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 26, 2014 – 03:05 PM GMT

PDB ID	:	3GC1
Title	:	Crystal structure of bovine lactoperoxidase
Authors	:	Singh, A.K.; Singh, N.; Sinha, M.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on	:	2009-02-21
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.312
Clashscore		44
Ramachandran outliers		3.5%
Sidechain outliers		17.0%
RSRZ outliers		15.3%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
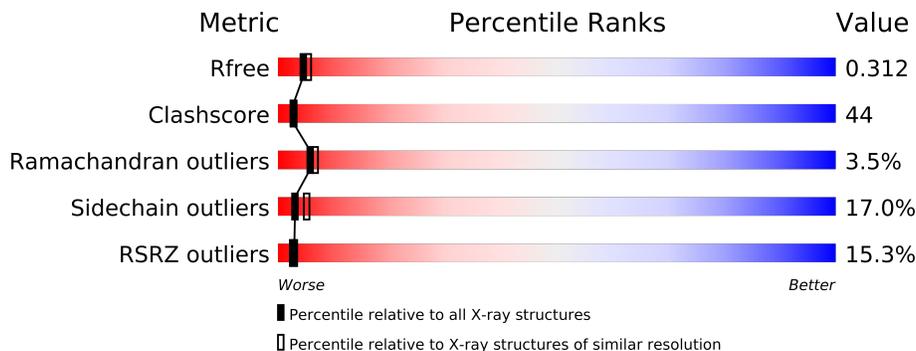
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HEM	A	605	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 5258 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			Total	C	N	O	P	S			
1	A	595	4774	3037	847	863	1	26	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
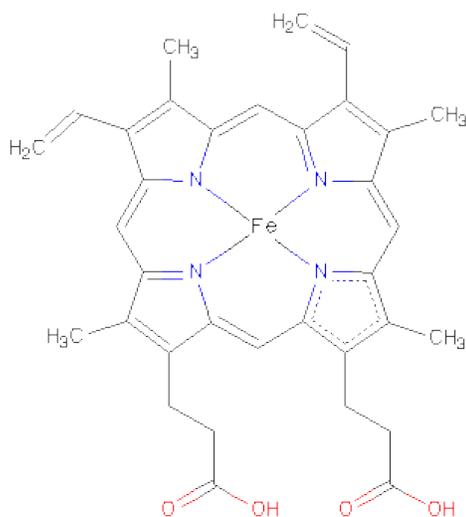
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

• Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 3	C 1	N 1	S 1	0	0

• Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

• Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

• Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	I 7	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	296	Total O 296 296		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 errors 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

Chain A:
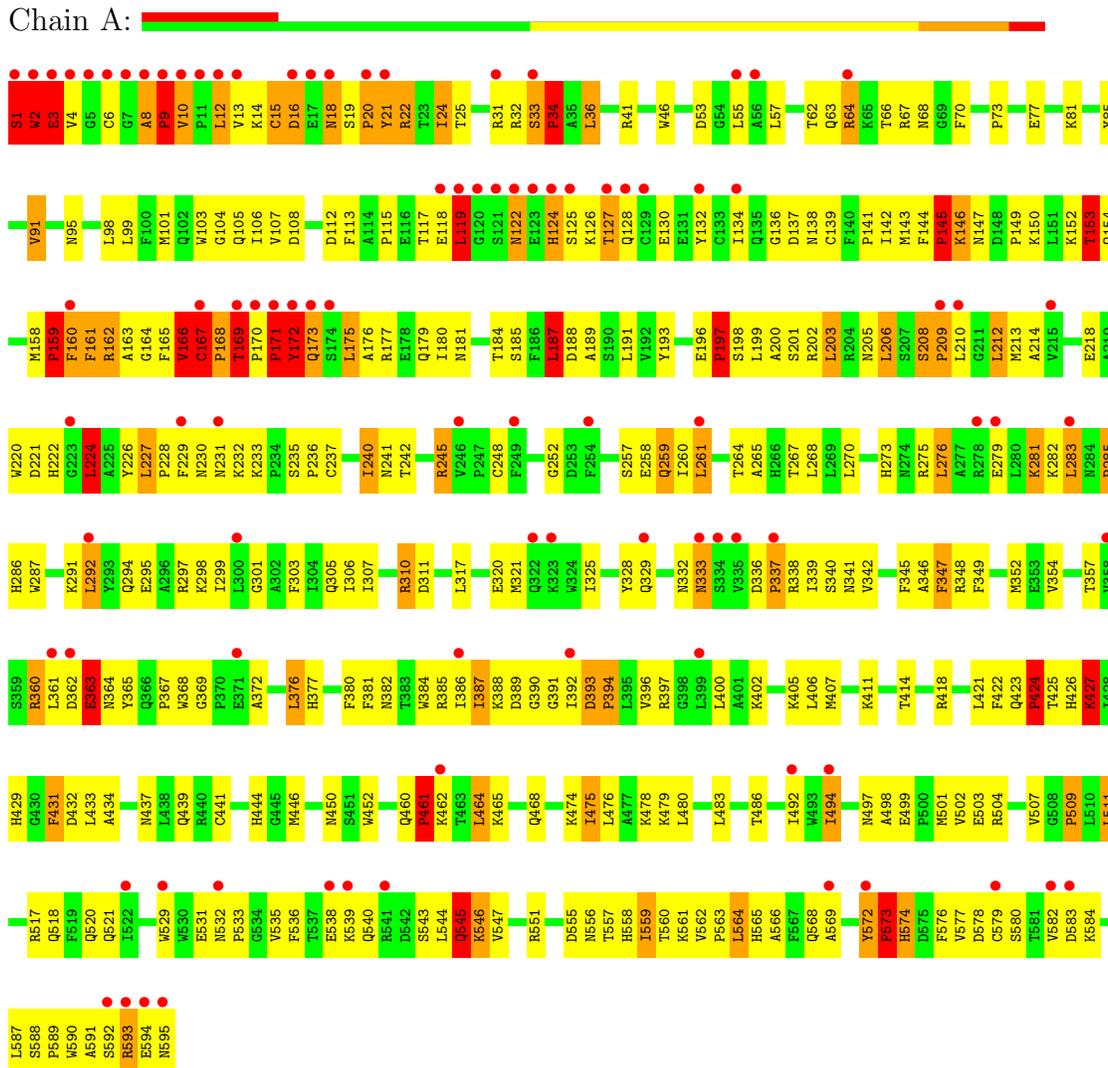
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.65Å 80.71Å 75.68Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	24.97 – 2.50 24.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.97-2.50) 95.4 (24.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.47 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.247 , 0.268 0.264 , 0.312	Depositor DCC
R_{free} test set	1073 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<\lvert L \rvert> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 20970 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]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: SCN, NAG, SEP, CA, NDG, HEM, IOD, 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	0.73	7/4891 (0.1%)	1.25	44/6634 (0.7%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	TRP	CB-CG	-6.67	1.38	1.50
1	A	145	PRO	CA-C	-6.62	1.39	1.52
1	A	461	PRO	CA-C	-6.30	1.40	1.52
1	A	171	PRO	N-CA	6.11	1.57	1.47
1	A	33	SER	C-N	5.38	1.44	1.34

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	PRO	CA-N-CD	-18.07	86.20	111.50
1	A	572	TYR	C-N-CD	-14.29	89.15	120.60
1	A	2	TRP	N-CA-C	13.15	146.51	111.00
1	A	573	PRO	N-CA-CB	13.11	119.03	103.30
1	A	572	TYR	C-N-CA	12.57	174.80	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4688	420	0
2	A	43	0	30	31	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	78	0	68	8	0
6	A	56	0	50	3	0
7	A	7	0	0	6	0
8	A	296	0	0	43	0
All	All	5258	0	4836	428	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

The worst 5 of 428 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:GLN:HB2	2:A:605:HEM:C2C	1.64	1.32
1:A:221:ASP:HB2	1:A:226:TYR:CZ	1.81	1.16
1:A:104:GLY:HA3	2:A:605:HEM:HBC1	1.26	1.09
1:A:22:ARG:CG	1:A:22:ARG:HH11	1.66	1.08
1:A:22:ARG:NH1	1:A:22:ARG:HG2	1.53	1.06

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	592/595 (100%)	505 (85%)	66 (11%)	21 (4%)	6	7

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	424	PRO

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	517/517 (100%)	429 (83%)	88 (17%)	3	5

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	LEU
1	A	279	GLU
1	A	538	GLU
1	A	218	GLU
1	A	240	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	A	468	GLN
1	A	558	HIS
1	A	429	HIS
1	A	568	GLN

5.3.3   RNA (i)

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	#$|Z| > 2$
1	SEP	A	198	1	9,9,10	8.35	3 (33%)	10,12,14	3.29	4 (40%)

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
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	24.12	1.28	1.11
1	A	198	SEP	CA-C	5.80	1.59	1.48
1	A	198	SEP	P-O1P	2.38	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	O3P-P-OG	6.78	125.35	106.65
1	A	198	SEP	O2P-P-OG	-4.74	93.57	106.65
1	A	198	SEP	C-CA-N	-4.45	109.38	113.83
1	A	198	SEP	O3P-P-O1P	-3.33	99.57	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

10 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	#$|Z| > 2$
5	NDG	A	596	1,5	12,14,15	1.33	2 (16%)	15,19,21	1.31	1 (6%)
5	NAG	A	597	5	12,14,15	1.69	3 (25%)	15,19,21	2.79	5 (33%)
5	MAN	A	598	5	10,11,12	0.63	0	11,15,17	1.43	1 (9%)
6	NAG	A	599	1,6	12,14,15	1.00	0	15,19,21	1.72	5 (33%)
6	NAG	A	600	6	12,14,15	0.58	0	15,19,21	1.34	2 (13%)
5	NDG	A	601	1,5	12,14,15	0.81	0	15,19,21	1.99	7 (46%)
5	NAG	A	602	5	12,14,15	0.62	0	15,19,21	1.12	1 (6%)
5	MAN	A	603	5	10,11,12	0.61	0	11,15,17	0.67	0
6	NAG	A	604	1,6	12,14,15	1.32	2 (16%)	15,19,21	1.40	1 (6%)
6	NAG	A	607	6	12,14,15	0.73	0	15,19,21	1.09	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
5	NDG	A	596	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	597	5	-	0/6/23/26	0/1/1/1
5	MAN	A	598	5	-	0/2/19/22	0/1/1/1
6	NAG	A	599	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	600	6	-	0/6/23/26	0/1/1/1
5	NDG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	1/1/1/1
5	MAN	A	603	5	-	0/2/19/22	0/1/1/1
6	NAG	A	604	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	607	6	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	597	NAG	C8-C7	3.03	1.57	1.50
5	A	597	NAG	C2-N2	-2.74	1.43	1.46
6	A	604	NAG	C2-N2	-2.32	1.43	1.46
5	A	596	NDG	C4-C3	2.23	1.58	1.52
6	A	604	NAG	C4-C5	2.18	1.57	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	597	NAG	C3-C2-N2	-7.75	99.95	111.76
5	A	598	MAN	C4-C3-C2	4.11	116.02	110.50
5	A	597	NAG	C2-N2-C7	-4.04	116.31	123.09
5	A	597	NAG	C6-C5-C4	-3.96	103.43	113.00
5	A	596	NDG	C3-C4-C5	-3.95	103.15	110.20

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	605	1	49,50,50	4.84	29 (59%)	46,82,82	2.35	14 (30%)
4	SCN	A	615	-	2,2,2	2.57	1 (50%)	1,1,1	0.26	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

wwPDB X-ray Structure Validation Summary Report

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	605	1	-	0/14/114/114	0/0/8/8
4	SCN	A	615	-	-	0/0/0/0	0/0/0/0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C2B-C1B	21.20	1.49	1.44
2	A	605	HEM	FE-NC	13.90	2.50	1.97
2	A	605	HEM	C3D-C4D	8.20	1.46	1.44
2	A	605	HEM	C4A-C3A	7.76	1.49	1.40
2	A	605	HEM	C3B-CAB	6.82	1.62	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	CBD-CAD-C3D	-6.98	99.13	114.37
2	A	605	HEM	CHD-C4C-NC	-5.13	120.27	124.73
2	A	605	HEM	CHC-C1C-NC	5.11	129.17	124.73
2	A	605	HEM	CHD-C1D-ND	5.10	128.82	124.58
2	A	605	HEM	CHA-C4D-ND	4.81	130.92	124.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	595/595 (100%)	0.90	91 (15%)	3	2	28, 47, 86, 100	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	HIS	7.5
1	A	12	LEU	7.1
1	A	172	TYR	6.7
1	A	2	TRP	6.6
1	A	9	PRO	6.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	A	198	10/11	0.19	-0.40	31,48,50,50	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
5	NAG	A	597	14/15	0.52	5.00	83,87,89,91	0
6	NAG	A	604	14/15	0.32	1.50	71,74,77,82	0
5	NDG	A	596	14/15	0.29	0.76	68,70,74,78	0
5	NAG	A	602	14/15	0.26	0.13	64,66,70,74	0
5	NDG	A	601	14/15	0.21	-0.09	56,57,58,62	0
6	NAG	A	599	14/15	0.18	-1.01	72,73,75,77	0
5	MAN	A	598	11/12	0.39	-	94,95,96,96	0
6	NAG	A	607	14/15	0.55	-	86,89,91,91	0
6	NAG	A	600	14/15	0.40	-	80,82,83,84	0
5	MAN	A	603	11/12	0.56	-	78,80,81,82	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
2	HEM	A	605	43/43	0.25	2.10	22,27,34,38	0
7	IOD	A	614	1/1	0.19	1.51	54,54,54,54	0
4	SCN	A	615	3/3	0.18	-1.33	17,17,21,25	0
7	IOD	A	608	1/1	0.12	-1.42	43,43,43,43	0
7	IOD	A	609	1/1	0.04	-2.24	60,60,60,60	0
3	CA	A	606	1/1	0.09	-2.34	44,44,44,44	0
7	IOD	A	613	1/1	0.05	-2.37	85,85,85,85	0
7	IOD	A	612	1/1	0.06	-2.48	75,75,75,75	0
7	IOD	A	610	1/1	0.02	-3.10	56,56,56,56	0
7	IOD	A	611	1/1	0.05	-5.07	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.