



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 05:24 pm GMT

PDB ID : 4HG5  
Title : Structural insights into yeast Nit2: wild-type yeast Nit2 in complex with oxaloacetate  
Authors : Liu, H.; Qiu, X.; Zhang, M.; Gao, Y.; Niu, L.; Teng, M.  
Deposited on : 2012-10-07  
Resolution : 1.91 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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

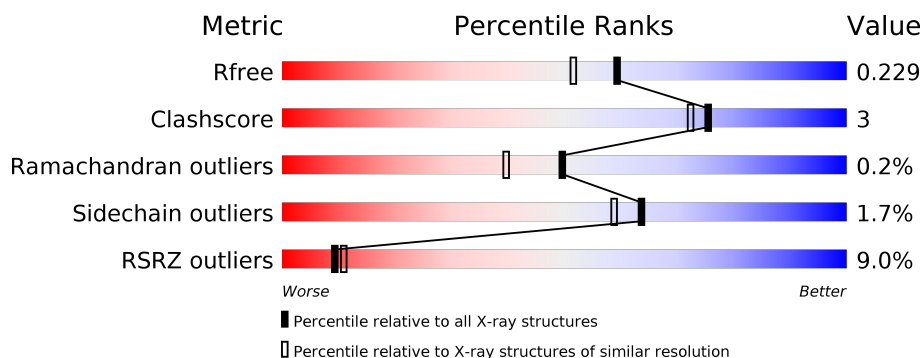
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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))
$R_{free}$	111664	6904 (1.94-1.90)
Clashscore	122126	7577 (1.94-1.90)
Ramachandran outliers	120053	7491 (1.94-1.90)
Sidechain outliers	120020	7491 (1.94-1.90)
RSRZ outliers	108989	6759 (1.94-1.90)

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 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.

Mol	Chain	Length	Quality of chain
1	A	341	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>11%</div> </div> </div>
1	B	341	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>11%</div> </div> </div>
1	C	341	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>
1	D	341	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9845 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 Probable hydrolase NIT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	2	0
			2374	1510	413	440	11			
1	B	302	Total	C	N	O	S	0	3	0
			2378	1512	413	442	11			
1	C	301	Total	C	N	O	S	0	2	0
			2336	1484	403	438	11			
1	D	293	Total	C	N	O	S	0	3	0
			2275	1451	395	419	10			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	EXPRESSION TAG	UNP P47016
A	-32	GLY	-	EXPRESSION TAG	UNP P47016
A	-31	SER	-	EXPRESSION TAG	UNP P47016
A	-30	SER	-	EXPRESSION TAG	UNP P47016
A	-29	HIS	-	EXPRESSION TAG	UNP P47016
A	-28	HIS	-	EXPRESSION TAG	UNP P47016
A	-27	HIS	-	EXPRESSION TAG	UNP P47016
A	-26	HIS	-	EXPRESSION TAG	UNP P47016
A	-25	HIS	-	EXPRESSION TAG	UNP P47016
A	-24	HIS	-	EXPRESSION TAG	UNP P47016
A	-23	SER	-	EXPRESSION TAG	UNP P47016
A	-22	SER	-	EXPRESSION TAG	UNP P47016
A	-21	GLY	-	EXPRESSION TAG	UNP P47016
A	-20	LEU	-	EXPRESSION TAG	UNP P47016
A	-19	VAL	-	EXPRESSION TAG	UNP P47016
A	-18	PRO	-	EXPRESSION TAG	UNP P47016
A	-17	ARG	-	EXPRESSION TAG	UNP P47016
A	-16	GLY	-	EXPRESSION TAG	UNP P47016
A	-15	SER	-	EXPRESSION TAG	UNP P47016
A	-14	HIS	-	EXPRESSION TAG	UNP P47016
A	-13	MET	-	EXPRESSION TAG	UNP P47016

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	EXPRESSION TAG	UNP P47016
A	-11	SER	-	EXPRESSION TAG	UNP P47016
A	-10	MET	-	EXPRESSION TAG	UNP P47016
A	-9	THR	-	EXPRESSION TAG	UNP P47016
A	-8	GLY	-	EXPRESSION TAG	UNP P47016
A	-7	GLY	-	EXPRESSION TAG	UNP P47016
A	-6	GLN	-	EXPRESSION TAG	UNP P47016
A	-5	GLN	-	EXPRESSION TAG	UNP P47016
A	-4	MET	-	EXPRESSION TAG	UNP P47016
A	-3	GLY	-	EXPRESSION TAG	UNP P47016
A	-2	ARG	-	EXPRESSION TAG	UNP P47016
A	-1	GLY	-	EXPRESSION TAG	UNP P47016
A	0	SER	-	EXPRESSION TAG	UNP P47016
B	-33	MET	-	EXPRESSION TAG	UNP P47016
B	-32	GLY	-	EXPRESSION TAG	UNP P47016
B	-31	SER	-	EXPRESSION TAG	UNP P47016
B	-30	SER	-	EXPRESSION TAG	UNP P47016
B	-29	HIS	-	EXPRESSION TAG	UNP P47016
B	-28	HIS	-	EXPRESSION TAG	UNP P47016
B	-27	HIS	-	EXPRESSION TAG	UNP P47016
B	-26	HIS	-	EXPRESSION TAG	UNP P47016
B	-25	HIS	-	EXPRESSION TAG	UNP P47016
B	-24	HIS	-	EXPRESSION TAG	UNP P47016
B	-23	SER	-	EXPRESSION TAG	UNP P47016
B	-22	SER	-	EXPRESSION TAG	UNP P47016
B	-21	GLY	-	EXPRESSION TAG	UNP P47016
B	-20	LEU	-	EXPRESSION TAG	UNP P47016
B	-19	VAL	-	EXPRESSION TAG	UNP P47016
B	-18	PRO	-	EXPRESSION TAG	UNP P47016
B	-17	ARG	-	EXPRESSION TAG	UNP P47016
B	-16	GLY	-	EXPRESSION TAG	UNP P47016
B	-15	SER	-	EXPRESSION TAG	UNP P47016
B	-14	HIS	-	EXPRESSION TAG	UNP P47016
B	-13	MET	-	EXPRESSION TAG	UNP P47016
B	-12	ALA	-	EXPRESSION TAG	UNP P47016
B	-11	SER	-	EXPRESSION TAG	UNP P47016
B	-10	MET	-	EXPRESSION TAG	UNP P47016
B	-9	THR	-	EXPRESSION TAG	UNP P47016
B	-8	GLY	-	EXPRESSION TAG	UNP P47016
B	-7	GLY	-	EXPRESSION TAG	UNP P47016
B	-6	GLN	-	EXPRESSION TAG	UNP P47016
B	-5	GLN	-	EXPRESSION TAG	UNP P47016

*Continued on next page...*

*Continued from previous page...*

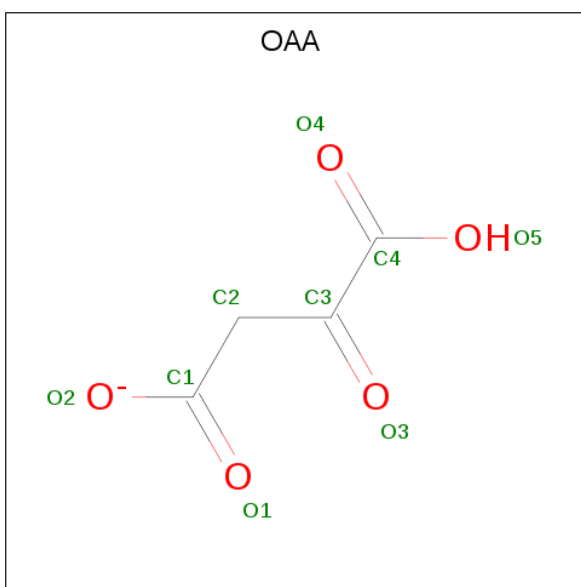
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	EXPRESSION TAG	UNP P47016
B	-3	GLY	-	EXPRESSION TAG	UNP P47016
B	-2	ARG	-	EXPRESSION TAG	UNP P47016
B	-1	GLY	-	EXPRESSION TAG	UNP P47016
B	0	SER	-	EXPRESSION TAG	UNP P47016
C	-33	MET	-	EXPRESSION TAG	UNP P47016
C	-32	GLY	-	EXPRESSION TAG	UNP P47016
C	-31	SER	-	EXPRESSION TAG	UNP P47016
C	-30	SER	-	EXPRESSION TAG	UNP P47016
C	-29	HIS	-	EXPRESSION TAG	UNP P47016
C	-28	HIS	-	EXPRESSION TAG	UNP P47016
C	-27	HIS	-	EXPRESSION TAG	UNP P47016
C	-26	HIS	-	EXPRESSION TAG	UNP P47016
C	-25	HIS	-	EXPRESSION TAG	UNP P47016
C	-24	HIS	-	EXPRESSION TAG	UNP P47016
C	-23	SER	-	EXPRESSION TAG	UNP P47016
C	-22	SER	-	EXPRESSION TAG	UNP P47016
C	-21	GLY	-	EXPRESSION TAG	UNP P47016
C	-20	LEU	-	EXPRESSION TAG	UNP P47016
C	-19	VAL	-	EXPRESSION TAG	UNP P47016
C	-18	PRO	-	EXPRESSION TAG	UNP P47016
C	-17	ARG	-	EXPRESSION TAG	UNP P47016
C	-16	GLY	-	EXPRESSION TAG	UNP P47016
C	-15	SER	-	EXPRESSION TAG	UNP P47016
C	-14	HIS	-	EXPRESSION TAG	UNP P47016
C	-13	MET	-	EXPRESSION TAG	UNP P47016
C	-12	ALA	-	EXPRESSION TAG	UNP P47016
C	-11	SER	-	EXPRESSION TAG	UNP P47016
C	-10	MET	-	EXPRESSION TAG	UNP P47016
C	-9	THR	-	EXPRESSION TAG	UNP P47016
C	-8	GLY	-	EXPRESSION TAG	UNP P47016
C	-7	GLY	-	EXPRESSION TAG	UNP P47016
C	-6	GLN	-	EXPRESSION TAG	UNP P47016
C	-5	GLN	-	EXPRESSION TAG	UNP P47016
C	-4	MET	-	EXPRESSION TAG	UNP P47016
C	-3	GLY	-	EXPRESSION TAG	UNP P47016
C	-2	ARG	-	EXPRESSION TAG	UNP P47016
C	-1	GLY	-	EXPRESSION TAG	UNP P47016
C	0	SER	-	EXPRESSION TAG	UNP P47016
D	-33	MET	-	EXPRESSION TAG	UNP P47016
D	-32	GLY	-	EXPRESSION TAG	UNP P47016
D	-31	SER	-	EXPRESSION TAG	UNP P47016

*Continued on next page...*

*Continued from previous page...*

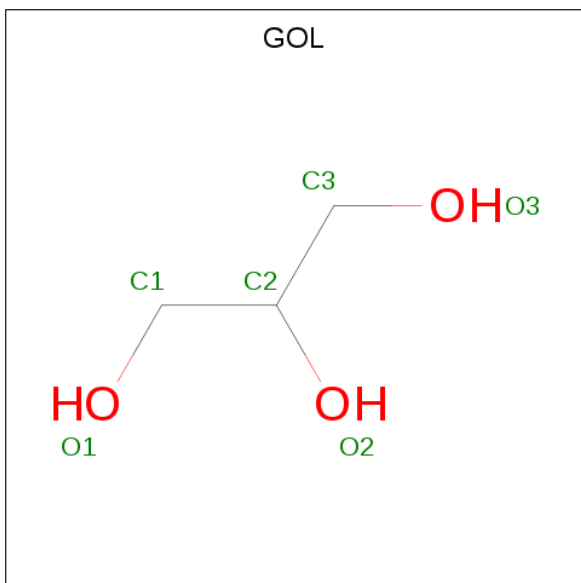
Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	SER	-	EXPRESSION TAG	UNP P47016
D	-29	HIS	-	EXPRESSION TAG	UNP P47016
D	-28	HIS	-	EXPRESSION TAG	UNP P47016
D	-27	HIS	-	EXPRESSION TAG	UNP P47016
D	-26	HIS	-	EXPRESSION TAG	UNP P47016
D	-25	HIS	-	EXPRESSION TAG	UNP P47016
D	-24	HIS	-	EXPRESSION TAG	UNP P47016
D	-23	SER	-	EXPRESSION TAG	UNP P47016
D	-22	SER	-	EXPRESSION TAG	UNP P47016
D	-21	GLY	-	EXPRESSION TAG	UNP P47016
D	-20	LEU	-	EXPRESSION TAG	UNP P47016
D	-19	VAL	-	EXPRESSION TAG	UNP P47016
D	-18	PRO	-	EXPRESSION TAG	UNP P47016
D	-17	ARG	-	EXPRESSION TAG	UNP P47016
D	-16	GLY	-	EXPRESSION TAG	UNP P47016
D	-15	SER	-	EXPRESSION TAG	UNP P47016
D	-14	HIS	-	EXPRESSION TAG	UNP P47016
D	-13	MET	-	EXPRESSION TAG	UNP P47016
D	-12	ALA	-	EXPRESSION TAG	UNP P47016
D	-11	SER	-	EXPRESSION TAG	UNP P47016
D	-10	MET	-	EXPRESSION TAG	UNP P47016
D	-9	THR	-	EXPRESSION TAG	UNP P47016
D	-8	GLY	-	EXPRESSION TAG	UNP P47016
D	-7	GLY	-	EXPRESSION TAG	UNP P47016
D	-6	GLN	-	EXPRESSION TAG	UNP P47016
D	-5	GLN	-	EXPRESSION TAG	UNP P47016
D	-4	MET	-	EXPRESSION TAG	UNP P47016
D	-3	GLY	-	EXPRESSION TAG	UNP P47016
D	-2	ARG	-	EXPRESSION TAG	UNP P47016
D	-1	GLY	-	EXPRESSION TAG	UNP P47016
D	0	SER	-	EXPRESSION TAG	UNP P47016

- Molecule 2 is OXALOACETATE ION (three-letter code: OAA) (formula: C<sub>4</sub>H<sub>3</sub>O<sub>5</sub>).



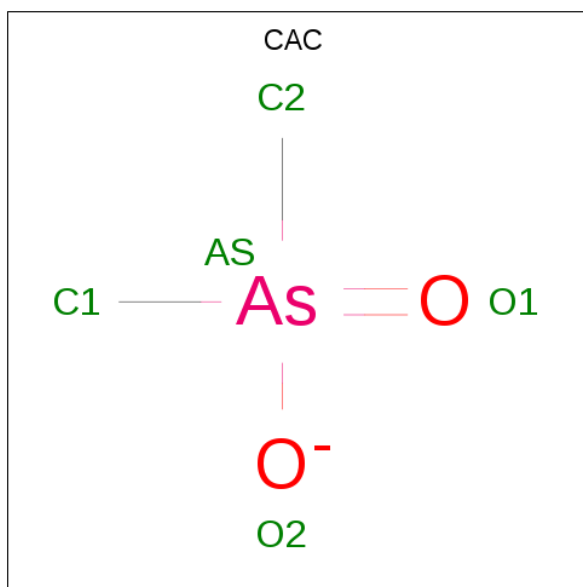
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	4	4		
2	B	1	Total	C	O	0	0
			8	4	4		
2	C	1	Total	C	O	0	0
			8	4	4		
2	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is water.

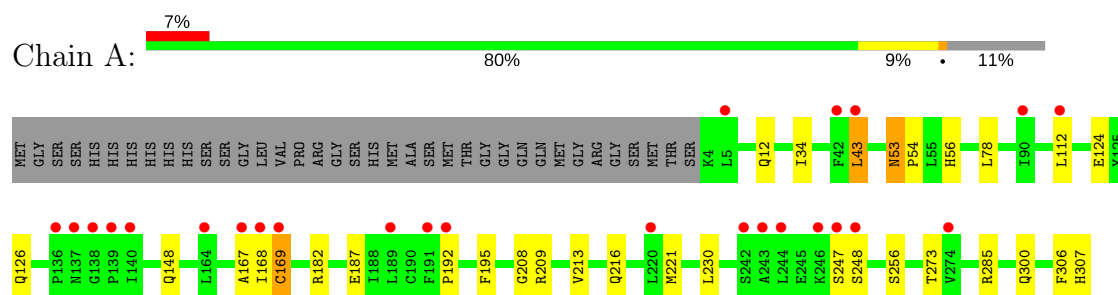


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total 112	O 112	0	0
5	B	115	Total 115	O 115	0	0
5	C	102	Total 102	O 102	0	0
5	D	57	Total 57	O 57	0	0

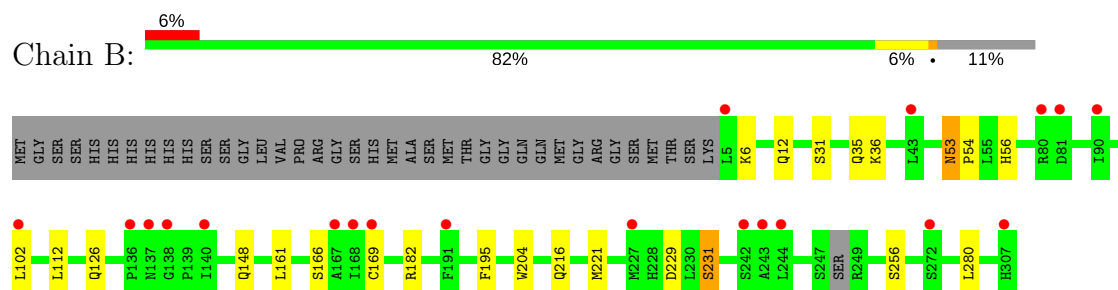
### 3 Residue-property plots [i](#)

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.

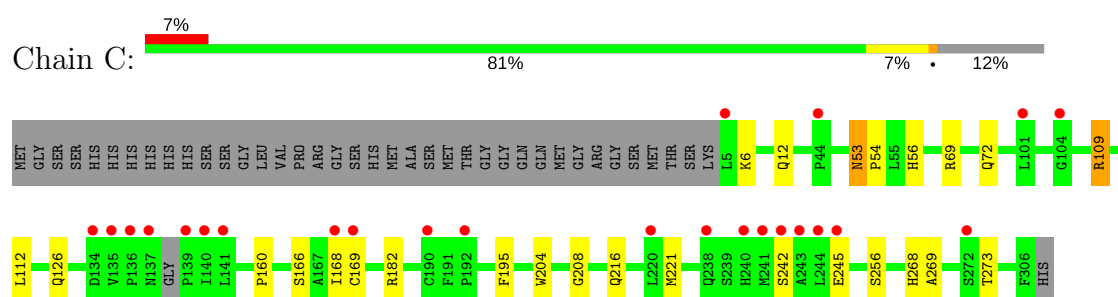
#### • Molecule 1: Probable hydrolase NIT2



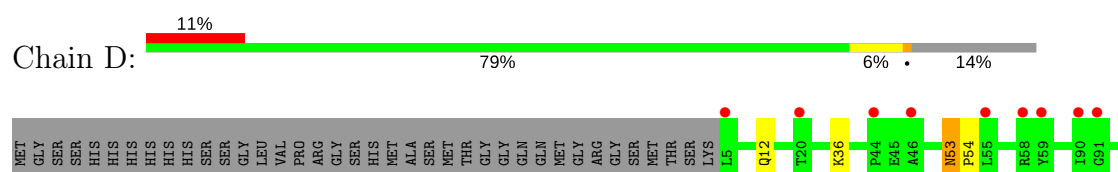
#### • Molecule 1: Probable hydrolase NIT2

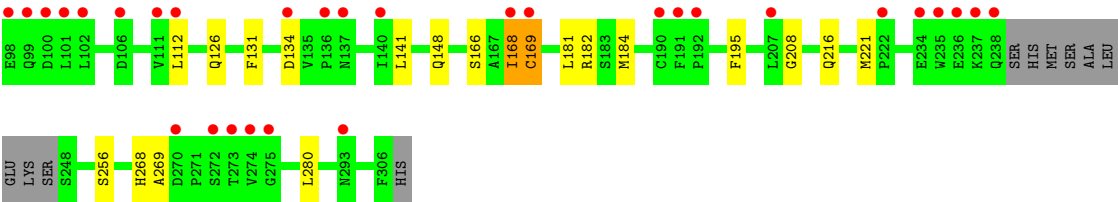


#### • Molecule 1: Probable hydrolase NIT2



#### • Molecule 1: Probable hydrolase NIT2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.50Å 125.84Å 77.88Å 90.00° 95.41° 90.00°	Depositor
Resolution (Å)	32.75 – 1.91 32.75 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.5 (32.75-1.91) 95.5 (32.75-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.200 , 0.229 0.202 , 0.229	Depositor DCC
$R_{free}$ test set	4648 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, GOL, OAA

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	0.41	1/2430 (0.0%)	0.56	1/3293 (0.0%)
1	B	0.38	1/2437 (0.0%)	0.54	0/3304
1	C	0.37	1/2390 (0.0%)	0.56	1/3243 (0.0%)
1	D	0.34	0/2332	0.55	3/3168 (0.1%)
All	All	0.38	3/9589 (0.0%)	0.55	5/13008 (0.0%)

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	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	CYS	CB-SG	-5.65	1.72	1.81
1	A	169	CYS	CB-SG	-5.26	1.73	1.81
1	B	169	CYS	CB-SG	-5.20	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ILE	O-C-N	-9.16	108.04	122.70
1	C	168	ILE	C-N-CA	5.85	136.32	121.70
1	A	43	LEU	CA-CB-CG	5.34	127.59	115.30
1	D	168	ILE	C-N-CA	5.24	134.79	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	CYS	N-CA-CB	-5.12	101.38	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	ILE	Mainchain
1	D	168	ILE	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	2374	0	2343	16	0
1	B	2378	0	2363	16	0
1	C	2336	0	2282	18	0
1	D	2275	0	2233	14	0
2	A	8	0	2	0	0
2	B	8	0	2	0	0
2	C	8	0	2	0	0
2	D	8	0	2	0	0
3	A	12	0	16	0	0
3	B	24	0	32	3	0
3	C	12	0	16	1	0
3	D	6	0	8	0	0
4	A	10	0	0	1	0
5	A	112	0	0	0	0
5	B	115	0	0	0	0
5	C	102	0	0	1	0
5	D	57	0	0	0	0
All	All	9845	0	9301	64	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 3.

The worst 5 of 64 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:D:181:LEU:HA	1:D:184:MET:HE2	1.61	0.82
1:A:182:ARG:HH12	1:A:216:GLN:HE21	1.38	0.70
1:C:182:ARG:HH12	1:C:216:GLN:HE21	1.37	0.70
1:B:182:ARG:HH12	1:B:216:GLN:HE21	1.39	0.70
1:B:31:SER:O	1:B:35:GLN:HG2	1.92	0.69

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	304/341 (89%)	300 (99%)	3 (1%)	1 (0%)	43	32
1	B	301/341 (88%)	299 (99%)	2 (1%)	0	100	100
1	C	299/341 (88%)	288 (96%)	11 (4%)	0	100	100
1	D	292/341 (86%)	289 (99%)	2 (1%)	1 (0%)	43	32
All	All	1196/1364 (88%)	1176 (98%)	18 (2%)	2 (0%)	49	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	169	CYS
1	A	169	CYS

### 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	255/300 (85%)	249 (98%)	6 (2%)	52	44
1	B	261/300 (87%)	257 (98%)	4 (2%)	67	64
1	C	250/300 (83%)	246 (98%)	4 (2%)	65	61
1	D	242/300 (81%)	239 (99%)	3 (1%)	74	71
All	All	1008/1200 (84%)	991 (98%)	17 (2%)	63	59

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	LEU
1	B	195	PHE
1	C	273	THR
1	B	53	ASN
1	D	53	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	C	12	GLN
1	D	148	GLN
1	B	268	HIS
1	A	216	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

15 ligands 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
2	OAA	A	401	1	3,7,8	0.49	0	3,8,10	1.95	1 (33%)
3	GOL	A	402	-	5,5,5	0.40	0	5,5,5	0.18	0
3	GOL	A	403	-	5,5,5	0.36	0	5,5,5	0.29	0
4	CAC	A	404	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	A	405	-	0,4,4	0.00	-	0,6,6	0.00	-
2	OAA	B	401	1	3,7,8	0.55	0	3,8,10	1.96	1 (33%)
3	GOL	B	402	-	5,5,5	0.39	0	5,5,5	0.31	0
3	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.42	0
3	GOL	B	405	-	5,5,5	0.36	0	5,5,5	0.30	0
2	OAA	C	401	1	3,7,8	0.51	0	3,8,10	1.48	1 (33%)
3	GOL	C	402	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	C	403	-	5,5,5	0.36	0	5,5,5	0.37	0
2	OAA	D	401	1	3,7,8	0.55	0	3,8,10	2.82	2 (66%)
3	GOL	D	402	-	5,5,5	0.35	0	5,5,5	0.37	0

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
2	OAA	A	401	1	-	0/1/7/8	0/0/0/0
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	A	403	-	-	0/4/4/4	0/0/0/0
4	CAC	A	404	-	-	0/0/0/0	0/0/0/0
4	CAC	A	405	-	-	0/0/0/0	0/0/0/0
2	OAA	B	401	1	-	0/1/7/8	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	B	404	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	405	-	-	0/4/4/4	0/0/0/0
2	OAA	C	401	1	-	0/1/7/8	0/0/0/0
3	GOL	C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	C	403	-	-	0/4/4/4	0/0/0/0
2	OAA	D	401	1	-	0/1/7/8	0/0/0/0
3	GOL	D	402	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	OAA	O1-C1-C2	-2.96	118.01	126.65
2	D	401	OAA	O1-C1-C2	-2.96	118.01	126.65
2	B	401	OAA	O1-C1-C2	-2.89	118.23	126.65
2	C	401	OAA	O1-C1-C2	-2.25	120.09	126.65
2	D	401	OAA	O3-C3-C2	3.88	125.09	120.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	CAC	1	0
3	B	402	GOL	3	0
3	C	402	GOL	1	0

## 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, 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	304/341 (89%)	0.37	25 (8%) 11 13	18, 23, 36, 47	0
1	B	302/341 (88%)	0.33	20 (6%) 18 21	19, 24, 37, 50	0
1	C	301/341 (88%)	0.43	24 (7%) 12 14	19, 25, 42, 49	0
1	D	293/341 (85%)	0.69	39 (13%) 3 3	22, 35, 45, 56	0
All	All	1200/1364 (87%)	0.46	108 (9%) 9 11	18, 26, 42, 56	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	VAL	6.6
1	B	243	ALA	6.1
1	C	137	ASN	5.9
1	C	5	LEU	5.5
1	C	240	HIS	5.2

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	402	6/6	0.65	0.28	50,51,51,52	0
2	OAA	C	401	8/9	0.77	0.24	35,37,39,39	0
2	OAA	B	401	8/9	0.79	0.23	37,40,40,41	0
2	OAA	A	401	8/9	0.80	0.17	34,37,37,38	0
3	GOL	C	403	6/6	0.81	0.22	49,50,51,51	0
3	GOL	C	402	6/6	0.82	0.25	38,42,43,43	0
3	GOL	B	402	6/6	0.82	0.15	39,42,42,43	0
2	OAA	D	401	8/9	0.85	0.16	42,43,43,44	0
3	GOL	B	404	6/6	0.85	0.15	42,43,43,43	0
3	GOL	A	403	6/6	0.87	0.18	39,39,40,40	0
3	GOL	B	403	6/6	0.88	0.14	41,41,41,42	0
4	CAC	A	405	5/5	0.94	0.26	29,29,30,32	5
3	GOL	B	405	6/6	0.96	0.11	26,28,28,28	0
4	CAC	A	404	5/5	0.96	0.20	30,31,32,34	5
3	GOL	A	402	6/6	0.97	0.09	25,25,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.