



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:02 AM GMT

PDB ID : 2VR5
Title : Crystal structure of Trex from Sulfolobus Solfataricus in complex with acarbose intermediate and glucose
Authors : Song, H.-N.; Yoon, S.-M.; Lee, S.-J.; Cha, H.-J.; Park, K.-H.; Woo, E.-J.
Deposited on : 2008-03-26
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

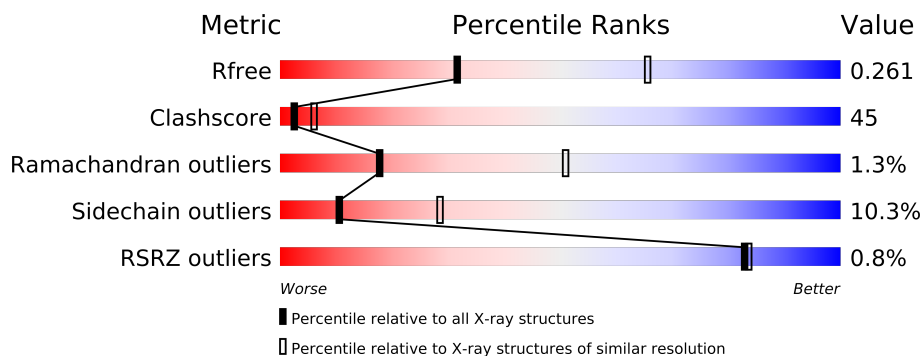
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	718	
1	B	718	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GLC	A	1719	-	X
2	GLC	A	1720	-	X
2	GLC	A	1721	-	X
2	GLC	B	1719	-	X
3	A16	A	1722	-	X
3	A16	B	1720	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	1723	-	X
5	GOL	A	1724	-	X

2 Entry composition i

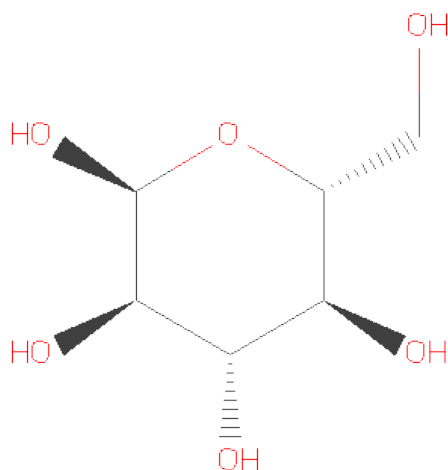
There are 6 unique types of molecules in this entry. The entry contains 12209 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

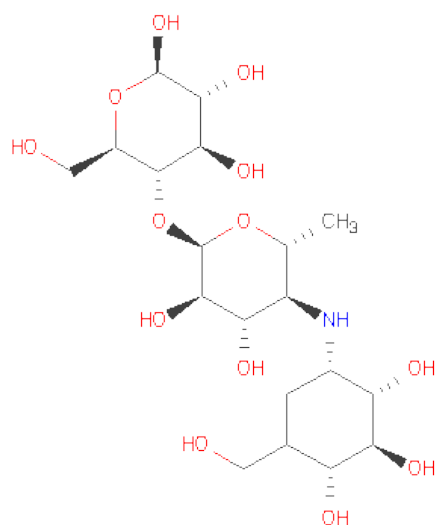
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5848	3753	985	1091	19			
1	B	714	Total	C	N	O	S	0	0	0
			5837	3744	984	1090	19			

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



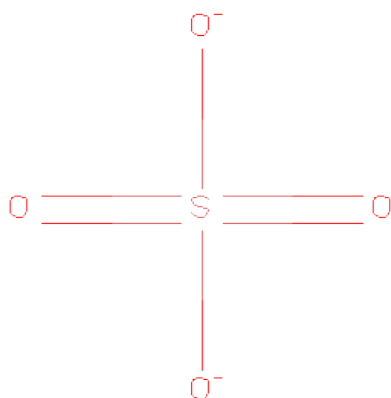
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 4-O-(4,6-DIDEOXY-4-[(1S,2S,3S,4R,5S)-2,3,4-TRIHYDROXY-5-(HYDROXYMETHYL)CYCLOHEXYL]AMINO}-ALPHA-D-GLUCOPYRANOSYL)-BETA-D-GLUCOPYRANOSE (three-letter code: A16) (formula: C₁₉H₃₅NO₁₃).



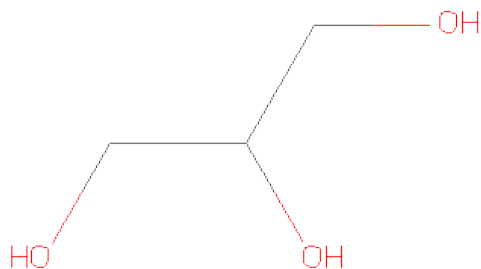
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	19	1	12		
3	B	1	Total	C	N	O	0	0
			32	19	1	12		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	B	188	Total	O	0	0
			188	188		





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.81Å 204.81Å 89.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.80 44.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.85-2.80) 96.6 (44.45-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.266 0.211 , 0.261	Depositor DCC
R_{free} test set	2573 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.8	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 51526 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12209	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GLC, A16, SO4

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	0.21	0/6002	0.32	0/8136
1	B	0.21	0/5990	0.32	0/8120
All	All	0.21	0/11992	0.32	0/16256

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	2	11
1	B	1	12
All	All	3	23

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	161	GLU	CA
1	A	261	CYS	CA
1	B	372	LEU	CA

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	GLY	Peptide
1	A	161	GLU	Peptide
1	A	165	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	259	THR	Peptide
1	A	56	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5848	0	5662	540	2
1	B	5837	0	5651	503	2
2	A	36	0	36	2	0
2	B	12	0	12	1	0
3	A	32	0	32	1	0
3	B	32	0	32	1	0
4	A	5	0	0	3	0
5	A	6	0	8	3	0
6	A	213	0	0	17	0
6	B	188	0	0	15	0
All	All	12209	0	11433	1043	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

The worst 5 of 1043 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:LYS:HB2	1:A:461:PHE:CE1	1.61	1.35
1:B:135:LEU:HD21	1:B:321:ARG:NH1	1.42	1.32
1:B:135:LEU:CD2	1:B:321:ARG:HH11	1.49	1.25
1:B:372:LEU:HD12	1:B:373:TYR:N	1.50	1.23
1:B:135:LEU:CD2	1:B:321:ARG:NH1	2.08	1.15

All (2) 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	Distance(Å)	Clash(Å)
1:A:653:ARG:O	1:B:654:ILE:O[2_565]	1.79	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:653:ARG:NH2	1:B:656:ASP:O[2_565]	2.18	0.02

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	713/718 (99%)	589 (83%)	113 (16%)	11 (2%)	15	46
1	B	712/718 (99%)	612 (86%)	92 (13%)	8 (1%)	21	57
All	All	1425/1436 (99%)	1201 (84%)	205 (14%)	19 (1%)	18	51

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ILE
1	A	121	ASP
1	A	164	ILE
1	B	195	ILE
1	B	515	ASN

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	631/636 (99%)	559 (89%)	72 (11%)	8	24
1	B	630/636 (99%)	572 (91%)	58 (9%)	13	36
All	All	1261/1272 (99%)	1131 (90%)	130 (10%)	10	28

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	603	LYS
1	B	7	THR
1	B	554	ASN
1	A	619	GLU
1	A	681	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	633	GLN
1	B	133	GLN
1	B	535	GLN
1	A	664	ASN
1	A	669	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	1719	-	12,12,12	0.98	0	17,17,17	0.72	0
2	GLC	A	1720	-	12,12,12	1.01	0	17,17,17	0.72	0
2	GLC	A	1721	-	12,12,12	0.99	0	17,17,17	0.72	0
3	A16	A	1722	1	33,34,35	1.93	9 (27%)	46,50,52	2.26	9 (19%)
4	SO4	A	1723	-	4,4,4	0.63	0	6,6,6	0.10	0
5	GOL	A	1724	-	5,5,5	0.39	0	5,5,5	0.32	0
2	GLC	B	1719	-	12,12,12	0.96	0	17,17,17	0.72	0
3	A16	B	1720	1	33,34,35	1.92	11 (33%)	46,50,52	2.28	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	1719	-	-	0/2/22/22	0/1/1/1
2	GLC	A	1720	-	-	0/2/22/22	0/1/1/1
2	GLC	A	1721	-	-	0/2/22/22	0/1/1/1
3	A16	A	1722	1	1/1/14/16	0/12/69/72	0/3/3/3
4	SO4	A	1723	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1724	-	-	0/4/4/4	0/0/0/0
2	GLC	B	1719	-	-	0/2/22/22	0/1/1/1
3	A16	B	1720	1	1/1/14/16	0/12/69/72	1/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1722	A16	C7A-C5A	-5.55	1.38	1.53
3	B	1720	A16	C7A-C5A	-5.35	1.39	1.53
3	B	1720	A16	C2A-C1A	3.52	1.61	1.52
3	A	1722	A16	C2A-C1A	3.49	1.61	1.52
3	A	1722	A16	O5B-C1B	3.31	1.50	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1720	A16	C1A-N4B-C4B	8.22	128.56	116.31
3	A	1722	A16	C1A-N4B-C4B	7.96	128.17	116.31
3	A	1722	A16	C7A-C5A-C4A	6.35	118.30	110.26
3	B	1720	A16	C7A-C5A-C4A	6.35	118.30	110.26
3	A	1722	A16	C5A-C7A-C1A	6.22	117.83	108.59

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1722	A16	C5A
3	B	1720	A16	C5A

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1720	A16	C1A-C2A-C3A-C4A-C5A-C7A

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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, 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	715/718 (99%)	-0.28	7 (0%) 79 79	19, 50, 80, 110	0
1	B	714/718 (99%)	-0.32	5 (0%) 84 85	23, 47, 80, 106	1 (0%)
All	All	1429/1436 (99%)	-0.30	12 (0%) 83 83	19, 49, 80, 110	1 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	3.9
1	B	621	ARG	2.7
1	B	674	PHE	2.7
1	B	373	TYR	2.5
1	A	690	ILE	2.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GLC	B	1719	12/12	0.30	38.33	85,102,104,105	0
2	GLC	A	1720	12/12	0.38	14.41	80,104,110,111	0
2	GLC	A	1721	12/12	0.41	11.75	93,99,107,108	0
5	GOL	A	1724	6/6	0.44	8.30	78,82,90,90	0
3	A16	B	1720	32/33	0.40	7.14	85,134,146,148	0
2	GLC	A	1719	12/12	0.42	4.89	85,101,105,110	0
4	SO4	A	1723	5/5	0.31	3.09	112,118,133,135	0
3	A16	A	1722	32/33	0.32	2.97	94,124,132,140	0

6.5 Other polymers ⓘ

There are no such residues in this entry.