



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:08 am BST

PDB ID : 4U48  
Title : Crystal structure of Salmonella alpha-2-macroglobulin  
Authors : Wong, S.G.; Dessen, A.  
Deposited on : 2014-07-23  
Resolution : 2.95 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

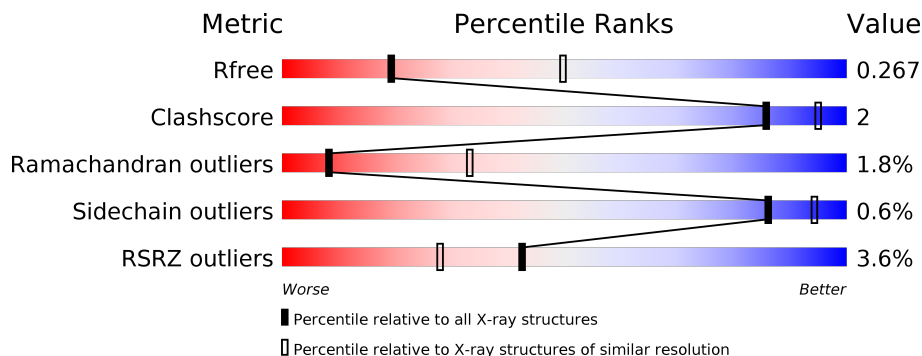
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 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	1647	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 23672 atoms, of which 11792 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 Putative inner membrane lipoprotein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	1538	23672	7487	11792	2090	2280	1	22	0	0	0

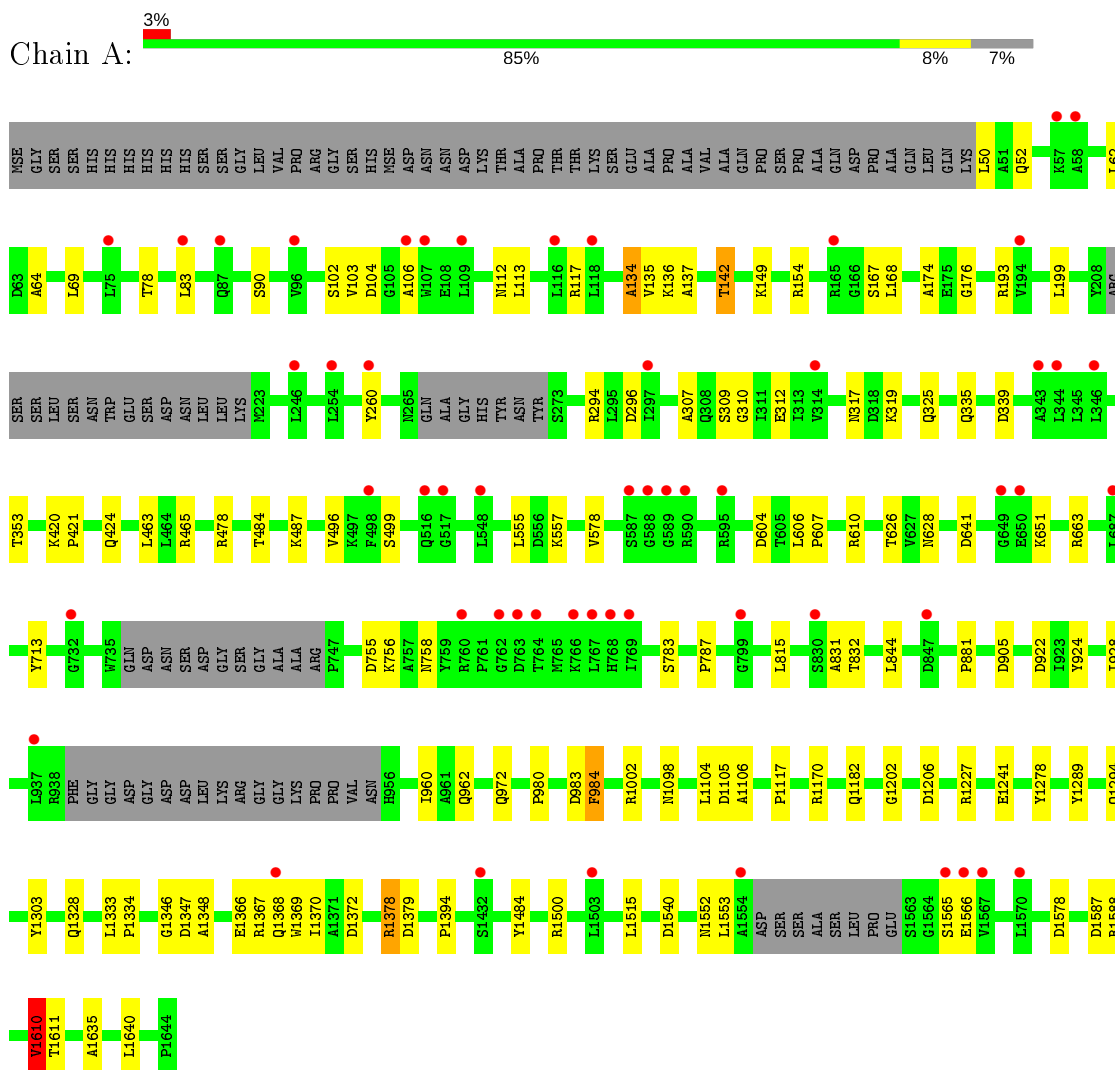
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	expression tag	UNP Q8ZN46
A	-1	GLY	-	expression tag	UNP Q8ZN46
A	0	SER	-	expression tag	UNP Q8ZN46
A	1	SER	-	expression tag	UNP Q8ZN46
A	2	HIS	-	expression tag	UNP Q8ZN46
A	3	HIS	-	expression tag	UNP Q8ZN46
A	4	HIS	-	expression tag	UNP Q8ZN46
A	5	HIS	-	expression tag	UNP Q8ZN46
A	6	HIS	-	expression tag	UNP Q8ZN46
A	7	HIS	-	expression tag	UNP Q8ZN46
A	8	SER	-	expression tag	UNP Q8ZN46
A	9	SER	-	expression tag	UNP Q8ZN46
A	10	GLY	-	expression tag	UNP Q8ZN46
A	11	LEU	-	expression tag	UNP Q8ZN46
A	12	VAL	-	expression tag	UNP Q8ZN46
A	13	PRO	-	expression tag	UNP Q8ZN46
A	14	ARG	-	expression tag	UNP Q8ZN46
A	15	GLY	-	expression tag	UNP Q8ZN46
A	16	SER	-	expression tag	UNP Q8ZN46
A	17	HIS	-	expression tag	UNP Q8ZN46
A	18	MSE	-	expression tag	UNP Q8ZN46
A	98	ALA	LYS	engineered mutation	UNP Q8ZN46
A	99	ALA	LYS	engineered mutation	UNP Q8ZN46

### 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: Putative inner membrane lipoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.55Å 82.18Å 99.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.71 – 2.95 59.14 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.71-2.95) 100.0 (59.14-2.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.224 , 0.265 0.230 , 0.267	Depositor DCC
$R_{free}$ test set	2244 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtrriage
Anisotropy	0.714	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/12099	0.41	0/16448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	11880	11792	11774	52	1
All	All	11880	11792	11774	52	1

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 2.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ARG:NH2	1:A:641:ASP:OD2	2.21	0.72
1:A:1372:ASP:O	1:A:1378:ARG:NH2	2.24	0.69
1:A:1294:GLN:OE1	1:A:1328:GLN:NE2	2.29	0.65
1:A:484:THR:OG1	1:A:499:SER:OG	2.15	0.64
1:A:1378:ARG:NH1	1:A:1379:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:NH2	1:A:335:GLN:OE1	2.32	0.63
1:A:1241:GLU:OE2	1:A:1278:TYR:OH	2.12	0.62
1:A:1289:TYR:OH	1:A:1578:ASP:OD2	2.10	0.61
1:A:1366:GLU:O	1:A:1368:GLN:N	2.33	0.60
1:A:663:ARG:NH1	1:A:713:TYR:OH	2.35	0.59
1:A:1105:ASP:OD1	1:A:1106:ALA:N	2.38	0.57
1:A:755:ASP:OD1	1:A:756:LYS:N	2.38	0.57
1:A:134:ALA:O	1:A:136:LYS:N	2.35	0.55
1:A:463:LEU:O	1:A:465:ARG:NH1	2.40	0.55
1:A:1587:ASP:OD2	1:A:1588:ARG:NH1	2.40	0.54
1:A:1552:ASN:OD1	1:A:1553:LEU:N	2.39	0.53
1:A:922:ASP:OD2	1:A:924:TYR:N	2.43	0.52
1:A:962:GLN:NE2	1:A:980:PRO:O	2.42	0.51
1:A:1500:ARG:NH1	1:A:1540:ASP:OD1	2.44	0.50
1:A:1565:SER:OG	1:A:1566:GLU:OE1	2.27	0.50
1:A:317:ASN:O	1:A:319:LYS:N	2.43	0.49
1:A:64:ALA:O	1:A:149:LYS:NZ	2.42	0.48
1:A:606:LEU:HB2	1:A:607:PRO:HD2	1.96	0.48
1:A:325:GLN:OE1	1:A:325:GLN:N	2.48	0.47
1:A:972:GLN:OE1	1:A:972:GLN:N	2.47	0.47
1:A:604:ASP:OD1	1:A:604:ASP:N	2.47	0.47
1:A:103:VAL:HG22	1:A:104:ASP:H	1.80	0.46
1:A:1346:GLY:O	1:A:1348:ALA:N	2.49	0.46
1:A:626:THR:HG21	1:A:905:ASP:OD2	2.15	0.46
1:A:628:ASN:OD1	1:A:1002:ARG:NH2	2.45	0.46
1:A:167:SER:OG	1:A:168:LEU:N	2.49	0.45
1:A:555:LEU:O	1:A:557:LYS:N	2.44	0.45
1:A:199:LEU:HD21	1:A:353:THR:HG21	1.99	0.45
1:A:1515:LEU:HD12	1:A:1640:LEU:HD11	1.98	0.45
1:A:312:GLU:OE1	1:A:312:GLU:N	2.50	0.45
1:A:1610:VAL:HG23	1:A:1611:THR:H	1.82	0.45
1:A:309:SER:OG	1:A:310:GLY:N	2.50	0.44
1:A:83:LEU:HA	1:A:137:ALA:HA	2.00	0.44
1:A:112:ASN:OD1	1:A:113:LEU:N	2.50	0.44
1:A:69:LEU:HD11	1:A:117:ARG:NH1	2.33	0.44
1:A:62:LEU:N	1:A:78:THR:O	2.51	0.43
1:A:960:ILE:HG13	1:A:984:PHE:HB2	2.00	0.43
1:A:1333:LEU:HB3	1:A:1334:PRO:HD3	2.01	0.42
1:A:193:ARG:NH2	1:A:260:TYR:OH	2.53	0.42
1:A:420:LYS:HB2	1:A:421:PRO:HD2	2.01	0.41
1:A:424:GLN:NE2	1:A:1227:ARG:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASP:OD2	1:A:787:PRO:HG3	2.20	0.41
1:A:1170:ARG:NH2	1:A:1202:GLY:O	2.54	0.41
1:A:1117:PRO:HG2	1:A:1484:TYR:CZ	2.56	0.41
1:A:496:VAL:HG21	1:A:578:VAL:HG11	2.03	0.41
1:A:50:LEU:HD13	1:A:52:GLN:H	1.86	0.41
1:A:783:SER:HB3	1:A:815:LEU:HD23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:OG	1:A:339:ASP:OD2[2_675]	1.98	0.22

## 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	1525/1647 (93%)	1382 (91%)	115 (8%)	28 (2%)	<b>8</b> 33

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	881	PRO
1	A	928	ILE
1	A	1098	ASN
1	A	1104	LEU
1	A	1347	ASP
1	A	1367	ARG
1	A	1370	ILE
1	A	90	SER
1	A	134	ALA

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Mol	Chain	Res	Type
1	A	142	THR
1	A	154	ARG
1	A	176	GLY
1	A	651	LYS
1	A	983	ASP
1	A	1635	ALA
1	A	307	ALA
1	A	487	LYS
1	A	831	ALA
1	A	832	THR
1	A	984	PHE
1	A	1206	ASP
1	A	1369	TRP
1	A	106	ALA
1	A	174	ALA
1	A	758	ASN
1	A	1394	PRO
1	A	1610	VAL

### 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	1260/1324 (95%)	1253 (99%)	7 (1%)	<a href="#">86</a> <a href="#">94</a>

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	THR
1	A	478	ARG
1	A	844	LEU
1	A	1182	GLN
1	A	1303	TYR
1	A	1378	ARG
1	A	1610	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1328	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	264:MSE	C	265:ASN	N	4.38

## 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	1516/1647 (92%)	0.41	54 (3%) 42 28	41, 83, 133, 158	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	GLY	4.5
1	A	767	LEU	4.2
1	A	344	LEU	4.0
1	A	517	GLY	3.8
1	A	116	LEU	3.7
1	A	1567	VAL	3.5
1	A	57	LYS	3.4
1	A	343	ALA	3.4
1	A	764	THR	3.3
1	A	1570	LEU	3.1
1	A	766	LYS	3.1
1	A	548	LEU	3.1
1	A	768	HIS	3.1
1	A	106	ALA	3.0
1	A	649	GLY	3.0
1	A	830	SER	3.0
1	A	83	LEU	2.9
1	A	58	ALA	2.9
1	A	1554	ALA	2.8
1	A	937	LEU	2.8
1	A	75	LEU	2.7
1	A	498	PHE	2.7
1	A	587	SER	2.7
1	A	107	TRP	2.7
1	A	589	GLY	2.6
1	A	254	LEU	2.6
1	A	760	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	732	GLY	2.5
1	A	96	VAL	2.5
1	A	650	GLU	2.4
1	A	595	ARG	2.4
1	A	118	LEU	2.4
1	A	1565	SER	2.4
1	A	799	GLY	2.3
1	A	590	ARG	2.3
1	A	763	ASP	2.3
1	A	260	TYR	2.3
1	A	847	ASP	2.3
1	A	165	ARG	2.3
1	A	1566	GLU	2.3
1	A	194	VAL	2.3
1	A	687	LEU	2.3
1	A	762	GLY	2.2
1	A	87	GLN	2.2
1	A	314	VAL	2.2
1	A	516	GLN	2.2
1	A	1432	SER	2.2
1	A	346	LEU	2.1
1	A	1503	LEU	2.1
1	A	297	ILE	2.1
1	A	769	ILE	2.1
1	A	246	LEU	2.1
1	A	109	LEU	2.1
1	A	1368	GLN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.