



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:12 PM GMT

PDB ID : 3DDC  
Title : Crystal Structure of NORE1A in Complex with RAS  
Authors : Stieglitz, B.; Bee, C.; Schwarz, D.; Yildiz, O.; Moshnikova, A.; Khokhlatchev, A.; Herrmann, C.  
Deposited on : 2008-06-05  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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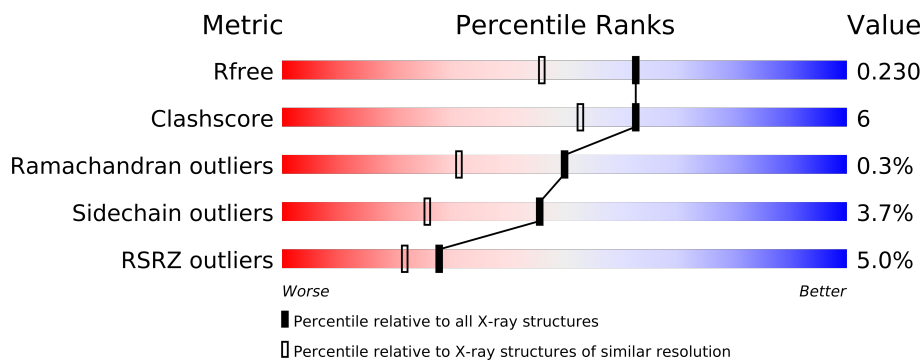
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. 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	166	
2	B	163	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2542 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 GTPase HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1323	826	229	261	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLU	ASP	ENGINEERED MUTATION	UNP P01112
A	31	LYS	GLU	ENGINEERED MUTATION	UNP P01112

- Molecule 2 is a protein called Ras association domain-containing family protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1071	695	179	193	4			

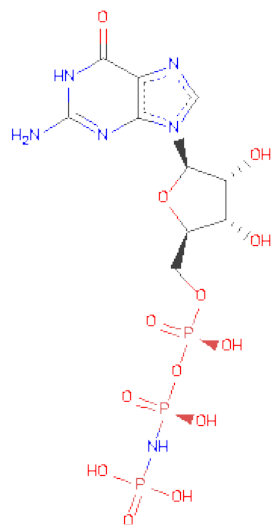
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	GLY	-	EXPRESSION TAG	UNP Q5EBH1
B	196	SER	-	EXPRESSION TAG	UNP Q5EBH1
B	197	PRO	-	EXPRESSION TAG	UNP Q5EBH1
B	198	GLU	-	EXPRESSION TAG	UNP Q5EBH1
B	199	PHE	-	EXPRESSION TAG	UNP Q5EBH1
B	285	MET	LEU	ENGINEERED MUTATION	UNP Q5EBH1
B	302	ASP	LYS	ENGINEERED MUTATION	UNP Q5EBH1

- 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		

- 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
			Total	C	N	O	P		
4	A	1	32	10	6	13	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	50	Total	O	0	0
			50	50		

### 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.

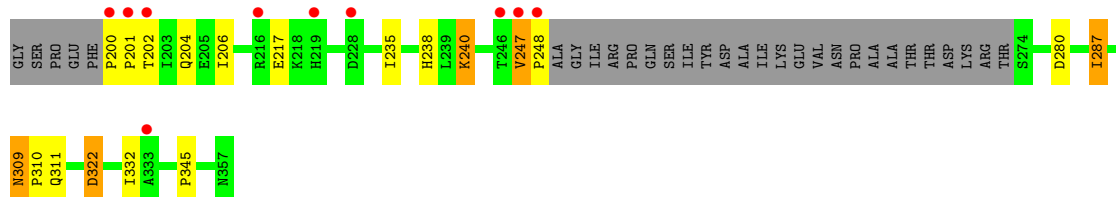
- Molecule 1: GTPase HRas

Chain A: 



- Molecule 2: Ras association domain-containing family protein 5

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.60Å 88.00Å 56.50Å 90.00° 125.00° 90.00°	Depositor
Resolution (Å)	19.59 – 1.80 19.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.59-1.80) 99.3 (19.59-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.193 , 0.230 0.192 , 0.230	Depositor DCC
$R_{free}$ test set	1466 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29320 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 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	0.71	0/1342	0.72	1/1810 (0.1%)
2	B	0.67	0/1093	0.72	0/1474
All	All	0.69	0/2435	0.72	1/3284 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	LEU	CA-CB-CG	5.04	126.89	115.30

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	1323	0	1303	11	0
2	B	1071	0	1112	16	0
3	A	1	0	0	0	0
4	A	32	0	13	0	0
5	A	65	0	0	1	0
5	B	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2542	0	2428	27	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 6.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:GLU:H	1:A:30:GLU:CD	1.74	0.91
2:B:247:VAL:HB	2:B:248:PRO:CD	2.15	0.75
1:A:63:GLU:OE1	5:A:638:HOH:O	2.05	0.74
2:B:247:VAL:HB	2:B:248:PRO:HD3	1.82	0.62
2:B:238:HIS:HE1	2:B:280:ASP:OD1	1.85	0.59
1:A:41:ARG:HG2	1:A:54:ASP:OD1	2.04	0.58
1:A:47:ASP:HB2	1:A:164:ARG:HH22	1.69	0.56
2:B:309:ASN:HD22	2:B:309:ASN:C	2.13	0.52
2:B:240:LYS:HE3	2:B:280:ASP:OD2	2.10	0.52
2:B:235:ILE:HG12	2:B:287:ILE:HD12	1.92	0.51
2:B:217:GLU:HG2	2:B:345:PRO:HB3	1.91	0.51
1:A:70:GLN:CD	1:A:70:GLN:H	2.14	0.50
1:A:56:LEU:CD2	1:A:71:TYR:HB2	2.43	0.49
2:B:201:PRO:HG2	2:B:206:ILE:HD11	1.94	0.49
1:A:108:ASP:O	1:A:166:HIS:NE2	2.46	0.49
2:B:200:PRO:N	2:B:201:PRO:HA	2.29	0.48
1:A:22:GLN:HE21	1:A:149:ARG:HH11	1.62	0.47
2:B:202:THR:HG22	2:B:204:GLN:H	1.80	0.47
2:B:235:ILE:HG23	2:B:287:ILE:HD11	1.97	0.46
1:A:22:GLN:HE21	1:A:149:ARG:NH1	2.14	0.46
2:B:309:ASN:ND2	2:B:311:GLN:H	2.15	0.45
2:B:309:ASN:HD22	2:B:310:PRO:N	2.15	0.45
1:A:72:MET:SD	1:A:99:GLN:HG2	2.57	0.44
2:B:322:ASP:OD1	2:B:322:ASP:N	2.51	0.44
2:B:202:THR:HG22	2:B:204:GLN:N	2.35	0.41
1:A:111:MET:HB3	1:A:111:MET:HE3	1.79	0.41
2:B:287:ILE:N	2:B:287:ILE:HD13	2.36	0.41

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	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
2	B	129/163 (79%)	127 (98%)	1 (1%)	1 (1%)	27	9
All	All	293/329 (89%)	287 (98%)	5 (2%)	1 (0%)	50	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	247	VAL

### 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	144/144 (100%)	139 (96%)	5 (4%)	48	28
2	B	123/147 (84%)	118 (96%)	5 (4%)	41	21
All	All	267/291 (92%)	257 (96%)	10 (4%)	45	26

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	30	GLU
1	A	32	TYR
1	A	63	GLU
1	A	107	ASP
2	B	240	LYS
2	B	287	ILE
2	B	309	ASN

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Mol	Chain	Res	Type
2	B	322	ASP
2	B	332	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	GLN
1	A	61	GLN
1	A	129	GLN
2	B	208	GLN
2	B	238	HIS
2	B	309	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	500	3	34,34,34	1.53	6 (17%)	50,54,54	3.90	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	500	3	-	0/18/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	GNP	PG-O1G	4.04	1.51	1.46
4	A	500	GNP	PB-N3B	-3.28	1.61	1.64
4	A	500	GNP	PB-O1B	3.16	1.50	1.46
4	A	500	GNP	C2-N2	2.63	1.36	1.32
4	A	500	GNP	PG-O3G	-2.53	1.47	1.55
4	A	500	GNP	C8-N7	-2.01	1.30	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	GNP	C6-C5-N7	-26.19	130.61	134.14
4	A	500	GNP	C6-N1-C2	3.01	124.77	119.51
4	A	500	GNP	C2-N3-C4	-2.86	111.07	115.09
4	A	500	GNP	C5-C4-N3	2.27	129.23	125.94
4	A	500	GNP	C8-N9-C4	-2.19	105.23	106.90
4	A	500	GNP	O1G-PG-N3B	-2.10	108.66	111.83
4	A	500	GNP	O3'-C3'-C2'	2.09	118.64	111.83

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	166/166 (100%)	0.17	5 (3%)	48	40	17, 24, 36, 54	0
2	B	133/163 (81%)	0.30	10 (7%)	14	10	17, 24, 44, 51	0
All	All	299/329 (90%)	0.23	15 (5%)	28	22	17, 24, 39, 54	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	PRO	7.5
2	B	200	PRO	5.8
2	B	247	VAL	5.7
1	A	166	HIS	5.1
2	B	246	THR	4.7
2	B	201	PRO	4.0
1	A	107	ASP	3.7
1	A	108	ASP	3.2
2	B	219	HIS	2.8
2	B	202	THR	2.6
2	B	216	ARG	2.5
1	A	122	ALA	2.4
2	B	228	ASP	2.3
1	A	105	ASP	2.1
2	B	333	ALA	2.0

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	GNP	A	500	32/32	0.08	-0.66	13,18,20,22	0
3	MG	A	600	1/1	0.07	-1.46	14,14,14,14	0

## 6.5 Other polymers

There are no such residues in this entry.