



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 03:25 AM EDT

PDB ID : 2IKC
Title : Crystal structure of sheep lactoperoxidase at 3.25 Å resolution reveals the binding sites for formate
Authors : Sheikh, I.A.; Singh, N.; Singh, A.K.; Sharma, S.; Singh, T.P.
Deposited on : unknown
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

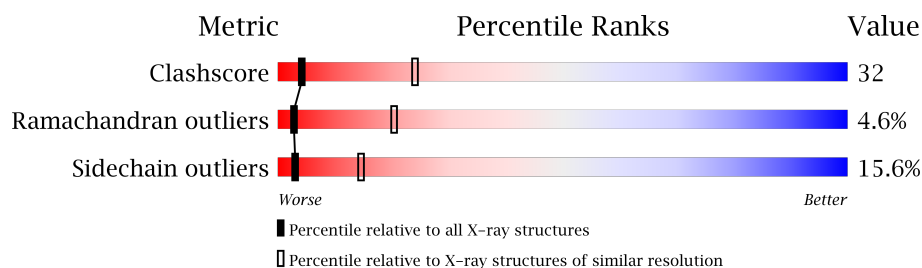
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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))
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	595	
1	B	595	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FMT	A	3002	-	-	X	-

2 Entry composition [i](#)

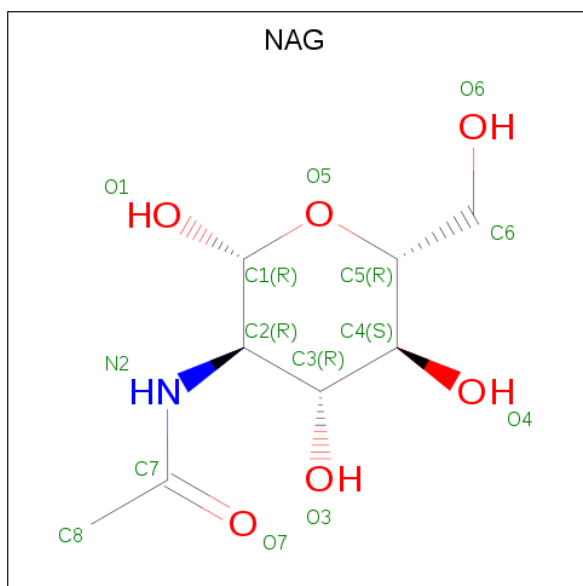
There are 8 unique types of molecules in this entry. The entry contains 10008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 milk lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4764	3024	853	861	26			
1	B	595	Total	C	N	O	S	0	0	0
			4764	3024	853	861	26			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



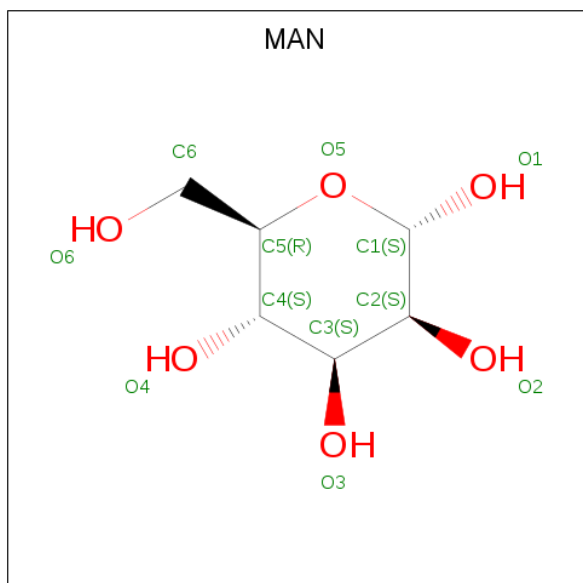
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

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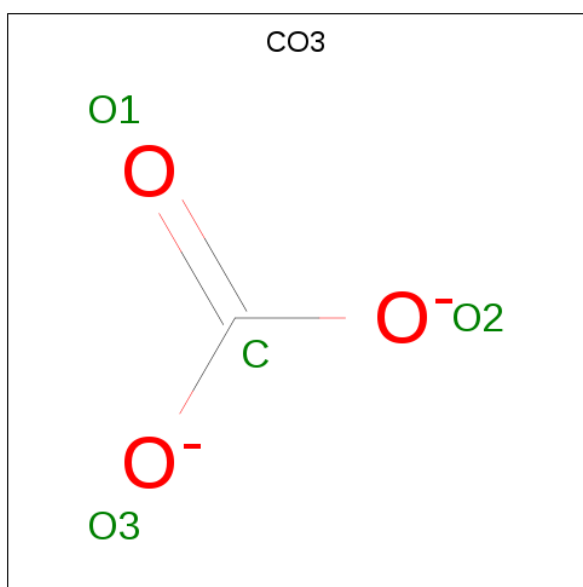
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			11	6	5		

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

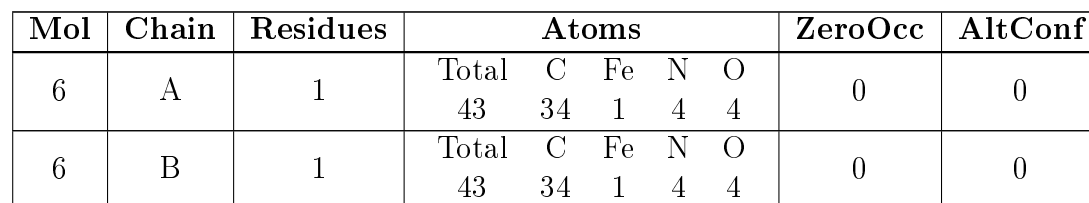
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



- FMT
-
- The diagram shows the chemical structure of formic acid (FMT). It consists of a central carbon atom (C) double-bonded to an oxygen atom (O) and single-bonded to a hydroxyl group (OH). The carbon atom is labeled 'C' in green. The double-bonded oxygen atom is labeled 'O1' in green. The single-bonded oxygen atom is labeled 'O2' in green. The hydrogen atom is labeled 'H' in red. The bonds are shown as gray lines, with the double bond represented by two parallel lines. The oxygen and hydrogen atoms are shown in red.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 3 1 2	0	0
7	A	1	Total C O 3 1 2	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 3	C 1	O 2	0	0
7	B	1	Total 3	C 1	O 2	0	0
7	B	1	Total 3	C 1	O 2	0	0
7	B	1	Total 3	C 1	O 2	0	0

- Molecule 8 is water.

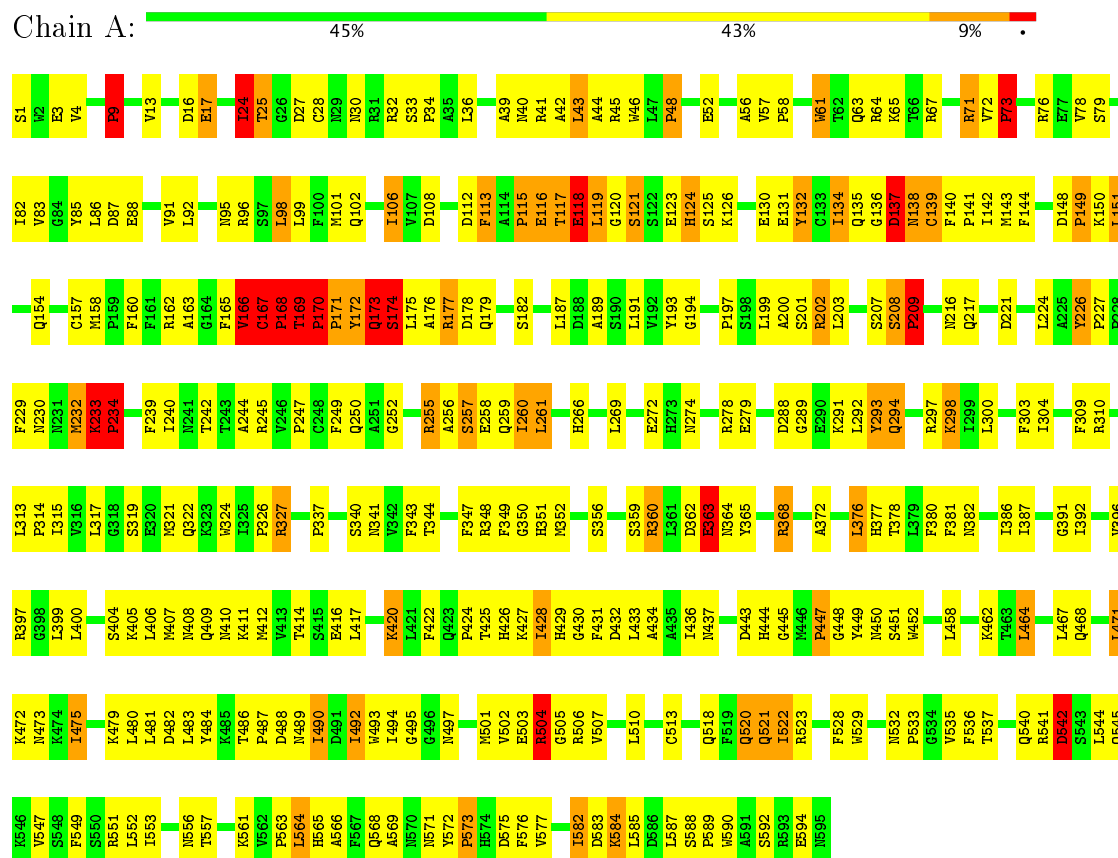
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	86	Total 86	O 86	0	0
8	B	62	Total 62	O 62	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: milk lactoperoxidase





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.08 Å 72.59 Å 84.47 Å 85.20° 84.07° 75.41°	Depositor
Resolution (Å)	19.97 – 3.25	Depositor
% Data completeness (in resolution range)	96.4 (19.97-3.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.187 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10008	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, NAG, FMT, HEM, CA, MAN

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	0.64	7/4889 (0.1%)	1.10	36/6629 (0.5%)
1	B	0.64	3/4889 (0.1%)	1.04	24/6629 (0.4%)
All	All	0.64	10/9778 (0.1%)	1.07	60/13258 (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	B	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	ARG	N-CA	18.38	1.83	1.46
1	A	24	ILE	N-CA	6.80	1.59	1.46
1	A	9	PRO	N-CA	6.63	1.58	1.47
1	A	172	TYR	N-CA	6.18	1.58	1.46
1	A	118	GLU	N-CA	-5.61	1.35	1.46

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	LYS	C-N-CD	-19.31	78.12	120.60
1	B	67	ARG	N-CA-CB	-17.09	79.85	110.60
1	A	233	LYS	C-N-CD	-14.78	88.09	120.60
1	A	172	TYR	CB-CG-CD2	-14.67	112.20	121.00
1	A	172	TYR	CB-CG-CD1	14.37	129.62	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	570	ASN	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	4764	0	4684	315	0
1	B	4764	0	4683	304	0
2	A	98	0	87	13	0
2	B	98	0	87	0	0
3	A	11	0	10	1	0
3	B	11	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	43	0	30	8	0
6	B	43	0	30	16	0
7	A	9	0	4	2	0
7	B	9	0	3	1	0
8	A	86	0	0	10	0
8	B	62	0	0	4	0
All	All	10008	0	9628	631	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 32.

The worst 5 of 631 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:67:ARG:CA	1:B:67:ARG:N	1.83	1.40
1:A:108:ASP:OD2	6:A:605:HEM:HMD1	1.25	1.33
1:A:233:LYS:HB3	1:A:234:PRO:HD2	1.31	1.11
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PRO:O	1:A:289:GLY:HA2	1.50	1.08

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%)	494 (83%)	75 (13%)	24 (4%)	3	24
1	B	593/595 (100%)	492 (83%)	70 (12%)	31 (5%)	2	17
All	All	1186/1190 (100%)	986 (83%)	145 (12%)	55 (5%)	3	20

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	117	THR
1	A	137	ASP
1	A	169	THR
1	A	174	SER

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	518/518 (100%)	430 (83%)	88 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	518/518 (100%)	444 (86%)	74 (14%)	4	18
All	All	1036/1036 (100%)	874 (84%)	162 (16%)	3	14

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	ILE
1	B	11	PRO
1	B	481	LEU
1	A	482	ASP
1	A	523	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	GLN
1	A	570	ASN
1	B	439	GLN
1	A	558	HIS
1	A	565	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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
5	CO3	A	2001	-	0,3,3	0.00	-	0,3,3	0.00	-
7	FMT	A	3001	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	3002	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	3003	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAG	A	596	1,2	14,14,15	1.10	1 (7%)	15,19,21	2.70	5 (33%)
2	NAG	A	597	2	14,14,15	1.24	1 (7%)	15,19,21	2.13	3 (20%)
2	NAG	A	598	1,2	14,14,15	0.66	0	15,19,21	1.03	0
2	NAG	A	599	2	14,14,15	0.75	0	15,19,21	0.80	0
2	NAG	A	600	1,2	14,14,15	0.55	0	15,19,21	0.89	0
2	NAG	A	601	3,2	14,14,15	0.85	0	15,19,21	0.89	1 (6%)
3	MAN	A	602	2	11,11,12	0.64	0	13,15,17	0.34	0
2	NAG	A	603	1	14,14,15	0.80	0	15,19,21	1.59	2 (13%)
6	HEM	A	605	1	28,50,50	2.38	9 (32%)	17,82,82	2.50	7 (41%)
5	CO3	B	2002	-	0,3,3	0.00	-	0,3,3	0.00	-
7	FMT	B	3004	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	3006	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAG	B	596	1,2	14,14,15	0.64	0	15,19,21	0.76	0
2	NAG	B	597	2	14,14,15	0.64	0	15,19,21	1.63	2 (13%)
2	NAG	B	598	1,2	14,14,15	0.66	0	15,19,21	0.91	0
2	NAG	B	599	2	14,14,15	0.84	1 (7%)	15,19,21	0.86	0
2	NAG	B	600	1,2	14,14,15	0.76	1 (7%)	15,19,21	1.47	2 (13%)
2	NAG	B	601	3,2	14,14,15	0.83	0	15,19,21	1.64	3 (20%)
3	MAN	B	602	2	11,11,12	0.81	0	13,15,17	1.74	2 (15%)
2	NAG	B	603	1	14,14,15	0.82	1 (7%)	15,19,21	1.48	2 (13%)
6	HEM	B	605	1	28,50,50	2.45	11 (39%)	17,82,82	2.21	7 (41%)

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
5	CO3	A	2001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FMT	A	3001	-	-	0/0/0/0	0/0/0/0
7	FMT	A	3002	-	-	0/0/0/0	0/0/0/0
7	FMT	A	3003	-	-	0/0/0/0	0/0/0/0
2	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	NAG	A	598	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	599	2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	601	3,2	-	0/6/23/26	0/1/1/1
3	MAN	A	602	2	-	0/2/19/22	1/1/1/1
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	HEM	A	605	1	-	0/6/54/54	0/0/8/8
5	CO3	B	2002	-	-	0/0/0/0	0/0/0/0
7	FMT	B	3004	-	-	0/0/0/0	0/0/0/0
7	FMT	B	3005	-	-	0/0/0/0	0/0/0/0
7	FMT	B	3006	-	-	0/0/0/0	0/0/0/0
2	NAG	B	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	597	2	-	0/6/23/26	0/1/1/1
2	NAG	B	598	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	599	2	-	0/6/23/26	0/1/1/1
2	NAG	B	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	601	3,2	-	0/6/23/26	0/1/1/1
3	MAN	B	602	2	-	0/2/19/22	1/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
6	HEM	B	605	1	-	0/6/54/54	0/0/8/8

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	HEM	C3B-C2B	-3.98	1.35	1.40
6	B	605	HEM	C3B-C2B	-3.05	1.36	1.40
6	A	605	HEM	C1C-NC	2.08	1.39	1.36
2	B	603	NAG	C4-C3	2.09	1.57	1.52
6	B	605	HEM	C1D-ND	2.11	1.40	1.36

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	596	NAG	C2-N2-C7	-5.29	115.23	122.94
2	A	596	NAG	C4-C3-C2	-5.27	103.30	111.02
6	A	605	HEM	CAD-CBD-CGD	-5.01	104.09	112.66
6	A	605	HEM	CBA-CAA-C2A	-4.39	104.10	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	605	HEM	CAD-CBD-CGD	-4.34	105.25	112.66

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	MAN	C1-C2-C3-C4-C5-O5
3	A	602	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3002	FMT	2	0
2	A	596	NAG	2	0
2	A	597	NAG	2	0
2	A	598	NAG	2	0
2	A	600	NAG	2	0
2	A	601	NAG	6	0
3	A	602	MAN	1	0
6	A	605	HEM	8	0
7	B	3004	FMT	1	0
3	B	602	MAN	1	0
6	B	605	HEM	16	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.