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

wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2024 – 04:50 PM JST

PDB ID	:	6KK8
Title	:	XN joint refinement of manganese catalase from Thermus Thermophilus HB27
Authors	:	Yamada, T.; Yano, N.; Kusaka, K.
Deposited on	:	2019-07-24
Resolution	:	1.37 Å(reported)

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

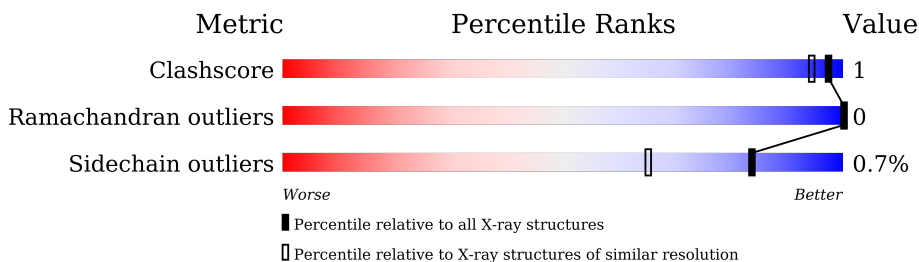|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.37 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
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		0.7%

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))
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	302	97%
1	B	302	97%

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
3	O	A	1004[B]	-	-	X	-
3	O	B	1004[A]	-	-	X	-
3	O	B	1005[B]	-	-	X	-

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2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 10509 atoms, of which 4431 are hydrogens and 1169 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 Pseudocatalase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	299	Total 4979	C 1489	D 437	H 2230	N 381	O 427	S 15	64	281	0
1	B	300	Total 4911	C 1476	D 430	H 2189	N 381	O 423	S 12	63	282	0

- Molecule 2 is MANGANESE (III) ION (three-letter code: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 5	O 5	0	2
3	B	3	Total 5	O 5	0	2

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	D	H	O	0	1
			12	2	2	6	2		
4	B	1	Total	C	D	H	O	0	1
			12	2	2	6	2		

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

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

• Molecule 6 is water.

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	141	Total 293	D 151	O 142	0	1
6	B	134	Total 283	D 147	O 136	0	2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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 failed to run properly.

• Molecule 1: Pseudocatalase

Chain A:

97%

• Molecule 1: Pseudocatalase

Chain B:

97%

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	133.40Å 133.40Å 133.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.47 – 1.37	Depositor
% Data completeness (in resolution range)	100.0 (44.47-1.37)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.37Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.122 , 0.133	Depositor
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
Total number of atoms	10509	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

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: MN3, EDO, O, DOD, SO4

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	0.56	4/4552 (0.1%)	0.75	6/6179 (0.1%)
1	B	0.55	4/4532 (0.1%)	0.77	10/6157 (0.2%)
All	All	0.55	8/9084 (0.1%)	0.76	16/12336 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167[A]	GLU	CD-OE1	-6.40	1.18	1.25
1	A	167[B]	GLU	CD-OE1	-6.40	1.18	1.25
1	B	280[A]	GLU	CD-OE1	-6.25	1.18	1.25
1	B	280[B]	GLU	CD-OE1	-6.25	1.18	1.25
1	B	167[A]	GLU	CD-OE1	-5.84	1.19	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	260[A]	VAL	CG1-CB-CG2	8.49	124.49	110.90
1	B	260[B]	VAL	CG1-CB-CG2	8.49	124.49	110.90
1	A	173[A]	VAL	CG1-CB-CG2	6.86	121.87	110.90
1	A	173[B]	VAL	CG1-CB-CG2	6.86	121.87	110.90
1	B	84[A]	LEU	CB-CG-CD2	6.68	122.36	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2749	2230	206	0	0
1	B	2722	2189	170	1	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	3	0
3	B	5	0	0	4	0
4	A	6	6	0	0	0
4	B	6	6	0	0	0
5	A	5	0	0	0	0
6	A	293	0	0	0	0
6	B	283	0	0	0	0
All	All	6078	4431	376	7	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 1.

The worst 5 of 7 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)
3:B:1004[B]:O:O	3:B:1005[B]:O:O	2.09	0.70
3:A:1004[A]:O:O	3:A:1005[A]:O:O	2.17	0.61
3:A:1004[B]:O:O	3:A:1005[B]:O:O	2.27	0.52
1:B:162[B]:LYS:NZ	3:B:1005[B]:O:O	2.44	0.51
3:B:1004[A]:O:O	3:B:1005[A]:O:O	2.34	0.45

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	576/302 (191%)	568 (99%)	8 (1%)	0	100	100
1	B	578/302 (191%)	568 (98%)	10 (2%)	0	100	100
All	All	1154/604 (191%)	1136 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	436/241 (181%)	432 (99%)	4 (1%)	78	56
1	B	432/241 (179%)	430 (100%)	2 (0%)	88	74
All	All	868/482 (180%)	862 (99%)	6 (1%)	84	65

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263[B]	ASP
1	B	122[A]	ASN
1	B	122[B]	ASN
1	A	122[B]	ASN
1	A	122[A]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	SO4	A	1007	-	4,4,4	0.36	0	6,6,6	0.38	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.