



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2021 – 11:11 am GMT

PDB ID : 7A3N  
Title : Crystal structure of Zika virus envelope glycoprotein in complex with the Fab fragment of the broadly neutralizing human antibody EDE1 C10  
Authors : Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.  
Deposited on : 2020-08-18  
Resolution : 2.10 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  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

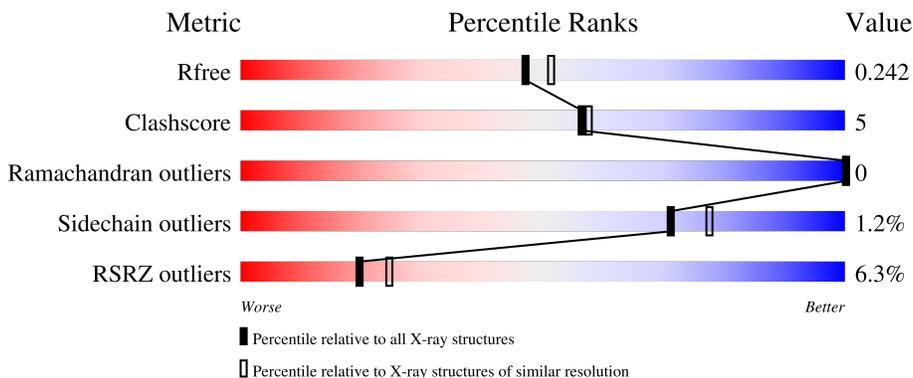
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	414	 88% 7% 5%
2	H	268	 6% 71% 10% 13%
3	L	217	 16% 84% 11% 5%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6542 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3019	1887	527	579	26	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	GLY	-	expression tag	UNP A0A1U9YHM2
A	411	LEU	-	expression tag	UNP A0A1U9YHM2
A	412	VAL	-	expression tag	UNP A0A1U9YHM2
A	413	PRO	-	expression tag	UNP A0A1U9YHM2
A	414	ARG	-	expression tag	UNP A0A1U9YHM2

- Molecule 2 is a protein called EDE1 C10 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1703	1083	283	330	7	0	1	0

- Molecule 3 is a protein called EDE1 C10 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	207	1507	943	251	308	5	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

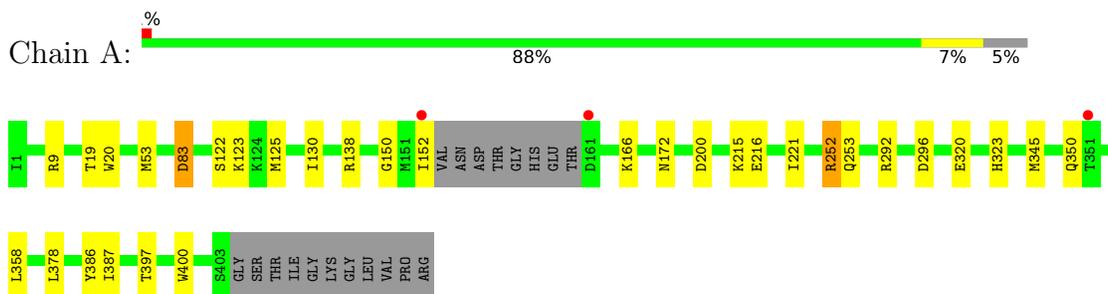
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	203	Total 203	O 203	0	0
5	H	41	Total 41	O 41	0	0
5	L	68	Total 68	O 68	0	0

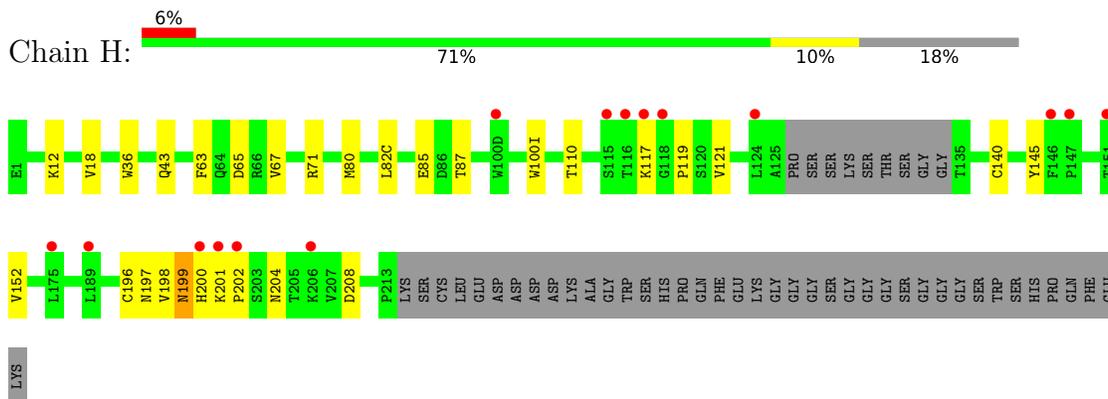
### 3 Residue-property plots [i](#)

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.

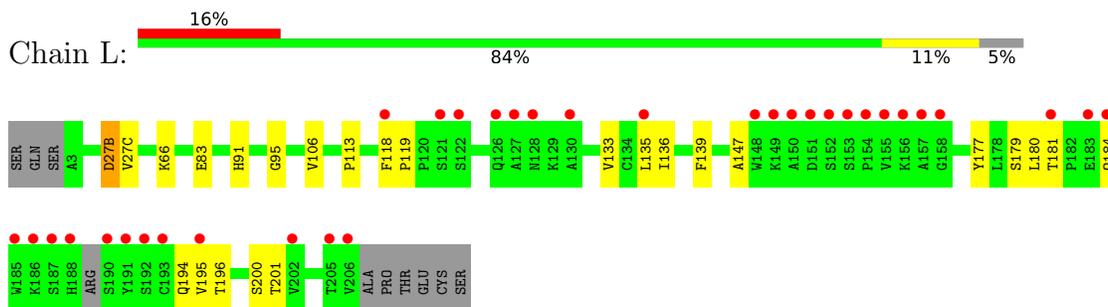
- Molecule 1: Core protein



- Molecule 2: EDE1 C10 Fab



- Molecule 3: EDE1 C10 Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.96Å 168.61Å 220.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.10 46.58 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.91-2.10) 98.9 (46.58-1.99)	Depositor EDS
$R_{merge}$	0.66	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.66 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.203 , 0.240 0.206 , 0.242	Depositor DCC
$R_{free}$ test set	2000 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.35	0/3082	0.57	0/4173
2	H	0.34	0/1752	0.56	0/2389
3	L	0.36	0/1544	0.53	0/2108
All	All	0.35	0/6378	0.56	0/8670

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

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	3019	0	2958	26	0
2	H	1703	0	1645	21	0
3	L	1507	0	1434	17	0
4	A	1	0	0	0	0
5	A	203	0	0	3	0
5	H	41	0	0	0	0
5	L	68	0	0	1	0
All	All	6542	0	6037	61	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 5.

All (61) 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:138:ARG:HE	1:A:166:LYS:HD2	1.44	0.80
2:H:12:LYS:HG3	2:H:18:VAL:HG22	1.65	0.77
2:H:18:VAL:HG23	2:H:82(C):LEU:HD11	1.69	0.74
2:H:152:VAL:HG22	2:H:198:VAL:HG12	1.70	0.72
1:A:83:ASP:OD1	5:A:601:HOH:O	2.13	0.66
3:L:181:THR:HG23	3:L:184:GLN:H	1.63	0.64
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.81	0.62
1:A:150:GLY:HA2	2:H:100(I):TRP:HZ3	1.67	0.60
1:A:252:ARG:CD	1:A:253:GLN:H	2.20	0.55
2:H:117:LYS:O	2:H:200:HIS:HE1	1.91	0.54
1:A:83:ASP:OD2	5:A:602:HOH:O	2.18	0.54
1:A:150:GLY:HA2	2:H:100(I):TRP:CZ3	2.41	0.54
1:A:152:ILE:HG23	2:H:100(I):TRP:CD1	2.43	0.53
3:L:83:GLU:HG3	3:L:106:VAL:HG23	1.90	0.53
2:H:87:THR:HG23	2:H:110:THR:HA	1.90	0.53
1:A:252:ARG:HD2	1:A:253:GLN:H	1.74	0.51
3:L:147:ALA:HB3	3:L:194:GLN:HG3	1.92	0.50
1:A:216:GLU:H	1:A:216:GLU:CD	2.15	0.50
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.46	0.50
3:L:136:ILE:HG12	3:L:195:VAL:HG21	1.94	0.49
1:A:358:LEU:HD22	1:A:378:LEU:HD23	1.93	0.49
2:H:121:VAL:HG21	2:H:198:VAL:HG21	1.94	0.49
2:H:65:ASP:OD1	2:H:65:ASP:N	2.34	0.49
1:A:320:GLU:HB2	1:A:400:TRP:HZ2	1.79	0.48
1:A:320:GLU:HB2	1:A:400:TRP:CZ2	2.50	0.47
1:A:350:GLN:OE1	1:A:350:GLN:N	2.48	0.47
2:H:197:ASN:ND2	2:H:208:ASP:OD1	2.44	0.46
3:L:66:LYS:NZ	5:L:302:HOH:O	2.42	0.46
1:A:200:ASP:HA	1:A:215:LYS:HE3	1.97	0.45
2:H:201:LYS:O	2:H:204:ASN:N	2.44	0.45
3:L:118:PHE:HE2	3:L:135:LEU:HD12	1.81	0.45
1:A:172:ASN:ND2	5:A:610:HOH:O	2.49	0.45
3:L:136:ILE:HG22	3:L:139:PHE:CD1	2.52	0.45
1:A:345:MET:HA	1:A:386:TYR:O	2.17	0.44
3:L:113:PRO:HB2	3:L:136:ILE:HG23	2.00	0.44
1:A:125:MET:CE	1:A:221:ILE:HD13	2.48	0.44
1:A:9:ARG:HB3	1:A:323:HIS:CE1	2.53	0.44
3:L:195:VAL:O	3:L:201:THR:HA	2.18	0.43
1:A:19:THR:HG22	1:A:296:ASP:OD1	2.18	0.43
3:L:118:PHE:HE2	3:L:135:LEU:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:179:SER:O	3:L:180:LEU:HD23	2.18	0.43
1:A:53:MET:HE3	1:A:130:ILE:HG12	2.00	0.43
2:H:200:HIS:HE2	2:H:202:PRO:HB2	1.84	0.43
2:H:201:LYS:C	2:H:204:ASN:H	2.21	0.43
3:L:196:THR:HA	3:L:200:SER:O	2.19	0.42
3:L:136:ILE:HG22	3:L:139:PHE:CE1	2.54	0.42
1:A:387:ILE:O	1:A:397:THR:HA	2.20	0.42
1:A:20:TRP:CE3	1:A:292:ARG:HG2	2.55	0.42
1:A:252:ARG:HD3	1:A:252:ARG:HA	1.73	0.42
2:H:199:ASN:C	2:H:199:ASN:HD22	2.23	0.41
2:H:85:GLU:OE2	2:H:85:GLU:N	2.53	0.41
2:H:119:PRO:HD3	2:H:200:HIS:ND1	2.34	0.41
3:L:27(B):ASP:OD1	3:L:27(C):VAL:N	2.49	0.41
2:H:63:PHE:HB3	2:H:67:VAL:CG2	2.51	0.41
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.92	0.41
1:A:122:SER:O	1:A:123:LYS:HD2	2.21	0.41
2:H:200:HIS:HD2	2:H:202:PRO:HD2	1.86	0.41
3:L:133:VAL:HG22	3:L:177:TYR:HD2	1.86	0.41
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.85	0.40
3:L:91:HIS:CE1	3:L:95:GLY:HA2	2.56	0.40
1:A:53:MET:CE	1:A:130:ILE:HG12	2.52	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	391/414 (94%)	385 (98%)	6 (2%)	0	100	100
2	H	216/268 (81%)	213 (99%)	3 (1%)	0	100	100
3	L	203/217 (94%)	198 (98%)	5 (2%)	0	100	100
All	All	810/899 (90%)	796 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	330/345 (96%)	328 (99%)	2 (1%)	86	90
2	H	188/223 (84%)	183 (97%)	5 (3%)	44	48
3	L	167/182 (92%)	166 (99%)	1 (1%)	86	90
All	All	685/750 (91%)	677 (99%)	8 (1%)	71	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	252	ARG
2	H	43	GLN
2	H	71	ARG
2	H	140	CYS
2	H	196	CYS
2	H	199	ASN
3	L	27(B)	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	395/414 (95%)	0.04	3 (0%) 86 88	22, 39, 75, 107	0
2	H	219/268 (81%)	0.41	15 (6%) 17 21	23, 64, 101, 116	0
3	L	207/217 (95%)	0.68	34 (16%) 1 2	22, 46, 124, 152	0
All	All	821/899 (91%)	0.30	52 (6%) 20 24	22, 46, 103, 152	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	185	TRP	6.7
3	L	127	ALA	6.5
3	L	191	TYR	6.0
3	L	122	SER	5.2
3	L	190	SER	5.2
3	L	183	GLU	5.1
3	L	202	VAL	5.1
3	L	187	SER	4.9
2	H	202	PRO	4.8
3	L	150	ALA	4.7
3	L	151	ASP	4.7
3	L	155	VAL	4.0
3	L	181	THR	3.9
3	L	118	PHE	3.5
3	L	154	PRO	3.4
3	L	205	THR	3.4
3	L	195	VAL	3.3
2	H	175	LEU	3.2
3	L	121	SER	3.2
2	H	117	LYS	3.1
3	L	149	LYS	3.0
3	L	128	ASN	3.0
1	A	351	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	116	THR	2.9
2	H	115	SER	2.9
3	L	157	ALA	2.8
2	H	146	PHE	2.8
3	L	148	TRP	2.8
3	L	206	VAL	2.8
1	A	152	ILE	2.8
3	L	153	SER	2.7
3	L	156	LYS	2.7
3	L	186	LYS	2.6
2	H	118	GLY	2.6
2	H	201	LYS	2.5
3	L	184	GLN	2.5
3	L	135	LEU	2.4
2	H	200	HIS	2.4
3	L	158	GLY	2.4
2	H	100(D)	TRP	2.3
3	L	152	SER	2.3
2	H	189	LEU	2.3
3	L	130	ALA	2.3
3	L	192	SER	2.3
2	H	151	THR	2.2
3	L	126	GLN	2.2
2	H	147	PRO	2.2
2	H	206	LYS	2.1
1	A	161	ASP	2.1
2	H	124	LEU	2.1
3	L	193	CYS	2.1
3	L	188	HIS	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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	A	501	1/1	0.99	0.12	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.