wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2024 – 04:16 PM JST

PDB ID	:	8WIN
Title	:	Durio zibethinus trypsin inhibitor DzTI-12
Authors	:	Deentanya, P.; Wangkanont, K.
Deposited on	:	2023-09-25
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

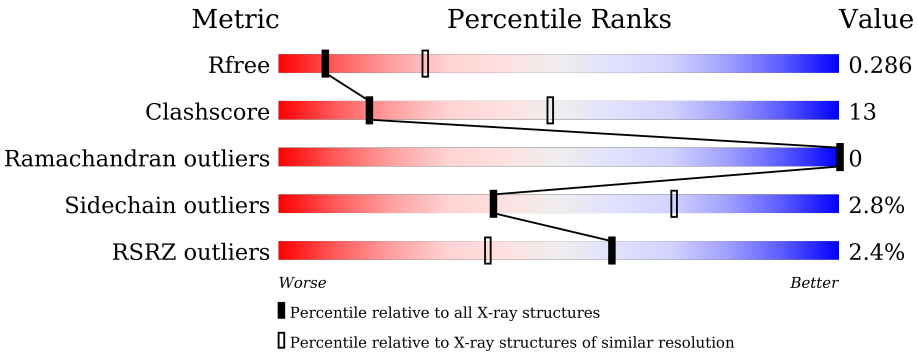
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

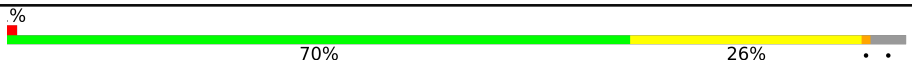
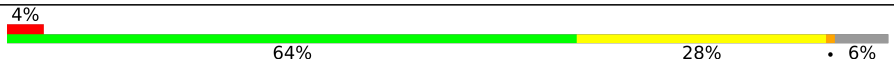
The reported resolution of this entry is 3.00 Å.

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 <=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	194	
1	B	194	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2895 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 21 kDa seed protein-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1461	928	247	280	6			
1	B	182	Total	C	N	O	S	0	0	0
			1434	912	243	273	6			

There are 24 discrepancies between the modelled and reference sequences:

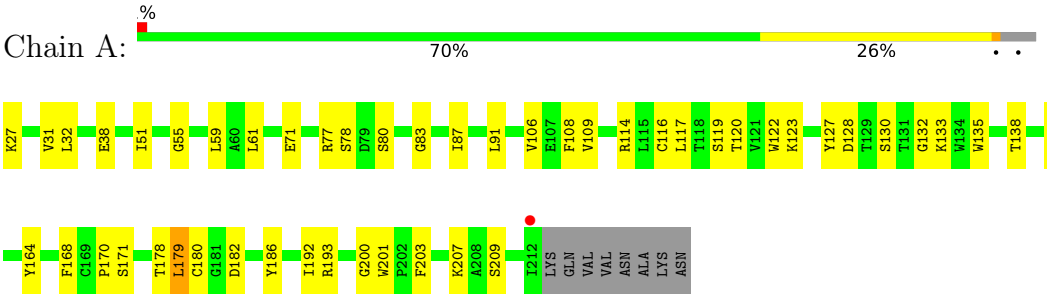
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LYS	GLN	conflict	UNP A0A6P5Y2I1
A	139	ASP	ASN	conflict	UNP A0A6P5Y2I1
A	142	LYS	ILE	conflict	UNP A0A6P5Y2I1
A	148	HIS	GLN	conflict	UNP A0A6P5Y2I1
A	162	PHE	LEU	conflict	UNP A0A6P5Y2I1
A	177	ILE	VAL	conflict	UNP A0A6P5Y2I1
A	181	GLY	SER	conflict	UNP A0A6P5Y2I1
A	188	HIS	ASP	conflict	UNP A0A6P5Y2I1
A	199	SER	ARG	conflict	UNP A0A6P5Y2I1
A	206	GLN	LYS	conflict	UNP A0A6P5Y2I1
A	215	VAL	ILE	conflict	UNP A0A6P5Y2I1
A	217	ASN	TYR	conflict	UNP A0A6P5Y2I1
B	133	LYS	GLN	conflict	UNP A0A6P5Y2I1
B	139	ASP	ASN	conflict	UNP A0A6P5Y2I1
B	142	LYS	ILE	conflict	UNP A0A6P5Y2I1
B	148	HIS	GLN	conflict	UNP A0A6P5Y2I1
B	162	PHE	LEU	conflict	UNP A0A6P5Y2I1
B	177	ILE	VAL	conflict	UNP A0A6P5Y2I1
B	181	GLY	SER	conflict	UNP A0A6P5Y2I1
B	188	HIS	ASP	conflict	UNP A0A6P5Y2I1
B	199	SER	ARG	conflict	UNP A0A6P5Y2I1
B	206	GLN	LYS	conflict	UNP A0A6P5Y2I1
B	215	VAL	ILE	conflict	UNP A0A6P5Y2I1
B	217	ASN	TYR	conflict	UNP A0A6P5Y2I1

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.

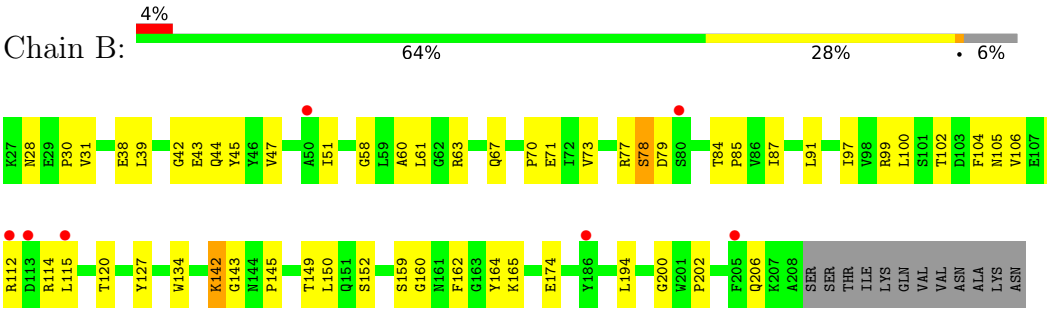
• Molecule 1: 21 kDa seed protein-like

Chain A:



• Molecule 1: 21 kDa seed protein-like

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	197.57Å 197.57Å 91.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.74 – 3.00 29.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.74-3.00) 99.8 (29.74-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.239 , 0.276 0.242 , 0.286	Depositor DCC
R_{free} test set	700 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	95.8	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2895	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.51	0/1499	0.74	0/2037
1	B	0.52	0/1472	0.74	0/2000
All	All	0.52	0/2971	0.74	0/4037

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

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	1461	0	1398	35	0
1	B	1434	0	1370	38	0
All	All	2895	0	2768	73	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 73 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:108:PHE:HB2	1:B:120:THR:HB	1.67	0.77
1:B:110:PRO:HB3	1:B:114:ARG:HH11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HB2	1:B:112:ARG:HH21	1.61	0.65
1:A:71:GLU:OE1	1:A:114:ARG:NH2	2.31	0.63
1:B:61:LEU:HB2	1:B:112:ARG:NH2	2.15	0.62

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	184/194 (95%)	172 (94%)	12 (6%)	0	100	100
1	B	180/194 (93%)	160 (89%)	20 (11%)	0	100	100
All	All	364/388 (94%)	332 (91%)	32 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	160/167 (96%)	157 (98%)	3 (2%)	52	79
1	B	156/167 (93%)	150 (96%)	6 (4%)	28	62
All	All	316/334 (95%)	307 (97%)	9 (3%)	38	70

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	115	LEU
1	B	142	LYS
1	B	43	GLU
1	B	51	ILE
1	B	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	ASN

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 oligosaccharides 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, 95^{th} 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	186/194 (95%)	0.06	1 (0%)	87	75	80, 99, 133, 158	0
1	B	182/194 (93%)	0.45	8 (4%)	39	23	89, 111, 136, 162	0
All	All	368/388 (94%)	0.25	9 (2%)	59	37	80, 105, 136, 162	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	ILE	3.5
1	B	186	TYR	2.9
1	B	205	PHE	2.7
1	B	113	ASP	2.6
1	B	115	LEU	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.