



wwPDB X-ray Structure Validation Summary Report

Sep 29, 2014 – 06:11 PM EDT

PDB ID : 4KVG
Title : Crystal structure of RIAM RA-PH domains in complex with GTP bound Rap1
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Deposited on : 2013-05-22
Resolution : 1.65 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

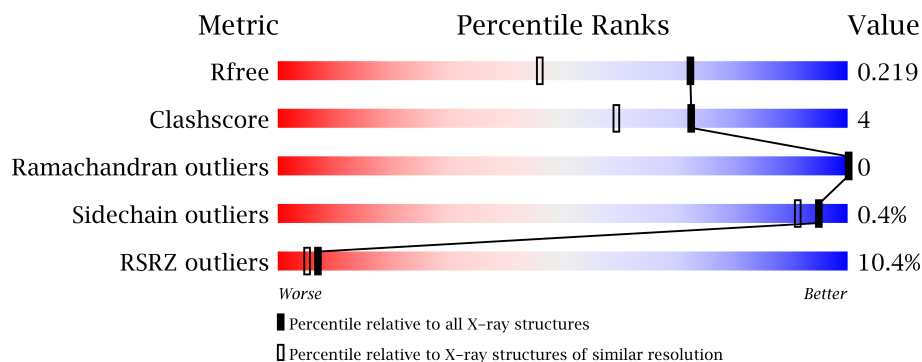
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
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) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 1.65 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	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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	168	
1	C	168	
2	B	260	
2	D	260	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7731 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 Ras-related protein Rap-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	10	0
			1378	868	237	263	10			
1	C	160	Total	C	N	O	S	0	1	0
			1282	804	219	250	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP P62834
A	12	VAL	GLY	ENGINEERED MUTATION	UNP P62834
A	63	GLU	GLN	ENGINEERED MUTATION	UNP P62834
C	0	HIS	-	EXPRESSION TAG	UNP P62834
C	12	VAL	GLY	ENGINEERED MUTATION	UNP P62834
C	63	GLU	GLN	ENGINEERED MUTATION	UNP P62834

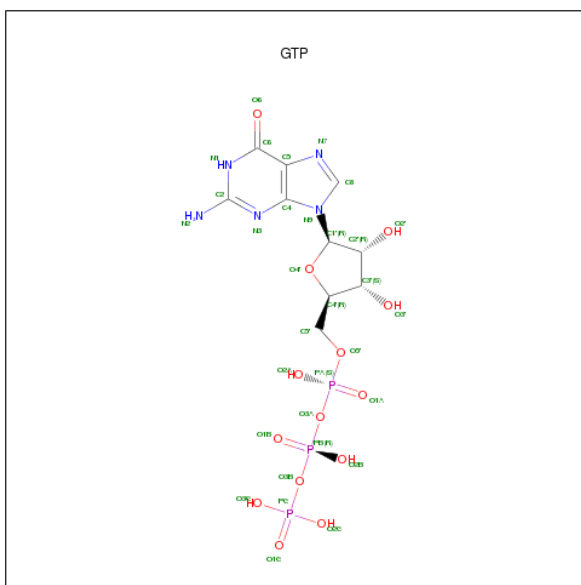
- Molecule 2 is a protein called Amyloid beta A4 precursor protein-binding family B member 1-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	17	0
			2138	1384	349	388	17			
2	D	247	Total	C	N	O	S	0	12	0
			2125	1373	348	387	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	178	MET	-	EXPRESSION TAG	UNP Q8R5A3
D	178	MET	-	EXPRESSION TAG	UNP Q8R5A3

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

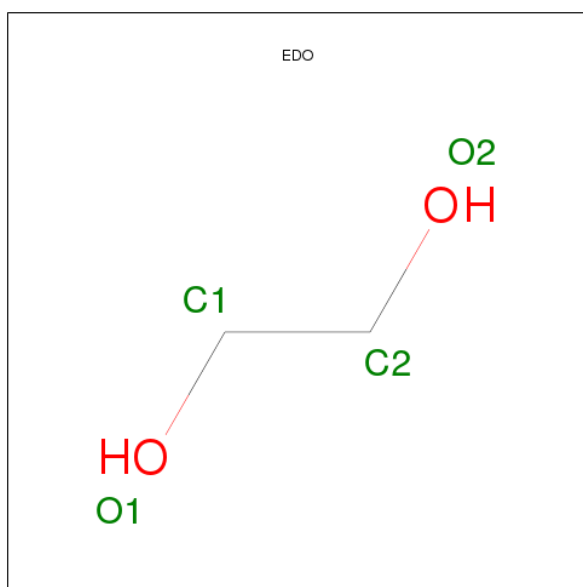


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total	O	0	0
			113	113		
6	B	290	Total	O	0	6
			296	296		
6	C	33	Total	O	0	0
			33	33		
6	D	289	Total	O	0	3
			292	292		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.47Å 85.85Å 160.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.82 – 1.65 47.82 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.82-1.65) 99.3 (47.82-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.219 0.196 , 0.219	Depositor DCC
R_{free} test set	6891 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
Estimated twinning fraction	0.002 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 137213 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7731	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, EDO

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	0.35	1/1418 (0.1%)	0.50	0/1904
1	C	0.33	0/1299	0.47	0/1748
2	B	0.45	2/2233 (0.1%)	0.58	0/3005
2	D	0.44	1/2209 (0.0%)	0.58	0/2971
All	All	0.41	4/7159 (0.1%)	0.55	0/9628

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	250	TRP	CD2-CE2	5.24	1.47	1.41
1	A	138	TRP	CD2-CE2	5.10	1.47	1.41
2	D	330	TRP	CD2-CE2	5.08	1.47	1.41
2	B	330	TRP	CD2-CE2	5.07	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1378	0	1407	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1282	0	1282	9	0
2	B	2138	0	2185	24	0
2	D	2125	0	2155	21	0
3	A	32	0	12	0	0
3	C	32	0	12	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	A	113	0	0	0	0
6	B	296	0	0	3	0
6	C	33	0	0	0	0
6	D	292	0	0	1	0
All	All	7731	0	7065	60	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 4.

The worst 5 of 60 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:311[B]:ILE:HD11	2:B:424[B]:LYS:CG	1.66	1.23
2:B:311[B]:ILE:HD11	2:B:424[B]:LYS:HG2	1.19	1.11
2:B:311[B]:ILE:CD1	2:B:424[B]:LYS:HG3	1.79	1.10
2:D:342[B]:ILE:HG22	2:D:360:ILE:HG22	1.34	1.10
2:B:311[B]:ILE:CD1	2:B:424[B]:LYS:CG	2.33	1.06

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	171/168 (102%)	168 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	157/168 (94%)	154 (98%)	3 (2%)	0	100	100
2	B	259/260 (100%)	255 (98%)	4 (2%)	0	100	100
2	D	256/260 (98%)	250 (98%)	6 (2%)	0	100	100
All	All	843/856 (98%)	827 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	157/150 (105%)	157 (100%)	0	100	100
1	C	144/150 (96%)	143 (99%)	1 (1%)	91	80
2	B	243/239 (102%)	242 (100%)	1 (0%)	95	91
2	D	240/239 (100%)	239 (100%)	1 (0%)	95	91
All	All	784/778 (101%)	781 (100%)	3 (0%)	95	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	351	LYS
1	C	69	ASP
2	D	261	LEU

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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
3	GTP	A	201	4	34,34,34	1.29	5 (14%)	52,54,54	2.70	8 (15%)
5	EDO	B	501	-	3,3,3	0.50	0	2,2,2	0.23	0
3	GTP	C	201	4	34,34,34	1.26	5 (14%)	52,54,54	2.99	9 (17%)
5	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.07	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
3	GTP	A	201	4	-	0/22/38/38	0/3/3/3
5	EDO	B	501	-	-	0/1/1/1	0/0/0/0
3	GTP	C	201	4	-	0/22/38/38	0/3/3/3
5	EDO	D	501	-	-	0/1/1/1	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GTP	C4-N9	-3.33	1.32	1.37
3	C	201	GTP	C5-C4	3.26	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GTP	C5-C4	3.06	1.47	1.40
3	A	201	GTP	C2-N2	2.73	1.36	1.32
3	C	201	GTP	C4-N9	-2.66	1.33	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	GTP	C6-C5-N7	17.50	136.50	134.14
3	A	201	GTP	C6-C5-N7	15.45	136.22	134.14
3	C	201	GTP	C5-C4-N3	-6.16	118.97	126.07
3	C	201	GTP	N3-C4-N9	5.32	134.72	126.91
3	A	201	GTP	C5-C4-N3	-5.29	119.97	126.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	165/168 (98%)	0.04	8 (4%) 29 27	15, 25, 45, 64	0
1	C	160/168 (95%)	1.15	43 (26%) 1 1	25, 54, 98, 113	0
2	B	246/260 (94%)	0.46	15 (6%) 21 18	11, 18, 41, 78	0
2	D	247/260 (95%)	0.45	19 (7%) 13 12	10, 19, 39, 71	0
All	All	818/856 (95%)	0.51	85 (10%) 7 5	10, 22, 75, 113	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	348	GLY	9.9
2	D	353	SER	9.4
2	B	350	THR	9.1
2	B	353	SER	8.0
1	C	108	ASP	7.7

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 ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	B	501	4/4	0.09	1.62	18,19,19,20	0
5	EDO	D	501	4/4	0.12	0.96	19,19,20,22	0
3	GTP	C	201	32/32	0.12	-0.13	29,38,39,39	0
3	GTP	A	201	32/32	0.07	-0.42	15,19,20,21	0
4	MG	A	202	1/1	0.07	-0.71	15,15,15,15	0
4	MG	C	202	1/1	0.07	-0.80	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.