



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID : 2WAU
Title : Structure of DBL6 epsilon domain from VAR2CSA
Authors : Khunrae, P.; Higgins, M.K.
Deposited on : 2009-02-16
Resolution : 3.00 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

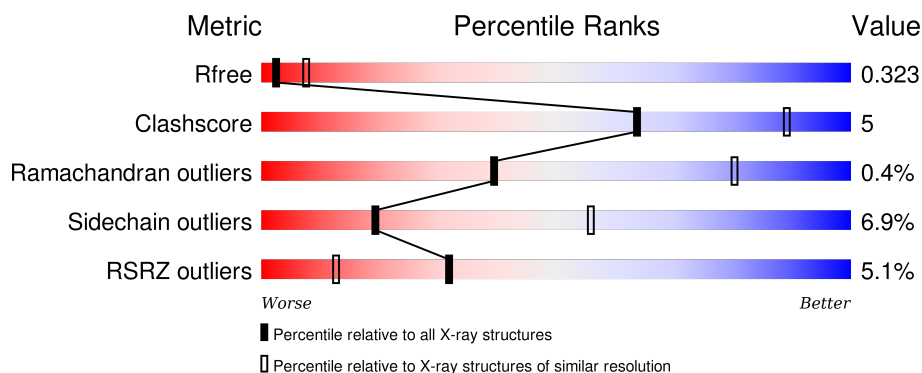
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	302	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	B	302	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 10%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4541 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 ERYTHROCYTE MEMBRANE PROTEIN 1 (PFEMP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	1
			2290	1437	386	447	20			
1	B	271	Total	C	N	O	S	0	0	0
			2251	1415	377	440	19			

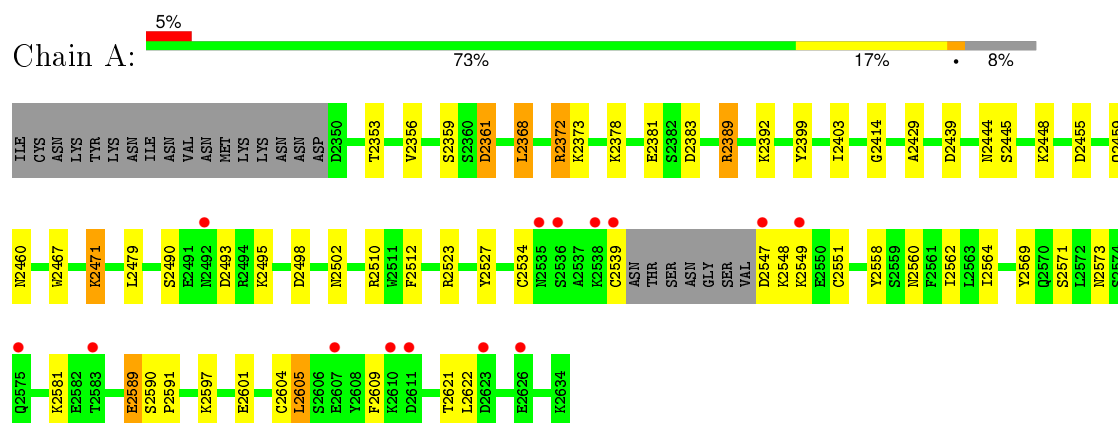
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2480	SER	CYS	ENGINEERED MUTATION	UNP Q8I639
B	2480	SER	CYS	ENGINEERED MUTATION	UNP Q8I639

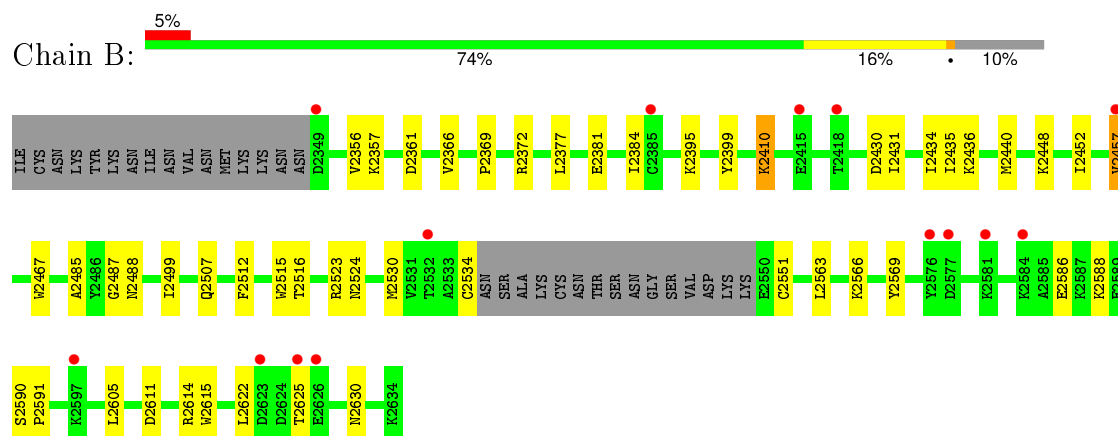
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ERYTHROCYTE MEMBRANE PROTEIN 1 (PFEMP1)



• Molecule 1: ERYTHROCYTE MEMBRANE PROTEIN 1 (PFEMP1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.94Å 62.94Å 334.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.62 – 3.00 83.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (83.62-3.00) 99.8 (83.57-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.289 , 0.325 0.284 , 0.323	Depositor DCC
R_{free} test set	723 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	88.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 14403 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4541	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.33	0/2337	0.48	1/3133 (0.0%)
1	B	0.32	0/2298	0.47	0/3079
All	All	0.32	0/4635	0.48	1/6212 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2368	LEU	CA-CB-CG	5.53	128.02	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	2290	0	2199	25	0
1	B	2251	0	2165	22	0
All	All	4541	0	4364	46	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 5.

All (46) 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:A:2490:SER:HB2	1:A:2493:ASP:HB2	1.55	0.88
1:A:2590:SER:HB3	1:A:2591:PRO:HD3	1.74	0.70
1:B:2566:LYS:HG3	1:B:2615:TRP:HB3	1.73	0.69
1:A:2560:ASN:O	1:A:2564:ILE:HG12	1.96	0.65
1:B:2591:PRO:HA	1:B:2605:LEU:HB3	1.76	0.65
1:B:2410:LYS:HG3	1:B:2485:ALA:HB1	1.80	0.63
1:B:2440:MET:H	1:B:2507:GLN:HE22	1.47	0.61
1:A:2381:GLU:HG2	1:A:2448:LYS:HE3	1.83	0.61
1:B:2436:LYS:HE3	1:B:2467:TRP:CD1	2.36	0.60
1:B:2395:LYS:O	1:B:2399:TYR:HD1	1.84	0.60
1:B:2381:GLU:O	1:B:2384:ILE:HG12	2.02	0.59
1:A:2389:ARG:HA	1:A:2389:ARG:HE	1.67	0.59
1:A:2459:GLN:HG3	1:A:2460:ASN:H	1.71	0.56
1:A:2502:ASN:HB3	1:A:2510:ARG:HD3	1.88	0.56
1:A:2361:ASP:N	1:A:2361:ASP:OD1	2.40	0.55
1:B:2357:LYS:HE2	1:B:2440:MET:HA	1.90	0.54
1:B:2369:PRO:HG2	1:B:2372:ARG:HB3	1.90	0.53
1:B:2440:MET:N	1:B:2507:GLN:HE22	2.07	0.53
1:A:2372:ARG:NH2	1:A:2439:ASP:OD1	2.44	0.51
1:B:2590:SER:N	1:B:2591:PRO:HD2	2.26	0.51
1:B:2515:TRP:CH2	1:B:2569:TYR:HB2	2.46	0.51
1:A:2581:LYS:HE2	1:A:2589:GLU:HA	1.93	0.51
1:B:2430:ASP:O	1:B:2434:ILE:HG12	2.10	0.50
1:B:2356:VAL:HG21	1:B:2366:VAL:HG13	1.93	0.50
1:B:2611:ASP:HB3	1:B:2614:ARG:HG3	1.93	0.49
1:A:2445:SER:HB2	1:A:2448:LYS:HD2	1.96	0.48
1:A:2467:TRP:O	1:A:2471:LYS:HG2	2.14	0.47
1:A:2527:TYR:HE1	1:A:2622:LEU:HG	1.79	0.47
1:B:2516:THR:HG23	1:B:2605:LEU:HD23	1.95	0.47
1:A:2368:LEU:CD1	1:A:2373:LYS:HB2	2.44	0.47
1:A:2368:LEU:HD11	1:A:2373:LYS:HB2	1.97	0.47
1:A:2534:CYS:HB3	1:A:2551:CYS:HB2	1.64	0.45
1:B:2448:LYS:O	1:B:2452:ILE:HG12	2.16	0.45
1:B:2431:ILE:O	1:B:2435:ILE:HG12	2.17	0.44
1:B:2530:MET:O	1:B:2534:CYS:HB3	2.17	0.44
1:A:2353:THR:HG21	1:B:2563:LEU:HD13	2.00	0.44
1:B:2487:GLY:HA2	1:B:2488:ASN:HA	1.52	0.44
1:A:2356:VAL:HG23	1:A:2359:SER:HB3	2.00	0.44
1:A:2429:ALA:HB2	1:A:2502:ASN:HB2	2.00	0.43
1:B:2586:GLU:HB3	1:B:2588:LYS:HE3	2.01	0.43
1:A:2548:LYS:HB3	1:A:2549:LYS:H	1.71	0.43
1:A:2569:TYR:CE1	1:A:2605:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2558:TYR:O	1:A:2562:ILE:HG12	2.20	0.41
1:A:2609:PHE:CE1	1:A:2621:THR:HG21	2.56	0.41
1:A:2372:ARG:HH22	1:A:2439:ASP:CG	2.23	0.40
1:A:2399:TYR:O	1:A:2403:ILE:HG12	2.21	0.40

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	274/302 (91%)	248 (90%)	25 (9%)	1 (0%)	39	80
1	B	267/302 (88%)	240 (90%)	26 (10%)	1 (0%)	39	80
All	All	541/604 (90%)	488 (90%)	51 (9%)	2 (0%)	39	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2414	GLY
1	B	2457	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/281 (91%)	233 (91%)	23 (9%)	12	41
1	B	252/281 (90%)	240 (95%)	12 (5%)	31	71
All	All	508/562 (90%)	473 (93%)	35 (7%)	19	56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2361	ASP
1	A	2372	ARG
1	A	2378	LYS
1	A	2383	ASP
1	A	2389	ARG
1	A	2392	LYS
1	A	2444	ASN
1	A	2455	ASP
1	A	2471	LYS
1	A	2479	LEU
1	A	2495	LYS
1	A	2498	ASP
1	A	2512	PHE
1	A	2523	ARG
1	A	2539	CYS
1	A	2547	ASP
1	A	2571	SER
1	A	2573	ASN
1	A	2589	GLU
1	A	2597	LYS
1	A	2601	GLU
1	A	2604	CYS
1	A	2605	LEU
1	B	2361	ASP
1	B	2377	LEU
1	B	2410	LYS
1	B	2457	VAL
1	B	2499	ILE
1	B	2512	PHE
1	B	2523	ARG
1	B	2524	ASN
1	B	2551	CYS

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Mol	Chain	Res	Type
1	B	2622	LEU
1	B	2625	THR
1	B	2630	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2444	ASN
1	A	2470	ASN
1	A	2501	ASN
1	A	2502	ASN
1	A	2507	GLN
1	A	2557	ASN
1	A	2573	ASN
1	B	2374	ASN
1	B	2459	GLN
1	B	2507	GLN
1	B	2524	ASN
1	B	2573	ASN
1	B	2579	ASN
1	B	2629	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

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, 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	278/302 (92%)	0.37	14 (5%) 32 13	53, 88, 136, 153	0
1	B	271/302 (89%)	0.50	14 (5%) 31 12	55, 100, 140, 163	0
All	All	549/604 (90%)	0.44	28 (5%) 32 12	53, 94, 138, 163	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2623	ASP	5.2
1	B	2626	GLU	5.1
1	A	2535	ASN	5.1
1	B	2625	THR	4.8
1	A	2492	ASN	4.4
1	A	2536	SER	4.1
1	A	2611	ASP	3.8
1	A	2547	ASP	3.4
1	B	2349	ASP	3.0
1	B	2597	LYS	3.0
1	A	2539	CYS	3.0
1	B	2577	ASP	3.0
1	A	2610	LYS	2.8
1	B	2418	THR	2.6
1	B	2532	THR	2.6
1	A	2607	GLU	2.4
1	A	2549	LYS	2.4
1	A	2623	ASP	2.4
1	B	2457	VAL	2.3
1	B	2584	LYS	2.3
1	B	2581	LYS	2.3
1	B	2415	GLU	2.2
1	A	2538	LYS	2.1
1	A	2583	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2576	TYR	2.1
1	A	2626	GLU	2.0
1	B	2385	CYS	2.0
1	A	2575	GLN	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.