wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:48 AM GMT

PDB ID	:	2EFB
Title	:	Crystal structure of the complex of goat lactoperoxidase with phosphate at 2.94 A resolution
Authors	:	Singh, A.K.; Hariprasad, G.; Prem Kumar, R.; Singh, N.; Bhushan, A.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-02-22
Resolution	:	2.94 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 (i) symbol.

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

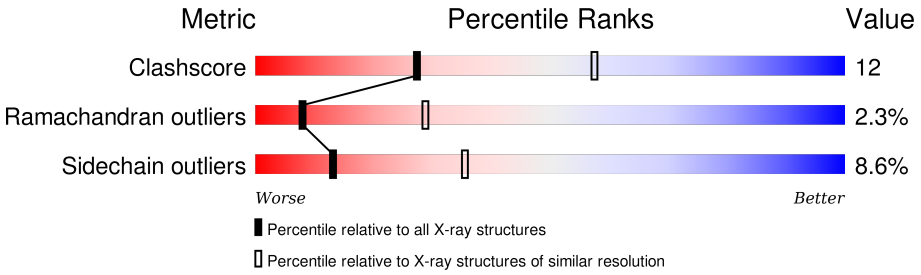
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.94 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	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)

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	75% 21%
1	B	595	77% 19%

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
5	PO4	A	2001	-	-	X	-
5	PO4	B	2003	-	-	X	-
5	PO4	B	2004	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CYN	A	2011	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10287 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	C	N	O	S	0	0	0
			4754	3021	844	863	26			
1	B	595	Total	C	N	O	S	0	0	0
			4754	3021	844	863	26			

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

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

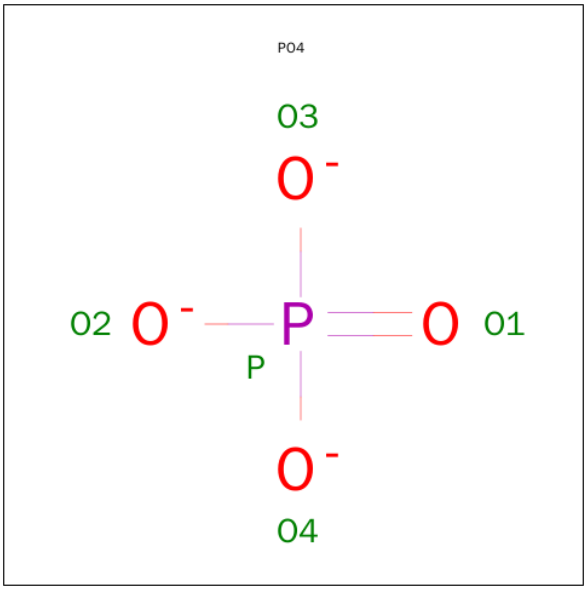
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

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

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

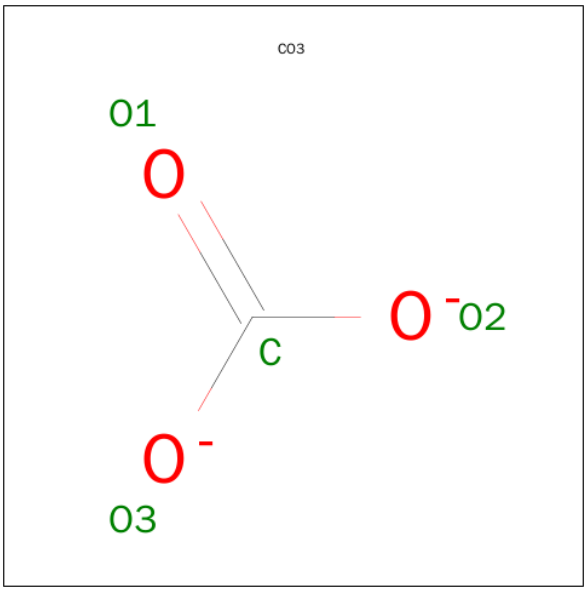
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

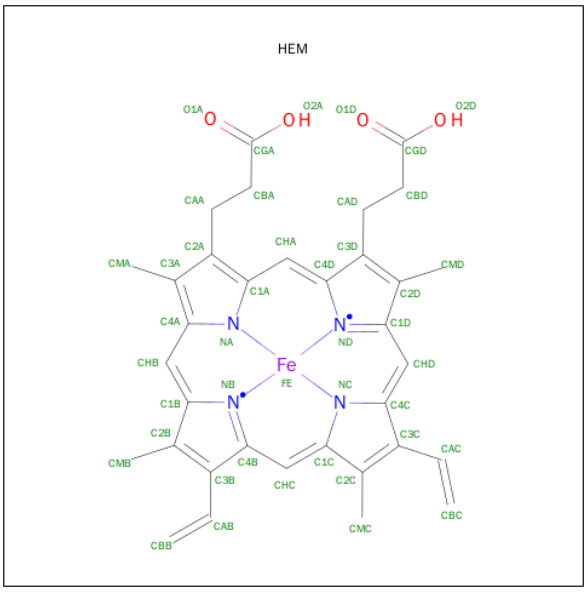


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

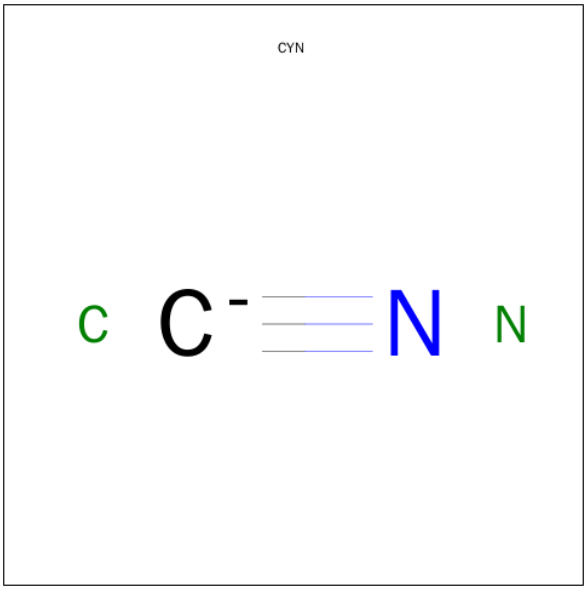
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



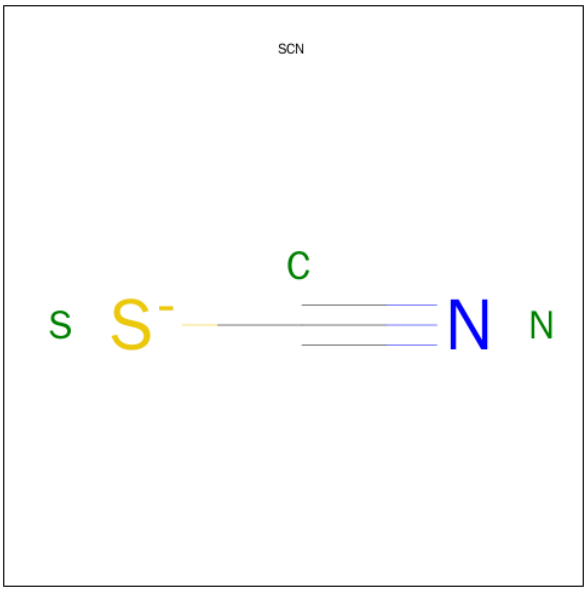
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
8	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 9 is CYANIDE ION (three-letter code: CYN) (formula: CN).



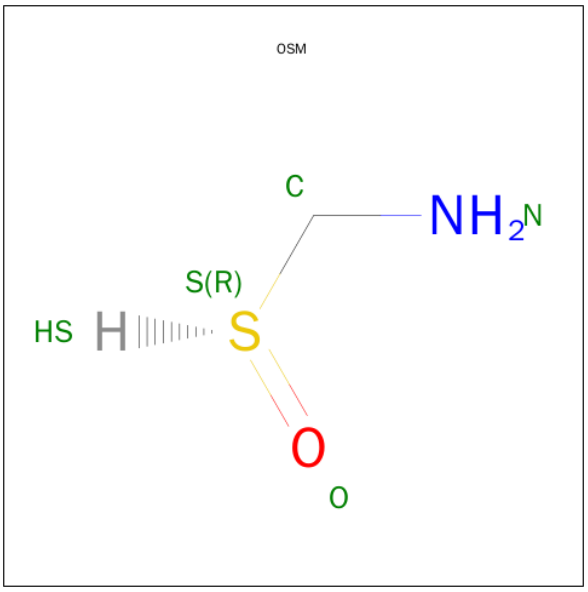
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N		0	0
			2	1	1			

- Molecule 10 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 11 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	B	1	4	1	1	1	1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	188	Total O 188 188	0	0
12	B	171	Total O 171 171	0	0

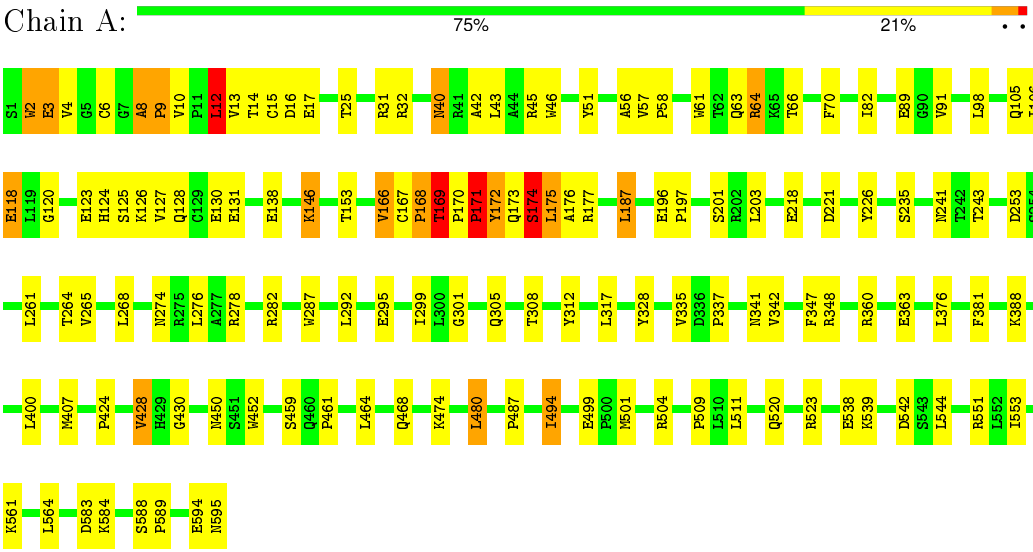
3 Residue-property plots (i)

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.

Note EDS was not executed.

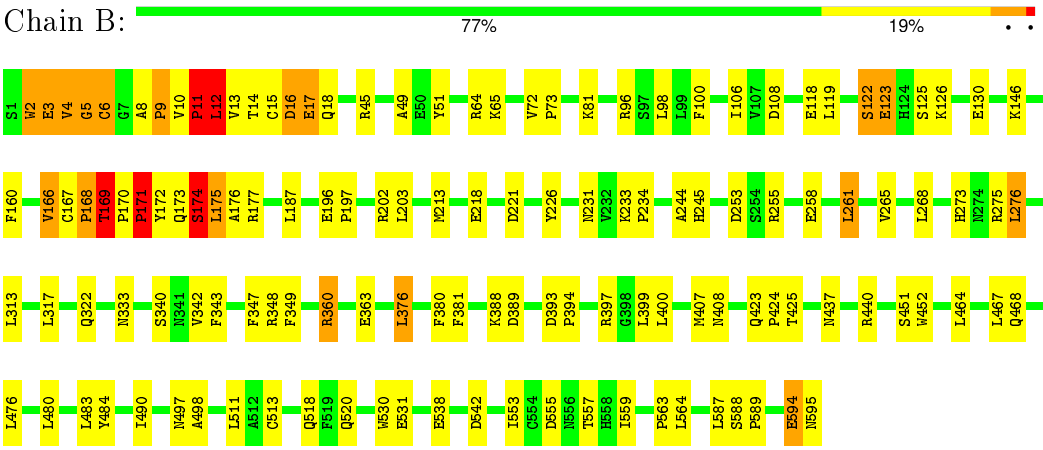
- Molecule 1: Lactoperoxidase

Chain A:



- Molecule 1: Lactoperoxidase

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.20Å 75.59Å 83.81Å 79.93° 77.86° 72.50°	Depositor
Resolution (Å)	20.00 – 2.94	Depositor
% Data completeness (in resolution range)	95.3 (20.00-2.94)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10287	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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, PO4, BMA, OSM, HEM, CA, CYN, 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	0.55	2/4883 (0.0%)	0.70	5/6632 (0.1%)
1	B	0.52	0/4883	0.67	3/6632 (0.0%)
All	All	0.54	2/9766 (0.0%)	0.69	8/13264 (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	3
1	B	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	GLY	N-CA	7.09	1.56	1.46
1	A	63	GLN	C-N	6.13	1.48	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	SER	O-C-N	-8.93	108.41	122.70
1	B	174	SER	N-CA-C	6.19	127.72	111.00
1	A	174	SER	CA-C-N	5.86	130.09	117.20
1	A	63	GLN	C-N-CA	5.54	135.54	121.70
1	A	171	PRO	N-CA-C	5.53	126.48	112.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	LEU	Peptide
1	A	169	THR	Peptide
1	A	171	PRO	Peptide
1	B	12	LEU	Peptide
1	B	169	THR	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	4754	0	4645	101	0
1	B	4754	0	4645	122	0
2	A	78	0	68	2	0
2	B	39	0	34	0	0
3	A	39	0	34	0	0
3	B	78	0	68	0	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	15	0	0	5	0
5	B	10	0	0	6	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	43	0	30	14	0
8	B	43	0	30	15	0
9	A	2	0	0	3	0
10	A	3	0	0	1	0
11	B	4	0	5	1	0
12	A	188	0	0	12	0
12	B	171	0	0	16	0
All	All	10287	0	9609	233	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 12.

The worst 5 of 233 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:8:ALA:HB1	1:B:9:PRO:HD2	1.32	1.11
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.28	1.09
1:A:175:LEU:HD22	1:A:176:ALA:H	1.15	1.09
1:A:2:TRP:HZ3	1:A:174:SER:HB3	1.25	1.00
1:B:168:PRO:HB2	1:B:170:PRO:HD2	1.44	0.98

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%)	539 (91%)	38 (6%)	16 (3%)	6 24
1	B	593/595 (100%)	541 (91%)	41 (7%)	11 (2%)	10 34
All	All	1186/1190 (100%)	1080 (91%)	79 (7%)	27 (2%)	8 29

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	12	LEU
1	A	168	PRO
1	A	169	THR
1	A	171	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%)	471 (91%)	46 (9%)	12 34
1	B	517/517 (100%)	474 (92%)	43 (8%)	14 37
All	All	1034/1034 (100%)	945 (91%)	89 (9%)	13 35

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	GLN
1	B	11	PRO
1	B	511	LEU
1	A	538	GLU
1	A	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	GLN
1	A	497	ASN
1	B	333	ASN
1	A	429	HIS
1	A	437	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)

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	0.59	0	15,19,21	0.80	0
2	NAG	A	597	2	14,14,15	0.67	0	15,19,21	1.35	3 (20%)
2	MAN	A	598	2	11,11,12	0.66	0	14,15,17	1.49	2 (14%)
2	NAG	A	599	1,2	14,14,15	0.59	0	15,19,21	0.91	1 (6%)
2	NAG	A	600	2	14,14,15	0.53	0	15,19,21	1.67	3 (20%)
2	MAN	A	601	2	11,11,12	0.65	0	14,15,17	1.54	2 (14%)
3	NAG	A	602	1,3	14,14,15	0.63	0	15,19,21	1.45	2 (13%)
3	NAG	A	603	3	14,14,15	0.55	0	15,19,21	1.19	1 (6%)
3	BMA	A	604	3	11,11,12	0.59	0	14,15,17	1.84	2 (14%)
4	NAG	A	605	1,4	14,14,15	0.63	0	15,19,21	1.37	2 (13%)
4	NAG	A	606	4	14,14,15	0.62	0	15,19,21	1.57	2 (13%)
2	NAG	B	596	1,2	14,14,15	0.77	0	15,19,21	1.33	1 (6%)
2	NAG	B	597	2	14,14,15	0.75	1 (7%)	15,19,21	2.69	2 (13%)
2	MAN	B	598	2	11,11,12	0.65	0	14,15,17	1.43	2 (14%)
3	NAG	B	599	1,3	14,14,15	0.54	0	15,19,21	1.27	2 (13%)
3	NAG	B	600	3	14,14,15	0.65	0	15,19,21	1.10	1 (6%)
3	BMA	B	601	3	11,11,12	0.61	0	14,15,17	2.23	2 (14%)
3	NAG	B	602	1,3	14,14,15	0.46	0	15,19,21	1.59	2 (13%)
3	NAG	B	603	3	14,14,15	0.53	0	15,19,21	1.96	1 (6%)
3	BMA	B	604	3	11,11,12	0.60	0	14,15,17	1.57	2 (14%)
4	NAG	B	605	1,4	14,14,15	0.62	0	15,19,21	1.47	2 (13%)
4	NAG	B	606	4	14,14,15	0.47	0	15,19,21	0.84	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	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	0/1/1/1
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)
2	B	597	NAG	C1-C2	2.10	1.55	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	NAG	O4-C4-C3	-2.82	103.98	110.34
3	B	599	NAG	O7-C7-C8	-2.40	117.65	122.06
3	B	601	BMA	C1-C2-C3	2.05	111.97	109.54
2	A	598	MAN	C1-C2-C3	2.11	112.04	109.54
2	A	597	NAG	C3-C4-C5	2.11	113.88	110.20

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

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

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	597	NAG	2	0

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
8	HEM	A	1001	1	30,50,50	2.24	7 (23%)	24,82,82	2.29	9 (37%)
5	PO4	A	2001	-	4,4,4	0.68	0	6,6,6	0.29	0
5	PO4	A	2002	-	4,4,4	0.46	0	6,6,6	0.27	0
5	PO4	A	2005	-	4,4,4	0.39	0	6,6,6	0.27	0
6	CO3	A	2006	-	0,3,3	0.00	-	0,3,3	0.00	-
9	CYN	A	2011	-	0,1,1	0.00	-	0,0,0	0.00	-
10	SCN	A	2012	-	2,2,2	2.08	1 (50%)	1,1,1	1.66	0
8	HEM	B	1021	1	30,50,50	2.42	8 (26%)	24,82,82	2.21	7 (29%)
5	PO4	B	2003	-	4,4,4	0.43	0	6,6,6	0.28	0
5	PO4	B	2004	-	4,4,4	0.57	0	6,6,6	0.28	0
6	CO3	B	2007	-	0,3,3	0.00	-	0,3,3	0.00	-
11	OSM	B	2021	-	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
8	HEM	A	1001	1	-	0/10/54/54	0/0/8/8
5	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
5	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
5	PO4	A	2005	-	-	0/0/0/0	0/0/0/0
6	CO3	A	2006	-	-	0/0/0/0	0/0/0/0
9	CYN	A	2011	-	-	0/0/0/0	0/0/0/0
10	SCN	A	2012	-	-	0/0/0/0	0/0/0/0
8	HEM	B	1021	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	B	2003	-	-	0/0/0/0	0/0/0/0
5	PO4	B	2004	-	-	0/0/0/0	0/0/0/0
6	CO3	B	2007	-	-	0/0/0/0	0/0/0/0
11	OSM	B	2021	-	-	0/0/1/1	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1001	HEM	C3B-C4B	-8.05	1.44	1.51
8	B	1021	HEM	C3B-C4B	-7.55	1.45	1.51
8	B	1021	HEM	C3D-C4D	-5.36	1.44	1.51
8	A	1001	HEM	C3D-C4D	-4.51	1.45	1.51
8	B	1021	HEM	C2C-C1C	-4.05	1.44	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	HEM	C3B-CAB-CBB	-3.18	119.58	124.46
8	A	1001	HEM	CAA-C2A-C1A	-3.06	123.68	127.01
8	B	1021	HEM	CBA-CAA-C2A	-2.23	108.53	112.53
8	B	1021	HEM	CAA-C2A-C1A	-2.21	124.61	127.01
8	A	1001	HEM	C2C-C1C-CHC	2.20	127.03	123.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	HEM	14	0
5	A	2001	PO4	5	0
9	A	2011	CYN	3	0
10	A	2012	SCN	1	0
8	B	1021	HEM	15	0
5	B	2003	PO4	2	0
5	B	2004	PO4	4	0
11	B	2021	OSM	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.