



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2021 – 04:05 PM EDT

PDB ID : 7N3I  
Title : Crystal structure of the SARS-CoV-2 receptor binding domain in complex with the human neutralizing antibody Fab fragment C098  
Authors : Flyak, A.I.; Bjorkman, P.J.; Barnes, C.O.  
Deposited on : 2021-06-01  
Resolution : 2.03 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 : 2.23.1  
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) : 2.23.1

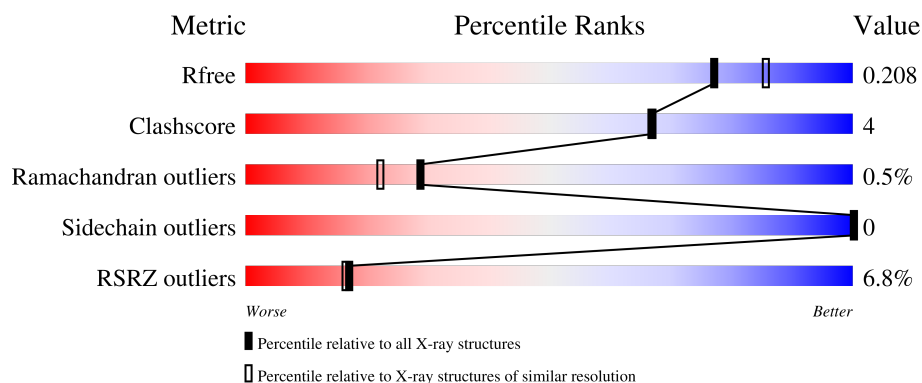
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 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	C	212	<div> <div>17%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>8%</div> </div> </div>
2	H	230	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>7%</div> </div> </div>
3	L	215	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5244 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	194	Total	C	N	O	S	0	0	0
			1533	983	254	288	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
C	538	HIS	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called C098 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1593	1000	268	318	7			

- Molecule 3 is a protein called C098 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1624	1014	276	330	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

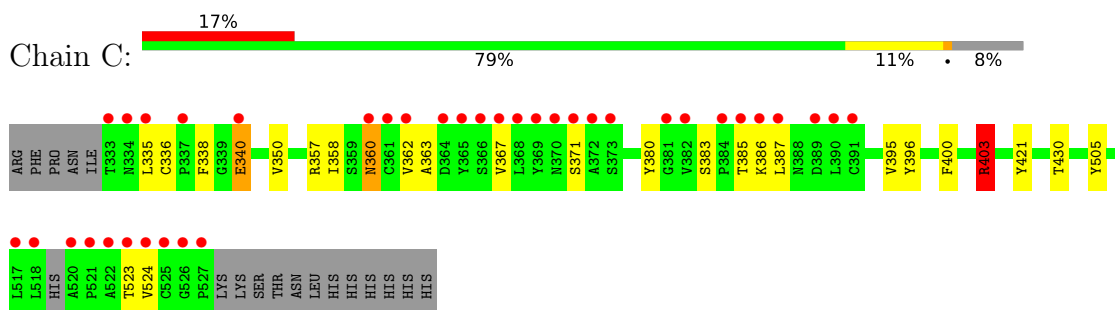
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	120	Total	O	0	0
			120	120		
5	H	208	Total	O	0	0
			208	208		
5	L	152	Total	O	0	0
			152	152		

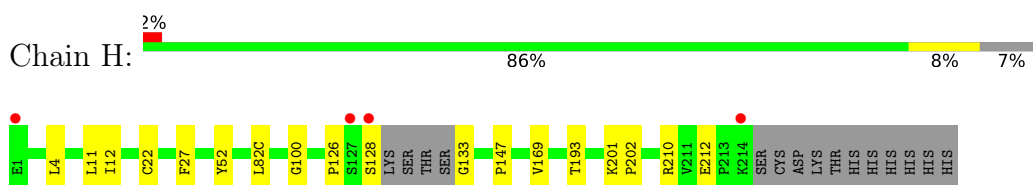
### 3 Residue-property plots

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.

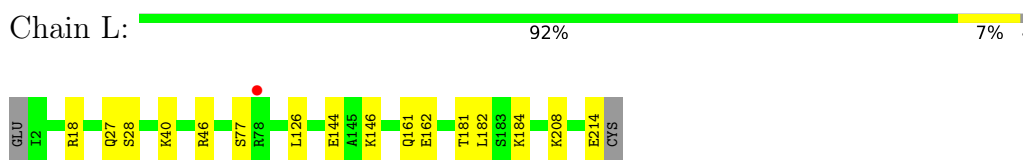
- Molecule 1: Spike protein S1



- Molecule 2: C098 Fab heavy chain



- Molecule 3: C098 Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.33Å 87.84Å 56.81Å 90.00° 99.79° 90.00°	Depositor
Resolution (Å)	44.32 – 2.03 44.32 – 2.03	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.32-2.03) 95.8 (44.32-2.03)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.179 , 0.208 0.179 , 0.208	Depositor DCC
$R_{free}$ test set	2870 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: NAG

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	C	0.49	1/1575 (0.1%)	0.71	6/2143 (0.3%)
2	H	0.49	2/1628 (0.1%)	0.66	0/2216
3	L	0.50	1/1659 (0.1%)	0.63	0/2252
All	All	0.50	4/4862 (0.1%)	0.67	6/6611 (0.1%)

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	C	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	162	GLU	CD-OE1	-10.39	1.14	1.25
1	C	340	GLU	CG-CD	-8.61	1.39	1.51
2	H	212	GLU	CD-OE2	-6.93	1.18	1.25
2	H	212	GLU	CB-CG	-6.34	1.40	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	GLU	CA-CB-CG	11.55	138.81	113.40
1	C	403	ARG	CD-NE-CZ	8.31	135.24	123.60
1	C	340	GLU	CB-CA-C	7.80	126.00	110.40
1	C	340	GLU	N-CA-CB	-6.34	99.18	110.60
1	C	340	GLU	CG-CD-OE2	-5.95	106.41	118.30
1	C	403	ARG	NE-CZ-NH1	-5.22	117.69	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	340	GLU	Sidechain
1	C	403	ARG	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	C	1533	0	1451	15	0
2	H	1593	0	1558	11	0
3	L	1624	0	1576	12	0
4	C	14	0	13	0	0
5	C	120	0	0	0	0
5	H	208	0	0	2	0
5	L	152	0	0	8	0
All	All	5244	0	4598	36	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 4.

All (36) 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:GLN:NE2	5:L:301:HOH:O	1.85	1.07
2:H:193:THR:HG23	2:H:210:ARG:HE	1.37	0.90
1:C:367:VAL:O	1:C:371:SER:N	2.22	0.72
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.72	0.71
3:L:144:GLU:OE2	5:L:303:HOH:O	2.10	0.68
2:H:128:SER:O	5:H:301:HOH:O	2.14	0.66
3:L:40:LYS:NZ	5:L:302:HOH:O	1.91	0.65
2:H:169:VAL:HG21	3:L:161:GLN:HB3	1.79	0.64
1:C:338:PHE:HE1	1:C:358:ILE:HD13	1.61	0.64
1:C:385:THR:HG23	1:C:386:LYS:HG3	1.80	0.64
1:C:403:ARG:HD2	1:C:505:TYR:HA	1.80	0.63
3:L:208:LYS:NZ	5:L:306:HOH:O	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:HD22	1:C:523:THR:HB	1.67	0.60
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.42	0.60
3:L:214:GLU:N	5:L:308:HOH:O	2.31	0.59
1:C:335:LEU:HD23	1:C:362:VAL:HG13	1.85	0.57
3:L:46:ARG:NH1	5:L:307:HOH:O	2.27	0.56
3:L:28:SER:OG	5:L:304:HOH:O	2.17	0.56
3:L:146:LYS:NZ	5:L:310:HOH:O	2.39	0.55
2:H:201:LYS:HB2	2:H:202:PRO:HD3	1.92	0.51
1:C:383:SER:O	1:C:387:LEU:HB2	2.12	0.50
2:H:12:ILE:HG21	2:H:82(C):LEU:HD13	1.95	0.49
2:H:133:GLY:N	5:H:307:HOH:O	2.45	0.49
2:H:11:LEU:HD21	2:H:147:PRO:HG3	1.94	0.48
3:L:181:THR:O	3:L:182:LEU:HD23	2.16	0.45
2:H:193:THR:HG23	2:H:210:ARG:NE	2.19	0.45
1:C:338:PHE:CE1	1:C:358:ILE:HD13	2.48	0.45
1:C:360:ASN:ND2	1:C:523:THR:HB	2.30	0.44
2:H:4:LEU:HD21	2:H:27:PHE:HZ	1.83	0.43
1:C:357:ARG:HG3	1:C:396:TYR:CE2	2.53	0.43
3:L:18:ARG:HG3	3:L:77:SER:HA	2.01	0.42
1:C:421:TYR:OH	2:H:52:TYR:HB3	2.20	0.42
1:C:350:VAL:HA	1:C:400:PHE:HB2	2.02	0.41
3:L:126:LEU:O	3:L:184:LYS:HD2	2.21	0.41
1:C:336:CYS:SG	1:C:363:ALA:HB2	2.61	0.41
1:C:380:TYR:O	1:C:430:THR:HA	2.20	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	C	190/212 (90%)	182 (96%)	7 (4%)	1 (0%)	29 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	211/230 (92%)	206 (98%)	3 (1%)	2 (1%)	17	10
3	L	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
All	All	612/657 (93%)	596 (97%)	13 (2%)	3 (0%)	29	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	360	ASN
2	H	100	GLY
2	H	126	PRO

### 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	C	167/185 (90%)	167 (100%)	0	100	100
2	H	179/194 (92%)	179 (100%)	0	100	100
3	L	183/185 (99%)	183 (100%)	0	100	100
All	All	529/564 (94%)	529 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	C	360	ASN

### 5.3.3 RNA ⓘ

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](#)

1 ligand is 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	$\# Z  > 2$
4	NAG	C	601	1	14,14,15	0.50	0	17,19,21	1.14	1 (5%)

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
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	O5-C5-C6	3.73	113.05	107.20

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 ⓘ

### 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	C	194/212 (91%)	0.84	37 (19%) 1 0	25, 40, 93, 103	0
2	H	215/230 (93%)	-0.12	4 (1%) 66 66	24, 34, 51, 76	0
3	L	213/215 (99%)	-0.10	1 (0%) 91 91	25, 36, 52, 67	0
All	All	622/657 (94%)	0.19	42 (6%) 17 16	24, 36, 83, 103	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	371	SER	8.0
1	C	517	LEU	7.9
1	C	385	THR	7.6
1	C	390	LEU	7.0
1	C	369	TYR	6.3
1	C	335	LEU	6.1
1	C	387	LEU	5.9
1	C	518	LEU	5.6
2	H	128	SER	5.2
1	C	333	THR	5.0
1	C	386	LYS	5.0
1	C	384	PRO	4.7
1	C	334	ASN	4.4
1	C	521	PRO	4.4
1	C	372	ALA	4.3
1	C	527	PRO	4.3
1	C	389	ASP	4.1
1	C	362	VAL	4.1
1	C	366	SER	4.0
1	C	370	ASN	3.9
1	C	367	VAL	3.8
2	H	127	SER	3.7
1	C	337	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	1	GLU	3.4
1	C	340	GLU	3.4
1	C	523	THR	3.4
1	C	391	CYS	3.3
1	C	360	ASN	3.0
1	C	522	ALA	3.0
1	C	381	GLY	2.8
2	H	214	LYS	2.7
1	C	525	CYS	2.6
1	C	520	ALA	2.5
1	C	365	TYR	2.5
1	C	526	GLY	2.4
3	L	78	ARG	2.3
1	C	361	CYS	2.3
1	C	364	ASP	2.3
1	C	368	LEU	2.3
1	C	524	VAL	2.2
1	C	373	SER	2.1
1	C	382	VAL	2.1

## 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	601	14/15	0.82	0.27	55,64,70,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.