Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2022 – 01:20 pm GMT

PDB ID	:	7OQV
Title	:	Crystal structure of the polymerising VEL domain of VIN3 (I575D mutant)
Authors	:	Fiedler, M.; Franco-Echevarria, E.; Dean, C.; Bienz, M.
Deposited on	:	2021-06-04
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

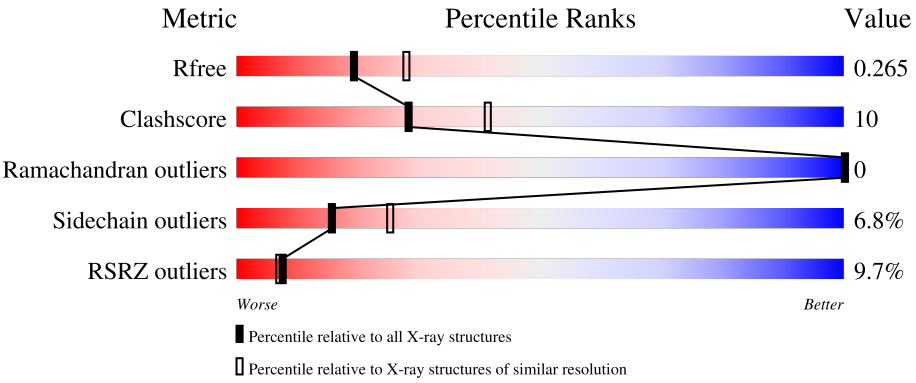
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	AAA	75	5% 73% 21%
1	BBB	75	9% 73% 20% 5%
1	CCC	75	12% 72% 17% 7%
1	DDD	75	9% 63% 24% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2357 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 Protein VERNALIZATION INSENSITIVE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	72	Total	C	N	O	S	0	0	0
			600	379	106	113	2			
1	BBB	71	Total	C	N	O	S	0	0	0
			589	373	102	112	2			
1	CCC	70	Total	C	N	O	S	0	0	0
			580	367	100	111	2			
1	DDD	66	Total	C	N	O	S	0	0	0
			550	348	96	104	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	575	ASP	ILE	engineered mutation	UNP Q9FIE3
BBB	575	ASP	ILE	engineered mutation	UNP Q9FIE3
CCC	575	ASP	ILE	engineered mutation	UNP Q9FIE3
DDD	575	ASP	ILE	engineered mutation	UNP Q9FIE3

- Molecule 2 is water.

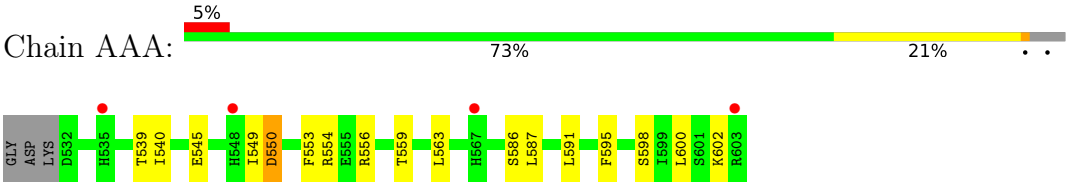
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	8	Total	O	0	0
			8	8		
2	BBB	11	Total	O	0	0
			11	11		
2	CCC	8	Total	O	0	0
			8	8		
2	DDD	11	Total	O	0	0
			11	11		

3 Residue-property plots (i)

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

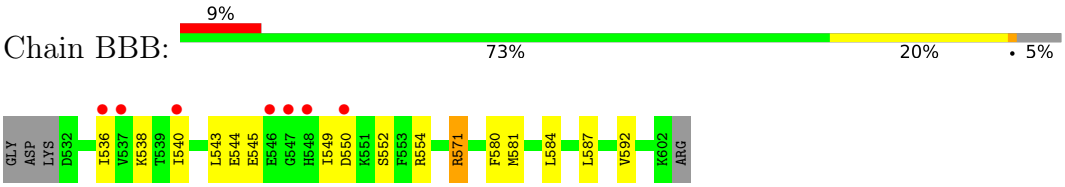
• Molecule 1: Protein VERNALIZATION INSENSITIVE 3

Chain AAA:



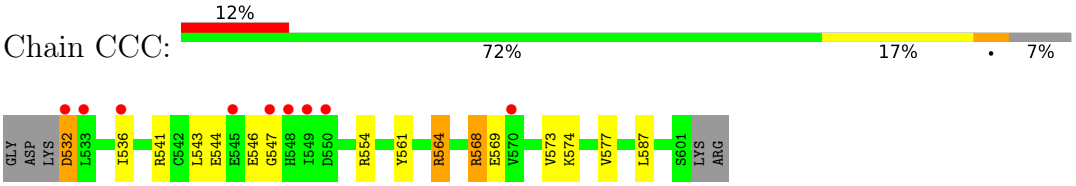
• Molecule 1: Protein VERNALIZATION INSENSITIVE 3

Chain BBB:



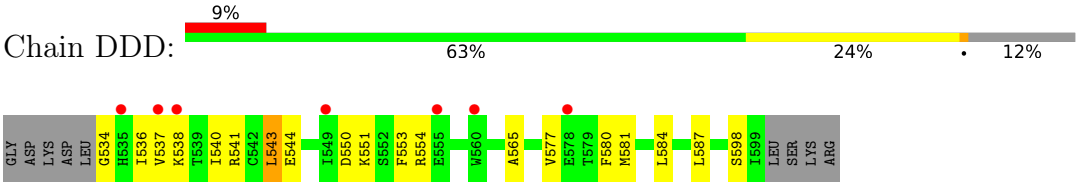
• Molecule 1: Protein VERNALIZATION INSENSITIVE 3

Chain CCC:



• Molecule 1: Protein VERNALIZATION INSENSITIVE 3

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	31.50Å 91.27Å 98.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.07 – 2.40 29.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.07-2.40) 100.0 (29.07-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.270 0.226 , 0.265	Depositor DCC
R_{free} test set	590 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2357	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	AAA	0.73	0/610	0.85	0/818
1	BBB	0.67	0/599	0.84	0/804
1	CCC	0.74	0/590	0.88	0/793
1	DDD	0.71	0/560	0.87	0/752
All	All	0.71	0/2359	0.86	0/3167

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	600	0	594	12	1
1	BBB	589	0	581	15	0
1	CCC	580	0	568	14	0
1	DDD	550	0	537	14	1
2	AAA	8	0	0	0	0
2	BBB	11	0	0	1	0
2	CCC	8	0	0	2	0
2	DDD	11	0	0	0	0
All	All	2357	0	2280	45	1

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.

All (45) 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:BBB:538:LYS:NZ	2:BBB:701:HOH:O	2.16	0.79
1:AAA:539:THR:HG21	1:CCC:587:LEU:HD21	1.68	0.76
1:CCC:564:ARG:HD2	2:CCC:702:HOH:O	1.87	0.74
1:AAA:549:ILE:HD11	1:AAA:553:PHE:HD2	1.51	0.74
1:BBB:544:GLU:OE1	1:BBB:554:ARG:HD3	1.98	0.64
1:BBB:580:PHE:CZ	1:DDD:584:LEU:HD13	2.34	0.63
1:AAA:539:THR:CG2	1:CCC:587:LEU:HD21	2.29	0.62
1:BBB:584:LEU:HD11	1:DDD:543:LEU:HD13	1.84	0.60
1:CCC:543:LEU:O	1:CCC:547:GLY:O	2.20	0.59
1:CCC:561:TYR:CE1	1:CCC:573:VAL:HG21	2.40	0.57
1:DDD:540:ILE:CG2	1:DDD:554:ARG:HG3	2.36	0.55
1:CCC:568:ARG:HH11	1:CCC:568:ARG:HG2	1.72	0.54
1:BBB:587:LEU:HD13	1:DDD:580:PHE:HB2	1.90	0.54
1:AAA:549:ILE:CD1	1:AAA:553:PHE:HD2	2.20	0.53
1:BBB:550:ASP:OD1	1:BBB:552:SER:HB3	2.10	0.52
1:BBB:580:PHE:HD2	1:BBB:581:MET:HE2	1.75	0.51
1:DDD:540:ILE:HG21	1:DDD:554:ARG:HG3	1.92	0.50
1:BBB:536:ILE:O	1:BBB:540:ILE:HG12	2.12	0.50
1:CCC:564:ARG:CD	2:CCC:702:HOH:O	2.50	0.50
1:DDD:544:GLU:OE1	1:DDD:551:LYS:CG	2.59	0.50
1:CCC:532:ASP:OD2	1:CCC:532:ASP:N	2.45	0.49
1:CCC:574:LYS:O	1:CCC:577:VAL:HG12	2.12	0.49
1:DDD:577:VAL:O	1:DDD:581:MET:HG2	2.12	0.49
1:DDD:534:GLY:O	1:DDD:537:VAL:HG22	2.13	0.49
1:CCC:574:LYS:HA	1:CCC:577:VAL:HG12	1.95	0.47
1:CCC:544:GLU:OE1	1:CCC:554:ARG:HD3	2.14	0.47
1:CCC:569:GLU:O	1:CCC:573:VAL:HG13	2.15	0.47
1:AAA:595:PHE:CZ	1:CCC:573:VAL:HG12	2.51	0.46
1:AAA:550:ASP:OD1	1:AAA:550:ASP:N	2.43	0.45
1:DDD:544:GLU:OE1	1:DDD:551:LYS:HG2	2.16	0.45
1:AAA:539:THR:CG2	1:CCC:587:LEU:CD2	2.95	0.44
1:BBB:543:LEU:HB3	1:BBB:549:ILE:HG12	1.99	0.44
1:BBB:580:PHE:CB	1:DDD:587:LEU:HD22	2.48	0.43
1:AAA:591:LEU:HD12	1:AAA:591:LEU:HA	1.81	0.43
1:BBB:571:ARG:HH11	1:BBB:571:ARG:HG2	1.84	0.43
1:AAA:549:ILE:HD11	1:AAA:553:PHE:CD2	2.41	0.42
1:AAA:559:THR:HG23	1:AAA:563:LEU:HD12	2.01	0.42
1:BBB:592:VAL:HG22	1:DDD:553:PHE:CZ	2.55	0.42
1:DDD:544:GLU:OE1	1:DDD:551:LYS:HG3	2.19	0.41
1:DDD:540:ILE:HG22	1:DDD:554:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:598:SER:O	1:AAA:602:LYS:HG3	2.20	0.41
1:BBB:580:PHE:HD2	1:BBB:581:MET:CE	2.34	0.41
1:BBB:584:LEU:CD1	1:DDD:543:LEU:HD13	2.48	0.41
1:BBB:545:GLU:HA	1:BBB:545:GLU:OE1	2.21	0.41
1:AAA:540:ILE:HG21	1:AAA:554:ARG:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:556:ARG:NH2	1:DDD:565:ALA:O[2_454]	2.14	0.06

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	AAA	70/75 (93%)	68 (97%)	2 (3%)	0	100	100
1	BBB	69/75 (92%)	69 (100%)	0	0	100	100
1	CCC	68/75 (91%)	67 (98%)	1 (2%)	0	100	100
1	DDD	64/75 (85%)	64 (100%)	0	0	100	100
All	All	271/300 (90%)	268 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	68/70 (97%)	63 (93%)	5 (7%)	13 22
1	BBB	67/70 (96%)	66 (98%)	1 (2%)	65 80
1	CCC	66/70 (94%)	60 (91%)	6 (9%)	9 14
1	DDD	62/70 (89%)	56 (90%)	6 (10%)	8 12
All	All	263/280 (94%)	245 (93%)	18 (7%)	16 25

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	545	GLU
1	AAA	550	ASP
1	AAA	586	SER
1	AAA	587	LEU
1	AAA	600	LEU
1	BBB	571	ARG
1	CCC	532	ASP
1	CCC	536	ILE
1	CCC	541	ARG
1	CCC	546	GLU
1	CCC	564	ARG
1	CCC	568	ARG
1	DDD	536	ILE
1	DDD	538	LYS
1	DDD	541	ARG
1	DDD	543	LEU
1	DDD	550	ASP
1	DDD	598	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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

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^{th} 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	AAA	72/75 (96%)	0.50	4 (5%)	24 23	40, 55, 85, 98	0
1	BBB	71/75 (94%)	0.85	7 (9%)	7 6	36, 53, 94, 111	0
1	CCC	70/75 (93%)	0.92	9 (12%)	3 3	37, 58, 94, 104	0
1	DDD	66/75 (88%)	0.90	7 (10%)	6 5	39, 56, 89, 93	0
All	All	279/300 (93%)	0.79	27 (9%)	7 7	36, 56, 92, 111	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	570	VAL	5.7
1	CCC	548	HIS	4.6
1	BBB	548	HIS	4.4
1	CCC	549	ILE	4.3
1	DDD	549	ILE	4.0
1	CCC	532	ASP	3.2
1	CCC	550	ASP	3.1
1	BBB	546	GLU	3.1
1	AAA	548	HIS	2.8
1	DDD	535	HIS	2.8
1	CCC	545	GLU	2.8
1	AAA	567	HIS	2.8
1	AAA	603	ARG	2.6
1	BBB	536	ILE	2.6
1	DDD	560	TRP	2.5
1	BBB	540	ILE	2.5
1	DDD	578	GLU	2.5
1	DDD	555	GLU	2.4
1	BBB	550	ASP	2.4
1	BBB	537	VAL	2.2
1	DDD	537	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	547	GLY	2.1
1	DDD	538	LYS	2.1
1	AAA	535	HIS	2.1
1	CCC	536	ILE	2.1
1	BBB	547	GLY	2.1
1	CCC	533	LEU	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 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.