLY	3.4
1	A	274	SER	3.3
1	B	294	ILE	3.1
1	B	30	ALA	3.1
1	B	270	ALA	2.9
1	B	272	LEU	2.9
1	B	211	ASP	2.7
1	B	217	ARG	2.6
1	A	29	ALA	2.4
1	B	277	GLU	2.4
1	A	213	PRO	2.2
1	A	327	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

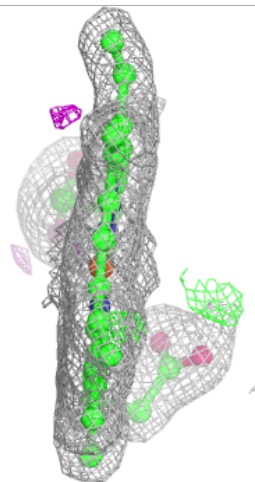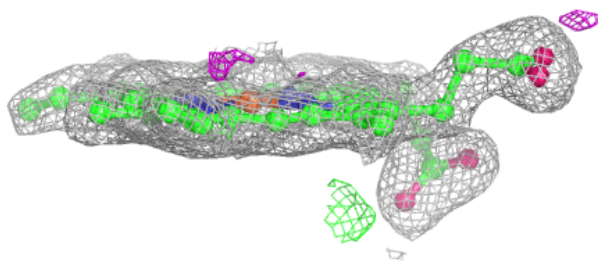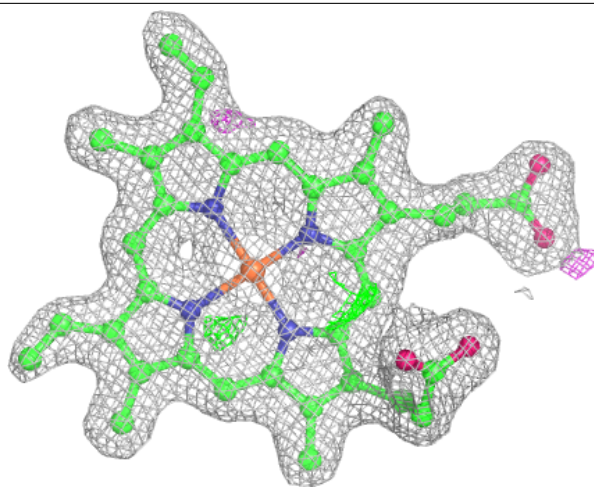There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
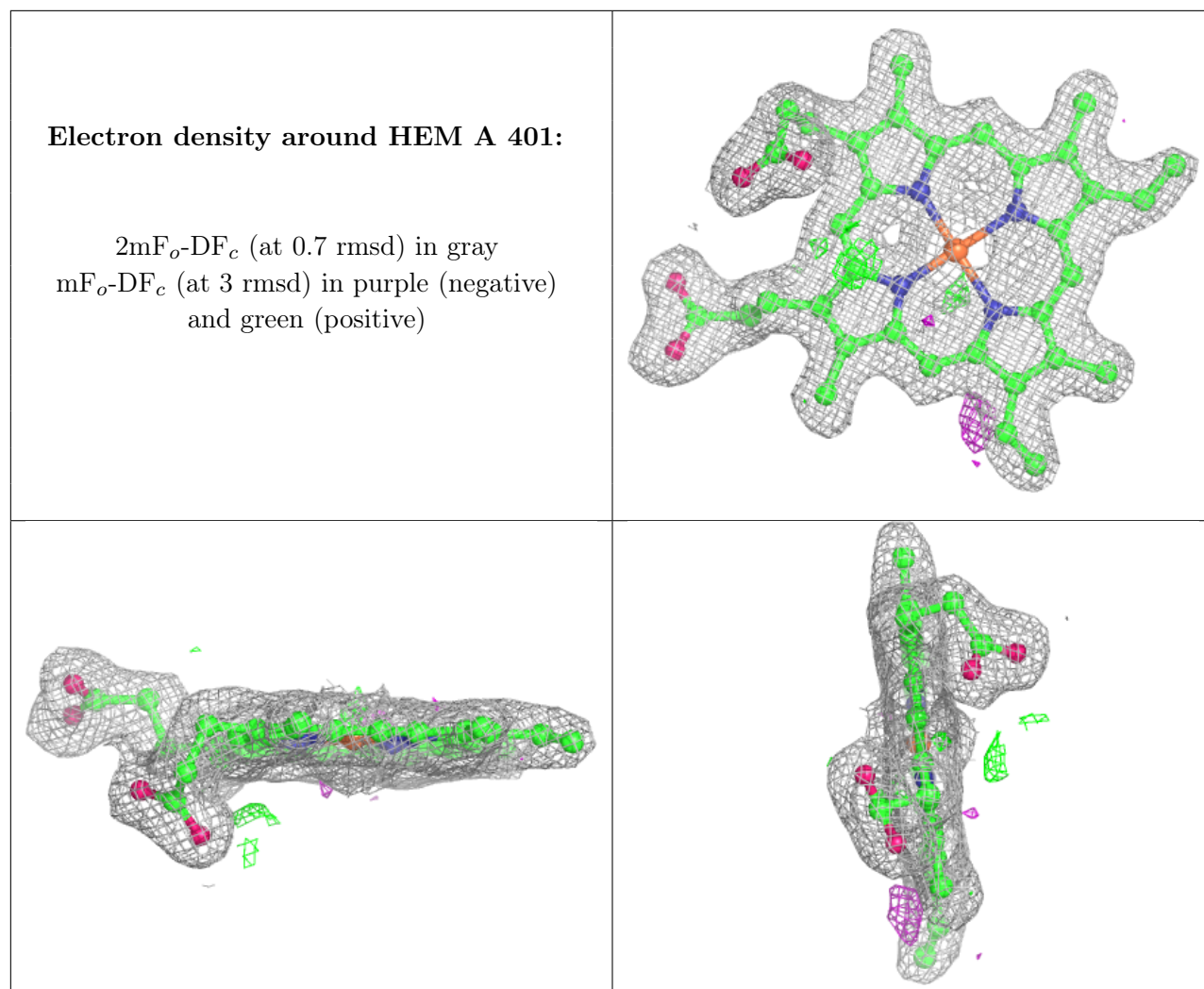
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OXY	A	402	2/2	0.86	0.16	29,29,29,36	0
3	OXY	B	402	2/2	0.87	0.25	44,44,44,46	0
2	HEM	B	401	43/43	0.96	0.10	21,26,34,38	0
2	HEM	A	401	43/43	0.98	0.09	19,23,28,30	0

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 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)

Electron density around HEM A 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.