



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:41 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

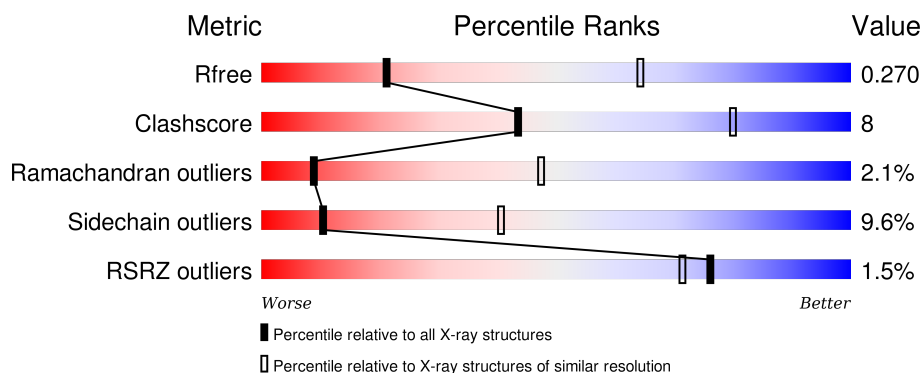
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	341	 68% 28% ..
1	B	341	 74% 23% ..
1	C	341	 74% 21% . .
2	D	167	 74% 20% 6%

2 Entry composition

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	A	336	Total	C	N	O	S	0	0	0
			2706	1744	453	498	11			
1	B	337	Total	C	N	O	S	0	0	0
			2709	1745	453	500	11			
1	C	332	Total	C	N	O	S	0	0	0
			2675	1725	448	491	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	ALA	GLN	ENGINEERED	UNP P47736
B	204	ALA	GLN	ENGINEERED	UNP P47736
C	204	ALA	GLN	ENGINEERED	UNP P47736

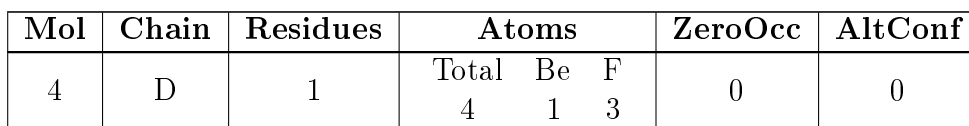
- Molecule 2 is a protein called Ras-related protein Rap-1b.

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

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

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

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

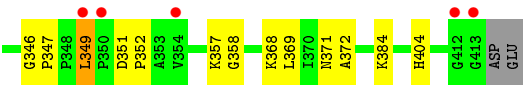


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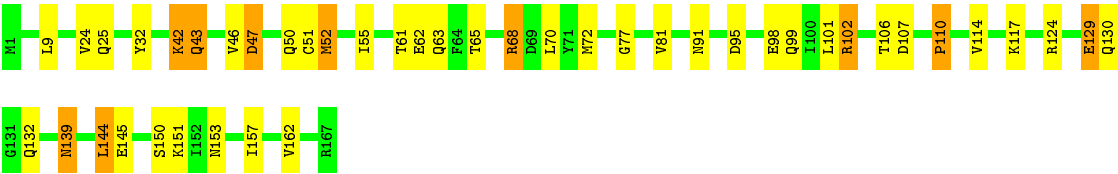
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.72Å 209.72Å 108.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 – 3.40 48.08 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.08-3.40) 99.2 (48.08-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.280 0.227 , 0.270	Depositor DCC
R_{free} test set	1878 reflections (5.25%)	DCC
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 , 43.3	EDS
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 37639 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9465	wwPDB-VP
Average B, all atoms (Å 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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: GDP, MG, BEF

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	0.39	0/2774	0.54	0/3756
1	B	0.40	0/2777	0.55	0/3760
1	C	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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	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	C	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	B	2709	0	2658	39	0
1	C	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	B	1	0	0	0	0
6	C	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	Interatomic distance (Å)	Clash overlap (Å)
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%)	11 50
1	B	335/341 (98%)	300 (90%)	28 (8%)	7 (2%)	9 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	328/341 (96%)	282 (86%)	40 (12%)	6 (2%)	11	50
2	D	165/167 (99%)	146 (88%)	14 (8%)	5 (3%)	5	39
All	All	1162/1190 (98%)	1033 (89%)	105 (9%)	24 (2%)	9	47

5 of 24 Ramachandran outliers are listed below:

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

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	295/300 (98%)	263 (89%)	32 (11%)	8	35
1	B	295/300 (98%)	267 (90%)	28 (10%)	11	41
1	C	291/300 (97%)	269 (92%)	22 (8%)	16	54
2	D	147/147 (100%)	130 (88%)	17 (12%)	7	31
All	All	1028/1047 (98%)	929 (90%)	99 (10%)	10	40

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

Mol	Chain	Res	Type
1	B	227	LEU
1	B	356	ARG
2	D	70	LEU
1	B	255	VAL
1	B	299	ASP

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

Mol	Chain	Res	Type
1	B	321	GLN
1	B	402	HIS
2	D	63	GLN
1	B	362	GLN
1	B	404	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 carbohydrates 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BEF	D	170	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	D	171	-	23,30,30	1.06	1 (4%)	30,47,47	1.67	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
4	BEF	D	170	-	-	0/0/0/0	0/0/0/0
5	GDP	D	171	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	171	GDP	C6-C5	3.54	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	171	GDP	C5-C6-N1	-3.95	118.19	123.59
5	D	171	GDP	N3-C2-N1	-3.84	121.59	127.44
5	D	171	GDP	C2'-C1'-N9	-2.96	109.78	114.29
5	D	171	GDP	PA-O3A-PB	-2.33	124.85	132.67
5	D	171	GDP	C6-C5-C4	-2.08	118.41	120.90

There are no chirality outliers.

There are no torsion outliers.

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

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, 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	336/341 (98%)	-0.07	1 (0%) 94 92	69, 102, 124, 128	0
1	B	337/341 (98%)	-0.12	3 (0%) 85 81	54, 80, 112, 126	0
1	C	332/341 (97%)	0.17	13 (3%) 43 38	61, 136, 163, 167	0
2	D	167/167 (100%)	-0.17	0 100 100	63, 76, 90, 94	0
All	All	1172/1190 (98%)	-0.03	17 (1%) 76 71	54, 91, 156, 167	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	PRO	3.6
1	B	327	PRO	3.3
1	C	282	LEU	3.2
1	C	296	VAL	3.2
1	C	317	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	D	172	1/1	0.98	0.21	0.36	68,68,68,68	0
4	BEF	D	170	4/4	0.99	0.20	-0.05	64,64,64,65	0
5	GDP	D	171	28/28	0.98	0.20	-0.35	62,63,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.