



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2021 – 12:19 PM EDT

PDB ID : 7JKT  
Title : Crystal structure of vaccine-elicited broadly neutralizing VRC01-class antibody 2413a in complex with HIV-1 gp120 core  
Authors : Zhou, T.; Chen, X.; Kwong, P.D.; Mascola, J.R.  
Deposited on : 2020-07-28  
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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	:	2.19
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)	:	2.19

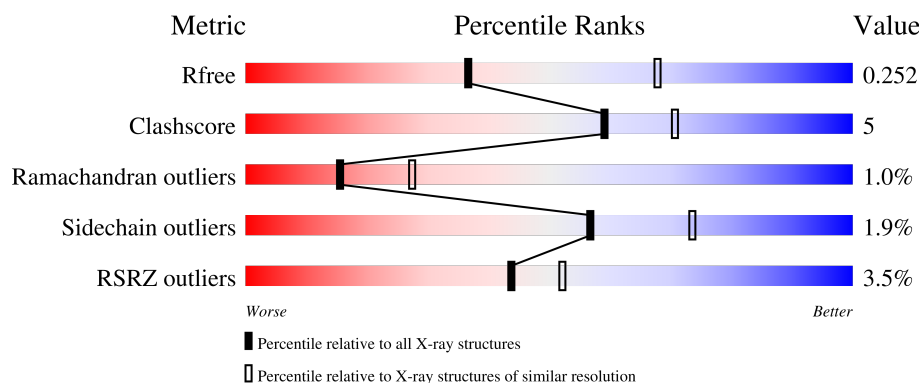
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	G	375	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>8%</div> </div> </div>
2	H	233	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>
3	L	213	<div> <div></div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	602	-	-	-	X
6	SO4	H	302	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6268 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 HIV-1 gp120 core from strain d45-01dG5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	344	2703	1695	470	517	21	0	0	0

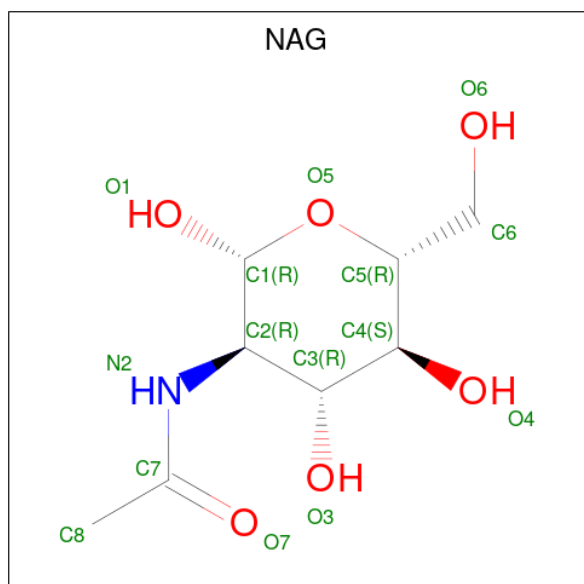
- Molecule 2 is a protein called Heavy chain of antibody 2413a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	225	1736	1105	289	333	9	0	0	0

- Molecule 3 is a protein called Light chain of antibody 2413a.

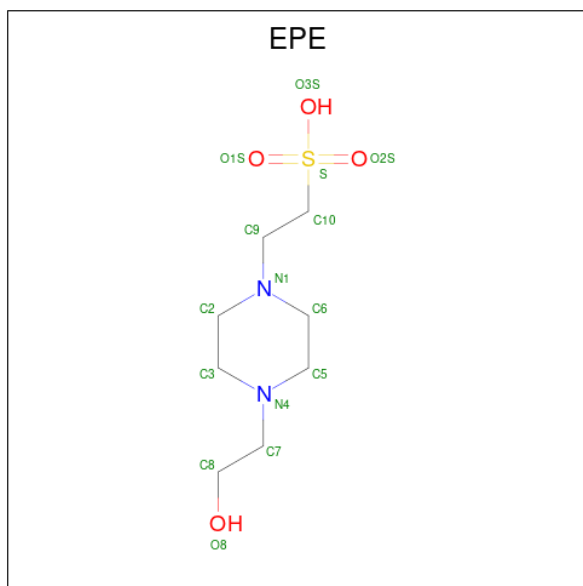
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	1647	1023	282	337	5	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

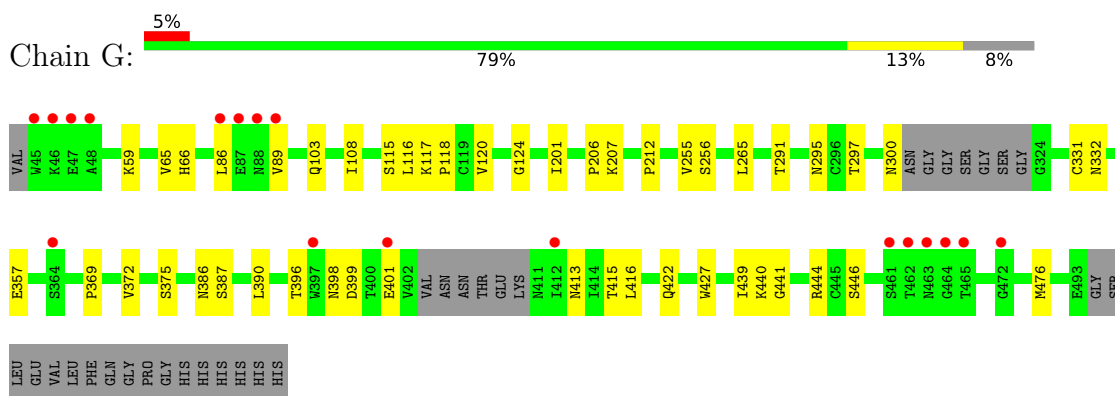
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	10	Total	O	0	0
			10	10		
7	H	14	Total	O	0	0
			14	14		
7	L	7	Total	O	0	0
			7	7		

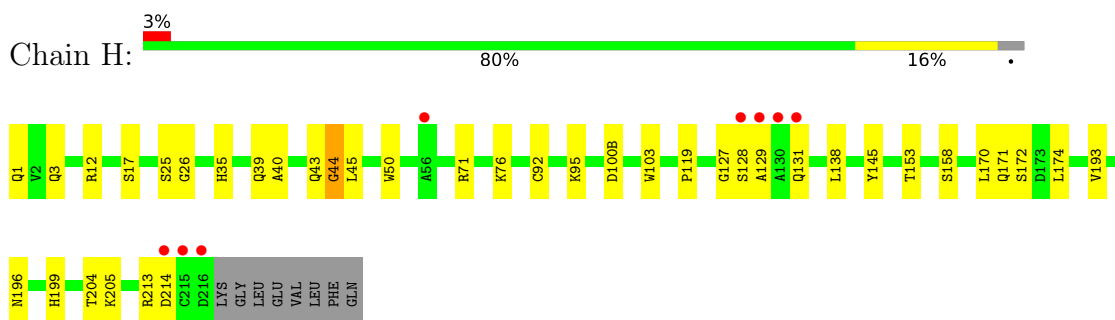
### 3 Residue-property plots

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.

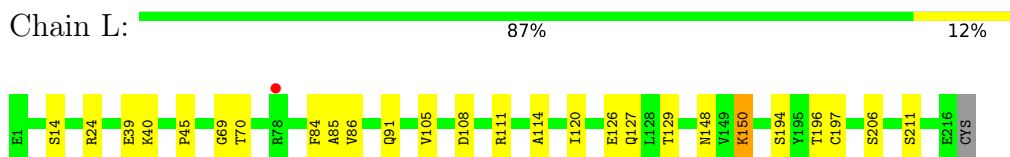
- Molecule 1: HIV-1 gp120 core from strain d45-01dG5



- Molecule 2: Heavy chain of antibody 2413a



- Molecule 3: Light chain of antibody 2413a



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.25Å 67.86Å 240.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.25 – 2.75 39.25 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.25-2.75) 97.2 (39.25-2.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.197 , 0.252 0.197 , 0.252	Depositor DCC
$R_{free}$ test set	1444 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EPE, 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	G	0.27	0/2760	0.46	0/3747
2	H	0.28	0/1788	0.49	0/2453
3	L	0.28	0/1683	0.47	0/2286
All	All	0.28	0/6231	0.47	0/8486

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	G	2703	0	2624	25	0
2	H	1736	0	1673	20	0
3	L	1647	0	1575	15	0
4	G	126	0	117	0	0
5	G	15	0	17	1	0
6	H	10	0	0	2	0
7	G	10	0	0	0	0
7	H	14	0	0	3	0
7	L	7	0	0	1	0
All	All	6268	0	6006	58	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.

The worst 5 of 58 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:G:300:ASN:OD1	1:G:440:LYS:HE3	1.49	1.10
1:G:300:ASN:OD1	1:G:440:LYS:CE	2.30	0.77
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.68	0.74
2:H:213:ARG:NH2	7:H:403:HOH:O	2.24	0.71
3:L:127:GLN:OE1	7:L:301:HOH:O	2.10	0.69

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	G	338/375 (90%)	317 (94%)	18 (5%)	3 (1%)	17	31
2	H	223/233 (96%)	211 (95%)	8 (4%)	4 (2%)	8	15
3	L	210/213 (99%)	197 (94%)	12 (6%)	1 (0%)	29	47
All	All	771/821 (94%)	725 (94%)	38 (5%)	8 (1%)	15	27

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	398	ASN
1	G	357	GLU
2	H	44	GLY
2	H	128	SER
2	H	131	GLN

### 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	G	304/328 (93%)	300 (99%)	4 (1%)	69	81
2	H	194/201 (96%)	189 (97%)	5 (3%)	46	66
3	L	186/187 (100%)	182 (98%)	4 (2%)	52	70
All	All	684/716 (96%)	671 (98%)	13 (2%)	57	73

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	205	LYS
2	H	214	ASP
3	L	206	SER
3	L	150	LYS
3	L	194	SER

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

12 ligands are 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	G	609	1	14,14,15	0.20	0	17,19,21	0.39	0
6	SO4	H	302	-	4,4,4	0.15	0	6,6,6	0.05	0
4	NAG	G	605	1	14,14,15	0.33	0	17,19,21	0.58	0
4	NAG	G	607	1	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	G	608	1	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	G	602	1	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
5	EPE	G	610	-	15,15,15	0.71	1 (6%)	18,20,20	1.88	4 (22%)
4	NAG	G	606	1	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	G	603	1	14,14,15	0.36	0	17,19,21	0.43	0
4	NAG	G	601	1	14,14,15	0.17	0	17,19,21	0.39	0
4	NAG	G	604	1	14,14,15	0.24	0	17,19,21	0.44	0
6	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.05	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	G	609	1	-	0/6/23/26	0/1/1/1
4	NAG	G	605	1	-	0/6/23/26	0/1/1/1
4	NAG	G	607	1	-	3/6/23/26	0/1/1/1
4	NAG	G	608	1	-	2/6/23/26	0/1/1/1
4	NAG	G	602	1	-	1/6/23/26	0/1/1/1
5	EPE	G	610	-	-	7/9/19/19	0/1/1/1
4	NAG	G	606	1	-	2/6/23/26	0/1/1/1
4	NAG	G	603	1	-	1/6/23/26	0/1/1/1
4	NAG	G	601	1	-	4/6/23/26	0/1/1/1
4	NAG	G	604	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	610	EPE	C10-S	2.35	1.80	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	610	EPE	C5-N4-C3	5.18	120.50	108.83
5	G	610	EPE	C7-N4-C5	2.82	118.44	111.23
5	G	610	EPE	O1S-S-C10	2.80	110.28	106.92
5	G	610	EPE	C7-N4-C3	2.71	118.16	111.23
4	G	602	NAG	C1-O5-C5	2.52	115.61	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	607	NAG	O5-C5-C6-O6
4	G	601	NAG	C8-C7-N2-C2
4	G	601	NAG	O7-C7-N2-C2
4	G	606	NAG	C8-C7-N2-C2
4	G	606	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	302	SO4	2	0
5	G	610	EPE	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 [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	G	344/375 (91%)	0.25	18 (5%)	27 33	43, 70, 119, 177	0
2	H	225/233 (96%)	0.14	8 (3%)	42 51	44, 72, 119, 143	0
3	L	212/213 (99%)	-0.03	1 (0%)	91 94	47, 73, 99, 129	0
All	All	781/821 (95%)	0.14	27 (3%)	44 52	43, 71, 113, 177	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	45	TRP	5.4
1	G	462	THR	4.3
1	G	397	TRP	3.9
1	G	46	LYS	3.7
1	G	463	ASN	3.5

### 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	G	602	14/15	0.77	0.44	112,124,128,132	0
4	NAG	G	603	14/15	0.79	0.35	109,129,150,156	0
4	NAG	G	608	14/15	0.83	0.25	83,99,112,114	0
6	SO4	H	302	5/5	0.89	0.24	143,143,145,146	0
4	NAG	G	607	14/15	0.90	0.16	86,99,107,109	0
4	NAG	G	604	14/15	0.92	0.21	75,90,98,99	0
4	NAG	G	609	14/15	0.92	0.19	77,90,106,107	0
6	SO4	H	301	5/5	0.92	0.21	123,129,131,132	0
4	NAG	G	601	14/15	0.92	0.16	80,92,109,118	0
4	NAG	G	606	14/15	0.93	0.15	78,92,104,107	0
4	NAG	G	605	14/15	0.96	0.13	53,65,79,86	0
5	EPE	G	610	15/15	0.97	0.19	50,69,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.