



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 03:31 PM GMT

PDB ID : 1IBR
Title : COMPLEX OF RAN WITH IMPORTIN BETA
Authors : Vetter, I.R.; Arndt, A.; Kutay, U.; Goerlich, D.; Wittinghofer, A.
Deposited on : 1999-05-14
Resolution : 2.30 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>

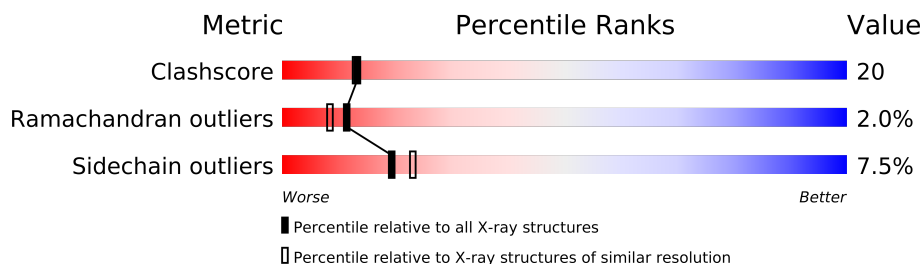
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	
1	C	216	
2	B	462	
2	D	462	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10117 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 GTP-binding nuclear protein RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	1
			1371	890	242	235	4			
1	C	169	Total	C	N	O	S	0	0	1
			1371	890	242	235	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	SER	CONFLICT	UNP P62826
C	129	ARG	SER	CONFLICT	UNP P62826

- Molecule 2 is a protein called Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	458	Total	C	N	O	S	0	0	0
			3573	2255	595	698	25			
2	D	438	Total	C	N	O	S	0	0	0
			3424	2158	573	669	24			

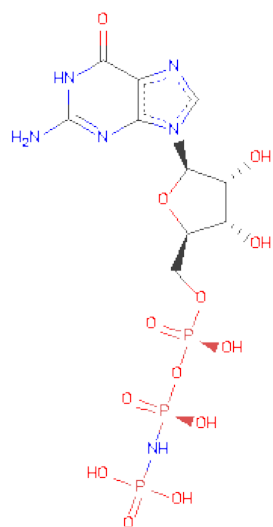
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLN	HIS	CONFLICT	UNP Q14974
D	97	GLN	HIS	CONFLICT	UNP Q14974

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

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

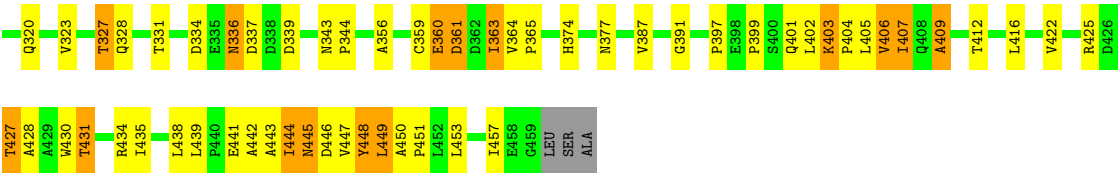
- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

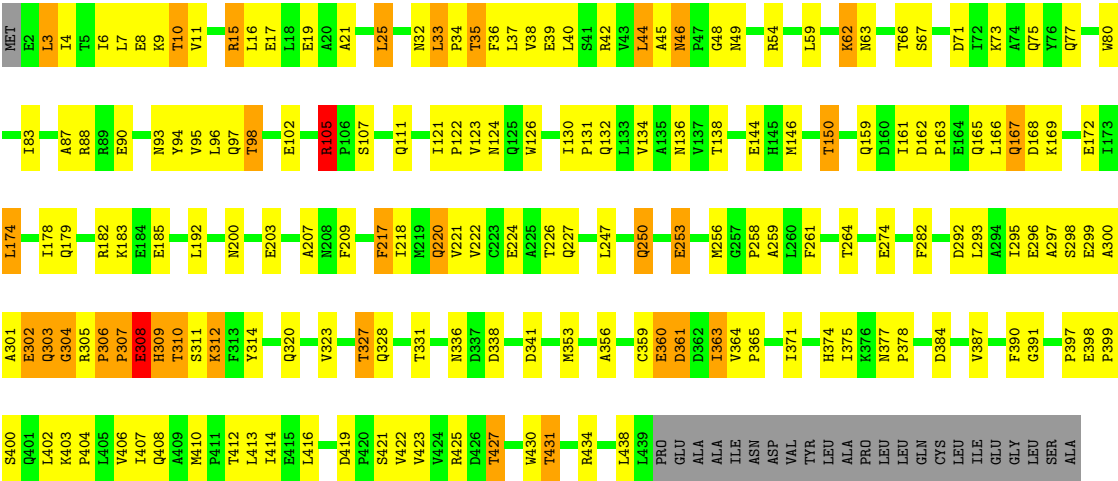
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	121	Total	O	0	0
			121	121		
5	C	29	Total	O	0	0
			29	29		
5	D	85	Total	O	0	0
			85	85		



• Molecule 2: Importin beta-1 subunit

Chain D:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.70Å 108.95Å 114.05Å 90.00° 100.66° 90.00°	Depositor
Resolution (Å)	28.70 – 2.30	Depositor
% Data completeness (in resolution range)	96.7 (28.70-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.245 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10117	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.42	0/1405	0.64	0/1897
1	C	0.41	0/1405	0.63	0/1897
2	B	0.36	0/3638	0.63	1/4954 (0.0%)
2	D	0.36	0/3486	0.63	4/4744 (0.1%)
All	All	0.38	0/9934	0.63	5/13492 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	306	PRO	C-N-CD	-7.15	104.87	120.60
2	D	306	PRO	N-CA-C	-7.15	93.51	112.10
2	D	312	LYS	N-CA-C	-6.19	94.29	111.00
2	D	310	THR	N-CA-C	-6.00	94.80	111.00
2	B	302	GLU	N-CA-C	5.42	125.64	111.00

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	1371	0	1393	49	0
1	C	1371	0	1393	48	0
2	B	3573	0	3564	154	1
2	D	3424	0	3413	158	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	13	4	0
4	C	32	0	13	2	0
5	A	77	0	0	5	0
5	B	121	0	0	6	0
5	C	29	0	0	3	0
5	D	85	0	0	3	0
All	All	10117	0	9789	400	1

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 20.

The worst 5 of 400 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:250:GLN:HE22	2:D:308:GLU:HB3	1.17	1.07
1:C:75:LEU:HD13	2:D:10:THR:HG22	1.37	1.05
2:B:406:VAL:HG23	2:B:407:ILE:H	1.25	0.99
2:D:250:GLN:HE22	2:D:308:GLU:CB	1.77	0.98
2:B:310:THR:HG22	2:B:312:LYS:HD3	1.51	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:164:GLU:OE1	2:D:144:GLU:OE2[2_645]	2.04	0.16

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/216 (77%)	157 (94%)	8 (5%)	2 (1%)	19	19
1	C	167/216 (77%)	156 (93%)	9 (5%)	2 (1%)	19	19
2	B	456/462 (99%)	415 (91%)	30 (7%)	11 (2%)	9	6
2	D	436/462 (94%)	403 (92%)	24 (6%)	9 (2%)	11	8
All	All	1226/1356 (90%)	1131 (92%)	71 (6%)	24 (2%)	11	8

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	303	GLN
2	B	307	PRO
2	B	360	GLU
2	B	407	ILE
2	B	444	ILE

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	148/185 (80%)	143 (97%)	5 (3%)	49	64
1	C	148/185 (80%)	143 (97%)	5 (3%)	49	64
2	B	395/398 (99%)	359 (91%)	36 (9%)	14	15
2	D	379/398 (95%)	345 (91%)	34 (9%)	14	15
All	All	1070/1166 (92%)	990 (92%)	80 (8%)	19	23

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	427	THR
1	C	95	ARG
2	D	361	ASP
2	B	431	THR
2	B	449	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	374	HIS
1	C	114	ASN
2	D	328	GLN
1	C	69	GLN
1	C	100	ASN

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 4 ligands modelled in this entry, 2 are 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	GNP	A	250	3	34,34,34	1.53	7 (20%)	50,54,54	3.28	7 (14%)
4	GNP	C	252	3	34,34,34	1.55	7 (20%)	50,54,54	3.15	7 (14%)

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	GNP	A	250	3	-	1/18/38/38	0/1/3/3
4	GNP	C	252	3	-	1/18/38/38	0/1/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	250	GNP	C2-N3	4.02	1.38	1.33
4	C	252	GNP	C2-N3	3.80	1.38	1.33
4	C	252	GNP	C6-C5	3.23	1.46	1.41
4	A	250	GNP	C6-C5	3.20	1.46	1.41
4	C	252	GNP	PG-O2G	-2.97	1.46	1.55

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	250	GNP	C6-C5-N7	-20.70	131.35	134.14
4	C	252	GNP	C6-C5-N7	-19.64	131.50	134.14
4	C	252	GNP	PB-N3B-PG	-4.98	121.69	130.07
4	A	250	GNP	PB-N3B-PG	-4.43	122.62	130.07
4	A	250	GNP	O3G-PG-O1G	-4.15	102.93	113.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	250	GNP	O1B-PB-N3B-PG
4	C	252	GNP	O1B-PB-N3B-PG

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.