

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3P8C
Title	:	Structure and Control of the Actin Regulatory WAVE Complex
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Deposited on	:	2010-10-13
Resolution	:	2.29 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.29 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$				
R _{free}	130704	5042 (2.30-2.30)				
Clashscore	141614	5643 (2.30-2.30)				
Ramachandran outliers	138981	5575(2.30-2.30)				
Sidechain outliers	138945	5575(2.30-2.30)				
RSRZ outliers	127900	4938 (2.30-2.30)				

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	А	1253	5% 88%	5% 6%
2	В	1128	4% 91%	5% •
3	D	279	9% 69% •	27%
4	Е	75	3%	9% 15%
5	F	159	% 96%	• •



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	А	1255	-	-	-	Х
7	CL	А	1256	-	-	-	Х



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23017 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 Cytoplasmic FMR1-interacting protein 1.

Mol	Chain	Residues		Atoms					AltConf	Trace
1	А	1175	Total 9753	C 6235	N 1681	O 1768	S 69	0	14	0

• Molecule 2 is a protein called Nck-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	1086	Total 8782	C 5605	N 1473	0 1634	S 70	0	10	0

• Molecule 3 is a protein called Wiskott-Aldrich syndrome protein family member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	204	Total 1690	C 1060	N 296	O 330	${S \atop 4}$	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	187	GLY	-	linker	UNP Q92558
D	188	GLY	-	linker	UNP Q92558
D	189	SER	-	linker	UNP Q92558
D	190	GLY	-	linker	UNP Q92558
D	191	GLY	-	linker	UNP Q92558
D	192	SER	-	linker	UNP Q92558
D	193	GLY	-	linker	UNP Q92558
D	194	GLY	-	linker	UNP Q92558
D	195	SER	-	linker	UNP Q92558
D	196	GLY	-	linker	UNP Q92558
D	197	GLY	-	linker	UNP Q92558
D	198	SER	-	linker	UNP Q92558
D	199	GLY	-	linker	UNP Q92558
D	200	GLY	-	linker	UNP Q92558



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Chain	Residue	Modelled	Actual	Comment	Reference
D	201	SER	-	linker	UNP Q92558
D	202	GLY	-	linker	UNP Q92558
D	203	GLY	-	linker	UNP Q92558
D	204	SER	-	linker	UNP Q92558

• Molecule 4 is a protein called Probable protein BRICK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Е	64	Total 541	C 337	N 99	0 103	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	1	0

• Molecule 5 is a protein called Abl interactor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	156	Total 1255	C 779	N 227	0 244	${ m S}{ m 5}$	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP B4DSN1

• Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	А	1	Total 8	C 4	N 1	O 3	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	4	Total Cl 4 4	0	0
7	В	3	Total Cl 3 3	0	0

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 9 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	404	Total O 404 404	0	0
9	В	426	Total O 426 426	0	0
9	D	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
9	Е	12	Total O 12 12	0	0
9	F	58	Total O 58 58	0	0



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.









15%

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• Molecule 3: Wiskott-Aldrich syndrome protein family member 1



SER GLU PHE ASP GLU VAL ASP TRP LEU CLU

• Molecule 4: Probable protein BRICK1







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	97.01Å 113.98Å 327.19Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(Å)	47.98 - 2.29	Depositor
Resolution (A)	47.98 - 2.29	EDS
% Data completeness	86.9 (47.98-2.29)	Depositor
(in resolution range)	86.9(47.98-2.29)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$3.57 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
B B.	0.188 , 0.237	Depositor
II, II, <i>free</i>	0.206 , 0.251	DCC
R_{free} test set	7144 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	31.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 27.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23017	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, TRS

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).

Mal	Mol Chain	Bond	lengths	Bond angles	
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.35	0/9960	0.46	0/13440
2	В	0.34	0/8956	0.47	0/12108
3	D	0.34	0/1713	0.46	0/2301
4	Е	0.32	0/548	0.46	0/735
5	F	0.30	0/1270	0.46	0/1716
All	All	0.34	0/22447	0.46	0/30300

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 (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	А	9753	0	9748	42	0
2	В	8782	0	8827	32	0
3	D	1690	0	1698	8	0
4	Е	541	0	541	6	0
5	F	1255	0	1273	3	0
6	А	8	0	12	2	0
7	А	4	0	0	0	0
7	В	3	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	А	18	0	24	1	0
8	В	6	0	8	1	0
9	А	404	0	0	1	0
9	В	426	0	0	0	0
9	D	57	0	0	0	0
9	Ε	12	0	0	0	0
9	F	58	0	0	0	0
All	All	23017	0	22131	79	0

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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 2.

The worst 5 of 79 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:660:MET:HE3	2:B:1117:HIS:HD2	1.45	0.82
1:A:660:MET:CE	2:B:1117:HIS:CD2	2.71	0.73
1:A:660:MET:HE3	2:B:1117:HIS:CD2	2.23	0.72
1:A:498:GLN:HE22	1:A:585:GLU:HG3	1.58	0.67
1:A:660:MET:HE1	2:B:1117:HIS:CD2	2.35	0.60

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	Perce	ntiles
1	А	1175/1253~(94%)	1150 (98%)	24 (2%)	1 (0%)	51	64
2	В	1086/1128~(96%)	1066 (98%)	20 (2%)	0	100	100
3	D	199/279~(71%)	193 (97%)	6 (3%)	0	100	100
4	Е	63/75~(84%)	63 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
5	F	155/159~(98%)	154 (99%)	1 (1%)	0	100	100
All	All	2678/2894~(92%)	2626 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1089	GLY

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	Perce	ntiles
1	А	1080/1131~(96%)	1072 (99%)	8 (1%)	84	92
2	В	992/1021~(97%)	980~(99%)	12 (1%)	71	84
3	D	192/252~(76%)	191 (100%)	1 (0%)	88	95
4	Ε	59/67~(88%)	59~(100%)	0	100	100
5	F	138/140~(99%)	138 (100%)	0	100	100
All	All	2461/2611~(94%)	2440 (99%)	21 (1%)	78	89

5 of 21 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	В	688	SER
2	В	930	TYR
3	D	63	SER
2	В	1002	PHE
2	В	860	SER

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such side chains are listed below:

Mol	Chain	Res	Type
2	В	1117	HIS
	<i>a</i>	-	



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Mol	Chain	Res	Type
2	В	1038	GLN
2	В	774	GLN
2	В	766	ASN
2	В	889	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

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).

Mal	Mol Turno Chair		Res	Link	Bond lengths			Bond angles		
mor Type	Chain	Counts			RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
6	TRS	А	1254	-	7,7,7	0.29	0	9,9,9	0.33	0
8	GOL	А	1259	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.27	0
8	GOL	А	1260	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.26	0
8	GOL	А	1261	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.30	0
8	GOL	В	1132	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	А	1254	-	-	3/9/9/9	-
8	GOL	А	1259	-	-	2/4/4/4	-
8	GOL	А	1260	-	-	2/4/4/4	-
8	GOL	А	1261	-	-	0/4/4/4	-
8	GOL	В	1132	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	1254	TRS	C1-C-C3-O3
6	А	1254	TRS	N-C-C3-O3
8	В	1132	GOL	O1-C1-C2-C3
8	А	1259	GOL	O1-C1-C2-C3
8	А	1260	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	1254	TRS	2	0
8	А	1261	GOL	1	0
8	В	1132	GOL	1	0

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, 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	А	1175/1253~(93%)	0.10	66 (5%) 24 30	2, 12, 46, 99	0
2	В	1086/1128~(96%)	0.03	46 (4%) 36 43	2, 11, 41, 74	0
3	D	204/279~(73%)	0.54	24 (11%) 4 6	5, 27, 92, 110	0
4	Е	64/75~(85%)	-0.02	2 (3%) 49 56	3, 17, 55, 66	0
5	F	156/159~(98%)	-0.06	2 (1%) 77 81	10, 21, 40, 55	0
All	All	2685/2894~(92%)	0.09	140 (5%) 27 34	2, 13, 48, 110	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	234	VAL	8.0
3	D	184	LEU	7.4
3	D	181	GLN	6.7
1	А	198	MET	6.0
1	А	380	ALA	5.7

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)

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,



3P8C	
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	В	1132	6/6	0.59	0.27	62,68,75,91	0
6	TRS	А	1254	8/8	0.60	0.25	67,83,93,94	0
7	CL	А	1256	1/1	0.75	0.50	$93,\!93,\!93,\!93$	0
7	CL	А	1255	1/1	0.78	0.74	86,86,86,86	0
8	GOL	А	1261	6/6	0.79	0.37	72,75,81,84	0
7	CL	В	1129	1/1	0.81	0.37	94,94,94,94	0
8	GOL	А	1259	6/6	0.84	0.30	$63,\!71,\!82,\!83$	0
7	CL	В	1130	1/1	0.87	0.36	$77,\!77,\!77,\!77$	0
7	CL	А	1258	1/1	0.89	0.32	89,89,89,89	0
7	CL	A	1257	1/1	0.90	0.47	103,103,103,103	0
8	GOL	А	1260	6/6	0.93	0.14	82,88,89,95	0
7	CL	В	1131	1/1	0.96	0.46	55, 55, 55, 55	0

median, 95^{th} 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.

6.5 Other polymers (i)

There are no such residues in this entry.

