



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 06:04 PM EDT

PDB ID : 35UJ / pdb_000035uj
Title : Crystal structure of TFPI K2 domain in complex with 4D8 Fab fragment
Authors : Juo, Z.S.; Mosyak, L.
Deposited on : 2026-05-18
Resolution : 2.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

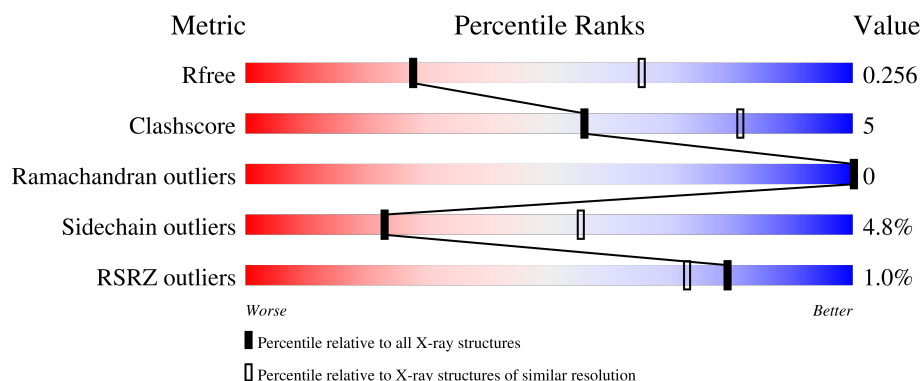
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	H	221	
2	L	213	
3	T	71	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3775 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 4D8 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1597	1016	255	320	6			

- Molecule 2 is a protein called 4D8 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1646	1030	280	328	8			

- Molecule 3 is a protein called Tissue factor pathway inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	59	Total	C	N	O	S	0	0	0
			483	299	80	97	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	151	GLY	-	expression tag	UNP Q2PFV4
T	152	GLY	-	expression tag	UNP Q2PFV4
T	153	SER	-	expression tag	UNP Q2PFV4
T	154	GLY	-	expression tag	UNP Q2PFV4
T	155	GLY	-	expression tag	UNP Q2PFV4
T	156	GLY	-	expression tag	UNP Q2PFV4
T	157	LEU	-	expression tag	UNP Q2PFV4
T	158	ASN	-	expression tag	UNP Q2PFV4

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	27	Total	O	0	0
			27	27		

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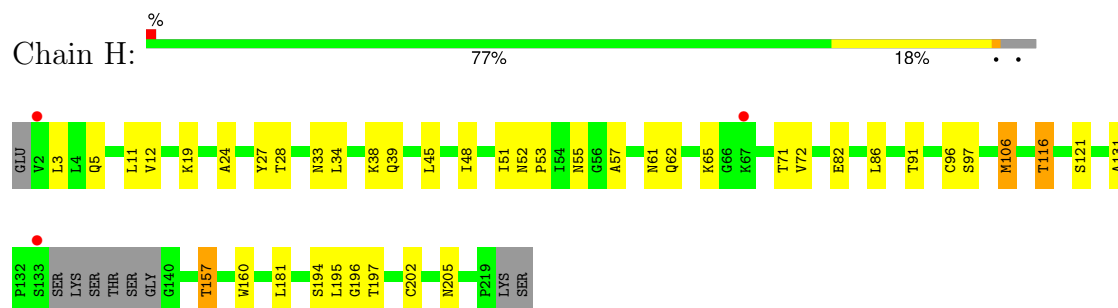
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	14	Total 14	O 14	0	0
4	T	8	Total 8	O 8	0	0

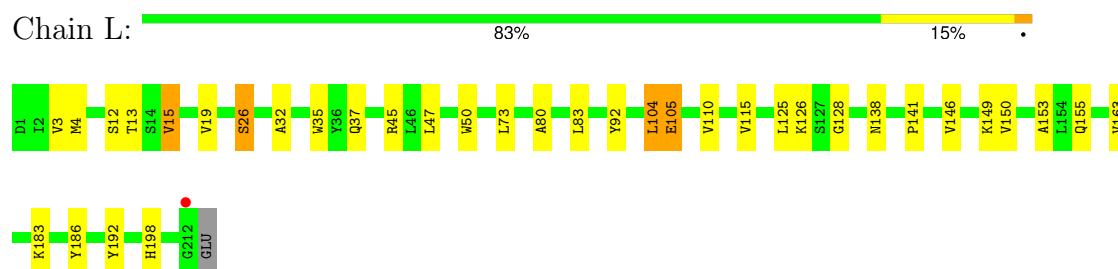
3 Residue-property plots [i](#)

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.

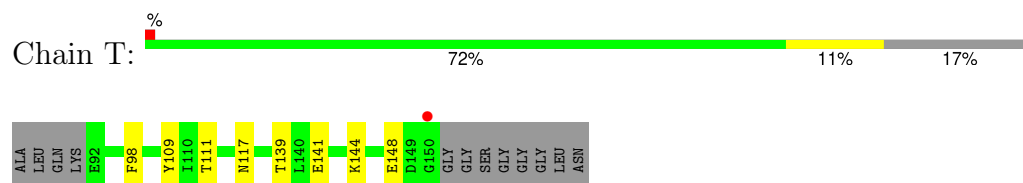
- Molecule 1: 4D8 Heavy chain



- Molecule 2: 4D8 Light chain



- Molecule 3: Tissue factor pathway inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.10Å 82.28Å 103.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.85 – 2.90 43.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.85-2.90) 99.5 (43.85-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.171 , 0.242 0.183 , 0.256	Depositor DCC
R_{free} test set	586 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3775	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	0.85	0/1637	1.29	7/2235 (0.3%)
2	L	0.83	1/1684 (0.1%)	1.32	7/2288 (0.3%)
3	T	0.82	0/493	1.30	1/659 (0.2%)
All	All	0.84	1/3814 (0.0%)	1.30	15/5182 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	MET	SD-CE	-5.26	1.66	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	138	ASN	N-CA-C	11.18	126.51	111.30
2	L	15	VAL	CB-CA-C	8.25	120.35	111.35
1	H	131	ALA	N-CA-C	6.74	119.41	109.50
2	L	198	HIS	CA-C-N	6.43	128.90	120.28
2	L	198	HIS	C-N-CA	6.43	128.90	120.28
2	L	126	LYS	N-CA-C	-6.05	105.66	113.16
1	H	196	GLY	CA-C-N	5.98	128.54	120.65
1	H	196	GLY	C-N-CA	5.98	128.54	120.65
1	H	96	CYS	N-CA-C	-5.90	101.27	110.42
3	T	109	TYR	N-CA-C	5.47	118.51	110.30
1	H	61	ASN	N-CA-C	-5.32	101.77	109.59
1	H	121	SER	CA-C-N	5.26	129.63	121.26
1	H	121	SER	C-N-CA	5.26	129.63	121.26
2	L	50	TRP	CA-C-N	5.07	131.21	121.54
2	L	50	TRP	C-N-CA	5.07	131.21	121.54

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	H	1597	0	1554	16	0
2	L	1646	0	1591	14	0
3	T	483	0	429	4	0
4	H	27	0	0	0	0
4	L	14	0	0	0	0
4	T	8	0	0	0	0
All	All	3775	0	3574	34	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 (34) 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:H:52:ASN:HB3	1:H:55:ASN:OD1	1.99	0.62
2:L:149:LYS:HA	2:L:153:ALA:O	1.99	0.61
2:L:19:VAL:HG21	2:L:104:LEU:HD21	1.83	0.59
1:H:157:THR:HB	1:H:205:ASN:HB3	1.85	0.58
2:L:3:VAL:H	2:L:26:SER:HB3	1.71	0.56
2:L:125:LEU:HD12	2:L:183:LYS:HG3	1.88	0.56
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.89	0.55
2:L:186:TYR:HA	2:L:192:TYR:OH	2.09	0.52
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.91	0.51
3:T:139:THR:HG22	3:T:141:GLU:H	1.75	0.51
2:L:128:GLY:O	2:L:183:LYS:HB2	2.11	0.51
1:H:194:SER:HA	1:H:197:THR:HB	1.92	0.50
1:H:91:THR:HG23	1:H:116:THR:HA	1.94	0.48
3:T:139:THR:HG22	3:T:141:GLU:N	2.30	0.47
2:L:12:SER:HA	2:L:105:GLU:HG3	1.97	0.46
1:H:3:LEU:HD21	1:H:5:GLN:HG2	1.97	0.46
1:H:19:LYS:HG3	1:H:82:GLU:HG3	1.98	0.45
1:H:160:TRP:CH2	1:H:202:CYS:HB3	2.52	0.44
2:L:19:VAL:HG11	2:L:104:LEU:HD11	1.98	0.44
3:T:98:PHE:HD1	3:T:117:ASN:HD21	1.66	0.44
3:T:144:LYS:HA	3:T:148:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:110:VAL:HG22	2:L:141:PRO:HD3	1.99	0.44
1:H:97:SER:OG	1:H:106:MET:HB2	2.18	0.43
2:L:80:ALA:O	2:L:83:LEU:HB2	2.19	0.43
1:H:34:LEU:HD23	1:H:53:PRO:HG3	2.00	0.43
1:H:24:ALA:HB1	1:H:27:TYR:CE1	2.54	0.43
1:H:11:LEU:HD23	1:H:116:THR:HB	2.01	0.42
2:L:32:ALA:HB3	2:L:92:TYR:HB2	2.02	0.42
2:L:150:VAL:HB	2:L:155:GLN:HE21	1.85	0.41
1:H:62:GLN:NE2	1:H:65:LYS:HD3	2.36	0.41
1:H:51:ILE:HA	1:H:57:ALA:O	2.21	0.41
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.56	0.41
1:H:195:LEU:HD12	1:H:195:LEU:HA	1.88	0.40
1:H:38:LYS:HB2	1:H:48:ILE:HD11	2.04	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	Percentiles	
1	H	208/221 (94%)	203 (98%)	5 (2%)	0	100	100
2	L	210/213 (99%)	200 (95%)	10 (5%)	0	100	100
3	T	57/71 (80%)	54 (95%)	3 (5%)	0	100	100
All	All	475/505 (94%)	457 (96%)	18 (4%)	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	H	181/189 (96%)	171 (94%)	10 (6%)	19	50
2	L	186/187 (100%)	177 (95%)	9 (5%)	23	55
3	T	53/59 (90%)	52 (98%)	1 (2%)	50	79
All	All	420/435 (97%)	400 (95%)	20 (5%)	23	55

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	VAL
1	H	28	THR
1	H	33	ASN
1	H	71	THR
1	H	72	VAL
1	H	86	LEU
1	H	106	MET
1	H	116	THR
1	H	157	THR
1	H	181	LEU
2	L	13	THR
2	L	15	VAL
2	L	26	SER
2	L	45	ARG
2	L	104	LEU
2	L	105	GLU
2	L	115	VAL
2	L	146	VAL
2	L	163	VAL
3	T	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	62	GLN
1	H	198	GLN
1	H	205	ASN
2	L	37	GLN
2	L	38	GLN

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Mol	Chain	Res	Type
2	L	155	GLN
2	L	158	ASN
2	L	189	HIS
3	T	117	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 oligosaccharides 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, 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	H	212/221 (95%)	-0.31	3 (1%) 73 65	31, 51, 76, 91	0
2	L	212/213 (99%)	-0.13	1 (0%) 87 83	36, 67, 104, 126	0
3	T	59/71 (83%)	-0.39	1 (1%) 69 61	32, 49, 81, 94	0
All	All	483/505 (95%)	-0.24	5 (1%) 79 73	31, 57, 94, 126	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	150	GLY	3.6
1	H	133	SER	2.3
1	H	67	LYS	2.3
2	L	212	GLY	2.3
1	H	2	VAL	2.3

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 oligosaccharides 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.