



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:22 AM GMT

PDB ID : 2RKO
Title : Crystal Structure of the Vps4p-dimer
Authors : Hartmann, C.; Gruetter, M.G.
Deposited on : 2007-10-17
Resolution : 3.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

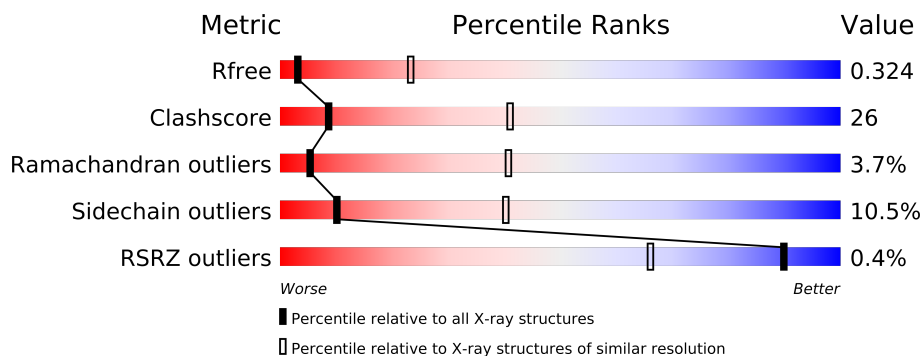
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.35 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}	66092	1141 (3.50-3.22)
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	331	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2173 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Vacuolar protein sorting-associated protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	337	0	0
			2173	1380	366	419	8			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MET	-	EXPRESSION TAG	UNP P52917
A	108	GLY	-	EXPRESSION TAG	UNP P52917
A	109	HIS	-	EXPRESSION TAG	UNP P52917
A	110	HIS	-	EXPRESSION TAG	UNP P52917
A	111	HIS	-	EXPRESSION TAG	UNP P52917
A	112	HIS	-	EXPRESSION TAG	UNP P52917
A	113	HIS	-	EXPRESSION TAG	UNP P52917
A	114	HIS	-	EXPRESSION TAG	UNP P52917
A	115	SER	-	EXPRESSION TAG	UNP P52917
A	116	ARG	-	EXPRESSION TAG	UNP P52917
A	117	GLY	-	EXPRESSION TAG	UNP P52917
A	118	LEU	-	EXPRESSION TAG	UNP P52917
A	119	VAL	-	EXPRESSION TAG	UNP P52917
A	120	PRO	-	EXPRESSION TAG	UNP P52917
A	121	ARG	-	EXPRESSION TAG	UNP P52917
A	122	GLY	-	EXPRESSION TAG	UNP P52917
A	123	SER	-	EXPRESSION TAG	UNP P52917

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	109.12Å 109.12Å 176.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.35 94.50 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-3.35) 99.1 (94.50-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.298 0.285 , 0.324	Depositor DCC
R_{free} test set	472 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	129.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 183.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 9403 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2173	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	1.41	37/2208 (1.7%)	0.97	20/2983 (0.7%)

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

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLU	CB-CG	-22.34	1.09	1.52
1	A	363	VAL	CB-CG1	19.45	1.93	1.52
1	A	363	VAL	CB-CG2	-16.57	1.18	1.52
1	A	287	ARG	CB-CG	-13.31	1.16	1.52
1	A	146	LYS	CB-CG	-12.89	1.17	1.52
1	A	167	SER	CA-CB	-12.73	1.33	1.52
1	A	134	ASP	CA-CB	-12.15	1.27	1.53
1	A	304	ARG	CA-CB	-11.62	1.28	1.53
1	A	204	SER	CA-CB	-10.81	1.36	1.52
1	A	293	ARG	CA-CB	-10.73	1.30	1.53
1	A	430	ARG	CA-CB	-10.12	1.31	1.53
1	A	288	ARG	CA-CB	-9.80	1.32	1.53
1	A	360	PHE	CB-CG	-8.89	1.36	1.51
1	A	164	LYS	CA-CB	-8.85	1.34	1.53
1	A	133	GLU	CB-CG	-8.79	1.35	1.52
1	A	394	ASP	CA-CB	-8.13	1.36	1.53
1	A	300	ASP	CA-CB	-8.09	1.36	1.53
1	A	393	ALA	CA-CB	-7.79	1.36	1.52
1	A	237	LEU	CA-CB	-7.74	1.35	1.53
1	A	418	ASN	CA-CB	-7.66	1.33	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	LYS	CA-CB	-7.48	1.37	1.53
1	A	380	ASP	CA-CB	-7.48	1.37	1.53
1	A	423	LEU	CA-CB	-7.43	1.36	1.53
1	A	181	TYR	CA-CB	-7.40	1.37	1.53
1	A	248	ALA	CA-CB	7.40	1.68	1.52
1	A	404	LYS	CA-CB	-7.36	1.37	1.53
1	A	233	GLU	CB-CG	-7.34	1.38	1.52
1	A	292	ARG	CB-CG	7.02	1.71	1.52
1	A	147	GLU	CB-CG	6.62	1.64	1.52
1	A	254	THR	CB-OG1	6.45	1.56	1.43
1	A	426	GLU	CA-CB	-6.39	1.39	1.53
1	A	291	GLU	CA-CB	-5.97	1.40	1.53
1	A	215	LYS	CB-CG	-5.40	1.38	1.52
1	A	421	ASP	CA-CB	-5.27	1.42	1.53
1	A	249	SER	CA-CB	5.25	1.60	1.52
1	A	211	GLU	CA-CB	-5.25	1.42	1.53
1	A	309	GLU	CB-CG	5.16	1.61	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	LYS	CB-CG-CD	9.68	136.77	111.60
1	A	363	VAL	CA-CB-CG2	9.59	125.29	110.90
1	A	146	LYS	CA-CB-CG	9.46	134.21	113.40
1	A	147	GLU	CA-CB-CG	-8.97	93.67	113.40
1	A	363	VAL	CA-CB-CG1	-8.39	98.31	110.90
1	A	223	GLU	CA-CB-CG	8.23	131.50	113.40
1	A	248	ALA	N-CA-CB	-7.18	100.05	110.10
1	A	414	ARG	CB-CA-C	-7.04	96.31	110.40
1	A	302	ALA	CB-CA-C	6.94	120.51	110.10
1	A	404	LYS	N-CA-CB	6.85	122.93	110.60
1	A	282	LEU	CB-CG-CD1	-6.77	99.49	111.00
1	A	395	GLU	N-CA-CB	6.40	122.12	110.60
1	A	282	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	287	ARG	CA-CB-CG	5.89	126.36	113.40
1	A	261	ASN	N-CA-CB	5.82	121.07	110.60
1	A	225	LYS	CB-CA-C	5.61	121.62	110.40
1	A	249	SER	N-CA-CB	5.51	118.77	110.50
1	A	302	ALA	N-CA-CB	-5.40	102.55	110.10
1	A	134	ASP	CA-CB-CG	-5.33	101.68	113.40
1	A	314	ASP	N-CA-CB	5.26	120.07	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	GLY	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2173	0	2202	91	0
All	All	2173	0	2202	91	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (91) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:315:THR:HG21	1:A:347:LEU:HD22	1.32	1.10
1:A:298:LEU:HD21	1:A:417:VAL:HG21	1.43	0.95
1:A:193:THR:HG1	1:A:195:PHE:HE1	1.10	0.93
1:A:338:ASP:O	1:A:341:VAL:HG13	1.79	0.82
1:A:298:LEU:HD12	1:A:422:LEU:HD12	1.65	0.79
1:A:298:LEU:HD11	1:A:417:VAL:HG11	1.69	0.73
1:A:403:ILE:HD12	1:A:403:ILE:H	1.55	0.72
1:A:403:ILE:N	1:A:403:ILE:HD12	2.04	0.71
1:A:257:LEU:HD21	1:A:286:ILE:HD13	1.72	0.71
1:A:298:LEU:HD12	1:A:422:LEU:CD1	2.22	0.70
1:A:132:TRP:CD1	1:A:189:GLU:HG3	2.27	0.69
1:A:311:ASN:HD22	1:A:311:ASN:N	1.89	0.68
1:A:132:TRP:CG	1:A:189:GLU:HG3	2.29	0.68
1:A:182:LEU:HD23	1:A:296:ILE:HD13	1.77	0.67
1:A:138:LEU:HB2	1:A:141:ALA:HB3	1.77	0.67
1:A:169:ILE:HB	1:A:273:LEU:HD22	1.76	0.66
1:A:298:LEU:CD1	1:A:417:VAL:HG11	2.27	0.65
1:A:318:VAL:O	1:A:318:VAL:HG12	1.96	0.64
1:A:310:ILE:O	1:A:312:VAL:N	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:VAL:HG11	1:A:190:ALA:HB1	1.81	0.62
1:A:298:LEU:CD1	1:A:422:LEU:HD12	2.28	0.62
1:A:300:ASP:O	1:A:302:ALA:N	2.33	0.62
1:A:146:LYS:HA	1:A:150:ILE:HD12	1.80	0.62
1:A:178:GLY:O	1:A:181:TYR:N	2.32	0.61
1:A:362:ASP:HA	1:A:373:LEU:HD23	1.82	0.61
1:A:309:GLU:HA	1:A:324:TYR:CE2	2.35	0.61
1:A:351:ILE:HD13	1:A:351:ILE:H	1.67	0.60
1:A:298:LEU:CD2	1:A:417:VAL:HG21	2.25	0.59
1:A:187:ALA:HB2	1:A:228:ILE:HD12	1.84	0.57
1:A:216:GLN:O	1:A:219:ALA:HB3	2.04	0.57
1:A:254:THR:O	1:A:258:VAL:HG23	2.04	0.57
1:A:384:ILE:CG2	1:A:386:MET:HE2	2.36	0.56
1:A:384:ILE:HG22	1:A:386:MET:HE2	1.89	0.54
1:A:347:LEU:O	1:A:350:PRO:HD2	2.08	0.54
1:A:310:ILE:C	1:A:312:VAL:H	2.09	0.54
1:A:135:VAL:HG21	1:A:182:LEU:HD13	1.90	0.54
1:A:305:THR:HG23	1:A:324:TYR:C	2.29	0.53
1:A:146:LYS:O	1:A:150:ILE:HB	2.08	0.52
1:A:403:ILE:CD1	1:A:403:ILE:H	2.16	0.52
1:A:311:ASN:N	1:A:311:ASN:ND2	2.58	0.52
1:A:348:MET:SD	1:A:351:ILE:HD11	2.49	0.51
1:A:384:ILE:HG21	1:A:386:MET:CE	2.42	0.50
1:A:138:LEU:H	1:A:138:LEU:HD13	1.75	0.50
1:A:330:MET:CE	1:A:330:MET:HA	2.41	0.50
1:A:138:LEU:H	1:A:138:LEU:HD22	1.76	0.50
1:A:315:THR:CG2	1:A:347:LEU:HD22	2.24	0.49
1:A:343:VAL:HG13	1:A:406:PHE:HE2	1.78	0.49
1:A:227:SER:OG	1:A:270:VAL:HG22	2.12	0.49
1:A:315:THR:HG21	1:A:347:LEU:CD2	2.24	0.49
1:A:311:ASN:OD1	1:A:340:ALA:CB	2.60	0.49
1:A:374:THR:HG23	1:A:375:PRO:HD2	1.95	0.48
1:A:349:GLN:HB2	1:A:350:PRO:HD3	1.96	0.48
1:A:384:ILE:HG21	1:A:386:MET:HE3	1.96	0.47
1:A:172:TYR:HA	1:A:276:THR:O	2.14	0.47
1:A:306:THR:O	1:A:309:GLU:HB2	2.16	0.46
1:A:322:GLU:O	1:A:325:ARG:N	2.49	0.46
1:A:331:THR:HB	1:A:334:TYR:HB2	1.98	0.45
1:A:195:PHE:HB3	1:A:217:LEU:HD11	1.98	0.45
1:A:384:ILE:CG2	1:A:386:MET:CE	2.95	0.45
1:A:308:PHE:CE1	1:A:339:ILE:HG23	2.52	0.45
1:A:347:LEU:HD23	1:A:401:LEU:HD11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:ASP:C	1:A:302:ALA:N	2.69	0.44
1:A:300:ASP:C	1:A:302:ALA:H	2.21	0.44
1:A:354:ILE:HD13	1:A:375:PRO:HG2	1.99	0.44
1:A:221:ALA:CB	1:A:229:ILE:HD11	2.47	0.44
1:A:179:LYS:HD2	1:A:179:LYS:N	2.31	0.44
1:A:187:ALA:CB	1:A:228:ILE:HD12	2.47	0.44
1:A:135:VAL:O	1:A:136:ALA:C	2.55	0.43
1:A:342:VAL:HG12	1:A:413:THR:HG21	2.00	0.43
1:A:384:ILE:O	1:A:386:MET:HG2	2.18	0.43
1:A:354:ILE:HD13	1:A:375:PRO:CG	2.49	0.43
1:A:317:CYS:HA	1:A:401:LEU:HB2	2.00	0.42
1:A:256:LEU:HD12	1:A:260:MET:HG3	2.02	0.42
1:A:343:VAL:O	1:A:347:LEU:HG	2.20	0.42
1:A:300:ASP:O	1:A:303:ALA:N	2.52	0.41
1:A:132:TRP:CE3	1:A:135:VAL:HG11	2.55	0.41
1:A:177:THR:H	1:A:179:LYS:HE3	1.85	0.41
1:A:325:ARG:O	1:A:328:GLY:N	2.53	0.41
1:A:406:PHE:O	1:A:410:ILE:HG13	2.19	0.41
1:A:312:VAL:O	1:A:313:GLY:C	2.59	0.41
1:A:178:GLY:O	1:A:179:LYS:C	2.58	0.41
1:A:178:GLY:O	1:A:180:SER:N	2.54	0.41
1:A:339:ILE:O	1:A:343:VAL:HG23	2.20	0.41
1:A:145:LEU:HB3	1:A:186:VAL:HG21	2.02	0.41
1:A:331:THR:HG23	1:A:410:ILE:HD13	2.01	0.41
1:A:318:VAL:CG1	1:A:318:VAL:O	2.67	0.41
1:A:144:ALA:CB	1:A:294:ILE:HD12	2.51	0.41
1:A:330:MET:HA	1:A:330:MET:HE3	2.01	0.40
1:A:374:THR:CG2	1:A:375:PRO:HD2	2.51	0.40
1:A:138:LEU:N	1:A:138:LEU:HD13	2.37	0.40
1:A:144:ALA:HB1	1:A:294:ILE:CD1	2.51	0.40

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	270/331 (82%)	224 (83%)	36 (13%)	10 (4%)	5	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLY
1	A	179	LYS
1	A	301	LEU
1	A	225	LYS
1	A	313	GLY
1	A	223	GLU
1	A	311	ASN
1	A	154	LYS
1	A	155	PHE
1	A	310	ILE

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	239/282 (85%)	214 (90%)	25 (10%)	10	40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	164	LYS
1	A	179	LYS
1	A	180	SER
1	A	182	LEU
1	A	189	GLU
1	A	229	ILE
1	A	268	GLN
1	A	278	ILE
1	A	281	GLN
1	A	292	ARG
1	A	311	ASN
1	A	331	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	335	SER
1	A	341	VAL
1	A	342	VAL
1	A	351	ILE
1	A	352	ARG
1	A	380	ASP
1	A	391	ILE
1	A	398	GLU
1	A	402	THR
1	A	403	ILE
1	A	411	LYS
1	A	430	ARG

Some 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 chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	279/331 (84%)	0.07	1 (0%)	90 66	94, 129, 152, 167	77 (27%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	LEU	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.