



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2023 – 08:16 AM EDT

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

<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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

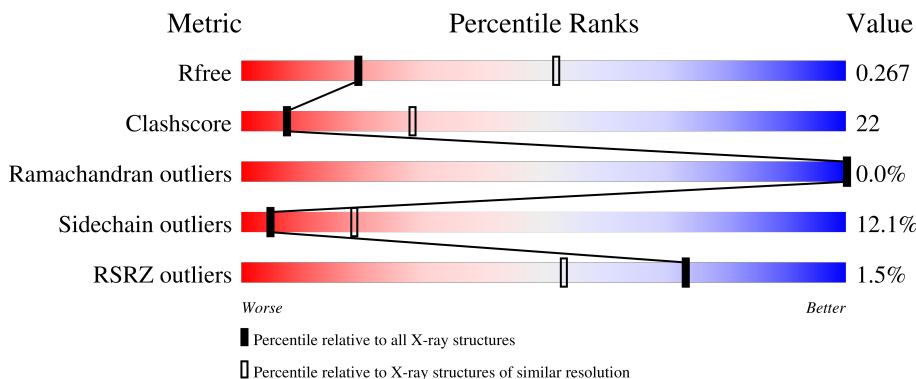
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (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 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	A	207	
1	B	207	
1	C	207	
1	D	207	
1	E	207	

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

2 Entry composition [i](#)

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

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	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	L	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	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0

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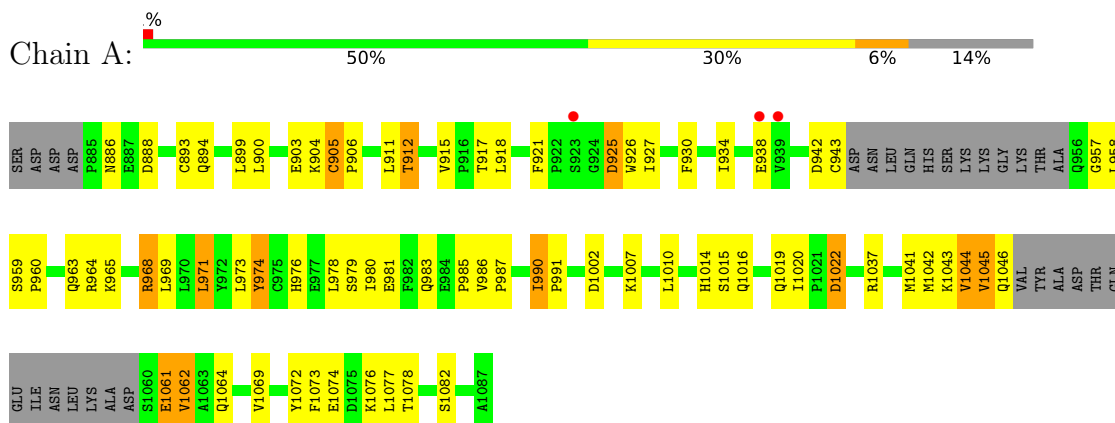
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total 2	Ca 2	0	0
3	E	2	Total 2	Ca 2	0	0
3	F	2	Total 2	Ca 2	0	0
3	I	2	Total 2	Ca 2	0	0

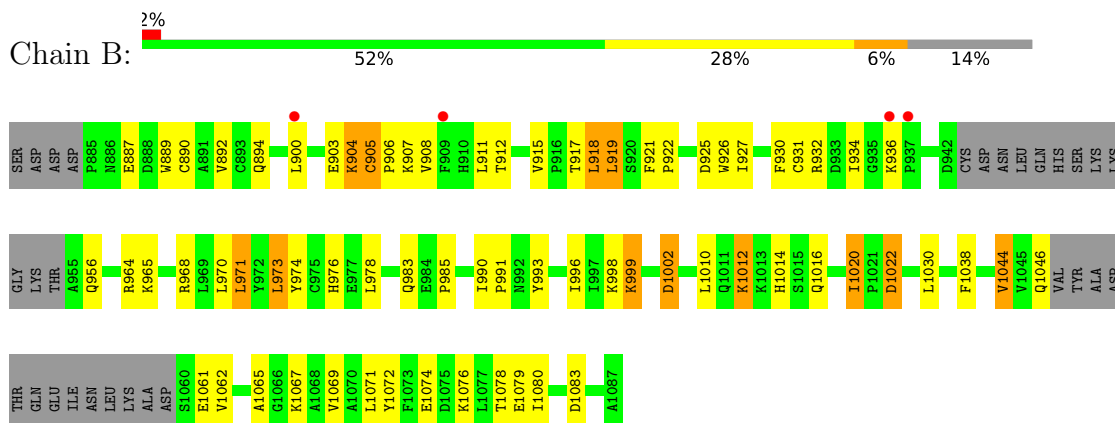
3 Residue-property plots [i](#)

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.

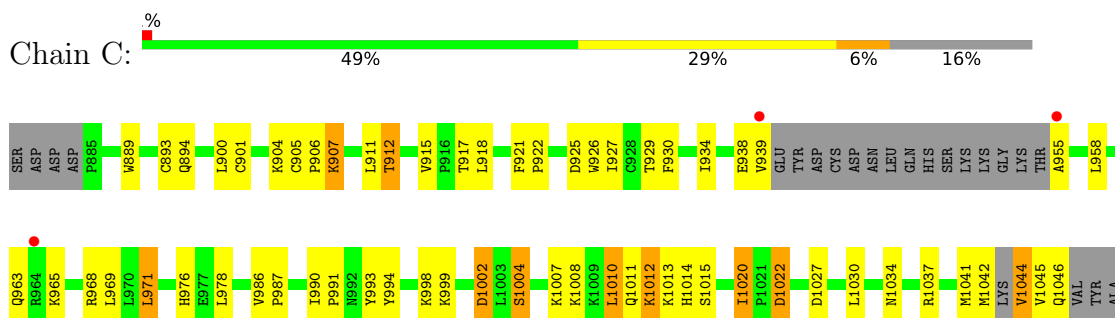
- Molecule 1: E3 ubiquitin-protein ligase TRIM33

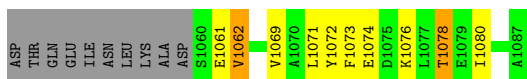


- Molecule 1: E3 ubiquitin-protein ligase TRIM33



- Molecule 1: E3 ubiquitin-protein ligase TRIM33

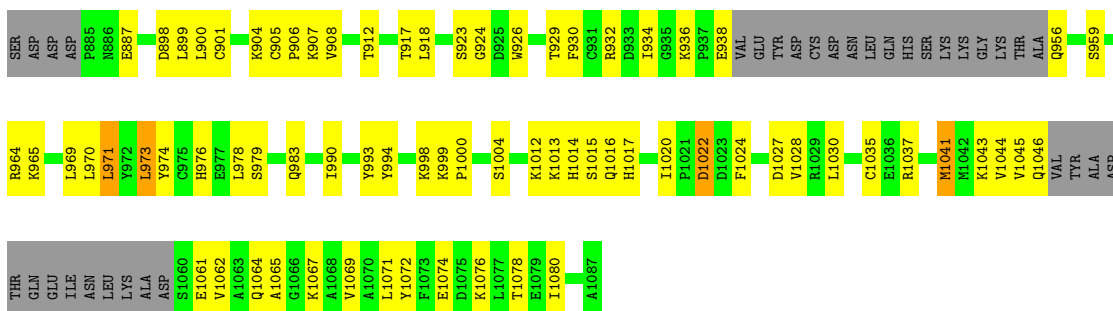




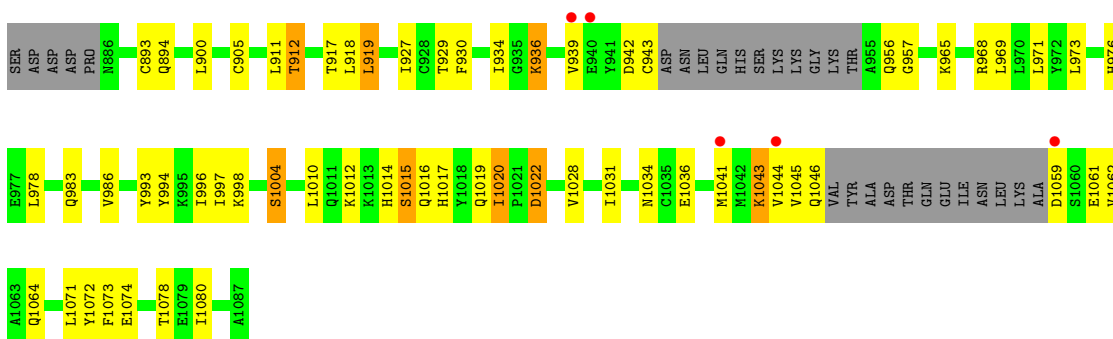
- Molecule 1: E3 ubiquitin-protein ligase TRIM33



- Molecule 1: E3 ubiquitin-protein ligase TRIM33

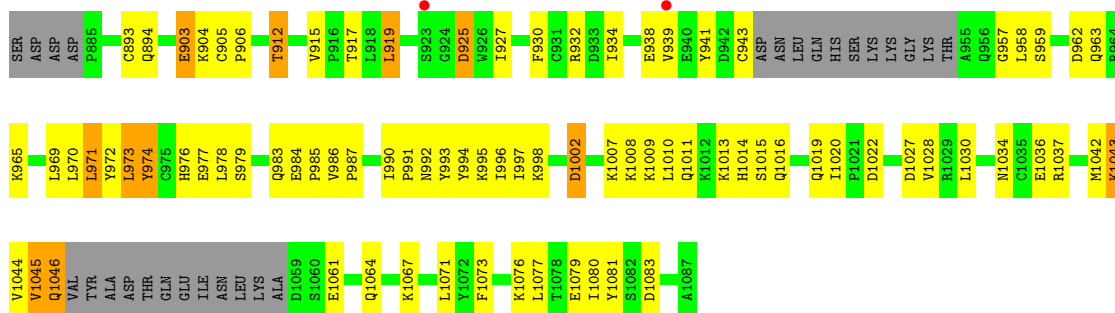


- Molecule 1: E3 ubiquitin-protein ligase TRIM33

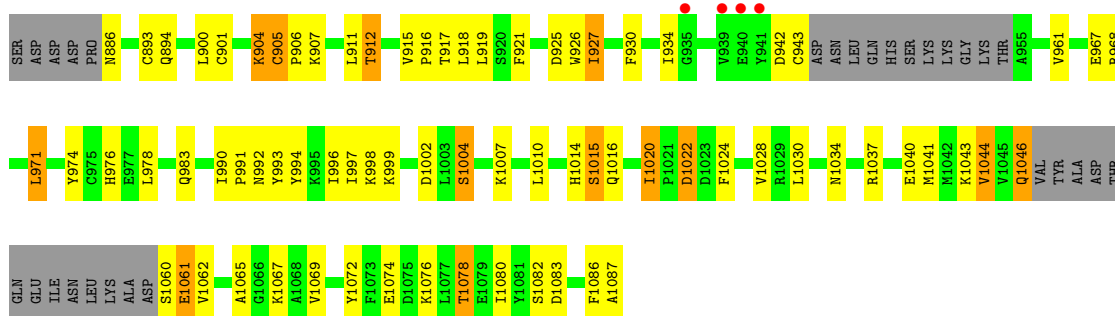


- Molecule 1: E3 ubiquitin-protein ligase TRIM33

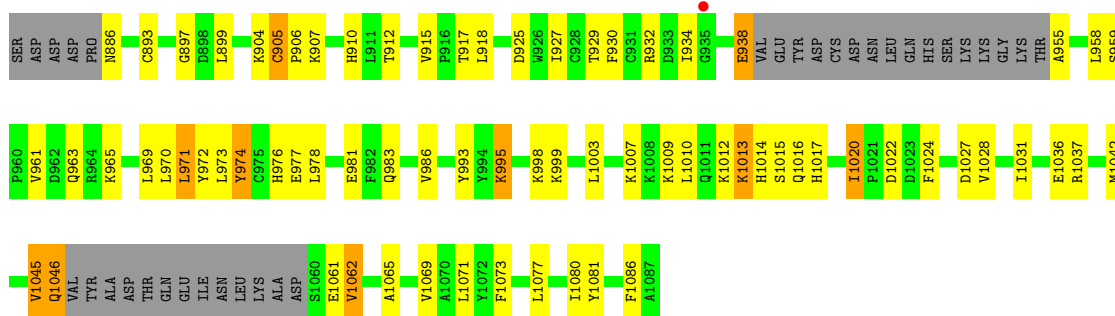




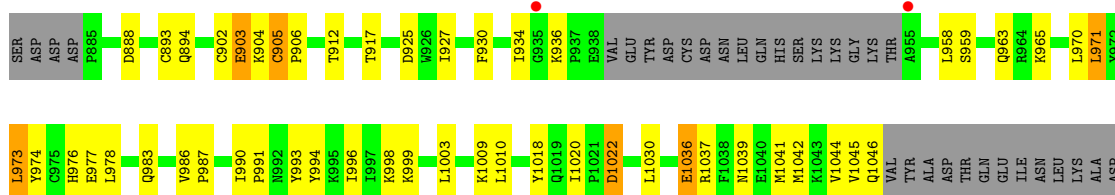
● Molecule 1: E3 ubiquitin-protein ligase TRIM33



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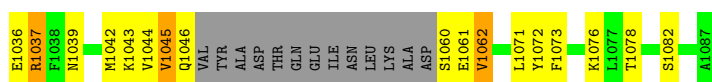


● Molecule 1: E3 ubiquitin-protein ligase TRIM33

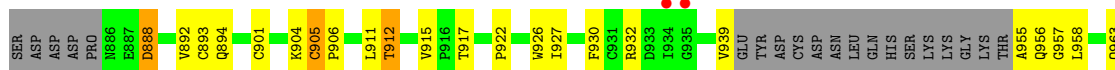




● Molecule 1: E3 ubiquitin-protein ligase TRIM33



● 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) 90.8 (27.36-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.207 , 0.293 0.192 , 0.267	Depositor DCC
R_{free} test set	1963 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	122.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
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 0.389 for h,h-k,-l 0.407 for -k,-h,-l 0.417 for -h,-k,l 0.429 for -h+k,k,-l 0.426 for h-k,-k,-l 0.400 for -h,-h+k,-l 0.387 for k,h,-l	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 3.74% 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: CA, 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	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 [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	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:HE2	1:G:998:LYS:HA	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%)	25	57
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%)	3	13
1	B	163/189 (86%)	146 (90%)	17 (10%)	7	25
1	C	159/189 (84%)	143 (90%)	16 (10%)	7	26
1	D	163/189 (86%)	149 (91%)	14 (9%)	10	36
1	E	159/189 (84%)	141 (89%)	18 (11%)	6	22
1	F	164/189 (87%)	142 (87%)	22 (13%)	4	15
1	G	165/189 (87%)	145 (88%)	20 (12%)	5	19
1	H	163/189 (86%)	145 (89%)	18 (11%)	6	23
1	I	158/189 (84%)	138 (87%)	20 (13%)	4	17
1	J	159/189 (84%)	139 (87%)	20 (13%)	4	17
1	K	160/189 (85%)	134 (84%)	26 (16%)	2	9
1	L	160/189 (85%)	140 (88%)	20 (12%)	4	17
All	All	1937/2268 (85%)	1702 (88%)	235 (12%)	5	19

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

Mol	Chain	Res	Type
1	G	959	SER
1	L	977	GLU
1	H	1022	ASP
1	L	969	LEU
1	K	971	LEU

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

Mol	Chain	Res	Type
1	K	976	HIS
1	K	983	GLN
1	L	1014	HIS
1	F	1014	HIS

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Mol	Chain	Res	Type
1	F	983	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	178/207 (85%)	-0.28	3 (1%) 70 48	106, 144, 198, 220	0
1	B	178/207 (85%)	-0.23	4 (2%) 62 39	110, 142, 200, 223	0
1	C	174/207 (84%)	-0.24	3 (1%) 70 48	105, 141, 189, 210	0
1	D	177/207 (85%)	-0.25	2 (1%) 80 62	108, 141, 196, 217	0
1	E	173/207 (83%)	-0.33	0 100 100	108, 143, 188, 217	0
1	F	179/207 (86%)	-0.22	5 (2%) 53 28	112, 144, 205, 239	0
1	G	180/207 (86%)	-0.28	2 (1%) 80 62	111, 145, 202, 235	0
1	H	178/207 (85%)	-0.21	4 (2%) 62 39	108, 145, 197, 237	0
1	I	173/207 (83%)	-0.28	1 (0%) 89 77	104, 144, 191, 211	0
1	J	174/207 (84%)	-0.22	2 (1%) 80 62	106, 142, 191, 219	0
1	K	175/207 (84%)	-0.24	3 (1%) 70 48	109, 142, 190, 213	0
1	L	175/207 (84%)	-0.24	3 (1%) 70 48	106, 142, 198, 233	0
All	All	2114/2484 (85%)	-0.25	32 (1%) 73 53	104, 143, 196, 239	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	939	VAL	5.9
1	A	939	VAL	4.6
1	H	940	GLU	4.4
1	F	1059	ASP	4.1
1	K	939	VAL	4.0

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](#)

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(\AA^2)	Q<0.9
3	CA	I	3	1/1	0.73	0.16	132,132,132,132	0
2	ZN	L	2	1/1	0.85	0.12	155,155,155,155	0
2	ZN	I	1	1/1	0.86	0.11	149,149,149,149	0
2	ZN	E	1	1/1	0.87	0.15	149,149,149,149	0
3	CA	F	3	1/1	0.89	0.23	142,142,142,142	0
3	CA	A	1088	1/1	0.91	0.31	133,133,133,133	0
2	ZN	G	2	1/1	0.92	0.15	156,156,156,156	0
3	CA	B	1088	1/1	0.92	0.26	127,127,127,127	0
2	ZN	A	2	1/1	0.92	0.14	148,148,148,148	0
2	ZN	A	1	1/1	0.92	0.11	149,149,149,149	0
3	CA	B	3	1/1	0.94	0.25	138,138,138,138	0
2	ZN	F	1	1/1	0.94	0.15	150,150,150,150	0
2	ZN	K	1	1/1	0.95	0.12	148,148,148,148	0
3	CA	F	1088	1/1	0.95	0.25	135,135,135,135	0
2	ZN	K	2	1/1	0.95	0.17	147,147,147,147	0
2	ZN	J	1	1/1	0.96	0.14	149,149,149,149	0
3	CA	A	3	1/1	0.96	0.25	129,129,129,129	0
2	ZN	E	2	1/1	0.96	0.13	146,146,146,146	0
2	ZN	B	2	1/1	0.96	0.21	148,148,148,148	0
2	ZN	J	2	1/1	0.97	0.17	154,154,154,154	0
3	CA	E	3	1/1	0.97	0.18	138,138,138,138	0
2	ZN	B	1	1/1	0.97	0.14	156,156,156,156	0
2	ZN	H	1	1/1	0.97	0.14	151,151,151,151	0
2	ZN	L	1	1/1	0.97	0.17	160,160,160,160	0
3	CA	I	1088	1/1	0.97	0.26	142,142,142,142	0
3	CA	C	3	1/1	0.98	0.30	134,134,134,134	0
2	ZN	G	1	1/1	0.98	0.11	154,154,154,154	0
2	ZN	C	1	1/1	0.98	0.15	151,151,151,151	0
2	ZN	C	2	1/1	0.98	0.15	146,146,146,146	0
2	ZN	D	2	1/1	0.98	0.12	147,147,147,147	0
2	ZN	I	2	1/1	0.98	0.17	149,149,149,149	0
3	CA	E	1088	1/1	0.99	0.23	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	H	2	1/1	0.99	0.12	153,153,153,153	0
2	ZN	F	2	1/1	0.99	0.10	144,144,144,144	0
3	CA	C	1088	1/1	0.99	0.18	135,135,135,135	0
2	ZN	D	1	1/1	0.99	0.12	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.