



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2022 – 01:09 pm BST

PDB ID : 7ZA5
Title : GSTF sh101 mutant
Authors : Papageorgiou, A.C.
Deposited on : 2022-03-22
Resolution : 1.87 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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

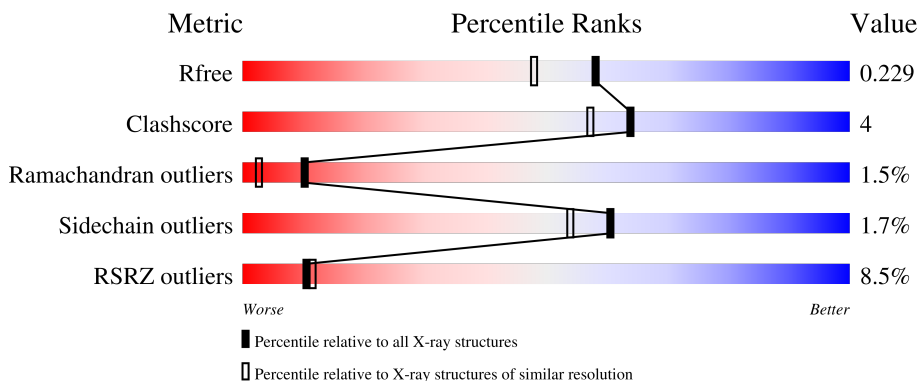
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	225	
1	B	225	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3312 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 Glutathione transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	202	Total 1619	C 1053	N 264	O 294	S 8	0	0	0
1	A	199	Total 1592	C 1036	N 260	O 288	S 8	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	90	GLY	SER	conflict	UNP Q9ZS17
B	93	LYS	GLU	conflict	UNP Q9ZS17
B	119	GLU	GLN	conflict	UNP Q9ZS17
B	122	ILE	PHE	conflict	UNP Q9ZS17
B	125	LEU	MET	conflict	UNP Q9ZS17
B	132	ASN	ASP	conflict	UNP Q9ZS17
B	133	GLN	GLU	conflict	UNP Q9ZS17
B	134	THR	LYS	conflict	UNP Q9ZS17
B	137	ASP	ALA	conflict	UNP Q9ZS17
B	156	GLN	LYS	conflict	UNP Q9ZS17
B	158	LYS	SER	conflict	UNP Q9ZS17
B	220	HIS	-	expression tag	UNP Q9ZS17
B	221	HIS	-	expression tag	UNP Q9ZS17
B	222	HIS	-	expression tag	UNP Q9ZS17
B	223	HIS	-	expression tag	UNP Q9ZS17
B	224	HIS	-	expression tag	UNP Q9ZS17
B	225	HIS	-	expression tag	UNP Q9ZS17
A	90	GLY	SER	conflict	UNP Q9ZS17
A	93	LYS	GLU	conflict	UNP Q9ZS17
A	119	GLU	GLN	conflict	UNP Q9ZS17
A	122	ILE	PHE	conflict	UNP Q9ZS17
A	125	LEU	MET	conflict	UNP Q9ZS17
A	132	ASN	ASP	conflict	UNP Q9ZS17
A	133	GLN	GLU	conflict	UNP Q9ZS17
A	134	THR	LYS	conflict	UNP Q9ZS17

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Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ASP	ALA	conflict	UNP Q9ZS17
A	156	GLN	LYS	conflict	UNP Q9ZS17
A	158	LYS	SER	conflict	UNP Q9ZS17
A	220	HIS	-	expression tag	UNP Q9ZS17
A	221	HIS	-	expression tag	UNP Q9ZS17
A	222	HIS	-	expression tag	UNP Q9ZS17
A	223	HIS	-	expression tag	UNP Q9ZS17
A	224	HIS	-	expression tag	UNP Q9ZS17
A	225	HIS	-	expression tag	UNP Q9ZS17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	61	Total O 61 61	0	0
2	A	40	Total O 40 40	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.45Å 46.38Å 110.82Å 90.00° 112.04° 90.00°	Depositor
Resolution (Å)	42.85 – 1.87 42.85 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.85-1.87) 90.0 (42.85-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 1.87Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.233 0.197 , 0.229	Depositor DCC
R_{free} test set	1813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.097	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3312	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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	0.39	0/1635	0.58	0/2227
1	B	0.44	0/1663	0.63	0/2266
All	All	0.42	0/3298	0.61	0/4493

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	A	1592	0	1584	20	0
1	B	1619	0	1602	8	0
2	A	40	0	0	2	0
2	B	61	0	0	3	0
All	All	3312	0	3186	27	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 4.

All (27) 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:175:TYR:OH	2:B:301:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:HA	1:A:122:ILE:HB	1.68	0.74
1:A:28:GLU:N	1:A:28:GLU:OE1	2.22	0.72
1:A:28:GLU:H	1:A:28:GLU:CD	1.96	0.66
1:A:89:GLU:OE2	2:A:301:HOH:O	2.14	0.65
1:B:89:GLU:OE2	2:B:302:HOH:O	2.15	0.63
1:A:93:LYS:HE2	1:A:93:LYS:H	1.65	0.60
1:A:127:ARG:HB3	1:A:129:LEU:HG	1.84	0.59
1:A:131:THR:O	1:A:133:GLN:N	2.40	0.55
1:B:34:ILE:HG22	1:B:35:ASP:N	2.22	0.55
1:A:91:ASN:OD1	1:A:93:LYS:HE2	2.07	0.54
1:A:209:LYS:NZ	2:A:305:HOH:O	2.42	0.53
1:A:33:ASN:HD22	1:A:33:ASN:C	2.13	0.52
1:A:13:THR:HG21	1:A:175:TYR:CZ	2.45	0.51
1:B:121:LEU:O	1:B:125:LEU:HB2	2.13	0.48
1:A:145:LYS:HA	1:A:148:GLU:HG3	1.95	0.48
1:A:215:VAL:H	1:A:216:PRO:CD	2.27	0.48
1:A:158:LYS:HD3	1:A:158:LYS:HA	1.63	0.45
1:B:67:GLU:OE1	1:A:103:GLU:HG3	2.16	0.45
1:A:7:PHE:HB2	1:A:57:ALA:HB3	2.00	0.44
1:B:158:LYS:NZ	2:B:307:HOH:O	2.48	0.42
1:A:127:ARG:HD2	1:A:129:LEU:HD21	2.01	0.42
1:A:93:LYS:H	1:A:93:LYS:CE	2.32	0.42
1:B:9:PRO:HB3	1:B:34:ILE:HG23	2.03	0.41
1:B:34:ILE:HG22	1:B:35:ASP:H	1.85	0.41
1:A:88:ARG:HA	1:A:88:ARG:HD3	1.74	0.41
1:A:76:LEU:HD22	1:A:86:LEU:HD12	2.03	0.41

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	195/225 (87%)	184 (94%)	8 (4%)	3 (2%)	10	3
1	B	198/225 (88%)	192 (97%)	3 (2%)	3 (2%)	10	3
All	All	393/450 (87%)	376 (96%)	11 (3%)	6 (2%)	10	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	34	ILE
1	A	132	ASN
1	A	215	VAL
1	B	67	GLU
1	A	67	GLU

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	A	171/195 (88%)	166 (97%)	5 (3%)	42	32
1	B	174/195 (89%)	173 (99%)	1 (1%)	86	86
All	All	345/390 (88%)	339 (98%)	6 (2%)	60	54

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	155	SER
1	A	33	ASN
1	A	80	LYS
1	A	82	ASP
1	A	127	ARG
1	A	145	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	GLN

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](#)

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

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	199/225 (88%)	0.66	27 (13%) 3 3	35, 58, 107, 128	0
1	B	202/225 (89%)	0.11	7 (3%) 44 45	31, 46, 64, 102	0
All	All	401/450 (89%)	0.38	34 (8%) 10 11	31, 51, 94, 128	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	PRO	16.6
1	A	129	LEU	11.3
1	B	35	ASP	9.1
1	B	34	ILE	7.1
1	A	125	LEU	5.9
1	B	36	PHE	5.5
1	A	127	ARG	4.9
1	A	130	PRO	4.9
1	A	126	MET	4.6
1	A	128	GLY	4.6
1	A	124	PRO	4.6
1	A	135	VAL	4.6
1	A	122	ILE	4.5
1	A	52	PHE	4.5
1	A	215	VAL	4.2
1	A	118	TYR	4.2
1	A	131	THR	3.8
1	A	121	LEU	3.8
1	A	134	THR	3.4
1	A	34	ILE	3.3
1	A	123	ASN	3.2
1	B	216	PRO	3.2
1	A	136	VAL	3.1
1	B	33	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.9
1	A	133	GLN	2.9
1	A	140	LEU	2.8
1	B	52	PHE	2.4
1	B	66	TRP	2.4
1	A	51	PRO	2.3
1	A	141	GLU	2.2
1	A	142	LYS	2.2
1	A	11	MET	2.1
1	A	120	CYS	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.