



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q43  
Title : Ensemble refinement of the protein crystal structure of IAA-aminoacid hydrolase from Arabidopsis thaliana gene At5g56660  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

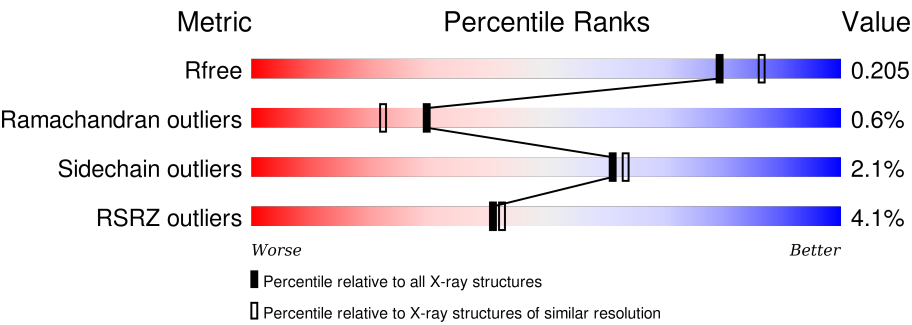
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



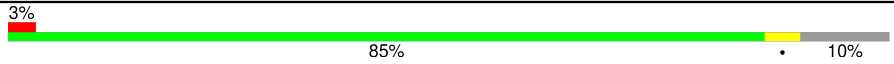
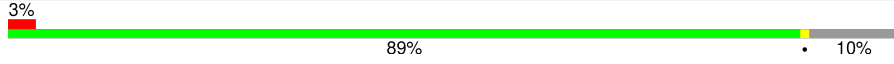
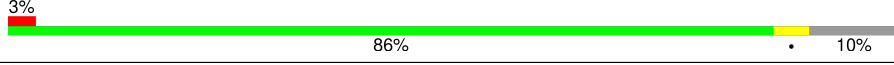
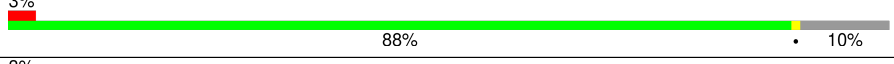
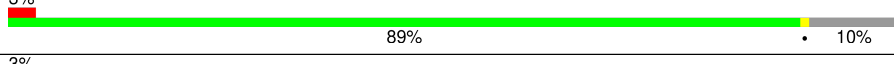
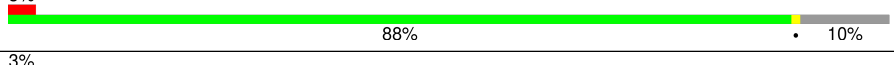
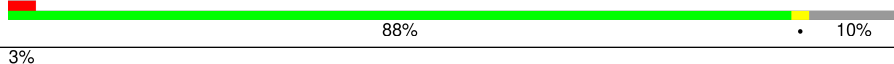
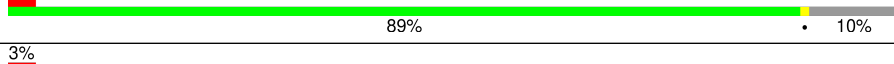
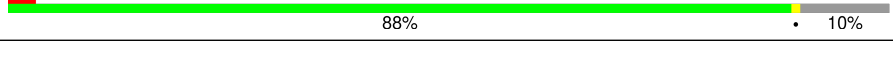
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	1-A	418	<div><div>3%</div><div>88%</div><div>10%</div></div>
1	10-A	418	<div><div>3%</div><div>88%</div><div>10%</div></div>
1	11-A	418	<div><div>3%</div><div>88%</div><div>10%</div></div>
1	12-A	418	<div><div>3%</div><div>87%</div><div>10%</div></div>
1	13-A	418	<div><div>3%</div><div>87%</div><div>10%</div></div>
1	14-A	418	<div><div>3%</div><div>87%</div><div>10%</div></div>
1	15-A	418	<div><div>3%</div><div>86%</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
1	16-A	418	
1	2-A	418	
1	3-A	418	
1	4-A	418	
1	5-A	418	
1	6-A	418	
1	7-A	418	
1	8-A	418	
1	9-A	418	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50784 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 IAA-amino acid hydrolase ILR1-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	2-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	3-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	4-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	5-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	6-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	7-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	8-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	9-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	10-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	11-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	12-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	13-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	14-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	15-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	16-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			

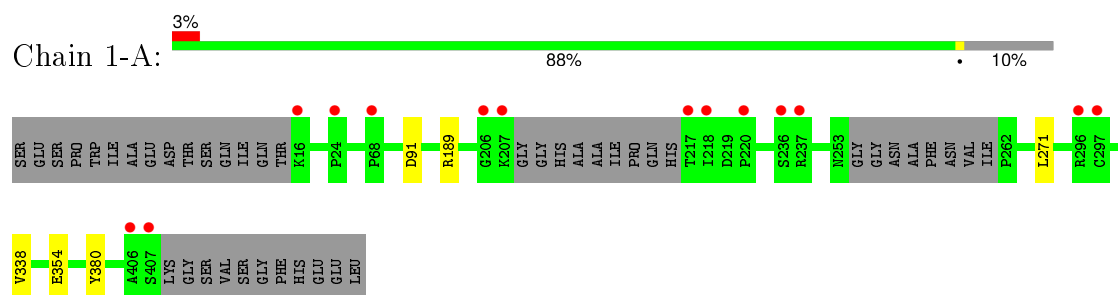
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	285	Total 285	O 285	0	0
2	2-A	285	Total 285	O 285	0	0
2	3-A	285	Total 285	O 285	0	0
2	4-A	285	Total 285	O 285	0	0
2	5-A	285	Total 285	O 285	0	0
2	6-A	285	Total 285	O 285	0	0
2	7-A	285	Total 285	O 285	0	0
2	8-A	285	Total 285	O 285	0	0
2	9-A	285	Total 285	O 285	0	0
2	10-A	285	Total 285	O 285	0	0
2	11-A	285	Total 285	O 285	0	0
2	12-A	285	Total 285	O 285	0	0
2	13-A	285	Total 285	O 285	0	0
2	14-A	285	Total 285	O 285	0	0
2	15-A	285	Total 285	O 285	0	0
2	16-A	285	Total 285	O 285	0	0

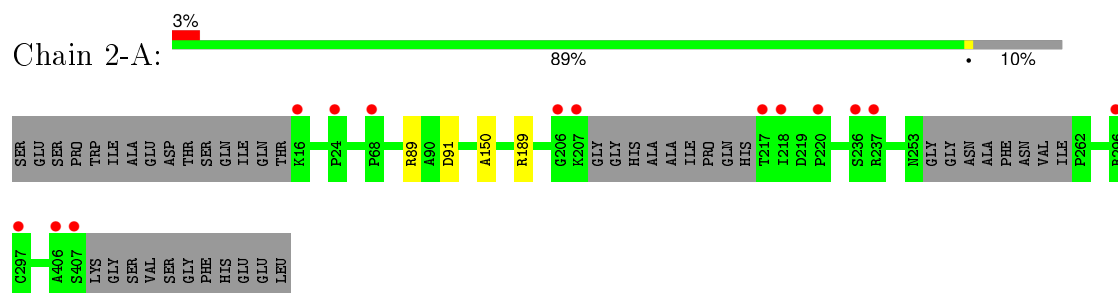
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

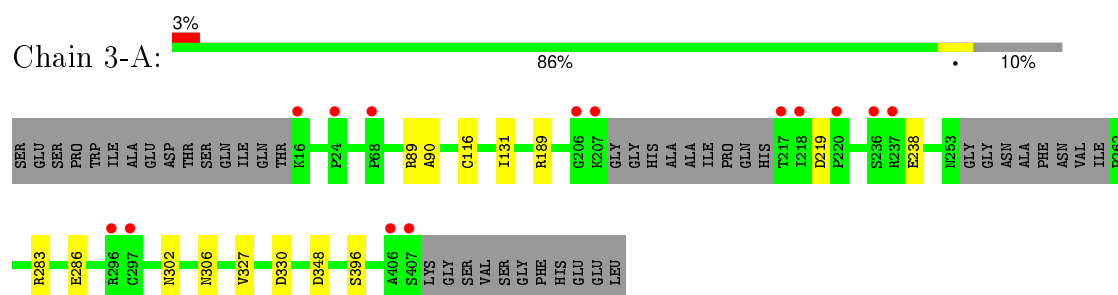
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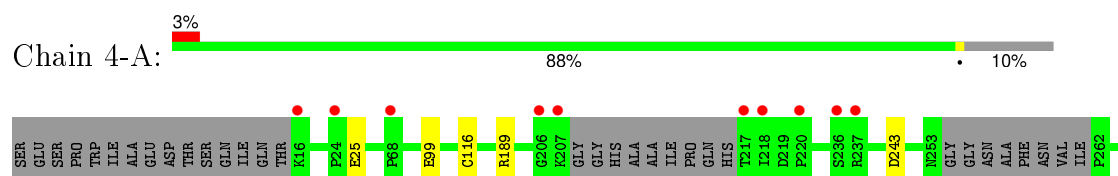
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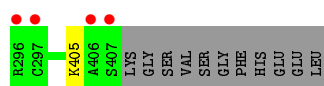


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

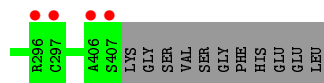
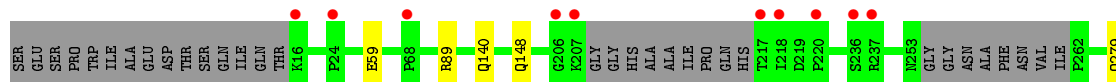
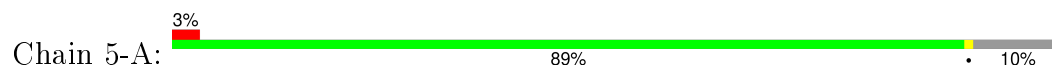


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

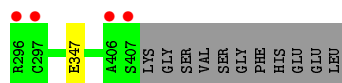
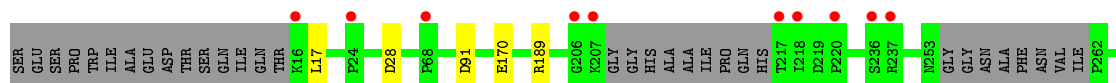
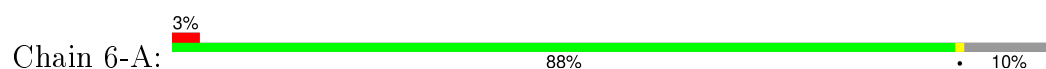




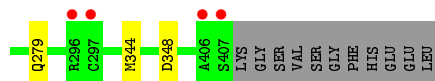
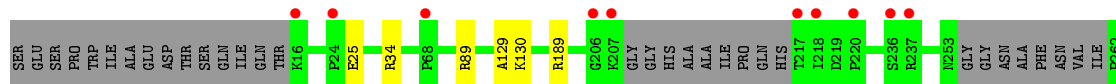
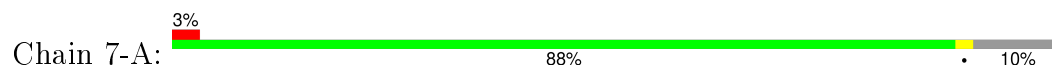
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2



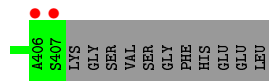
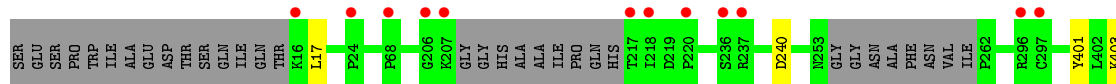
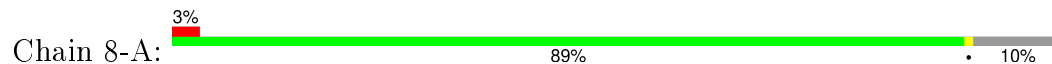
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2



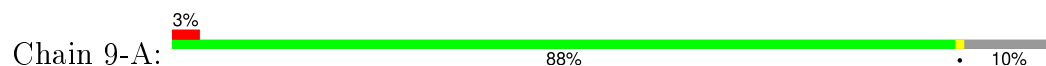
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

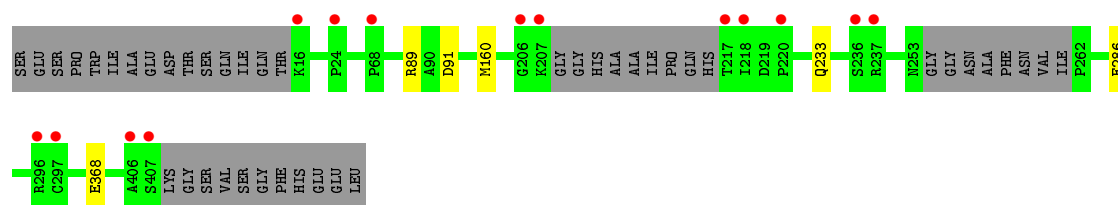


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

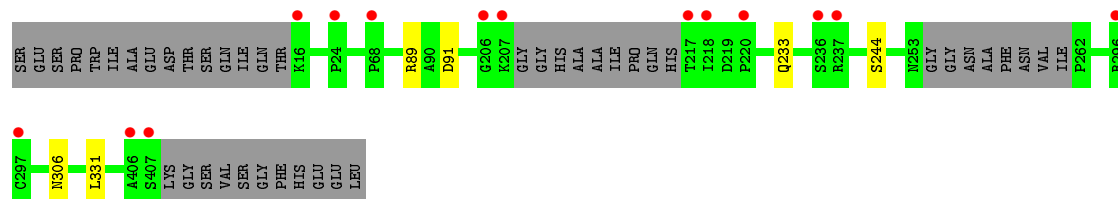


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

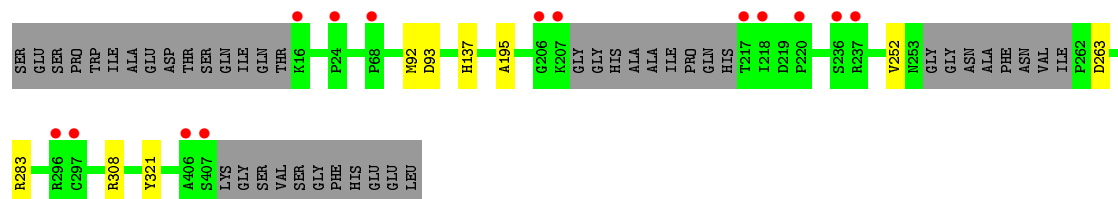
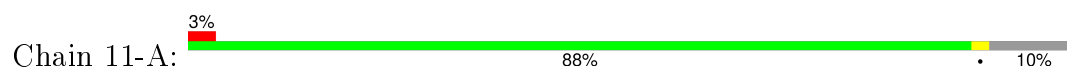




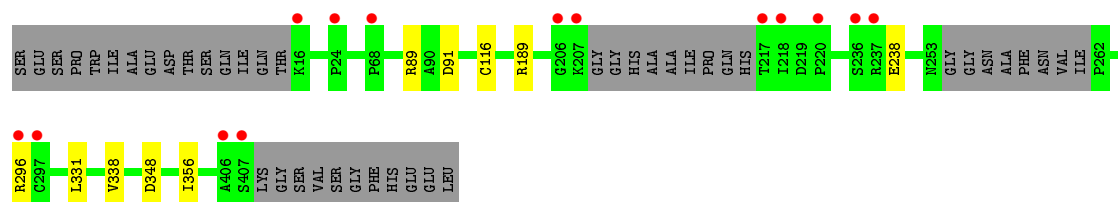
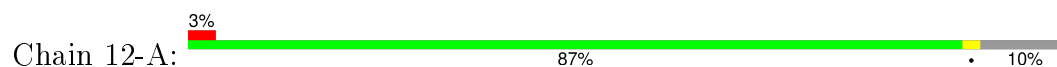
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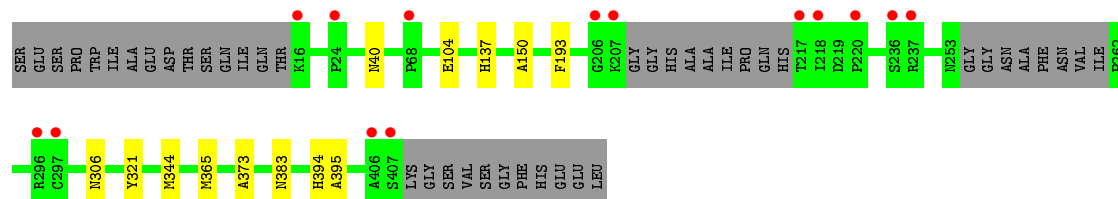
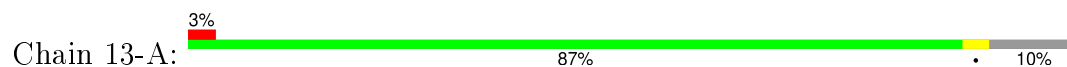
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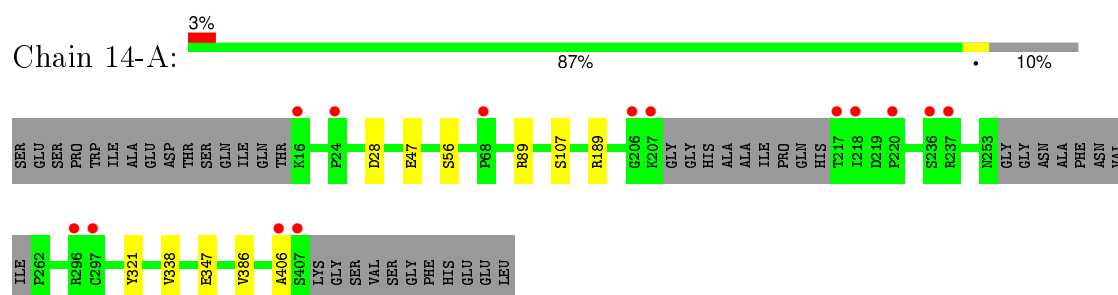


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

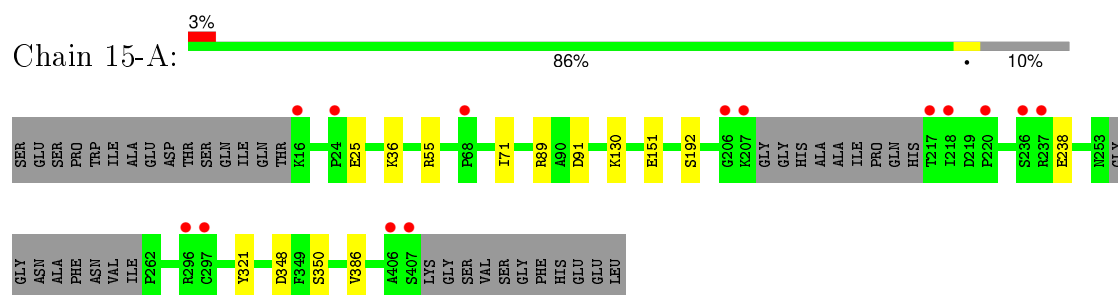


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

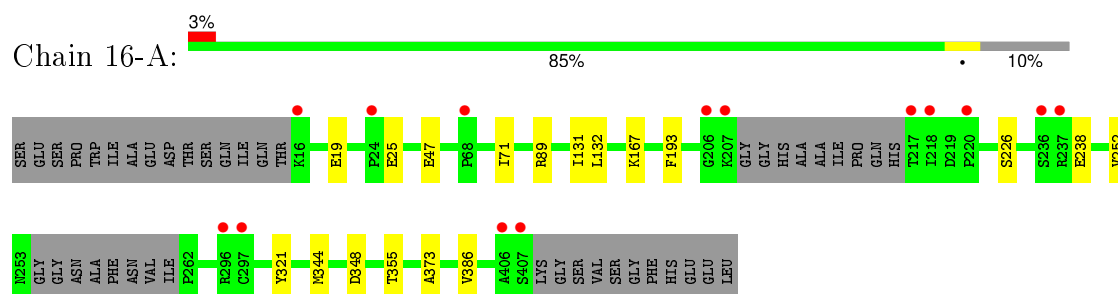




- Molecule 1: IAA-amino acid hydrolase ILR1-like 2



- Molecule 1: IAA-amino acid hydrolase ILR1-like 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.26 Å 75.26 Å 130.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.09 – 2.00 24.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.09-2.00) 99.9 (24.21-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.99 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.149 , 0.204 0.155 , 0.205	Depositor DCC
$R_{free}$ test set	1504 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 68.1	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29630 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	50784	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 4.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	1-A	0.45	0/2948	0.63	0/3984
1	2-A	0.45	0/2948	0.63	0/3984
1	3-A	0.45	0/2948	0.63	0/3984
1	4-A	0.45	0/2948	0.63	0/3984
1	5-A	0.46	0/2948	0.62	0/3984
1	6-A	0.46	0/2948	0.62	0/3984
1	7-A	0.46	0/2948	0.61	0/3984
1	8-A	0.46	0/2948	0.61	0/3984
1	9-A	0.45	0/2948	0.61	0/3984
1	10-A	0.46	0/2948	0.62	0/3984
1	11-A	0.45	0/2948	0.62	0/3984
1	12-A	0.44	0/2948	0.62	0/3984
1	13-A	0.54	0/2948	0.70	0/3984
1	14-A	0.52	0/2948	0.71	1/3984 (0.0%)
1	15-A	0.52	0/2948	0.70	0/3984
1	16-A	0.51	0/2948	0.70	0/3984
All	All	0.47	0/47168	0.64	1/63744 (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	16-A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	189	ARG	NE-CZ-NH1	-5.11	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	16-A	321	TYR	Sidechain

## 5.2 Too-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 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	1-A	2889	0	2919	0	0
1	2-A	2889	0	2919	0	0
1	3-A	2889	0	2919	0	0
1	4-A	2889	0	2919	0	0
1	5-A	2889	0	2919	0	0
1	6-A	2889	0	2919	0	0
1	7-A	2889	0	2919	0	0
1	8-A	2889	0	2919	0	0
1	9-A	2889	0	2919	0	0
1	10-A	2889	0	2919	0	0
1	11-A	2889	0	2919	0	0
1	12-A	2889	0	2919	0	0
1	13-A	2889	0	2919	0	0
1	14-A	2889	0	2919	0	0
1	15-A	2889	0	2919	0	0
1	16-A	2889	0	2919	0	0
2	1-A	285	0	0	0	0
2	2-A	285	0	0	0	0
2	3-A	285	0	0	0	0
2	4-A	285	0	0	0	0
2	5-A	285	0	0	0	0
2	6-A	285	0	0	0	0
2	7-A	285	0	0	0	0
2	8-A	285	0	0	0	0
2	9-A	285	0	0	0	0
2	10-A	285	0	0	0	0
2	11-A	285	0	0	0	0
2	12-A	285	0	0	0	0
2	13-A	285	0	0	0	0
2	14-A	285	0	0	0	0
2	15-A	285	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	16-A	285	0	0	0	0
All	All	50784	0	46704	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	369/418 (88%)	348 (94%)	20 (5%)	1 (0%)	46	41
1	2-A	369/418 (88%)	348 (94%)	20 (5%)	1 (0%)	46	41
1	3-A	369/418 (88%)	338 (92%)	27 (7%)	4 (1%)	17	9
1	4-A	369/418 (88%)	354 (96%)	15 (4%)	0	100	100
1	5-A	369/418 (88%)	357 (97%)	12 (3%)	0	100	100
1	6-A	369/418 (88%)	352 (95%)	17 (5%)	0	100	100
1	7-A	369/418 (88%)	340 (92%)	27 (7%)	2 (0%)	34	26
1	8-A	369/418 (88%)	354 (96%)	13 (4%)	2 (0%)	34	26
1	9-A	369/418 (88%)	356 (96%)	13 (4%)	0	100	100
1	10-A	369/418 (88%)	355 (96%)	13 (4%)	1 (0%)	46	41
1	11-A	369/418 (88%)	348 (94%)	16 (4%)	5 (1%)	14	6
1	12-A	369/418 (88%)	345 (94%)	23 (6%)	1 (0%)	46	41
1	13-A	369/418 (88%)	341 (92%)	23 (6%)	5 (1%)	14	6
1	14-A	369/418 (88%)	349 (95%)	16 (4%)	4 (1%)	17	9
1	15-A	369/418 (88%)	347 (94%)	21 (6%)	1 (0%)	46	41
1	16-A	369/418 (88%)	340 (92%)	21 (6%)	8 (2%)	8	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5904/6688 (88%)	5572 (94%)	297 (5%)	35 (1%)	30	22

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	150	ALA
1	11-A	195	ALA
1	11-A	263	ASP
1	11-A	308	ARG
1	13-A	373	ALA
1	15-A	71	ILE
1	16-A	131	ILE
1	3-A	238	GLU
1	7-A	130	LYS
1	12-A	331	LEU
1	13-A	394	HIS
1	13-A	395	ALA
1	14-A	107	SER
1	16-A	132	LEU
1	16-A	238	GLU
1	3-A	90	ALA
1	8-A	403	LYS
1	10-A	331	LEU
1	11-A	137	HIS
1	13-A	137	HIS
1	14-A	47	GLU
1	14-A	406	ALA
1	16-A	373	ALA
1	1-A	380	TYR
1	3-A	396	SER
1	7-A	129	ALA
1	16-A	167	LYS
1	8-A	401	TYR
1	13-A	150	ALA
1	16-A	47	GLU
1	14-A	347	GLU
1	16-A	71	ILE
1	3-A	131	ILE
1	16-A	252	VAL
1	11-A	252	VAL

### 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	1-A	308/341 (90%)	303 (98%)	5 (2%)	70	73
1	2-A	308/341 (90%)	305 (99%)	3 (1%)	82	85
1	3-A	308/341 (90%)	297 (96%)	11 (4%)	42	39
1	4-A	308/341 (90%)	302 (98%)	6 (2%)	65	67
1	5-A	308/341 (90%)	303 (98%)	5 (2%)	70	73
1	6-A	308/341 (90%)	302 (98%)	6 (2%)	65	67
1	7-A	308/341 (90%)	301 (98%)	7 (2%)	58	60
1	8-A	308/341 (90%)	306 (99%)	2 (1%)	90	93
1	9-A	308/341 (90%)	302 (98%)	6 (2%)	65	67
1	10-A	308/341 (90%)	303 (98%)	5 (2%)	70	73
1	11-A	308/341 (90%)	304 (99%)	4 (1%)	76	79
1	12-A	308/341 (90%)	299 (97%)	9 (3%)	50	49
1	13-A	308/341 (90%)	300 (97%)	8 (3%)	54	54
1	14-A	308/341 (90%)	302 (98%)	6 (2%)	65	67
1	15-A	308/341 (90%)	295 (96%)	13 (4%)	36	31
1	16-A	308/341 (90%)	299 (97%)	9 (3%)	50	49
All	All	4928/5456 (90%)	4823 (98%)	105 (2%)	61	63

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	91	ASP
1	1-A	189	ARG
1	1-A	271	LEU
1	1-A	338	VAL
1	1-A	354	GLU
1	2-A	89	ARG
1	2-A	91	ASP
1	2-A	189	ARG

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Mol	Chain	Res	Type
1	3-A	89	ARG
1	3-A	116	CYS
1	3-A	189	ARG
1	3-A	219	ASP
1	3-A	283	ARG
1	3-A	286	GLU
1	3-A	302	ASN
1	3-A	306	ASN
1	3-A	327	VAL
1	3-A	330	ASP
1	3-A	348	ASP
1	4-A	25	GLU
1	4-A	99	GLU
1	4-A	116	CYS
1	4-A	189	ARG
1	4-A	243	ASP
1	4-A	405	LYS
1	5-A	59	GLU
1	5-A	89	ARG
1	5-A	140	GLN
1	5-A	148	GLN
1	5-A	279	GLN
1	6-A	17	LEU
1	6-A	28	ASP
1	6-A	91	ASP
1	6-A	170	GLU
1	6-A	189	ARG
1	6-A	347	GLU
1	7-A	25	GLU
1	7-A	34	ARG
1	7-A	89	ARG
1	7-A	189	ARG
1	7-A	279	GLN
1	7-A	344	MET
1	7-A	348	ASP
1	8-A	17	LEU
1	8-A	240	ASP
1	9-A	89	ARG
1	9-A	91	ASP
1	9-A	160	MET
1	9-A	233	GLN
1	9-A	286	GLU

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Mol	Chain	Res	Type
1	9-A	368	GLU
1	10-A	89	ARG
1	10-A	91	ASP
1	10-A	233	GLN
1	10-A	244	SER
1	10-A	306	ASN
1	11-A	92	MET
1	11-A	93	ASP
1	11-A	283	ARG
1	11-A	321	TYR
1	12-A	89	ARG
1	12-A	91	ASP
1	12-A	116	CYS
1	12-A	189	ARG
1	12-A	238	GLU
1	12-A	296	ARG
1	12-A	338	VAL
1	12-A	348	ASP
1	12-A	356	ILE
1	13-A	40	ASN
1	13-A	104	GLU
1	13-A	193	PHE
1	13-A	306	ASN
1	13-A	321	TYR
1	13-A	344	MET
1	13-A	365	MET
1	13-A	383	ASN
1	14-A	28	ASP
1	14-A	56	SER
1	14-A	89	ARG
1	14-A	321	TYR
1	14-A	338	VAL
1	14-A	386	VAL
1	15-A	25	GLU
1	15-A	36	LYS
1	15-A	55	ARG
1	15-A	89	ARG
1	15-A	91	ASP
1	15-A	130	LYS
1	15-A	151	GLU
1	15-A	192	SER
1	15-A	238	GLU

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Mol	Chain	Res	Type
1	15-A	321	TYR
1	15-A	348	ASP
1	15-A	350	SER
1	15-A	386	VAL
1	16-A	19	GLU
1	16-A	25	GLU
1	16-A	89	ARG
1	16-A	193	PHE
1	16-A	226	SER
1	16-A	344	MET
1	16-A	348	ASP
1	16-A	355	THR
1	16-A	386	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	133	HIS
1	1-A	233	GLN
1	1-A	281	GLN
1	1-A	298	ASN
1	1-A	316	ASN
1	2-A	114	HIS
1	2-A	133	HIS
1	2-A	233	GLN
1	2-A	281	GLN
1	2-A	298	ASN
1	2-A	316	ASN
1	2-A	334	GLN
1	2-A	359	HIS
1	2-A	370	ASN
1	2-A	400	GLN
1	3-A	233	GLN
1	3-A	281	GLN
1	3-A	298	ASN
1	3-A	302	ASN
1	3-A	306	ASN
1	3-A	316	ASN
1	3-A	334	GLN
1	3-A	370	ASN
1	4-A	133	HIS
1	4-A	233	GLN

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Mol	Chain	Res	Type
1	4-A	281	GLN
1	4-A	298	ASN
1	4-A	334	GLN
1	4-A	400	GLN
1	5-A	98	GLN
1	5-A	233	GLN
1	5-A	298	ASN
1	5-A	302	ASN
1	5-A	334	GLN
1	5-A	370	ASN
1	5-A	400	GLN
1	6-A	118	HIS
1	6-A	133	HIS
1	6-A	233	GLN
1	6-A	298	ASN
1	6-A	334	GLN
1	6-A	370	ASN
1	7-A	137	HIS
1	7-A	232	GLN
1	7-A	233	GLN
1	7-A	282	GLN
1	7-A	298	ASN
1	7-A	334	GLN
1	7-A	370	ASN
1	8-A	233	GLN
1	8-A	281	GLN
1	8-A	298	ASN
1	8-A	334	GLN
1	8-A	400	GLN
1	9-A	281	GLN
1	9-A	298	ASN
1	9-A	334	GLN
1	9-A	370	ASN
1	9-A	400	GLN
1	10-A	140	GLN
1	10-A	176	HIS
1	10-A	253	ASN
1	10-A	298	ASN
1	10-A	306	ASN
1	10-A	323	GLN
1	10-A	370	ASN
1	11-A	138	HIS

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Mol	Chain	Res	Type
1	11-A	233	GLN
1	11-A	298	ASN
1	11-A	316	ASN
1	11-A	334	GLN
1	11-A	370	ASN
1	11-A	400	GLN
1	12-A	140	GLN
1	12-A	168	ASN
1	12-A	233	GLN
1	12-A	282	GLN
1	12-A	298	ASN
1	12-A	306	ASN
1	12-A	359	HIS
1	12-A	370	ASN
1	13-A	40	ASN
1	13-A	98	GLN
1	13-A	176	HIS
1	13-A	233	GLN
1	13-A	281	GLN
1	13-A	291	GLN
1	13-A	298	ASN
1	13-A	334	GLN
1	13-A	376	HIS
1	13-A	394	HIS
1	13-A	400	GLN
1	14-A	133	HIS
1	14-A	233	GLN
1	14-A	282	GLN
1	14-A	291	GLN
1	14-A	298	ASN
1	14-A	316	ASN
1	14-A	334	GLN
1	14-A	376	HIS
1	15-A	140	GLN
1	15-A	168	ASN
1	15-A	233	GLN
1	15-A	282	GLN
1	15-A	298	ASN
1	15-A	334	GLN
1	15-A	400	GLN
1	16-A	98	GLN
1	16-A	140	GLN

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Mol	Chain	Res	Type
1	16-A	168	ASN
1	16-A	233	GLN
1	16-A	281	GLN
1	16-A	298	ASN
1	16-A	302	ASN
1	16-A	316	ASN
1	16-A	334	GLN
1	16-A	400	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 carbohydrates 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	1-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	2-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	3-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	4-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	5-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	6-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	7-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	8-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	9-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	10-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	11-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	12-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	13-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	14-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	15-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
1	16-A	375/418 (89%)	-0.16	14 (3%)	45	47	10, 23, 47, 66	375 (100%)
All	All	6000/6688 (89%)	-0.16	224 (3%)	41	47	10, 23, 48, 66	6000 (100%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	218	ILE	5.8
1	2-A	218	ILE	5.8
1	3-A	218	ILE	5.8
1	4-A	218	ILE	5.8
1	5-A	218	ILE	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	6-A	218	ILE	5.8
1	7-A	218	ILE	5.8
1	8-A	218	ILE	5.8
1	9-A	218	ILE	5.8
1	10-A	218	ILE	5.8
1	11-A	218	ILE	5.8
1	12-A	218	ILE	5.8
1	13-A	218	ILE	5.8
1	14-A	218	ILE	5.8
1	15-A	218	ILE	5.8
1	16-A	218	ILE	5.8
1	1-A	236	SER	4.7
1	2-A	236	SER	4.7
1	3-A	236	SER	4.7
1	4-A	236	SER	4.7
1	5-A	236	SER	4.7
1	6-A	236	SER	4.7
1	7-A	236	SER	4.7
1	8-A	236	SER	4.7
1	9-A	236	SER	4.7
1	10-A	236	SER	4.7
1	11-A	236	SER	4.7
1	12-A	236	SER	4.7
1	13-A	236	SER	4.7
1	14-A	236	SER	4.7
1	15-A	236	SER	4.7
1	16-A	236	SER	4.7
1	1-A	24	PRO	4.0
1	2-A	24	PRO	4.0
1	3-A	24	PRO	4.0
1	4-A	24	PRO	4.0
1	5-A	24	PRO	4.0
1	6-A	24	PRO	4.0
1	7-A	24	PRO	4.0
1	8-A	24	PRO	4.0
1	9-A	24	PRO	4.0
1	10-A	24	PRO	4.0
1	11-A	24	PRO	4.0
1	12-A	24	PRO	4.0
1	13-A	24	PRO	4.0
1	14-A	24	PRO	4.0
1	15-A	24	PRO	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	16-A	24	PRO	4.0
1	1-A	296	ARG	3.8
1	2-A	296	ARG	3.8
1	3-A	296	ARG	3.8
1	4-A	296	ARG	3.8
1	5-A	296	ARG	3.8
1	6-A	296	ARG	3.8
1	7-A	296	ARG	3.8
1	8-A	296	ARG	3.8
1	9-A	296	ARG	3.8
1	10-A	296	ARG	3.8
1	11-A	296	ARG	3.8
1	12-A	296	ARG	3.8
1	13-A	296	ARG	3.8
1	14-A	296	ARG	3.8
1	15-A	296	ARG	3.8
1	16-A	296	ARG	3.8
1	1-A	217	THR	2.9
1	2-A	217	THR	2.9
1	3-A	217	THR	2.9
1	4-A	217	THR	2.9
1	5-A	217	THR	2.9
1	6-A	217	THR	2.9
1	7-A	217	THR	2.9
1	8-A	217	THR	2.9
1	9-A	217	THR	2.9
1	10-A	217	THR	2.9
1	11-A	217	THR	2.9
1	12-A	217	THR	2.9
1	13-A	217	THR	2.9
1	14-A	217	THR	2.9
1	15-A	217	THR	2.9
1	16-A	217	THR	2.9
1	1-A	68	PRO	2.8
1	2-A	68	PRO	2.8
1	3-A	68	PRO	2.8
1	4-A	68	PRO	2.8
1	5-A	68	PRO	2.8
1	6-A	68	PRO	2.8
1	7-A	68	PRO	2.8
1	8-A	68	PRO	2.8
1	9-A	68	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	10-A	68	PRO	2.8
1	11-A	68	PRO	2.8
1	12-A	68	PRO	2.8
1	13-A	68	PRO	2.8
1	14-A	68	PRO	2.8
1	15-A	68	PRO	2.8
1	16-A	68	PRO	2.8
1	1-A	220	PRO	2.7
1	2-A	220	PRO	2.7
1	3-A	220	PRO	2.7
1	4-A	220	PRO	2.7
1	5-A	220	PRO	2.7
1	6-A	220	PRO	2.7
1	7-A	220	PRO	2.7
1	8-A	220	PRO	2.7
1	9-A	220	PRO	2.7
1	10-A	220	PRO	2.7
1	11-A	220	PRO	2.7
1	12-A	220	PRO	2.7
1	13-A	220	PRO	2.7
1	14-A	220	PRO	2.7
1	15-A	220	PRO	2.7
1	16-A	220	PRO	2.7
1	1-A	16	LYS	2.7
1	2-A	16	LYS	2.7
1	3-A	16	LYS	2.7
1	4-A	16	LYS	2.7
1	5-A	16	LYS	2.7
1	6-A	16	LYS	2.7
1	7-A	16	LYS	2.7
1	8-A	16	LYS	2.7
1	9-A	16	LYS	2.7
1	10-A	16	LYS	2.7
1	11-A	16	LYS	2.7
1	12-A	16	LYS	2.7
1	13-A	16	LYS	2.7
1	14-A	16	LYS	2.7
1	15-A	16	LYS	2.7
1	16-A	16	LYS	2.7
1	1-A	407	SER	2.7
1	2-A	407	SER	2.7
1	3-A	407	SER	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	4-A	407	SER	2.7
1	5-A	407	SER	2.7
1	6-A	407	SER	2.7
1	7-A	407	SER	2.7
1	8-A	407	SER	2.7
1	9-A	407	SER	2.7
1	10-A	407	SER	2.7
1	11-A	407	SER	2.7
1	12-A	407	SER	2.7
1	13-A	407	SER	2.7
1	14-A	407	SER	2.7
1	15-A	407	SER	2.7
1	16-A	407	SER	2.7
1	1-A	207	LYS	2.7
1	2-A	207	LYS	2.7
1	3-A	207	LYS	2.7
1	4-A	207	LYS	2.7
1	5-A	207	LYS	2.7
1	6-A	207	LYS	2.7
1	7-A	207	LYS	2.7
1	8-A	207	LYS	2.7
1	9-A	207	LYS	2.7
1	10-A	207	LYS	2.7
1	11-A	207	LYS	2.7
1	12-A	207	LYS	2.7
1	13-A	207	LYS	2.7
1	14-A	207	LYS	2.7
1	15-A	207	LYS	2.7
1	16-A	207	LYS	2.7
1	1-A	237	ARG	2.5
1	2-A	237	ARG	2.5
1	3-A	237	ARG	2.5
1	4-A	237	ARG	2.5
1	5-A	237	ARG	2.5
1	6-A	237	ARG	2.5
1	7-A	237	ARG	2.5
1	8-A	237	ARG	2.5
1	9-A	237	ARG	2.5
1	10-A	237	ARG	2.5
1	11-A	237	ARG	2.5
1	12-A	237	ARG	2.5
1	13-A	237	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	14-A	237	ARG	2.5
1	15-A	237	ARG	2.5
1	16-A	237	ARG	2.5
1	1-A	406	ALA	2.5
1	2-A	406	ALA	2.5
1	3-A	406	ALA	2.5
1	4-A	406	ALA	2.5
1	5-A	406	ALA	2.5
1	6-A	406	ALA	2.5
1	7-A	406	ALA	2.5
1	8-A	406	ALA	2.5
1	9-A	406	ALA	2.5
1	10-A	406	ALA	2.5
1	11-A	406	ALA	2.5
1	12-A	406	ALA	2.5
1	13-A	406	ALA	2.5
1	14-A	406	ALA	2.5
1	15-A	406	ALA	2.5
1	16-A	406	ALA	2.5
1	1-A	206	GLY	2.5
1	2-A	206	GLY	2.5
1	3-A	206	GLY	2.5
1	4-A	206	GLY	2.5
1	5-A	206	GLY	2.5
1	6-A	206	GLY	2.5
1	7-A	206	GLY	2.5
1	8-A	206	GLY	2.5
1	9-A	206	GLY	2.5
1	10-A	206	GLY	2.5
1	11-A	206	GLY	2.5
1	12-A	206	GLY	2.5
1	13-A	206	GLY	2.5
1	14-A	206	GLY	2.5
1	15-A	206	GLY	2.5
1	16-A	206	GLY	2.5
1	1-A	297	CYS	2.2
1	2-A	297	CYS	2.2
1	3-A	297	CYS	2.2
1	4-A	297	CYS	2.2
1	5-A	297	CYS	2.2
1	6-A	297	CYS	2.2
1	7-A	297	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	8-A	297	CYS	2.2
1	9-A	297	CYS	2.2
1	10-A	297	CYS	2.2
1	11-A	297	CYS	2.2
1	12-A	297	CYS	2.2
1	13-A	297	CYS	2.2
1	14-A	297	CYS	2.2
1	15-A	297	CYS	2.2
1	16-A	297	CYS	2.2

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.