W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:20 pm GMT

PDB ID	:	2EHA
Title	:	Crystal structure of goat lactoperoxidase complexed with formate anion at 3.3 A resolution
Authors	:	Singh, A.K.; Ethayathulla, A.S.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-03-06
Resolution	:	3.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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)	:	recalc28949

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 3.30 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.
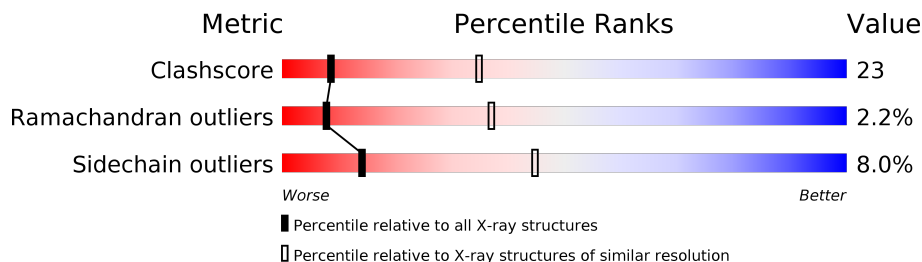
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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 <=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	61% / 34% / 5%
1	B	595	60% / 35% / 5% ·

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
10	FMT	A	2002	-	-	X	-
10	FMT	B	2003	-	-	X	-
7	SCN	A	3002	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	OSM	B	3021	-	-	X	-

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 10124 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total 4753	C 3021	N 844	O 862	S 26	0	0	0
1	B	595	Total 4753	C 3021	N 844	O 862	S 26	0	0	0

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total 39	C 22	N 2	O 15	0	0
2	A	3	Total 39	C 22	N 2	O 15	0	0
2	B	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total 39	C 22	N 2	O 15	0	0
3	B	3	Total 39	C 22	N 2	O 15	0	0
3	B	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total 28	C 16	N 2	O 10	0	0
4	B	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).
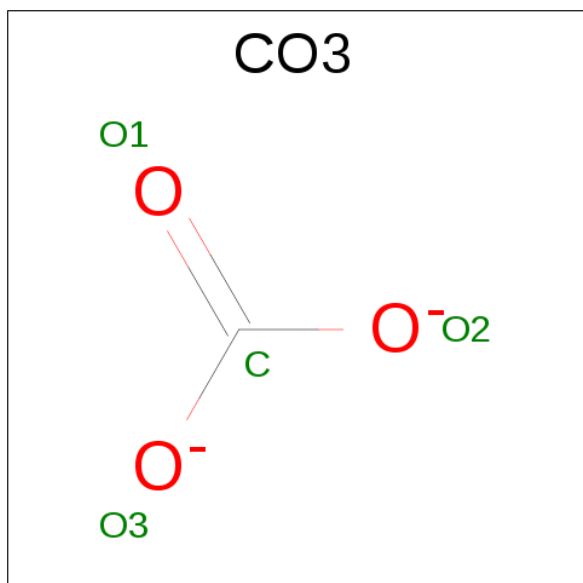
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).
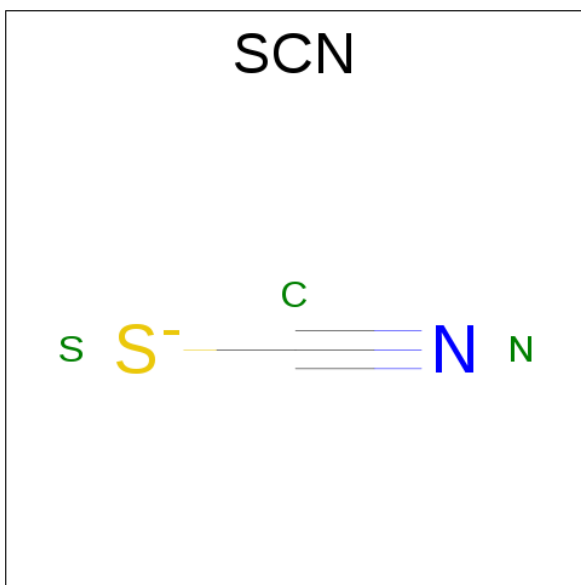
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
7	A	1	3	1	1	1	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
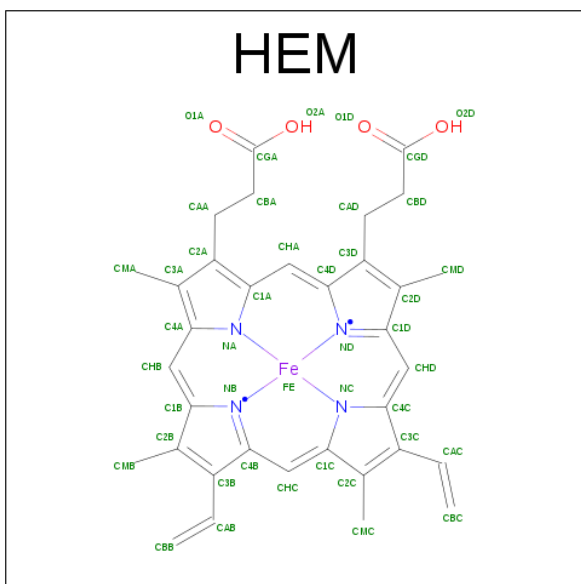
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	43	34	1	4	4	0	0
8	B	1	43	34	1	4	4	0	0

• Molecule 9 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).
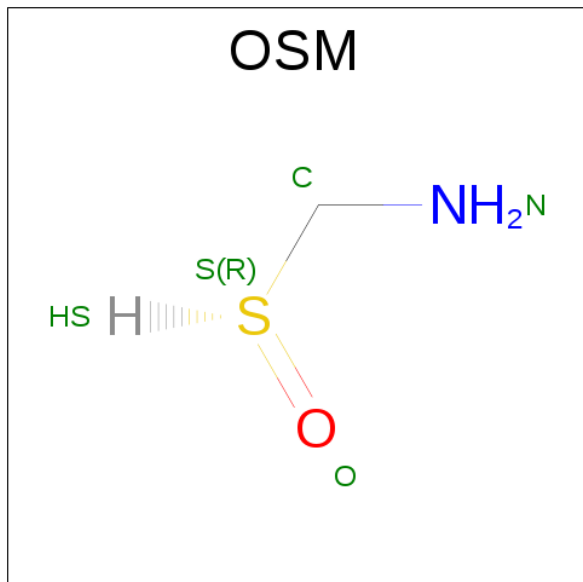
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	4	1	1	1	1	0	0

• Molecule 10 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

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

Continued on next page...

Continued from previous page...
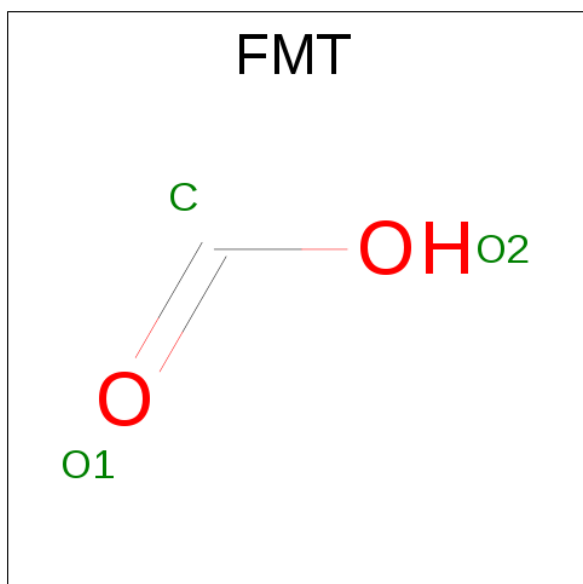
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 3	C 1	O 2	0	0
10	B	1	Total 3	C 1	O 2	0	0
10	B	1	Total 3	C 1	O 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	116	Total 116	O 116	0	0
11	B	97	Total 97	O 97	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: Lactoperoxidase

Chain A:

- Molecule 1: Lactoperoxidase

Chain B:

L376 H377 T378 L379 F380 F381 N382 T383 I386 I387 K388 D389 G390 G391 I392 D393 P394 L395 V396 R397 G398 L399 M407 N408 L417 T425 H426 F431 D432 L433 I436 N437 M446 P447 N450 S451 W452 Q460 P461 K462 T463 L464 K465 G466 L467 Q468 L471 V475

K478 K479 L483 P487 I490 D491 I492 N497 P500 M501 C513 R517 Q518 F519 Q520 Q521 I522 R523 D526 W529 F536 T537 E538 K539 Q540 L544 Q545 K546 V547 S548 F549 S550 R551 L552 I553 T557 H558 I559 L564 Q568 A569 K584 S588 P589

W590 R593 E594 N595

4 Data and refinement statistics (i)

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	57.99Å 72.27Å 83.65Å 85.45° 84.04° 75.89°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10124	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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, SCN, NAG, FMT, BMA, OSM, 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	0.44	0/4882	0.80	4/6632 (0.1%)
1	B	0.44	0/4882	0.82	7/6632 (0.1%)
All	All	0.44	0/9764	0.81	11/13264 (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.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	VAL	N-CA-C	8.08	132.83	111.00
1	B	174	SER	N-CA-C	6.67	129.02	111.00
1	A	166	VAL	N-CA-C	6.65	128.96	111.00
1	A	559	ILE	N-CA-C	-6.14	94.42	111.00
1	B	12	LEU	CA-CB-CG	5.94	128.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	TYR	Sidechain

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	4753	0	4646	228	0
1	B	4753	0	4646	226	0
2	A	78	0	68	0	0
2	B	39	0	34	7	0
3	A	39	0	34	0	0
3	B	78	0	68	2	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	3	0	0	3	0
8	A	43	0	30	11	0
8	B	43	0	30	7	0
9	B	4	0	5	2	0
10	A	6	0	4	3	0
10	B	6	0	4	3	0
11	A	116	0	0	20	0
11	B	97	0	0	8	0
All	All	10124	0	9619	446	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 23.

The worst 5 of 446 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:167:CYS:HB2	1:B:168:PRO:HD3	1.26	1.14
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.28	1.13
1:A:132:TYR:OH	1:B:120:GLY:HA2	1.58	1.04
1:A:124:HIS:HB2	1:B:137:ASP:CG	1.80	1.01
1:B:315:ILE:HG22	2:B:597:NAG:H82	1.40	1.01

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	593/595 (100%)	526 (89%)	54 (9%)	13 (2%)	8	37
1	B	593/595 (100%)	529 (89%)	51 (9%)	13 (2%)	8	37
All	All	1186/1190 (100%)	1055 (89%)	105 (9%)	26 (2%)	8	37

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	VAL
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	594	GLU

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	517/517 (100%)	476 (92%)	41 (8%)	14	45
1	B	517/517 (100%)	475 (92%)	42 (8%)	14	44
All	All	1034/1034 (100%)	951 (92%)	83 (8%)	14	45

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	546	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	71	ARG
1	B	464	LEU
1	A	564	LEU
1	B	6	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	497	ASN
1	A	595	ASN
1	B	521	GLN
1	A	545	GLN
1	A	565	HIS

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 ⓘ

22 carbohydrates 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	#$|Z| > 2$
2	NAG	A	596	1,2	14,14,15	0.65	0	15,19,21	0.59	0
2	NAG	A	597	2	14,14,15	0.81	0	15,19,21	1.09	1 (6%)
2	MAN	A	598	2	11,11,12	0.73	0	13,15,17	0.75	1 (7%)
2	NAG	A	599	1,2	14,14,15	0.57	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	A	600	2	14,14,15	0.66	0	15,19,21	1.26	1 (6%)
2	MAN	A	601	2	11,11,12	0.58	0	13,15,17	0.42	0
3	NAG	A	602	1,3	14,14,15	0.55	0	15,19,21	0.88	0
3	NAG	A	603	3	14,14,15	0.83	0	15,19,21	1.32	2 (13%)
3	BMA	A	604	3	11,11,12	0.69	0	13,15,17	1.26	2 (15%)
4	NAG	A	605	1,4	14,14,15	0.64	0	15,19,21	1.46	2 (13%)
4	NAG	A	606	4	14,14,15	0.60	0	15,19,21	1.45	3 (20%)
2	NAG	B	596	1,2	14,14,15	0.63	0	15,19,21	0.55	0
2	NAG	B	597	2	14,14,15	0.54	0	15,19,21	1.60	4 (26%)
2	MAN	B	598	2	11,11,12	0.67	0	13,15,17	1.01	1 (7%)
3	NAG	B	599	1,3	14,14,15	0.50	0	15,19,21	0.95	1 (6%)
3	NAG	B	600	3	14,14,15	0.94	1 (7%)	15,19,21	1.01	1 (6%)
3	BMA	B	601	3	11,11,12	0.86	0	13,15,17	1.93	4 (30%)
3	NAG	B	602	1,3	14,14,15	0.49	0	15,19,21	0.76	0
3	NAG	B	603	3	14,14,15	0.69	0	15,19,21	1.90	3 (20%)
3	BMA	B	604	3	11,11,12	0.67	0	13,15,17	1.02	2 (15%)
4	NAG	B	605	1,4	14,14,15	0.50	0	15,19,21	1.55	3 (20%)
4	NAG	B	606	4	14,14,15	0.50	0	15,19,21	0.88	1 (6%)

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	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	MAN	A	598	2	-	0/2/19/22	1/1/1/1
2	NAG	A	599	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	2	-	0/6/23/26	0/1/1/1
2	MAN	A	601	2	-	0/2/19/22	1/1/1/1
3	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	BMA	A	604	3	-	0/2/19/22	1/1/1/1
4	NAG	A	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	606	4	-	0/6/23/26	0/1/1/1
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	MAN	B	598	2	-	0/2/19/22	1/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	600	3	-	0/6/23/26	0/1/1/1
3	BMA	B	601	3	-	0/2/19/22	0/1/1/1
3	NAG	B	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	603	3	-	0/6/23/26	0/1/1/1
3	BMA	B	604	3	-	0/2/19/22	1/1/1/1
4	NAG	B	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	606	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	NAG	C1-C2	2.00	1.55	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	NAG	C4-C3-C2	-5.54	102.90	111.02
3	B	603	NAG	C2-N2-C7	-3.04	118.51	122.94
3	A	603	NAG	C4-C3-C2	-2.96	106.68	111.02
2	B	597	NAG	O5-C1-C2	-2.56	107.92	111.47
3	B	601	BMA	C2-C3-C4	-2.47	106.56	110.88

There are no chirality outliers.

There are no torsion outliers.

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MAN	C1-C2-C3-C4-C5-O5
2	A	598	MAN	C1-C2-C3-C4-C5-O5
3	B	604	BMA	C1-C2-C3-C4-C5-O5
2	B	598	MAN	C1-C2-C3-C4-C5-O5
3	A	604	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	596	NAG	1	0
2	B	597	NAG	6	0
3	B	599	NAG	1	0
3	B	600	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	NAG	1	0
3	B	604	BMA	1	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#|Z| > 2$
6	CO3	A	1001	-	0,3,3	0.00	-	0,3,3	0.00	-
10	FMT	A	2001	-	0,2,2	0.00	-	0,1,1	0.00	-
10	FMT	A	2002	-	0,2,2	0.00	-	0,1,1	0.00	-
7	SCN	A	3002	-	1,2,2	2.77	1 (100%)	0,1,1	0.00	-
8	HEM	A	3003	1	28,50,50	2.08	6 (21%)	17,82,82	1.61	5 (29%)
6	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
8	HEM	B	1003	1	28,50,50	2.74	11 (39%)	17,82,82	1.94	4 (23%)
10	FMT	B	2003	-	0,2,2	0.00	-	0,1,1	0.00	-
10	FMT	B	2004	-	0,2,2	0.00	-	0,1,1	0.00	-
9	OSM	B	3021	-	1,3,3	0.52	0	0,2,2	0.00	-

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
6	CO3	A	1001	-	-	0/0/0/0	0/0/0/0
10	FMT	A	2001	-	-	0/0/0/0	0/0/0/0
10	FMT	A	2002	-	-	0/0/0/0	0/0/0/0
7	SCN	A	3002	-	-	0/0/0/0	0/0/0/0
8	HEM	A	3003	1	-	0/6/54/54	0/0/8/8
6	CO3	B	1002	-	-	0/0/0/0	0/0/0/0
8	HEM	B	1003	1	-	0/6/54/54	0/0/8/8
10	FMT	B	2003	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FMT	B	2004	-	-	0/0/0/0	0/0/0/0
9	OSM	B	3021	-	-	0/0/1/1	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1003	HEM	C3B-C2B	-7.11	1.31	1.40
8	B	1003	HEM	C1A-CHA	-4.35	1.28	1.40
8	B	1003	HEM	C3C-C2C	-3.16	1.36	1.40
8	A	3003	HEM	C3B-C2B	-3.14	1.36	1.40
8	B	1003	HEM	CAD-C3D	2.22	1.56	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1003	HEM	C1D-C2D-C3D	-4.54	103.83	107.00
8	B	1003	HEM	CBD-CAD-C3D	-3.84	105.14	112.47
8	A	3003	HEM	CBD-CAD-C3D	-3.39	105.99	112.47
8	A	3003	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
8	A	3003	HEM	C1D-C2D-C3D	-2.24	105.44	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2001	FMT	1	0
10	A	2002	FMT	2	0
7	A	3002	SCN	3	0
8	A	3003	HEM	11	0
8	B	1003	HEM	7	0
10	B	2003	FMT	2	0
10	B	2004	FMT	1	0
9	B	3021	OSM	2	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.