



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 11:04 PM EDT

PDB ID : 3NIV
Title : The crystal structure of Glutathione S-transferase from Legionella pneumophila
Authors : Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-06-16
Resolution : 2.30 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

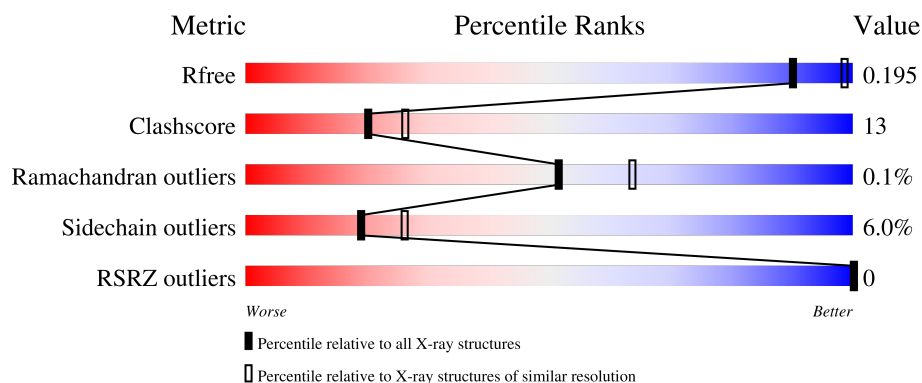
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	222	 66% 18% • 14%
1	B	222	 59% 24% • 15%
1	C	222	 59% 23% • 14%
1	D	222	 62% 21% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6308 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 S-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	Se	0	1	0
			1552	1006	256	279	5	6			
1	B	188	Total	C	N	O	S	Se	0	0	0
			1525	989	250	275	5	6			
1	C	191	Total	C	N	O	S	Se	0	0	0
			1550	1004	256	279	5	6			
1	D	192	Total	C	N	O	S	Se	0	1	0
			1552	1006	256	279	5	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q5ZT82
A	0	SER	-	expression tag	UNP Q5ZT82
A	1	LEU	-	expression tag	UNP Q5ZT82
A	213	GLU	-	expression tag	UNP Q5ZT82
A	214	GLY	-	expression tag	UNP Q5ZT82
A	215	HIS	-	expression tag	UNP Q5ZT82
A	216	HIS	-	expression tag	UNP Q5ZT82
A	217	HIS	-	expression tag	UNP Q5ZT82
A	218	HIS	-	expression tag	UNP Q5ZT82
A	219	HIS	-	expression tag	UNP Q5ZT82
A	220	HIS	-	expression tag	UNP Q5ZT82
B	-1	MSE	-	expression tag	UNP Q5ZT82
B	0	SER	-	expression tag	UNP Q5ZT82
B	1	LEU	-	expression tag	UNP Q5ZT82
B	213	GLU	-	expression tag	UNP Q5ZT82
B	214	GLY	-	expression tag	UNP Q5ZT82
B	215	HIS	-	expression tag	UNP Q5ZT82
B	216	HIS	-	expression tag	UNP Q5ZT82
B	217	HIS	-	expression tag	UNP Q5ZT82
B	218	HIS	-	expression tag	UNP Q5ZT82
B	219	HIS	-	expression tag	UNP Q5ZT82

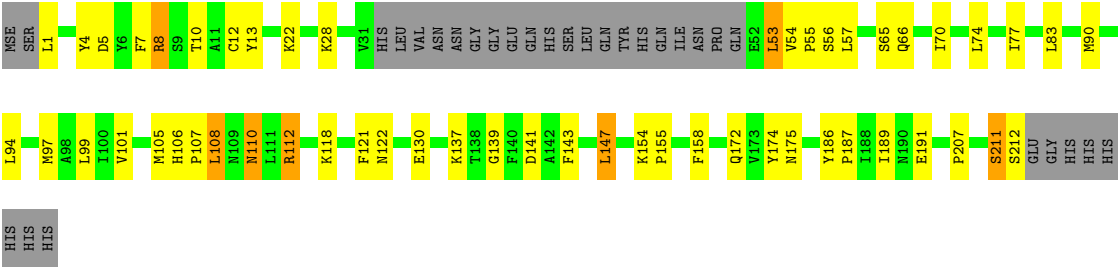
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Chain	Residue	Modelled	Actual	Comment	Reference
B	220	HIS	-	expression tag	UNP Q5ZT82
C	-1	MSE	-	expression tag	UNP Q5ZT82
C	0	SER	-	expression tag	UNP Q5ZT82
C	1	LEU	-	expression tag	UNP Q5ZT82
C	213	GLU	-	expression tag	UNP Q5ZT82
C	214	GLY	-	expression tag	UNP Q5ZT82
C	215	HIS	-	expression tag	UNP Q5ZT82
C	216	HIS	-	expression tag	UNP Q5ZT82
C	217	HIS	-	expression tag	UNP Q5ZT82
C	218	HIS	-	expression tag	UNP Q5ZT82
C	219	HIS	-	expression tag	UNP Q5ZT82
C	220	HIS	-	expression tag	UNP Q5ZT82
D	-1	MSE	-	expression tag	UNP Q5ZT82
D	0	SER	-	expression tag	UNP Q5ZT82
D	1	LEU	-	expression tag	UNP Q5ZT82
D	213	GLU	-	expression tag	UNP Q5ZT82
D	214	GLY	-	expression tag	UNP Q5ZT82
D	215	HIS	-	expression tag	UNP Q5ZT82
D	216	HIS	-	expression tag	UNP Q5ZT82
D	217	HIS	-	expression tag	UNP Q5ZT82
D	218	HIS	-	expression tag	UNP Q5ZT82
D	219	HIS	-	expression tag	UNP Q5ZT82
D	220	HIS	-	expression tag	UNP Q5ZT82

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	33	Total O 33 33	0	0
2	C	44	Total O 44 44	0	0
2	D	29	Total O 29 29	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.48Å 55.04Å 84.72Å 71.99° 84.33° 68.79°	Depositor
Resolution (Å)	80.56 – 2.30 80.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.2 (80.56-2.30) 91.2 (80.56-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.197 , 0.249 0.197 , 0.195	Depositor DCC
R_{free} test set	1678 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6308	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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	0.38	0/1589	0.53	0/2149
1	B	0.40	0/1557	0.53	0/2103
1	C	0.38	0/1583	0.51	0/2139
1	D	0.46	0/1588	0.53	0/2146
All	All	0.41	0/6317	0.53	0/8537

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	1552	0	1532	34	0
1	B	1525	0	1516	49	0
1	C	1550	0	1534	41	0
1	D	1552	0	1540	36	0
2	A	23	0	0	0	0
2	B	33	0	0	1	0
2	C	44	0	0	0	0
2	D	29	0	0	0	0
All	All	6308	0	6122	154	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 13.

The worst 5 of 154 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:D:118:LYS:O	1:D:122:ASN:HA	1.68	0.93
1:C:2:ILE:HG23	1:C:29:ILE:HD13	1.51	0.92
1:A:110:ASN:HD22	1:A:112:ARG:H	1.18	0.87
1:C:97:MSE:HE1	1:C:147:LEU:HD13	1.63	0.80
1:A:132:TYR:O	1:A:136:LEU:HD23	1.83	0.78

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	188/222 (85%)	179 (95%)	9 (5%)	0	100	100
1	B	184/222 (83%)	180 (98%)	4 (2%)	0	100	100
1	C	187/222 (84%)	184 (98%)	2 (1%)	1 (0%)	29	35
1	D	189/222 (85%)	183 (97%)	6 (3%)	0	100	100
All	All	748/888 (84%)	726 (97%)	21 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	GLN

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	169/190 (89%)	160 (95%)	9 (5%)	22	31
1	B	166/190 (87%)	160 (96%)	6 (4%)	35	49
1	C	169/190 (89%)	155 (92%)	14 (8%)	11	14
1	D	169/190 (89%)	158 (94%)	11 (6%)	17	23
All	All	673/760 (89%)	633 (94%)	40 (6%)	19	27

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	170	ILE
1	D	110	ASN
1	D	1	LEU
1	D	28	LYS
1	D	130	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	60	ASN
1	D	172	GLN
1	D	175	ASN
1	D	134	HIS
1	C	20	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 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 [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	185/222 (83%)	-0.19	0 100 100	24, 35, 49, 61	0
1	B	182/222 (81%)	-0.20	0 100 100	22, 33, 48, 63	0
1	C	185/222 (83%)	-0.27	0 100 100	24, 33, 47, 55	0
1	D	186/222 (83%)	-0.21	0 100 100	21, 33, 46, 57	0
All	All	738/888 (83%)	-0.22	0 100 100	21, 34, 48, 63	0

There are no RSRZ outliers to report.

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.