

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 20, 2023 – 09:43 PM JST

PDB ID : 7DMR

Title: Crystal structure of potassium induced heme modification in yak lactoperoxi-

dase at 2.20 A resolution

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Deposited on : 2020-12-06

Resolution : 2.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), 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)

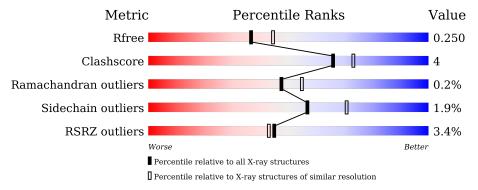
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.20 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	595	90%	10%			
2	В	2	50%				



## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5345 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 Lactoperoxidase.

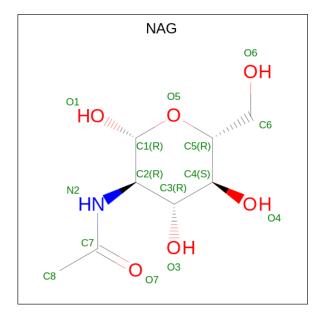
$\mathbf{Mol}$	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	595	Total 4770	C 3037	N 847	O 860	S 26	0	0	0

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



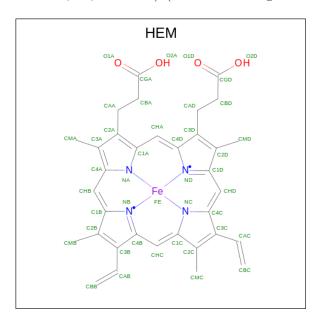


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

• Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	A	1	Total 48	C 37		N 4	O 6	0	1

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

 $\bullet$  Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0

• Molecule 9 is water.

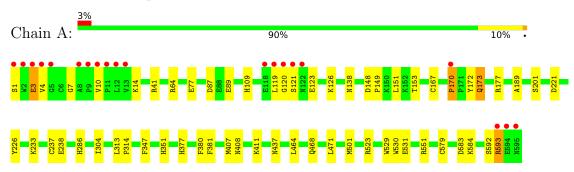
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	452	Total O 452 452	0	0



# 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: Lactoperoxidase



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50% 50%





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	80.24Å 85.31Å 98.93Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.61 - 2.20	Depositor
Resolution (A)	64.61 - 2.20	EDS
% Data completeness	99.7 (64.61-2.20)	Depositor
(in resolution range)	99.7 (64.61-2.20)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$< I/\sigma(I) > 1$	2.42 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.190 , 0.243	Depositor
$R, R_{free}$	0.195 , $0.250$	DCC
$R_{free}$ test set	1815 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 50.4	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5345	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: CL, K, ZN, CA, HEM, NAG

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).

Mal	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.66	0/4898	0.81	1/6645 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	170	PRO	N-CA-C	5.02	125.14	112.10

There are no chirality outliers.

There are no planarity outliers.

### 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	4770	0	4688	37	0
2	В	28	0	25	1	0
3	A	42	0	39	0	0
4	A	1	0	0	0	0
5	A	48	0	8	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	1	0
9	A	452	0	0	7	0
All	All	5345	0	4760	38	0



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
1:A:138:ASN:ND2	9:A:702:HOH:O	2.13	0.81
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.29	0.80
1:A:119:LEU:HD21	1:A:138:ASN:HB2	1.63	0.78
1:A:109:HIS:NE2	8:A:609:K:K	2.13	0.74
1:A:201:SER:OG	9:A:701:HOH:O	2.09	0.70
1:A:593:ARG:NH2	9:A:705:HOH:O	2.28	0.67
1:A:1:SER:N	1:A:177:ARG:HD2	2.16	0.61
1:A:119:LEU:HD21	1:A:138:ASN:CB	2.29	0.60
1:A:41:ARG:NE	9:A:707:HOH:O	2.35	0.58
1:A:121:SER:HB3	9:A:1012:HOH:O	2.04	0.57
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.86	0.57
9:A:1151:HOH:O	2:B:2:NAG:O4	2.19	0.52
1:A:87:ASP:OD1	1:A:89:GLU:HB2	2.10	0.52
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.45	0.51
1:A:123:GLU:HB3	1:A:126:LYS:H	1.75	0.51
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.46	0.51
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.46	0.50
1:A:1:SER:H3	1:A:177:ARG:HD2	1.77	0.49
1:A:286:HIS:CE1	1:A:592:SER:O	2.66	0.49
1:A:579:CYS:HB2	9:A:1064:HOH:O	2.12	0.48
1:A:551:ARG:HD3	1:A:583:ASP:O	2.14	0.48
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.47
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.96	0.47
1:A:7:GLY:HA3	1:A:167:CYS:SG	2.55	0.46
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.50	0.46
1:A:593:ARG:N	1:A:593:ARG:HD3	2.31	0.46
1:A:313:LEU:N	1:A:314:PRO:CD	2.79	0.46
1:A:464:LEU:O	1:A:468:GLN:HG3	2.17	0.45
1:A:3:GLU:O	1:A:3:GLU:HG3	2.18	0.44
1:A:593:ARG:HD3	1:A:593:ARG:H	1.83	0.43
1:A:148:ASP:O	1:A:151:LEU:HB2	2.18	0.43
1:A:407:MET:HB3	1:A:501:MET:CE	2.48	0.43
1:A:233:LYS:NZ	1:A:238:GLU:OE1	2.46	0.42
1:A:173:GLN:H	1:A:173:GLN:HG3	1.66	0.42
1:A:120:GLY:O	1:A:123:GLU:HG2	2.21	0.41
1:A:408:ASN:HB3	1:A:411:LYS:HB2	2.02	0.41
1:A:148:ASP:HA	1:A:149:PRO:HD2	1.95	0.40



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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)	
1:A:170:PRO:HA	1:A:172:TYR:CZ	2.57	0.40	

There are no symmetry-related clashes.

### 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	593/595 (100%)	571 (96%)	21 (4%)	1 (0%)	47 55	

### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	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.

Mo	l Cha	in	Analysed	Analysed Rotameric		Perce	ntiles
1	A		518/518 (100%)	508 (98%)	10 (2%)	57	71

#### All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	10	VAL



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Mol	Chain	Res	Type
1	A	14	LYS
1	A	64	ARG
1	A	77	GLU
1	A	153	THR
1	A	173	GLN
1	A	347	PHE
1	A	471	LEU
1	A	593	ARG

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	128	GLN
1	A	138	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)

2 monosaccharides 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	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain Res	Link	Bond lengths			Bond angles		
MIOI	туре		nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2																				
2	NAG	В	1	2,1	14,14,15	0.47	0	17,19,21	1.20	2 (11%)																				
2	NAG	В	2	2	14,14,15	0.37	0	17,19,21	1.51	2 (11%)																				



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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	NAG	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	2	NAG	C1-O5-C5	4.21	117.90	112.19
2	В	1	NAG	O5-C5-C6	3.83	113.21	107.20
2	В	2	NAG	C1-C2-N2	-3.52	104.48	110.49
2	В	1	NAG	C4-C3-C2	-2.34	107.59	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C8-C7-N2-C2
2	В	2	NAG	O5-C5-C6-O6
2	В	2	NAG	C4-C5-C6-O6

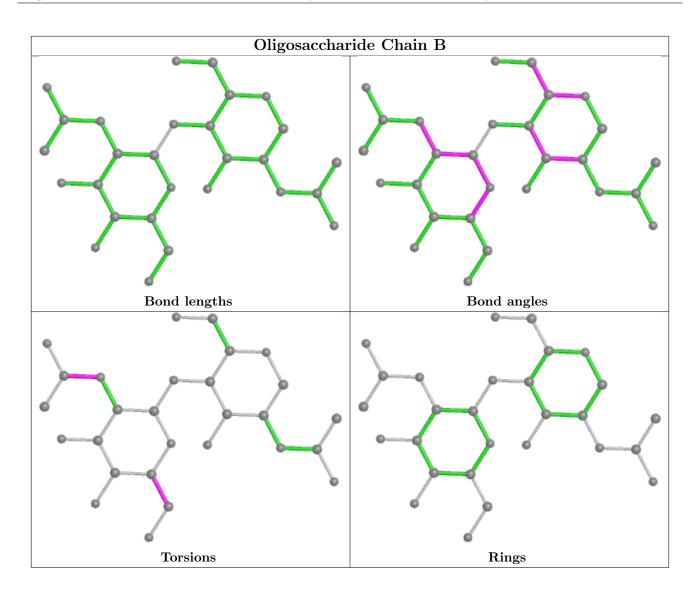
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2	NAG	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 oligosaccharide.





## 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	Trus	Chain	Dec	Link	Во	Bond lengths			Bond angles		
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	NAG	A	601	1	14,14,15	0.45	0	17,19,21	1.91	4 (23%)	
5	HEM	A	605[A]	8	41,50,50	1.50	7 (17%)	45,82,82	1.74	11 (24%)	
5	HEM	A	605[B]	-	41,50,50	1.52	7 (17%)	45,82,82	1.62	8 (17%)	



Mol	Trunc	Chain	Dec	Timle	Bond lengths			В	ond ang	gles
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	NAG	A	602	1	14,14,15	0.62	0	17,19,21	1.85	6 (35%)
3	NAG	A	603	1	14,14,15	0.73	0	17,19,21	2.00	3 (17%)

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	NAG	A	601	1	-	3/6/23/26	0/1/1/1
5	HEM	A	605[A]	8	-	5/12/54/54	-
5	HEM	A	605[B]	-	-	4/12/54/54	-
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	1/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
5	A	605[A]	HEM	FE-NB	3.72	2.15	1.96
5	A	605[B]	HEM	FE-NB	3.72	2.15	1.96
5	A	605[A]	HEM	C4D-C3D	3.58	1.51	1.45
5	A	605[B]	HEM	C4D-C3D	3.58	1.51	1.45
5	A	605[A]	HEM	C1D-C2D	3.03	1.50	1.44
5	A	605[B]	HEM	C1D-C2D	3.03	1.50	1.44
5	A	605[A]	HEM	C1B-NB	-2.82	1.35	1.40
5	A	605[B]	HEM	C1B-NB	-2.82	1.35	1.40
5	A	605[A]	HEM	C3B-C4B	2.71	1.50	1.44
5	A	605[B]	HEM	C3B-C4B	2.71	1.50	1.44
5	A	605[A]	HEM	C3C-C2C	-2.20	1.37	1.40
5	A	605[B]	HEM	C3C-C2C	-2.20	1.37	1.40
5	A	605[A]	HEM	C1A-CHA	-2.06	1.35	1.41
5	A	605[B]	HEM	C1A-CHA	-2.06	1.35	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
3	A	603	NAG	C1-O5-C5	6.21	120.60	112.19
3	A	601	NAG	C1-O5-C5	4.95	118.89	112.19
3	A	602	NAG	C1-C2-N2	-4.28	103.17	110.49
5	A	605[A]	HEM	O2A-CGA-O1A	-4.14	112.97	123.30
5	A	605[B]	HEM	O2A-CGA-O1A	-4.14	112.97	123.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	605[A]	HEM	O2A-CGA-CBA	3.54	125.40	114.03
5	A	605[B]	HEM	O2A-CGA-CBA	3.54	125.40	114.03
3	A	601	NAG	O5-C1-C2	-3.35	105.99	111.29
5	A	605[A]	HEM	O2D-CGD-CBD	3.12	124.05	114.03
5	A	605[A]	HEM	C4D-C3D-C2D	-2.86	102.74	106.90
5	A	605[B]	HEM	C4D-C3D-C2D	-2.86	102.74	106.90
3	A	602	NAG	O5-C1-C2	-2.78	106.91	111.29
3	A	603	NAG	C6-C5-C4	-2.69	106.70	113.00
5	A	605[A]	HEM	O2D-CGD-O1D	-2.62	116.77	123.30
5	A	605[A]	HEM	CBD-CAD-C3D	-2.58	105.46	112.63
5	A	605[A]	HEM	C1B-NB-C4B	2.56	107.72	105.07
5	A	605[B]	HEM	C1B-NB-C4B	2.56	107.72	105.07
5	A	605[A]	HEM	CHC-C4B-NB	2.50	127.14	124.43
5	A	605[B]	HEM	CHC-C4B-NB	2.50	127.14	124.43
3	A	603	NAG	C4-C3-C2	2.44	114.59	111.02
3	A	602	NAG	C4-C3-C2	2.42	114.56	111.02
5	A	605[A]	HEM	C3D-C4D-ND	2.40	112.84	110.17
5	A	605[B]	HEM	C3D-C4D-ND	2.40	112.84	110.17
3	A	601	NAG	C8-C7-N2	2.37	120.11	116.10
5	A	605[A]	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
5	A	605[B]	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
3	A	602	NAG	C3-C4-C5	-2.30	106.13	110.24
3	A	601	NAG	C4-C3-C2	-2.24	107.74	111.02
5	A	605[A]	HEM	C4B-CHC-C1C	2.17	125.42	122.56
5	A	605[B]	HEM	C4B-CHC-C1C	2.17	125.42	122.56
3	A	602	NAG	C2-N2-C7	2.04	125.81	122.90
3	A	602	NAG	O4-C4-C3	2.03	115.04	110.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605[A]	HEM	C3D-CAD-CBD-CGD
3	A	601	NAG	C8-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
3	A	601	NAG	O5-C5-C6-O6
3	A	603	NAG	C4-C5-C6-O6
5	A	605[A]	HEM	CAA-CBA-CGA-O2A
5	A	605[B]	HEM	CAA-CBA-CGA-O2A
5	A	605[A]	HEM	CAA-CBA-CGA-O1A
5	A	605[B]	HEM	CAA-CBA-CGA-O1A
5	A	605[A]	HEM	CAD-CBD-CGD-O1D



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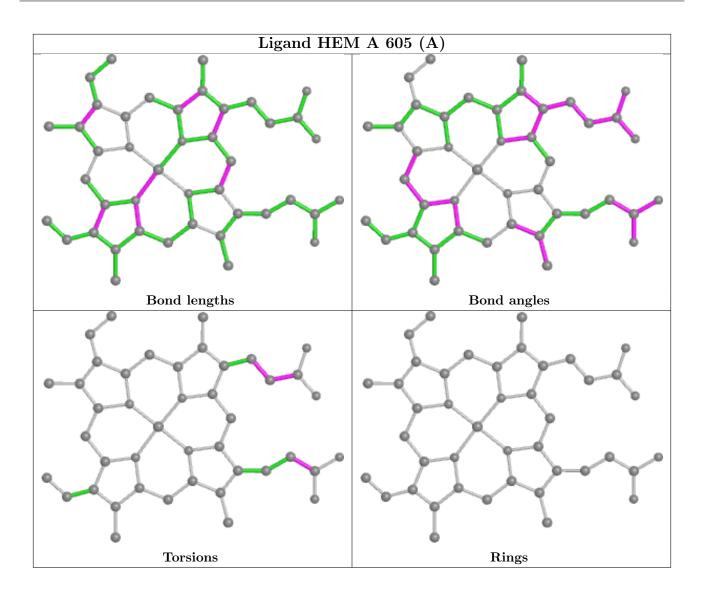
Mol	Chain	Res	Type	Atoms
5	A	605[A]	HEM	CAD-CBD-CGD-O2D
5	A	605[B]	HEM	CAD-CBD-CGD-O2D
5	A	605[B]	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

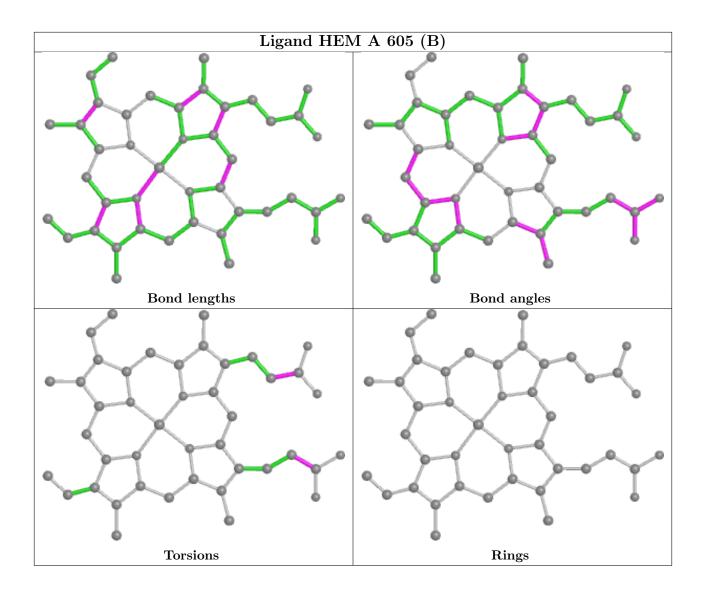
No monomer is involved in short contacts.

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.









# 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	595/595 (100%)	-0.17	20 (3%) 45 43	17, 28, 59, 135	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	GLU	13.5
1	A	2	TRP	12.1
1	A	1	SER	10.4
1	A	122	ASN	10.3
1	A	121	SER	9.6
1	A	119	LEU	8.7
1	A	120	GLY	7.8
1	A	11	PRO	7.7
1	A	595	ASN	7.6
1	A	9	PRO	7.3
1	A	10	VAL	5.3
1	A	12	LEU	4.8
1	A	170	PRO	3.7
1	A	5	GLY	3.6
1	A	13	VAL	3.5
1	A	4	VAL	3.3
1	A	3	GLU	3.1
1	A	593	ARG	2.9
1	A	118	GLU	2.4
1	A	8	ALA	2.3

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

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

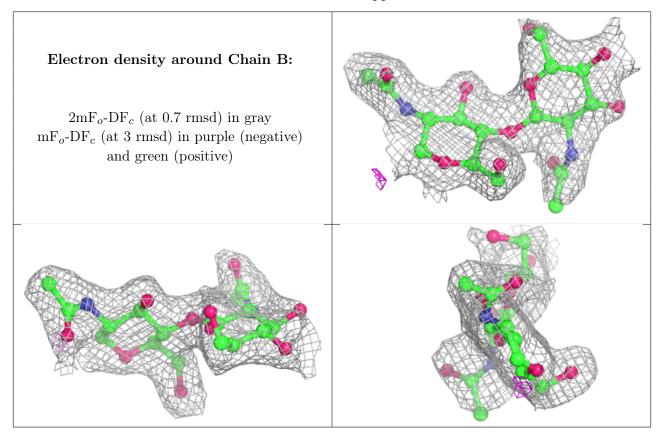


## 6.3 Carbohydrates (i)

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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	NAG	В	2	14/15	0.88	0.16	55,60,64,65	0
2	NAG	В	1	14/15	0.93	0.10	32,36,39,42	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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,  $95^{th}$  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.

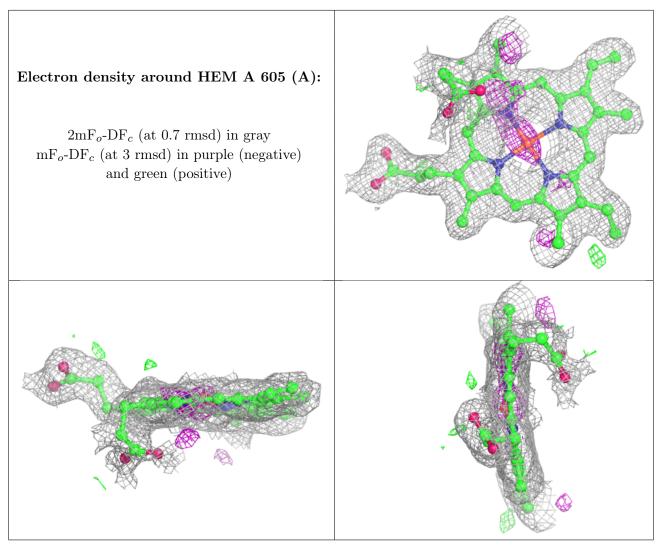
Mol	Type	Chain	$\operatorname{Res}$	Atoms	RSCC	RSR	$oxed{ \mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2) }$	Q<0.9
3	NAG	A	601	14/15	0.84	0.16	51,56,64,74	0



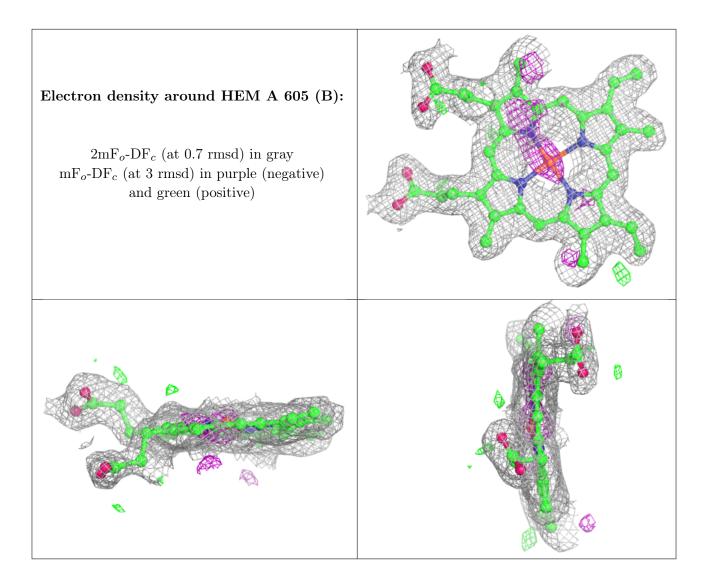
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	NAG	A	603	14/15	0.86	0.16	37,45,50,57	0
3	NAG	A	602	14/15	0.87	0.17	37,41,43,49	0
6	ZN	A	607	1/1	0.88	0.20	59,59,59,59	1
8	K	A	609	1/1	0.95	0.13	29,29,29,29	0
5	HEM	A	605[A]	43/43	0.96	0.12	20,22,26,28	5
5	HEM	A	605[B]	43/43	0.96	0.12	16,22,24,27	5
7	CL	A	608	1/1	0.97	0.07	27,27,27,27	0
4	CA	A	604	1/1	0.97	0.11	21,21,21,21	0
6	ZN	A	606	1/1	0.99	0.07	35,35,35,35	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.







## 6.5 Other polymers (i)

There are no such residues in this entry.

