wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:52 AM GMT

PDB ID	:	2YOR
Title	:	Crystallization of a 45 kDa peroxygenase- peroxidase from the mushroom Agrocybe aegerita and structure determination by SAD utilizing only the haem iron
Authors	:	Piontek, K.; Strittmatter, E.; Ullrich, R.; Plattner, D.A.; Hofrichter, M.
Deposited on	:	2012-10-26
Resolution	:	2.19 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 (1)) were used in the production of this report:

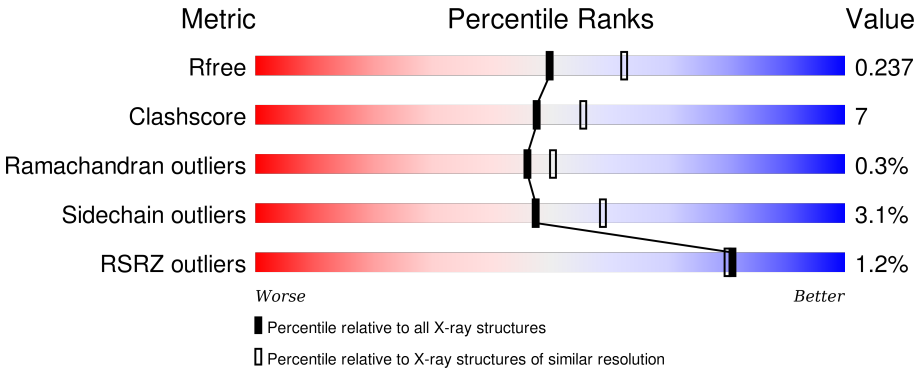
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.19 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))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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.

Mol	Chain	Length	Quality of chain
1	A	325	2% 89% 10%
1	B	325	% 86% 12%

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
12	NAG	B	372	-	-	-	X
12	NAG	B	391	-	-	-	X
12	NAG	B	401	X	-	-	-
6	NAG	A	372	-	-	-	X
6	MAN	A	374	-	-	-	X
7	NAG	A	391	-	-	-	X
7	NAG	B	511	-	-	-	X
8	BMA	A	501	-	-	-	X
8	BMA	B	501	-	-	-	X

2 Entry composition

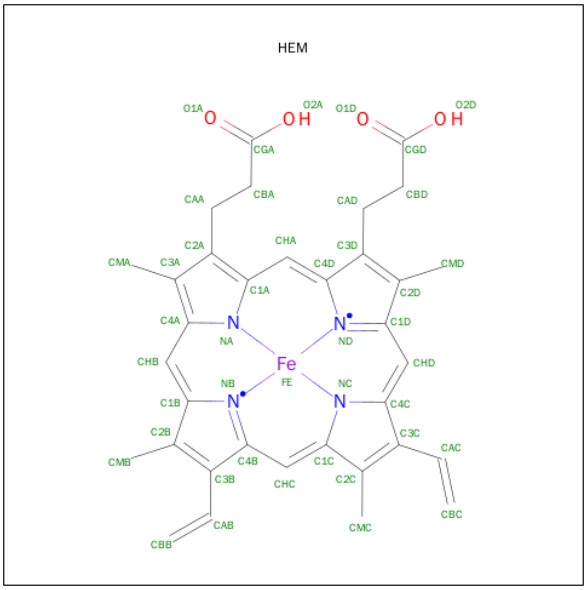
There are 14 unique types of molecules in this entry. The entry contains 6261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AROMATIC PEROXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2513	1590	438	477	8			
1	B	324	Total	C	N	O	S	0	2	0
			2521	1598	438	477	8			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

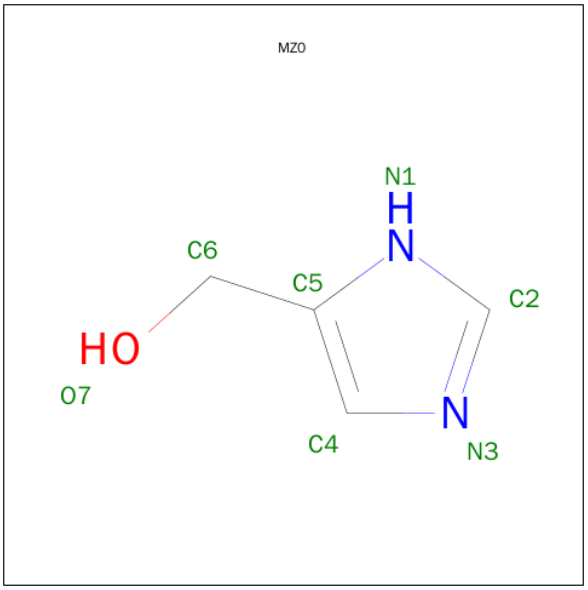


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is 1H-IMIDAZOL-5-YLMETHANOL (three-letter code: MZ0) (formula: $C_4H_6N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 7 4 2 1	0	0
4	B	1	Total C N O 7 4 2 1	0	0

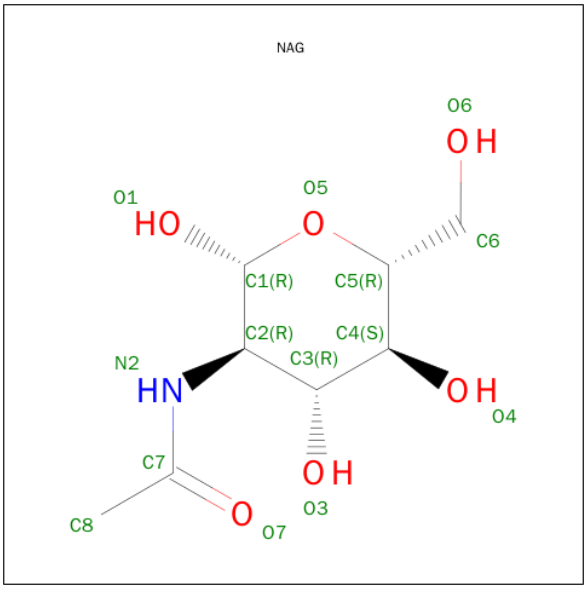
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

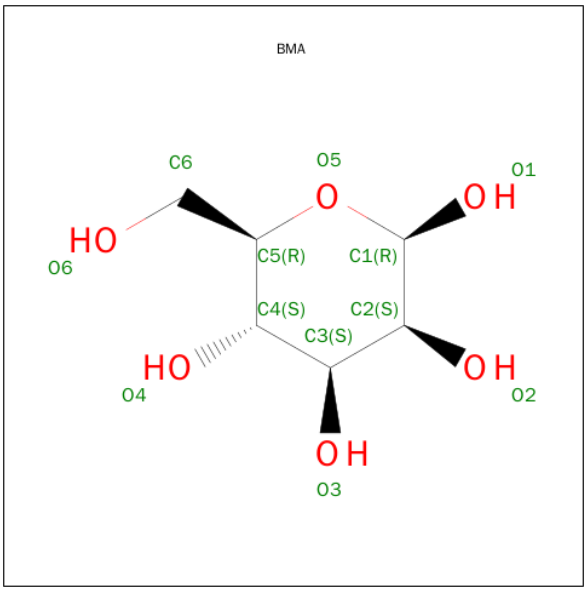
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



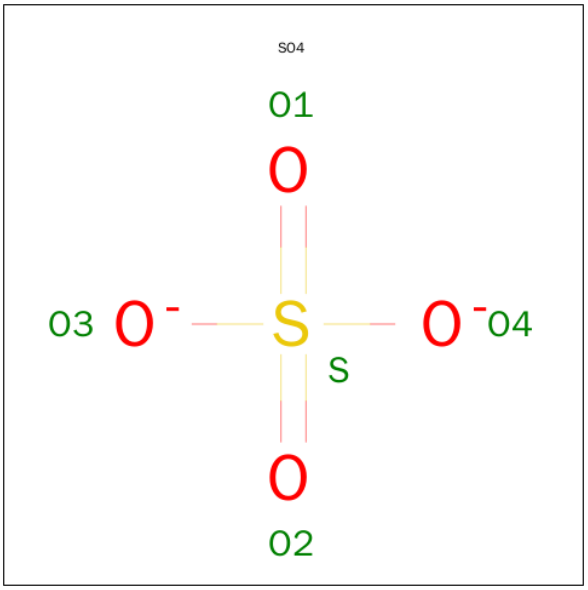
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 8 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 12 6 6	0	0
8	B	1	Total C O 12 6 6	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	3	Total Cl 3 3	0	0
10	A	1	Total Cl 1 1	0	0

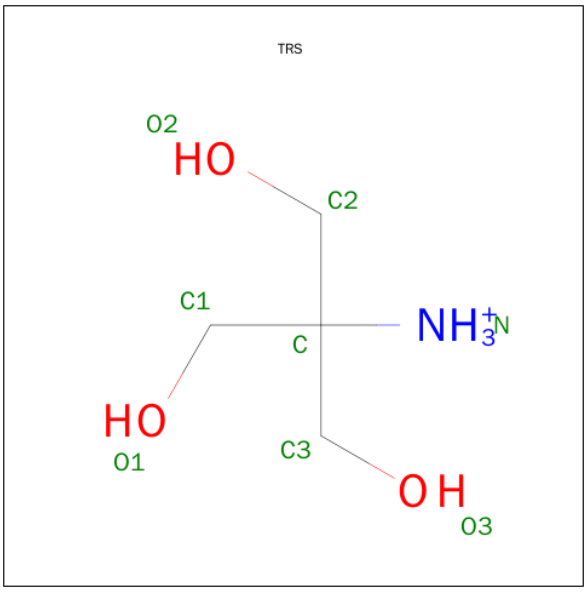
- Molecule 11 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	8	Total C N O 94 52 2 40	0	0

- Molecule 12 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 8 4 1 3	0	0

- Molecule 14 is water.

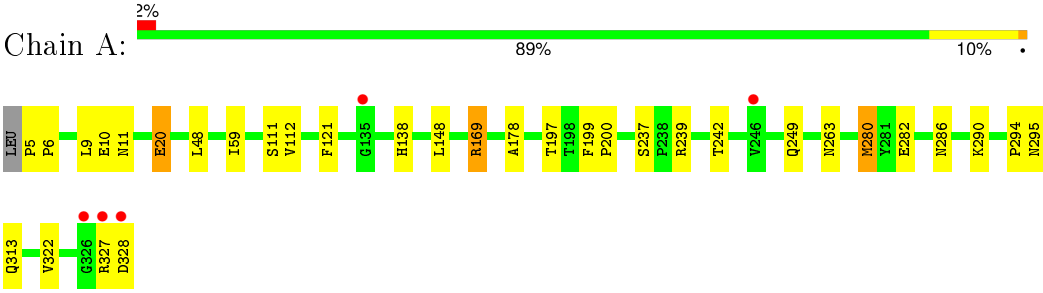
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	350	Total O 350 350	0	0
14	B	293	Total O 293 293	0	0

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.

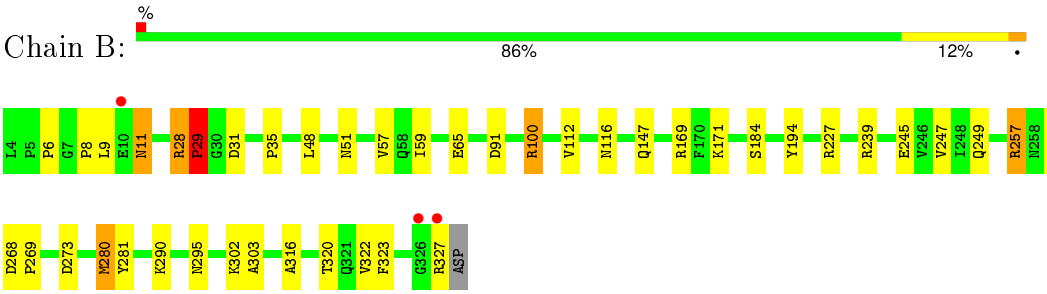
- Molecule 1: AROMATIC PEROXYGENASE

Chain A:



- Molecule 1: AROMATIC PEROXYGENASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.29Å 95.03Å 127.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.19 47.52 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.51-2.19) 98.0 (47.52-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.237 0.170 , 0.237	Depositor DCC
R_{free} test set	2384 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 47667 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6261	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, MZ0, NAG, CL, SO4, HEM, TRS, 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	0.76	0/2583	0.70	1/3514 (0.0%)
1	B	0.75	0/2597	0.69	1/3535 (0.0%)
All	All	0.76	0/5180	0.70	2/7049 (0.0%)

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
12	B	1	0
All	All	1	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	169	ARG	NE-CZ-NH1	-5.97	117.31	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	401	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	PRO	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	2513	0	2387	27	0
1	B	2521	0	2404	37	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	7	0	6	0	0
4	B	7	0	6	0	0
5	A	78	0	68	3	0
6	A	61	0	52	2	0
7	A	42	0	38	6	0
7	B	29	0	28	4	0
8	A	12	0	12	3	0
8	B	12	0	12	3	0
9	A	15	0	0	0	0
9	B	15	0	0	1	0
10	A	1	0	0	0	0
10	B	3	0	0	1	0
11	B	94	0	79	0	0
12	B	112	0	100	2	0
13	B	8	0	12	1	0
14	A	350	0	0	5	0
14	B	293	0	0	8	0
All	All	6261	0	5264	80	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 7.

The worst 5 of 80 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:303:ALA:HA	8:B:501:BMA:H62	1.35	1.04
2:A:350:HEM:HBC2	2:A:350:HEM:HMC2	1.44	0.95
1:A:294:PRO:HB2	7:A:401:NAG:H5	1.50	0.92
12:B:401:NAG:H4	12:B:402:NAG:N2	1.85	0.91
1:A:282:GLU:HG2	1:A:322:VAL:HG21	1.54	0.87

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	322/325 (99%)	307 (95%)	15 (5%)	0	100 100
1	B	324/325 (100%)	308 (95%)	14 (4%)	2 (1%)	30 29
All	All	646/650 (99%)	615 (95%)	29 (4%)	2 (0%)	46 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	PRO
1	B	11	ASN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/271 (100%)	262 (97%)	8 (3%)	48 60
1	B	272/271 (100%)	263 (97%)	9 (3%)	45 56
All	All	542/542 (100%)	525 (97%)	17 (3%)	47 59

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	LYS
1	B	28	ARG
1	B	280	MET
1	A	280	MET
1	B	290	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	147	GLN
1	B	71	ASN
1	A	263	ASN
1	A	313	GLN

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)

27 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	NAG	A	361	1,5	14,14,15	0.61	0	15,19,21	1.18	3 (20%)
5	NAG	A	362	5	14,14,15	0.39	0	15,19,21	1.66	4 (26%)
5	BMA	A	363	5	11,11,12	0.46	0	14,15,17	1.34	2 (14%)
6	NAG	A	371	1,6	14,14,15	0.86	1 (7%)	15,19,21	1.61	4 (26%)
6	NAG	A	372	6	14,14,15	0.61	0	15,19,21	1.68	5 (33%)
6	BMA	A	373	6	11,11,12	0.57	0	14,15,17	1.60	3 (21%)
6	MAN	A	374	6	11,11,12	0.52	0	14,15,17	0.88	1 (7%)
6	MAN	A	375	6	11,11,12	0.55	0	14,15,17	1.02	1 (7%)
5	NAG	A	381	1,5	14,14,15	0.41	0	15,19,21	1.80	4 (26%)
5	NAG	A	382	5	14,14,15	0.61	0	15,19,21	1.24	1 (6%)
5	BMA	A	383	5	11,11,12	0.86	0	14,15,17	2.47	6 (42%)
11	NAG	B	361	1,11	14,14,15	0.80	0	15,19,21	1.12	2 (13%)
11	NAG	B	362	11	14,14,15	0.82	0	15,19,21	1.02	1 (6%)
11	BMA	B	363	11	11,11,12	0.62	0	14,15,17	1.18	1 (7%)
11	MAN	B	364	11	11,11,12	0.63	0	14,15,17	0.97	0
11	MAN	B	365	11	11,11,12	0.57	0	14,15,17	1.08	1 (7%)
11	MAN	B	366	11	11,11,12	0.49	0	14,15,17	1.51	1 (7%)
11	MAN	B	367	11	11,11,12	0.42	0	14,15,17	1.52	3 (21%)
11	MAN	B	368	11	11,11,12	0.73	0	14,15,17	1.80	3 (21%)
12	NAG	B	371	1,12	14,14,15	0.75	0	15,19,21	1.65	4 (26%)
12	NAG	B	372	12	14,14,15	0.61	0	15,19,21	2.04	2 (13%)
12	NAG	B	381	1,12	14,14,15	0.75	0	15,19,21	1.48	2 (13%)
12	NAG	B	382	12	14,14,15	0.51	0	15,19,21	1.99	2 (13%)
12	NAG	B	391	1,12	14,14,15	0.55	0	15,19,21	2.51	4 (26%)
12	NAG	B	392	12	14,14,15	0.50	0	15,19,21	1.18	1 (6%)
12	NAG	B	401	1,12	14,14,15	0.48	0	15,19,21	0.81	0
12	NAG	B	402	12	14,14,15	0.66	0	15,19,21	0.69	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 no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	361	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	362	5	-	0/6/23/26	0/1/1/1
5	BMA	A	363	5	-	0/2/19/22	0/1/1/1
6	NAG	A	371	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	372	6	-	0/6/23/26	0/1/1/1
6	BMA	A	373	6	-	0/2/19/22	0/1/1/1
6	MAN	A	374	6	-	0/2/19/22	1/1/1/1
6	MAN	A	375	6	-	0/2/19/22	0/1/1/1
5	NAG	A	381	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	382	5	-	0/6/23/26	0/1/1/1
5	BMA	A	383	5	-	0/2/19/22	0/1/1/1
11	NAG	B	361	1,11	-	0/6/23/26	0/1/1/1
11	NAG	B	362	11	-	0/6/23/26	0/1/1/1
11	BMA	B	363	11	-	0/2/19/22	0/1/1/1
11	MAN	B	364	11	-	0/2/19/22	0/1/1/1
11	MAN	B	365	11	-	0/2/19/22	0/1/1/1
11	MAN	B	366	11	-	0/2/19/22	0/1/1/1
11	MAN	B	367	11	-	0/2/19/22	0/1/1/1
11	MAN	B	368	11	-	0/2/19/22	0/1/1/1
12	NAG	B	371	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	372	12	-	0/6/23/26	0/1/1/1
12	NAG	B	381	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	382	12	-	0/6/23/26	0/1/1/1
12	NAG	B	391	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	392	12	-	0/6/23/26	0/1/1/1
12	NAG	B	401	1,12	1/1/5/7	0/6/23/26	0/1/1/1
12	NAG	B	402	12	-	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)
6	A	371	NAG	C1-C2	2.25	1.55	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	372	NAG	C1-O5-C5	-6.31	104.24	112.25
12	B	391	NAG	C4-C3-C2	-5.88	102.09	111.23
5	A	383	BMA	C3-C4-C5	-5.02	101.45	110.20
11	B	366	MAN	C1-C2-C3	-4.22	104.55	109.54
5	A	383	BMA	C2-C3-C4	-4.12	104.05	111.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	401	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	374	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	362	NAG	2	0
5	A	363	BMA	2	0
6	A	373	BMA	2	0
6	A	375	MAN	2	0
5	A	381	NAG	1	0
12	B	401	NAG	2	0
12	B	402	NAG	2	0

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
9	SO4	A	1355	-	4,4,4	0.16	0	6,6,6	0.09	0
9	SO4	A	1357	-	4,4,4	0.38	0	6,6,6	0.33	0
9	SO4	A	1358	-	4,4,4	0.22	0	6,6,6	0.07	0
2	HEM	A	350	1,3,4	30,50,50	2.12	8 (26%)	24,82,82	2.88	13 (54%)
4	MZ0	A	354	2	3,7,7	0.51	0	3,8,8	1.50	0
7	NAG	A	391	1	14,14,15	0.54	0	15,19,21	0.59	0
7	NAG	A	401	1	14,14,15	0.56	0	15,19,21	3.79	2 (13%)
7	NAG	A	411	1	14,14,15	1.52	3 (21%)	15,19,21	2.14	4 (26%)
8	BMA	A	501	-	12,12,12	0.90	0	17,17,17	2.18	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	TRS	B	1355	-	7,7,7	0.96	1 (14%)	9,9,9	0.50	0
9	SO4	B	1357	-	4,4,4	0.20	0	6,6,6	0.32	0
9	SO4	B	1359	-	4,4,4	0.11	0	6,6,6	0.27	0
9	SO4	B	1360	-	4,4,4	0.20	0	6,6,6	0.16	0
2	HEM	B	350	1,3,4	30,50,50	2.28	6 (20%)	24,82,82	2.37	10 (41%)
4	MZ0	B	354	2	3,7,7	0.50	0	3,8,8	1.32	0
7	NAG	B	411	1	14,14,15	0.51	0	15,19,21	0.73	0
8	BMA	B	501	-	12,12,12	0.67	0	17,17,17	1.54	4 (23%)
7	NAG	B	511	-	15,15,15	0.78	1 (6%)	17,21,21	1.97	5 (29%)

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
9	SO4	A	1355	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1357	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1358	-	-	0/0/0/0	0/0/0/0
2	HEM	A	350	1,3,4	-	0/10/54/54	0/0/8/8
4	MZ0	A	354	2	-	0/0/2/2	0/1/1/1
7	NAG	A	391	1	-	0/6/23/26	0/1/1/1
7	NAG	A	401	1	-	0/6/23/26	0/1/1/1
7	NAG	A	411	1	-	0/6/23/26	0/1/1/1
8	BMA	A	501	-	-	0/2/22/22	0/1/1/1
13	TRS	B	1355	-	-	0/9/9/9	0/0/0/0
9	SO4	B	1357	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1359	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1360	-	-	0/0/0/0	0/0/0/0
2	HEM	B	350	1,3,4	-	0/10/54/54	0/0/8/8
4	MZ0	B	354	2	-	0/0/2/2	0/1/1/1
7	NAG	B	411	1	-	0/6/23/26	0/1/1/1
8	BMA	B	501	-	-	0/2/22/22	0/1/1/1
7	NAG	B	511	-	-	0/6/26/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	HEM	C3B-C4B	-7.21	1.45	1.51
2	B	350	HEM	C3D-C4D	-6.73	1.42	1.51
2	A	350	HEM	C3B-C4B	-6.18	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	HEM	C3D-C4D	-4.86	1.45	1.51
2	A	350	HEM	C2C-C1C	-4.10	1.44	1.52

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	350	HEM	C3B-CAB-CBB	-6.43	114.59	124.46
2	A	350	HEM	C3C-CAC-CBC	-4.81	117.08	124.46
2	A	350	HEM	CAA-C2A-C1A	-4.08	122.58	127.01
7	B	511	NAG	C3-C2-N2	-3.92	102.55	110.66
2	A	350	HEM	CAA-CBA-CGA	-3.26	106.77	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	HEM	4	0
7	A	401	NAG	6	0
8	A	501	BMA	3	0
13	B	1355	TRS	1	0
9	B	1357	SO4	1	0
2	B	350	HEM	2	0
8	B	501	BMA	3	0
7	B	511	NAG	4	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

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>2			OWAB(Å^2)	Q<0.9
1	A	324/325 (99%)	-0.33	5 (1%)	76	75	8, 18, 32, 77	0
1	B	324/325 (99%)	-0.31	3 (0%)	85	85	6, 16, 31, 68	0
All	All	648/650 (99%)	-0.32	8 (1%)	81	80	6, 17, 32, 77	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ARG	5.7
1	B	326	GLY	3.8
1	A	328	ASP	3.7
1	A	327	ARG	3.1
1	A	326	GLY	2.8

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

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

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, 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	LLDF	B-factors(Å^2)	Q<0.9
12	NAG	B	391	14/15	0.85	0.28	10.26	41,46,50,61	0
6	MAN	A	374	11/12	0.65	0.34	6.92	89,92,93,95	0
6	NAG	A	372	14/15	0.87	0.21	6.20	46,51,58,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	NAG	B	372	14/15	0.77	0.21	3.32	44,52,57,60	0
12	NAG	B	371	14/15	0.95	0.09	0.23	9,12,24,32	0
6	NAG	A	371	14/15	0.96	0.09	0.14	10,21,30,35	0
11	NAG	B	361	14/15	0.93	0.10	-0.11	21,24,27,28	0
11	MAN	B	367	11/12	0.79	0.32	-	53,57,60,63	0
11	MAN	B	364	11/12	0.91	0.19	-	38,42,43,43	0
5	NAG	A	381	14/15	0.89	0.25	-	39,50,57,65	0
11	MAN	B	365	11/12	0.91	0.19	-	40,44,47,50	0
6	BMA	A	373	11/12	0.73	0.27	-	74,78,83,84	0
5	NAG	A	361	14/15	0.94	0.13	-	30,35,41,48	0
11	NAG	B	362	14/15	0.94	0.15	-	30,32,38,39	0
11	MAN	B	366	11/12	0.90	0.25	-	46,48,52,59	0
12	NAG	B	401	14/15	0.48	0.60	-	77,83,86,91	0
12	NAG	B	381	14/15	0.87	0.20	-	41,51,58,65	0
11	BMA	B	363	11/12	0.92	0.23	-	39,42,44,46	0
12	NAG	B	382	14/15	0.69	0.42	-	72,75,76,77	0
5	NAG	A	382	14/15	0.71	0.33	-	72,76,79,84	0
5	NAG	A	362	14/15	0.88	0.21	-	43,51,59,64	0
12	NAG	B	402	14/15	0.14	0.67	-	95,96,97,97	0
5	BMA	A	383	11/12	0.50	0.56	-	89,90,92,93	0
11	MAN	B	368	11/12	0.52	0.62	-	67,71,72,73	0
6	MAN	A	375	11/12	0.46	0.28	-	80,82,84,84	0
5	BMA	A	363	11/12	0.80	0.42	-	70,72,74,74	0
12	NAG	B	392	14/15	0.70	0.44	-	68,73,76,77	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, 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	LLDF	B-factors(Å^2)	Q<0.9
8	BMA	B	501	12/12	0.66	0.36	15.37	48,55,57,57	0
8	BMA	A	501	12/12	0.83	0.37	13.37	22,37,43,45	0
7	NAG	B	511	15/15	0.71	0.40	10.62	48,54,60,61	0
7	NAG	A	391	14/15	0.70	0.28	9.04	39,54,65,66	0
9	SO4	B	1360	5/5	0.92	0.13	1.70	48,50,54,55	0
4	MZ0	B	354	7/7	0.96	0.15	0.63	15,18,26,33	0
3	MG	A	353	1/1	0.98	0.09	0.47	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	B	350	43/43	0.98	0.12	0.38	2,7,14,16	0
2	HEM	A	350	43/43	0.98	0.10	0.17	6,8,16,20	0
4	MZ0	A	354	7/7	0.96	0.12	-0.38	15,17,23,27	0
9	SO4	A	1357	5/5	0.99	0.09	-0.66	40,41,43,45	0
3	MG	B	353	1/1	0.98	0.07	-1.87	9,9,9,9	0
10	CL	A	1356	1/1	0.99	0.05	-2.00	35,35,35,35	0
10	CL	B	1356	1/1	0.98	0.05	-2.70	34,34,34,34	0
9	SO4	B	1357	5/5	0.97	0.08	-	44,45,46,48	0
9	SO4	B	1359	5/5	0.94	0.27	-	68,68,70,72	0
13	TRS	B	1355	8/8	0.58	0.47	-	88,89,90,90	0
7	NAG	B	411	14/15	0.62	0.66	-	71,77,81,81	0
7	NAG	A	411	14/15	0.80	0.37	-	57,61,66,68	0
10	CL	B	1358	1/1	0.91	0.05	-	68,68,68,68	0
9	SO4	A	1355	5/5	0.94	0.24	-	81,81,82,82	0
9	SO4	A	1358	5/5	0.96	0.14	-	75,76,77,77	0
7	NAG	A	401	14/15	0.68	0.47	-	66,70,72,73	0
10	CL	B	1361	1/1	0.95	0.06	-	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.