



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EWR
Title : CRYSTAL STRUCTURE OF TAQ MUTS
Authors : Obmolova, G.; Ban, C.; Hsieh, P.; Yang, W.
Deposited on : 2000-04-26
Resolution : 3.19 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

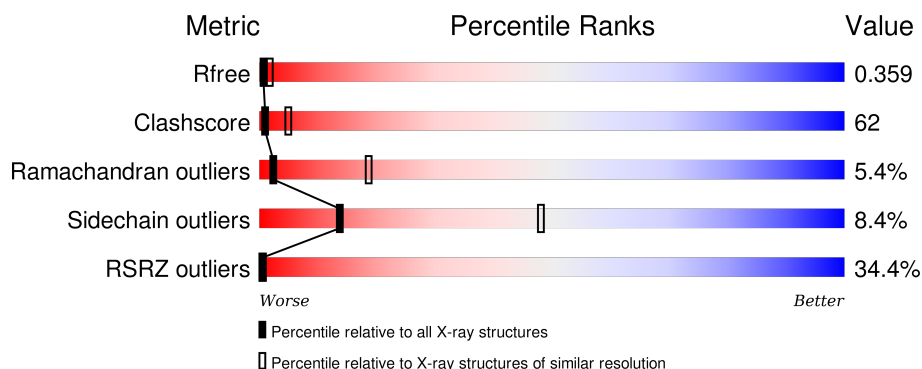
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	649	<div> <div>26%</div> <div>19%</div> <div>44%</div> <div>6%</div> <div>31%</div> </div>
1	B	649	<div> <div>25%</div> <div>22%</div> <div>52%</div> <div>7%</div> <div>18%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7593 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.

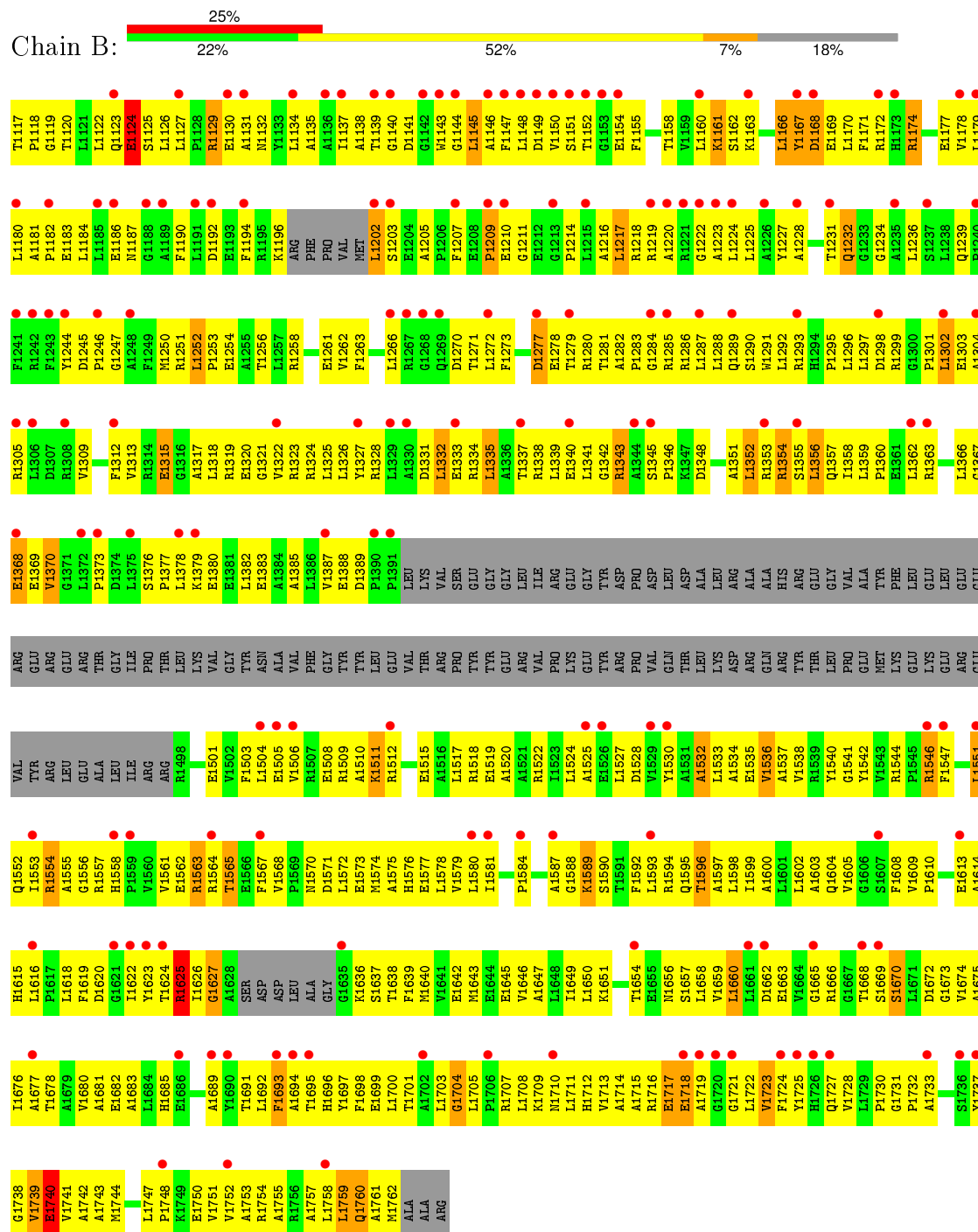
- Molecule 1 is a protein called DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	Se	0	0	0
			3468	2209	626	626	7			
1	B	529	Total	C	N	O	Se	0	0	0
			4125	2623	740	755	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	MSE	MET	MODIFIED	UNP Q56215
A	574	MSE	MET	MODIFIED	UNP Q56215
A	586	MSE	MET	MODIFIED	UNP Q56215
A	640	MSE	MET	MODIFIED	UNP Q56215
A	643	MSE	MET	MODIFIED	UNP Q56215
A	744	MSE	MET	MODIFIED	UNP Q56215
A	762	MSE	MET	MODIFIED	UNP Q56215
B	1250	MSE	MET	MODIFIED	UNP Q56215
B	1574	MSE	MET	MODIFIED	UNP Q56215
B	1586	MSE	MET	MODIFIED	UNP Q56215
B	1640	MSE	MET	MODIFIED	UNP Q56215
B	1643	MSE	MET	MODIFIED	UNP Q56215
B	1744	MSE	MET	MODIFIED	UNP Q56215
B	1762	MSE	MET	MODIFIED	UNP Q56215

● Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.73Å 96.73Å 427.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.19 19.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.94-3.19) 94.2 (19.94-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.22Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.331 , 0.361 0.332 , 0.359	Depositor DCC
R_{free} test set	1813 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	98.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.7	EDS
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 68672 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7593	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/3526	0.67	0/4757
1	B	0.51	0/4192	0.69	0/5662
All	All	0.50	0/7718	0.68	0/10419

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	3468	0	3513	435	0
1	B	4125	0	4200	526	0
All	All	7593	0	7713	949	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 62.

The worst 5 of 949 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:292:LEU:HD23	1:A:605:VAL:HG21	1.31	1.11
1:A:272:LEU:HD11	1:A:602:LEU:HD21	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PRO:HB2	1:A:218:ARG:HH21	1.16	1.04
1:A:557:ARG:HH21	1:A:610:PRO:HA	1.26	1.00
1:B:1557:ARG:HH21	1:B:1610:PRO:HA	1.23	0.99

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	437/649 (67%)	344 (79%)	69 (16%)	24 (6%)	2	18
1	B	521/649 (80%)	406 (78%)	87 (17%)	28 (5%)	2	19
All	All	958/1298 (74%)	750 (78%)	156 (16%)	52 (5%)	2	19

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	235	ALA
1	A	519	GLU
1	A	670	SER
1	A	704	GLY

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	346/515 (67%)	316 (91%)	30 (9%)	13	45
1	B	419/515 (81%)	385 (92%)	34 (8%)	15	51
All	All	765/1030 (74%)	701 (92%)	64 (8%)	14	48

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	759	LEU
1	B	1168	ASP
1	B	1693	PHE
1	A	760	GLN
1	B	1141	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1123	GLN
1	B	1173	HIS
1	B	1604	GLN
1	A	685	HIS
1	A	727	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	440/649 (67%)	1.89	168 (38%)	0 0	34, 104, 154, 181	0
1	B	522/649 (80%)	1.74	163 (31%)	1 0	14, 98, 158, 188	0
All	All	962/1298 (74%)	1.81	331 (34%)	0 0	14, 102, 156, 188	0

The worst 5 of 331 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1142	GLY	13.7
1	A	530	TYR	8.8
1	A	216	ALA	8.3
1	B	1726	HIS	8.2
1	B	1719	ALA	8.2

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 carbohydrates 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.