



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 11:55 pm BST

PDB ID : 3VGO
Title : Crystal structure of the N-terminal fragment of Cbl-b
Authors : Kobashigawa, Y.; Noda, N.N.; Inagaki, F.
Deposited on : 2011-08-18
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 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

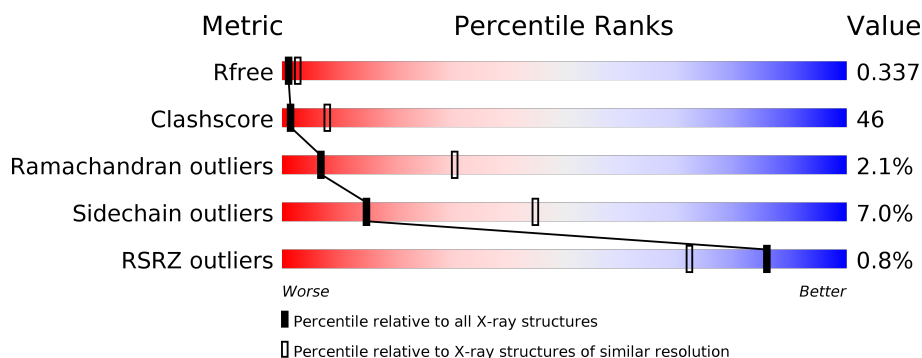
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 on 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	394	<div> <div>27%</div> <div>40%</div> <div>6%</div> <div>27%</div> </div>
1	B	394	<div> <div>27%</div> <div>45%</div> <div>•</div> <div>25%</div> </div>
1	C	394	<div> <div>2%</div> <div>31%</div> <div>39%</div> <div>•</div> <div>26%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6668 atoms, of which 0 are hydrogens and 0 are deuteriums.

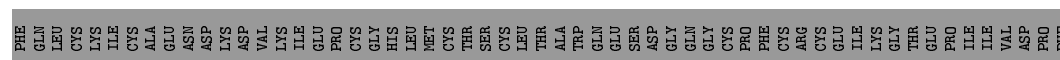
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase CBL-B.

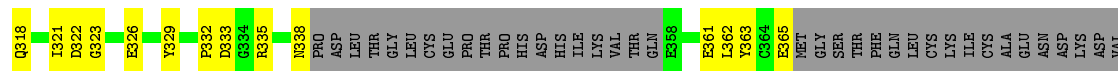
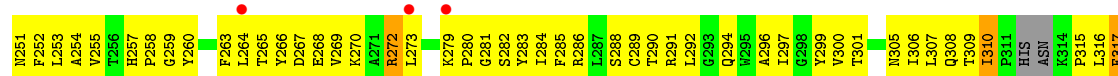
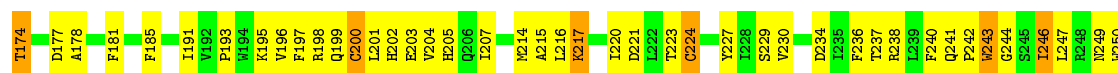
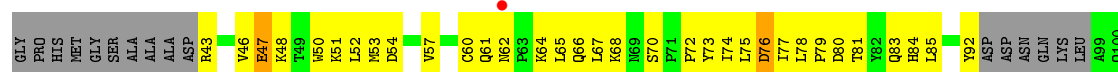
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2196	1430	371	385	10			
1	B	294	Total	C	N	O	S	0	0	0
			2252	1465	384	393	10			
1	C	292	Total	C	N	O	S	0	0	0
			2220	1450	370	391	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	EXPRESSION TAG	UNP Q13191
A	34	PRO	-	EXPRESSION TAG	UNP Q13191
A	35	HIS	-	EXPRESSION TAG	UNP Q13191
A	36	MET	-	EXPRESSION TAG	UNP Q13191
A	37	GLY	-	EXPRESSION TAG	UNP Q13191
A	38	SER	-	EXPRESSION TAG	UNP Q13191
B	33	GLY	-	EXPRESSION TAG	UNP Q13191
B	34	PRO	-	EXPRESSION TAG	UNP Q13191
B	35	HIS	-	EXPRESSION TAG	UNP Q13191
B	36	MET	-	EXPRESSION TAG	UNP Q13191
B	37	GLY	-	EXPRESSION TAG	UNP Q13191
B	38	SER	-	EXPRESSION TAG	UNP Q13191
C	33	GLY	-	EXPRESSION TAG	UNP Q13191
C	34	PRO	-	EXPRESSION TAG	UNP Q13191
C	35	HIS	-	EXPRESSION TAG	UNP Q13191
C	36	MET	-	EXPRESSION TAG	UNP Q13191
C	37	GLY	-	EXPRESSION TAG	UNP Q13191
C	38	SER	-	EXPRESSION TAG	UNP Q13191



• Molecule 1: E3 ubiquitin-protein ligase CBL-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	98.88Å 98.88Å 105.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.82 – 3.10 44.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.82-3.10) 96.4 (44.81-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.270 , 0.328 0.272 , 0.337	Depositor DCC
R_{free} test set	1909 reflections (8.28%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.074 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for h+k,-k,-l	Depositor
Outliers	0 of 23046 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6668	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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	0.69	0/2253	0.88	2/3063 (0.1%)
1	B	0.68	0/2308	0.84	0/3133
1	C	0.61	0/2275	0.80	0/3091
All	All	0.66	0/6836	0.84	2/9287 (0.0%)

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	SER	N-CA-C	-7.75	90.07	111.00
1	A	314	LYS	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	TYR	Sidechain
1	C	133	TYR	Sidechain

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	2196	0	2035	200	0
1	B	2252	0	2084	221	0
1	C	2220	0	2045	174	0
All	All	6668	0	6164	595	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 46.

The worst 5 of 595 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:C:77:ILE:HG23	1:C:154:LEU:HD22	1.22	1.14
1:C:174:THR:HG21	1:C:238:ARG:HD3	1.29	1.10
1:A:263:PHE:O	1:A:264:LEU:HD12	1.49	1.10
1:B:193:PRO:HG2	1:B:196:VAL:HB	1.40	1.03
1:A:52:LEU:HD21	1:A:119:LYS:HG2	1.41	1.01

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	281/394 (71%)	231 (82%)	41 (15%)	9 (3%)	4	22
1	B	284/394 (72%)	222 (78%)	59 (21%)	3 (1%)	14	46
1	C	282/394 (72%)	238 (84%)	38 (14%)	6 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	847/1182 (72%)	691 (82%)	138 (16%)	18 (2%)	7	30

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ILE
1	C	200	CYS
1	C	246	ILE
1	A	147	SER
1	A	184	LYS

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	208/352 (59%)	189 (91%)	19 (9%)	9	33
1	B	212/352 (60%)	201 (95%)	11 (5%)	23	55
1	C	208/352 (59%)	194 (93%)	14 (7%)	16	46
All	All	628/1056 (60%)	584 (93%)	44 (7%)	15	45

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	63	PRO
1	B	188	ASP
1	C	272	ARG
1	B	113	SER
1	B	148	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	HIS
1	B	305	ASN

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Mol	Chain	Res	Type
1	C	318	GLN
1	B	205	HIS
1	B	249	ASN

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](#)

There are no ligands in this entry.

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	287/394 (72%)	-0.37	0 100 100	43, 43, 46, 46	0
1	B	294/394 (74%)	-0.27	1 (0%) 94 88	40, 47, 55, 55	0
1	C	292/394 (74%)	-0.03	6 (2%) 63 43	47, 59, 101, 101	0
All	All	873/1182 (73%)	-0.22	7 (0%) 86 72	40, 47, 89, 101	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	GLU	3.8
1	C	62	ASN	3.1
1	C	273	LEU	2.5
1	B	45	THR	2.2
1	C	279	LYS	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.