



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:46 PM BST

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 Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

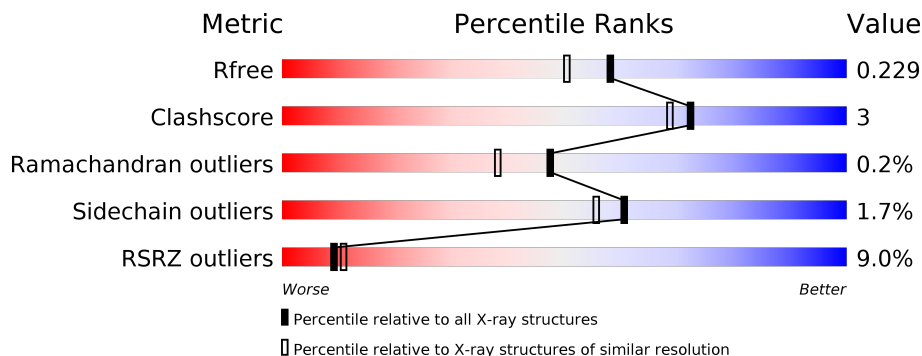
1 Overall quality at a glance

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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (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 ≥ 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	341	
1	B	341	
1	C	341	
1	D	341	

2 Entry composition i

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

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...

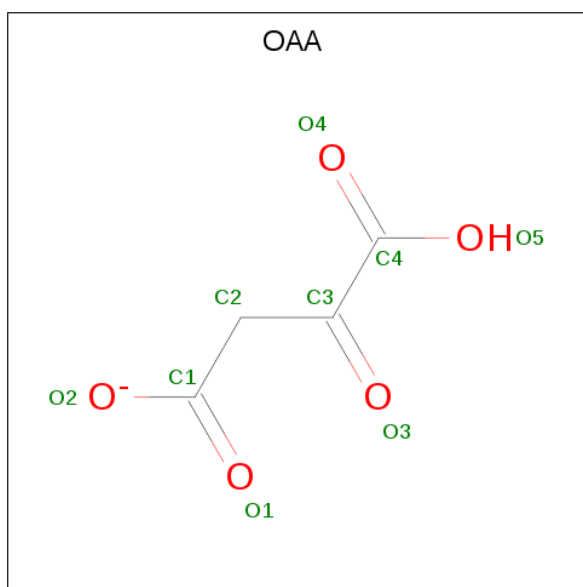
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	EXPRESSION TAG	UNP P47016
B	-3	GLY	-	EXPRESSION TAG	UNP P47016
B	-2	ARG	-	EXPRESSION TAG	UNP P47016
B	-1	GLY	-	EXPRESSION TAG	UNP P47016
B	0	SER	-	EXPRESSION TAG	UNP P47016
C	-33	MET	-	EXPRESSION TAG	UNP P47016
C	-32	GLY	-	EXPRESSION TAG	UNP 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...

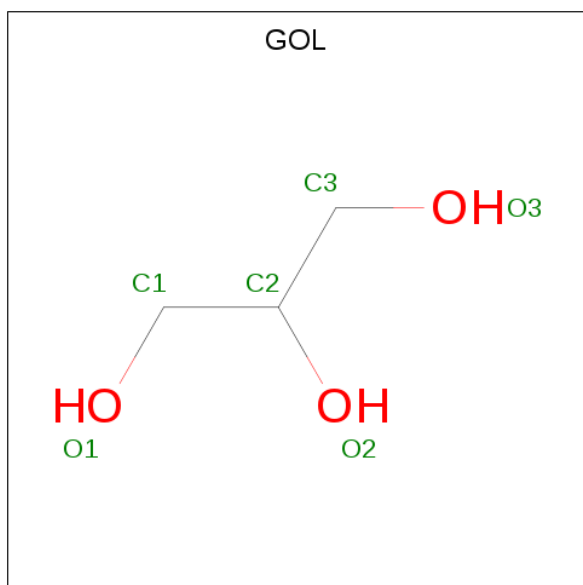
Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	SER	-	EXPRESSION TAG	UNP P47016
D	-29	HIS	-	EXPRESSION TAG	UNP P47016
D	-28	HIS	-	EXPRESSION TAG	UNP P47016
D	-27	HIS	-	EXPRESSION TAG	UNP P47016
D	-26	HIS	-	EXPRESSION TAG	UNP P47016
D	-25	HIS	-	EXPRESSION TAG	UNP P47016
D	-24	HIS	-	EXPRESSION TAG	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: C₄H₃O₅).



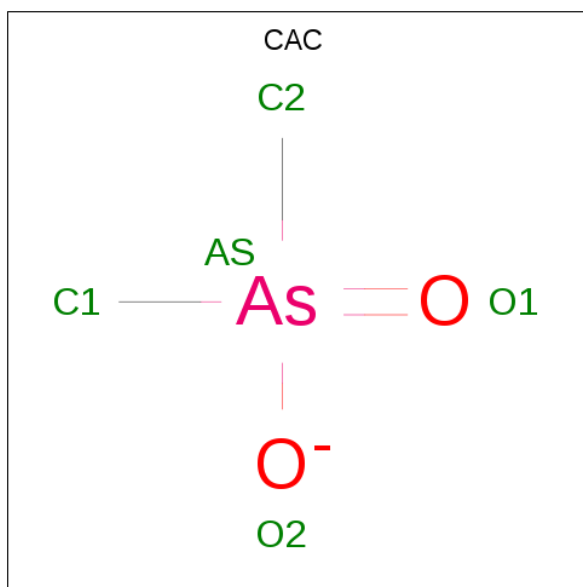
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			8	4 4		
2	B	1	Total	C O	0	0
			8	4 4		
2	C	1	Total	C O	0	0
			8	4 4		
2	D	1	Total	C O	0	0
			8	4 4		

- 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	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: C₂H₆AsO₂).



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		

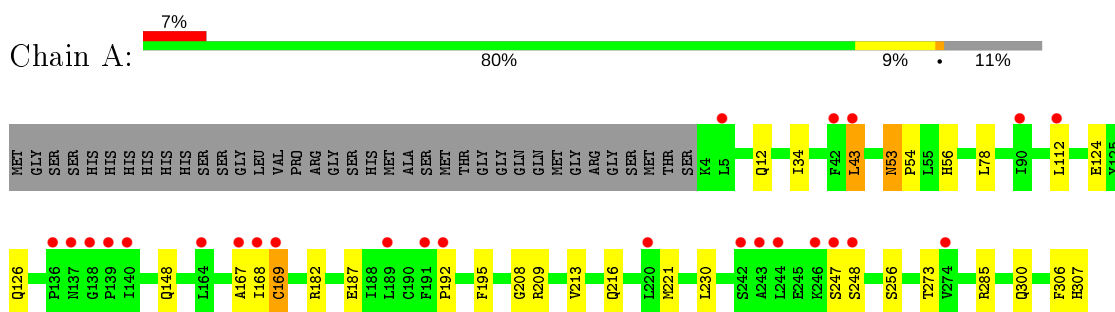
- Molecule 5 is water.

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

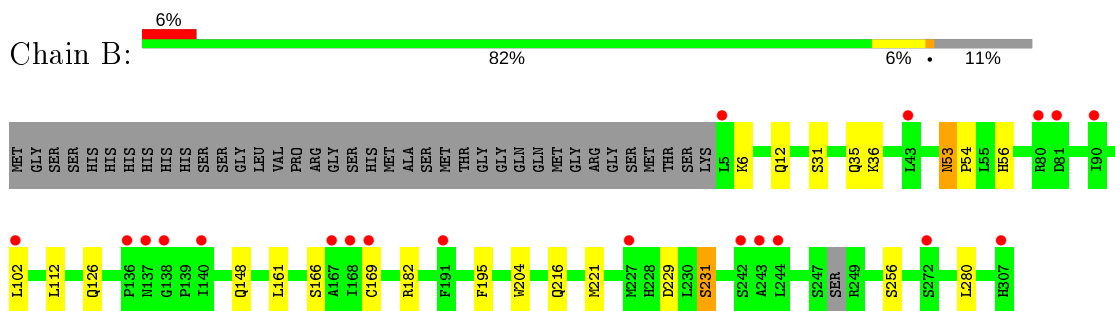
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

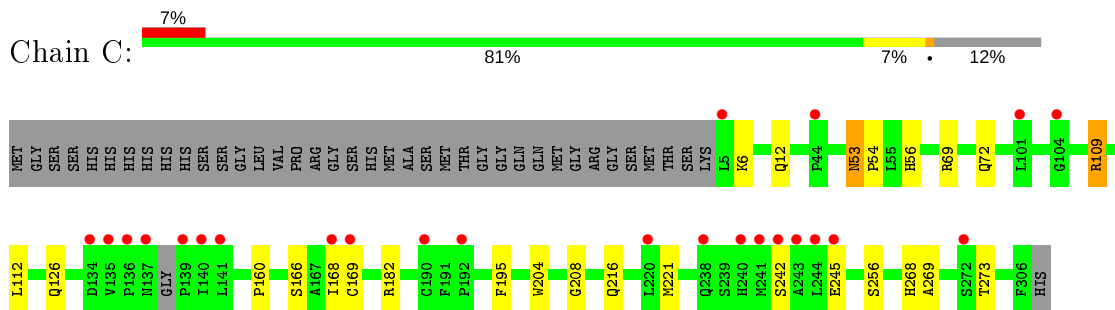
- Molecule 1: Probable hydrolase NIT2



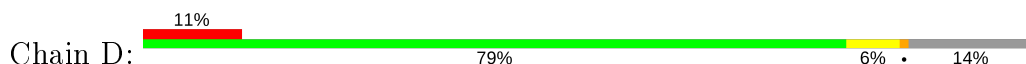
- Molecule 1: Probable hydrolase NIT2

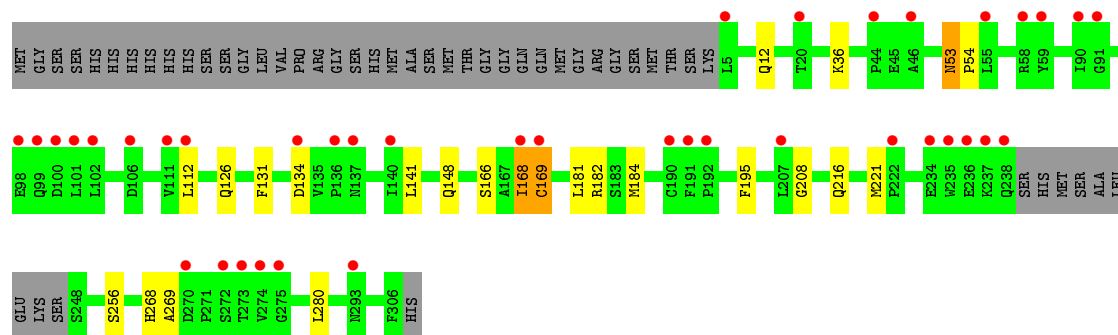


- Molecule 1: Probable hydrolase NIT2



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.91Å)	Xtrriage
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 ²)	26.3	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9845	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² 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](#)

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.

All (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
1:D:53:ASN:HB2	1:D:54:PRO:HD2	1.75	0.68
1:D:182:ARG:HH12	1:D:216:GLN:HE21	1.41	0.68
1:C:53:ASN:ND2	1:C:56:HIS:H	1.93	0.65
1:D:181:LEU:HD23	1:D:184:MET:HE1	1.77	0.64
1:C:12:GLN:NE2	1:C:256:SER:H	2.00	0.59
1:B:280:LEU:H	3:B:402:GOL:C1	2.15	0.59
1:C:6:LYS:HD3	1:C:160:PRO:O	2.04	0.58
1:D:12:GLN:NE2	1:D:256:SER:H	2.02	0.57
1:A:126:GLN:HE22	1:A:148:GLN:HE21	1.51	0.57
1:C:12:GLN:HE22	1:C:256:SER:H	1.51	0.57
1:D:53:ASN:HB2	1:D:54:PRO:CD	2.35	0.56
1:C:112:LEU:HD23	1:C:166:SER:HB3	1.87	0.56
1:B:12:GLN:HE22	1:B:256:SER:H	1.54	0.56
1:A:12:GLN:HE22	1:A:256:SER:H	1.53	0.55
1:A:12:GLN:NE2	1:A:256:SER:H	2.05	0.55
1:B:12:GLN:NE2	1:B:256:SER:H	2.05	0.54
1:B:36:LYS:HD3	1:B:280:LEU:HD11	1.89	0.54
1:C:53:ASN:HD22	1:C:53:ASN:C	2.10	0.54
1:B:53:ASN:HB2	1:B:54:PRO:HD2	1.89	0.54
1:C:53:ASN:HB2	1:C:54:PRO:CD	2.37	0.54
1:A:124:GLU:OE2	4:A:405:CAC:O1	2.26	0.53
1:D:181:LEU:HD23	1:D:184:MET:CE	2.39	0.53
1:B:53:ASN:HB2	1:B:54:PRO:CD	2.40	0.51
1:B:280:LEU:N	3:B:402:GOL:H11	2.26	0.51
1:C:53:ASN:HB2	1:C:54:PRO:HD2	1.93	0.51
1:A:230:LEU:HD12	1:A:248:SER:HB2	1.94	0.50
1:C:53:ASN:HD22	1:C:56:HIS:H	1.60	0.49
1:A:126:GLN:HE22	1:A:148:GLN:NE2	2.10	0.49
1:D:12:GLN:HE22	1:D:256:SER:H	1.61	0.49
1:A:306:PHE:O	1:A:307:HIS:CB	2.61	0.49
1:B:280:LEU:H	3:B:402:GOL:H11	1.77	0.48
1:B:126:GLN:HE22	1:B:148:GLN:HE21	1.62	0.48
1:B:112:LEU:HD23	1:B:166:SER:HB3	1.95	0.48
1:C:69:ARG:HA	1:C:72:GLN:HE21	1.79	0.48
1:B:53:ASN:ND2	1:B:56:HIS:H	2.13	0.46
1:C:204:TRP:CZ2	1:C:221[B]:MET:HB3	2.51	0.46
1:D:112:LEU:HD23	1:D:166:SER:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLU:OE2	1:A:285:ARG:NH2	2.49	0.45
1:C:204:TRP:CZ2	1:C:221[A]:MET:HB3	2.52	0.45
1:A:300:GLN:HB3	3:C:402:GOL:O3	2.18	0.44
1:A:209:ARG:O	1:A:213:VAL:HG13	2.17	0.44
1:D:126:GLN:HE22	1:D:148:GLN:HE21	1.65	0.44
1:D:131:PHE:HE2	1:D:141:LEU:HD12	1.83	0.44
1:A:53:ASN:ND2	1:A:56:HIS:H	2.16	0.43
1:B:6:LYS:HB3	1:B:161:LEU:HD23	2.01	0.42
1:C:109:ARG:HG2	1:C:126:GLN:CD	2.39	0.42
1:C:242:SER:O	1:C:245:GLU:HG2	2.19	0.42
1:D:268:HIS:HD2	1:D:269:ALA:O	2.02	0.42
1:C:268:HIS:HD2	1:C:269:ALA:O	2.02	0.42
1:A:167:ALA:O	1:A:192:PRO:HD2	2.20	0.41
1:B:204:TRP:CZ2	1:B:221[A]:MET:HB3	2.55	0.41
1:A:34:ILE:HD12	1:A:78:LEU:HB3	2.02	0.41
1:C:268:HIS:HE1	5:C:541:HOH:O	2.04	0.41
1:A:53:ASN:HB2	1:A:54:PRO:CD	2.51	0.41
1:A:208:GLY:HA3	1:A:221:MET:SD	2.61	0.41
1:C:208:GLY:HA3	1:C:221[A]:MET:SD	2.61	0.40
1:D:208:GLY:HA3	1:D:221[A]:MET:SD	2.61	0.40
1:D:36:LYS:HB3	1:D:280:LEU:HD11	2.03	0.40
1:B:229:ASP:OD1	1:B:231:SER:HB3	2.22	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	304/341 (89%)	300 (99%)	3 (1%)	1 (0%)	41	31
1	B	301/341 (88%)	299 (99%)	2 (1%)	0	100	100
1	C	299/341 (88%)	288 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	292/341 (86%)	289 (99%)	2 (1%)	1 (0%)	41 31
All	All	1196/1364 (88%)	1176 (98%)	18 (2%)	2 (0%)	47 38

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%)	49 41
1	B	261/300 (87%)	257 (98%)	4 (2%)	65 61
1	C	250/300 (83%)	246 (98%)	4 (2%)	62 58
1	D	242/300 (81%)	239 (99%)	3 (1%)	71 69
All	All	1008/1200 (84%)	991 (98%)	17 (2%)	60 55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	53	ASN
1	A	112	LEU
1	A	195	PHE
1	A	247	SER
1	A	273	THR
1	B	53	ASN
1	B	102	LEU
1	B	195	PHE
1	B	231	SER
1	C	53	ASN
1	C	109	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	195	PHE
1	C	273	THR
1	D	53	ASN
1	D	134	ASP
1	D	195	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	52	GLN
1	A	53	ASN
1	A	72	GLN
1	A	123	GLN
1	A	148	GLN
1	A	216	GLN
1	A	238	GLN
1	A	268	HIS
1	A	300	GLN
1	B	12	GLN
1	B	52	GLN
1	B	53	ASN
1	B	72	GLN
1	B	123	GLN
1	B	148	GLN
1	B	216	GLN
1	B	268	HIS
1	B	307	HIS
1	C	12	GLN
1	C	52	GLN
1	C	53	ASN
1	C	72	GLN
1	C	123	GLN
1	C	148	GLN
1	C	216	GLN
1	C	268	HIS
1	D	12	GLN
1	D	53	ASN
1	D	72	GLN
1	D	123	GLN
1	D	148	GLN
1	D	216	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	268	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	CAC	A	405	-	0,4,4	0.00	-	0,6,6	0.00	-
2	OAA	C	401	1	3,7,8	0.52	0	3,8,10	1.54	1 (33%)
3	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.42	0
3	GOL	A	402	-	5,5,5	0.41	0	5,5,5	0.18	0
3	GOL	C	402	-	5,5,5	0.36	0	5,5,5	0.33	0
2	OAA	A	401	1	3,7,8	0.51	0	3,8,10	2.02	1 (33%)
3	GOL	A	403	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	C	403	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	D	402	-	5,5,5	0.35	0	5,5,5	0.36	0
2	OAA	B	401	1	3,7,8	0.57	0	3,8,10	2.03	1 (33%)
2	OAA	D	401	1	3,7,8	0.57	0	3,8,10	2.90	2 (66%)
4	CAC	A	404	-	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	403	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GOL	B	405	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	B	402	-	5,5,5	0.40	0	5,5,5	0.31	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	C	401	1	-	0/1/7/8	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	C	402	-	-	4/4/4/4	-
2	OAA	A	401	1	-	0/1/7/8	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	C	403	-	-	1/4/4/4	-
3	GOL	D	402	-	-	3/4/4/4	-
2	OAA	B	401	1	-	0/1/7/8	-
2	OAA	D	401	1	-	0/1/7/8	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	OAA	O3-C3-C2	3.94	125.09	120.57
2	A	401	OAA	O1-C1-C2	-3.09	118.01	126.64
2	D	401	OAA	O1-C1-C2	-3.09	118.01	126.64
2	B	401	OAA	O1-C1-C2	-3.01	118.23	126.64
2	C	401	OAA	O1-C1-C2	-2.34	120.09	126.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	402	GOL	O1-C1-C2-O2
3	C	402	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	D	402	GOL	C1-C2-C3-O3
3	C	402	GOL	O2-C2-C3-O3
3	C	402	GOL	C1-C2-C3-O3
3	D	402	GOL	O1-C1-C2-C3
3	B	402	GOL	O1-C1-C2-C3
3	D	402	GOL	O2-C2-C3-O3
3	C	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3

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	C	402	GOL	1	0
3	B	402	GOL	3	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, 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	304/341 (89%)	0.37	25 (8%) 11 13	18, 23, 36, 47	0
1	B	302/341 (88%)	0.33	20 (6%) 18 20	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

All (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
1	B	136	PRO	4.7
1	C	136	PRO	4.7
1	A	243	ALA	4.7
1	A	274	VAL	4.5
1	B	307	HIS	4.5
1	C	169	CYS	4.3
1	A	248	SER	4.2
1	B	244	LEU	4.1
1	B	5	LEU	4.1
1	C	140	ILE	3.9
1	A	136	PRO	3.8
1	A	138	GLY	3.8
1	D	5	LEU	3.8
1	C	139	PRO	3.8
1	B	169	CYS	3.8
1	D	136	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	242	SER	3.7
1	D	235	TRP	3.7
1	D	273	THR	3.6
1	C	241	MET	3.5
1	D	272	SER	3.5
1	D	99	GLN	3.5
1	D	140	ILE	3.5
1	D	59	TYR	3.4
1	C	135	VAL	3.3
1	D	102	LEU	3.3
1	D	169	CYS	3.3
1	D	238	GLN	3.3
1	C	134	ASP	3.2
1	A	137	ASN	3.2
1	A	247	SER	3.2
1	D	234	GLU	3.1
1	A	164	LEU	3.1
1	A	244	LEU	3.1
1	D	90	ILE	3.1
1	B	227	MET	3.1
1	D	112	LEU	3.0
1	B	168	ILE	3.0
1	A	169	CYS	3.0
1	B	80	ARG	3.0
1	D	236	GLU	3.0
1	B	140	ILE	3.0
1	C	244	LEU	2.9
1	B	102	LEU	2.9
1	D	101	LEU	2.9
1	D	237	LYS	2.9
1	B	137	ASN	2.9
1	C	238	GLN	2.9
1	C	243	ALA	2.8
1	C	101	LEU	2.8
1	D	106	ASP	2.8
1	D	100	ASP	2.8
1	B	272	SER	2.8
1	D	46	ALA	2.7
1	B	167	ALA	2.7
1	D	190	CYS	2.6
1	D	168	ILE	2.6
1	C	141	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	139	PRO	2.6
1	C	220	LEU	2.6
1	C	242	SER	2.6
1	D	207	LEU	2.5
1	C	190	CYS	2.5
1	A	191	PHE	2.5
1	A	43	LEU	2.5
1	B	81	ASP	2.5
1	B	90	ILE	2.5
1	B	138	GLY	2.5
1	D	44	PRO	2.4
1	A	112	LEU	2.4
1	A	189	LEU	2.4
1	D	191	PHE	2.4
1	D	55	LEU	2.4
1	D	293[A]	ASN	2.4
1	C	245	GLU	2.4
1	C	168	ILE	2.4
1	D	270	ASP	2.3
1	D	192	PRO	2.3
1	C	272	SER	2.3
1	D	137	ASN	2.3
1	C	104	GLY	2.2
1	A	42	PHE	2.2
1	A	192	PRO	2.2
1	A	90	ILE	2.2
1	D	275	GLY	2.2
1	A	246	LYS	2.2
1	D	222	PRO	2.2
1	D	134	ASP	2.2
1	C	44	PRO	2.1
1	C	192	PRO	2.1
1	A	140	ILE	2.1
1	D	20	THR	2.1
1	D	91	GLY	2.1
1	A	242	SER	2.1
1	A	5	LEU	2.1
1	D	111	VAL	2.1
1	A	167	ALA	2.1
1	A	168	ILE	2.1
1	A	220	LEU	2.1
1	B	43	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	191	PHE	2.0
1	D	98	GLU	2.0
1	D	58	ARG	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](#)

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, 95th 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(Å 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.