



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:56 PM UTC

PDB ID : 3S7Y / pdb_00003s7y
Title : Crystal structure of mmNAGS in Space Group P3121 at 4.3 Å resolution
Authors : Shi, D.; Li, Y.; Cabrera-Luque, J.; Jin, Z.; Yu, X.; Allewell, N.M.; Tuchman, M.
Deposited on : 2011-05-27
Resolution : 4.31 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

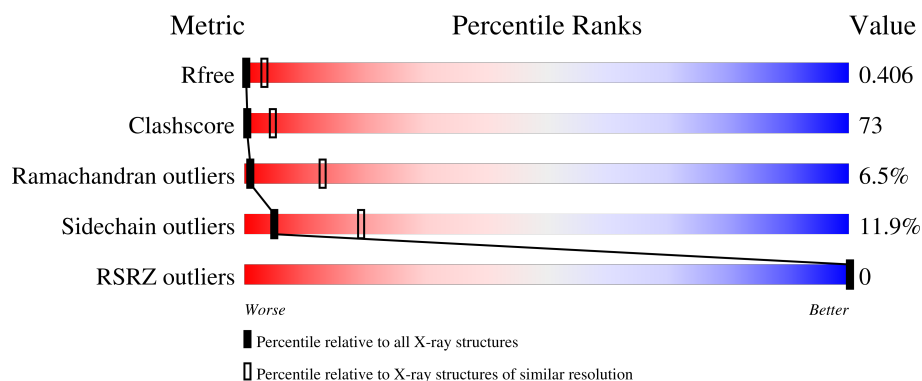
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.31 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}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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 ≥ 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	461	
1	X	461	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6683 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 N-acetylglutamate kinase / N-acetylglutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	1	0
			3349	2107	605	631	6			
1	X	435	Total	C	N	O	S	0	0	0
			3334	2097	601	630	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q0ASS9
A	-18	GLY	-	expression tag	UNP Q0ASS9
A	-17	SER	-	expression tag	UNP Q0ASS9
A	-16	SER	-	expression tag	UNP Q0ASS9
A	-15	HIS	-	expression tag	UNP Q0ASS9
A	-14	HIS	-	expression tag	UNP Q0ASS9
A	-13	HIS	-	expression tag	UNP Q0ASS9
A	-12	HIS	-	expression tag	UNP Q0ASS9
A	-11	HIS	-	expression tag	UNP Q0ASS9
A	-10	HIS	-	expression tag	UNP Q0ASS9
A	-9	SER	-	expression tag	UNP Q0ASS9
A	-8	SER	-	expression tag	UNP Q0ASS9
A	-7	GLY	-	expression tag	UNP Q0ASS9
A	-6	LEU	-	expression tag	UNP Q0ASS9
A	-5	VAL	-	expression tag	UNP Q0ASS9
A	-4	PRO	-	expression tag	UNP Q0ASS9
A	-3	ARG	-	expression tag	UNP Q0ASS9
A	-2	GLY	-	expression tag	UNP Q0ASS9
A	-1	SER	-	expression tag	UNP Q0ASS9
A	0	HIS	-	expression tag	UNP Q0ASS9
X	-19	MET	-	expression tag	UNP Q0ASS9
X	-18	GLY	-	expression tag	UNP Q0ASS9
X	-17	SER	-	expression tag	UNP Q0ASS9
X	-16	SER	-	expression tag	UNP Q0ASS9
X	-15	HIS	-	expression tag	UNP Q0ASS9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	-14	HIS	-	expression tag	UNP Q0ASS9
X	-13	HIS	-	expression tag	UNP Q0ASS9
X	-12	HIS	-	expression tag	UNP Q0ASS9
X	-11	HIS	-	expression tag	UNP Q0ASS9
X	-10	HIS	-	expression tag	UNP Q0ASS9
X	-9	SER	-	expression tag	UNP Q0ASS9
X	-8	SER	-	expression tag	UNP Q0ASS9
X	-7	GLY	-	expression tag	UNP Q0ASS9
X	-6	LEU	-	expression tag	UNP Q0ASS9
X	-5	VAL	-	expression tag	UNP Q0ASS9
X	-4	PRO	-	expression tag	UNP Q0ASS9
X	-3	ARG	-	expression tag	UNP Q0ASS9
X	-2	GLY	-	expression tag	UNP Q0ASS9
X	-1	SER	-	expression tag	UNP Q0ASS9
X	0	HIS	-	expression tag	UNP Q0ASS9

GLN	V372	L308	A173	Q238	I106	
	V373	D309	I174	A239		I108
	N374	N310	L175	I109		
	R375	L311	A176			
	A380	A315	G177		L113	
	P381	F316	L178	T114		
	Q382	G317	G179			Q115
	L383	R318	E180		A116	
	L384	E322	R247	T181		
	V385	G323	L248			P182
R386	Y324	K249	D183			
S387	W325	L250		G184		
R388	R327	E251			T185	
T389	D326	L186	V121			
N390	R327	K254		I124		
N391	L328	R255			I189	
P392	R329	L256	N190			
V393	S330	D258		A191		
N394	D331	D259			D192	
G395	R332	L260	V193			
F398	A333	P261		V195		
	F334	L262			R196	
	V335	S263	A197			
	C401	S264		H200		
	D402	S265			A201	
	G403	V266	L202			
	A404	S267		Q203		
	V405	L268			P204	
	R406	T269	Y205			
	R407	R270		K206		
D408	E273	V207				
E409	L274		V208			
W410	A275			F209		
T411	R276	L210				
V412	R347		T211			
F413	L348			G212		
W414	D349	L278				
P420	G350		F279			
	W351			T286		
	V352	L287				
	L353		I288			
	V423			R289		
	A424	R290				
	D425		G291			
	V426			E292		
	V427	V359				
	E428		L360			
K429	D361					
A430		D362				
F431			A363			
A432	R364					
L433		G365				
P434			E366			
P435	G367					
T436		L368				
L437			G369			
E438	R370					
A439		T371				
PR0			R307			
Q236	M237					
		A172				

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.11Å 95.11Å 253.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.13 – 4.31 31.13 – 4.31	Depositor EDS
% Data completeness (in resolution range)	92.1 (31.13-4.31) 89.1 (31.13-4.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.274 , 0.419 0.259 , 0.406	Depositor DCC
R_{free} test set	949 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	192.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 436.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6683	wwPDB-VP
Average B, all atoms (Å ²)	456.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.05	7/3412 (0.2%)	1.87	123/4639 (2.7%)
1	X	0.91	7/3393 (0.2%)	1.44	53/4613 (1.1%)
All	All	0.98	14/6805 (0.2%)	1.67	176/9252 (1.9%)

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	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ALA	CA-CB	-8.54	1.38	1.53
1	X	352	VAL	C-O	-8.33	1.15	1.24
1	A	174	ILE	CA-CB	-7.39	1.44	1.54
1	A	43	ILE	CA-CB	-7.22	1.44	1.54
1	A	95	VAL	CA-CB	6.92	1.63	1.54

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	134	VAL	CA-C-N	16.01	137.16	120.83
1	X	134	VAL	C-N-CA	16.01	137.16	120.83
1	A	344	ILE	N-CA-C	14.99	129.63	107.75
1	A	134	VAL	CA-C-N	14.06	137.91	120.89
1	A	134	VAL	C-N-CA	14.06	137.91	120.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLN	Sidechain
1	A	413	PHE	Mainchain

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	3349	0	3352	549	0
1	X	3334	0	3332	473	0
All	All	6683	0	6684	982	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 73.

The worst 5 of 982 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:296:ALA:O	1:A:297:THR:HG22	1.21	1.26
1:A:398:PHE:CD1	1:X:398:PHE:CD1	2.33	1.15
1:A:95:VAL:H	1:A:100:VAL:CG1	1.59	1.14
1:A:295:VAL:HG22	1:A:335:VAL:O	1.46	1.14
1:A:266:VAL:O	1:A:287:LEU:HA	1.47	1.14

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	435/461 (94%)	360 (83%)	46 (11%)	29 (7%)	1	12
1	X	433/461 (94%)	349 (81%)	57 (13%)	27 (6%)	1	13
All	All	868/922 (94%)	709 (82%)	103 (12%)	56 (6%)	1	13

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	89	ASP
1	A	95	VAL
1	A	96	ASP
1	A	99	ARG

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	346/367 (94%)	305 (88%)	41 (12%)	5	19
1	X	344/367 (94%)	302 (88%)	42 (12%)	5	19
All	All	690/734 (94%)	607 (88%)	83 (12%)	5	19

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	190	ASN
1	X	344	ILE
1	X	206	LYS
1	X	254	LYS
1	X	362	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	18	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	65	GLN
1	X	394	ASN
1	X	80	GLN
1	A	65	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	436/461 (94%)	-0.86	0 100 100	185, 421, 690, 893	1 (0%)
1	X	435/461 (94%)	-0.87	0 100 100	209, 472, 685, 784	0
All	All	871/922 (94%)	-0.87	0 100 100	185, 454, 688, 893	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.