



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:17 am GMT

PDB ID : 3RAN
Title : CANINE GDP-RAN Q69L MUTANT
Authors : Stewart, M.; Kent, H.M.; Mccoy, A.J.
Deposited on : 1998-10-19
Resolution : 2.15 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

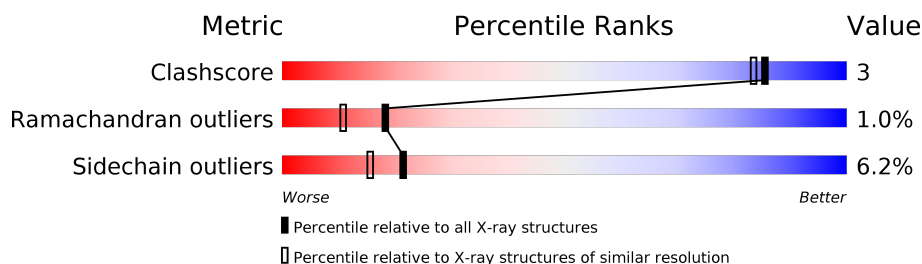
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	 78% 13% •• 7%
1	B	216	 77% 16% • 6%
1	C	216	 81% 10% • 6%
1	D	216	 77% 13% •• 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6829 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 PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	22	0	0
			1612	1045	278	283	6			
1	B	204	Total	C	N	O	S	39	0	0
			1635	1058	282	289	6			
1	C	203	Total	C	N	O	S	11	0	0
			1628	1054	281	287	6			
1	D	203	Total	C	N	O	S	48	0	0
			1628	1054	281	287	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	GLN	ENGINEERED	UNP P62825
B	69	LEU	GLN	ENGINEERED	UNP P62825
C	69	LEU	GLN	ENGINEERED	UNP P62825
D	69	LEU	GLN	ENGINEERED	UNP P62825

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 4 is water.

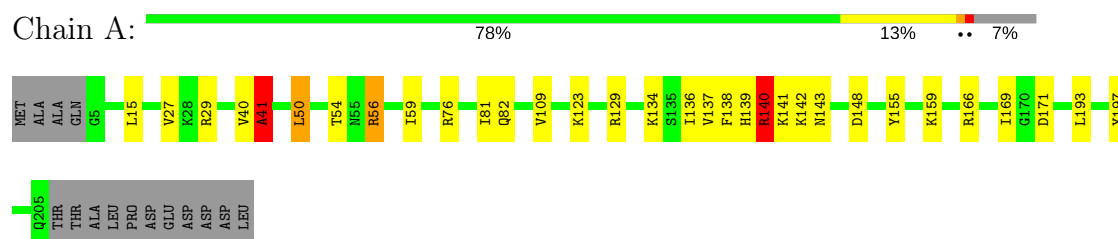
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	9	Total O 9 9	0	0
4	C	73	Total O 73 73	0	0
4	D	72	Total O 72 72	1	0

3 Residue-property plots [i](#)

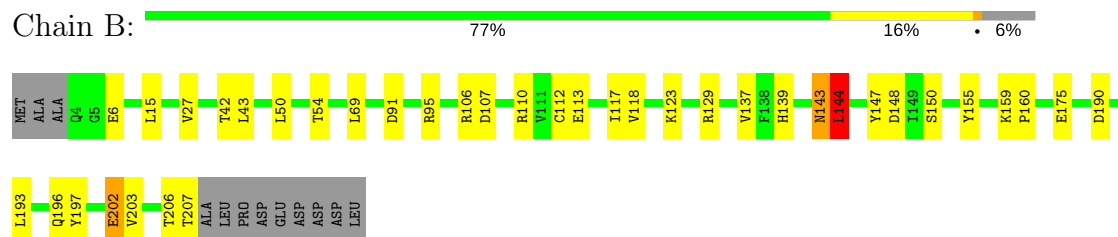
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

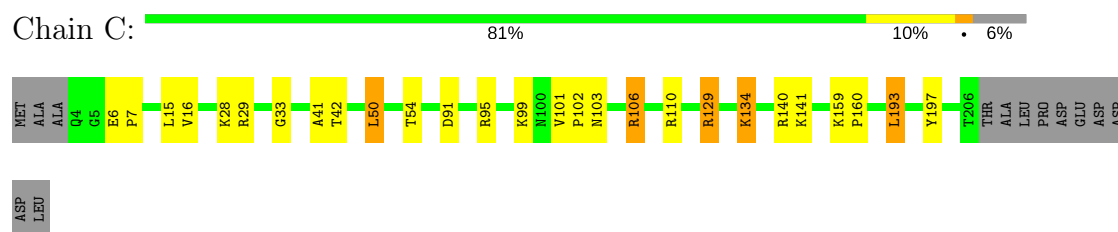
• Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)



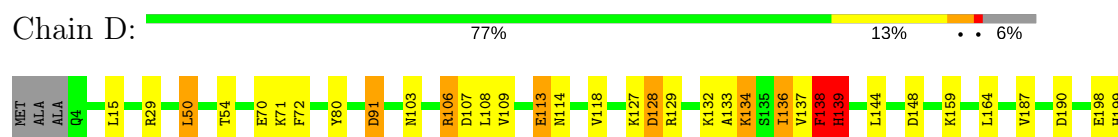
• Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)



• Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)



• Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)



T206	THR
	ALA
	LEU
	PRO
	ASP
	GLU
	ASP
	ASP
	ASP
	LEU

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.09Å 59.17Å 116.37Å 90.00° 100.68° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	94.7 (6.00-2.15)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6829	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

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

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	0.62	0/1653	1.51	14/2240 (0.6%)
1	B	0.60	0/1676	1.43	19/2272 (0.8%)
1	C	0.62	0/1669	1.54	10/2262 (0.4%)
1	D	0.64	0/1669	1.43	15/2262 (0.7%)
All	All	0.62	0/6667	1.48	58/9036 (0.6%)

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	A	0	4
1	B	0	4
1	C	0	2
1	D	0	3
All	All	0	13

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	ARG	CD-NE-CZ	27.00	161.41	123.60
1	A	137	VAL	C-N-CA	17.04	164.29	121.70
1	C	129	ARG	NE-CZ-NH2	15.72	128.16	120.30
1	D	137	VAL	O-C-N	12.87	143.29	122.70
1	A	56	ARG	CD-NE-CZ	11.83	140.16	123.60

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TYR	Mainchain
1	A	27	VAL	Mainchain
1	A	41	ALA	Mainchain
1	A	54	THR	Mainchain
1	B	27	VAL	Mainchain

5.2 Too-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 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	1612	0	1626	6	0
1	B	1635	0	1649	6	2
1	C	1628	0	1642	7	2
1	D	1628	0	1642	14	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	12	1	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	56	0	0	0	0
4	B	9	0	0	0	0
4	C	73	0	0	0	1
4	D	72	0	0	0	0
All	All	6829	0	6607	33	3

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 3.

The worst 5 of 33 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:D:136:ILE:HG22	1:D:136:ILE:O	1.82	0.78
1:D:134:LYS:H	1:D:134:LYS:HE2	1.49	0.78
1:D:138:PHE:O	1:D:138:PHE:HD1	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LYS:O	1:D:128:ASP:HB2	1.98	0.63
1:D:138:PHE:O	1:D:138:PHE:CD1	2.53	0.61

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:OE1	4:C:727:HOH:O[2_646]	1.51	0.69
1:C:28:LYS:NZ	1:D:113:GLU:OE1[2_656]	1.69	0.51
1:B:202:GLU:OE2	1:C:41:ALA:CB[2_646]	1.94	0.26

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	199/216 (92%)	183 (92%)	12 (6%)	4 (2%)	9	3
1	B	202/216 (94%)	191 (95%)	10 (5%)	1 (0%)	32	25
1	C	201/216 (93%)	198 (98%)	3 (2%)	0	100	100
1	D	201/216 (93%)	185 (92%)	13 (6%)	3 (2%)	12	5
All	All	803/864 (93%)	757 (94%)	38 (5%)	8 (1%)	18	11

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	B	137	VAL
1	D	128	ASP
1	D	138	PHE
1	A	140	ARG

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	173/185 (94%)	164 (95%)	9 (5%)	27	22
1	B	176/185 (95%)	166 (94%)	10 (6%)	24	18
1	C	175/185 (95%)	164 (94%)	11 (6%)	21	15
1	D	175/185 (95%)	162 (93%)	13 (7%)	16	10
All	All	699/740 (94%)	656 (94%)	43 (6%)	21	15

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	LEU
1	C	106	ARG
1	D	138	PHE
1	C	42	THR
1	C	50	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	GLN
1	B	103	ASN
1	D	10	GLN
1	B	62	ASN
1	C	105	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 8 ligands modelled in this entry, 4 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	GDP	A	704	2	25,30,30	1.52	5 (20%)	26,47,47	2.59	6 (23%)
3	GDP	B	705	2	25,30,30	1.41	4 (16%)	26,47,47	2.40	3 (11%)
3	GDP	C	706	2	25,30,30	1.47	4 (16%)	26,47,47	2.37	5 (19%)
3	GDP	D	707	2	25,30,30	1.48	4 (16%)	26,47,47	2.18	4 (15%)

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	GDP	A	704	2	-	0/12/32/32	0/3/3/3
3	GDP	B	705	2	-	0/12/32/32	0/3/3/3
3	GDP	C	706	2	-	0/12/32/32	0/3/3/3
3	GDP	D	707	2	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	GDP	PB-O3B	-2.20	1.45	1.54
3	C	706	GDP	C8-N7	-2.14	1.30	1.34
3	B	705	GDP	PB-O3A	2.18	1.63	1.60
3	A	704	GDP	C2-N1	2.25	1.39	1.35
3	D	707	GDP	C2-N1	2.27	1.39	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	704	GDP	C5-C6-N1	-9.87	109.43	123.48
3	B	705	GDP	C5-C6-N1	-9.20	110.38	123.48
3	C	706	GDP	C5-C6-N1	-8.62	111.20	123.48
3	D	707	GDP	C5-C6-N1	-8.25	111.74	123.48
3	B	705	GDP	C2-N3-C4	-2.97	111.69	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	GDP	1	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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.