



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 12:45 AM UTC

PDB ID : 6TNL / pdb_00006tnl
Title : GSTF1 from Alopecurus myosuroides
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Deposited on : 2019-12-09
Resolution : 1.95 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
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

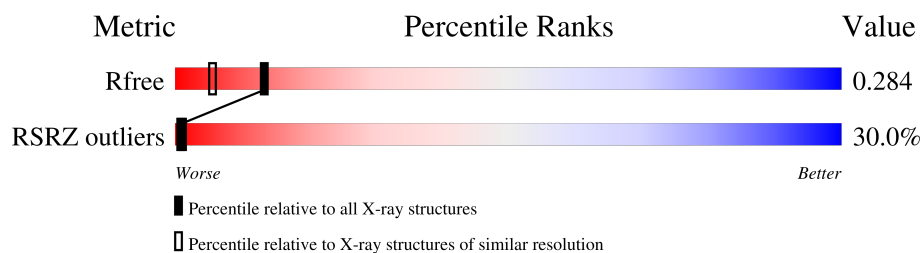
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

2 Entry composition [i](#)

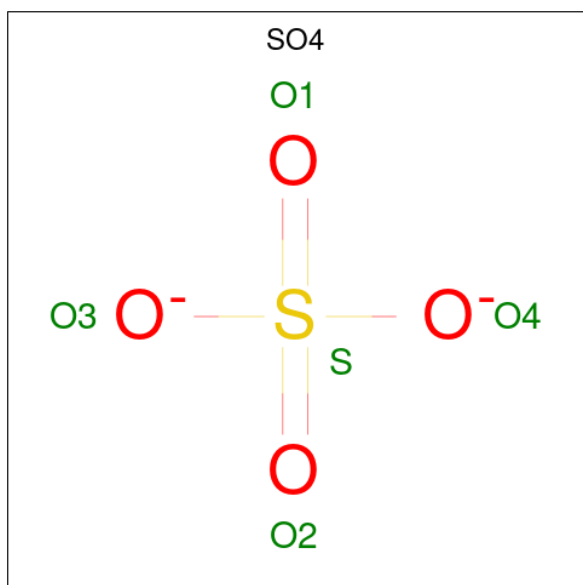
There are 3 unique types of molecules in this entry. The entry contains 18467 atoms, of which 8828 are hydrogens and 0 are deuteriums.

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 Glutathione transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	190	Total	C	H	N	O	S	55	0	0
			2946	975	1453	241	269	8			
1	BBB	190	Total	C	H	N	O	S	60	1	0
			2983	985	1475	243	272	8			
1	CCC	191	Total	C	H	N	O	S	57	0	0
			2982	984	1475	244	271	8			
1	DDD	189	Total	C	H	N	O	S	59	1	0
			2971	981	1467	244	271	8			
1	EEE	189	Total	C	H	N	O	S	58	2	0
			3000	988	1485	246	273	8			
1	FFF	192	Total	C	H	N	O	S	57	0	0
			2983	986	1473	244	272	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	CCC	1	Total O S 5 4 1	0	0
2	EEE	1	Total O S 5 4 1	0	0
2	FFF	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	57	Total O 57 57	0	0
3	BBB	117	Total O 117 117	0	0
3	CCC	76	Total O 76 76	0	0
3	DDD	105	Total O 105 105	0	0
3	EEE	113	Total O 113 113	0	0
3	FFF	119	Total O 119 119	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	180.78Å 180.78Å 237.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.95 – 1.95 41.95 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.95-1.95) 99.1 (41.95-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.260 , 0.284 0.260 , 0.284	Depositor DCC
R_{free} test set	5352 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18467	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 95.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5831e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

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](#)

MolProbity failed to run properly - this section is therefore empty.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSS	EEE	120	1	4,6,7	0.55	0	2,6,8	0.71	0
1	CSS	DDD	120	1	4,6,7	0.46	0	2,6,8	0.73	0
1	CSS	BBB	120	1	4,6,7	0.56	0	2,6,8	0.74	0
1	CSS	AAA	120	1	4,6,7	0.57	0	2,6,8	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSS	CCC	120	1	4,6,7	0.52	0	2,6,8	0.73	0
1	CSS	FFF	120	1	4,6,7	0.67	0	2,6,8	0.77	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
1	CSS	EEE	120	1	-	0/1/5/7	-
1	CSS	DDD	120	1	-	0/1/5/7	-
1	CSS	BBB	120	1	-	0/1/5/7	-
1	CSS	AAA	120	1	-	0/1/5/7	-
1	CSS	CCC	120	1	-	0/1/5/7	-
1	CSS	FFF	120	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

3 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	SO4	CCC	301	-	4,4,4	0.39	0	6,6,6	0.18	0
2	SO4	FFF	301	-	4,4,4	0.33	0	6,6,6	0.20	0
2	SO4	EEE	301	-	4,4,4	0.38	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	189/219 (86%)	3.11	150 (79%) 0 0	35, 47, 67, 88	0
1	BBB	189/219 (86%)	0.35	13 (6%) 23 26	19, 28, 54, 75	1 (0%)
1	CCC	190/219 (86%)	2.57	118 (62%) 0 0	29, 46, 67, 100	0
1	DDD	188/219 (85%)	0.48	18 (9%) 13 15	18, 30, 55, 92	1 (0%)
1	EEE	188/219 (85%)	0.36	19 (10%) 12 14	13, 28, 51, 75	2 (1%)
1	FFF	191/219 (87%)	0.46	22 (11%) 9 11	19, 28, 55, 91	0
All	All	1135/1314 (86%)	1.22	340 (29%) 1 1	13, 36, 63, 100	4 (0%)

The worst 5 of 340 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	123	ASN	11.6
1	CCC	123	ASN	8.8
1	FFF	124	PRO	8.3
1	DDD	37	ASN	7.3
1	AAA	59	GLN	7.2

5.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSS	AAA	120	7/8	0.78	0.20	58,60,76,76	1
1	CSS	BBB	120	7/8	0.85	0.14	41,44,63,63	1
1	CSS	DDD	120	7/8	0.85	0.15	50,52,69,69	1
1	CSS	EEE	120	7/8	0.85	0.14	43,46,67,67	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSS	FFF	120	7/8	0.87	0.14	42,44,64,64	1
1	CSS	CCC	120	7/8	0.88	0.14	46,48,66,66	1

5.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
2	SO4	CCC	301	5/5	0.79	0.14	60,77,81,82	0
2	SO4	EEE	301	5/5	0.89	0.10	61,63,65,67	0
2	SO4	FFF	301	5/5	0.91	0.09	54,56,62,72	0

5.5 Other polymers [i](#)

There are no such residues in this entry.