



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:27 pm GMT

PDB ID : 1SO7  
Title : Maltose-induced structure of the human cytosolic sialidase Neu2  
Authors : Chavas, L.M.G.; Fusi, P.; Tringali, C.; Venerando, B.; Tettamanti, G.; Kato, R.; Monti, E.; Wakatsuki, S.  
Deposited on : 2004-03-12  
Resolution : 1.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : **FAILED**  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

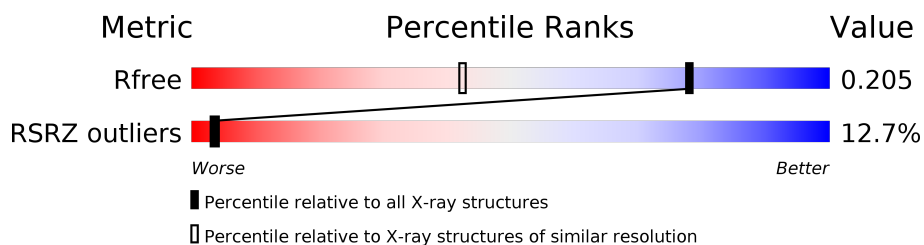
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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))
$R_{free}$	111664	2534 (1.50-1.50)
RSRZ outliers	108989	2481 (1.50-1.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3157 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 Sialidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	11	0
			2860	1809	511	526	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9Y3R4
A	0	SER	-	CLONING ARTIFACT	UNP Q9Y3R4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	296	Total	O	0	0
			296	296		

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### 3 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.69Å 145.69Å 64.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.49 45.06 – 1.49	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-1.49) 97.2 (45.06-1.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.67 (at 1.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.213 0.205 , 0.205	Depositor DCC
$R_{free}$ test set	3987 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

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

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### 4.5 Carbohydrates [i](#)

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### 4.6 Ligand geometry [i](#)

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### 4.7 Other polymers [i](#)

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## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	361/382 (94%)	0.77	46 (12%) 3 4	14, 23, 37, 45	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	THR	7.4
1	A	185	HIS	6.8
1	A	288	SER	5.8
1	A	187	ILE	5.7
1	A	111	GLU	5.5
1	A	49	ALA	5.2
1	A	225	GLU	4.8
1	A	115	LEU	4.5
1	A	375	ALA	4.3
1	A	217	LEU	4.0
1	A	191	ILE	3.9
1	A	78	ARG	3.9
1	A	270	GLN	3.9
1	A	109	VAL	3.5
1	A	289	PRO	3.4
1	A	152	ARG	3.4
1	A	377	TYR	3.3
1	A	4	LEU	3.1
1	A	16	GLY	3.0
1	A	229	GLN	2.9
1	A	110	THR	2.8
1	A	116	GLN	2.8
1	A	189	ARG	2.7
1	A	181	TYR	2.6
1	A	114	GLN	2.6
1	A	179	TYR	2.5
1	A	80	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	186	PRO	2.5
1	A	112	GLN	2.5
1	A	195	PHE	2.5
1	A	108	GLN	2.4
1	A	14	GLN	2.4
1	A	192	PRO	2.4
1	A	51	LEU	2.4
1	A	326	LEU	2.4
1	A	72	GLU	2.3
1	A	333	ALA	2.2
1	A	70	ALA	2.2
1	A	374	PRO	2.2
1	A	17	ALA	2.1
1	A	88[A]	CYS	2.1
1	A	144	ASP	2.1
1	A	159	VAL	2.1
1	A	219	CYS	2.1
1	A	221	VAL	2.1
1	A	214	GLN	2.0

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

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

## 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	381	1/1	0.98	0.08	27,27,27,27	0



## 5.5 Other polymers [i](#)

There are no such residues in this entry.