

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3BZV
Title	:	Crystal structural of the mutated T264A EscU C-terminal domain
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Deposited on	:	2008-01-18
Resolution	:	1.94 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

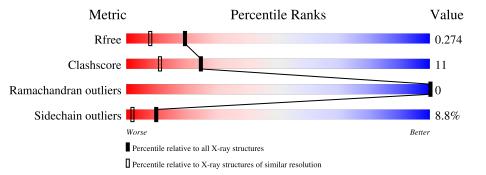
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.94 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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%

Mol	Chain	Length	Quality of chain					
1	А	54	30%	11% •	56%			
2	В	83		78%		13% • • •		



3BZV

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 875 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 EscU.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
1	А	24	Total 185	C 113	N 36	O 36	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	209	GLY	-	expression tag	UNP Q7DB59
А	210	SER	-	expression tag	UNP Q7DB59
А	211	HIS	-	expression tag	UNP Q7DB59
А	212	MET	-	expression tag	UNP Q7DB59
А	213	ALA	-	expression tag	UNP Q7DB59
А	214	SER	-	expression tag	UNP Q7DB59

• Molecule 2 is a protein called EscU.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	80	Total 659	C 437	N 104	0 116	S 2	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	264	ALA	THR	engineered mutation	UNP Q9AJ26

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	9	Total O 9 9	0	0
3	В	22	TotalO2222	0	0



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. 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. 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.

Chain A:	30%	11%	•	56%		
GLY SER HIS MET ALA ALA ALA SER MET SER LYS GLU VAL	ARG GLU ALA LYS ASP ASP GLY ASP GLY PRO	GLU GLY GLY	GLU ARG ARG ARG L240 L240 S242 E243 E243 E243 I244	L249 N252 1253 8256 N262		
• Molecule 2: Esc	U					
Chain B:		78%			13%	
PR0 A264 1283 1283 1294 1294 1294 1297 1297 1299 1300	Y301 D302 1303 P304 R313 K317 K317 D328	E331 D342	L343 ASP TYR			

• Molecule 1: EscU



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	52.09Å 52.09Å 155.18Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.13 - 1.94	Depositor
Resolution (A)	45.11 - 1.94	EDS
% Data completeness	99.8 (45.13-1.94)	Depositor
(in resolution range)	99.8 (45.11-1.94)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.33 (at 1.94 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.215 , 0.268	Depositor
R, R_{free}	0.220 , 0.274	DCC
R_{free} test set	474 reflections $(4.79%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 62.7	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	875	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.84% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.96	0/185	1.06	0/245	
2	В	1.02	0/678	0.97	2/921~(0.2%)	
All	All	1.01	0/863	0.99	2/1166~(0.2%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
2	В	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	313	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	В	328	ASP	CB-CG-OD2	-5.35	113.49	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	244	ILE	Peptide
2	В	342	ASP	Peptide



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	А	185	0	198	11	0
2	В	659	0	700	15	0
3	А	9	0	0	1	0
3	В	22	0	0	0	0
All	All	875	0	898	19	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 11.

All (19) 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:A:256:SER:OG	2:B:269[B]:CYS:SG	2.05	1.10
1:A:242:SER:HB3	1:A:244:ILE:HG13	1.68	0.75
1:A:252:ASN:HB3	2:B:283[A]:ILE:HD12	1.77	0.67
1:A:253:ILE:HD13	2:B:297:LEU:HB2	1.84	0.59
1:A:256:SER:OG	2:B:283[A]:ILE:HD11	2.04	0.58
2:B:300:LEU:C	2:B:300:LEU:HD23	2.26	0.55
2:B:304:PRO:HB3	2:B:343:LEU:HD12	1.90	0.52
1:A:253:ILE:O	2:B:303:ILE:CD1	2.58	0.51
2:B:313:ARG:O	2:B:317:LYS:HG3	2.13	0.48
2:B:299:GLU:OE2	2:B:299:GLU:HA	2.15	0.47
1:A:241:HIS:CD2	3:A:45:HOH:O	2.69	0.46
1:A:253:ILE:O	2:B:303:ILE:HD11	2.15	0.45
2:B:300:LEU:HD23	2:B:300:LEU:O	2.16	0.45
2:B:299:GLU:OE2	2:B:299:GLU:O	2.36	0.44
1:A:249:LEU:CD2	1:A:253:ILE:HD11	2.49	0.43
1:A:253:ILE:O	2:B:303:ILE:HD13	2.19	0.42
2:B:343:LEU:H	2:B:343:LEU:HD23	1.86	0.41
1:A:249:LEU:CD2	1:A:253:ILE:CD1	2.99	0.41
2:B:269[A]:CYS:SG	2:B:294:ILE:CG2	3.10	0.40

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	Perce	ntiles
1	А	22/54~(41%)	20 (91%)	2 (9%)	0	100	100
2	В	81/83~(98%)	78~(96%)	3~(4%)	0	100	100
All	All	103/137~(75%)	98~(95%)	5 (5%)	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	А	22/47~(47%)	20~(91%)	2 (9%)	9 1
2	В	72/72~(100%)	66~(92%)	6 (8%)	11 2
All	All	94/119~(79%)	86~(92%)	8 (8%)	10 2

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	243	GLU
1	А	249	LEU
2	В	299	GLU
2	В	302	ASP
2	В	313	ARG
2	В	328	ASP
2	В	331	GLU
2	В	342	ASP



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

Mol	Chain	Res	Type
2	В	293	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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

