



# Full wwPDB X-ray Structure Validation Report i

Oct 5, 2024 – 04:13 pm BST

PDB ID : 4TSC  
Title : Structure of a lysozyme antibody complex  
Authors : Wensley, B.  
Deposited on : 2014-06-18  
Resolution : 1.92 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

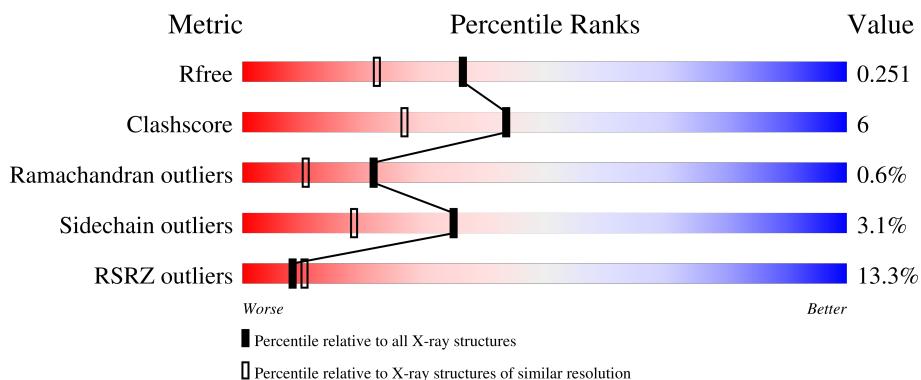
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

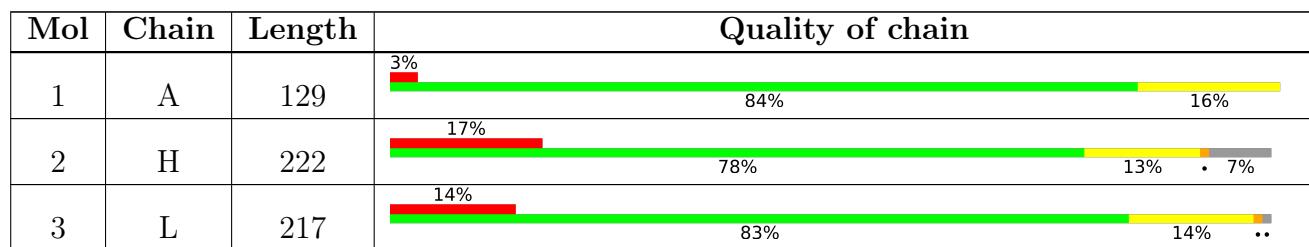
The reported resolution of this entry is 1.92 Å.

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))
$R_{free}$	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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 of 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.



## 2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 4316 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 Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1001	613	193	185	10	0	0	0

- Molecule 2 is a protein called FAB Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	206	1542	971	263	302	6	0	0	0

- Molecule 3 is a protein called FAB Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1579	986	267	321	5	0	0	0

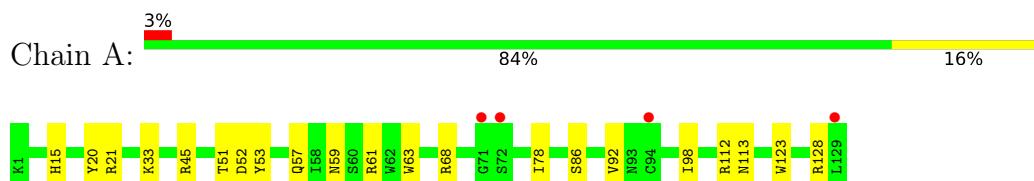
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	61	Total O 61 61	0	0
4	H	60	Total O 60 60	0	0
4	L	73	Total O 73 73	0	0

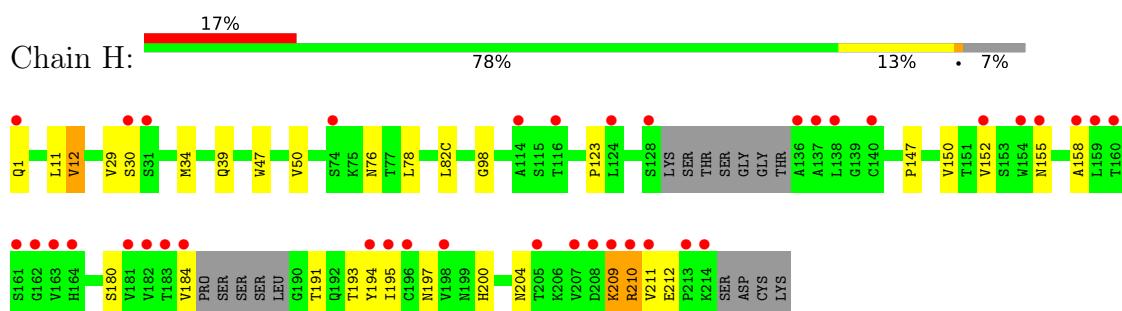
### 3 Residue-property plots [\(i\)](#)

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.

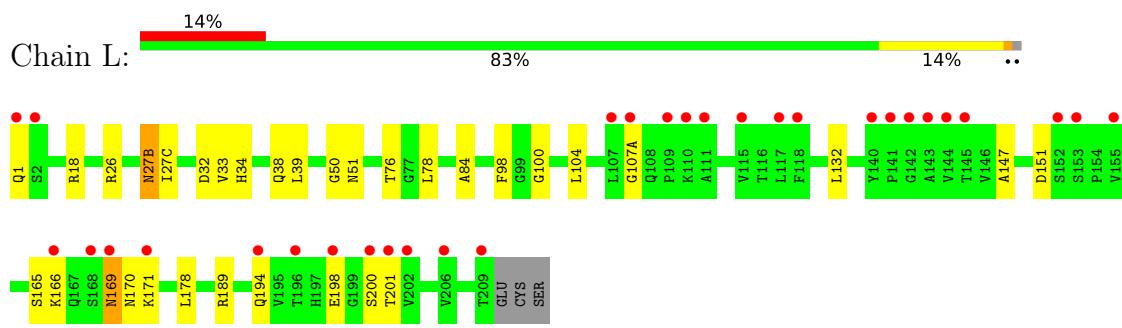
- Molecule 1: Lysozyme C



- Molecule 2: FAb Heavy Chain



- Molecule 3: FAb Light Chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.63Å 129.73Å 59.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.87 – 1.92 64.87 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.7 (64.87-1.92) 98.9 (64.87-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.26 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
$R$ , $R_{free}$	0.209 , 0.232 0.226 , 0.251	Depositor DCC
$R_{free}$ test set	2232 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.42$ , $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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  $< |L| >$ ,  $< L^2 >$  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	0.48	0/1021	0.68	0/1379
2	H	0.42	0/1575	0.70	0/2140
3	L	0.42	0/1617	0.66	0/2207
All	All	0.43	0/4213	0.68	0/5726

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	1001	0	959	11	0
2	H	1542	0	1514	21	0
3	L	1579	0	1539	23	0
4	A	61	0	0	0	0
4	H	60	0	0	2	0
4	L	73	0	0	0	0
All	All	4316	0	4012	49	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 6.

All (49) 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)
3:L:27(B):ASN:HD22	3:L:27(C):ILE:H	1.30	0.77
1:A:45:ARG:HD3	1:A:68:ARG:NH1	2.04	0.72
2:H:98:GLY:O	3:L:34:HIS:HE1	1.74	0.69
3:L:27(C):ILE:HD12	3:L:33:VAL:CG2	2.24	0.68
3:L:27(C):ILE:HD12	3:L:33:VAL:HG22	1.78	0.66
3:L:33:VAL:H	3:L:51:ASN:ND2	1.95	0.65
2:H:193:THR:HG23	2:H:210:ARG:HH21	1.62	0.64
3:L:166:LYS:HE3	3:L:170:ASN:HA	1.83	0.61
3:L:1:GLN:HA	3:L:98:PHE:O	2.01	0.61
1:A:113:ASN:HD21	3:L:32:ASP:H	1.48	0.60
2:H:39:GLN:HE22	3:L:38:GLN:HE22	1.47	0.60
3:L:18:ARG:HG3	3:L:76:THR:HG22	1.84	0.60
3:L:34:HIS:HD2	3:L:50:GLY:H	1.49	0.60
1:A:113:ASN:ND2	3:L:32:ASP:H	2.03	0.57
2:H:11:LEU:HB2	2:H:147:PRO:HG3	1.88	0.55
3:L:34:HIS:CD2	3:L:50:GLY:H	2.24	0.54
3:L:26:ARG:H	3:L:27(B):ASN:ND2	2.08	0.52
2:H:195:ILE:HG23	2:H:209:LYS:O	2.09	0.51
1:A:15:HIS:HB3	1:A:92:VAL:HG11	1.93	0.51
2:H:193:THR:CG2	2:H:210:ARG:HH21	2.24	0.51
1:A:59:ASN:OD1	1:A:61:ARG:HB3	2.11	0.50
2:H:184:VAL:HG21	2:H:194:TYR:OH	2.12	0.50
3:L:169:ASN:OD1	3:L:171:LYS:HB2	2.12	0.50
3:L:78:LEU:HD11	3:L:104:LEU:HD21	1.95	0.49
2:H:152:VAL:HG11	2:H:180:SER:HB2	1.93	0.49
1:A:20:TYR:CE2	1:A:21:ARG:HG2	2.48	0.48
2:H:1:GLN:N	4:H:301:HOH:O	2.44	0.48
2:H:123:PRO:HB3	2:H:211:VAL:HG22	1.94	0.48
2:H:150:VAL:HG12	2:H:200:HIS:CD2	2.49	0.47
1:A:51:THR:HB	1:A:53:TYR:CE1	2.50	0.47
2:H:29:VAL:H	2:H:76:ASN:HD21	1.63	0.47
3:L:198:GLU:C	3:L:200:SER:H	2.18	0.46
2:H:30:SER:HB3	4:H:347:HOH:O	2.15	0.46
3:L:147:ALA:HB3	3:L:194:GLN:HB2	1.98	0.45
1:A:33:LYS:HG2	1:A:123:TRP:CH2	2.52	0.45
2:H:98:GLY:O	3:L:34:HIS:CE1	2.63	0.44
1:A:112:ARG:O	2:H:98:GLY:HA2	2.18	0.43
2:H:155:ASN:HB2	2:H:158:ALA:HB3	2.01	0.43
3:L:132:LEU:HB2	3:L:178:LEU:HB3	2.00	0.43
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.99	0.43
3:L:39:LEU:HD23	3:L:84:ALA:HB2	2.00	0.43
1:A:63:TRP:CE2	1:A:98:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:VAL:H	3:L:51:ASN:HD22	1.66	0.42
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	2.02	0.42
2:H:47:TRP:HZ2	2:H:50:VAL:HG12	1.85	0.41
2:H:209:LYS:HA	2:H:209:LYS:HD3	1.73	0.41
3:L:1:GLN:HB2	3:L:100:GLY:HA2	2.02	0.40
1:A:52:ASP:HB3	1:A:57:GLN:HB3	2.02	0.40
2:H:29:VAL:H	2:H:76:ASN:ND2	2.19	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	127/129 (98%)	127 (100%)	0	0	100 100
2	H	200/222 (90%)	192 (96%)	8 (4%)	0	100 100
3	L	212/217 (98%)	200 (94%)	9 (4%)	3 (1%)	9 2
All	All	539/568 (95%)	519 (96%)	17 (3%)	3 (1%)	22 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	169	ASN
3	L	151	ASP
3	L	107(A)	GLY

### 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	105/105 (100%)	102 (97%)	3 (3%)	37 20
2	H	172/186 (92%)	165 (96%)	7 (4%)	26 11
3	L	177/180 (98%)	173 (98%)	4 (2%)	45 30
All	All	454/471 (96%)	440 (97%)	14 (3%)	35 18

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ILE
1	A	86	SER
1	A	128	ARG
2	H	12	VAL
2	H	191	THR
2	H	197	ASN
2	H	204	ASN
2	H	209	LYS
2	H	210	ARG
2	H	212	GLU
3	L	27(B)	ASN
3	L	165	SER
3	L	189	ARG
3	L	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
2	H	76	ASN
2	H	164	HIS
2	H	171	GLN
2	H	204	ASN
3	L	27(B)	ASN
3	L	34	HIS
3	L	38	GLN
3	L	51	ASN
3	L	167	GLN
3	L	170	ASN

### 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 oligosaccharides 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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	129/129 (100%)	0.13	4 (3%) 51 57	22, 30, 47, 83	0
2	H	206/222 (92%)	1.18	38 (18%) 4 5	24, 42, 88, 109	0
3	L	214/217 (98%)	0.83	31 (14%) 7 9	23, 38, 65, 77	0
All	All	549/568 (96%)	0.80	73 (13%) 8 10	22, 37, 74, 109	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	184	VAL	7.4
2	H	154	TRP	5.4
2	H	160	THR	5.1
2	H	211	VAL	4.8
2	H	194	TYR	4.0
2	H	159	LEU	3.8
2	H	136	ALA	3.8
2	H	163	VAL	3.6
2	H	30	SER	3.5
3	L	171	LYS	3.4
3	L	202	VAL	3.4
3	L	209	THR	3.3
2	H	138	LEU	3.3
3	L	1	GLN	3.3
2	H	152	VAL	3.2
2	H	214	LYS	3.2
3	L	143	ALA	3.2
2	H	182	VAL	3.2
2	H	195	ILE	3.2
3	L	144	VAL	3.2
2	H	128	SER	3.1
2	H	124	LEU	3.1
3	L	201	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	140	CYS	3.0
2	H	205	THR	3.0
3	L	109	PRO	3.0
3	L	141	PRO	2.9
2	H	162	GLY	2.9
2	H	158	ALA	2.9
3	L	111	ALA	2.9
3	L	168	SER	2.9
2	H	207	VAL	2.9
2	H	161	SER	2.9
3	L	152	SER	2.8
3	L	115	VAL	2.8
3	L	200	SER	2.8
3	L	206	VAL	2.7
1	A	129	LEU	2.7
2	H	213	PRO	2.6
2	H	198	VAL	2.6
3	L	166	LYS	2.6
2	H	196	CYS	2.5
2	H	116	THR	2.5
3	L	194	GLN	2.5
3	L	153	SER	2.5
3	L	140	TYR	2.5
2	H	183	THR	2.5
3	L	198	GLU	2.5
1	A	94	CYS	2.4
3	L	196	THR	2.4
2	H	1	GLN	2.4
2	H	31	SER	2.4
2	H	209	LYS	2.3
3	L	117	LEU	2.3
2	H	137	ALA	2.3
2	H	155	ASN	2.3
2	H	74	SER	2.3
3	L	145	THR	2.3
3	L	118	PHE	2.3
2	H	210	ARG	2.2
2	H	164	HIS	2.2
3	L	155	VAL	2.2
3	L	107	LEU	2.2
3	L	110	LYS	2.2
3	L	107(A)	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	169	ASN	2.2
1	A	71	GLY	2.1
2	H	208	ASP	2.1
1	A	72	SER	2.1
3	L	2	SER	2.1
3	L	142	GLY	2.1
2	H	181	VAL	2.0
2	H	114	ALA	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 [\(i\)](#)

There are no ligands in this entry.

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.