



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2023 – 02:45 AM EDT

PDB ID : 4WQO
Title : Structure of VHL-EloB-EloC-Cul2
Authors : Nguyen, H.C.; Xiong, Y.
Deposited on : 2014-10-22
Resolution : 3.20 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 : 2.35.1
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

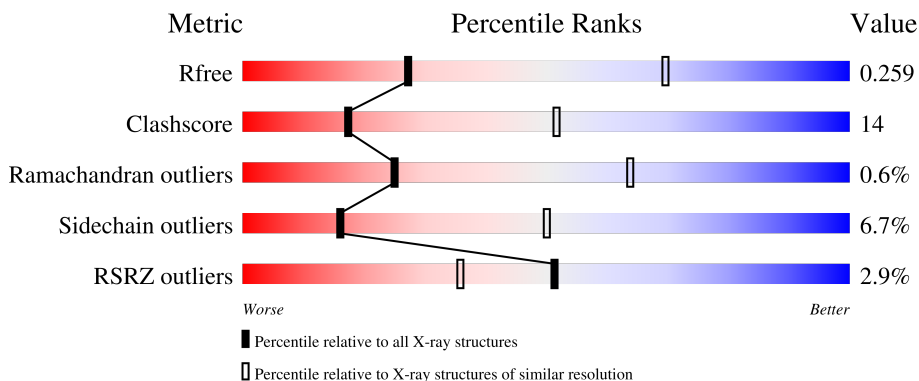
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	233	
2	B	118	
3	C	96	
4	D	186	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3902 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 Von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	148	1197	760	222	213	2	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P40337
A	-18	GLY	-	expression tag	UNP P40337
A	-17	SER	-	expression tag	UNP P40337
A	-16	SER	-	expression tag	UNP P40337
A	-15	HIS	-	expression tag	UNP P40337
A	-14	HIS	-	expression tag	UNP P40337
A	-13	HIS	-	expression tag	UNP P40337
A	-12	HIS	-	expression tag	UNP P40337
A	-11	HIS	-	expression tag	UNP P40337
A	-10	HIS	-	expression tag	UNP P40337
A	-9	SER	-	expression tag	UNP P40337
A	-8	SER	-	expression tag	UNP P40337
A	-7	GLY	-	expression tag	UNP P40337
A	-6	LEU	-	expression tag	UNP P40337
A	-5	VAL	-	expression tag	UNP P40337
A	-4	PRO	-	expression tag	UNP P40337
A	-3	ARG	-	expression tag	UNP P40337
A	-2	GLY	-	expression tag	UNP P40337
A	-1	SER	-	expression tag	UNP P40337
A	0	HIS	-	expression tag	UNP P40337

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	104	798	506	135	152	5	0	0	0

- Molecule 3 is a protein called Transcription elongation factor B polypeptide 1.

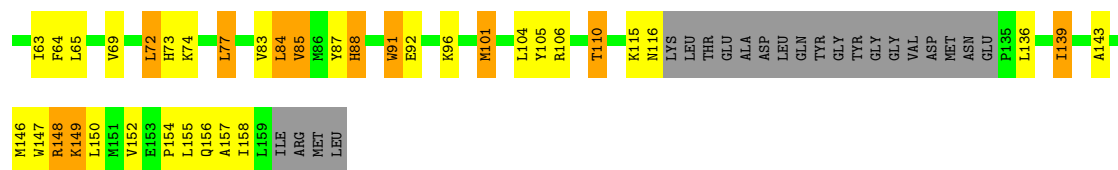
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	96	739	474	120	139	6	0	0	0

- Molecule 4 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	141	1168	759	195	206	8	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	MET	-	initiating methionine	UNP Q13617
D	-21	GLY	-	expression tag	UNP Q13617
D	-20	SER	-	expression tag	UNP Q13617
D	-19	SER	-	expression tag	UNP Q13617
D	-18	HIS	-	expression tag	UNP Q13617
D	-17	HIS	-	expression tag	UNP Q13617
D	-16	HIS	-	expression tag	UNP Q13617
D	-15	HIS	-	expression tag	UNP Q13617
D	-14	HIS	-	expression tag	UNP Q13617
D	-13	HIS	-	expression tag	UNP Q13617
D	-12	SER	-	expression tag	UNP Q13617
D	-11	GLN	-	expression tag	UNP Q13617
D	-10	ASP	-	expression tag	UNP Q13617
D	-9	PRO	-	expression tag	UNP Q13617
D	-8	THR	-	expression tag	UNP Q13617
D	-7	THR	-	expression tag	UNP Q13617
D	-6	VAL	-	expression tag	UNP Q13617
D	-5	LYS	-	expression tag	UNP Q13617
D	-4	LEU	-	expression tag	UNP Q13617
D	-3	GLN	-	expression tag	UNP Q13617
D	-2	ALA	-	expression tag	UNP Q13617
D	-1	GLY	-	expression tag	UNP Q13617
D	0	PHE	-	expression tag	UNP Q13617



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.28Å 108.28Å 213.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.30 – 3.20 48.30 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.30-3.20) 98.8 (48.30-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.19Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.249 0.232 , 0.259	Depositor DCC
R_{free} test set	1163 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtrriage
Anisotropy	0.068	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3902	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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](#)

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	0.58	0/1228	0.95	3/1676 (0.2%)
2	B	0.44	0/813	0.80	0/1100
3	C	0.60	0/755	0.92	0/1022
4	D	0.48	0/1197	0.63	0/1621
All	All	0.53	0/3993	0.83	3/5419 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	153	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	101	LEU	CA-CB-CG	5.16	127.17	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	1197	0	1187	36	0
2	B	798	0	793	16	0
3	C	739	0	724	19	0
4	D	1168	0	1143	46	0
All	All	3902	0	3847	107	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 14.

The worst 5 of 107 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:53:ALA:HA	4:D:32:ARG:HH12	1.32	0.91
1:A:120:ARG:NH1	1:A:125:HIS:O	2.11	0.83
1:A:133:THR:HG22	1:A:134:GLU:H	1.45	0.80
4:D:45:LEU:HD23	4:D:57:LEU:HD22	1.64	0.78
1:A:68:SER:OG	1:A:113:ARG:O	2.02	0.77

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	146/233 (63%)	137 (94%)	8 (6%)	1 (1%)	22	61
2	B	102/118 (86%)	98 (96%)	4 (4%)	0	100	100
3	C	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
4	D	137/186 (74%)	126 (92%)	9 (7%)	2 (2%)	10	44
All	All	479/633 (76%)	453 (95%)	23 (5%)	3 (1%)	25	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
4	D	84	LEU
4	D	157	ALA

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	133/202 (66%)	126 (95%)	7 (5%)	22	58
2	B	86/103 (84%)	85 (99%)	1 (1%)	71	88
3	C	80/85 (94%)	77 (96%)	3 (4%)	33	67
4	D	122/169 (72%)	105 (86%)	17 (14%)	3	16
All	All	421/559 (75%)	393 (93%)	28 (7%)	16	50

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	59	THR
4	D	155	LEU
4	D	85	VAL
4	D	139	ILE
4	D	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
3	C	35	HIS
3	C	61	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 monosaccharides 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	148/233 (63%)	0.26	3 (2%) 65 51	79, 107, 147, 184	0
2	B	104/118 (88%)	0.48	11 (10%) 6 3	99, 133, 180, 209	0
3	C	96/96 (100%)	0.33	0 100 100	84, 109, 191, 212	0
4	D	141/186 (75%)	0.12	0 100 100	91, 125, 169, 213	0
All	All	489/633 (77%)	0.28	14 (2%) 51 36	79, 119, 169, 213	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	LEU	3.5
2	B	79	PHE	2.8
2	B	77	LEU	2.7
2	B	62	PHE	2.6
2	B	78	ALA	2.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.