



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6HKI / pdb_00006hki
Title : Crystal structure of surface entropy mutant of human O-GlcNAc hydrolase
Authors : Males, A.; Davies, G.J.
Deposited on : 2018-09-06
Resolution : 3.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

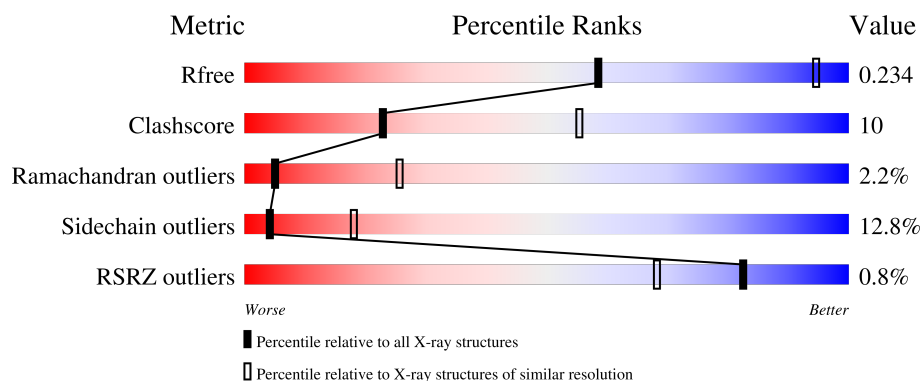
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	916	
1	B	916	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7880 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 Protein O-GlcNAcase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	2	0
			3965	2562	657	721	25			
1	B	486	Total	C	N	O	S	0	0	0
			3914	2531	650	708	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	602	ALA	GLU	engineered mutation	UNP O60502
A	605	ALA	GLU	engineered mutation	UNP O60502
B	602	ALA	GLU	engineered mutation	UNP O60502
B	605	ALA	GLU	engineered mutation	UNP O60502

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.17Å 222.17Å 72.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.40 – 3.30 192.40 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (192.40-3.30) 100.0 (192.40-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.169 , 0.234 0.177 , 0.234	Depositor DCC
R_{free} test set	1483 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7880	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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

5.1 Standard geometry

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	0.89	1/4080 (0.0%)	1.23	6/5536 (0.1%)
1	B	0.88	2/4021 (0.0%)	1.23	9/5453 (0.2%)
All	All	0.88	3/8101 (0.0%)	1.23	15/10989 (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	4
1	B	0	4
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	714	VAL	N-CA	6.92	1.54	1.46
1	B	594	VAL	N-CA	6.78	1.54	1.46
1	B	673	ILE	N-CA	5.04	1.52	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	CA-CB-CG	9.48	122.08	112.60
1	B	631	CYS	CB-CA-C	7.30	120.78	109.84
1	B	705	PRO	N-CA-C	6.64	118.80	110.70
1	B	549	THR	CA-CB-OG1	-5.80	100.89	109.60
1	A	317	GLU	CB-CG-CD	5.72	122.32	112.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	ARG	Sidechain
1	A	273	ARG	Sidechain
1	A	83[A]	ARG	Sidechain
1	A	83[B]	ARG	Sidechain
1	B	59	ARG	Sidechain

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	3965	0	3862	87	0
1	B	3914	0	3810	90	0
2	B	1	0	0	0	0
All	All	7880	0	7672	162	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 162 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:A:108:ARG:HH22	1:A:150:GLU:CD	1.92	0.78
1:B:110:MET:HB3	1:B:160:GLN:HE22	1.49	0.77
1:A:300:SER:O	1:A:303:LEU:HD22	1.88	0.74
1:B:585:LEU:HD21	1:B:611:ALA:HA	1.71	0.72
1:A:586:ARG:NH2	1:A:700:ASP:O	2.22	0.72

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	486/916 (53%)	425 (87%)	49 (10%)	12 (2%)	4	23
1	B	480/916 (52%)	431 (90%)	40 (8%)	9 (2%)	6	28
All	All	966/1832 (53%)	856 (89%)	89 (9%)	21 (2%)	5	26

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	699	ASN
1	B	593	SER
1	B	597	LYS
1	A	334	SER

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	426/795 (54%)	375 (88%)	51 (12%)	5	20
1	B	418/795 (53%)	359 (86%)	59 (14%)	3	14
All	All	844/1590 (53%)	734 (87%)	110 (13%)	4	17

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	153	THR
1	B	267	VAL
1	B	696	ASP
1	B	640	MET
1	B	159	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	595	ASN
1	B	630	ASN
1	A	537	GLN
1	A	395	HIS
1	B	633	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](#)

There are no oligosaccharides 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	490/916 (53%)	-0.50	3 (0%) 85 73	29, 68, 125, 179	2 (0%)
1	B	486/916 (53%)	-0.24	5 (1%) 79 63	44, 72, 116, 175	0
All	All	976/1832 (53%)	-0.37	8 (0%) 82 68	29, 70, 122, 179	2 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	699	ASN	3.7
1	A	602	ALA	3.6
1	A	699	ASN	3.0
1	A	713	LYS	2.6
1	B	178	HIS	2.5

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 oligosaccharides 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.