



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:23 am BST

PDB ID : 4A0C  
Title : Structure of the CAND1-CUL4B-RBX1 complex  
Authors : Scrima, A.; Fischer, E.S.; Faty, M.; Gut, H.; Thoma, N.H.  
Deposited on : 2011-09-08  
Resolution : 3.80 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](mailto: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.

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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	:	2.11
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)	:	2.11

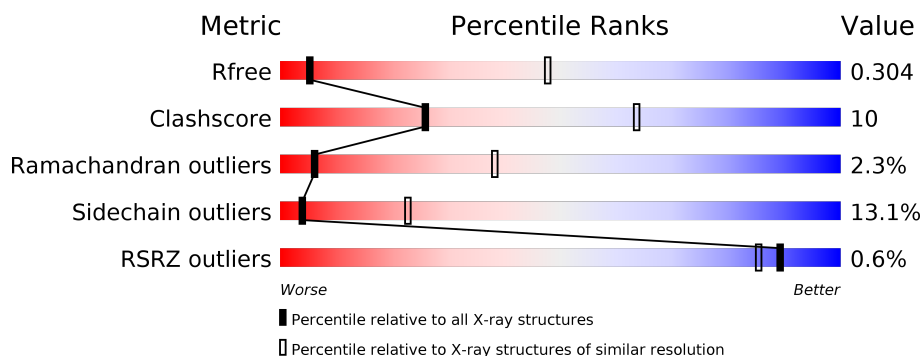
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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  $\geq 3$ , 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	1253	<div> <div>63%</div> <div>25%</div> <div>•</div> <div>8%</div> </div>
1	B	1253	<div> <div>63%</div> <div>24%</div> <div>•</div> <div>8%</div> </div>
2	C	741	<div>2%</div> <div> <div>62%</div> <div>26%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30804 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 CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1155	Total	C	N	O	S	0	0	0
			8963	5708	1517	1682	56			
1	B	1154	Total	C	N	O	S	0	0	0
			8975	5713	1519	1687	56			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q86VP6
A	-21	ALA	-	expression tag	UNP Q86VP6
A	-20	SER	-	expression tag	UNP Q86VP6
A	-19	TRP	-	expression tag	UNP Q86VP6
A	-18	SER	-	expression tag	UNP Q86VP6
A	-17	HIS	-	expression tag	UNP Q86VP6
A	-16	PRO	-	expression tag	UNP Q86VP6
A	-15	GLN	-	expression tag	UNP Q86VP6
A	-14	PHE	-	expression tag	UNP Q86VP6
A	-13	GLU	-	expression tag	UNP Q86VP6
A	-12	LYS	-	expression tag	UNP Q86VP6
A	-11	VAL	-	expression tag	UNP Q86VP6
A	-10	ASP	-	expression tag	UNP Q86VP6
A	-9	GLU	-	expression tag	UNP Q86VP6
A	-8	ASN	-	expression tag	UNP Q86VP6
A	-7	LEU	-	expression tag	UNP Q86VP6
A	-6	TYR	-	expression tag	UNP Q86VP6
A	-5	PHE	-	expression tag	UNP Q86VP6
A	-4	GLN	-	expression tag	UNP Q86VP6
A	-3	GLY	-	expression tag	UNP Q86VP6
A	-2	GLY	-	expression tag	UNP Q86VP6
A	-1	GLY	-	expression tag	UNP Q86VP6
A	0	ARG	-	expression tag	UNP Q86VP6
A	952	VAL	ALA	variant	UNP Q86VP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	expression tag	UNP Q86VP6
B	-21	ALA	-	expression tag	UNP Q86VP6
B	-20	SER	-	expression tag	UNP Q86VP6
B	-19	TRP	-	expression tag	UNP Q86VP6
B	-18	SER	-	expression tag	UNP Q86VP6
B	-17	HIS	-	expression tag	UNP Q86VP6
B	-16	PRO	-	expression tag	UNP Q86VP6
B	-15	GLN	-	expression tag	UNP Q86VP6
B	-14	PHE	-	expression tag	UNP Q86VP6
B	-13	GLU	-	expression tag	UNP Q86VP6
B	-12	LYS	-	expression tag	UNP Q86VP6
B	-11	VAL	-	expression tag	UNP Q86VP6
B	-10	ASP	-	expression tag	UNP Q86VP6
B	-9	GLU	-	expression tag	UNP Q86VP6
B	-8	ASN	-	expression tag	UNP Q86VP6
B	-7	LEU	-	expression tag	UNP Q86VP6
B	-6	TYR	-	expression tag	UNP Q86VP6
B	-5	PHE	-	expression tag	UNP Q86VP6
B	-4	GLN	-	expression tag	UNP Q86VP6
B	-3	GLY	-	expression tag	UNP Q86VP6
B	-2	GLY	-	expression tag	UNP Q86VP6
B	-1	GLY	-	expression tag	UNP Q86VP6
B	0	ARG	-	expression tag	UNP Q86VP6
B	952	VAL	ALA	variant	UNP Q86VP6

- Molecule 2 is a protein called CULLIN-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	692	Total	C	N	O	S	0	0	0
			5702	3636	973	1062	31			
2	E	696	Total	C	N	O	S	0	0	0
			5744	3663	978	1071	32			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	173	MET	-	expression tag	UNP Q13620
C	174	HIS	-	expression tag	UNP Q13620
C	175	HIS	-	expression tag	UNP Q13620
C	176	HIS	-	expression tag	UNP Q13620
C	177	HIS	-	expression tag	UNP Q13620
C	178	HIS	-	expression tag	UNP Q13620

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Chain	Residue	Modelled	Actual	Comment	Reference
C	179	HIS	-	expression tag	UNP Q13620
C	180	VAL	-	expression tag	UNP Q13620
C	181	ASP	-	expression tag	UNP Q13620
C	182	GLU	-	expression tag	UNP Q13620
C	183	ASN	-	expression tag	UNP Q13620
C	184	LEU	-	expression tag	UNP Q13620
C	185	TYR	-	expression tag	UNP Q13620
C	186	PHE	-	expression tag	UNP Q13620
C	187	GLN	-	expression tag	UNP Q13620
C	188	GLY	-	expression tag	UNP Q13620
C	189	GLY	-	expression tag	UNP Q13620
C	190	GLY	-	expression tag	UNP Q13620
C	191	ARG	-	expression tag	UNP Q13620
E	173	MET	-	expression tag	UNP Q13620
E	174	HIS	-	expression tag	UNP Q13620
E	175	HIS	-	expression tag	UNP Q13620
E	176	HIS	-	expression tag	UNP Q13620
E	177	HIS	-	expression tag	UNP Q13620
E	178	HIS	-	expression tag	UNP Q13620
E	179	HIS	-	expression tag	UNP Q13620
E	180	VAL	-	expression tag	UNP Q13620
E	181	ASP	-	expression tag	UNP Q13620
E	182	GLU	-	expression tag	UNP Q13620
E	183	ASN	-	expression tag	UNP Q13620
E	184	LEU	-	expression tag	UNP Q13620
E	185	TYR	-	expression tag	UNP Q13620
E	186	PHE	-	expression tag	UNP Q13620
E	187	GLN	-	expression tag	UNP Q13620
E	188	GLY	-	expression tag	UNP Q13620
E	189	GLY	-	expression tag	UNP Q13620
E	190	GLY	-	expression tag	UNP Q13620
E	191	ARG	-	expression tag	UNP Q13620

- Molecule 3 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total	C	N	O	S	0	0	0
			737	466	135	127	9			
3	F	80	Total	C	N	O	S	0	0	0
			677	434	125	109	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	11	MET	-	expression tag	UNP P62878
F	11	MET	-	expression tag	UNP P62878

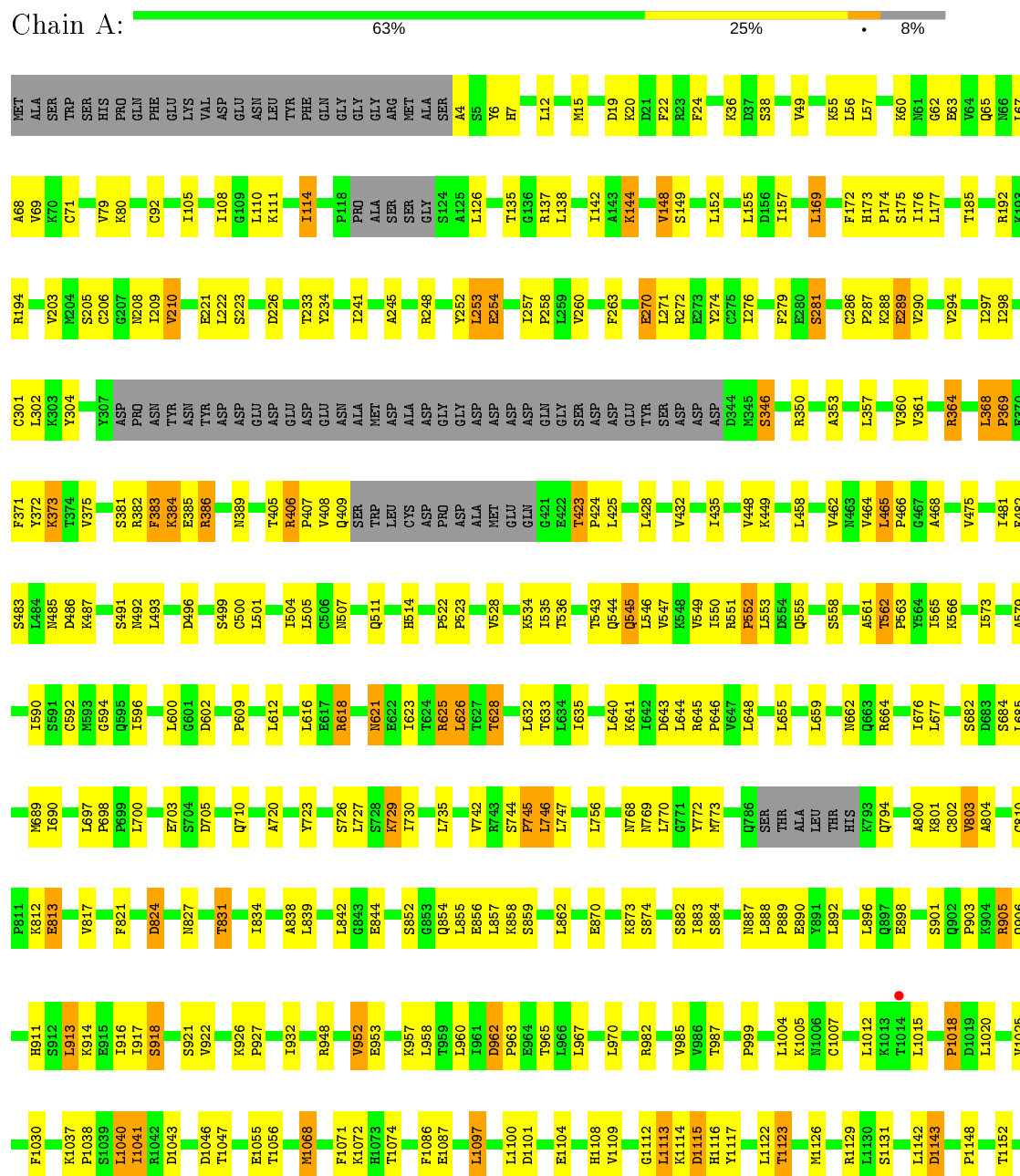
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

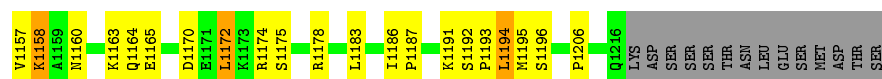
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Zn 3	0	0
4	F	3	Total 3	Zn 3	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

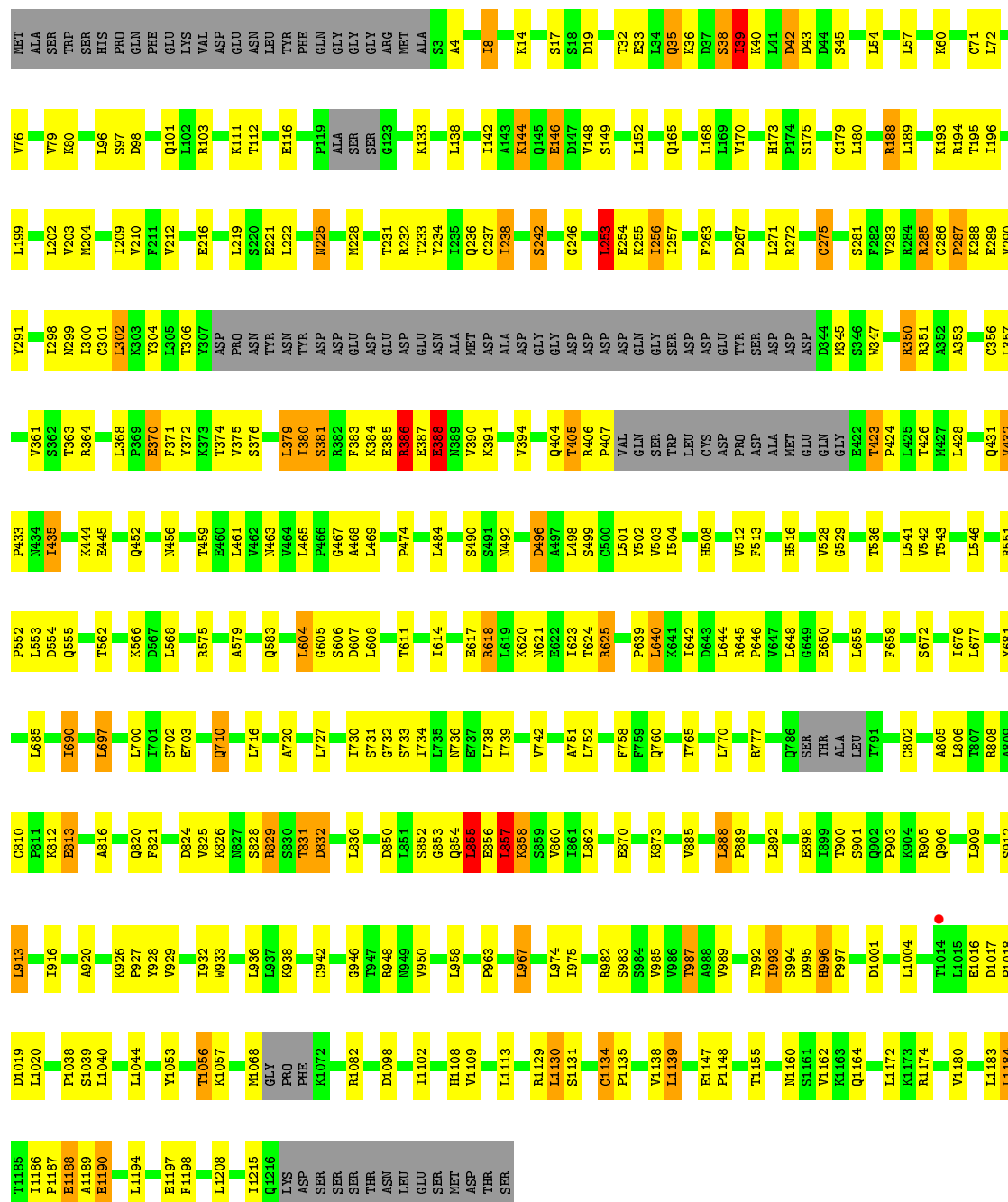
#### • Molecule 1: CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1





• Molecule 1: CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1

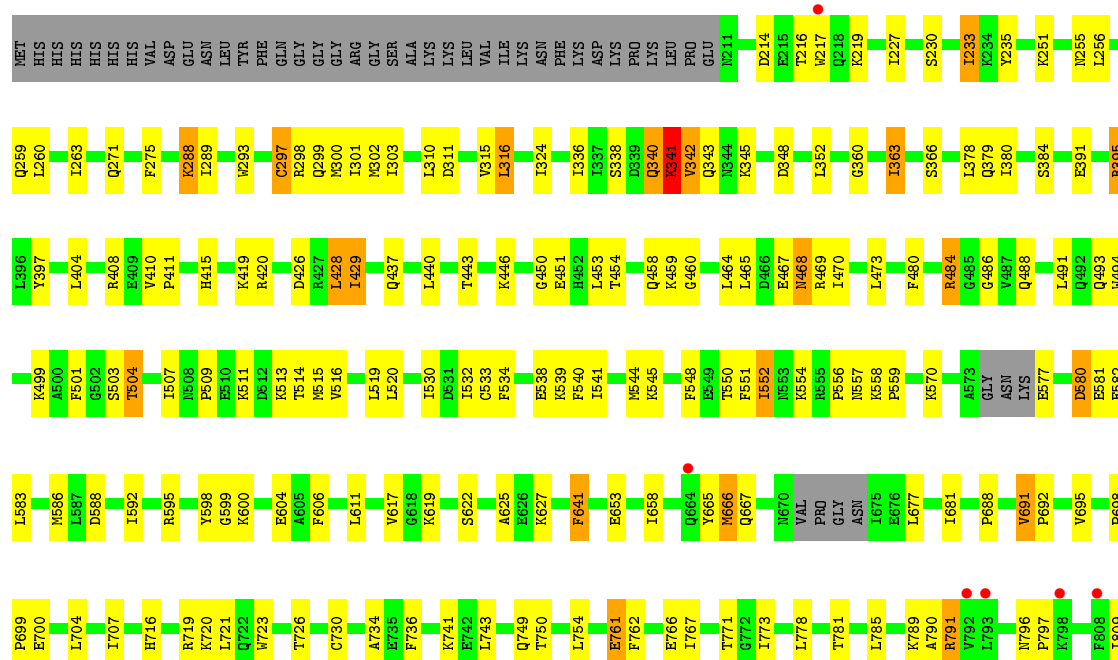
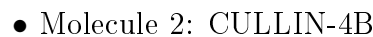
Chain B: 63% 24% 8%

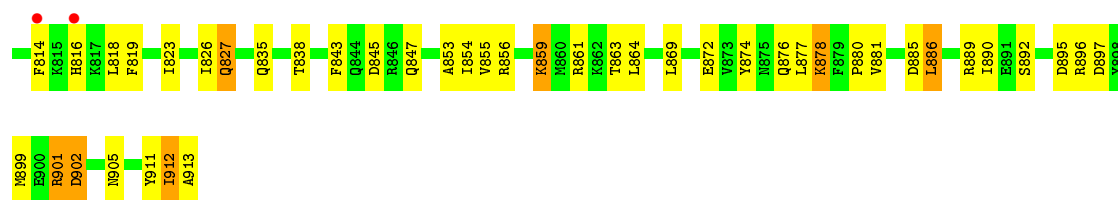


• Molecule 2: CULLIN-4B

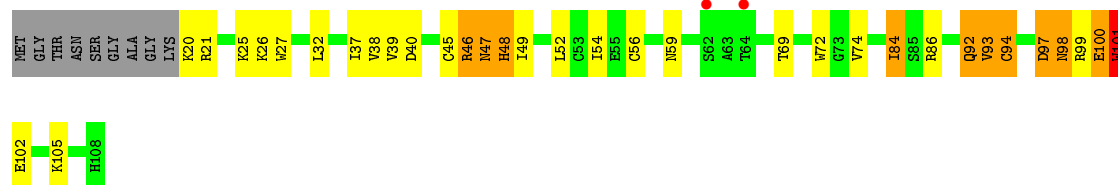
Chain C: 2% 62% 26% 5% 7%



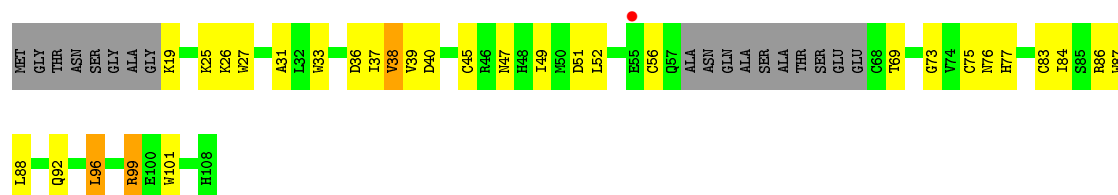




• Molecule 3: E3 UBIQUITIN-PROTEIN LIGASE RBX1



• Molecule 3: E3 UBIQUITIN-PROTEIN LIGASE RBX1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.09 Å 152.36 Å 263.01 Å 90.00° 89.37° 90.00°	Depositor
Resolution (Å)	47.76 – 3.80 47.76 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.76-3.80) 99.7 (47.76-3.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 3.77 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.238 , 0.319 0.230 , 0.304	Depositor DCC
$R_{free}$ test set	2990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.37	0/9101	0.56	0/12327
1	B	0.38	0/9113	0.58	2/12340 (0.0%)
2	C	0.39	0/5794	0.57	1/7776 (0.0%)
2	E	0.38	0/5836	0.55	0/7832
3	D	0.40	0/759	0.52	0/1029
3	F	0.37	0/698	0.50	0/943
All	All	0.38	0/31301	0.56	3/42247 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	280	LEU	CA-CB-CG	5.98	129.06	115.30
1	B	857	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	253	LEU	CA-CB-CG	5.59	128.16	115.30

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	8963	0	9308	208	0
1	B	8975	0	9328	192	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5702	0	5801	137	0
2	E	5744	0	5841	110	0
3	D	737	0	687	17	0
3	F	677	0	642	13	0
4	D	3	0	0	0	0
4	F	3	0	0	1	0
All	All	30804	0	31607	653	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 10.

The worst 5 of 653 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:A:982:ARG:HH21	1:A:1018:PRO:HB3	1.25	1.00
1:A:423:THR:HG22	1:A:424:PRO:HD2	1.45	0.99
1:B:386:ARG:HG3	1:B:387:GLU:H	1.35	0.90
3:D:72:TRP:HB2	3:D:105:LYS:HB3	1.52	0.89
1:A:862:LEU:HB3	1:A:905:ARG:HH21	1.40	0.86

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	1145/1253 (91%)	1001 (87%)	122 (11%)	22 (2%)	8	42
1	B	1142/1253 (91%)	991 (87%)	129 (11%)	22 (2%)	8	42
2	C	686/741 (93%)	589 (86%)	83 (12%)	14 (2%)	7	41
2	E	690/741 (93%)	611 (89%)	63 (9%)	16 (2%)	6	38
3	D	87/98 (89%)	62 (71%)	16 (18%)	9 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	76/98 (78%)	48 (63%)	23 (30%)	5 (7%)	1	19
All	All	3826/4184 (91%)	3302 (86%)	436 (11%)	88 (2%)	6	38

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	226	ASP
1	A	290	VAL
1	A	386	ARG
1	A	552	PRO

### 5.3.2 Protein sidechains ⓘ

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	1028/1118 (92%)	904 (88%)	124 (12%)	5	25
1	B	1033/1118 (92%)	893 (86%)	140 (14%)	3	22
2	C	632/675 (94%)	548 (87%)	84 (13%)	4	22
2	E	637/675 (94%)	556 (87%)	81 (13%)	4	23
3	D	78/83 (94%)	62 (80%)	16 (20%)	1	8
3	F	72/83 (87%)	60 (83%)	12 (17%)	2	15
All	All	3480/3752 (93%)	3023 (87%)	457 (13%)	4	23

5 of 457 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	672	SER
1	B	1172	LEU
2	E	666	MET
1	B	738	LEU
1	B	892	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	760	GLN
2	C	340	GLN
2	E	827	GLN
1	B	820	GLN
1	B	1108	HIS

### 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 6 ligands modelled in this entry, 6 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1155/1253 (92%)	-0.31	1 (0%) 95 95	103, 127, 153, 165	0
1	B	1154/1253 (92%)	-0.31	1 (0%) 95 95	90, 115, 159, 179	0
2	C	692/741 (93%)	-0.07	12 (1%) 70 62	86, 129, 188, 201	0
2	E	696/741 (93%)	-0.10	8 (1%) 80 74	98, 141, 173, 177	0
3	D	89/98 (90%)	-0.08	2 (2%) 62 54	111, 132, 148, 149	0
3	F	80/98 (81%)	-0.15	1 (1%) 77 70	141, 155, 168, 170	0
All	All	3866/4184 (92%)	-0.22	25 (0%) 89 85	86, 125, 170, 201	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	795	LYS	3.7
2	C	794	ALA	3.5
2	C	792	VAL	3.2
2	C	221	LYS	2.9
2	C	809	ILE	2.9

### 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

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
4	ZN	F	4003	1/1	0.95	0.04	144,144,144,144	0
4	ZN	F	4001	1/1	0.97	0.10	113,113,113,113	0
4	ZN	F	4002	1/1	0.98	0.06	120,120,120,120	0
4	ZN	D	4001	1/1	0.99	0.09	104,104,104,104	0
4	ZN	D	4003	1/1	0.99	0.11	104,104,104,104	0
4	ZN	D	4002	1/1	1.00	0.12	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.