



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 2VUY / pdb_00002vuy
Title : Crystal structure of Glycogen Debranching exzyme TreX from Sulfolobus sol-
fatarius
Authors : Song, H.-N.; Yoon, S.-M.; Cha, H.-J.; Park, K.-H.; Woo, E.-J.
Deposited on : 2008-06-02
Resolution : 3.00 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

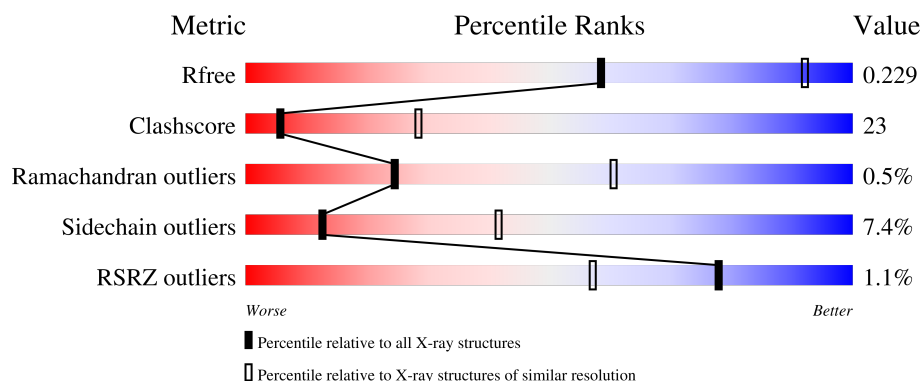
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	718	
1	B	718	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11634 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 GLYCOGEN OPERON PROTEIN GLGX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	0	0
			5826	3735	983	1089	19			
1	B	711	Total	C	N	O	S	0	0	0
			5808	3725	978	1086	19			

I683	S684	S685	T686	L687	R688	E689	I690	R695	E700	E706	G707	R708	T709	A710	L711	V712	R715	I716	E717	L718																																
L578	K583	M584	I585	Y588	R589	A590	H591	P592	R595	R596	E597	R598	Y599	K603	M608	K611	D612	E619	V623	E625	K626	T627	F637	E640	V643	E646	I647	R648	R653	I654	A655	D656	I661	N669	K673	F674	K678	L681	V682													
V479	S480	M486	A487	N488	N489	N492	N493	S502	Q503	N504	C505	G506	T511	N512	D513	I518	C519	R520	E521	K522	R525	I529	L532	V533	S534	Q535	L541	D544	E545	L546	S547	R548	T549	Q550	R551	N554	Q559	D560	N561	E562	I563	T564	W565	W568	N569	L570						
F382	I383	I390	K395	L396	I397	A398	E399	P400	W401	D402	V403	G407	Y408	Q409	F413	P414	Y415	Q416	W417	K423	Y424	R425	D426	R429	L437	E441	I442	R445	L446	L447	G448	S449	P450	Y453	L454	N457	K458	F461	Y466	V467	T468	T474	D477	L478								
N290	H291	T292	A293	E294	H297	L298	G299	P300	T301	L302	S303	F304	R305	G306	I307	Y313	M314	L315	N319	K320	R321	Y322	Y323	L324	D325	F326	T327	T332	P338	R339	Q342	M343	V344	Y350	T353	E354	R361	L364	A365	A366	L372	Y373	K377	L378	T380	F381						
L105	P108	Y109	R108	A110	K111	I118	W119	N120	V123	F124	G125	Y126	K127	I128	G129	D130	Q131	N132	Q133	D134	L135	S142	G143	E144	Y145	K148	S149	V150	N153	P154	Y155	F156	E157	W158	D159	D160	E161	D162	F163	I164	K165	K168	L171	K172	D173	T174	V175	I176	Y177	E178	V179	H180
V181	K182	L187	L189	D190	L191	P192	E193	Y199	S204	E205	Q206	N207	I208	K212	D213	I216	T217	T218	M222	P223	V224	F225	H226	F227	Q230	R231	F232	L233	K236	T247	F250	E253	Y256	Q263	V266	L267	H277	E282	V287	V288	Y289											

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.63Å 203.63Å 89.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 3.00 29.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.86-3.00) 92.9 (29.86-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.56 (at 3.01Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.206 , 0.231 0.204 , 0.229	Depositor DCC
R_{free} test set	2004 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11634	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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	0.38	0/5978	0.89	13/8104 (0.2%)
1	B	0.37	0/5960	0.89	13/8080 (0.2%)
All	All	0.37	0/11938	0.89	26/16184 (0.2%)

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	1	2
1	B	0	3
All	All	1	5

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	297	HIS	N-CA-C	-7.84	100.77	110.41
1	A	297	HIS	N-CA-C	-7.69	100.95	110.41
1	A	373	TYR	N-CA-C	6.59	120.42	112.38
1	B	373	TYR	N-CA-C	6.59	120.42	112.38
1	B	474	THR	N-CA-C	-6.56	100.27	110.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	THR	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	ALA	Peptide
1	A	7	THR	Peptide
1	B	398	ALA	Peptide
1	B	417	TRP	Peptide
1	B	9	ASP	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	5826	0	5642	280	0
1	B	5808	0	5622	258	0
All	All	11634	0	11264	534	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 23.

The worst 5 of 534 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:6:ARG:NH1	1:A:7:THR:HG22	1.29	1.43
1:A:6:ARG:CG	1:A:7:THR:H	1.59	1.15
1:A:511:THR:HG22	1:A:513:ASP:H	1.13	1.10
1:B:8:ARG:O	1:B:8:ARG:HG2	1.51	1.10
1:B:292:THR:HG22	1:B:294:GLU:H	1.17	1.08

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	711/718 (99%)	644 (91%)	64 (9%)	3 (0%)	30	65
1	B	709/718 (99%)	643 (91%)	62 (9%)	4 (1%)	21	56
All	All	1420/1436 (99%)	1287 (91%)	126 (9%)	7 (0%)	24	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	700	GLU
1	B	156	PHE
1	B	414	PRO
1	B	700	GLU

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	629/636 (99%)	581 (92%)	48 (8%)	12	41
1	B	627/636 (99%)	582 (93%)	45 (7%)	13	43
All	All	1256/1272 (99%)	1163 (93%)	93 (7%)	13	42

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	LEU
1	B	492	ASN
1	B	213	ASP
1	B	319	ASN
1	B	533	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	554	ASN
1	B	559	GLN
1	A	550	GLN
1	A	526	ASN
1	B	561	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	713/718 (99%)	-0.17	9 (1%) 75 53	16, 32, 53, 100	0
1	B	711/718 (99%)	-0.15	6 (0%) 82 64	13, 34, 58, 83	0
All	All	1424/1436 (99%)	-0.16	15 (1%) 78 57	13, 33, 55, 100	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	THR	7.9
1	B	164	ILE	3.3
1	A	6	ARG	3.2
1	B	159	ASP	3.1
1	B	160	ASP	2.9

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.