



wwPDB X-ray Structure Validation Summary Report

Apr 7, 2014 – 10:26 PM EDT

PDB ID : 4KTU
Title : Bovine trypsin in complex with microviridin J at pH 6.5
Authors : Quitterer, F.; Groll, M.; Hertweck, C.; Dittmann, E.
Deposited on : 2013-05-21
Resolution : 1.35 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

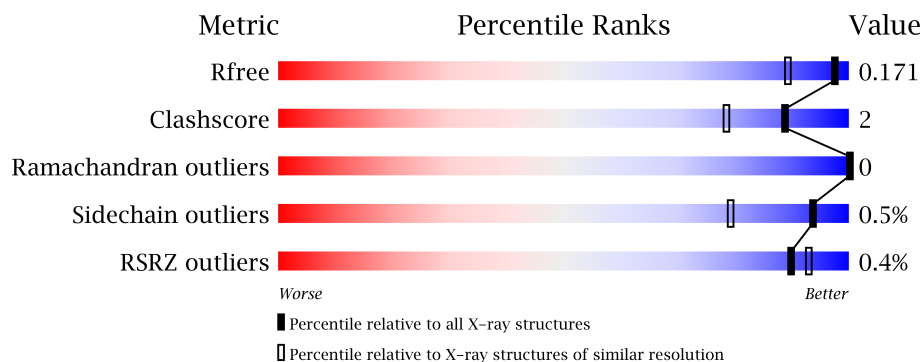
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance



The reported resolution of this entry is 1.35 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}	66092	1519 (1.40-1.32)
Clashscore	79885	1707 (1.40-1.32)
Ramachandran outliers	78287	1662 (1.40-1.32)
Sidechain outliers	78261	1661 (1.40-1.32)
RSRZ outliers	66119	1519 (1.40-1.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	223	
2	B	14	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1991 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is a protein called microviridin j.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			106	69	17	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ACE	-	ACETYLATION	UNP B2G3C8

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	241	Total	O	0	0
			241	241		
4	B	14	Total	O	0	0
			14	14		

i

- Molecule 1: Cationic trypsin

Amino Acid	Relative Abundance (approx.)
I16	10
H40	15
I63	15
R66	15
V76	20
F82	15
N97	15
T125	15
S130	15
K159	15
D189	15
S195	15
S217	15
G219	15
C220	15
N245	15

- Molecule 2: microviridin j

?	1	2	3	4	5	6	7	8
	I1	I2	S3	T4	R5		E13	TRP

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.23Å 71.23Å 72.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 1.35 35.62 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (15.00-1.35) 99.4 (35.62-1.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.135 , 0.160 0.145 , 0.171	Depositor DCC
R_{free} test set	2351 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.5	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 47008 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1991	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACE

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	1.03	5/1660 (0.3%)	0.97	3/2250 (0.1%)
2	B	1.59	1/107 (0.9%)	1.32	0/143
All	All	1.07	6/1767 (0.3%)	1.00	3/2393 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	SER	CB-OG	-10.81	1.28	1.42
1	A	125	THR	C-N	7.65	1.51	1.34
1	A	130	SER	C-N	6.09	1.48	1.34
1	A	130	SER	CB-OG	6.03	1.50	1.42
1	A	220	CYS	CA-CB	5.21	1.65	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	82	PHE	CB-CG-CD1	5.28	124.49	120.80
1	A	189	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1629	0	0	4	0
2	B	106	0	0	1	0
3	A	1	0	0	0	0
4	A	241	0	0	3	1
4	B	14	0	0	0	0
All	All	1991	0	0	4	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:ILE:CD1	4:A:494:HOH:O	2.36	0.73
1:A:159:LYS:NZ	4:A:540:HOH:O	2.36	0.57
1:A:40:HIS:N	4:A:461:HOH:O	2.50	0.43
1:A:195:SER:OG	2:B:5:ARG:C	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:563:HOH:O	4:A:563:HOH:O[5_557]	1.29	0.91

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
2	B	11/14 (79%)	11 (100%)	0	0	100	100
All	All	232/237 (98%)	229 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	184/184 (100%)	183 (100%)	1 (0%)	94	79
2	B	10/13 (77%)	10 (100%)	0	100	100
All	All	194/197 (98%)	193 (100%)	1 (0%)	94	79

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASN

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

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	223/223 (100%)	-0.04	1 (0%) 90 93	9, 18, 30, 42	0
2	B	13/14 (92%)	-0.12	0 100 100	11, 13, 28, 38	0
All	All	236/237 (99%)	-0.04	1 (0%) 90 93	9, 18, 30, 42	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	VAL	2.1

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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	A	301	1/1	0.03	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.