



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:03 AM UTC

PDB ID : 5F7T / pdb_00005f7t
Title : TRIM5 B-box2 and coiled-coil chimera
Authors : Wagner, J.M.; Doss, G.; Pornillos, O.
Deposited on : 2015-12-08
Resolution : 2.29 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

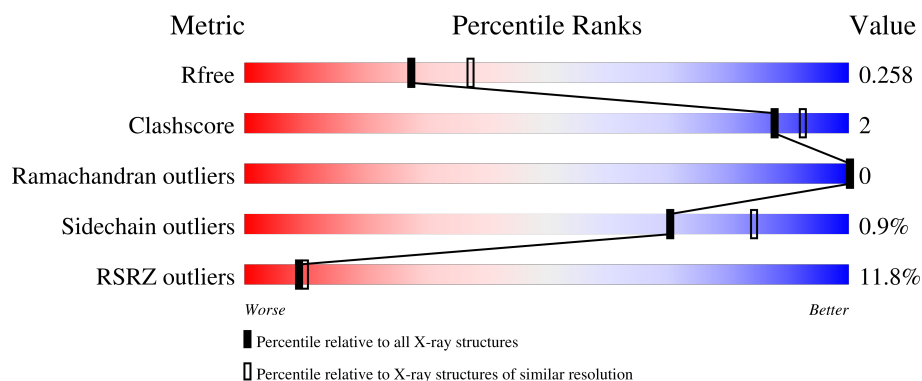
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	E	141	11% 83% 12% 5%
1	F	141	9% 86% 8% 6%
1	H	141	9% 91% • 6%
1	L	141	15% 89% 5% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8557 atoms, of which 4208 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 Tripartite motif-containing protein 5, Serine-tRNA ligase, Tripartite motif-containing protein 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	134	Total	C	H	N	O	S	0	0	0
			2125	663	1050	199	203	10			
1	F	132	Total	C	H	N	O	S	0	0	0
			2130	661	1058	199	202	10			
1	H	133	Total	C	H	N	O	S	0	0	0
			2129	662	1054	199	204	10			
1	L	133	Total	C	H	N	O	S	0	0	0
			2113	658	1046	199	200	10			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	L	2	Total	Zn	0	0
			2	2		

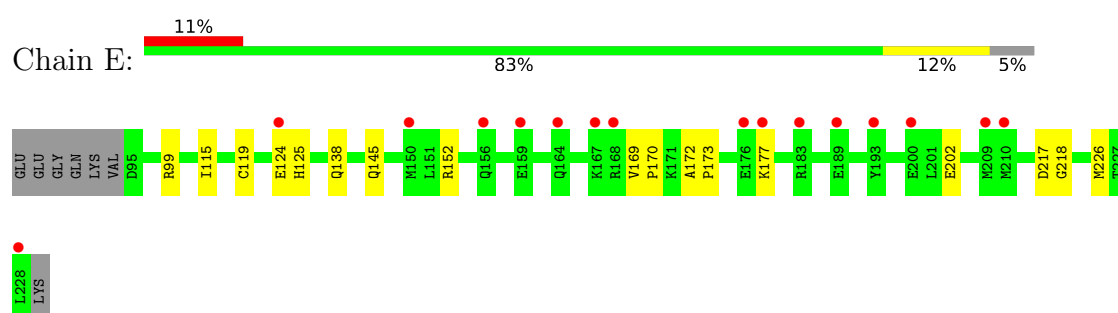
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	13	Total	O	0	0
			13	13		
3	F	16	Total	O	0	0
			16	16		
3	H	15	Total	O	0	0
			15	15		
3	L	8	Total	O	0	0
			8	8		

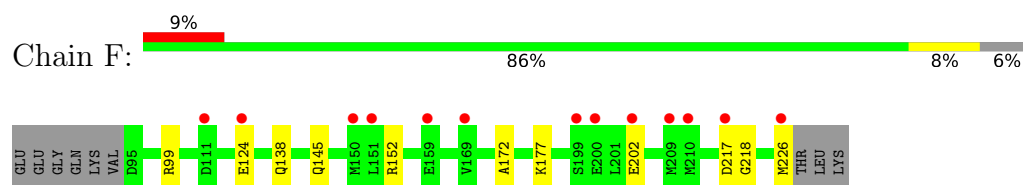
3 Residue-property plots [i](#)

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.

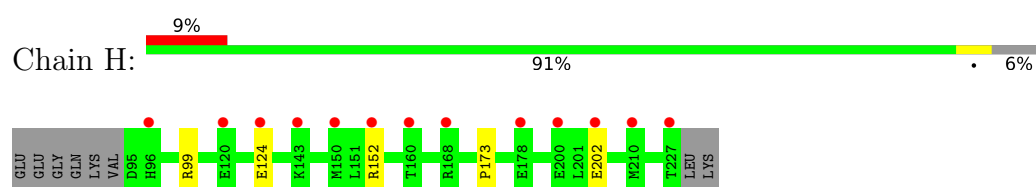
- Molecule 1: Tripartite motif-containing protein 5,Serine-tRNA ligase,Tripartite motif-containing protein 5



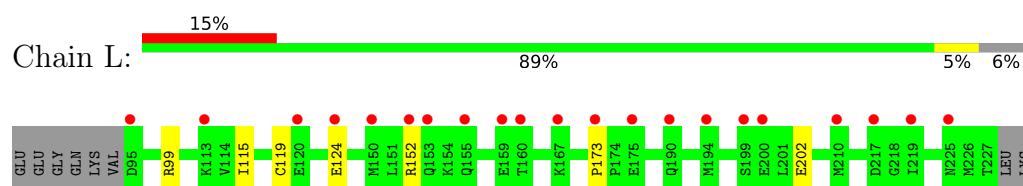
- Molecule 1: Tripartite motif-containing protein 5,Serine-tRNA ligase,Tripartite motif-containing protein 5



- Molecule 1: Tripartite motif-containing protein 5,Serine-tRNA ligase,Tripartite motif-containing protein 5



- Molecule 1: Tripartite motif-containing protein 5,Serine-tRNA ligase,Tripartite motif-containing protein 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.80Å 52.33Å 69.69Å 94.77° 105.54° 103.02°	Depositor
Resolution (Å)	35.05 – 2.29 35.05 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.4 (35.05-2.29) 93.4 (35.05-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.256 0.231 , 0.258	Depositor DCC
R_{free} test set	1305 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8557	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	E	0.33	0/1090	0.68	2/1463 (0.1%)
1	F	0.35	0/1087	0.65	0/1455
1	H	0.33	0/1090	0.64	2/1461 (0.1%)
1	L	0.34	0/1082	0.66	2/1451 (0.1%)
All	All	0.34	0/4349	0.66	6/5830 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	173	PRO	CA-C-N	6.23	125.72	119.24
1	L	173	PRO	C-N-CA	6.23	125.72	119.24
1	E	173	PRO	CA-C-N	6.09	125.57	119.24
1	E	173	PRO	C-N-CA	6.09	125.57	119.24
1	H	173	PRO	CA-C-N	5.15	124.59	119.24
1	H	173	PRO	C-N-CA	5.15	124.59	119.24

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	E	1075	1050	1050	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1072	1058	1058	5	0
1	H	1075	1054	1054	2	0
1	L	1067	1046	1046	3	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	H	2	0	0	0	0
2	L	2	0	0	0	0
3	E	13	0	0	0	0
3	F	16	0	0	0	0
3	H	15	0	0	0	0
3	L	8	0	0	0	0
All	All	4349	4208	4208	17	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 2.

All (17) 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:F:152:ARG:NH2	1:F:202:GLU:OE2	2.15	0.78
1:E:152:ARG:NH2	1:E:202:GLU:OE2	2.21	0.74
1:H:152:ARG:NH2	1:H:202:GLU:OE2	2.24	0.70
1:L:152:ARG:NH2	1:L:202:GLU:OE2	2.27	0.67
1:F:99:ARG:NH2	1:F:124:GLU:OE2	2.30	0.64
1:E:172:ALA:O	1:E:177:LYS:NZ	2.27	0.61
1:L:99:ARG:NH2	1:L:124:GLU:OE1	2.36	0.59
1:F:172:ALA:O	1:F:177:LYS:NZ	2.37	0.57
1:E:99:ARG:NH2	1:E:124:GLU:OE2	2.38	0.56
1:F:217:ASP:OD1	1:F:218:GLY:N	2.39	0.56
1:H:99:ARG:NH2	1:H:124:GLU:OE2	2.39	0.55
1:E:217:ASP:OD1	1:E:218:GLY:N	2.49	0.46
1:L:115:ILE:HB	1:L:119:CYS:HB2	2.01	0.43
1:E:169:VAL:HB	1:E:170:PRO:HD3	2.01	0.42
1:E:115:ILE:HB	1:E:119:CYS:HB2	2.02	0.41
1:E:124:GLU:HG3	1:E:125:HIS:CD2	2.55	0.41
1:E:145:GLN:OE1	1:F:145:GLN:NE2	2.48	0.41

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	E	132/141 (94%)	131 (99%)	1 (1%)	0	100	100
1	F	130/141 (92%)	129 (99%)	1 (1%)	0	100	100
1	H	131/141 (93%)	130 (99%)	1 (1%)	0	100	100
1	L	131/141 (93%)	130 (99%)	1 (1%)	0	100	100
All	All	524/564 (93%)	520 (99%)	4 (1%)	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	E	114/124 (92%)	112 (98%)	2 (2%)	51	70
1	F	115/124 (93%)	113 (98%)	2 (2%)	53	72
1	H	115/124 (93%)	115 (100%)	0	100	100
1	L	113/124 (91%)	113 (100%)	0	100	100
All	All	457/496 (92%)	453 (99%)	4 (1%)	70	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	138	GLN
1	E	226	MET

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Mol	Chain	Res	Type
1	F	138	GLN
1	F	226	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	164	GLN
1	L	109	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	E	134/141 (95%)	1.08	16 (11%) 9 10	33, 59, 97, 117	0
1	F	132/141 (93%)	0.91	13 (9%) 13 14	36, 57, 92, 138	0
1	H	133/141 (94%)	0.98	13 (9%) 13 14	38, 61, 95, 113	0
1	L	133/141 (94%)	1.15	21 (15%) 5 5	39, 62, 99, 112	0
All	All	532/564 (94%)	1.03	63 (11%) 9 10	33, 60, 97, 138	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	209	MET	4.1
1	F	226	MET	3.9
1	E	228	LEU	3.8
1	F	200	GLU	3.7
1	L	225	ASN	3.7
1	L	150	MET	3.6
1	F	150	MET	3.5
1	E	193	TYR	3.3
1	L	217	ASP	3.2
1	E	159	GLU	3.1
1	E	124	GLU	3.1
1	L	120	GLU	3.0
1	L	210	MET	2.9
1	H	178	GLU	2.8
1	L	175	GLU	2.8
1	L	190	GLN	2.8
1	L	219	ILE	2.8
1	L	173	PRO	2.8
1	E	200	GLU	2.7
1	F	159	GLU	2.7
1	F	210	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	167	LYS	2.7
1	H	160	THR	2.7
1	L	113	LYS	2.6
1	H	200	GLU	2.6
1	E	168	ARG	2.6
1	L	200	GLU	2.6
1	L	155	GLN	2.6
1	L	159	GLU	2.6
1	L	124	GLU	2.6
1	L	160	THR	2.5
1	H	210	MET	2.4
1	L	194	MET	2.4
1	H	202	GLU	2.4
1	F	199	SER	2.3
1	F	124	GLU	2.3
1	H	124	GLU	2.3
1	L	95	ASP	2.3
1	H	150	MET	2.3
1	L	167	LYS	2.3
1	H	227	THR	2.3
1	L	199	SER	2.3
1	E	177	LYS	2.3
1	H	143	LYS	2.3
1	H	152	ARG	2.3
1	E	156	GLN	2.3
1	H	120	GLU	2.2
1	F	217	ASP	2.2
1	E	183	ARG	2.2
1	H	96	HIS	2.2
1	F	111	ASP	2.2
1	E	210	MET	2.2
1	E	176	GLU	2.2
1	F	151	LEU	2.1
1	E	150	MET	2.1
1	E	209	MET	2.1
1	L	153	GLN	2.1
1	E	164	GLN	2.1
1	F	169	VAL	2.1
1	F	202	GLU	2.0
1	E	189	GLU	2.0
1	H	168	ARG	2.0
1	L	152	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	E	701	1/1	0.97	0.04	38,38,38,38	0
2	ZN	E	702	1/1	0.97	0.04	40,40,40,40	0
2	ZN	L	701	1/1	0.97	0.04	53,53,53,53	0
2	ZN	H	701	1/1	0.98	0.06	49,49,49,49	0
2	ZN	F	702	1/1	0.98	0.15	67,67,67,67	0
2	ZN	L	702	1/1	0.98	0.04	40,40,40,40	0
2	ZN	F	701	1/1	0.99	0.03	41,41,41,41	0
2	ZN	H	702	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.