



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:56 PM GMT

PDB ID : 3FY1  
Title : The Acidic Mammalian Chitinase catalytic domain in complex with methylal-  
losamidin  
Authors : Olland, A.M.  
Deposited on : 2009-01-21  
Resolution : 1.70 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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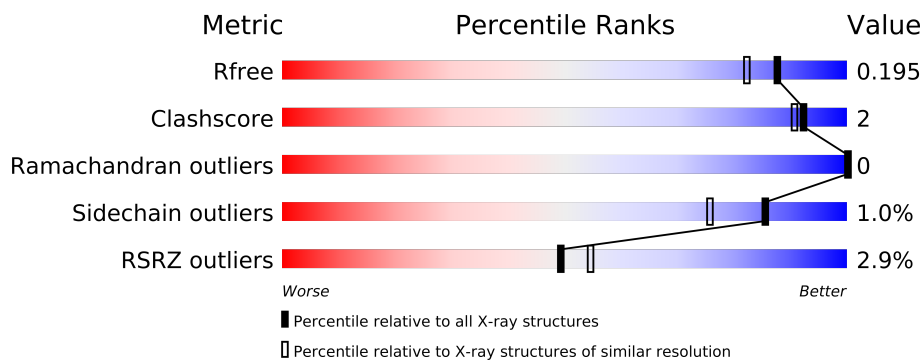
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	395	
1	B	395	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6620 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.

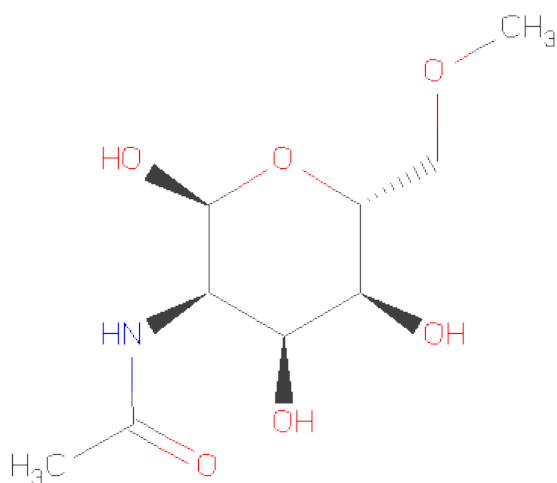
- Molecule 1 is a protein called Acidic mammalian chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	1	0
			2987	1927	485	560	15			
1	B	373	Total	C	N	O	S	0	1	0
			2963	1912	481	555	15			

There are 24 discrepancies between the modelled and reference sequences:

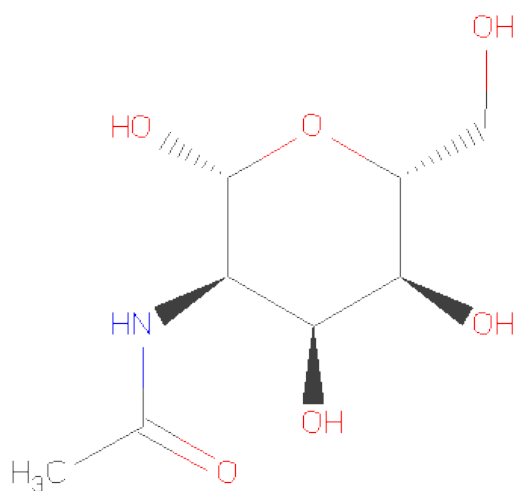
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASP	ASN	SEE REMARK 999	UNP Q9BZP6
A	47	ASN	ASP	SEE REMARK 999	UNP Q9BZP6
A	61	MET	ARG	SEE REMARK 999	UNP Q9BZP6
A	339	VAL	ILE	variant	UNP Q9BZP6
A	409	GLY	-	EXPRESSION TAG	UNP Q9BZP6
A	410	SER	-	EXPRESSION TAG	UNP Q9BZP6
A	411	HIS	-	EXPRESSION TAG	UNP Q9BZP6
A	412	HIS	-	EXPRESSION TAG	UNP Q9BZP6
A	413	HIS	-	EXPRESSION TAG	UNP Q9BZP6
A	414	HIS	-	EXPRESSION TAG	UNP Q9BZP6
A	415	HIS	-	EXPRESSION TAG	UNP Q9BZP6
A	416	HIS	-	EXPRESSION TAG	UNP Q9BZP6
B	45	ASP	ASN	SEE REMARK 999	UNP Q9BZP6
B	47	ASN	ASP	SEE REMARK 999	UNP Q9BZP6
B	61	MET	ARG	SEE REMARK 999	UNP Q9BZP6
B	339	VAL	ILE	variant	UNP Q9BZP6
B	409	GLY	-	EXPRESSION TAG	UNP Q9BZP6
B	410	SER	-	EXPRESSION TAG	UNP Q9BZP6
B	411	HIS	-	EXPRESSION TAG	UNP Q9BZP6
B	412	HIS	-	EXPRESSION TAG	UNP Q9BZP6
B	413	HIS	-	EXPRESSION TAG	UNP Q9BZP6
B	414	HIS	-	EXPRESSION TAG	UNP Q9BZP6
B	415	HIS	-	EXPRESSION TAG	UNP Q9BZP6
B	416	HIS	-	EXPRESSION TAG	UNP Q9BZP6

- Molecule 2 is METHYL N-ACETYL ALLOSAMINE (three-letter code: NA1) (formula:  $C_9H_{17}NO_6$ ).



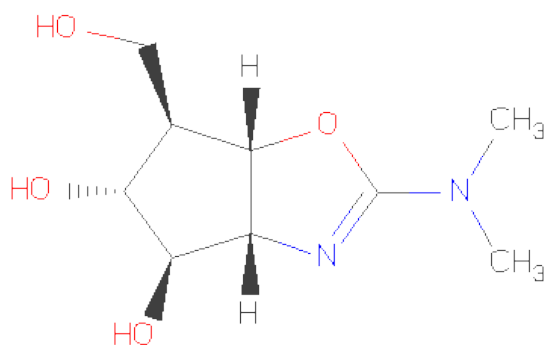
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	1	5		
2	B	1	Total	C	N	O	0	0
			15	9	1	5		

- Molecule 3 is SUGAR (N-ACETYL-D-ALLOSAMINE) (three-letter code: NAA) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALLOSAMIZOLINE (three-letter code: AMI) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	9	2	4		
4	B	1	Total	C	N	O	0	0
			15	9	2	4		

- Molecule 5 is water.

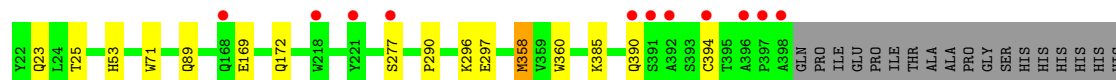
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	307	Total	O	0	0
			307	307		
5	B	275	Total	O	0	0
			275	275		

### 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.

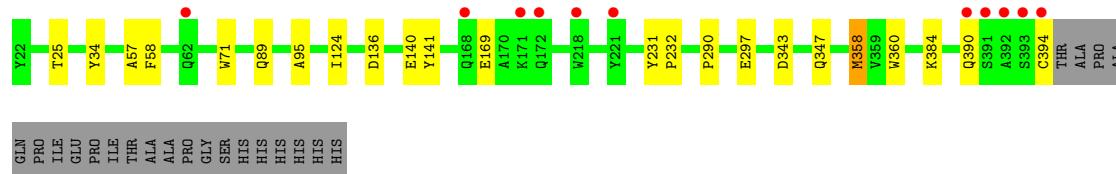
- Molecule 1: Acidic mammalian chitinase

Chain A: 



- Molecule 1: Acidic mammalian chitinase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.69Å 89.29Å 126.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 29.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-1.70) 89.6 (29.85-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.175 , 0.194 0.175 , 0.195	Depositor DCC
$R_{free}$ test set	3586 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71824 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: AMI, NAA, NA1

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	0/3083	0.52	0/4203
1	B	0.42	1/3058 (0.0%)	0.53	0/4167
All	All	0.41	1/6141 (0.0%)	0.52	0/8370

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	B	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	CYS	C-O	5.16	1.33	1.23

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	394	CYS	CA

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	2987	0	2835	11	0
1	B	2963	0	2811	13	0
2	A	15	0	15	1	0
2	B	15	0	15	1	0
3	A	14	0	12	0	0
3	B	14	0	12	0	0
4	A	15	0	15	1	0
4	B	15	0	15	1	0
5	A	307	0	0	0	0
5	B	275	0	0	0	0
All	All	6620	0	5730	21	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 2.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:LYS:HA	1:A:390:GLN:HG2	1.74	0.69
1:B:297:GLU:HG2	2:B:801:NA1:H9C2	1.92	0.51
1:A:23:GLN:OE1	1:A:53:HIS:CE1	2.64	0.51
1:A:25:THR:O	1:A:358:MET:HA	2.12	0.48
1:B:360:TRP:CE2	4:B:803:AMI:H5	2.50	0.47
1:B:25:THR:O	1:B:358:MET:HA	2.14	0.47
1:A:297:GLU:HG2	2:A:801:NA1:H9C2	1.97	0.47
1:B:231:TYR:CG	1:B:232:PRO:HD2	2.51	0.45
1:B:57:ALA:HA	1:B:58:PHE:HA	1.81	0.45
1:B:343:ASP:O	1:B:347:GLN:HG2	2.18	0.44
1:A:71:TRP:CD2	1:B:290:PRO:HA	2.53	0.44
1:A:360:TRP:CE2	4:A:803:AMI:H5	2.53	0.44
1:B:384:LYS:HE3	1:B:390:GLN:HA	2.01	0.43
1:A:296:LYS:HD3	1:B:34:TYR:HB3	2.01	0.43
1:A:169:GLU:HA	1:A:172:GLN:HG2	2.01	0.42
1:A:169:GLU:O	1:A:172:GLN:HG2	2.20	0.41
1:B:124:ILE:HG21	1:B:169:GLU:HG3	2.01	0.41
1:A:290:PRO:HA	1:B:71:TRP:CD2	2.55	0.41
1:A:23:GLN:OE1	1:A:53:HIS:HE1	2.02	0.40
1:B:95:ALA:HA	1:B:136:ASP:O	2.21	0.40
1:B:140:GLU:HA	1:B:141:TYR:CD2	2.57	0.40

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	376/395 (95%)	370 (98%)	6 (2%)	0	100	100
1	B	372/395 (94%)	366 (98%)	6 (2%)	0	100	100
All	All	748/790 (95%)	736 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	313/327 (96%)	309 (99%)	4 (1%)	80	66
1	B	311/327 (95%)	309 (99%)	2 (1%)	92	87
All	All	624/654 (95%)	618 (99%)	6 (1%)	85	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	277	SER
1	A	358	MET
1	A	394	CYS
1	B	89	GLN
1	B	358	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 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 ⓘ

6 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	NA1	A	801	3	13,15,16	1.22	1 (7%)	16,20,22	1.69	2 (12%)
3	NAA	A	802	2,4	12,14,15	1.50	2 (16%)	15,19,21	1.14	1 (6%)
4	AMI	A	803	3	16,16,16	1.72	4 (25%)	24,24,24	2.00	3 (12%)
2	NA1	B	801	3	13,15,16	1.26	1 (7%)	16,20,22	1.66	1 (6%)
3	NAA	B	802	2,4	12,14,15	1.47	2 (16%)	15,19,21	1.05	1 (6%)
4	AMI	B	803	3	16,16,16	1.63	4 (25%)	24,24,24	1.80	4 (16%)

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	NA1	A	801	3	1/1/5/7	0/7/24/27	0/1/1/1
3	NAA	A	802	2,4	-	0/6/23/26	0/1/1/1
4	AMI	A	803	3	-	0/6/34/34	0/0/2/2
2	NA1	B	801	3	1/1/5/7	0/7/24/27	0/1/1/1
3	NAA	B	802	2,4	-	0/6/23/26	0/1/1/1
4	AMI	B	803	3	-	0/6/34/34	0/0/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	AMI	C2-N2	-4.09	1.43	1.47
4	B	803	AMI	C2-N2	-3.75	1.43	1.47
4	A	803	AMI	C6-C5	3.49	1.58	1.52
4	B	803	AMI	C6-C5	3.23	1.57	1.52
3	A	802	NAA	C4-C3	3.22	1.61	1.52
3	B	802	NAA	C4-C3	3.15	1.60	1.52
2	B	801	NA1	C4-C5	3.06	1.59	1.53
4	B	803	AMI	C7-N2	3.02	1.34	1.29
2	A	801	NA1	C4-C5	2.94	1.59	1.53
4	A	803	AMI	C7-N2	2.92	1.34	1.29
3	B	802	NAA	C2-N2	2.74	1.49	1.46
3	A	802	NAA	C2-N2	2.63	1.49	1.46
4	A	803	AMI	O7-C7	2.38	1.38	1.34
4	B	803	AMI	O7-C7	2.25	1.37	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	AMI	O7-C7-N2	-7.19	113.10	117.70
4	B	803	AMI	O7-C7-N2	-5.64	114.09	117.70
2	A	801	NA1	O5-C5-C4	-5.22	104.03	110.65
2	B	801	NA1	O5-C5-C4	-5.16	104.11	110.65
4	A	803	AMI	C5-C4-C3	-4.76	98.31	103.67
4	B	803	AMI	C5-C4-C3	-4.47	98.64	103.67
3	A	802	NAA	O5-C5-C4	-3.27	106.50	110.65
3	B	802	NAA	O5-C5-C4	-2.84	107.05	110.65
4	B	803	AMI	O4-C4-C5	-2.44	105.19	112.43
2	A	801	NA1	C2-N2-C7	2.26	126.89	123.09
4	A	803	AMI	O4-C4-C5	-2.10	106.21	112.43
4	B	803	AMI	O7-C7-N7	2.01	121.84	117.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	801	NA1	C1
2	A	801	NA1	C1

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	377/395 (95%)	-0.09	11 (2%) 49 54	7, 11, 20, 31	0
1	B	373/395 (94%)	-0.12	11 (2%) 49 54	8, 12, 22, 34	0
All	All	750/790 (94%)	-0.11	22 (2%) 49 54	7, 12, 22, 34	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	391	SER	6.3
1	B	390	GLN	5.6
1	B	393	SER	5.5
1	A	391	SER	5.0
1	B	392	ALA	4.7
1	A	398	ALA	4.6
1	B	394	CYS	4.3
1	A	396	ALA	3.5
1	A	390	GLN	3.3
1	A	221	TYR	3.2
1	A	392	ALA	3.0
1	B	62	GLN	2.7
1	B	172	GLN	2.6
1	A	277	SER	2.6
1	B	168	GLN	2.6
1	B	221	TYR	2.5
1	A	394	CYS	2.4
1	A	218	TRP	2.2
1	B	171	LYS	2.2
1	A	168	GLN	2.1
1	A	397	PRO	2.1
1	B	218	TRP	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
3	NAA	A	802	14/15	0.09	0.90	9,9,10,10	0
4	AMI	B	803	15/15	0.10	0.62	7,8,10,11	0
4	AMI	A	803	15/15	0.10	0.60	8,9,10,11	0
3	NAA	B	802	14/15	0.08	0.10	8,9,9,10	0
2	NA1	B	801	15/16	0.07	-0.17	9,11,13,14	0
2	NA1	A	801	15/16	0.07	-0.45	9,10,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.