Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 04:58 PM EDT

PDB ID	:	6FLN
Title	:	Crystal structure of the human TRIM25 coiled-coil and PRYSPRY domains
Authors	:	Cusack, S.; Lethier, M.
Deposited on	:	2018-01-26
Resolution	:	3.60 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:

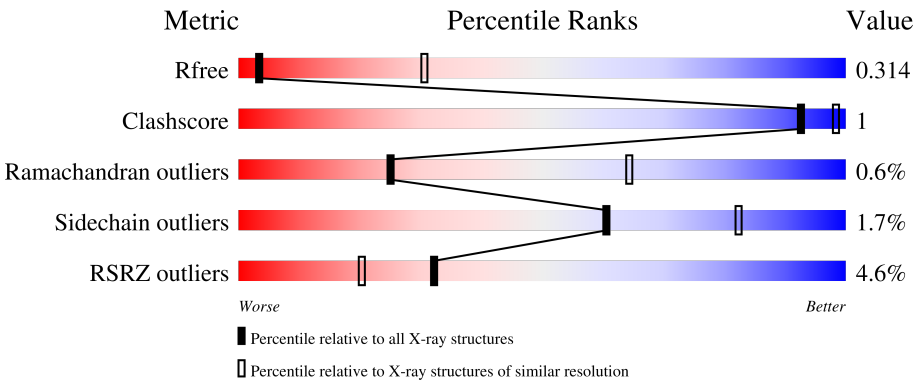
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	445	% 77% • • 18%
1	B	445	3% 76% 6% 18%
1	E	445	7% 80% • 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8861 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 E3 ubiquitin/ISG15 ligase TRIM25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2957	1878	515	549	15	0	0	0
1	B	367	2964	1881	516	551	16	0	0	0
1	E	364	2940	1866	513	546	15	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

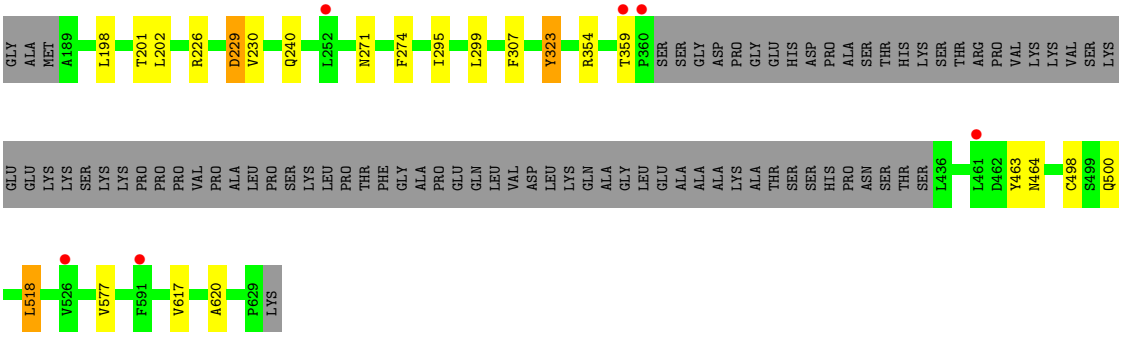
Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	-	expression tag	UNP Q14258
A	187	ALA	-	expression tag	UNP Q14258
A	188	MET	-	expression tag	UNP Q14258
B	186	GLY	-	expression tag	UNP Q14258
B	187	ALA	-	expression tag	UNP Q14258
B	188	MET	-	expression tag	UNP Q14258
E	186	GLY	-	expression tag	UNP Q14258
E	187	ALA	-	expression tag	UNP Q14258
E	188	MET	-	expression tag	UNP Q14258

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.

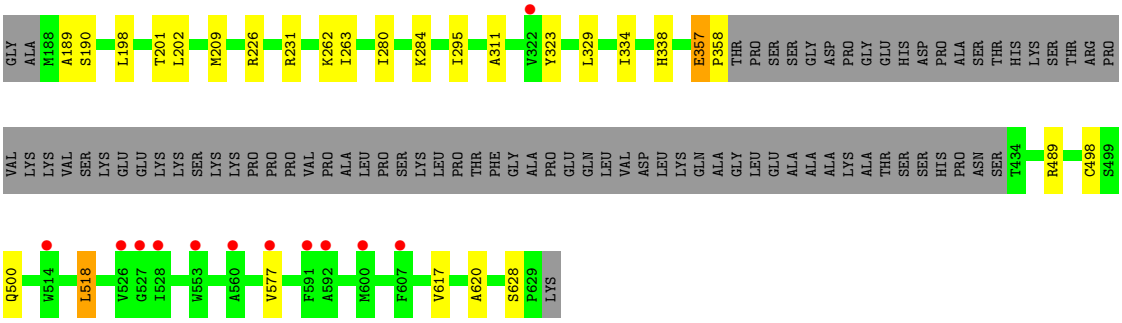
• Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25

Chain A:



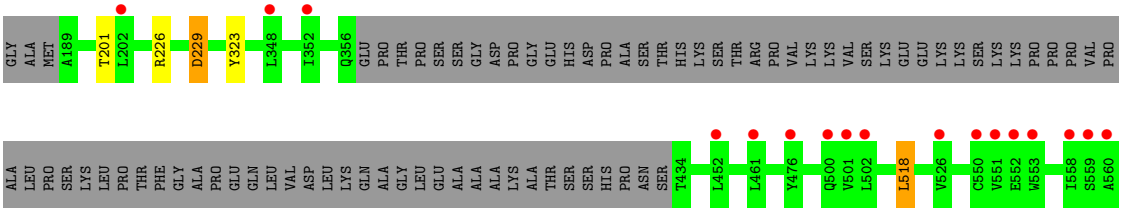
• Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25

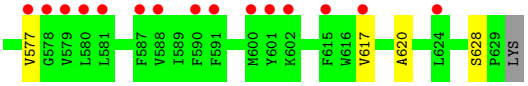
Chain B:



• Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25

Chain E:




V577
G578
V579
L580
L581
F587
V588
I589
F590
F591
M600
Y601
K602
F615
W616
V617
A620
L624
S628
P629
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	89.92Å 89.92Å 827.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	137.85 – 3.60 49.27 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (137.85-3.60) 99.4 (49.27-3.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.287 , 0.318 0.289 , 0.314	Depositor DCC
R_{free} test set	1255 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	138.3	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 172.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8861	wwPDB-VP
Average B, all atoms (Å^2)	225.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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	A	0.41	0/3016	0.56	0/4070
1	B	0.41	0/3022	0.57	0/4076
1	E	0.41	0/2997	0.55	0/4042
All	All	0.41	0/9035	0.56	0/12188

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 (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	2957	0	2978	20	0
1	B	2964	0	2985	21	0
1	E	2940	0	2963	2	0
All	All	8861	0	8926	26	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 1.

All (26) 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:E:518:LEU:HD21	1:E:577:VAL:HG23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LEU:HD21	1:B:577:VAL:HG23	1.72	0.72
1:A:518:LEU:HD21	1:A:577:VAL:HG23	1.71	0.72
1:A:295:ILE:HD12	1:B:209:MET:HE1	1.85	0.58
1:A:463:TYR:CE2	1:B:280:ILE:HG21	2.42	0.54
1:A:230:VAL:HG13	1:B:329:LEU:HD22	1.88	0.54
1:A:359:THR:O	1:B:262:LYS:NZ	2.41	0.54
1:A:295:ILE:HG23	1:B:202:LEU:HD11	1.92	0.52
1:A:271:ASN:HD21	1:B:231:ARG:HG3	1.77	0.50
1:A:274:PHE:CZ	1:B:226:ARG:HD2	2.50	0.47
1:A:299:LEU:HD21	1:B:202:LEU:HD23	1.96	0.47
1:B:357:GLU:HG3	1:B:358:PRO:HD3	1.98	0.46
1:A:464:ASN:HD21	1:B:284:LYS:HE2	1.82	0.45
1:A:323:TYR:CD1	1:B:489:ARG:HD2	2.52	0.45
1:A:307:PHE:CE2	1:B:198:LEU:HD23	2.52	0.45
1:A:464:ASN:ND2	1:B:284:LYS:HD3	2.33	0.43
1:A:307:PHE:CZ	1:B:198:LEU:HD23	2.53	0.43
1:A:464:ASN:HD21	1:B:284:LYS:CE	2.32	0.43
1:A:498:CYS:SG	1:A:500:GLN:NE2	2.92	0.42
1:E:226:ARG:HA	1:E:229:ASP:HB2	1.99	0.42
1:B:498:CYS:SG	1:B:500:GLN:NE2	2.92	0.42
1:A:226:ARG:HA	1:A:229:ASP:HB3	2.00	0.42
1:A:202:LEU:HD11	1:B:295:ILE:HG23	2.01	0.41
1:B:263:ILE:HG12	1:B:334:ILE:HD12	2.02	0.41
1:A:198:LEU:HD21	1:B:311:ALA:HB3	2.02	0.41
1:A:240:GLN:HB3	1:B:338:HIS:NE2	2.37	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	A	362/445 (81%)	343 (95%)	18 (5%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	363/445 (82%)	343 (94%)	17 (5%)	3 (1%)	19	59
1	E	360/445 (81%)	342 (95%)	16 (4%)	2 (1%)	25	64
All	All	1085/1335 (81%)	1028 (95%)	51 (5%)	6 (1%)	25	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	ALA
1	B	620	ALA
1	E	620	ALA
1	B	189	ALA
1	B	628	SER
1	E	628	SER

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	327/392 (83%)	321 (98%)	6 (2%)	59	81
1	B	328/392 (84%)	322 (98%)	6 (2%)	59	81
1	E	325/392 (83%)	320 (98%)	5 (2%)	65	84
All	All	980/1176 (83%)	963 (98%)	17 (2%)	60	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	THR
1	A	229	ASP
1	A	323	TYR
1	A	354	ARG
1	A	518	LEU
1	A	617	VAL
1	B	190	SER
1	B	201	THR

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Mol	Chain	Res	Type
1	B	323	TYR
1	B	357	GLU
1	B	518	LEU
1	B	617	VAL
1	E	201	THR
1	E	229	ASP
1	E	323	TYR
1	E	518	LEU
1	E	617	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	A	240	GLN
1	A	271	ASN
1	A	500	GLN
1	A	522	ASN
1	A	563	ASN
1	B	240	GLN
1	B	271	ASN
1	B	500	GLN
1	B	522	ASN
1	B	563	ASN
1	E	522	ASN
1	E	563	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, 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	366/445 (82%)	-0.01	6 (1%)	72	57	144, 207, 260, 326	0
1	B	367/445 (82%)	0.04	12 (3%)	46	31	160, 214, 265, 315	0
1	E	364/445 (81%)	0.29	32 (8%)	10	6	186, 250, 286, 312	0
All	All	1097/1335 (82%)	0.11	50 (4%)	32	20	144, 223, 279, 326	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	PRO	4.4
1	E	588	VAL	4.1
1	E	526	VAL	3.6
1	E	578	GLY	3.6
1	E	617	VAL	3.6
1	B	526	VAL	3.5
1	E	577	VAL	3.4
1	B	560	ALA	3.1
1	E	591	PHE	3.0
1	E	601	TYR	3.0
1	E	558	ILE	2.9
1	A	359	THR	2.8
1	E	560	ALA	2.8
1	E	553	TRP	2.8
1	E	602	LYS	2.8
1	E	500	GLN	2.7
1	A	526	VAL	2.7
1	E	580	LEU	2.6
1	E	587	PHE	2.6
1	E	452	LEU	2.6
1	E	476	TYR	2.6
1	B	600	MET	2.5
1	E	615	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	514	TRP	2.5
1	E	461	LEU	2.5
1	E	551	VAL	2.5
1	E	352	ILE	2.4
1	E	348	LEU	2.4
1	B	577	VAL	2.4
1	E	579	VAL	2.4
1	E	502	LEU	2.3
1	E	550	CYS	2.3
1	B	607	PHE	2.2
1	E	202	LEU	2.2
1	E	600	MET	2.2
1	A	252	LEU	2.2
1	B	592	ALA	2.2
1	B	322	VAL	2.2
1	B	527	GLY	2.1
1	E	559	SER	2.1
1	E	552	GLU	2.1
1	B	553	TRP	2.1
1	E	581	LEU	2.1
1	B	591	PHE	2.1
1	E	501	VAL	2.1
1	E	590	PHE	2.1
1	A	591	PHE	2.1
1	E	624	LEU	2.0
1	B	528	ILE	2.0
1	A	461	LEU	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.