

Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 - 06:00 PM EDT

PDB ID : 3EBM

Title : Crystal structure of human translationally controlled tumour associated pro-

tein (hTCTP) mutant E12V

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Deposited on : 2008-08-28

Resolution : 2.60 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

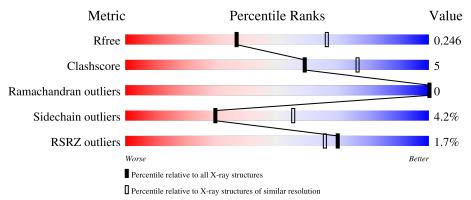
Validation Pipeline (wwPDB-VP) : 2.36

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 2.60 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	180	67%	13%	•	18%
1	В	180	73%	8%	6 •	18%
1	С	180	70%	8%		19%
1	D	180	71%	8%		20%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4825 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 Translationally-controlled tumor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	147	Total	С	N	O	S	0	0	0
1	A	141	1206	775	197	222	12	0	U	0
1	B	147	Total	С	N	О	S	0	0	0
1	Б	141	1212	777	202	221	12	0	U	0
1	С	145	Total	С	N	О	S	0	0	0
1		140	1192	766	195	219	12	0	U	0
1	D	144	Total	С	N	О	S	0	0	0
1	ע	144	1178	757	190	219	12		U	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	VAL	GLU	engineered mutation	UNP P13693
A	173	LEU	-	expression tag	UNP P13693
A	174	GLU	-	expression tag	UNP P13693
A	175	HIS	-	expression tag	UNP P13693
A	176	HIS	-	expression tag	UNP P13693
A	177	HIS	-	expression tag	UNP P13693
A	178	HIS	-	expression tag	UNP P13693
A	179	HIS	-	expression tag	UNP P13693
A	180	HIS	-	expression tag	UNP P13693
В	12	VAL	GLU	engineered mutation	UNP P13693
В	173	LEU	-	expression tag	UNP P13693
В	174	GLU	-	expression tag	UNP P13693
В	175	HIS	-	expression tag	UNP P13693
В	176	HIS	-	expression tag	UNP P13693
В	177	HIS	-	expression tag	UNP P13693
В	178	HIS	-	expression tag	UNP P13693
В	179	HIS	-	expression tag	UNP P13693
В	180	HIS	-	expression tag	UNP P13693
С	12	VAL	GLU	engineered mutation	UNP P13693
С	173	LEU	-	expression tag	UNP P13693
С	174	GLU	-	expression tag	UNP P13693

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Chain	Residue	Modelled	Actual	Actual Comment	
С	175	HIS	-	expression tag	UNP P13693
С	176	HIS	-	expression tag	UNP P13693
С	177	HIS	-	expression tag	UNP P13693
С	178	HIS	-	expression tag	UNP P13693
С	179	HIS	-	expression tag	UNP P13693
С	180	HIS	-	expression tag	UNP P13693
D	12	VAL	GLU	engineered mutation	UNP P13693
D	173	LEU	-	expression tag	UNP P13693
D	174	GLU	-	expression tag	UNP P13693
D	175	HIS	-	expression tag	UNP P13693
D	176	HIS	-	expression tag	UNP P13693
D	177	HIS	-	expression tag	UNP P13693
D	178	HIS	-	expression tag	UNP P13693
D	179	HIS	-	expression tag	UNP P13693
D	180	HIS	-	expression tag	UNP P13693

• Molecule 2 is water.

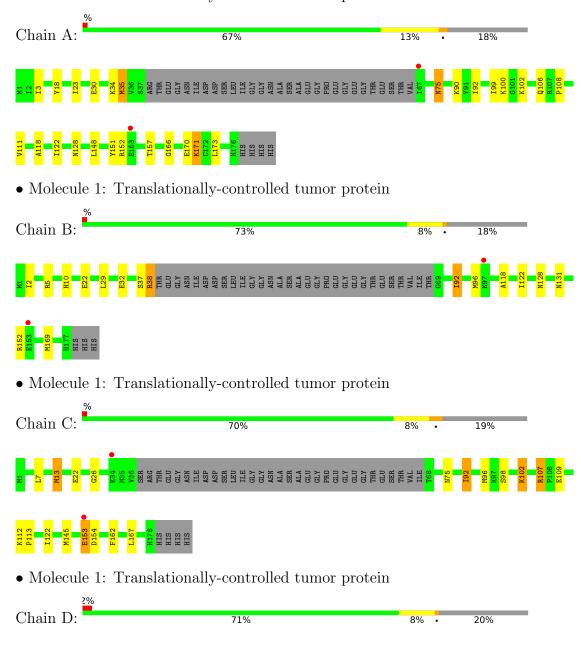
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	В	4	Total O 4 4	0	0
2	С	9	Total O 9 9	0	0
2	D	19	Total O 19 19	0	0



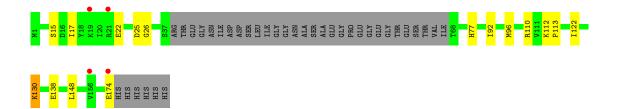
3 Residue-property plots (i)

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 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: Translationally-controlled tumor protein









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	78.19Å 81.54Å 139.92Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 - 2.60	Depositor
rtesolution (A)	35.95 - 2.60	EDS
% Data completeness	97.4 (36.00-2.60)	Depositor
(in resolution range)	97.6 (35.95-2.60)	EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	2.84 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
υ .	0.237 , 0.280	Depositor
R, R_{free}	0.235 , 0.246	DCC
R_{free} test set	1391 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 35.2	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4825	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 17.79% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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		Bo	nd lengths	Bond	angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.41	0/1230	0.48	0/1646
1	В	0.42	0/1237	0.48	0/1654
1	С	0.36	0/1216	0.48	0/1627
1	D	0.59	3/1200 (0.2%)	0.47	0/1605
All	All	0.45	3/4883 (0.1%)	0.48	0/6532

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
1	D	130	LYS	CE-NZ	11.34	1.77	1.49
1	D	130	LYS	C-O	5.17	1.33	1.23
1	D	174	GLU	C-O	5.02	1.32	1.23

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	1206	0	1201	14	0
1	В	1212	0	1202	10	0
1	С	1192	0	1184	11	0
1	D	1178	0	1176	10	0
2	A	5	0	0	0	0
2	В	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	9	0	0	0	0
2	D	19	0	0	0	0
All	All	4825	0	4763	45	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 5.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:D:130:LYS:CE	1:D:130:LYS:NZ	1.77	1.45
1:D:92:ILE:HG12	1:D:122:ILE:HD11	1.51	0.90
1:B:118:ALA:O	1:B:122:ILE:HG12	1.83	0.78
1:C:96:MET:HE1	1:C:122:ILE:HD11	1.69	0.73
1:D:92:ILE:O	1:D:96:MET:HG2	1.91	0.71
1:A:3:ILE:HG13	1:A:170:GLU:HB3	1.71	0.71
1:A:118:ALA:O	1:A:122:ILE:HG12	1.90	0.70
1:A:35:MET:HE3	1:A:157:THR:HA	1.73	0.69
1:A:35:MET:SD	1:A:35:MET:N	2.53	0.68
1:D:92:ILE:HG12	1:D:122:ILE:CD1	2.22	0.66
1:C:92:ILE:HG23	1:C:96:MET:HE3	1.86	0.58
1:C:153:GLU:H	1:C:153:GLU:CD	2.08	0.56
1:B:5:ARG:HD2	1:B:10:HIS:O	2.05	0.56
1:D:112:LYS:HB3	1:D:113:PRO:HD3	1.91	0.53
1:A:92:ILE:HG12	1:A:122:ILE:HD12	1.91	0.52
1:A:171:LYS:HE3	1:A:173:LEU:HD11	1.91	0.52
1:A:92:ILE:HG12	1:A:122:ILE:CD1	2.41	0.51
1:A:3:ILE:CG1	1:A:170:GLU:HB3	2.38	0.51
1:C:107:ARG:HG3	1:C:109:GLU:OE1	2.13	0.49
1:D:22:GLU:HG2	1:D:26:GLY:HA2	1.96	0.47
1:D:77:HIS:O	1:D:138:GLU:HB3	2.15	0.47
1:C:13:MET:HG3	1:C:162:PHE:HE2	1.81	0.46
1:C:145:MET:HE1	1:C:167:LEU:HG	2.00	0.44
1:B:37:SER:O	1:B:38:ARG:HB2	2.17	0.44
1:D:130:LYS:NZ	1:D:130:LYS:CD	2.72	0.44
1:A:151:TYR:HA	1:A:157:THR:O	2.18	0.43
1:B:128:ASN:HB3	1:B:131:ASN:HD22	1.82	0.43
1:C:22:GLU:HG2	1:C:26:GLY:HA2	2.01	0.43
1:C:112:LYS:N	1:C:113:PRO:HD2	2.34	0.43
1:C:92:ILE:HD13	1:C:92:ILE:HA	1.84	0.42
1:B:37:SER:O	1:B:38:ARG:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:A:108:PRO:O	1:A:111:VAL:HG22	2.19	0.42
1:D:110:ARG:C	1:D:113:PRO:HD2	2.40	0.42
1:B:2:ILE:HG21	1:B:169:MET:HE3	2.02	0.42
1:C:98:SER:O	1:C:102:LYS:HG2	2.19	0.42
1:A:99:ILE:HD12	1:A:166:GLY:HA2	2.01	0.41
1:D:15:SER:OG	1:D:17:ILE:HG12	2.20	0.41
1:A:30:GLU:OE1	1:A:152:ARG:NH1	2.52	0.41
1:B:92:ILE:HD13	1:B:92:ILE:HA	1.86	0.41
1:B:32:GLU:HG3	1:B:152:ARG:HH21	1.85	0.41
1:B:92:ILE:HG13	1:B:122:ILE:HD12	2.03	0.40
1:A:18:TYR:OH	1:A:75:ASN:ND2	2.47	0.40
1:A:102:LYS:O	1:A:106:GLN:HG2	2.20	0.40
1:B:22:GLU:HG2	1:B:29:LEU:HD23	2.04	0.40
1:C:13:MET:HG3	1:C:162:PHE:CE2	2.56	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	entiles
1	A	143/180 (79%)	138 (96%)	5 (4%)	0	100	100
1	В	143/180 (79%)	140 (98%)	3 (2%)	0	100	100
1	С	141/180 (78%)	138 (98%)	3 (2%)	0	100	100
1	D	140/180 (78%)	135 (96%)	5 (4%)	0	100	100
All	All	567/720 (79%)	551 (97%)	16 (3%)	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	132/157 (84%)	123 (93%)	9 (7%)	16 32
1	В	132/157 (84%)	129 (98%)	3 (2%)	50 75
1	С	130/157 (83%)	122 (94%)	8 (6%)	18 37
1	D	129/157 (82%)	127 (98%)	2 (2%)	62 82
All	All	523/628 (83%)	501 (96%)	22 (4%)	30 55

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	34	LYS
1	A	35	MET
1	A	75	ASN
1	A	90	LYS
1	A	100	LYS
1	A	128	ASN
1	A	148	LEU
1	A	171	LYS
1	В	38	ARG
1	В	92	ILE
1	В	96	MET
1	С	7	LEU
1	С	13	MET
1	С	75	ASN
1	С	92	ILE
1	С	102	LYS
1	С	107	ARG
1	C C C C C C	153	GLU
1		154	ASP
1	D	25	ASP
1	D	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:



Mol	Chain	Res	Type
1	В	121	GLN
1	В	131	ASN
1	С	75	ASN
1	С	131	ASN
1	С	139	ASN
1	D	131	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 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, 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	147/180 (81%)	-0.08	2 (1%) 75 71	32, 51, 78, 119	0
1	В	147/180 (81%)	0.05	2 (1%) 75 71	33, 55, 76, 100	0
1	С	145/180 (80%)	-0.08	2 (1%) 75 71	34, 52, 71, 98	0
1	D	144/180 (80%)	0.19	4 (2%) 53 46	35, 57, 84, 119	0
All	All	583/720 (80%)	0.02	10 (1%) 70 66	32, 54, 78, 119	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ILE	3.8
1	A	153	GLU	3.8
1	D	21	ARG	3.7
1	D	156	VAL	3.2
1	В	153	GLU	2.7
1	В	97	LYS	2.3
1	D	19	LYS	2.3
1	С	153	GLU	2.3
1	С	34	LYS	2.1
1	D	174	GLU	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.

