



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:03 PM UTC

PDB ID : 1U6G / pdb_00001u6g
Title : Crystal Structure of The Cand1-Cul1-Roc1 Complex
Authors : Goldenberg, S.J.; Shumway, S.D.; Cascio, T.C.; Garbutt, K.C.; Liu, J.; Xiong, Y.; Zheng, N.
Deposited on : 2004-07-29
Resolution : 3.10 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	:	4-5-2 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

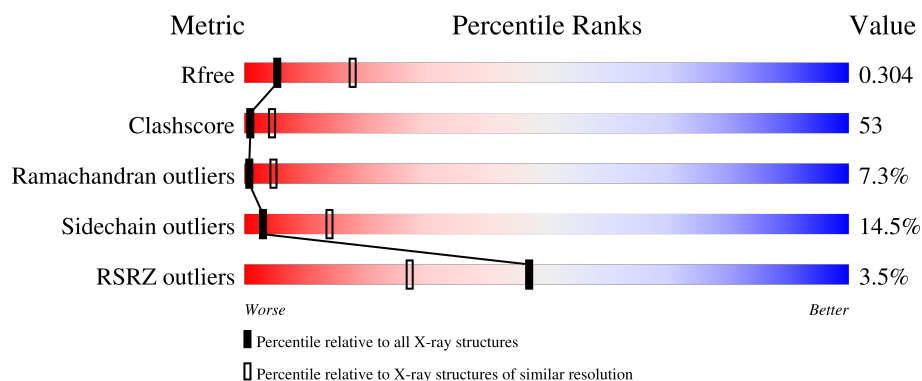
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	776	4% 35% 41% 14% • 8%
2	B	108	25% 40% 15% • 19%
3	C	1230	3% 26% 49% 16% • 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15511 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 homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5855	3719	998	1109	29			

- Molecule 2 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			731	464	133	125	9			

- Molecule 3 is a protein called TIP120 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1146	Total	C	N	O	S	0	0	0
			8904	5667	1509	1672	56			

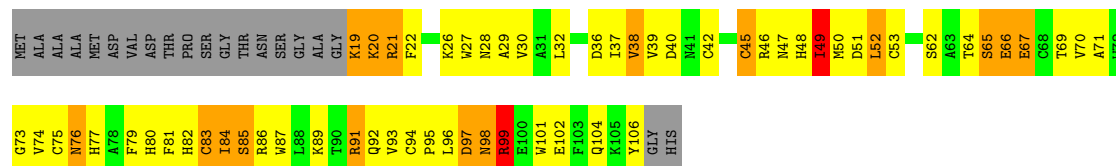
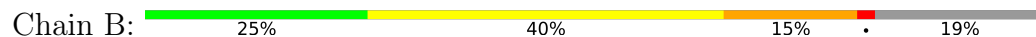
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Zn	0	0
			3	3		

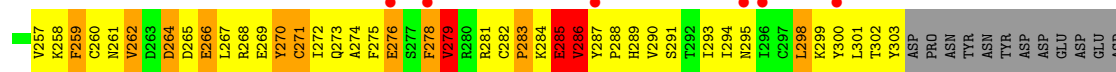
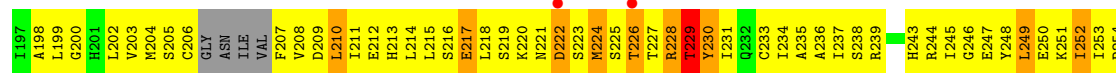
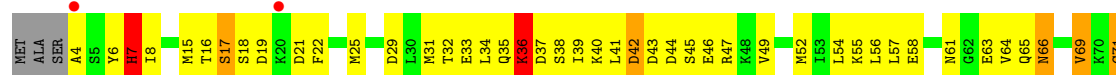
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	3	Total	O	0	0
			3	3		
5	C	5	Total	O	0	0
			5	5		

- Molecule 2: RING-box protein 1



- Molecule 3: TIP120 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.47Å 151.33Å 215.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 94.5 (50.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.317 0.236 , 0.304	Depositor DCC
R_{free} test set	3108 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15511	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.65	4/5949 (0.1%)	1.49	71/8007 (0.9%)
2	B	0.68	1/752 (0.1%)	1.27	9/1020 (0.9%)
3	C	0.59	5/9041 (0.1%)	1.25	113/12243 (0.9%)
All	All	0.62	10/15742 (0.1%)	1.35	193/21270 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	2
All	All	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	ASP	C-N	14.71	1.52	1.33
1	A	437	GLU	C-N	-14.37	1.13	1.33
3	C	601	GLY	C-N	-10.52	1.19	1.34
1	A	630	ILE	CG1-CD1	8.57	1.85	1.51
3	C	490	SER	N-CA	-8.11	1.36	1.46

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	GLU	O-C-N	-72.55	6.91	123.00
1	A	476	GLN	N-CA-C	18.73	137.54	109.07
1	A	142	ARG	N-CA-C	14.29	128.83	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	ARG	N-CA-C	-14.03	88.06	109.24
3	C	487	LYS	CB-CA-C	12.51	135.31	110.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLU	Mainchain
3	C	599	ASN	Mainchain
3	C	601	GLY	Mainchain

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	5855	0	5900	541	0
2	B	731	0	689	81	0
3	C	8904	0	9249	1098	0
4	B	3	0	0	0	0
5	A	10	0	0	0	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
All	All	15511	0	15838	1668	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 53.

The worst 5 of 1668 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)
3:C:373:LYS:CE	3:C:427:MET:HE3	1.25	1.60
3:C:373:LYS:HE3	3:C:427:MET:CE	1.36	1.54
3:C:373:LYS:CG	3:C:427:MET:HE1	1.36	1.52
1:A:630:ILE:CG1	1:A:630:ILE:CD1	1.85	1.51
3:C:373:LYS:CE	3:C:427:MET:CE	1.84	1.48

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	705/776 (91%)	584 (83%)	91 (13%)	30 (4%)	2	12
2	B	86/108 (80%)	68 (79%)	13 (15%)	5 (6%)	1	8
3	C	1134/1230 (92%)	793 (70%)	236 (21%)	105 (9%)	0	3
All	All	1925/2114 (91%)	1445 (75%)	340 (18%)	140 (7%)	1	5

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TRP
1	A	145	VAL
1	A	646	LYS
1	A	652	ASP
1	A	674	TYR

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	650/698 (93%)	561 (86%)	89 (14%)	3	15
2	B	78/90 (87%)	62 (80%)	16 (20%)	1	5
3	C	1022/1098 (93%)	874 (86%)	148 (14%)	3	14
All	All	1750/1886 (93%)	1497 (86%)	253 (14%)	3	14

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	116	GLU
3	C	1006	ASN
3	C	364	ARG
3	C	1004	LEU
3	C	1111	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	472	HIS
3	C	736	ASN
3	C	511	GLN
3	C	599	ASN
3	C	902	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	601:GLY	C	602:ASP	N	1.19
1	A	437:GLU	C	438:GLU	N	1.13

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	715/776 (92%)	-0.04	30 (4%) 40 22	13, 46, 129, 197	0
2	B	88/108 (81%)	-0.25	0 100 100	3, 38, 76, 151	0
3	C	1146/1230 (93%)	0.07	39 (3%) 48 28	14, 61, 122, 190	0
All	All	1949/2114 (92%)	0.01	69 (3%) 47 27	3, 55, 124, 197	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	SER	5.7
1	A	176	ASN	5.2
3	C	278	PHE	5.1
1	A	477	ASN	5.0
3	C	490	SER	4.9

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
4	ZN	B	1230	1/1	0.97	0.05	56,56,56,56	0
4	ZN	B	1229	1/1	0.99	0.03	42,42,42,42	0
4	ZN	B	1231	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.