



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:13 PM UTC

PDB ID : 1XWI / pdb_00001xwi
Title : Crystal Structure of VPS4B
Authors : Scott, A.; Sundquist, W.I.; Hill, C.P.
Deposited on : 2004-11-01
Resolution : 2.80 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

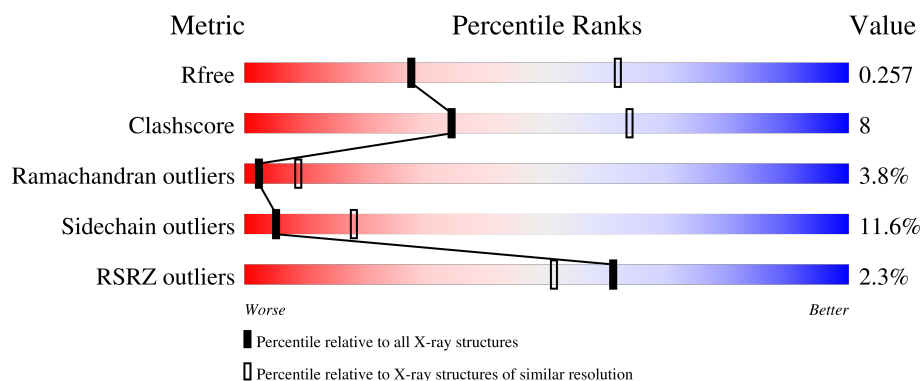
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	322	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2527 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 SKD1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	158	0	0
			2508	1591	438	470	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

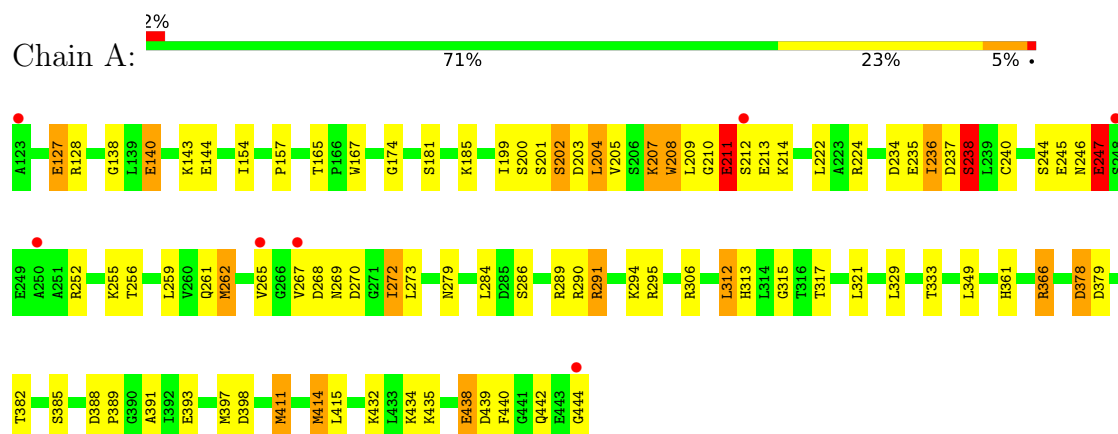
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

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: SKD1 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	88.06Å 88.06Å 112.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.70 – 2.80 76.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (76.70-2.80) 98.8 (76.26-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.32 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.260 0.193 , 0.257	Depositor DCC
R_{free} test set	1190 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2527	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.71	14/2560 (0.5%)	2.33	33/3464 (1.0%)

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	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLU	C-N	-60.10	0.42	1.33
1	A	199	ILE	C-N	-14.23	1.14	1.33
1	A	211	GLU	C-N	-14.21	1.13	1.33
1	A	205	VAL	N-CA	10.95	1.58	1.46
1	A	204	LEU	CA-C	10.07	1.66	1.52
1	A	204	LEU	C-N	9.61	1.44	1.33
1	A	238	SER	C-N	-6.57	1.24	1.33
1	A	203	ASP	N-CA	6.47	1.53	1.45
1	A	201	SER	CA-C	6.32	1.61	1.52
1	A	202	SER	N-CA	6.10	1.54	1.46
1	A	247	GLU	N-CA	-5.52	1.39	1.46
1	A	245	GLU	CA-C	5.33	1.59	1.52
1	A	246	ASN	CA-C	-5.14	1.45	1.52
1	A	244	SER	CA-C	5.08	1.59	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLU	CA-C-N	-64.41	21.12	122.24
1	A	247	GLU	C-N-CA	-64.41	21.12	122.24
1	A	238	SER	O-C-N	-55.01	51.96	122.37
1	A	211	GLU	O-C-N	-28.18	84.61	122.36
1	A	199	ILE	O-C-N	-20.16	100.01	123.00
1	A	247	GLU	O-C-N	-16.99	100.00	122.59
1	A	205	VAL	CB-CA-C	-8.83	100.75	111.08
1	A	201	SER	N-CA-C	7.51	121.36	111.75
1	A	246	ASN	CA-C-N	-7.41	107.39	121.54
1	A	246	ASN	C-N-CA	-7.41	107.39	121.54
1	A	199	ILE	CA-C-N	-7.16	112.89	122.99
1	A	199	ILE	C-N-CA	-7.16	112.89	122.99
1	A	205	VAL	N-CA-C	6.94	118.81	108.54
1	A	213	GLU	N-CA-C	6.86	118.76	111.28
1	A	211	GLU	N-CA-C	-6.72	101.85	110.19
1	A	204	LEU	O-C-N	-6.45	114.85	122.20
1	A	245	GLU	CB-CA-C	6.44	123.23	110.42
1	A	208	TRP	CA-C-N	-6.31	113.44	122.77
1	A	208	TRP	C-N-CA	-6.31	113.44	122.77
1	A	211	GLU	CA-C-N	-6.20	109.70	121.54
1	A	211	GLU	C-N-CA	-6.20	109.70	121.54
1	A	208	TRP	N-CA-C	6.07	123.73	110.80
1	A	204	LEU	CA-C-O	-5.96	113.52	120.20
1	A	209	LEU	CA-C-N	5.94	133.05	121.41
1	A	209	LEU	C-N-CA	5.94	133.05	121.41
1	A	209	LEU	CA-C-O	5.74	127.81	121.39
1	A	207	LYS	CA-C-N	-5.54	110.95	121.54
1	A	207	LYS	C-N-CA	-5.54	110.95	121.54
1	A	238	SER	N-CA-C	-5.22	107.08	112.93
1	A	209	LEU	O-C-N	5.16	128.93	122.63
1	A	209	LEU	CB-CA-C	5.06	120.12	111.68
1	A	411	MET	CA-C-N	-5.06	112.08	120.68
1	A	411	MET	C-N-CA	-5.06	112.08	120.68

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	GLU	Mainchain,Peptide
1	A	238	SER	Mainchain
1	A	247	GLU	Mainchain,Peptide

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	A	2508	0	2542	36	0
2	A	10	0	0	0	0
3	A	9	0	0	0	0
All	All	2527	0	2542	36	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 8.

All (36) 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:259:LEU:HD23	1:A:291:ARG:HD2	1.61	0.82
1:A:379:ASP:N	1:A:379:ASP:OD1	2.16	0.76
1:A:411:MET:CE	1:A:414:MET:HB2	2.23	0.68
1:A:411:MET:HE2	1:A:415:LEU:HG	1.78	0.65
1:A:317:THR:HG21	1:A:349:LEU:HD22	1.80	0.63
1:A:286:SER:O	1:A:290:ARG:HG3	1.99	0.62
1:A:329:LEU:HD21	1:A:411:MET:HE1	1.81	0.61
1:A:127:GLU:OE1	1:A:185:LYS:HE3	2.02	0.60
1:A:411:MET:HE3	1:A:414:MET:HB2	1.84	0.59
1:A:289:ARG:NH1	1:A:444:GLY:O	2.36	0.58
1:A:329:LEU:HD11	1:A:411:MET:HE1	1.88	0.56
1:A:255:LYS:O	1:A:259:LEU:HD12	2.06	0.55
1:A:366:ARG:HD3	1:A:378:ASP:OD1	2.07	0.55
1:A:411:MET:HE3	1:A:411:MET:HA	1.91	0.53
1:A:167:TRP:CE2	1:A:294:LYS:HE3	2.44	0.52
1:A:262:MET:HE3	1:A:262:MET:HA	1.91	0.52
1:A:312:LEU:O	1:A:315:GLY:N	2.43	0.52
1:A:295:ARG:NH2	1:A:444:GLY:H	2.09	0.50
1:A:306:ARG:HD2	1:A:333:THR:OG1	2.11	0.49
1:A:140:GLU:H	1:A:140:GLU:CD	2.21	0.49
1:A:236:ILE:HG23	1:A:284:LEU:HD11	1.95	0.49
1:A:154:ILE:O	1:A:157:PRO:HD3	2.14	0.48
1:A:388:ASP:HB2	1:A:391:ALA:HB2	1.95	0.48
1:A:224:ARG:HA	1:A:272:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASP:O	1:A:235:GLU:C	2.57	0.47
1:A:295:ARG:HH22	1:A:444:GLY:H	1.62	0.47
1:A:361:HIS:CD2	1:A:393:GLU:HB2	2.50	0.47
1:A:268:ASP:OD2	1:A:270:ASP:HB3	2.15	0.47
1:A:261:GLN:O	1:A:269:ASN:ND2	2.48	0.46
1:A:414:MET:HA	1:A:414:MET:HE3	1.98	0.46
1:A:438:GLU:O	1:A:440:PHE:N	2.50	0.44
1:A:174:GLY:O	1:A:279:ASN:HA	2.17	0.44
1:A:138:GLY:O	1:A:143:LYS:HE3	2.19	0.43
1:A:289:ARG:NH1	1:A:444:GLY:C	2.78	0.41
1:A:235:GLU:HG2	1:A:238:SER:HB3	2.01	0.41
1:A:237:ASP:HA	1:A:284:LEU:HD12	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	320/322 (99%)	290 (91%)	18 (6%)	12 (4%)	2 9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	CYS
1	A	312	LEU
1	A	202	SER
1	A	210	GLY
1	A	212	SER
1	A	265	VAL
1	A	313	HIS
1	A	247	GLU
1	A	439	ASP

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Mol	Chain	Res	Type
1	A	208	TRP
1	A	438	GLU
1	A	389	PRO

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	276/276 (100%)	244 (88%)	32 (12%)	5 18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLU
1	A	128	ARG
1	A	140	GLU
1	A	144	GLU
1	A	165	THR
1	A	181	SER
1	A	200	SER
1	A	204	LEU
1	A	207	LYS
1	A	211	GLU
1	A	214	LYS
1	A	222	LEU
1	A	236	ILE
1	A	252	ARG
1	A	256	THR
1	A	262	MET
1	A	267	VAL
1	A	272	ILE
1	A	273	LEU
1	A	291	ARG
1	A	321	LEU
1	A	366	ARG
1	A	378	ASP

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Mol	Chain	Res	Type
1	A	382	THR
1	A	385	SER
1	A	397	MET
1	A	398	ASP
1	A	414	MET
1	A	432	LYS
1	A	434	LYS
1	A	435	LYS
1	A	442	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
1	A	357	GLN
1	A	420	ASN
1	A	428	HIS
1	A	442	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	601	-	4,4,4	0.36	0	6,6,6	0.44	0
2	SO4	A	602	-	4,4,4	0.17	0	6,6,6	0.24	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	199:ILE	C	200:SER	N	1.14
1	A	211:GLU	C	212:SER	N	1.13
1	A	247:GLU	C	248:SER	N	0.42

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	301/322 (93%)	-0.20	7 (2%) 61 51	30, 46, 87, 105	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	VAL	5.8
1	A	123	ALA	3.7
1	A	444	GLY	3.4
1	A	265	VAL	2.6
1	A	212	SER	2.5
1	A	248	SER	2.4
1	A	250	ALA	2.2

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	SO4	A	601	5/5	0.97	0.07	49,49,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	602	5/5	0.99	0.05	38,38,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.