

# wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID 2BWQ

Title : Crystal Structure of the RIM2 C2A-domain at 1.4 angstrom Resolution Authors Dai, H.; Tomchick, D.R.; Garcia, J.; Sudhof, T.C.; Machius, M.; Rizo, J.

2005-07-15 Deposited on

1.41 Å(reported) Resolution

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

> 1.8.4, CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

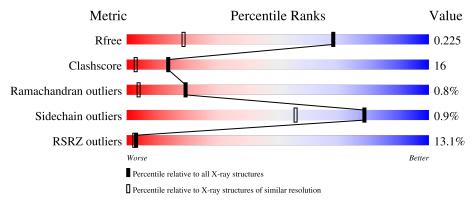
Validation Pipeline (wwPDB-VP) 2.36

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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		
	4	100	12%		
1	Α	129	72%	21%	• 5%

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
2	SO4	A	901	-	-	X	-



## 2 Entry composition (i)

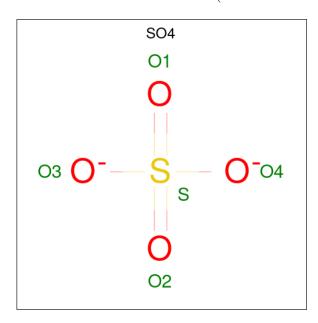
There are 3 unique types of molecules in this entry. The entry contains 1238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 REGULATING SYNAPTIC MEMBRANE EXOCYTOSIS PROTEIN 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	122	Total 1118	C 726	N 194	O 197	S 1	0	9	0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

• Molecule 3 is water.

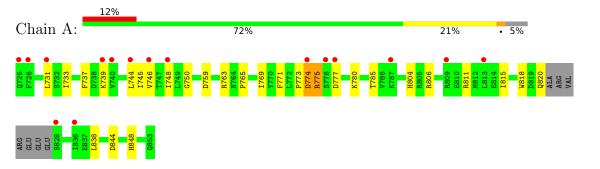
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	110	Total O 110 110	0	2



### 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: REGULATING SYNAPTIC MEMBRANE EXOCYTOSIS PROTEIN 2





## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	25.45Å 44.81Å 55.76Å	Donositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $103.86^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	20.00 - 1.41	Depositor	
resolution (A)	20.91 - 1.41	EDS	
% Data completeness	99.2 (20.00-1.41)	Depositor	
(in resolution range)	99.2 (20.91-1.41)	EDS	
$R_{merge}$	0.02	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	3.88 (at 1.41Å)	Xtriage	
Refinement program	REFMAC 5.2.0003	Depositor	
$R, R_{free}$	0.181 , $0.213$	Depositor	
it, it free	0.199 , $0.225$	DCC	
$R_{free}$ test set	1383 reflections $(5.94\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage	
Anisotropy	0.355	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.41, 57.8	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.33$	Xtriage	
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage	
$F_o, F_c$ correlation	0.96	EDS	
Total number of atoms	1238	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.80% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: 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).

Mal	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.91	0/1145	0.99	4/1543 (0.3%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	A	759	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	777	ASP	CB-CG-OD2	6.48	124.14	118.30
1	A	774	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	763	ARG	NE-CZ-NH2	-5.57	117.52	120.30

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	1118	0	1128	36	0
2	A	10	0	0	3	0
3	A	110	0	0	3	0
All	All	1238	0	1128	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 16.



The worst 5 of 36 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:A:731[A]:LEU:HD11	1:A:748[A]:ILE:CD1	1.90	1.01
1:A:731[A]:LEU:HD11	1:A:748[A]:ILE:HD11	1.02	0.99
1:A:731[A]:LEU:CD1	1:A:748[A]:ILE:HD11	1.94	0.96
1:A:804[B]:HIS:HD2	2:A:901:SO4:O4	1.52	0.90
1:A:748[B]:ILE:HD11	1:A:769:ILE:HD11	1.60	0.84

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	126/129 (98%)	124 (98%)	1 (1%)	1 (1%)	19 4

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	774	ASP

#### 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.

Mo	l Chain	Analysed	Analysed Rotameric		Percentiles		
1	A	124/121 (102%)	123 (99%)	1 (1%)	81 61		



All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	775	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	743	GLN
1	A	848	HIS
1	A	853	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)

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		Dec	Res Link	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	902	-	4,4,4	0.45	0	6,6,6	1.24	1 (16%)
2	SO4	A	901	-	4,4,4	0.33	0	6,6,6	0.30	0



There are no bond length outliers.

All (1) bond angle outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	902	SO4	O3-S-O2	-2.21	97.78	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SO4	1	0
2	A	901	SO4	2	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 $>$	$\# \mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q<0.9	
1	A	122/129 (94%)	0.49	16 (13%)	3	2	10, 15, 27, 33	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	740	VAL	4.6
1	A	725	GLN	4.4
1	A	774	ASP	4.2
1	A	726	PHE	3.0
1	A	809	ARG	2.9

#### 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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	SO4	A	901	5/5	0.91	0.12	25,28,38,39	0
2	SO4	A	902	5/5	0.98	0.15	20,24,29,29	0



## 6.5 Other polymers (i)

There are no such residues in this entry.

