



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:56 am GMT

PDB ID : 1DCE
Title : CRYSTAL STRUCTURE OF RAB GERANYLGERANYLTRANSFERASE
FROM RAT BRAIN
Authors : Zhang, H.; Seabra, M.C.; Deisenhofer, H.
Deposited on : 1999-11-04
Resolution : 2.00 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

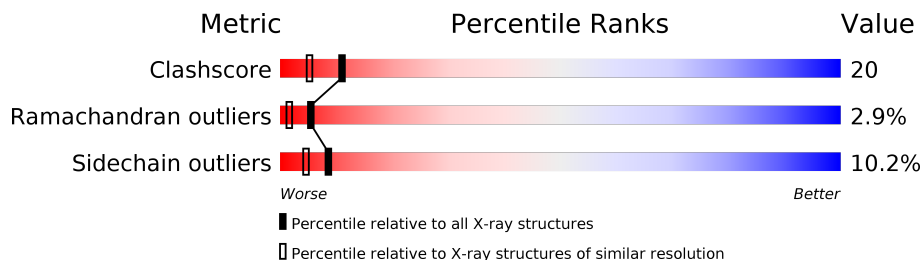
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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	567	
1	C	567	
2	B	331	
2	D	331	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14982 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 (RAB GERANYLGERANYLTRANSFERASE ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	0	0
			4494	2833	794	838	29			
1	C	567	Total	C	N	O	S	0	0	0
			4509	2845	797	838	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	FME	MET	MODIFIED RESIDUE	UNP Q08602
C	1	FME	MET	MODIFIED RESIDUE	UNP Q08602

- Molecule 2 is a protein called PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2574	1642	426	486	20			
2	D	329	Total	C	N	O	S	0	0	0
			2574	1642	426	486	20			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

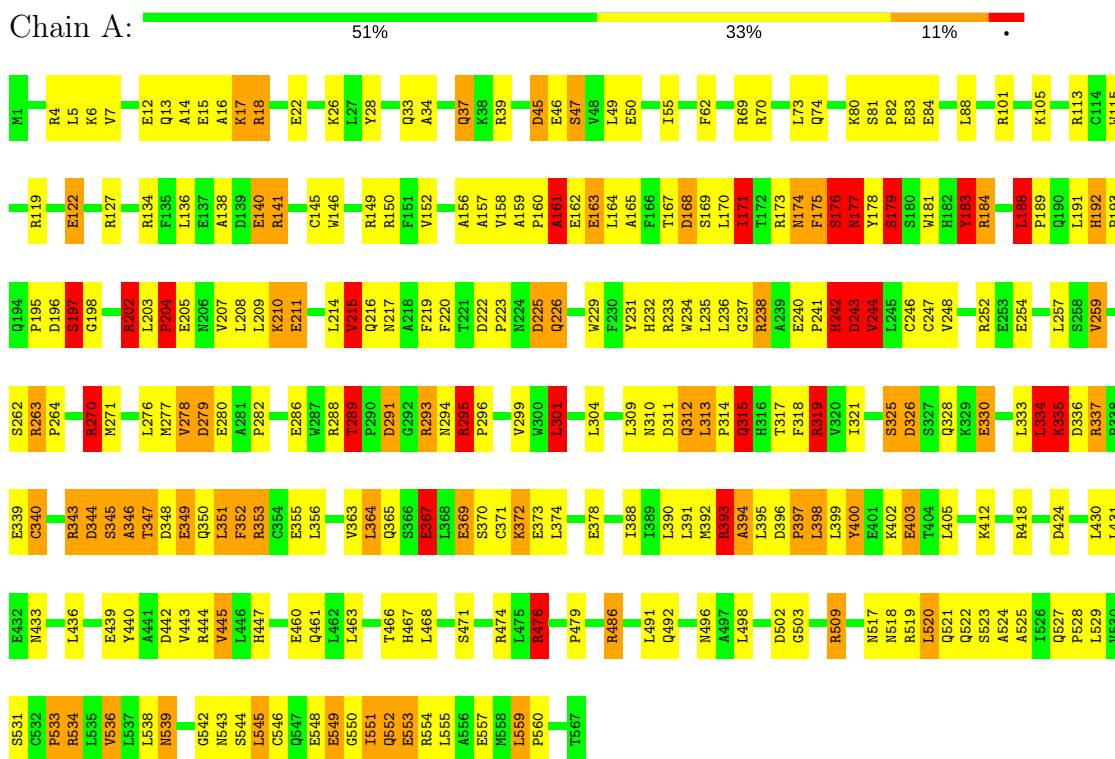
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	280	Total 280	O 280	0	0
4	B	165	Total 165	O 165	0	0
4	C	239	Total 239	O 239	0	0
4	D	145	Total 145	O 145	0	0

3 Residue-property plots

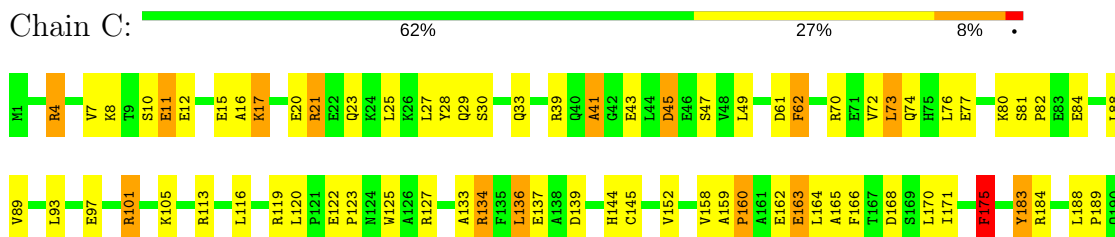
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

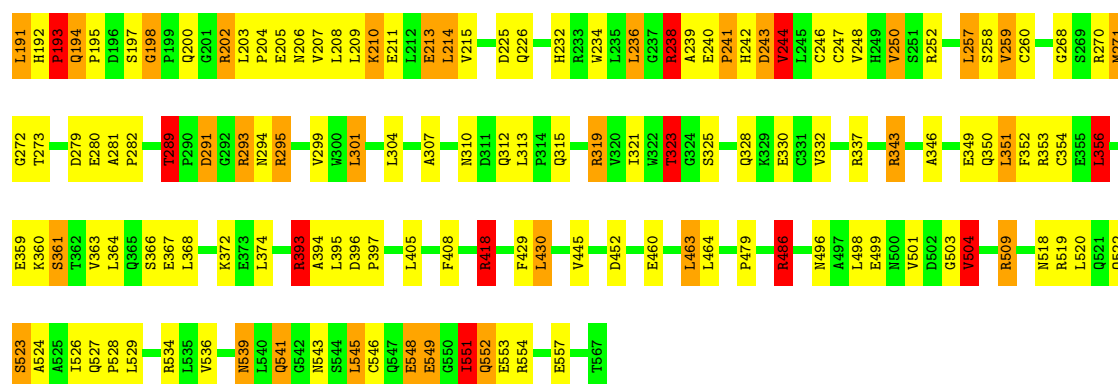
Note EDS was not executed.

- Molecule 1: PROTEIN (RAB GERANYLGERANYLTRANSFERASE ALPHA SUB-UNIT)



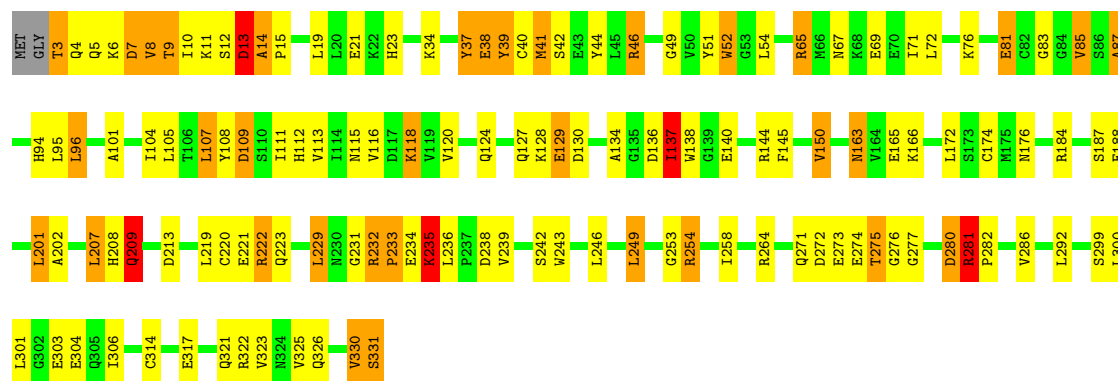
- Molecule 1: PROTEIN (RAB GERANYLGERANYLTRANSFERASE ALPHA SUB-UNIT)





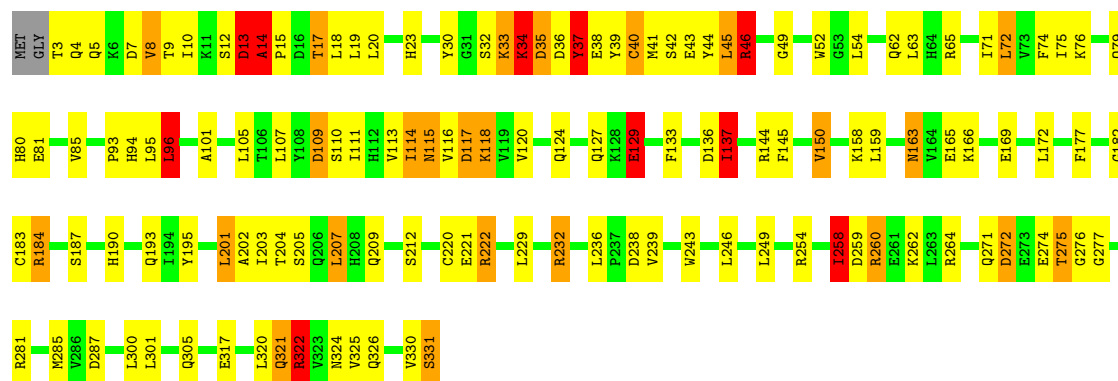
• Molecule 2: PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT)

Chain B: 60% 28% 10% ..



• Molecule 2: PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT)

Chain D: 59% 30% 7% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.86Å 77.44Å 121.78Å 74.60° 79.91° 67.89°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.4 (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14982	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: ZN, FME

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	0.81	0/4581	1.92	135/6235 (2.2%)
1	C	0.73	0/4596	1.79	78/6251 (1.2%)
2	B	0.81	1/2633 (0.0%)	1.64	38/3568 (1.1%)
2	D	0.77	0/2633	1.69	49/3568 (1.4%)
All	All	0.78	1/14443 (0.0%)	1.79	300/19622 (1.5%)

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	9
1	C	0	8
2	B	0	5
2	D	0	4
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	CYS	CB-SG	-5.20	1.73	1.81

The worst 5 of 300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ARG	CD-NE-CZ	34.32	171.65	123.60
1	C	393	ARG	NE-CZ-NH2	-27.36	106.62	120.30
1	C	337	ARG	NE-CZ-NH1	25.95	133.27	120.30
1	A	393	ARG	NE-CZ-NH2	-22.51	109.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	486	ARG	NE-CZ-NH2	-20.90	109.85	120.30

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ALA	Mainchain
1	A	176	SER	Peptide
1	A	211	GLU	Mainchain
1	A	215	VAL	Mainchain
1	A	238	ARG	Peptide

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	4494	0	4406	222	0
1	C	4509	0	4448	150	0
2	B	2574	0	2521	102	0
2	D	2574	0	2521	103	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	280	0	0	35	0
4	B	165	0	0	13	0
4	C	239	0	0	20	0
4	D	145	0	0	14	0
All	All	14982	0	13896	563	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 20.

The worst 5 of 563 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:272:GLY:HA2	1:C:323:THR:HG22	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HB3	1:A:207:VAL:HG13	1.48	0.93
1:A:242:HIS:HA	1:A:263:ARG:HH22	1.28	0.93
2:D:94:HIS:HD2	2:D:96:LEU:H	1.17	0.93
1:A:498:LEU:H	1:A:518:ASN:HD22	1.17	0.92

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	565/567 (100%)	492 (87%)	48 (8%)	25 (4%)	3	1
1	C	565/567 (100%)	503 (89%)	45 (8%)	17 (3%)	5	1
2	B	327/331 (99%)	310 (95%)	12 (4%)	5 (2%)	12	5
2	D	327/331 (99%)	309 (94%)	13 (4%)	5 (2%)	12	5
All	All	1784/1796 (99%)	1614 (90%)	118 (7%)	52 (3%)	5	1

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	158	VAL
1	A	174	ASN
1	A	176	SER
1	A	197	SER

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	490/507 (97%)	437 (89%)	53 (11%)	7	4
1	C	494/507 (97%)	453 (92%)	41 (8%)	13	8
2	B	283/284 (100%)	252 (89%)	31 (11%)	7	4
2	D	283/284 (100%)	250 (88%)	33 (12%)	6	3
All	All	1550/1582 (98%)	1392 (90%)	158 (10%)	8	4

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	163	ASN
1	C	122	GLU
2	D	163	ASN
2	B	207	LEU
2	B	249	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	326	GLN
1	C	217	ASN
2	D	176	ASN
1	C	74	GLN
1	C	232	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	FME	A	1	1	9,9,10	0.99	0	7,9,11	2.51	3 (42%)
1	FME	C	1	1	9,9,10	0.96	0	7,9,11	2.66	3 (42%)

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
1	FME	A	1	1	-	0/6/9/11	0/0/0/0
1	FME	C	1	1	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-5.36	112.65	125.15
1	C	1	FME	O-C-CA	-4.61	114.39	125.15
1	C	1	FME	CA-N-CN	-3.15	117.98	122.82
1	A	1	FME	CA-N-CN	-2.26	119.34	122.82
1	A	1	FME	CB-CA-C	2.93	116.48	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.