



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:31 am GMT

PDB ID : 2VNC
Title : CRYSTAL STRUCTURE OF GLYCOGEN DEBRANCHING ENZYME
TREX FROM SULFOLOBUS SOLFATARICUS
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Deposited on : 2008-02-04
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

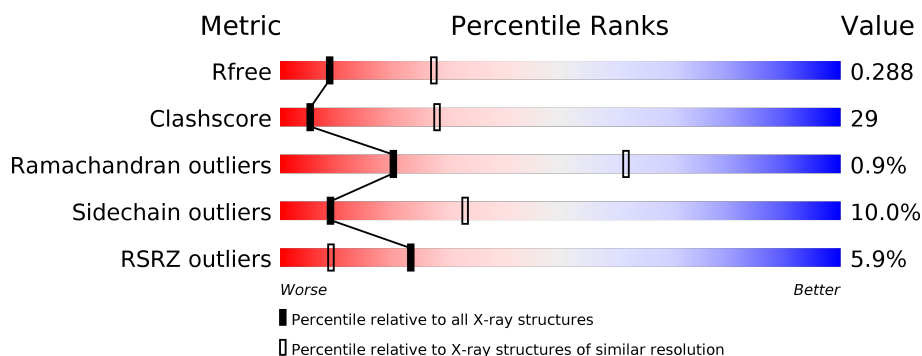
1 Overall quality at a glance

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>68%</div> <div>26%</div> <div>• •</div> </div>
1	B	718	<div> <div>9%</div> <div>47%</div> <div>36%</div> <div>8%</div> <div>• 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11284 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	699	Total	C	N	O	S	0	0	0
			5711	3661	959	1073	18			
1	B	666	Total	C	N	O	S	0	0	0
			5443	3490	919	1018	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	30	Total	O	0	0
			30	30		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.08Å 136.08Å 173.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 3.00 29.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-3.00) 99.8 (29.91-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.12 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.287 0.221 , 0.288	Depositor DCC
R_{free} test set	1909 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11284	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	0.51	0/5860	0.64	0/7948
1	B	0.47	0/5582	0.59	2/7566 (0.0%)
All	All	0.49	0/11442	0.62	2/15514 (0.0%)

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	3
1	B	0	23
All	All	0	26

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	459	THR	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	VAL	Peptide
1	A	404	GLY	Peptide
1	A	405	GLN	Peptide
1	B	10	ARG	Peptide
1	B	8	ARG	Peptide

5.2 Too-close contacts

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	5711	0	5508	157	1
1	B	5443	0	5242	486	12
2	A	100	0	0	4	0
2	B	30	0	0	6	0
All	All	11284	0	10750	635	13

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 29.

The worst 5 of 635 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:473:PHE:HB3	1:B:478:LEU:CD2	1.54	1.35
1:B:476:GLU:CG	1:B:479:VAL:HG13	1.58	1.31
1:B:9:ASP:CB	1:B:10:ARG:HA	1.63	1.25
1:B:476:GLU:HG2	1:B:479:VAL:CG1	1.72	1.18
1:B:9:ASP:HB3	1:B:10:ARG:CA	1.71	1.18

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ASN:C	1:B:572:GLU:OE2[5_554]	0.89	1.31
1:B:571:ASP:OD1	1:B:571:ASP:OD1[5_554]	1.34	0.86
1:B:569:ASN:CA	1:B:572:GLU:OE2[5_554]	1.47	0.73
1:B:569:ASN:ND2	1:B:572:GLU:OE1[5_554]	1.58	0.62
1:B:569:ASN:O	1:B:572:GLU:OE2[5_554]	1.61	0.59

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	695/718 (97%)	629 (90%)	62 (9%)	4 (1%)	28	70
1	B	652/718 (91%)	531 (81%)	113 (17%)	8 (1%)	15	53
All	All	1347/1436 (94%)	1160 (86%)	175 (13%)	12 (1%)	20	62

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	ILE
1	B	517	VAL
1	B	234	THR
1	B	190	ASP
1	B	420	TRP

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	617/636 (97%)	572 (93%)	45 (7%)	16	50
1	B	589/636 (93%)	513 (87%)	76 (13%)	5	22
All	All	1206/1272 (95%)	1085 (90%)	121 (10%)	9	33

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	130	ASP

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Mol	Chain	Res	Type
1	B	232	PHE
1	B	682	VAL
1	B	137	TYR
1	B	188	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	591	HIS
1	B	102	ASN
1	B	514	GLN
1	A	633	GLN
1	A	668	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 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	699/718 (97%)	-0.17	17 (2%) 59 30	25, 52, 83, 92	3 (0%)
1	B	666/718 (92%)	0.36	63 (9%) 9 3	34, 82, 122, 128	2 (0%)
All	All	1365/1436 (95%)	0.09	80 (5%) 23 9	25, 61, 118, 128	5 (0%)

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	LEU	4.8
1	A	455	GLY	4.7
1	B	631	PRO	4.5
1	A	718	LEU	4.4
1	B	506	GLY	4.2

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.