



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2020 – 06:02 PM EST

PDB ID : 6VY5  
Title : Crystal structure of Nipah receptor binding protein head domain in complex with human neutralizing antibody HENV-26  
Authors : Dong, J.; Crowe, J.E.  
Deposited on : 2020-02-25  
Resolution : 3.40 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	:	2.16
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)	:	2.16

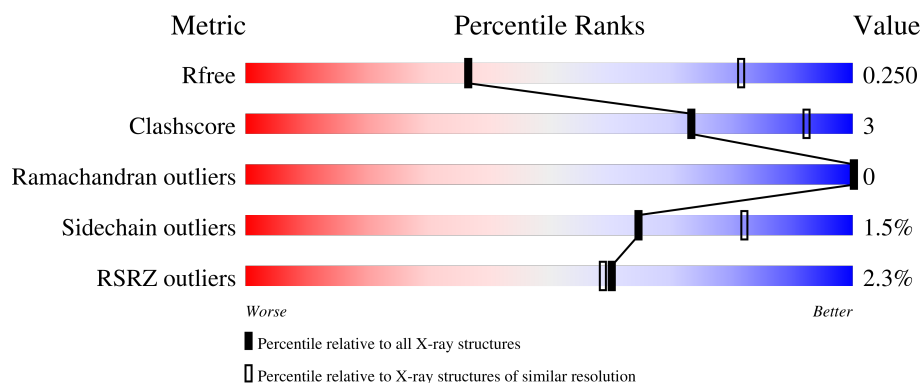
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	H	230	<div> <div>3%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
2	L	214	<div> <div>6%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
3	A	433	<div> <div>82%</div> <div>12%</div> <div>6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6252 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 Anti-Hendra receptor binding protein antibody HENV-26 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1575	999	270	299	7			

- Molecule 2 is a protein called Anti-Hendra receptor binding protein antibody HENV-26 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	208	Total	C	N	O	S	0	0	0
			1431	889	248	290	4			

- Molecule 3 is a protein called receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	409	Total	C	N	O	S	0	0	0
			3176	2029	538	589	20			

There are 13 discrepancies between the modelled and reference sequences:

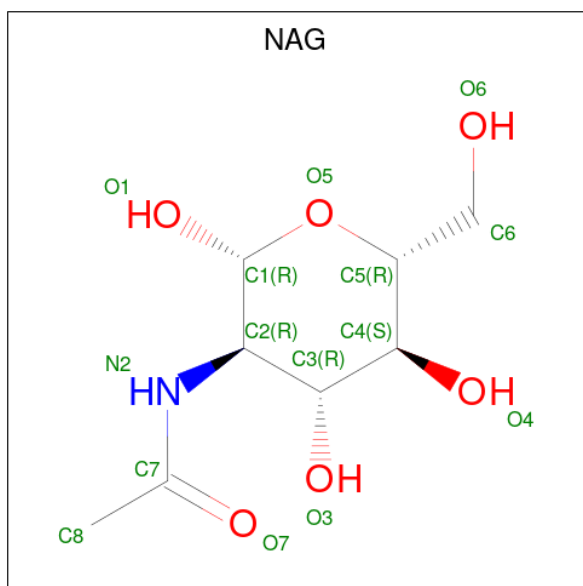
Chain	Residue	Modelled	Actual	Comment	Reference
A	603	GLU	-	expression tag	UNP Q9IH62
A	604	ASN	-	expression tag	UNP Q9IH62
A	605	LEU	-	expression tag	UNP Q9IH62
A	606	TYR	-	expression tag	UNP Q9IH62
A	607	PHE	-	expression tag	UNP Q9IH62
A	608	GLN	-	expression tag	UNP Q9IH62
A	609	GLY	-	expression tag	UNP Q9IH62
A	610	HIS	-	expression tag	UNP Q9IH62
A	611	HIS	-	expression tag	UNP Q9IH62
A	612	HIS	-	expression tag	UNP Q9IH62
A	613	HIS	-	expression tag	UNP Q9IH62
A	614	HIS	-	expression tag	UNP Q9IH62

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Chain	Residue	Modelled	Actual	Comment	Reference
A	615	HIS	-	expression tag	UNP Q9IH62

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

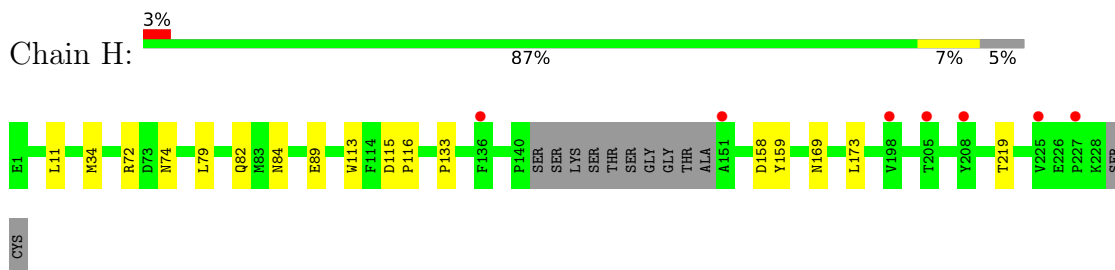


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

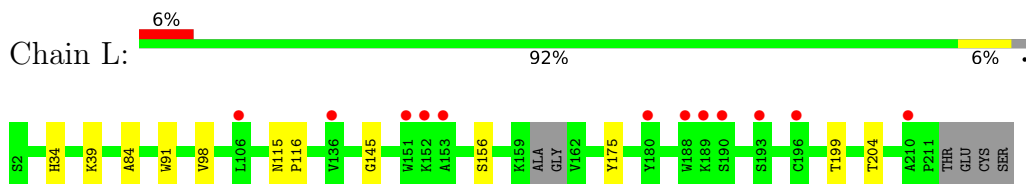
### 3 Residue-property plots [i](#)

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.

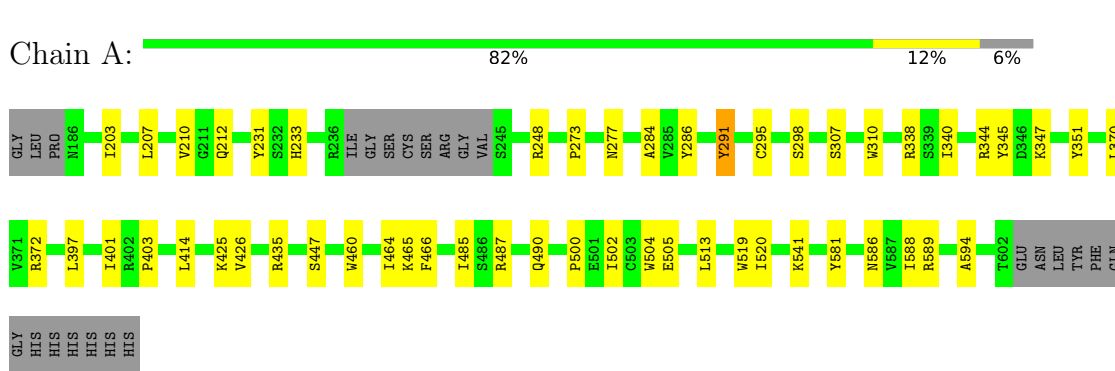
- Molecule 1: Anti-Hendra receptor binding protein antibody HENV-26 Fab heavy chain



- Molecule 2: Anti-Hendra receptor binding protein antibody HENV-26 Fab light chain



- Molecule 3: receptor binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.70Å 186.70Å 81.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.92 – 3.40 48.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.92-3.40) 100.0 (48.85-3.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.208 , 0.250 0.209 , 0.250	Depositor DCC
$R_{free}$ test set	1159 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.4	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 70.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: 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	H	0.25	0/1620	0.47	1/2215 (0.0%)
2	L	0.24	0/1469	0.43	0/2023
3	A	0.25	0/3254	0.45	0/4432
All	All	0.25	0/6343	0.45	1/8670 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	LEU	CA-CB-CG	5.29	127.46	115.30

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	H	1575	0	1409	9	0
2	L	1431	0	1170	6	1
3	A	3176	0	3017	25	0
4	A	70	0	65	0	0
All	All	6252	0	5661	39	1

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 3.

All (39) 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:A:207:LEU:HD12	3:A:210:VAL:HG23	1.62	0.82
1:H:133:PRO:HB3	1:H:159:TYR:HB3	1.74	0.69
1:H:133:PRO:HD2	1:H:219:THR:HG21	1.83	0.59
2:L:91:TRP:HE3	2:L:98:VAL:HG12	1.68	0.59
3:A:212:GLN:O	3:A:589:ARG:NH1	2.38	0.56
3:A:372:ARG:HH12	3:A:397:LEU:HA	1.72	0.54
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.90	0.53
3:A:231:TYR:OH	3:A:233:HIS:ND1	2.39	0.52
3:A:203:ILE:HD13	3:A:594:ALA:HB2	1.91	0.51
3:A:435:ARG:O	3:A:465:LYS:NZ	2.43	0.51
3:A:464:ILE:HB	3:A:485:ILE:HG22	1.93	0.50
1:H:113:TRP:HB3	2:L:34:HIS:CD2	2.47	0.49
3:A:345:TYR:CD2	3:A:370:LEU:HB2	2.49	0.47
3:A:307:SER:O	3:A:347:LYS:NZ	2.46	0.47
3:A:284:ALA:HB1	3:A:291:TYR:CE2	2.50	0.47
3:A:490:GLN:HB2	3:A:505:GLU:CD	2.36	0.46
3:A:460:TRP:CG	3:A:500:PRO:HA	2.50	0.46
3:A:403:PRO:HG3	3:A:502:ILE:HG21	1.97	0.46
1:H:89:GLU:OE1	1:H:89:GLU:N	2.49	0.46
1:H:82:GLN:OE1	1:H:84:ASN:ND2	2.47	0.45
3:A:581:TYR:OH	3:A:586:ASN:OD1	2.26	0.45
1:H:115:ASP:HA	1:H:116:PRO:HA	1.77	0.45
3:A:447:SER:OG	3:A:513:LEU:O	2.34	0.45
2:L:39:LYS:HG2	2:L:84:ALA:HB2	1.98	0.44
3:A:581:TYR:HA	3:A:588:ILE:HA	1.99	0.44
3:A:286:TYR:HB2	3:A:291:TYR:CE1	2.53	0.44
1:H:72:ARG:HD3	1:H:74:ASN:OD1	2.18	0.43
2:L:145:GLY:HA3	2:L:175:TYR:CG	2.53	0.43
2:L:199:THR:HA	2:L:204:THR:HA	2.01	0.43
3:A:338:ARG:HG3	3:A:425:LYS:HB3	2.01	0.42
3:A:248:ARG:O	3:A:273:PRO:HD2	2.19	0.42
3:A:460:TRP:CD2	3:A:500:PRO:HA	2.55	0.42
3:A:520:ILE:HG12	3:A:541:LYS:HG2	2.03	0.41
3:A:298:SER:HB2	3:A:310:TRP:CD1	2.56	0.41
3:A:340:ILE:HG23	3:A:426:VAL:HG23	2.02	0.41
3:A:414:LEU:HD23	3:A:414:LEU:HA	1.93	0.41
1:H:169:ASN:HB2	1:H:173:LEU:HB3	2.02	0.41
3:A:401:ILE:HG22	3:A:504:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:115:ASN:HA	2:L:116:PRO:HD3	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:156:SER:OG	2:L:156:SER:OG[5_554]	2.15	0.05

## 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	H	214/230 (93%)	202 (94%)	12 (6%)	0	100	100
2	L	204/214 (95%)	192 (94%)	12 (6%)	0	100	100
3	A	405/433 (94%)	369 (91%)	36 (9%)	0	100	100
All	All	823/877 (94%)	763 (93%)	60 (7%)	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	H	152/192 (79%)	151 (99%)	1 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	126/180 (70%)	126 (100%)	0	100	100
3	A	339/388 (87%)	331 (98%)	8 (2%)	49	74
All	All	617/760 (81%)	608 (98%)	9 (2%)	65	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	158	ASP
3	A	277	ASN
3	A	291	TYR
3	A	295	CYS
3	A	344	ARG
3	A	351	TYR
3	A	466	PHE
3	A	487	ARG
3	A	519	TRP

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

5 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	A	705	3	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	703	3	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	A	704	3	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	A	701	3	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	A	702	3	14,14,15	0.21	0	17,19,21	0.45	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	705	3	-	2/6/23/26	0/1/1/1
4	NAG	A	703	3	-	2/6/23/26	0/1/1/1
4	NAG	A	704	3	-	2/6/23/26	0/1/1/1
4	NAG	A	701	3	-	0/6/23/26	0/1/1/1
4	NAG	A	702	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	NAG	O5-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6
4	A	703	NAG	O5-C5-C6-O6
4	A	705	NAG	C4-C5-C6-O6
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
4	A	702	NAG	O5-C5-C6-O6
4	A	703	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	H	218/230 (94%)	0.04	7 (3%) 47 46	54, 88, 156, 196	0
2	L	208/214 (97%)	0.33	12 (5%) 23 24	57, 108, 162, 208	0
3	A	409/433 (94%)	-0.25	0 100 100	42, 66, 110, 159	0
All	All	835/877 (95%)	-0.03	19 (2%) 60 59	42, 77, 149, 208	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	193	SER	4.9
2	L	196	CYS	4.8
2	L	210	ALA	3.4
2	L	190	SER	3.4
1	H	198	VAL	3.3
2	L	180	TYR	3.1
2	L	106	LEU	3.1
1	H	227	PRO	3.0
2	L	151	TRP	2.7
1	H	225	VAL	2.5
2	L	188	TRP	2.4
2	L	153	ALA	2.3
1	H	151	ALA	2.3
2	L	189	LYS	2.3
2	L	152	LYS	2.2
1	H	208	TYR	2.2
2	L	136	VAL	2.2
1	H	136	PHE	2.1
1	H	205	THR	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	A	701	14/15	0.92	0.20	103,113,127,130	0
4	NAG	A	703	14/15	0.93	0.24	75,86,106,108	0
4	NAG	A	702	14/15	0.94	0.18	89,104,110,118	0
4	NAG	A	704	14/15	0.95	0.16	86,94,103,108	0
4	NAG	A	705	14/15	0.96	0.18	48,61,72,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.