wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:36 PM GMT

PDB ID	:	3U5M
Title	:	Crystal structure of TRIM33 PHD-Bromo in the free state
Authors	:	Wang, Z.; Patel, D.J.
Deposited on	:	2011-10-11
Resolution	:	3.08 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

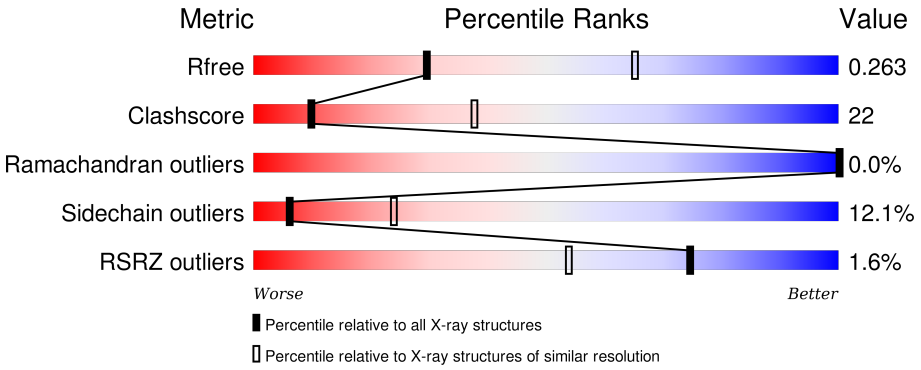
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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 <=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	207	2% 50% 30% 6% 14%
1	B	207	2% 52% 28% 6% 14%
1	C	207	% 49% 29% 6% 16%
1	D	207	% 51% 31% • 14%
1	E	207	48% 33% • 16%

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Mol	Chain	Length	Quality of chain
1	F	207	2% 57% 26% 14%
1	G	207	46% 35% 5% 13%
1	H	207	2% 50% 30% 6% 14%
1	I	207	48% 30% 5% 16%
1	J	207	53% 27% 16%
1	K	207	48% 29% 7% 15%
1	L	207	48% 30% 6% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17117 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-protein ligase TRIM33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1441	923	238	265	15			
1	B	178	Total	C	N	O	S	0	0	0
			1440	923	238	265	14			
1	C	174	Total	C	N	O	S	0	0	0
			1402	899	233	256	14			
1	D	177	Total	C	N	O	S	0	0	0
			1435	920	237	264	14			
1	E	173	Total	C	N	O	S	0	0	0
			1399	897	233	255	14			
1	F	179	Total	C	N	O	S	0	0	0
			1447	925	239	268	15			
1	G	180	Total	C	N	O	S	0	0	0
			1454	930	240	269	15			
1	H	178	Total	C	N	O	S	0	0	0
			1439	921	238	265	15			
1	I	173	Total	C	N	O	S	0	0	0
			1397	895	233	255	14			
1	J	174	Total	C	N	O	S	0	0	0
			1404	900	234	256	14			
1	K	175	Total	C	N	O	S	0	0	0
			1411	905	235	257	14			
1	L	175	Total	C	N	O	S	0	0	0
			1412	904	235	259	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
B	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
C	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
D	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
E	881	SER	-	EXPRESSION TAG	UNP Q9UPN9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
G	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
H	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
I	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
J	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
K	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
L	881	SER	-	EXPRESSION TAG	UNP Q9UPN9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0

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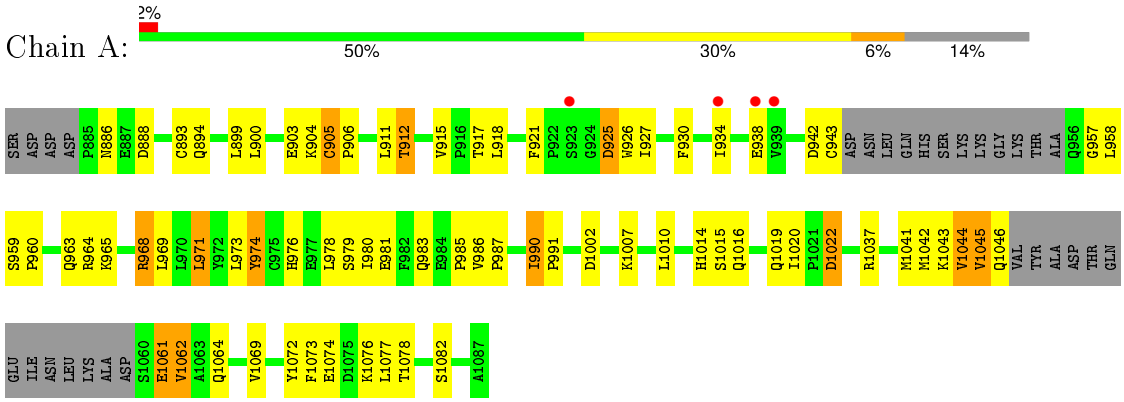
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0

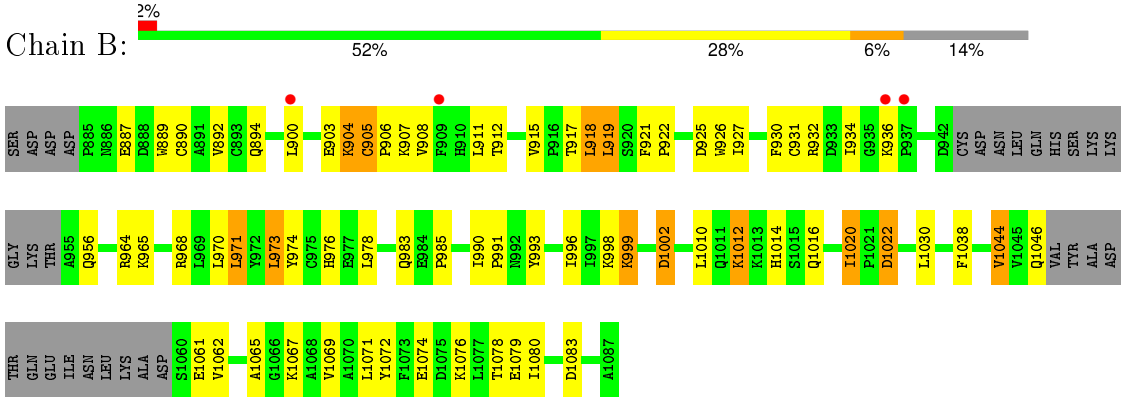
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

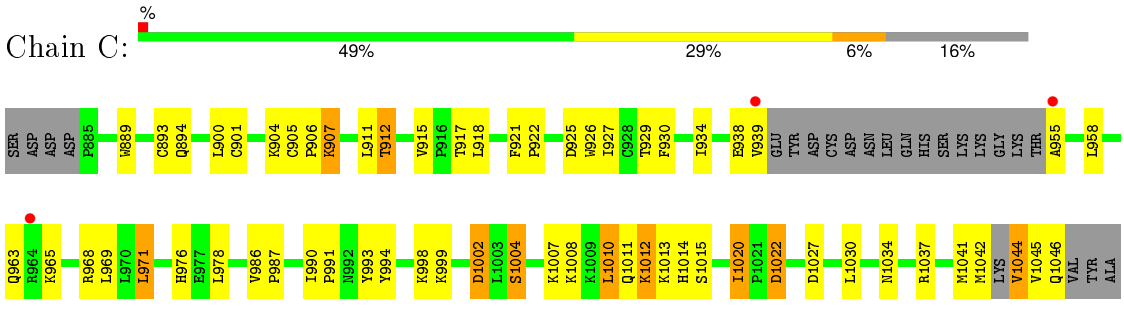
- Molecule 1: E3 ubiquitin-protein ligase TRIM33

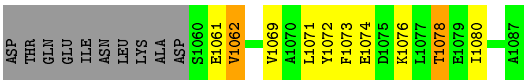


- Molecule 1: E3 ubiquitin-protein ligase TRIM33



- Molecule 1: E3 ubiquitin-protein ligase TRIM33



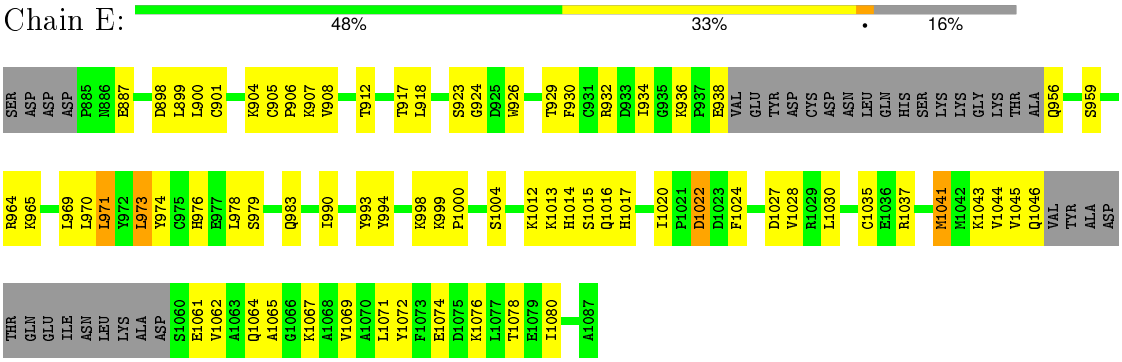


• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain D:

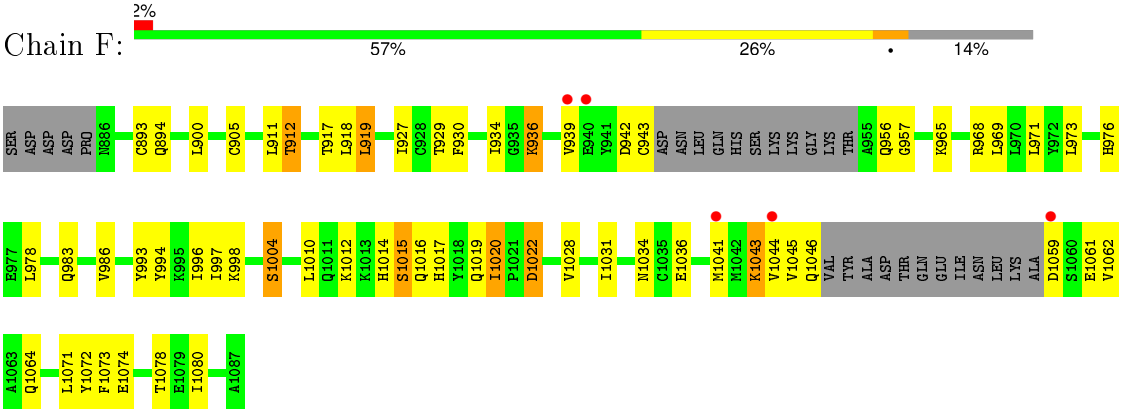
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain E:



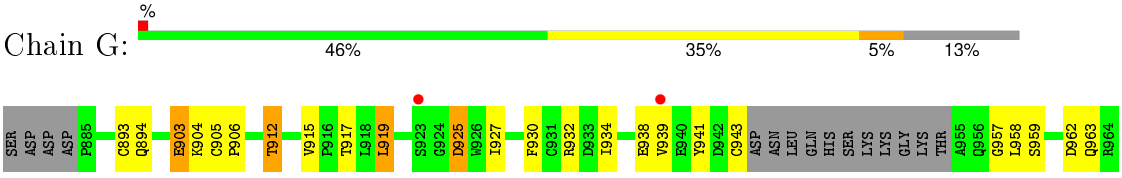
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

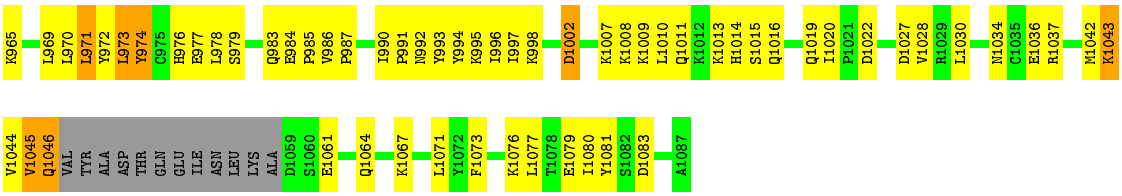
Chain F:



• Molecule 1: E3 ubiquitin-protein ligase TRIM33

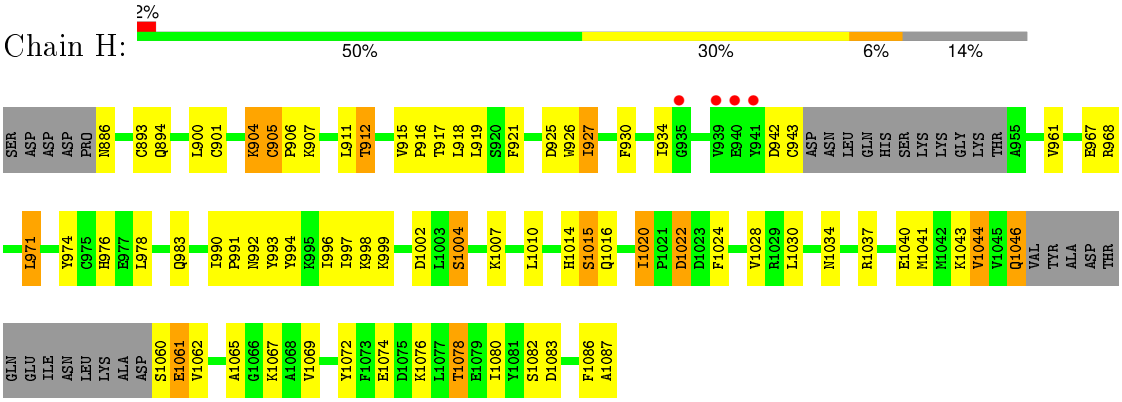
Chain G:





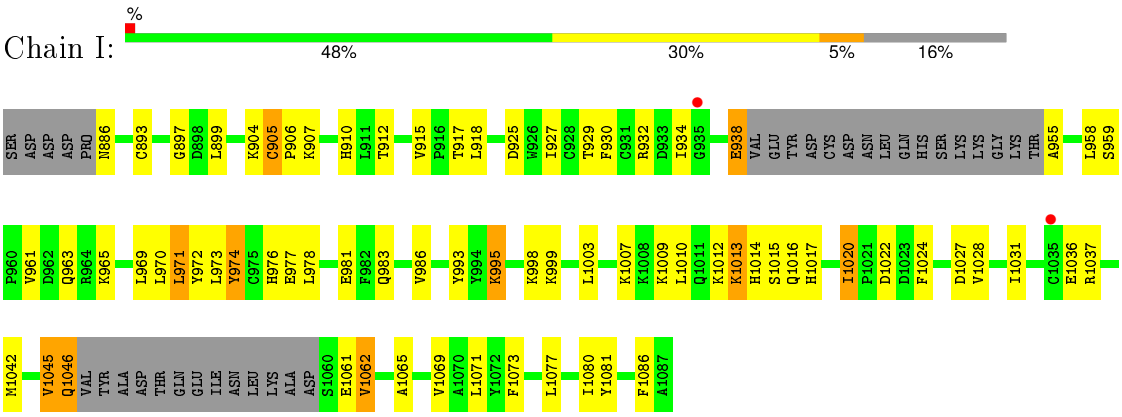
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain H:



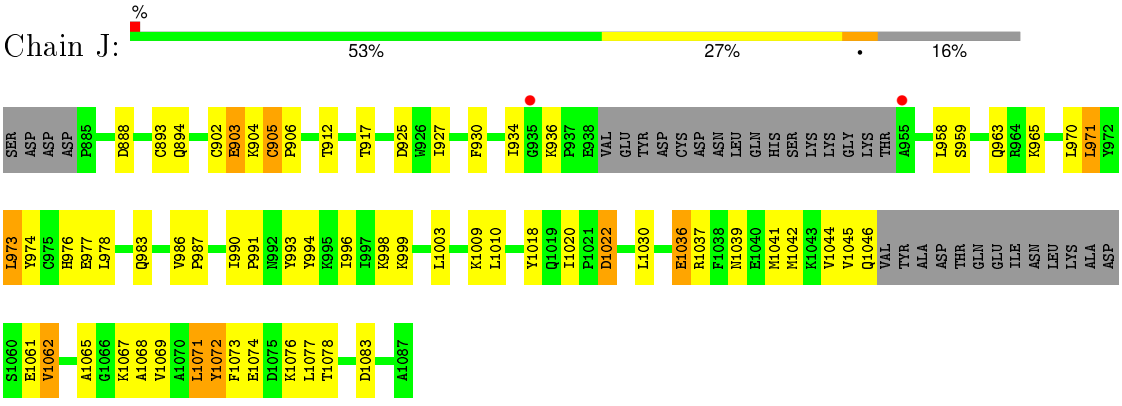
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain I:



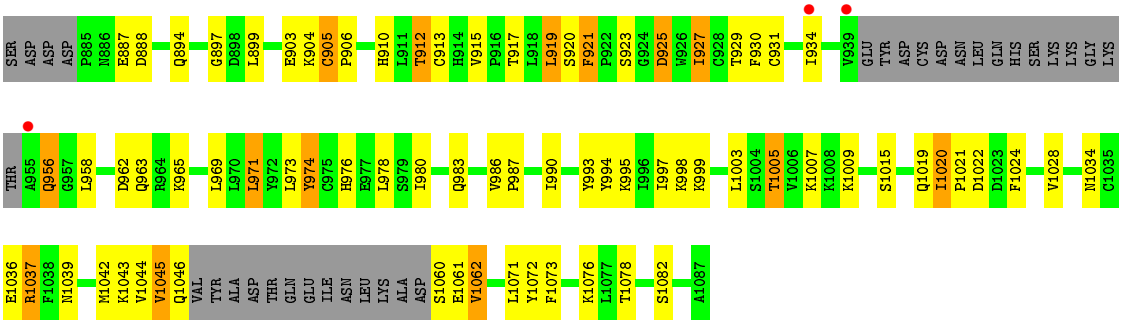
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain J:

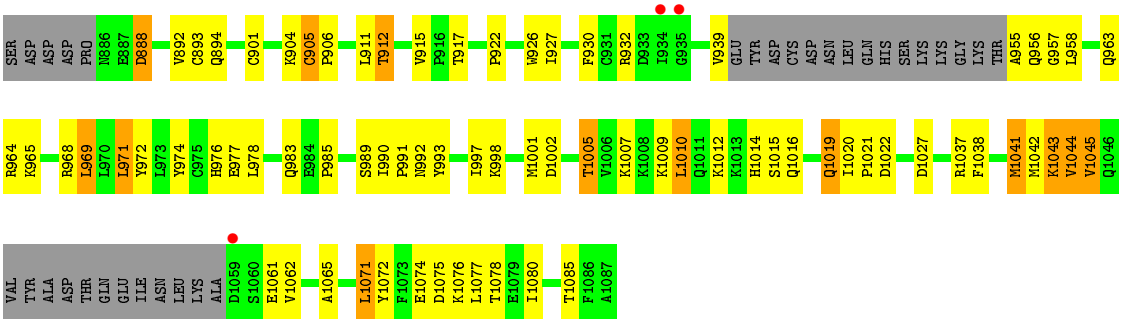


• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain K:



- Molecule 1: E3 ubiquitin-protein ligase TRIM33



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.53Å 79.78Å 134.16Å 89.90° 89.96° 59.97°	Depositor
Resolution (Å)	27.36 – 3.08 27.36 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.9 (27.36-3.08) 91.0 (27.36-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.207 , 0.293 0.189 , 0.263	Depositor DCC
R_{free} test set	1867 reflections (3.89%)	DCC
Wilson B-factor (Å^2)	123.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.397 for k,-h+k,l 0.397 for h-k,h,l 0.387 for -h+k,-h,l 0.387 for -k,h-k,l 0.388 for h,h-k,-l 0.407 for -k,-h,-l 0.417 for -h,-k,l 0.428 for -h+k,k,-l 0.427 for h-k,-k,-l 0.399 for -h,-h+k,-l 0.380 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 50455 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17117	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.46	0/1475	0.62	0/1991
1	B	0.44	0/1474	0.61	0/1990
1	C	0.47	0/1434	0.62	0/1935
1	D	0.46	0/1469	0.61	0/1983
1	E	0.45	0/1432	0.61	0/1932
1	F	0.43	0/1480	0.61	0/1998
1	G	0.47	0/1488	0.62	0/2009
1	H	0.45	0/1472	0.63	0/1987
1	I	0.44	0/1429	0.63	0/1928
1	J	0.46	0/1437	0.61	0/1939
1	K	0.47	0/1444	0.63	0/1949
1	L	0.46	0/1444	0.61	0/1949
All	All	0.46	0/17478	0.62	0/23590

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	1441	0	1415	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1440	0	1415	62	0
1	C	1402	0	1381	67	0
1	D	1435	0	1410	58	0
1	E	1399	0	1382	59	0
1	F	1447	0	1415	54	0
1	G	1454	0	1423	76	0
1	H	1439	0	1411	65	0
1	I	1397	0	1379	51	0
1	J	1404	0	1388	60	0
1	K	1411	0	1396	64	0
1	L	1412	0	1392	81	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	I	2	0	0	0	0
All	All	17117	0	16807	751	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 22.

The worst 5 of 751 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:L:1019:GLN:OE1	1:L:1019:GLN:HA	1.43	1.10
1:A:912:THR:HA	1:A:917:THR:HG23	1.37	1.06
1:G:998:LYS:HA	1:G:998:LYS:HE2	1.39	1.05
1:J:912:THR:HA	1:J:917:THR:HG23	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:976:HIS:HD2	1:J:1072:TYR:CD2	1.79	1.00

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	172/207 (83%)	162 (94%)	10 (6%)	0	100	100
1	B	172/207 (83%)	166 (96%)	6 (4%)	0	100	100
1	C	166/207 (80%)	156 (94%)	10 (6%)	0	100	100
1	D	171/207 (83%)	164 (96%)	7 (4%)	0	100	100
1	E	167/207 (81%)	163 (98%)	4 (2%)	0	100	100
1	F	173/207 (84%)	164 (95%)	9 (5%)	0	100	100
1	G	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
1	H	172/207 (83%)	162 (94%)	10 (6%)	0	100	100
1	I	167/207 (81%)	157 (94%)	10 (6%)	0	100	100
1	J	168/207 (81%)	161 (96%)	7 (4%)	0	100	100
1	K	169/207 (82%)	164 (97%)	5 (3%)	0	100	100
1	L	169/207 (82%)	160 (95%)	8 (5%)	1 (1%)	30	68
All	All	2040/2484 (82%)	1941 (95%)	98 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	922	PRO

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	164/189 (87%)	140 (85%)	24 (15%)	4 16
1	B	163/189 (86%)	146 (90%)	17 (10%)	9 32
1	C	159/189 (84%)	143 (90%)	16 (10%)	9 34
1	D	163/189 (86%)	149 (91%)	14 (9%)	13 45
1	E	159/189 (84%)	141 (89%)	18 (11%)	7 29
1	F	164/189 (87%)	142 (87%)	22 (13%)	5 20
1	G	165/189 (87%)	145 (88%)	20 (12%)	6 24
1	H	163/189 (86%)	145 (89%)	18 (11%)	8 30
1	I	158/189 (84%)	138 (87%)	20 (13%)	5 22
1	J	159/189 (84%)	139 (87%)	20 (13%)	5 22
1	K	160/189 (85%)	134 (84%)	26 (16%)	3 12
1	L	160/189 (85%)	140 (88%)	20 (12%)	6 22
All	All	1937/2268 (85%)	1702 (88%)	235 (12%)	6 24

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1059	ASP
1	H	904	LYS
1	L	911	LEU
1	F	1064	GLN
1	G	974	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	983	GLN
1	H	1014	HIS
1	L	886	ASN
1	G	1014	HIS

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Mol	Chain	Res	Type
1	G	1046	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

Of 36 ligands modelled in this entry, 36 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

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	178/207 (85%)	-0.26	4 (2%)	65	42	106, 144, 198, 220	0
1	B	178/207 (85%)	-0.21	4 (2%)	65	42	110, 142, 200, 223	0
1	C	174/207 (84%)	-0.22	3 (1%)	73	51	105, 141, 189, 210	0
1	D	177/207 (85%)	-0.23	2 (1%)	82	65	108, 141, 196, 217	0
1	E	173/207 (83%)	-0.31	0	100	100	108, 143, 188, 217	0
1	F	179/207 (86%)	-0.20	5 (2%)	56	31	112, 144, 205, 239	0
1	G	180/207 (86%)	-0.26	2 (1%)	82	65	111, 145, 202, 235	0
1	H	178/207 (85%)	-0.19	4 (2%)	65	42	108, 145, 197, 237	0
1	I	173/207 (83%)	-0.26	2 (1%)	81	63	104, 144, 191, 211	0
1	J	174/207 (84%)	-0.20	2 (1%)	82	65	106, 142, 191, 219	0
1	K	175/207 (84%)	-0.22	3 (1%)	73	51	109, 142, 190, 213	0
1	L	175/207 (84%)	-0.22	3 (1%)	73	51	106, 143, 198, 233	0
All	All	2114/2484 (85%)	-0.23	34 (1%)	74	54	104, 143, 196, 239	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	939	VAL	6.0
1	A	939	VAL	4.7
1	H	940	GLU	4.5
1	F	1059	ASP	4.2
1	K	939	VAL	4.1

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

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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	J	2	1/1	0.97	0.17	0.28	154,154,154,154	0
2	ZN	A	2	1/1	0.92	0.14	0.24	148,148,148,148	0
2	ZN	K	2	1/1	0.95	0.17	0.21	147,147,147,147	0
2	ZN	B	2	1/1	0.96	0.21	-0.05	148,148,148,148	0
2	ZN	H	1	1/1	0.97	0.15	-0.10	151,151,151,151	0
2	ZN	G	2	1/1	0.92	0.15	-0.17	156,156,156,156	0
2	ZN	E	2	1/1	0.96	0.13	-0.38	146,146,146,146	0
2	ZN	C	2	1/1	0.97	0.15	-0.43	146,146,146,146	0
2	ZN	I	1	1/1	0.86	0.11	-0.49	149,149,149,149	0
2	ZN	J	1	1/1	0.96	0.14	-0.51	149,149,149,149	0
2	ZN	L	2	1/1	0.85	0.12	-0.64	155,155,155,155	0
2	ZN	H	2	1/1	0.99	0.12	-0.79	153,153,153,153	0
2	ZN	F	2	1/1	0.99	0.10	-0.80	144,144,144,144	0
2	ZN	D	2	1/1	0.98	0.12	-0.86	147,147,147,147	0
3	CA	F	3	1/1	0.89	0.23	-	142,142,142,142	0
2	ZN	I	2	1/1	0.98	0.17	-	149,149,149,149	0
2	ZN	E	1	1/1	0.88	0.15	-	149,149,149,149	0
3	CA	F	1088	1/1	0.95	0.25	-	135,135,135,135	0
2	ZN	G	1	1/1	0.98	0.11	-	154,154,154,154	0
2	ZN	F	1	1/1	0.94	0.15	-	150,150,150,150	0
3	CA	I	3	1/1	0.73	0.15	-	132,132,132,132	0
2	ZN	D	1	1/1	0.99	0.12	-	147,147,147,147	0
2	ZN	L	1	1/1	0.97	0.17	-	160,160,160,160	0
3	CA	C	3	1/1	0.98	0.30	-	134,134,134,134	0
2	ZN	B	1	1/1	0.97	0.14	-	156,156,156,156	0
2	ZN	A	1	1/1	0.92	0.11	-	149,149,149,149	0
3	CA	B	1088	1/1	0.92	0.26	-	127,127,127,127	0
2	ZN	C	1	1/1	0.98	0.15	-	151,151,151,151	0
3	CA	I	1088	1/1	0.97	0.26	-	142,142,142,142	0
3	CA	B	3	1/1	0.94	0.25	-	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	E	1088	1/1	0.99	0.22	-	129,129,129,129	0
3	CA	C	1088	1/1	0.99	0.18	-	135,135,135,135	0
3	CA	A	1088	1/1	0.91	0.31	-	133,133,133,133	0
3	CA	A	3	1/1	0.97	0.24	-	129,129,129,129	0
3	CA	E	3	1/1	0.97	0.18	-	138,138,138,138	0
2	ZN	K	1	1/1	0.95	0.11	-	148,148,148,148	0

6.5 Other polymers

There are no such residues in this entry.