

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 3BRW

Title: Structure of the Rap-RapGAP complex

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Deposited on : 2007-12-21

Resolution : 3.40 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

buster-report : 1.1.7 (2018)

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)

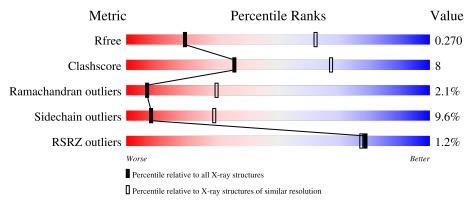
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	A	341	68%	28%	
1	В	341	74%	23%	
1	С	341	74%	21%	
2	D	167	74%	20%	6%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9465 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 Rap1 GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	336	Total	С	N	О	S	0	0	0
1	A	330	2706	1744	453	498	11	0	0	
1	В	337	Total	С	N	О	S	0	0	0
1	Б	337	2709	1745	453	500	11	0	U	
1	С	332	Total	С	N	О	S	0	0	0
1		332	2675	1725	448	491	11	U	U	U

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	ALA	GLN	engineered mutation	UNP P47736
В	204	ALA	GLN	engineered mutation	UNP P47736
С	204	ALA	GLN	engineered mutation	UNP P47736

• Molecule 2 is a protein called Ras-related protein Rap-1b.

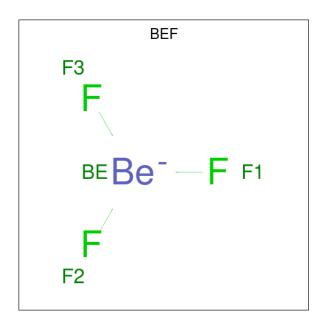
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	167	Total 1332	C 833	N 228	O 263	S 8	0	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0

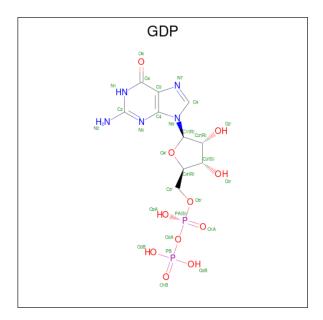
• Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 4	Be 1	F 3	0	0

 \bullet Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
5	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

• Molecule 6 is water.



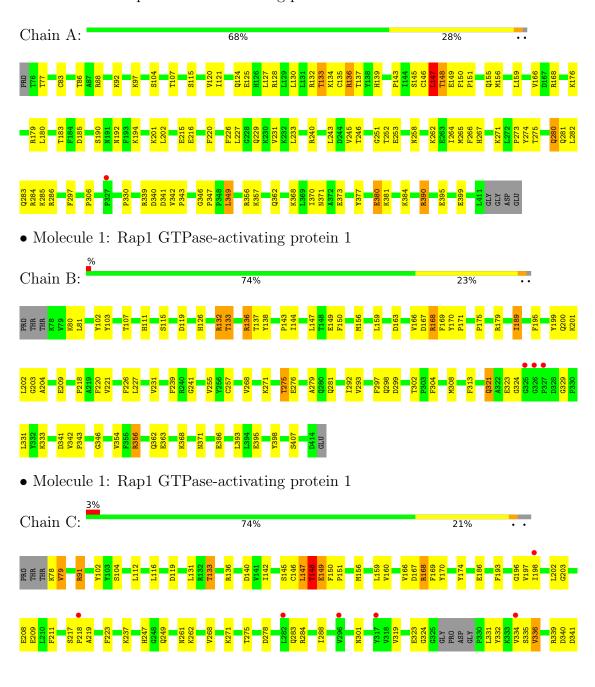
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	В	1	Total O 1 1	0	0
6	С	3	Total O 3 3	0	0
6	D	4	Total O 4 4	0	0



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.

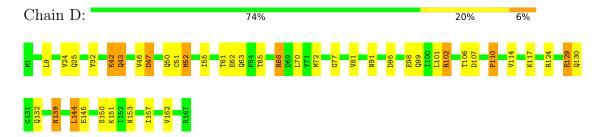
• Molecule 1: Rap1 GTPase-activating protein 1







• Molecule 2: Ras-related protein Rap-1b





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	209.72Å 209.72Å 108.22Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 - 3.40	Depositor
Resolution (A)	48.08 - 3.40	EDS
% Data completeness	99.2 (48.08-3.40)	Depositor
(in resolution range)	99.2 (48.08-3.40)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	3.22 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.234 , 0.280	Depositor
it, it free	0.227 , 0.270	DCC
R_{free} test set	1878 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	86.4	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.27, 43.2	EDS
L-test for twinning ²	$< L > = 0.44, < L^2> = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9465	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: MG, BEF, GDP

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.39	0/2774	0.54	0/3756	
1	В	0.40	0/2777	0.55	0/3760	
1	С	0.40	0/2741	0.52	0/3708	
2	D	0.38	0/1348	0.61	0/1814	
All	All	0.40	0/9640	0.55	0/13038	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	148	THR	Peptide

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	2706	0	2659	50	0
1	В	2709	0	2658	39	0
1	С	2675	0	2628	44	0
2	D	1332	0	1320	25	0
3	D	1	0	0	0	0
4	D	4	0	0	0	0
5	D	28	0	12	2	0
6	A	2	0	0	0	0
6	В	1	0	0	0	0
6	С	3	0	0	0	0
6	D	4	0	0	0	0
All	All	9465	0	9277	151	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.

The worst 5 of 151 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:C:148:THR:HB	1:C:149:GLU:HA	1.23	1.18
1:C:148:THR:CB	1:C:149:GLU:HA	1.98	0.94
1:C:148:THR:HB	1:C:149:GLU:CA	2.04	0.86
1:C:319:VAL:HB	1:C:335:SER:CB	2.18	0.73
1:C:319:VAL:HB	1:C:335:SER:HB3	1.70	0.72

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	$334/341 \ (98\%)$	305 (91%)	23 (7%)	6 (2%)	8 32
1	В	335/341 (98%)	300 (90%)	28 (8%)	7 (2%)	7 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	$\overline{\mathbf{s}}$
1	С	328/341 (96%)	282 (86%)	40 (12%)	6 (2%)	8 32	
2	D	165/167~(99%)	146 (88%)	14 (8%)	5 (3%)	4 23	
All	All	1162/1190 (98%)	1033 (89%)	105 (9%)	24 (2%)	7 30	

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	329	GLY
1	С	79	VAL
1	С	340	ASP
2	D	151	LYS
1	A	134	LYS

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	Percentiles
1	A	$295/300\ (98\%)$	263 (89%)	32 (11%)	6 24
1	В	295/300~(98%)	267 (90%)	28 (10%)	8 29
1	С	$291/300\ (97\%)$	269 (92%)	22 (8%)	13 41
2	D	147/147 (100%)	130 (88%)	17 (12%)	5 20
All	All	1028/1047 (98%)	929 (90%)	99 (10%)	8 29

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	363	GLU
1	С	202	LEU
1	В	393	LEU
1	С	147	LEU
1	С	261	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	362	GLN
2	D	137	GLN
1	В	404	HIS
2	D	43	GLN
1	В	402	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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 Type C		Type Chain Res Lin		Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
4	BEF	D	170	-	0,3,3	-	-	-				
5	GDP	D	171	-	24,30,30	0.89	0	30,47,47	1.37	7 (23%)		

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
5	GDP	D	171	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
5	D	171	GDP	O6-C6-C5	-2.60	119.30	124.37
5	D	171	GDP	C2-N1-C6	-2.58	120.36	125.10
5	D	171	GDP	C5-C6-N1	2.40	118.19	113.95
5	D	171	GDP	O2B-PB-O1B	2.38	120.00	110.68
5	D	171	GDP	PA-O3A-PB	-2.32	124.85	132.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	171	GDP	PA-O3A-PB-O2B

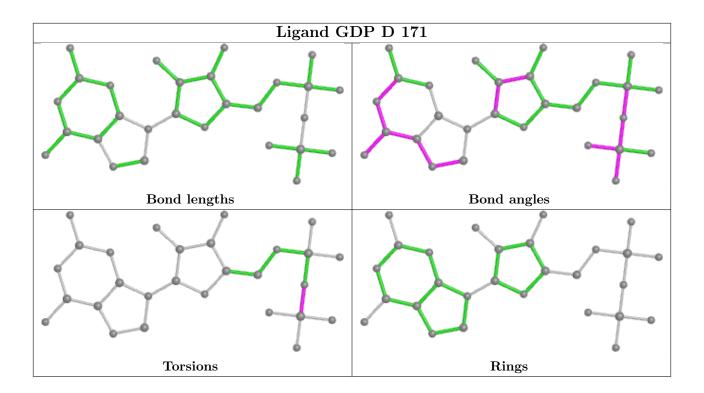
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	171	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	336/341 (98%)	-0.09	1 (0%) 94 93	69, 102, 124, 128	0
1	В	337/341 (98%)	-0.15	3 (0%) 84 83	54, 80, 112, 126	0
1	С	332/341 (97%)	0.14	10 (3%) 50 49	61, 136, 163, 167	0
2	D	167/167 (100%)	-0.19	0 100 100	63, 76, 90, 94	0
All	All	1172/1190 (98%)	-0.06	14 (1%) 79 77	54, 91, 156, 167	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	218	PRO	3.4
1	В	327	PRO	3.2
1	С	282	LEU	3.1
1	С	296	VAL	3.1
1	С	317	TYR	2.7

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.

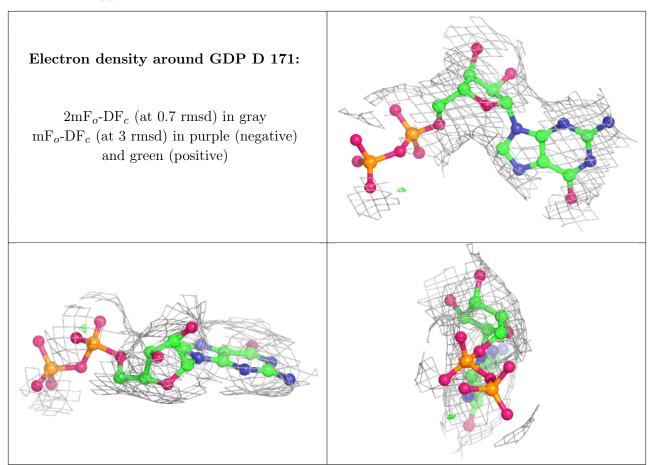
6.4 Ligands (i)

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, 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
3	MG	D	172	1/1	0.98	0.21	68,68,68,68	0
5	GDP	D	171	28/28	0.98	0.20	62,63,63,64	0
4	BEF	D	170	4/4	0.99	0.20	64,64,64,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

