



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2020 – 02:08 PM BST

PDB ID : 6ZJ7
Title : Trehalose transferase (TreT) from *Thermoproteus uzoniensis* soaked with Mg
Authors : Bento, I.; Mestrom, L.; Marsden, S.R.; van der Eijk, H.; Laustsen, J.U.; Jeffries, C.M.; Svergun, D.I.; Hagedoorn, P.-H.; Hanefeld, U.
Deposited on : 2020-06-28
Resolution : 2.15 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

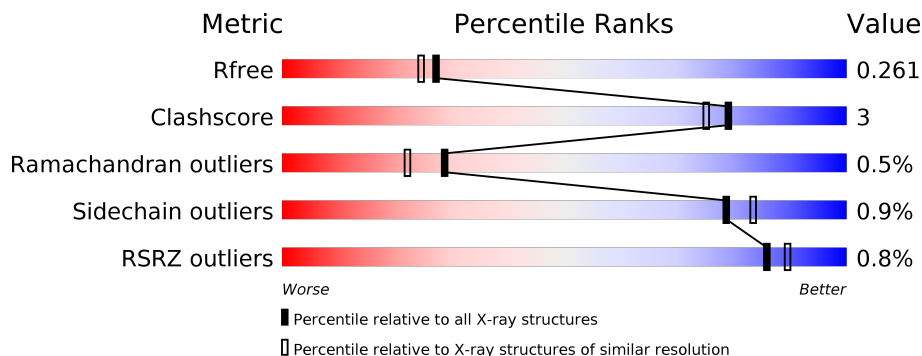
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	AAA	400	

2 Entry composition [i](#)

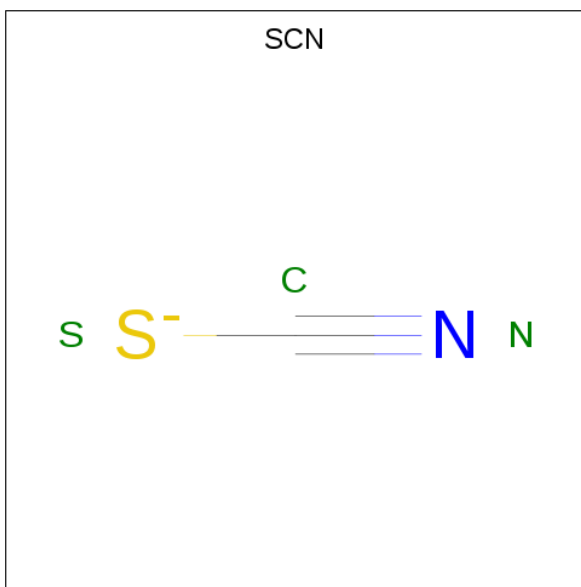
There are 5 unique types of molecules in this entry. The entry contains 6564 atoms, of which 3267 are hydrogens and 0 are deuteriums.

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 Trehalose phosphorylase/synthase.

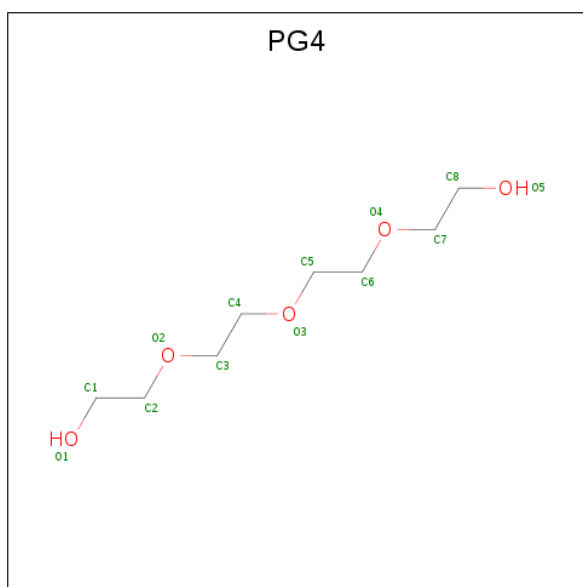
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	393	6405	2042	3233	558	563	9	122	2	0

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	AAA	1	3	1	1	1	0	0
2	AAA	1	3	1	1	1	0	0
2	AAA	1	3	1	1	1	0	0
2	AAA	1	3	1	1	1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	AAA	1	31	8	18	5	1	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0

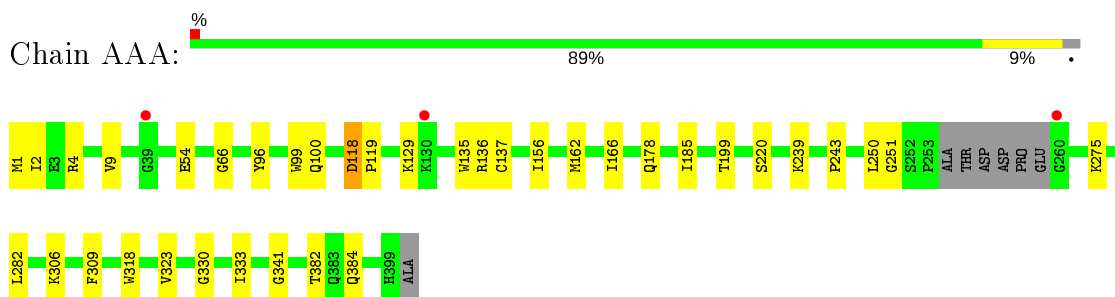
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	88	Total 88	O 88	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Trehalose phosphorylase/synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.57Å 69.28Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.76 – 2.15 58.69 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (58.76-2.15) 98.5 (58.69-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0258, REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.261 0.203 , 0.261	Depositor DCC
R_{free} test set	1306 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtrriage
Anisotropy	0.454	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6564	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, SCN

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	AAA	0.65	0/3254	0.74	0/4406

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	3172	3233	3222	18	0
2	AAA	12	0	0	2	0
3	AAA	13	18	18	0	0
4	AAA	12	16	16	0	0
5	AAA	88	0	0	0	0
All	All	3297	3267	3256	18	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 3.

All (18) 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:AAA:166:ILE:HG22	1:AAA:333:ILE:HD13	1.79	0.65
1:AAA:66:GLY:HA2	1:AAA:99:TRP:CZ3	2.41	0.55
1:AAA:306:LYS:O	2:AAA:502:SCN:S	2.65	0.54
1:AAA:135:TRP:CD2	1:AAA:156:ILE:HD12	2.44	0.52
1:AAA:9:VAL:HG11	1:AAA:382:THR:OG1	2.11	0.51
1:AAA:309:PHE:HA	1:AAA:330:GLY:HA3	1.92	0.51
1:AAA:96:TYR:O	1:AAA:100:GLN:HG2	2.13	0.48
1:AAA:2:ILE:HG22	1:AAA:54:GLU:OE2	2.14	0.47
1:AAA:220:SER:O	1:AAA:251:GLY:HA2	2.15	0.46
1:AAA:1:MET:HA	1:AAA:4:ARG:HD2	1.98	0.45
1:AAA:135:TRP:CZ3	1:AAA:137:CYS:HB2	2.51	0.45
1:AAA:118:ASP:HB3	1:AAA:119:PRO:CD	2.48	0.43
1:AAA:323:VAL:O	1:AAA:341:GLY:HA3	2.19	0.43
1:AAA:185:ILE:HD11	1:AAA:318:TRP:CG	2.54	0.42
1:AAA:239:LYS:NZ	1:AAA:243:PRO:O	2.50	0.42
1:AAA:384:GLN:HA	2:AAA:501:SCN:S	2.60	0.41
1:AAA:250:LEU:HD21	1:AAA:282:LEU:HD22	2.02	0.40
1:AAA:162:MET:HE1	1:AAA:178:GLN:OE1	2.21	0.40

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	AAA	391/400 (98%)	380 (97%)	9 (2%)	2 (0%)	29 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	129	LYS
1	AAA	118	ASP

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	AAA	341/344 (99%)	338 (99%)	3 (1%)	78 83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	136	ARG
1	AAA	199	THR
1	AAA	275	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	SCN	AAA	504	-	1,2,2	0.73	0	0,1,1	0.00	-
2	SCN	AAA	501	-	1,2,2	0.59	0	0,1,1	0.00	-
4	GOL	AAA	507	-	5,5,5	0.09	0	5,5,5	0.41	0
2	SCN	AAA	502	-	1,2,2	0.54	0	0,1,1	0.00	-
2	SCN	AAA	505	-	1,2,2	0.70	0	0,1,1	0.00	-
4	GOL	AAA	506	-	5,5,5	0.13	0	5,5,5	0.32	0
3	PG4	AAA	503	-	12,12,12	0.18	0	11,11,11	0.17	0

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
4	GOL	AAA	506	-	-	3/4/4/4	-
4	GOL	AAA	507	-	-	2/4/4/4	-
3	PG4	AAA	503	-	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	507	GOL	C1-C2-C3-O3
4	AAA	506	GOL	C1-C2-C3-O3
4	AAA	507	GOL	O2-C2-C3-O3
4	AAA	506	GOL	O2-C2-C3-O3
3	AAA	503	PG4	O1-C1-C2-O2
3	AAA	503	PG4	O3-C5-C6-O4
4	AAA	506	GOL	O1-C1-C2-O2
3	AAA	503	PG4	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	501	SCN	1	0
2	AAA	502	SCN	1	0

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	AAA	393/400 (98%)	0.18	3 (0%) 86 89	34, 52, 85, 125	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	260	GLY	3.7
1	AAA	130	LYS	2.8
1	AAA	39	GLY	2.2

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 monosaccharides in this entry.

6.4 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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SCN	AAA	504	3/3	0.80	0.26	59,59,64,68	3
4	GOL	AAA	507	6/6	0.83	0.29	20,54,63,63	14
3	PG4	AAA	503	13/13	0.85	0.23	48,51,54,59	31
4	GOL	AAA	506	6/6	0.91	0.20	20,65,67,68	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SCN	AAA	505	3/3	0.93	0.33	57,57,58,62	3
2	SCN	AAA	501	3/3	0.95	0.27	41,41,46,50	3
2	SCN	AAA	502	3/3	0.96	0.20	47,47,53,56	3

6.5 Other polymers [i](#)

There are no such residues in this entry.