



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:35 pm BST

PDB ID : 1AY1
Title : ANTI TAQ FAB TP7
Authors : Murali, R.; Helmer-Citterich, M.; Sharkey, D.J.; Scalice, E.R.; Daiss, J.L.;
Sullivan, M.A.; Murthy, H.M.K.
Deposited on : 1997-11-13
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

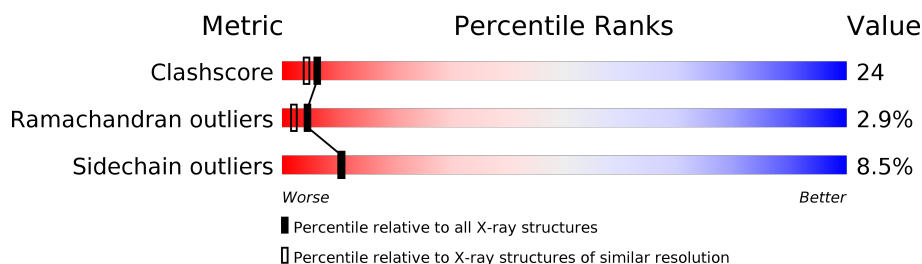
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	210	
2	H	213	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3282 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 TP7 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1617	1007	267	333	10			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	17	GLU	GLN	CONFLICT	UNP Q91W12
L	21	MET	ILE	CONFLICT	UNP Q91W12
L	?	-	SER	DELETION	UNP Q91W12
L	?	-	ARG	DELETION	UNP Q91W12
L	32	TYR	PHE	CONFLICT	UNP Q91W12
L	33	MET	LEU	CONFLICT	UNP Q91W12
L	34	TYR	HIS	CONFLICT	UNP Q91W12
L	40	PRO	SER	CONFLICT	UNP Q91W12
L	42	SER	ALA	CONFLICT	UNP Q91W12
L	45	ARG	LYS	CONFLICT	UNP Q91W12
L	47	LEU	TRP	CONFLICT	UNP Q91W12
L	51	SER	THR	CONFLICT	UNP Q91W12
L	52	THR	SER	CONFLICT	UNP Q91W12
L	53	ASN	LYS	CONFLICT	UNP Q91W12
L	56	SER	PRO	CONFLICT	UNP Q91W12
L	60	VAL	ALA	CONFLICT	UNP Q91W12
L	77	ARG	SER	CONFLICT	UNP Q91W12
L	85	THR	SER	CONFLICT	UNP Q91W12
L	87	TYR	PHE	CONFLICT	UNP Q91W12
L	89	GLN	HIS	CONFLICT	UNP Q91W12
L	93	THR	SER	CONFLICT	UNP Q91W12

- Molecule 2 is a protein called TP7 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total 1665	C 1067	N 264	O 329	S 5	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

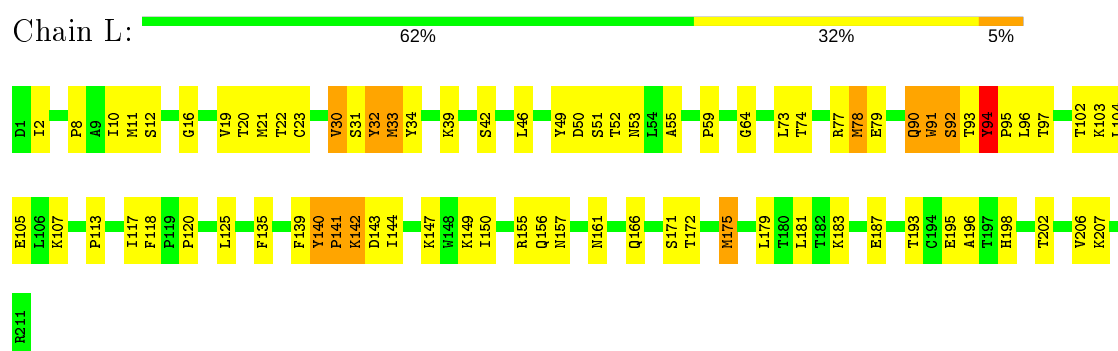
Chain	Residue	Modelled	Actual	Comment	Reference
H	15	TYR	SER	CONFLICT	GB 1513182
H	21	SER	THR	CONFLICT	GB 1513182
H	29	ILE	VAL	CONFLICT	GB 1513182
H	31A	ASP	GLU	CONFLICT	GB 1513182
H	48	MET	LEU	CONFLICT	GB 1513182
H	52	THR	ASN	CONFLICT	GB 1513182
H	55	THR	SER	CONFLICT	GB 1513182
H	57	ASP	SER	CONFLICT	GB 1513182
H	?	-	ASP	DELETION	GB 1513182
H	95	TYR	-	INSERTION	GB 1513182
H	96	TYR	-	INSERTION	GB 1513182
H	97	TYR	-	INSERTION	GB 1513182
H	98	GLY	-	INSERTION	GB 1513182
H	99	TYR	SER	CONFLICT	GB 1513182
H	101	TYR	-	INSERTION	GB 1513182
H	103	ASP	ALA	CONFLICT	GB 1513182
H	104	VAL	TYR	CONFLICT	GB 1513182
H	110	THR	LEU	CONFLICT	GB 1513182
H	111	LEU	VAL	CONFLICT	GB 1513182
H	115	SER	ALA	CONFLICT	GB 1513182
H	120	ALA	PRO	CONFLICT	GB 1513182
H	129	VAL	GLY	CONFLICT	GB 1513182
H	?	-	ALA	DELETION	GB 1513182
H	?	-	ALA	DELETION	GB 1513182
H	?	-	GLN	DELETION	GB 1513182
H	?	-	THR	DELETION	GB 1513182
H	?	-	ASN	DELETION	GB 1513182
H	?	-	MET	DELETION	GB 1513182
H	148	LEU	VAL	CONFLICT	GB 1513182
H	180	THR	PRO	CONFLICT	GB 1513182
H	187	GLN	GLU	CONFLICT	GB 1513182
H	188	SER	THR	CONFLICT	GB 1513182
H	189	ILE	VAL	CONFLICT	GB 1513182
H	207	GLU	VAL	CONFLICT	GB 1513182

3 Residue-property plots

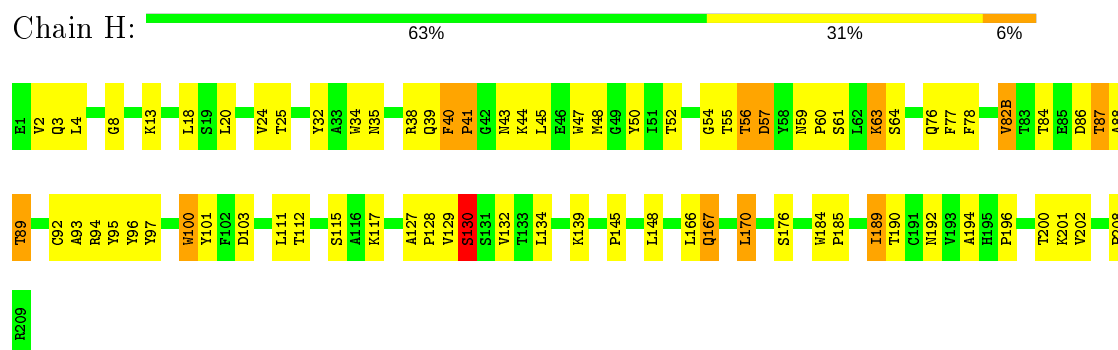
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: TP7 FAB



• Molecule 2: TP7 FAB



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.50 Å 72.70 Å 82.20 Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	82.5 (7.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3282	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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	L	0.47	0/1655	0.81	2/2249 (0.1%)
2	H	0.54	0/1715	0.81	1/2353 (0.0%)
All	All	0.51	0/3370	0.81	3/4602 (0.1%)

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	L	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	38	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	L	33	MET	CG-SD-CE	6.25	110.20	100.20
1	L	94	TYR	CB-CG-CD1	-5.33	117.80	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	127	ALA	Peptide
1	L	94	TYR	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	L	1617	0	1546	72	0
2	H	1665	0	1605	88	0
All	All	3282	0	3151	157	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 24.

The worst 5 of 157 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)
2:H:34:TRP:CZ3	2:H:94:ARG:CD	2.01	1.42
2:H:34:TRP:CZ3	2:H:94:ARG:HD3	1.59	1.33
2:H:34:TRP:CH2	2:H:94:ARG:HD2	1.72	1.25
1:L:140:TYR:HB3	1:L:141:PRO:HD3	1.37	1.03
2:H:32:TYR:HE1	2:H:97:TYR:H	1.04	0.94

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	L	208/210 (99%)	191 (92%)	12 (6%)	5 (2%)	6	3
2	H	211/213 (99%)	188 (89%)	16 (8%)	7 (3%)	4	2
All	All	419/423 (99%)	379 (90%)	28 (7%)	12 (3%)	4	2

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	92	SER
1	L	142	LYS
2	H	100	TRP
1	L	32	TYR
2	H	61	SER

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	L	185/185 (100%)	171 (92%)	14 (8%)	13	14
2	H	191/191 (100%)	173 (91%)	18 (9%)	8	8
All	All	376/376 (100%)	344 (92%)	32 (8%)	10	10

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	24	VAL
2	H	57	ASP
2	H	189	ILE
2	H	43	ASN
2	H	63	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
2	H	167	GLN
2	H	43	ASN
1	L	157	ASN
2	H	80	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 carbohydrates 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.