



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GND  
Title : GUANINE NUCLEOTIDE DISSOCIATION INHIBITOR, ALPHA-ISOFORM  
Authors : Schalk, I.; Zeng, K.; Wu, S.-K.; Stura, E.A.; Metteson, J.; Huang, M.; Tandon, A.; Wilson, I.A.; Balch, W.E.  
Deposited on : 1996-07-10  
Resolution : 1.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

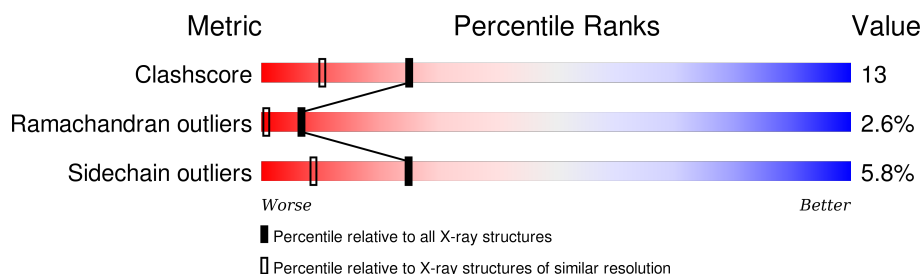
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)

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  $\geq 3$ , 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	447	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3823 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 GUANINE NUCLEOTIDE DISSOCIATION INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3405	2164	560	658	23			

- Molecule 2 is water.

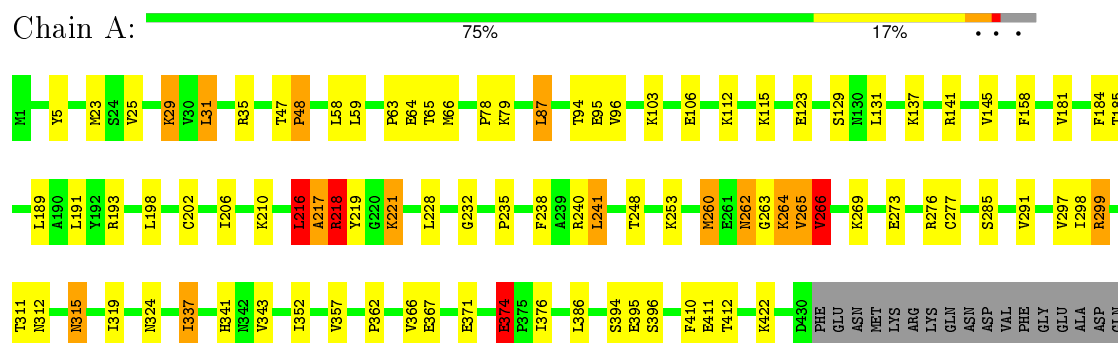
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	418	Total	O	0	0
			418	418		

### 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 errors 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: GUANINE NUCLEOTIDE DISSOCIATION INHIBITOR



## 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, $\alpha$ , $\beta$ , $\gamma$	91.80 Å   43.50 Å   63.20 Å 90.00°   104.50°   90.00°	Depositor
Resolution (Å)	6.00 – 1.81	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.81)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.198 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.50	0/3474	0.75	4/4701 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	374	GLU	N-CA-C	5.43	125.66	111.00
1	A	311	THR	N-CA-C	-5.27	96.76	111.00
1	A	216	LEU	N-CA-C	5.22	125.09	111.00
1	A	241	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3405	0	3370	86	0
2	A	418	0	0	23	0
All	All	3823	0	3370	86	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 13.

All (86) 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:A:219:TYR:CD1	1:A:221:LYS:HE3	2.21	0.76
1:A:141:ARG:O	1:A:145:VAL:HG23	1.85	0.76
1:A:216:LEU:HD12	1:A:217:ALA:H	1.56	0.70
1:A:411:GLU:HB2	2:A:500:HOH:O	1.92	0.70
1:A:79:LYS:HG2	2:A:731:HOH:O	1.94	0.67
1:A:367:GLU:O	1:A:371:GLU:HG3	1.96	0.65
1:A:218:ARG:NH1	1:A:219:TYR:HD2	1.94	0.65
1:A:48:PRO:HB3	2:A:717:HOH:O	1.96	0.64
1:A:265:VAL:O	1:A:266:VAL:HG13	1.97	0.64
1:A:232:GLY:O	1:A:235:PRO:HD2	1.98	0.63
1:A:123:GLU:CD	1:A:145:VAL:HG22	2.19	0.62
1:A:298:ILE:HG21	2:A:742:HOH:O	2.00	0.61
1:A:221:LYS:HD3	2:A:807:HOH:O	2.03	0.58
1:A:263:GLY:O	1:A:265:VAL:HG23	2.04	0.57
1:A:78:PRO:HG3	1:A:352:ILE:HD13	1.86	0.57
1:A:260:MET:HB2	1:A:264:LYS:O	2.04	0.57
1:A:202:CYS:SG	2:A:655:HOH:O	2.57	0.57
1:A:298:ILE:CG1	1:A:357:VAL:HG22	2.35	0.57
1:A:299:ARG:NH1	2:A:727:HOH:O	2.37	0.56
1:A:216:LEU:HA	2:A:656:HOH:O	2.06	0.55
1:A:218:ARG:HH12	1:A:219:TYR:HD2	1.53	0.55
1:A:366:VAL:HG12	1:A:366:VAL:O	2.07	0.54
1:A:185:THR:HA	1:A:189:LEU:HD12	1.89	0.54
1:A:315:ASN:HD22	1:A:315:ASN:C	2.12	0.53
1:A:218:ARG:HD3	1:A:219:TYR:HB2	1.91	0.53
1:A:79:LYS:CD	2:A:843:HOH:O	2.58	0.52
1:A:394:SER:O	1:A:395:GLU:HB2	2.10	0.52
1:A:79:LYS:HD3	2:A:843:HOH:O	2.11	0.51
1:A:29:LYS:HD3	2:A:451:HOH:O	2.10	0.51
1:A:206:ILE:HD11	2:A:743:HOH:O	2.09	0.51
1:A:47:THR:O	1:A:47:THR:HG22	2.12	0.50
1:A:158:PHE:CD1	1:A:158:PHE:N	2.79	0.50
1:A:29:LYS:HE2	2:A:536:HOH:O	2.10	0.50
1:A:411:GLU:HG2	1:A:412:THR:HG23	1.94	0.50
1:A:319:ILE:HG21	2:A:748:HOH:O	2.12	0.49
1:A:262:ASN:ND2	2:A:696:HOH:O	2.46	0.49
1:A:129:SER:O	1:A:137:LYS:HE2	2.13	0.48
1:A:218:ARG:NH1	1:A:219:TYR:CD2	2.78	0.48
1:A:5:TYR:O	1:A:277:CYS:HA	2.13	0.48
1:A:298:ILE:HG13	1:A:357:VAL:HG22	1.95	0.47
1:A:298:ILE:HD13	1:A:362:PRO:O	2.14	0.47
1:A:35:ARG:NH2	1:A:285:SER:OG	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:N	1:A:411:GLU:OE1	2.47	0.47
1:A:96:VAL:HG11	1:A:238:PHE:CD1	2.50	0.47
1:A:299:ARG:NH2	2:A:727:HOH:O	2.43	0.47
1:A:218:ARG:NH1	1:A:219:TYR:HB2	2.29	0.46
1:A:106:GLU:HG3	1:A:221:LYS:HD2	1.96	0.46
1:A:181:VAL:HA	1:A:184:PHE:CE2	2.51	0.46
1:A:374:GLU:O	1:A:376:ILE:N	2.48	0.46
1:A:337:ILE:HG13	1:A:343:VAL:HG21	1.98	0.46
1:A:141:ARG:NH2	2:A:756:HOH:O	2.48	0.45
1:A:129:SER:OG	1:A:131:LEU:HB2	2.16	0.45
1:A:264:LYS:HB2	1:A:396:SER:HA	1.99	0.45
1:A:216:LEU:O	1:A:217:ALA:HB3	2.17	0.45
1:A:262:ASN:HB3	2:A:697:HOH:O	2.16	0.45
1:A:262:ASN:C	1:A:264:LYS:H	2.21	0.44
1:A:411:GLU:HG2	1:A:412:THR:N	2.33	0.44
1:A:264:LYS:CB	1:A:396:SER:HA	2.47	0.44
1:A:94:THR:O	1:A:95:GLU:HB2	2.15	0.44
1:A:219:TYR:CE1	1:A:221:LYS:HE3	2.53	0.44
1:A:374:GLU:O	1:A:376:ILE:HG13	2.17	0.44
1:A:78:PRO:O	1:A:79:LYS:HG2	2.18	0.44
1:A:253:LYS:HE2	1:A:253:LYS:HB3	1.73	0.44
1:A:31:LEU:HD23	1:A:248:THR:OG1	2.18	0.44
1:A:297:VAL:HG13	1:A:386:LEU:HD11	2.00	0.44
1:A:47:THR:HB	1:A:48:PRO:HD3	2.00	0.43
1:A:299:ARG:NH1	2:A:495:HOH:O	2.50	0.43
1:A:64:GLU:HG2	1:A:65:THR:HG23	2.00	0.43
1:A:23:MET:HA	1:A:23:MET:CE	2.48	0.43
1:A:411:GLU:CG	1:A:412:THR:N	2.82	0.43
1:A:5:TYR:CZ	1:A:31:LEU:HG	2.54	0.42
1:A:58:LEU:HA	1:A:58:LEU:HD12	1.88	0.42
1:A:319:ILE:CG2	2:A:748:HOH:O	2.67	0.42
1:A:269:LYS:HA	1:A:273:GLU:O	2.20	0.42
1:A:228:LEU:HD12	1:A:228:LEU:HA	1.89	0.42
1:A:217:ALA:HB2	2:A:547:HOH:O	2.21	0.41
1:A:25:VAL:HG21	1:A:94:THR:HA	2.02	0.41
1:A:312:ASN:HB3	2:A:674:HOH:O	2.21	0.41
1:A:96:VAL:HG11	1:A:238:PHE:CE1	2.55	0.41
1:A:103:LYS:HB3	1:A:341:HIS:NE2	2.36	0.41
1:A:63:PRO:HD2	1:A:66:MET:HG3	2.03	0.41
1:A:87:LEU:HD13	1:A:410:PHE:HB3	2.02	0.41
1:A:158:PHE:N	1:A:158:PHE:HD1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG2	1:A:65:THR:N	2.37	0.40
1:A:263:GLY:HA3	2:A:828:HOH:O	2.21	0.40
1:A:394:SER:O	1:A:395:GLU:CB	2.69	0.40

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	428/447 (96%)	401 (94%)	16 (4%)	11 (3%)	<b>7</b> <b>1</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	218	ARG
1	A	262	ASN
1	A	374	GLU
1	A	265	VAL
1	A	48	PRO
1	A	266	VAL
1	A	217	ALA
1	A	221	LYS
1	A	260	MET
1	A	264	LYS

### 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	378/393 (96%)	356 (94%)	22 (6%)	25 9

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	31	LEU
1	A	59	LEU
1	A	87	LEU
1	A	112	LYS
1	A	115	LYS
1	A	191	LEU
1	A	193	ARG
1	A	198	LEU
1	A	210	LYS
1	A	218	ARG
1	A	240	ARG
1	A	241	LEU
1	A	266	VAL
1	A	276	ARG
1	A	291	VAL
1	A	299	ARG
1	A	315	ASN
1	A	324	ASN
1	A	337	ILE
1	A	374	GLU
1	A	422	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	73	ASN
1	A	130	ASN
1	A	207	ASN
1	A	262	ASN
1	A	310	ASN
1	A	315	ASN
1	A	325	GLN

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Mol	Chain	Res	Type
1	A	378	GLN
1	A	409	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](#)

There are no ligands in this entry.

### 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 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.