



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 12:08 PM EST

PDB ID : 2R6Z  
Title : Crystal structure of the SAM-dependent methyltransferase NGO1261 from *Neisseria gonorrhoeae*, Northeast Structural Genomics Consortium Target NgR48  
Authors : Forouhar, F.; Abashidze, M.; Seetharaman, J.; Mao, L.; Nwosu, C.; Fang, Y.; Xiao, R.; Baran, M.C.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2007-09-06  
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

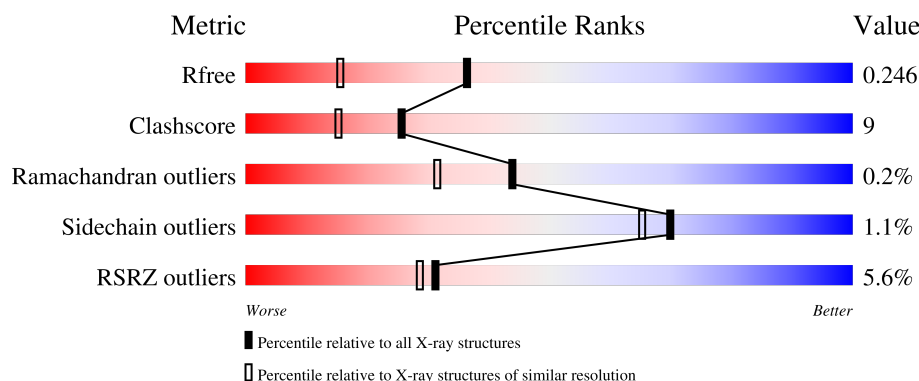
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	258	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>13%</div> </div> </div>
1	B	258	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4051 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 UPF0341 protein in rsp 3' region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	Se	0	0	0
			1734	1100	305	325	1	3			
1	B	242	Total	C	N	O	S	Se	0	0	0
			1864	1179	334	347	1	3			

There are 16 discrepancies between the modelled and reference sequences:

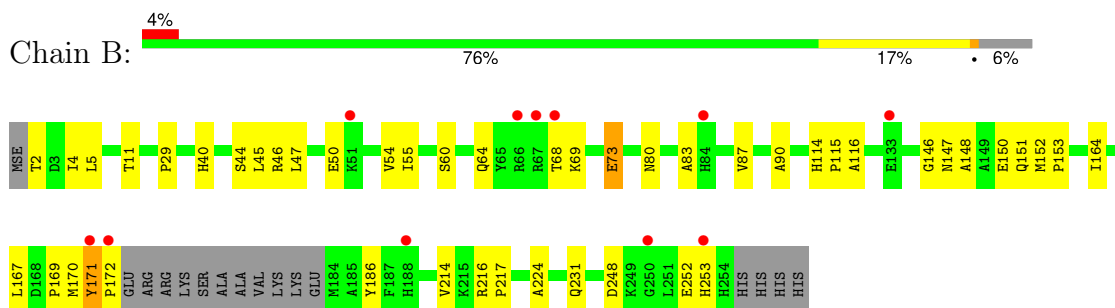
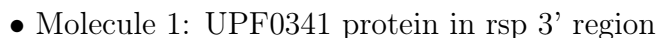
Chain	Residue	Modelled	Actual	Comment	Reference
A	251	LEU	-	expression tag	UNP P72077
A	252	GLU	-	expression tag	UNP P72077
A	253	HIS	-	expression tag	UNP P72077
A	254	HIS	-	expression tag	UNP P72077
A	255	HIS	-	expression tag	UNP P72077
A	256	HIS	-	expression tag	UNP P72077
A	257	HIS	-	expression tag	UNP P72077
A	258	HIS	-	expression tag	UNP P72077
B	251	LEU	-	expression tag	UNP P72077
B	252	GLU	-	expression tag	UNP P72077
B	253	HIS	-	expression tag	UNP P72077
B	254	HIS	-	expression tag	UNP P72077
B	255	HIS	-	expression tag	UNP P72077
B	256	HIS	-	expression tag	UNP P72077
B	257	HIS	-	expression tag	UNP P72077
B	258	HIS	-	expression tag	UNP P72077

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	193	Total	O	0	0
			193	193		
2	B	260	Total	O	0	0
			260	260		



- Molecule 1: UPF0341 protein in rsp 3' region



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.23Å 43.19Å 103.57Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	26.82 – 1.80 26.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.4 (26.82-1.80) 92.0 (26.82-1.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 1.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.215 , 0.231 0.230 , 0.246	Depositor DCC
$R_{free}$ test set	4569 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.28	0/1766	0.54	0/2401
1	B	0.31	0/1902	0.60	0/2585
All	All	0.30	0/3668	0.57	0/4986

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1734	0	1742	31	0
1	B	1864	0	1863	40	0
2	A	193	0	0	2	0
2	B	260	0	0	5	0
All	All	4051	0	3605	68	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 9.

All (68) 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:B:45:LEU:HB3	1:B:54:VAL:HG22	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:HD21	1:A:149:ALA:HB3	1.43	0.83
1:B:45:LEU:HB3	1:B:54:VAL:CG2	2.08	0.82
1:B:171:TYR:H	1:B:172:PRO:HD2	1.52	0.75
1:A:131:ASN:HD21	1:A:133:GLU:HG3	1.52	0.73
1:A:188:HIS:HE1	1:B:170:MSE:HG2	1.60	0.67
1:B:90:ALA:HB3	1:B:167:LEU:HD23	1.80	0.64
1:B:171:TYR:N	1:B:172:PRO:HD2	2.11	0.64
1:B:64:GLN:O	1:B:68:THR:HG23	1.98	0.63
1:A:90:ALA:HB3	1:A:167:LEU:HD23	1.82	0.62
1:A:88:TRP:HB3	1:A:152:MSE:HE2	1.85	0.58
1:A:152:MSE:O	1:A:156:VAL:HG23	2.02	0.58
1:A:107:THR:HG22	2:A:382:HOH:O	2.04	0.57
1:B:69:LYS:HA	1:B:73:GLU:OE1	2.05	0.56
1:A:51:LYS:N	1:A:51:LYS:HD2	2.19	0.56
1:A:131:ASN:ND2	1:A:133:GLU:HG3	2.22	0.55
1:A:147:ASN:ND2	1:A:149:ALA:HB3	2.18	0.55
1:B:5:LEU:HD22	1:B:29:PRO:HG3	1.88	0.55
1:A:92:ALA:HB2	1:A:110:ALA:HB1	1.89	0.55
1:B:171:TYR:H	1:B:172:PRO:CD	2.19	0.54
1:A:90:ALA:HB3	1:A:167:LEU:CD2	2.38	0.54
1:B:148:ALA:O	1:B:152:MSE:HG3	2.07	0.54
1:A:31:GLU:HG2	1:A:32:GLN:HG3	1.89	0.54
1:B:46:ARG:NE	2:B:372:HOH:O	2.43	0.52
1:A:88:TRP:HB3	1:A:152:MSE:CE	2.40	0.52
1:A:74:LEU:HD22	1:A:234:GLY:HA3	1.92	0.52
1:B:171:TYR:N	1:B:172:PRO:CD	2.73	0.52
1:A:131:ASN:HD21	1:A:133:GLU:CG	2.22	0.51
1:B:224:ALA:HA	2:B:331:HOH:O	2.11	0.51
1:A:184:MSE:HE3	1:B:170:MSE:SE	2.60	0.50
1:B:47:LEU:HD23	1:B:50:GLU:HG3	1.92	0.50
1:B:231:GLN:HG3	2:B:436:HOH:O	2.10	0.50
1:A:152:MSE:HB2	1:A:153:PRO:HD3	1.96	0.48
1:B:44:SER:HB3	1:B:55:ILE:HG12	1.96	0.48
1:B:68:THR:C	1:B:69:LYS:HD2	2.34	0.48
1:A:114:HIS:HD2	1:A:116:ALA:H	1.61	0.48
1:A:16:THR:HA	1:A:19:ARG:HH11	1.79	0.47
1:B:171:TYR:CD2	1:B:172:PRO:HD3	2.50	0.47
1:A:15:ARG:O	1:A:19:ARG:HG3	2.16	0.46
1:A:42:THR:HG23	2:A:379:HOH:O	2.15	0.46
1:B:44:SER:CB	1:B:55:ILE:HG12	2.46	0.46
1:A:155:LEU:HD11	1:A:159:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HG2	1:B:216:ARG:NH2	2.32	0.45
1:B:46:ARG:HD3	2:B:286:HOH:O	2.17	0.45
1:B:90:ALA:HB3	1:B:167:LEU:CD2	2.46	0.44
1:B:146:GLY:HA3	1:B:151:GLN:OE1	2.17	0.44
1:B:80:ASN:ND2	1:B:83:ALA:HB2	2.32	0.44
1:A:235:LYS:HG3	1:A:236:SER:H	1.83	0.43
1:B:248:ASP:O	1:B:252:GLU:HG2	2.19	0.43
1:A:92:ALA:CB	1:A:110:ALA:HB1	2.49	0.43
1:B:152:MSE:N	1:B:153:PRO:CD	2.82	0.42
1:B:11:THR:HG23	1:B:40:HIS:O	2.20	0.42
1:B:172:PRO:HB2	1:B:217:PRO:HG2	2.02	0.42
1:A:17:LEU:C	1:A:17:LEU:HD23	2.40	0.42
1:B:4:ILE:O	1:B:4:ILE:HG23	2.19	0.42
1:B:60:SER:O	1:B:64:GLN:HG2	2.20	0.42
1:A:165:VAL:HG23	1:A:208:ALA:HB2	2.02	0.42
1:B:147:ASN:OD1	1:B:150:GLU:HG3	2.20	0.41
1:B:186:TYR:HB3	2:B:432:HOH:O	2.18	0.41
1:B:167:LEU:HD12	1:B:214:VAL:HG22	2.01	0.41
1:B:2:THR:HG21	1:B:116:ALA:HB2	2.03	0.41
1:B:46:ARG:HE	1:B:46:ARG:HB3	1.75	0.41
1:B:87:VAL:HG22	1:B:164:ILE:HB	2.02	0.41
1:A:161:LYS:HB3	1:A:209:LYS:HG3	2.01	0.41
1:A:169:PRO:O	1:A:170:MSE:HG2	2.21	0.41
1:A:188:HIS:ND1	1:B:170:MSE:HE3	2.36	0.40
1:B:114:HIS:HA	1:B:115:PRO:HD3	1.94	0.40
1:A:45:LEU:HB2	1:A:120:LEU:HD11	2.04	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	219/258 (85%)	210 (96%)	9 (4%)	0	100	100
1	B	238/258 (92%)	233 (98%)	4 (2%)	1 (0%)	30	19
All	All	457/516 (89%)	443 (97%)	13 (3%)	1 (0%)	44	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	TYR

### 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	184/205 (90%)	182 (99%)	2 (1%)	70	65
1	B	195/205 (95%)	193 (99%)	2 (1%)	73	68
All	All	379/410 (92%)	375 (99%)	4 (1%)	70	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	LYS
1	A	231	GLN
1	B	73	GLU
1	B	253	HIS

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

Mol	Chain	Res	Type
1	A	40	HIS
1	A	81	HIS
1	A	114	HIS
1	A	131	ASN
1	A	142	ASN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	188	HIS
1	A	226	GLN
1	B	202	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 oligosaccharides 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

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	222/258 (86%)	0.46	15 (6%) 25 22	12, 27, 44, 55	0
1	B	239/258 (92%)	0.24	11 (4%) 38 35	11, 23, 40, 56	0
All	All	461/516 (89%)	0.34	26 (5%) 31 29	11, 25, 42, 56	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	TYR	6.8
1	B	253	HIS	4.0
1	A	218	ARG	3.5
1	A	158	THR	3.2
1	B	172	PRO	3.2
1	B	84	HIS	3.1
1	A	82	THR	2.9
1	B	188	HIS	2.7
1	A	188	HIS	2.7
1	A	131	ASN	2.7
1	B	67	ARG	2.7
1	B	66	ARG	2.6
1	A	84	HIS	2.5
1	A	51	LYS	2.5
1	B	51	LYS	2.5
1	A	237	THR	2.4
1	B	133	GLU	2.4
1	A	185	ALA	2.4
1	B	250	GLY	2.4
1	A	150	GLU	2.4
1	A	142	ASN	2.3
1	A	252	GLU	2.2
1	B	68	THR	2.1
1	A	156	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	220	GLY	2.0
1	A	246	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.