



wwPDB X-ray Structure Validation Summary Report

Feb 15, 2017 – 03:01 am GMT

PDB ID : 1U6G
Title : Crystal Structure of The Cand1-Cull1-Roc1 Complex
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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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

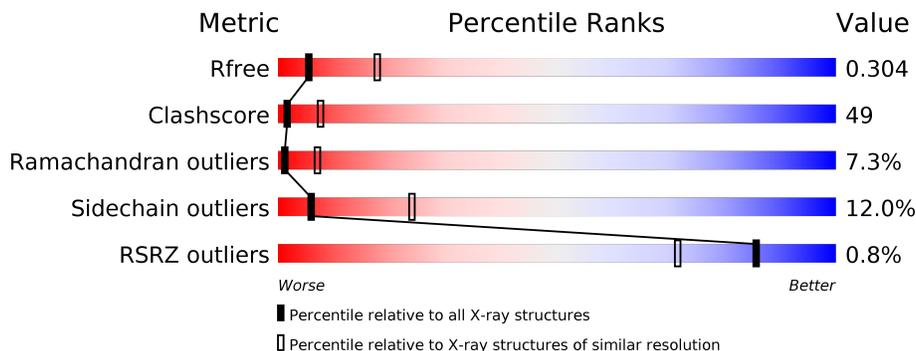
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 $\leq 5\%$. 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	 0% 41% 40% 10% • 8%
2	B	108	 2% 31% 38% 11% • 19%
3	C	1230	 0% 30% 50% 11% • 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
			Total	C	N	O	S			
1	A	715	5855	3719	998	1109	29	0	0	0

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

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

- Molecule 3 is a protein called TIP120 protein.

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

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

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

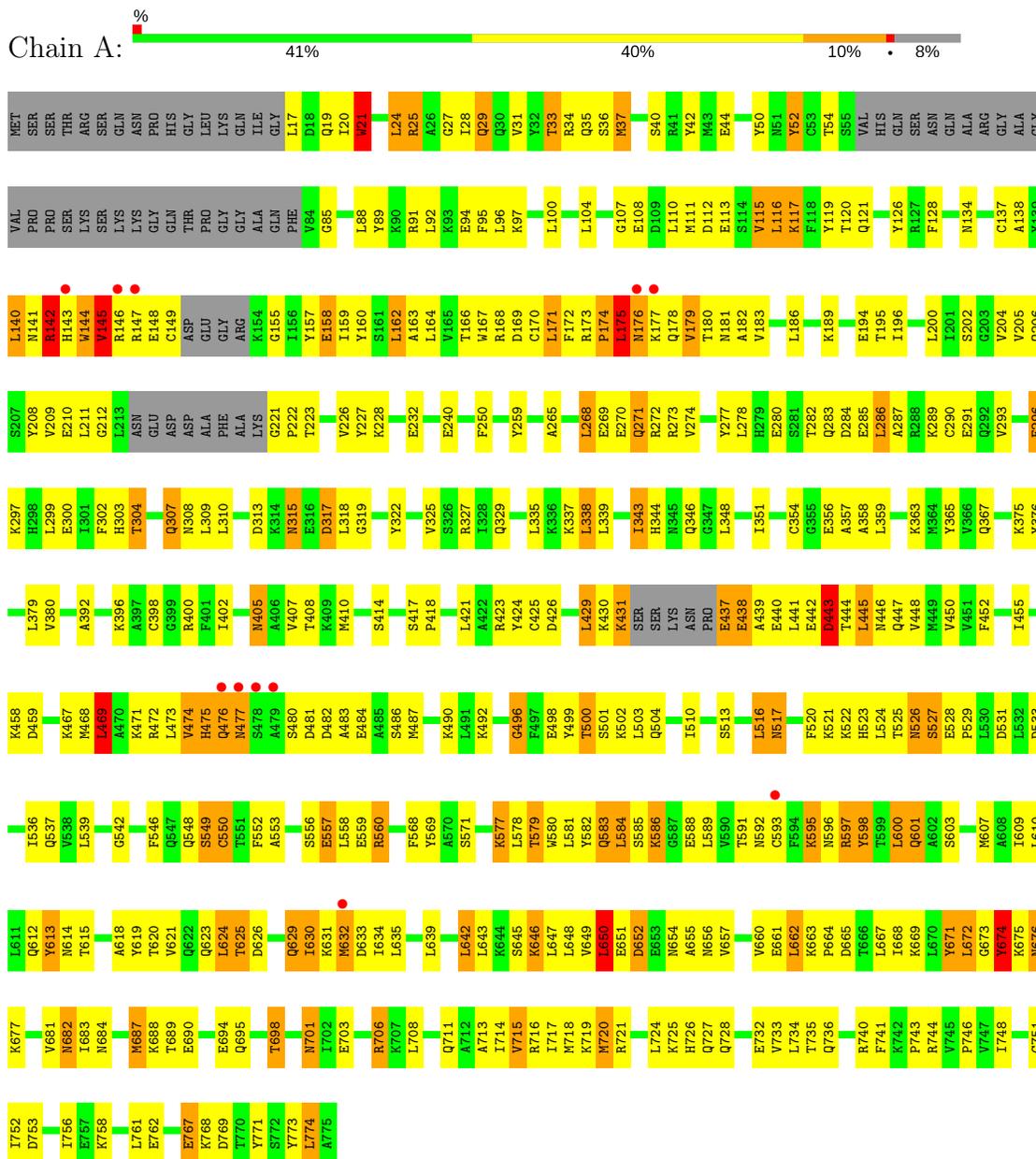
- Molecule 5 is water.

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		

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 homolog 1



- Molecule 2: RING-box protein 1

GLU	Q1164	D1098	D1019	C954	I883
SER	E1165	R1099	L1020	L958	S884
MET	F1166	L1100	M1021	T959	N887
ASP	E1167	D1101	V1022	T959	L888
THR	K1168	F1102	R1023	L961	P889
SER	Q1169	F1103	R1024	D962	F890
	D1170	E1104	V1026	P963	L891
	E1171	M1107	A1027	E964	L892
	R1174	H1108	V1028	P965	F893
	S1175	V1109	T1029	L966	F894
	A1176	E1110	F1030	L967	V895
	M1177	D1111	M1031	P968	L896
	R1178	G1112	S1032	R969	G897
	A1179	L1113	A1033	L970	E898
	V1180	Y1117	A1034	K971	L899
	A1181	H1035	H1036	G972	T900
	A1182	K1120	N1037	L973	S901
	L1183	M1121	K1037	L974	Q902
	L1184	L1122	P1038	L975	P903
	T1185	T1123	S1039	S976	R904
	I1186	M1126	L1040	G977	R905
	P1187	L1127	I1041	S978	Q906
	E1188	V1128	L1044	S979	L913
	A1189	R1129	T1047	Y980	K914
	E1190	L1130	V1048	A981	E915
	K1191	S1131	L1049	R982	L916
	S1192	P1132	P1050	V985	L917
	L1194	L1133	H1051	V986	S918
	M1195	C1134	L1052	T987	S919
	S1196	P1135	Y1053	R988	A920
	E1197	V1138	M1054	V989	S921
	F1198	L1139	E1055	K990	V922
	Q1199	Q1140	T1056	F991	V923
	S1200	R1141	R1064	T992	G924
	I1202	L1142	E1065	T993	L925
	S1203	D1143	V1066	S994	K926
	N1205	R1144	E1067	D995	P927
	P1206	L1145	M1068	H996	Y928
	E1207	V1146	H1073	P999	I932
	L1208	E1147	L1079	I1000	A933
	A1209	P1148	D1080	D1001	A934
	A1210	L1149	I1081	P1002	L935
	ILE	R1150	R1082	L1003	L936
	PHE	A1151	K1083	K1005	L937
	GLU	T1152	C1088	I1008	E941
	SER	C1153	M1089	G1009	C942
	ILE	T1154	Y1090	G1009	A943
	GLN	T1155	C1088	I1010	E944
	LYS	K1156	M1089	F1011	E945
	ASP	V1157	Y1090	L1012	G946
	SER	K1158	L1093	K1013	T947
	SER	A1159	D1094	T1014	R948
	SER	M1160	S1095	L1015	V951
	THR	S1161	C1096	D1017	A952
	ASN	V1162	L1097	P1018	E953
	LEU	K1163			

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 49.68 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 73.1 (49.68-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.48Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.317 0.236 , 0.304	Depositor DCC
R_{free} test set	3108 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	56.5	Xtrriage
Anisotropy	0.413	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.49	3/5949 (0.1%)	1.14	14/8007 (0.2%)
2	B	0.51	0/752	0.86	1/1020 (0.1%)
3	C	0.45	1/9041 (0.0%)	0.86	31/12243 (0.3%)
All	All	0.47	4/15742 (0.0%)	0.97	46/21270 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	GLU	C-N	-8.90	1.13	1.34
1	A	443	ASP	C-N	7.93	1.52	1.34
3	C	601	GLY	C-N	-6.35	1.19	1.34
1	A	630	ILE	CG1-CD1	5.03	1.85	1.50

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	GLU	O-C-N	-72.37	6.91	122.70
3	C	117	LEU	C-N-CD	-20.01	76.58	120.60
3	C	117	LEU	C-N-CA	13.74	179.69	122.00
3	C	487	LYS	CB-CA-C	12.45	135.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	PRO	CA-N-CD	-10.61	96.64	111.50

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 [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	5855	0	5900	502	0
2	B	731	0	689	76	0
3	C	8904	0	9248	998	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	15837	1525	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 49.

The worst 5 of 1525 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:HE1	1.31	1.56
3:C:373:LYS:HE3	3:C:427:MET:CE	1.36	1.54
1:A:630:ILE:CD1	1:A:630:ILE:CG1	1.85	1.51
3:C:373:LYS:CE	3:C:427:MET:CE	1.84	1.48
3:C:373:LYS:CD	3:C:427:MET:HE1	1.53	1.37

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

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%)	575 (88%)	75 (12%)	6	27
2	B	78/90 (87%)	65 (83%)	13 (17%)	2	11
3	C	1022/1098 (93%)	900 (88%)	122 (12%)	6	25
All	All	1750/1886 (93%)	1540 (88%)	210 (12%)	6	24

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	96	LEU
3	C	298	LEU
3	C	1102	ILE
3	C	144	LYS
3	C	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	676	ASN
3	C	66	ASN
3	C	1036	ASN
1	A	682	ASN
1	A	736	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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](#)

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	715/776 (92%)	-0.57	11 (1%) 74 54	13, 46, 129, 197	0
2	B	88/108 (81%)	-0.62	2 (2%) 61 39	3, 38, 76, 151	0
3	C	1146/1230 (93%)	-0.68	2 (0%) 94 89	14, 61, 122, 190	0
All	All	1949/2114 (92%)	-0.64	15 (0%) 86 71	3, 55, 124, 197	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	SER	16.0
1	A	477	ASN	10.7
1	A	479	ALA	4.6
1	A	176	ASN	4.1
2	B	20	LYS	3.7

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 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, 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	LLDF	B-factors(\AA^2)	Q < 0.9
4	ZN	B	1230	1/1	0.93	0.14	-0.61	56,56,56,56	0
4	ZN	B	1229	1/1	0.95	0.12	-1.25	42,42,42,42	0
4	ZN	B	1231	1/1	0.97	0.10	-2.00	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.