



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 01:58 am BST

PDB ID : 5TKE
Title : Crystal Structure of Eukaryotic Hydrolase
Authors : Li, B.; Jiang, J.
Deposited on : 2016-10-06
Resolution : 2.48 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

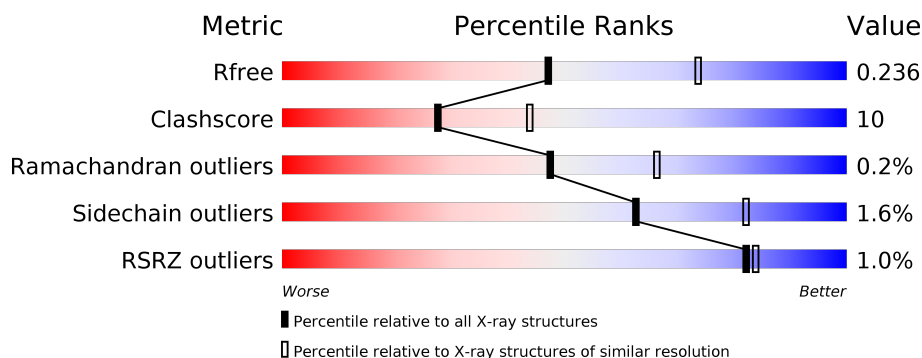
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 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 $\leq 5\%$. 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	504	<div> <div></div> <div> <div></div> <div>65%</div> <div>17%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	504	<div> <div></div> <div> <div></div> <div>68%</div> <div>14%</div> <div>•</div> <div>16%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7289 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 O-GlcNAcase: chimera construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3444	2233	564	624	23			
1	B	422	Total	C	N	O	S	0	0	0
			3461	2244	570	626	21			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	HIS	-	expression tag	UNP O60502
A	543	GLY	-	linker	UNP O60502
A	544	GLY	-	linker	UNP O60502
A	545	GLY	-	linker	UNP O60502
A	546	GLY	-	linker	UNP O60502
A	547	SER	-	linker	UNP O60502
A	548	GLY	-	linker	UNP O60502
A	549	GLY	-	linker	UNP O60502
A	550	GLY	-	linker	UNP O60502
A	551	GLY	-	linker	UNP O60502
A	552	SER	-	linker	UNP O60502
B	59	HIS	-	expression tag	UNP O60502
B	543	GLY	-	linker	UNP O60502
B	544	GLY	-	linker	UNP O60502
B	545	GLY	-	linker	UNP O60502
B	546	GLY	-	linker	UNP O60502
B	547	SER	-	linker	UNP O60502
B	548	GLY	-	linker	UNP O60502
B	549	GLY	-	linker	UNP O60502
B	550	GLY	-	linker	UNP O60502
B	551	GLY	-	linker	UNP O60502
B	552	SER	-	linker	UNP O60502

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	210	Total 210	O 210	0	0
2	B	174	Total 174	O 174	0	0

- Molecule 1: O-GlcNAcase: chimera construct



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.06 Å 96.58 Å 89.28 Å 90.00° 115.04° 90.00°	Depositor
Resolution (Å)	44.25 – 2.48 48.29 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.5 (44.25-2.48) 87.3 (48.29-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.48 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.181 , 0.236 0.181 , 0.236	Depositor DCC
R_{free} test set	2015 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.50	0/3534	0.64	1/4779 (0.0%)
1	B	0.48	0/3554	0.71	4/4808 (0.1%)
All	All	0.49	0/7088	0.67	5/9587 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	650	ILE	CG1-CB-CG2	-9.92	89.58	111.40
1	B	306	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	306	ARG	CA-CB-CG	6.88	128.53	113.40
1	B	381	LYS	CD-CE-NZ	6.64	126.98	111.70
1	A	290	ARG	NE-CZ-NH1	-6.21	117.19	120.30

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	3444	0	3376	76	0
1	B	3461	0	3391	64	0
2	A	210	0	0	13	0
2	B	174	0	0	7	0
All	All	7289	0	6767	136	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 10.

The worst 5 of 136 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:650:ILE:CD1	1:B:682:ARG:HH21	1.50	1.22
1:A:101:TYR:HD2	1:A:106:PHE:CD2	1.84	0.95
1:A:101:TYR:CD2	1:A:106:PHE:HD2	1.86	0.94
1:A:74:VAL:H	1:A:77:GLN:HE21	1.13	0.93
1:B:650:ILE:CD1	1:B:682:ARG:NH2	2.31	0.93

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	408/504 (81%)	399 (98%)	8 (2%)	1 (0%)	47	66
1	B	412/504 (82%)	401 (97%)	10 (2%)	1 (0%)	47	66
All	All	820/1008 (81%)	800 (98%)	18 (2%)	2 (0%)	47	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	PRO
1	B	314	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	372/442 (84%)	367 (99%)	5 (1%)	69	86
1	B	373/442 (84%)	366 (98%)	7 (2%)	57	78
All	All	745/884 (84%)	733 (98%)	12 (2%)	62	82

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	HIS
1	B	71	ARG
1	B	156	ARG
1	A	656	SER
1	B	127	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	559	GLN
1	B	195	GLN
1	B	313	ASN
1	A	396	GLN
1	B	204	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	420/504 (83%)	-0.23	6 (1%) 75 77	22, 43, 70, 102	0
1	B	422/504 (83%)	-0.23	2 (0%) 91 91	28, 50, 73, 94	0
All	All	842/1008 (83%)	-0.23	8 (0%) 82 84	22, 48, 71, 102	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	604	ILE	3.6
1	A	186	GLU	3.3
1	B	604	ILE	3.2
1	A	187	VAL	2.4
1	A	101	TYR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.