



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2022 – 02:02 PM EDT

PDB ID : 7TTX  
Title : Crystal structure of potent neutralizing antibody 10-40 in complex with Sarbecovirus bat RaTG13 receptor-binding domain  
Authors : Reddem, E.R.; Shapiro, L.  
Deposited on : 2022-02-02  
Resolution : 2.80 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.

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 ⓘ](#)) 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	:	2.29
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)	:	2.29

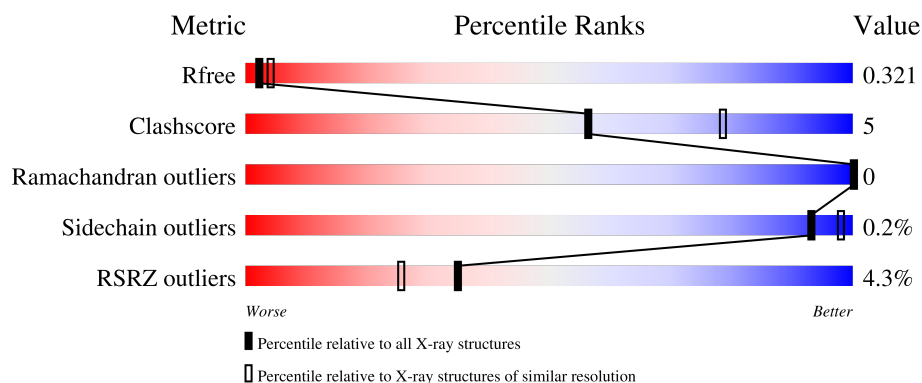
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	231	<div> <div>3%</div> <div>74%</div> <div>10%</div> <div>16%</div> </div>
2	H	237	<div> <div>6%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
3	L	216	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4910 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1546	994	255	289	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	538	GLY	CYS	conflict	UNP A0A6B9WHD3
A	542	HIS	-	expression tag	UNP A0A6B9WHD3
A	543	HIS	-	expression tag	UNP A0A6B9WHD3
A	544	HIS	-	expression tag	UNP A0A6B9WHD3
A	545	HIS	-	expression tag	UNP A0A6B9WHD3
A	546	HIS	-	expression tag	UNP A0A6B9WHD3
A	547	HIS	-	expression tag	UNP A0A6B9WHD3
A	548	HIS	-	expression tag	UNP A0A6B9WHD3
A	549	HIS	-	expression tag	UNP A0A6B9WHD3

- Molecule 2 is a protein called 1040 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	3	0
			1729	1103	282	339	5			

- Molecule 3 is a protein called 1040 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	2	0
			1621	1007	270	338	6			

- 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>).

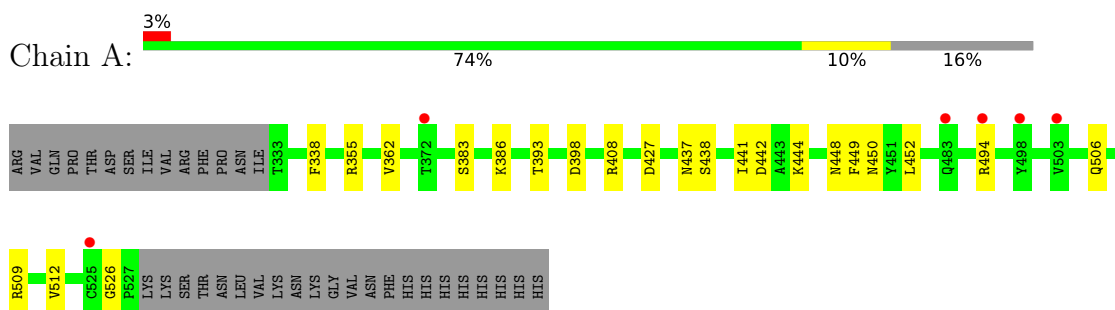


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

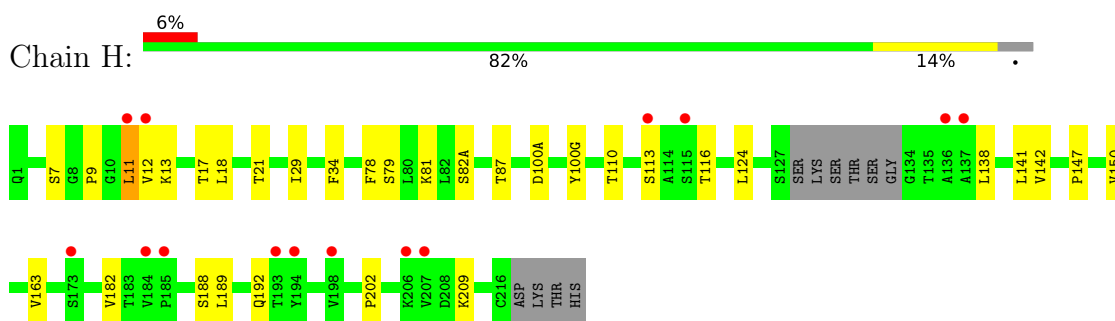
### 3 Residue-property plots [i](#)

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.

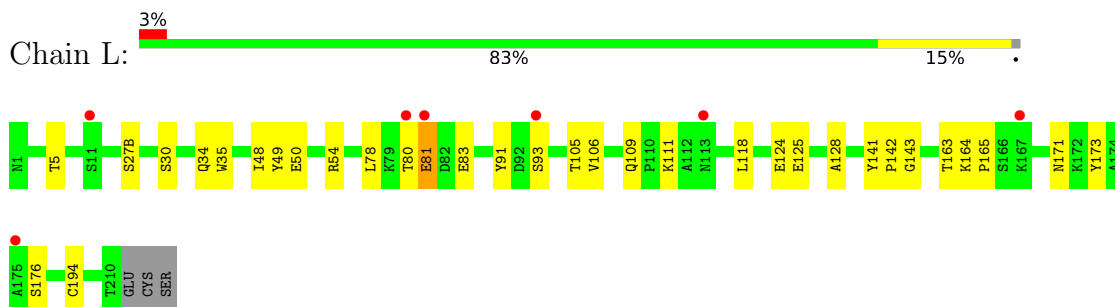
- Molecule 1: Spike glycoprotein



- Molecule 2: 1040 heavy chain



- Molecule 3: 1040 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.17Å 76.82Å 117.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.32 – 2.80 64.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (64.32-2.80) 99.3 (64.32-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.222 , 0.321 0.223 , 0.321	Depositor DCC
$R_{free}$ test set	849 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 30.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	A	0.65	0/1591	0.86	1/2167 (0.0%)
2	H	0.63	0/1782	0.91	2/2435 (0.1%)
3	L	0.69	3/1664 (0.2%)	1.34	5/2270 (0.2%)
All	All	0.66	3/5037 (0.1%)	1.06	8/6872 (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	A	0	1
3	L	0	4
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	125	GLU	CD-OE2	7.79	1.34	1.25
3	L	81	GLU	CD-OE1	5.56	1.31	1.25
3	L	93	SER	CA-C	5.55	1.67	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	125	GLU	OE1-CD-OE2	-39.16	76.31	123.30
3	L	125	GLU	CG-CD-OE1	20.01	158.33	118.30
3	L	125	GLU	CG-CD-OE2	-17.19	83.92	118.30
2	H	189	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	452	LEU	CA-CB-CG	6.79	130.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	138	LEU	CA-CB-CG	5.56	128.09	115.30
3	L	5	THR	C-N-CA	5.32	135.00	121.70
3	L	125	GLU	CB-CG-CD	5.16	128.13	114.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	393	THR	Peptide
3	L	128	ALA	Peptide
3	L	50	GLU	Sidechain
3	L	81	GLU	Sidechain
3	L	91	TYR	Peptide

## 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	1546	0	1467	15	0
2	H	1729	0	1690	21	0
3	L	1621	0	1553	16	0
4	A	14	0	13	1	0
All	All	4910	0	4723	48	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 (48) 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)
2:H:11:LEU:HD23	2:H:147:PRO:HG3	1.68	0.75
2:H:12:VAL:HG21	2:H:18:LEU:HD13	1.73	0.71
1:A:383:SER:HB3	1:A:386:LYS:HG3	1.74	0.69
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.86	0.57
2:H:87:THR:HG23	2:H:110:THR:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:SER:HB2	2:H:192:GLN:HB3	1.88	0.55
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.39	0.55
2:H:116[B]:THR:HG21	2:H:202:PRO:O	2.07	0.54
1:A:338:PHE:HB3	4:A:601:NAG:H81	1.89	0.54
1:A:448:ASN:OD1	1:A:450:ASN:ND2	2.42	0.53
1:A:383:SER:H	1:A:386:LYS:HE3	1.74	0.52
2:H:12:VAL:CG2	2:H:18:LEU:HD13	2.40	0.51
3:L:80:THR:O	3:L:171:ASN:ND2	2.44	0.50
2:H:12:VAL:HG21	2:H:18:LEU:HB2	1.93	0.49
1:A:398:ASP:HB2	1:A:512:VAL:HB	1.95	0.49
1:A:444:LYS:HD3	1:A:448:ASN:HB2	1.95	0.49
2:H:163:VAL:HG22	2:H:182:VAL:HG22	1.97	0.47
1:A:355:ARG:NE	1:A:398:ASP:OD1	2.48	0.47
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.48	0.46
2:H:13:LYS:NZ	2:H:113:SER:O	2.40	0.46
2:H:209:LYS:NZ	3:L:124:GLU:OE1	2.43	0.46
1:A:362:VAL:HG23	1:A:526:GLY:HA2	1.98	0.46
2:H:12:VAL:HG21	2:H:18:LEU:CD1	2.44	0.46
2:H:142:VAL:HG11	2:H:150:VAL:HG11	1.98	0.45
2:H:79[A]:SER:OG	2:H:81:LYS:NZ	2.44	0.45
3:L:83:GLU:HG3	3:L:105:THR:HA	1.97	0.44
3:L:118:LEU:HD22	3:L:194:CYS:HB2	2.00	0.44
3:L:163:THR:HG22	3:L:176:SER:H	1.82	0.44
2:H:11:LEU:HA	2:H:11:LEU:HD22	1.62	0.44
2:H:124:LEU:HD11	2:H:141:LEU:HB2	2.00	0.43
2:H:9:PRO:C	2:H:11:LEU:H	2.20	0.43
2:H:29:ILE:HD11	2:H:78:PHE:HB3	2.01	0.43
1:A:408:ARG:HH22	3:L:54:ARG:CZ	2.32	0.43
3:L:34:GLN:HG3	3:L:49:TYR:HA	2.00	0.43
3:L:164:LYS:HA	3:L:165:PRO:HD3	1.89	0.43
3:L:111:LYS:HE2	3:L:111:LYS:HB2	1.86	0.42
3:L:27(B):SER:O	3:L:30:SER:OG	2.37	0.42
3:L:78:LEU:HD22	3:L:106:VAL:HG13	2.00	0.42
1:A:408:ARG:CZ	3:L:54:ARG:H	2.32	0.42
1:A:427:ASP:HB3	2:H:34:PHE:HE2	1.85	0.41
2:H:100(A):ASP:HB3	2:H:100(G):TYR:HE1	1.85	0.41
1:A:449:PHE:HB3	1:A:494:ARG:HE	1.85	0.41
3:L:80:THR:HG23	3:L:109:GLN:NE2	2.36	0.40
3:L:143:GLY:HA3	3:L:173:TYR:CG	2.56	0.40
1:A:438:SER:HB2	1:A:441:ILE:HG23	2.02	0.40
2:H:7:SER:N	2:H:21:THR:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:141:TYR:HA	3:L:142:PRO:C	2.41	0.40
2:H:17:THR:HA	2:H:82(A):SER:HA	2.04	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	193/231 (84%)	171 (89%)	22 (11%)	0	100	100
2	H	226/237 (95%)	215 (95%)	11 (5%)	0	100	100
3	L	213/216 (99%)	205 (96%)	8 (4%)	0	100	100
All	All	632/684 (92%)	591 (94%)	41 (6%)	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	167/202 (83%)	167 (100%)	0	100	100
2	H	197/205 (96%)	196 (100%)	1 (0%)	88	96
3	L	188/189 (100%)	188 (100%)	0	100	100
All	All	552/596 (93%)	551 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	5	GLN
2	H	77	GLN
3	L	109	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 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	A	601	1	14,14,15	1.57	2 (14%)	17,19,21	0.66	0

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	A	601	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	4.43	1.50	1.43
4	A	601	NAG	C1-C2	3.56	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	1	0

## 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	A	195/231 (84%)	0.07	6 (3%)	49 39	56, 85, 119, 137	0
2	H	227/237 (95%)	0.22	14 (6%)	20 13	49, 76, 110, 122	0
3	L	213/216 (98%)	0.06	7 (3%)	46 36	51, 78, 102, 110	0
All	All	635/684 (92%)	0.12	27 (4%)	35 25	49, 78, 112, 137	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	136	ALA	5.3
2	H	184	VAL	3.9
1	A	483	GLN	3.7
3	L	167	LYS	3.4
3	L	113	ASN	3.3
3	L	93	SER	3.1
2	H	206	LYS	2.9
2	H	185	PRO	2.9
2	H	193	THR	2.9
2	H	113	SER	2.8
2	H	207	VAL	2.7
2	H	115	SER	2.5
1	A	498	TYR	2.5
2	H	11	LEU	2.4
2	H	194	TYR	2.4
2	H	12	VAL	2.3
2	H	198	VAL	2.3
3	L	11	SER	2.2
2	H	137	ALA	2.2
3	L	175	ALA	2.2
1	A	372	THR	2.2
3	L	80	THR	2.2
3	L	81	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	503	VAL	2.1
2	H	173	SER	2.0
1	A	525	CYS	2.0
1	A	494	ARG	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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	601	14/15	0.65	0.25	104,128,133,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.