



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:55 AM GMT

PDB ID : 3NGB  
Title : Crystal structure of broadly and potently neutralizing antibody VRC01 in complex with HIV-1 gp120  
Authors : Zhou, T.; Kwong, P.D.  
Deposited on : 2010-06-11  
Resolution : 2.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

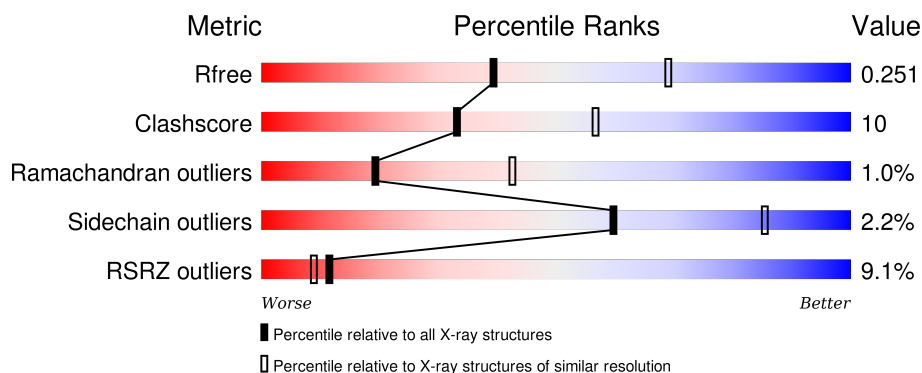
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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))
$R_{free}$	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	353	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	D	353	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	G	353	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	I	353	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>..</div> </div> </div>
2	B	224	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	224	
2	H	224	
2	J	224	
3	C	210	
3	F	210	
3	K	210	
3	L	210	

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	A	948	-	-	-	X
4	NAG	D	588	-	-	-	X
5	BGC	A	506	-	-	-	X
5	BGC	A	508	-	-	-	X
5	BGC	D	505	-	-	-	X
5	BGC	G	503	-	-	-	X
5	BGC	I	401	-	-	-	X
7	TRS	K	405	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25808 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	347	Total	C	N	O	S	0	0	0
			2713	1700	472	518	23			
1	A	349	Total	C	N	O	S	0	0	0
			2723	1705	474	521	23			
1	D	350	Total	C	N	O	S	0	0	0
			2727	1707	475	522	23			
1	I	349	Total	C	N	O	S	0	0	0
			2721	1704	474	520	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	LINKER	UNP Q0ED31
G	198	GLY	-	LINKER	UNP Q0ED31
G	318	GLY	-	LINKER	UNP Q0ED31
G	319	GLY	-	LINKER	UNP Q0ED31
G	320	SER	-	LINKER	UNP Q0ED31
G	321	GLY	-	LINKER	UNP Q0ED31
G	322	SER	-	LINKER	UNP Q0ED31
G	323	GLY	-	LINKER	UNP Q0ED31
A	124	GLY	-	LINKER	UNP Q0ED31
A	198	GLY	-	LINKER	UNP Q0ED31
A	318	GLY	-	LINKER	UNP Q0ED31
A	319	GLY	-	LINKER	UNP Q0ED31
A	320	SER	-	LINKER	UNP Q0ED31
A	321	GLY	-	LINKER	UNP Q0ED31
A	322	SER	-	LINKER	UNP Q0ED31
A	323	GLY	-	LINKER	UNP Q0ED31
D	124	GLY	-	LINKER	UNP Q0ED31
D	198	GLY	-	LINKER	UNP Q0ED31
D	318	GLY	-	LINKER	UNP Q0ED31
D	319	GLY	-	LINKER	UNP Q0ED31
D	320	SER	-	LINKER	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	321	GLY	-	LINKER	UNP Q0ED31
D	322	SER	-	LINKER	UNP Q0ED31
D	323	GLY	-	LINKER	UNP Q0ED31
I	124	GLY	-	LINKER	UNP Q0ED31
I	198	GLY	-	LINKER	UNP Q0ED31
I	302	GLY	-	LINKER	UNP Q0ED31
I	319	GLY	-	LINKER	UNP Q0ED31
I	320	SER	-	LINKER	UNP Q0ED31
I	321	GLY	-	LINKER	UNP Q0ED31
I	322	SER	-	LINKER	UNP Q0ED31
I	323	GLY	-	LINKER	UNP Q0ED31

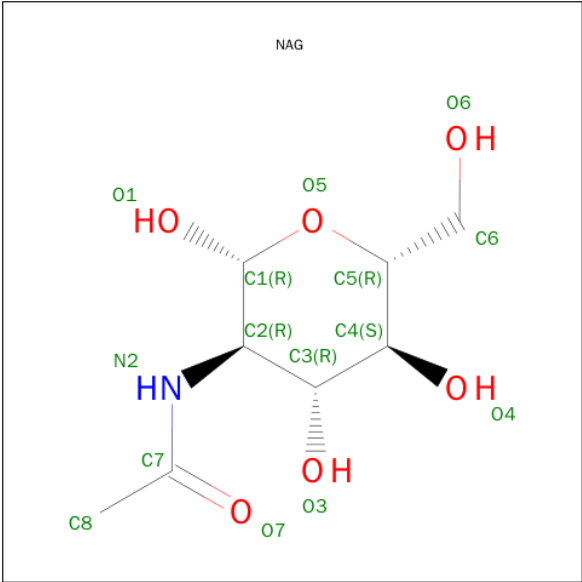
- Molecule 2 is a protein called Antigen binding fragment of heavy chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	B	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	E	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	J	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			

- Molecule 3 is a protein called Antigen binding fragment of light chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1615	1011	277	322	5			
3	C	210	Total	C	N	O	S	0	0	0
			1632	1022	279	326	5			
3	F	208	Total	C	N	O	S	0	0	0
			1615	1011	277	322	5			
3	K	210	Total	C	N	O	S	0	0	0
			1632	1022	279	326	5			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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		
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		

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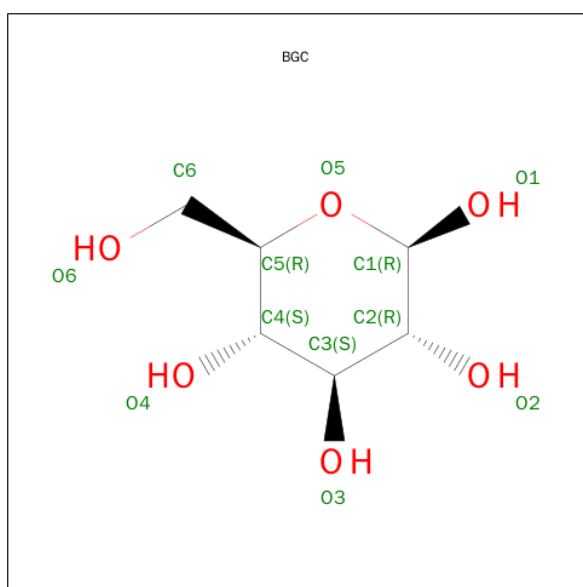
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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

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

- Molecule 5 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



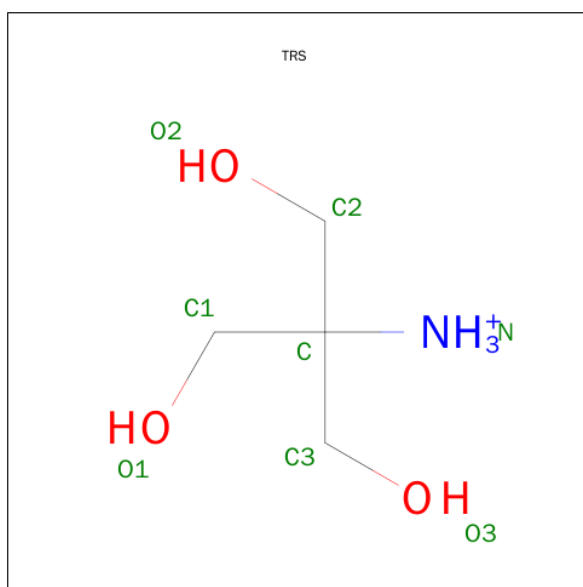


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		
5	C	1	Total	C	O	0	0
			12	6	6		
5	D	1	Total	C	O	0	0
			12	6	6		
5	E	1	Total	C	O	0	0
			12	6	6		
5	I	1	Total	C	O	0	0
			12	6	6		
5	I	1	Total	C	O	0	0
			12	6	6		
5	J	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	5	Total	C	N	O	0	0
			61	34	2	25		
6	C	5	Total	C	N	O	0	0
			61	34	2	25		
6	K	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	I	1	Total	C	N	O	0	0
			8	4	1	3		
7	J	1	Total	C	N	O	0	0
			8	4	1	3		
7	K	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	68	Total	O	0	0
			68	68		

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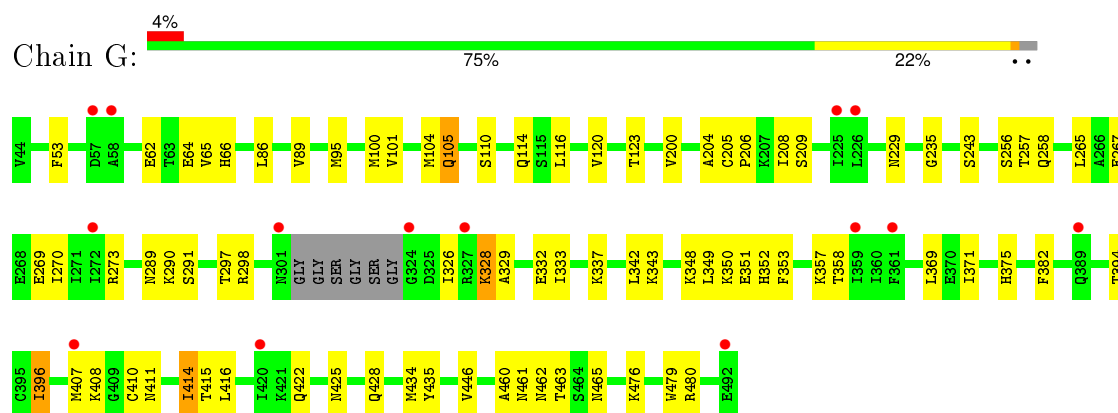
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	52	Total 52	O 52	0	0
9	L	44	Total 44	O 44	0	0
9	A	89	Total 89	O 89	0	0
9	B	46	Total 46	O 46	0	0
9	C	33	Total 33	O 33	0	0
9	D	60	Total 60	O 60	0	0
9	E	29	Total 29	O 29	0	0
9	F	7	Total 7	O 7	0	0
9	I	44	Total 44	O 44	0	0
9	J	24	Total 24	O 24	0	0
9	K	27	Total 27	O 27	0	0

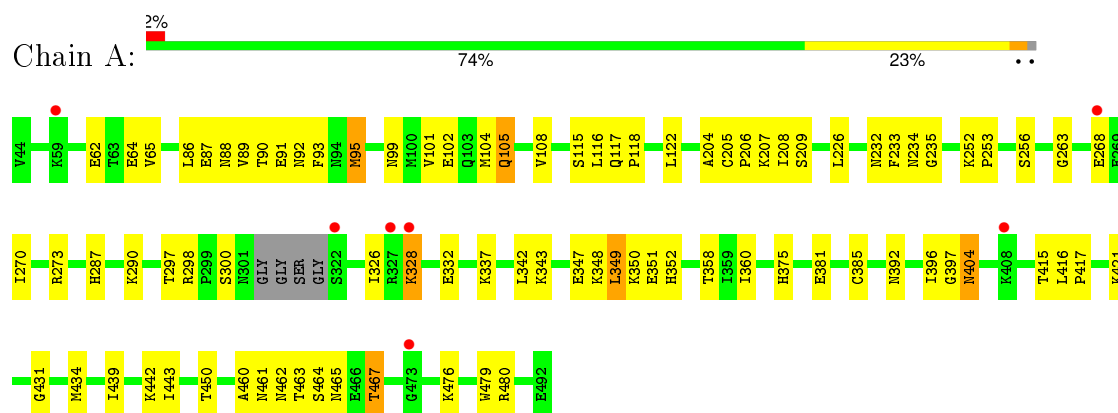
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

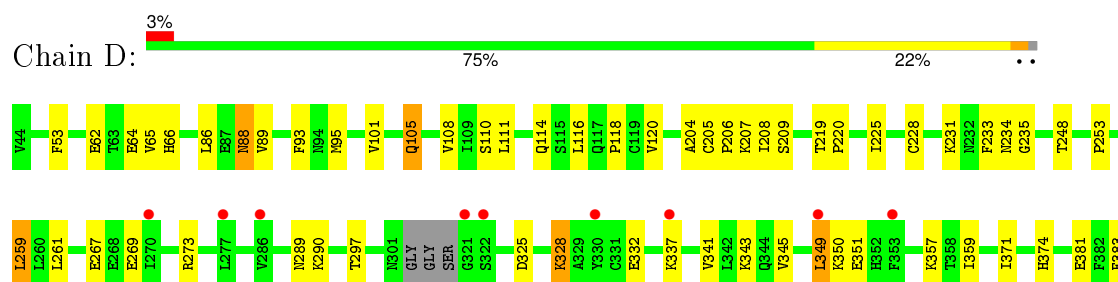
#### • Molecule 1: Envelope glycoprotein gp160

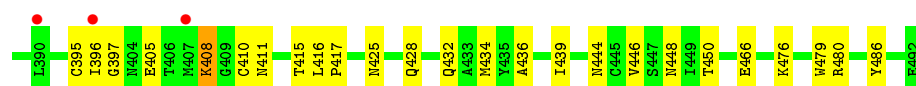


#### • Molecule 1: Envelope glycoprotein gp160

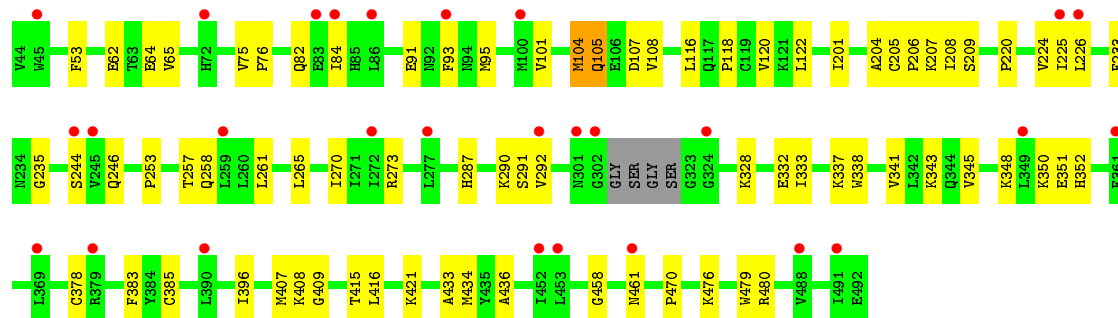
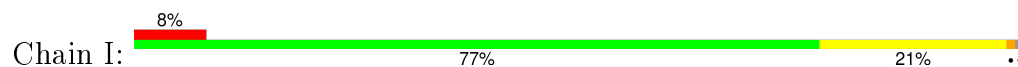


#### • Molecule 1: Envelope glycoprotein gp160

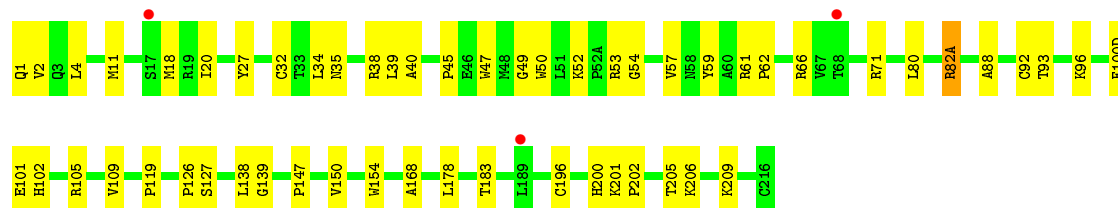
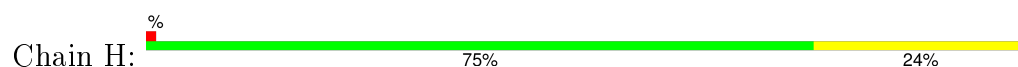




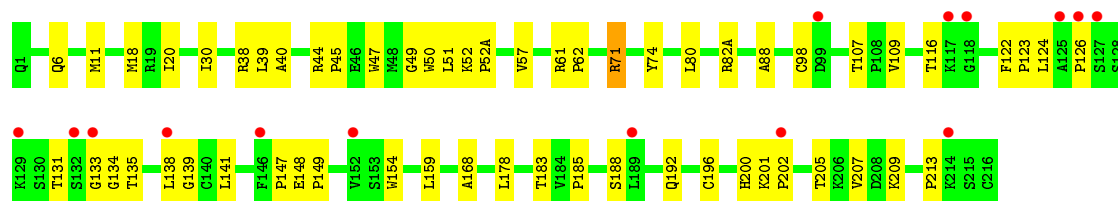
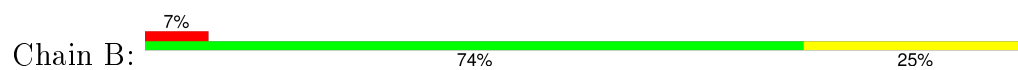
- Molecule 1: Envelope glycoprotein gp160



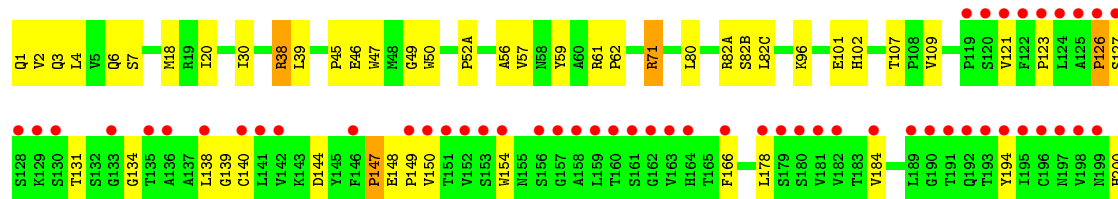
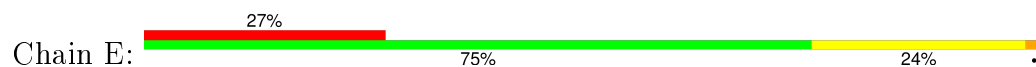
- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

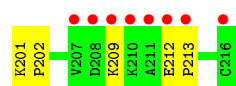


- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

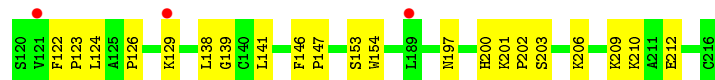
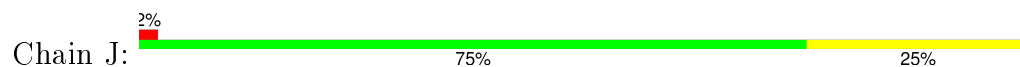


- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

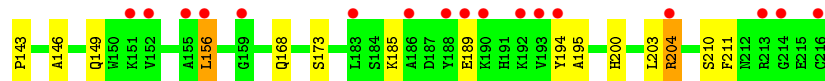
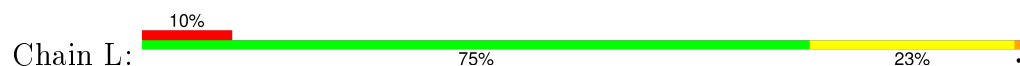




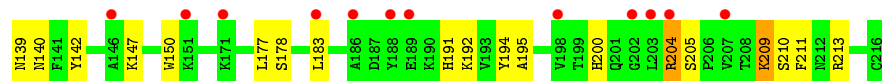
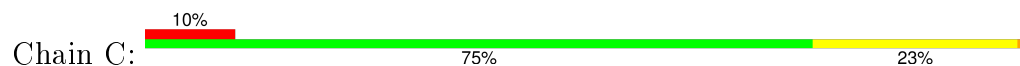
- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01



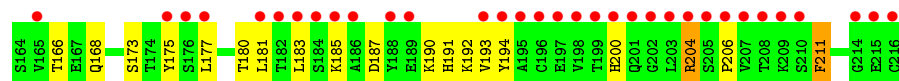
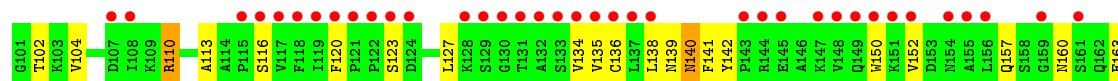
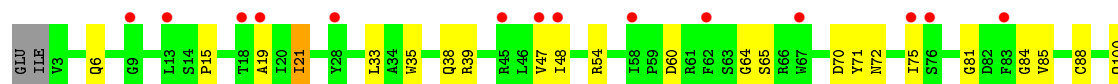
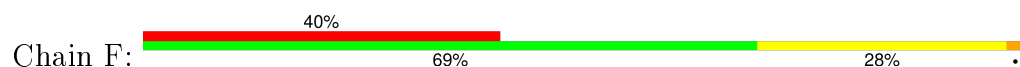
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



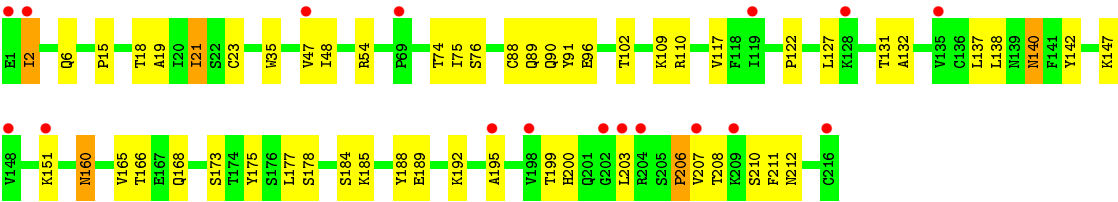
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.63 Å 98.28 Å 205.26 Å 90.00° 99.68° 90.00°	Depositor
Resolution (Å)	49.73 – 2.68 49.73 – 2.68	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.73-2.68) 81.3 (49.73-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.69 Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.197 , 0.256 0.194 , 0.251	Depositor DCC
$R_{free}$ test set	4868 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.6	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 68.1	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 97172 reflections	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BGC, TRS, BMA, NAG, MAN

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	0.21	0/2780	0.39	0/3773
1	D	0.21	0/2784	0.38	0/3778
1	G	0.21	0/2770	0.39	0/3760
1	I	0.21	0/2778	0.37	0/3770
2	B	0.21	0/1755	0.40	0/2387
2	E	0.21	0/1755	0.39	0/2387
2	H	0.22	0/1755	0.41	0/2387
2	J	0.21	0/1755	0.40	0/2387
3	C	0.21	0/1669	0.38	0/2265
3	F	0.20	0/1652	0.36	0/2242
3	K	0.21	0/1669	0.38	0/2265
3	L	0.21	0/1652	0.37	0/2242
All	All	0.21	0/24774	0.39	0/33643

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	A	2723	0	2649	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2727	0	2652	56	0
1	G	2713	0	2642	53	0
1	I	2721	0	2648	56	0
2	B	1710	0	1680	45	0
2	E	1710	0	1680	34	0
2	H	1710	0	1680	34	0
2	J	1710	0	1680	44	0
3	C	1632	0	1573	38	0
3	F	1615	0	1553	41	0
3	K	1632	0	1573	40	0
3	L	1615	0	1553	35	0
4	A	168	0	156	2	0
4	D	168	0	156	1	0
4	G	154	0	143	1	0
4	I	154	0	142	1	0
5	A	48	0	48	6	0
5	B	24	0	24	1	0
5	C	12	0	12	0	0
5	D	12	0	12	0	0
5	E	12	0	12	0	0
5	G	12	0	12	1	0
5	I	24	0	24	1	0
5	J	12	0	12	1	0
6	C	61	0	52	1	0
6	K	61	0	52	0	0
6	L	61	0	52	0	0
7	A	16	0	24	0	0
7	D	16	0	24	1	0
7	I	8	0	12	2	0
7	J	8	0	12	0	0
7	K	8	0	12	1	0
8	F	28	0	25	1	0
9	A	89	0	0	1	0
9	B	46	0	0	1	0
9	C	33	0	0	2	0
9	D	60	0	0	0	0
9	E	29	0	0	1	0
9	F	7	0	0	0	0
9	G	68	0	0	2	0
9	H	52	0	0	2	0
9	I	44	0	0	2	0
9	J	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	27	0	0	0	0
9	L	44	0	0	1	0
All	All	25808	0	24581	514	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 10.

The worst 5 of 514 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:105:GLN:HG3	1:G:476:LYS:HG2	1.47	0.96
1:A:342:LEU:HD23	1:A:396:ILE:HD11	1.54	0.88
1:I:105:GLN:HG3	1:I:476:LYS:HG2	1.56	0.87
1:A:95:MET:HE1	1:A:235:GLY:HA3	1.56	0.86
3:F:6:GLN:HE21	3:F:21:ILE:HD11	1.42	0.85

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	345/353 (98%)	312 (90%)	30 (9%)	3 (1%)	21	46
1	D	346/353 (98%)	314 (91%)	30 (9%)	2 (1%)	30	56
1	G	343/353 (97%)	315 (92%)	25 (7%)	3 (1%)	21	46
1	I	345/353 (98%)	311 (90%)	31 (9%)	3 (1%)	21	46
2	B	222/224 (99%)	203 (91%)	19 (9%)	0	100	100
2	E	222/224 (99%)	192 (86%)	25 (11%)	5 (2%)	8	19
2	H	222/224 (99%)	201 (90%)	19 (9%)	2 (1%)	21	46
2	J	222/224 (99%)	206 (93%)	14 (6%)	2 (1%)	21	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	208/210 (99%)	178 (86%)	28 (14%)	2 (1%)	19	42
3	F	206/210 (98%)	176 (85%)	26 (13%)	4 (2%)	10	23
3	K	208/210 (99%)	188 (90%)	16 (8%)	4 (2%)	10	23
3	L	206/210 (98%)	192 (93%)	12 (6%)	2 (1%)	19	42
All	All	3095/3148 (98%)	2788 (90%)	275 (9%)	32 (1%)	19	42

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	SER
2	E	147	PRO
1	G	410	CYS
2	H	100(D)	PHE
3	L	140	ASN

### 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	A	310/311 (100%)	301 (97%)	9 (3%)	50	78
1	D	310/311 (100%)	301 (97%)	9 (3%)	50	78
1	G	309/311 (99%)	299 (97%)	10 (3%)	46	75
1	I	309/311 (99%)	304 (98%)	5 (2%)	70	90
2	B	192/192 (100%)	190 (99%)	2 (1%)	82	94
2	E	192/192 (100%)	189 (98%)	3 (2%)	70	90
2	H	192/192 (100%)	185 (96%)	7 (4%)	42	71
2	J	192/192 (100%)	191 (100%)	1 (0%)	92	98
3	C	182/182 (100%)	178 (98%)	4 (2%)	60	85
3	F	180/182 (99%)	175 (97%)	5 (3%)	51	79
3	K	182/182 (100%)	180 (99%)	2 (1%)	80	94
3	L	180/182 (99%)	177 (98%)	3 (2%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2730/2740 (100%)	2670 (98%)	60 (2%)	60 85

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	LEU
3	C	204	ARG
1	I	328	LYS
2	B	71	ARG
1	D	88	ASN

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

Mol	Chain	Res	Type
1	G	389	GLN
1	A	92	ASN
1	A	362	GLN

### 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 ⓘ

17 carbohydrates 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
6	NAG	C	570	3,6	14,14,15	0.56	0	15,19,21	0.73	0
6	NAG	C	571	6	14,14,15	0.56	0	15,19,21	0.66	0
6	BMA	C	572	6	11,11,12	0.60	0	14,15,17	0.80	1 (7%)
6	MAN	C	573	6	11,11,12	0.61	0	14,15,17	0.54	0
6	MAN	C	574	6	11,11,12	0.64	0	14,15,17	0.65	0
8	NAG	F	570	8,3	14,14,15	0.46	0	15,19,21	0.92	1 (6%)
8	NAG	F	571	8	14,14,15	0.50	0	15,19,21	0.63	0
6	NAG	K	570	3,6	14,14,15	0.55	0	15,19,21	0.75	0
6	NAG	K	571	6	14,14,15	0.53	0	15,19,21	0.81	0
6	BMA	K	572	6	11,11,12	0.66	0	14,15,17	1.04	1 (7%)
6	MAN	K	573	6	11,11,12	0.59	0	14,15,17	0.59	0
6	MAN	K	574	6	11,11,12	0.63	0	14,15,17	0.67	0
6	NAG	L	570	3,6	14,14,15	0.54	0	15,19,21	0.72	0
6	NAG	L	571	6	14,14,15	0.51	0	15,19,21	0.76	0
6	BMA	L	572	6	11,11,12	0.61	0	14,15,17	0.83	1 (7%)
6	MAN	L	573	6	11,11,12	0.65	0	14,15,17	0.63	0
6	MAN	L	574	6	11,11,12	0.60	0	14,15,17	0.64	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
6	NAG	C	570	3,6	-	0/6/23/26	0/1/1/1
6	NAG	C	571	6	-	0/6/23/26	0/1/1/1
6	BMA	C	572	6	-	0/2/19/22	0/1/1/1
6	MAN	C	573	6	-	0/2/19/22	0/1/1/1
6	MAN	C	574	6	-	0/2/19/22	0/1/1/1
8	NAG	F	570	8,3	-	0/6/23/26	0/1/1/1
8	NAG	F	571	8	-	0/6/23/26	0/1/1/1
6	NAG	K	570	3,6	-	0/6/23/26	0/1/1/1
6	NAG	K	571	6	-	0/6/23/26	0/1/1/1
6	BMA	K	572	6	-	0/2/19/22	0/1/1/1
6	MAN	K	573	6	-	0/2/19/22	0/1/1/1
6	MAN	K	574	6	-	0/2/19/22	0/1/1/1
6	NAG	L	570	3,6	-	0/6/23/26	0/1/1/1
6	NAG	L	571	6	-	0/6/23/26	0/1/1/1
6	BMA	L	572	6	-	0/2/19/22	0/1/1/1
6	MAN	L	573	6	-	0/2/19/22	0/1/1/1
6	MAN	L	574	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	570	NAG	O5-C5-C6	2.06	111.81	107.35
6	C	572	BMA	C1-C2-C3	2.07	111.99	109.54
6	L	572	BMA	C1-C2-C3	2.55	112.56	109.54
6	K	572	BMA	C1-C2-C3	3.36	113.51	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	572	BMA	1	0
6	C	574	MAN	1	0
8	F	570	NAG	1	0
8	F	571	NAG	1	0

## 5.6 Ligand geometry

66 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	$\# Z  > 2$
7	TRS	A	403	-	7,7,7	0.96	1 (14%)	9,9,9	0.57	0
7	TRS	A	493	-	7,7,7	0.97	1 (14%)	9,9,9	0.51	0
5	BGC	A	494	-	12,12,12	0.54	0	17,17,17	0.50	0
5	BGC	A	495	-	12,12,12	0.53	0	17,17,17	0.52	0
5	BGC	A	506	-	12,12,12	0.53	0	17,17,17	0.45	0
5	BGC	A	508	-	12,12,12	0.55	0	17,17,17	0.57	0
4	NAG	A	588	1	14,14,15	0.53	0	15,19,21	0.65	0
4	NAG	A	734	1	14,14,15	0.51	0	15,19,21	0.73	0
4	NAG	A	741	1	14,14,15	0.50	0	15,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	762	1	14,14,15	0.53	0	15,19,21	0.96	1 (6%)
4	NAG	A	776	1	14,14,15	0.51	0	15,19,21	0.80	1 (6%)
4	NAG	A	789	1	14,14,15	0.51	0	15,19,21	0.84	1 (6%)
4	NAG	A	795	1	14,14,15	0.48	0	15,19,21	0.82	0
4	NAG	A	834	1	14,14,15	0.51	0	15,19,21	0.65	0
4	NAG	A	855	1	14,14,15	0.53	0	15,19,21	0.53	0
4	NAG	A	886	1	14,14,15	0.54	0	15,19,21	0.77	0
4	NAG	A	892	1	14,14,15	0.50	0	15,19,21	0.76	0
4	NAG	A	948	1	14,14,15	0.51	0	15,19,21	0.65	0
5	BGC	B	406	-	12,12,12	0.54	0	17,17,17	0.49	0
5	BGC	B	407	-	12,12,12	0.54	0	17,17,17	0.47	0
5	BGC	C	504	-	12,12,12	0.54	0	17,17,17	0.49	0
7	TRS	D	402	-	7,7,7	0.95	1 (14%)	9,9,9	0.56	0
7	TRS	D	500	-	7,7,7	0.99	1 (14%)	9,9,9	0.47	0
5	BGC	D	505	-	12,12,12	0.53	0	17,17,17	0.43	0
4	NAG	D	588	1	14,14,15	0.52	0	15,19,21	0.60	0
4	NAG	D	734	1	14,14,15	0.52	0	15,19,21	0.62	0
4	NAG	D	741	1	14,14,15	0.51	0	15,19,21	0.62	0
4	NAG	D	762	1	14,14,15	0.57	0	15,19,21	0.75	0
4	NAG	D	776	1	14,14,15	0.56	0	15,19,21	0.53	0
4	NAG	D	789	1	14,14,15	0.53	0	15,19,21	0.65	0
4	NAG	D	795	1	14,14,15	0.54	0	15,19,21	0.68	0
4	NAG	D	834	1	14,14,15	0.51	0	15,19,21	0.74	1 (6%)
4	NAG	D	855	1	14,14,15	0.53	0	15,19,21	0.63	0
4	NAG	D	886	1	14,14,15	0.54	0	15,19,21	0.69	0
4	NAG	D	892	1	14,14,15	0.52	0	15,19,21	0.74	0
4	NAG	D	948	1	14,14,15	0.52	0	15,19,21	0.57	0
5	BGC	E	511	-	12,12,12	0.53	0	17,17,17	0.50	0
5	BGC	G	503	-	12,12,12	0.54	0	17,17,17	0.48	0
4	NAG	G	588	1	14,14,15	0.50	0	15,19,21	0.59	0
4	NAG	G	734	1	14,14,15	0.51	0	15,19,21	0.66	0
4	NAG	G	741	1	14,14,15	0.51	0	15,19,21	0.73	0
4	NAG	G	762	1	14,14,15	0.51	0	15,19,21	1.12	1 (6%)
4	NAG	G	776	1	14,14,15	0.51	0	15,19,21	0.88	1 (6%)
4	NAG	G	789	1	14,14,15	0.46	0	15,19,21	0.99	1 (6%)
4	NAG	G	795	1	14,14,15	0.51	0	15,19,21	0.72	0
4	NAG	G	834	1	14,14,15	0.53	0	15,19,21	0.71	0
4	NAG	G	886	1	14,14,15	0.56	0	15,19,21	0.65	0
4	NAG	G	892	1	14,14,15	0.52	0	15,19,21	0.67	0
4	NAG	G	948	1	14,14,15	0.53	0	15,19,21	0.61	0
5	BGC	I	400	-	12,12,12	0.55	0	17,17,17	0.50	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BGC	I	401	-	12,12,12	0.55	0	17,17,17	0.55	0
7	TRS	I	502	-	7,7,7	0.96	1 (14%)	9,9,9	0.59	0
4	NAG	I	588	1	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
4	NAG	I	734	1	14,14,15	0.49	0	15,19,21	0.73	0
4	NAG	I	741	1	14,14,15	0.53	0	15,19,21	0.54	0
4	NAG	I	762	1	14,14,15	0.52	0	15,19,21	0.73	0
4	NAG	I	776	1	14,14,15	0.54	0	15,19,21	0.56	0
4	NAG	I	789	1	14,14,15	0.48	0	15,19,21	1.03	1 (6%)
4	NAG	I	795	1	14,14,15	0.52	0	15,19,21	0.55	0
4	NAG	I	834	1	14,14,15	0.54	0	15,19,21	0.55	0
4	NAG	I	886	1	14,14,15	0.53	0	15,19,21	0.72	0
4	NAG	I	892	1	14,14,15	0.50	0	15,19,21	0.84	1 (6%)
4	NAG	I	948	1	14,14,15	0.56	0	15,19,21	1.36	1 (6%)
7	TRS	J	501	-	7,7,7	0.97	1 (14%)	9,9,9	0.51	0
5	BGC	J	507	-	12,12,12	0.54	0	17,17,17	0.52	0
7	TRS	K	405	-	7,7,7	0.99	1 (14%)	9,9,9	0.49	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
7	TRS	A	403	-	-	0/9/9/9	0/0/0/0
7	TRS	A	493	-	-	0/9/9/9	0/0/0/0
5	BGC	A	494	-	-	0/2/22/22	0/1/1/1
5	BGC	A	495	-	-	0/2/22/22	0/1/1/1
5	BGC	A	506	-	-	0/2/22/22	0/1/1/1
5	BGC	A	508	-	-	0/2/22/22	0/1/1/1
4	NAG	A	588	1	-	0/6/23/26	0/1/1/1
4	NAG	A	734	1	-	0/6/23/26	0/1/1/1
4	NAG	A	741	1	-	0/6/23/26	0/1/1/1
4	NAG	A	762	1	-	0/6/23/26	0/1/1/1
4	NAG	A	776	1	-	0/6/23/26	0/1/1/1
4	NAG	A	789	1	-	0/6/23/26	0/1/1/1
4	NAG	A	795	1	-	0/6/23/26	0/1/1/1
4	NAG	A	834	1	-	0/6/23/26	0/1/1/1
4	NAG	A	855	1	-	0/6/23/26	0/1/1/1
4	NAG	A	886	1	-	0/6/23/26	0/1/1/1
4	NAG	A	892	1	-	0/6/23/26	0/1/1/1
4	NAG	A	948	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BGC	B	406	-	-	0/2/22/22	0/1/1/1
5	BGC	B	407	-	-	0/2/22/22	0/1/1/1
5	BGC	C	504	-	-	0/2/22/22	0/1/1/1
7	TRS	D	402	-	-	0/9/9/9	0/0/0/0
7	TRS	D	500	-	-	0/9/9/9	0/0/0/0
5	BGC	D	505	-	-	0/2/22/22	0/1/1/1
4	NAG	D	588	1	-	0/6/23/26	0/1/1/1
4	NAG	D	734	1	-	0/6/23/26	0/1/1/1
4	NAG	D	741	1	-	0/6/23/26	0/1/1/1
4	NAG	D	762	1	-	0/6/23/26	0/1/1/1
4	NAG	D	776	1	-	0/6/23/26	0/1/1/1
4	NAG	D	789	1	-	0/6/23/26	0/1/1/1
4	NAG	D	795	1	-	0/6/23/26	0/1/1/1
4	NAG	D	834	1	-	0/6/23/26	0/1/1/1
4	NAG	D	855	1	-	0/6/23/26	0/1/1/1
4	NAG	D	886	1	-	0/6/23/26	0/1/1/1
4	NAG	D	892	1	-	0/6/23/26	0/1/1/1
4	NAG	D	948	1	-	0/6/23/26	0/1/1/1
5	BGC	E	511	-	-	0/2/22/22	0/1/1/1
5	BGC	G	503	-	-	0/2/22/22	0/1/1/1
4	NAG	G	588	1	-	0/6/23/26	0/1/1/1
4	NAG	G	734	1	-	0/6/23/26	0/1/1/1
4	NAG	G	741	1	-	0/6/23/26	0/1/1/1
4	NAG	G	762	1	-	0/6/23/26	0/1/1/1
4	NAG	G	776	1	-	0/6/23/26	0/1/1/1
4	NAG	G	789	1	-	0/6/23/26	0/1/1/1
4	NAG	G	795	1	-	0/6/23/26	0/1/1/1
4	NAG	G	834	1	-	0/6/23/26	0/1/1/1
4	NAG	G	886	1	-	0/6/23/26	0/1/1/1
4	NAG	G	892	1	-	0/6/23/26	0/1/1/1
4	NAG	G	948	1	-	2/6/23/26	0/1/1/1
5	BGC	I	400	-	-	0/2/22/22	0/1/1/1
5	BGC	I	401	-	-	0/2/22/22	0/1/1/1
7	TRS	I	502	-	-	0/9/9/9	0/0/0/0
4	NAG	I	588	1	-	0/6/23/26	0/1/1/1
4	NAG	I	734	1	-	0/6/23/26	0/1/1/1
4	NAG	I	741	1	-	0/6/23/26	0/1/1/1
4	NAG	I	762	1	-	0/6/23/26	0/1/1/1
4	NAG	I	776	1	-	0/6/23/26	0/1/1/1
4	NAG	I	789	1	-	0/6/23/26	0/1/1/1
4	NAG	I	795	1	-	0/6/23/26	0/1/1/1
4	NAG	I	834	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	886	1	-	0/6/23/26	0/1/1/1
4	NAG	I	892	1	-	0/6/23/26	0/1/1/1
4	NAG	I	948	1	-	0/6/23/26	0/1/1/1
7	TRS	J	501	-	-	0/9/9/9	0/0/0/0
5	BGC	J	507	-	-	0/2/22/22	0/1/1/1
7	TRS	K	405	-	-	0/9/9/9	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	500	TRS	C-N	-2.58	1.46	1.50
7	K	405	TRS	C-N	-2.58	1.46	1.50
7	J	501	TRS	C-N	-2.53	1.47	1.50
7	A	493	TRS	C-N	-2.52	1.47	1.50
7	A	403	TRS	C-N	-2.51	1.47	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	789	NAG	C2-N2-C7	-2.03	120.43	123.04
4	D	834	NAG	C1-O5-C5	2.13	114.95	112.25
4	A	776	NAG	C1-O5-C5	2.33	115.20	112.25
4	G	776	NAG	C1-O5-C5	2.40	115.29	112.25
4	A	762	NAG	C1-O5-C5	2.43	115.33	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	948	NAG	C8-C7-N2-C2
4	G	948	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	495	BGC	1	0
5	A	506	BGC	3	0
5	A	508	BGC	2	0
4	A	776	NAG	1	0
4	A	795	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	407	BGC	1	0
7	D	402	TRS	1	0
4	D	795	NAG	1	0
5	G	503	BGC	1	0
4	G	795	NAG	1	0
5	I	401	BGC	1	0
7	I	502	TRS	2	0
4	I	789	NAG	1	0
5	J	507	BGC	1	0
7	K	405	TRS	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	349/353 (98%)	0.19	7 (2%) 68 68	55, 89, 141, 225	0
1	D	350/353 (99%)	0.25	12 (3%) 49 48	64, 97, 168, 273	0
1	G	347/353 (98%)	0.41	14 (4%) 42 40	68, 103, 160, 241	0
1	I	349/353 (98%)	0.44	28 (8%) 15 12	74, 118, 181, 249	0
2	B	224/224 (100%)	0.36	15 (6%) 21 19	59, 102, 172, 208	0
2	E	224/224 (100%)	1.89	61 (27%) 1 0	70, 118, 264, 292	0
2	H	224/224 (100%)	0.48	3 (1%) 79 79	59, 85, 117, 165	0
2	J	224/224 (100%)	0.19	4 (1%) 71 71	66, 101, 134, 202	0
3	C	210/210 (100%)	0.59	20 (9%) 10 8	61, 116, 173, 216	0
3	F	208/210 (99%)	2.12	84 (40%) 0 0	88, 181, 245, 270	0
3	K	210/210 (100%)	0.52	17 (8%) 15 12	78, 114, 163, 210	0
3	L	208/210 (99%)	0.44	21 (10%) 9 6	71, 112, 154, 228	0
All	All	3127/3148 (99%)	0.60	286 (9%) 11 9	55, 105, 206, 292	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	181	VAL	15.1
3	F	155	ALA	15.1
2	E	125	ALA	13.7
2	E	141	LEU	13.0
2	E	210	LYS	12.4

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

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

### 6.3 Carbohydrates

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	K	570	14/15	0.86	0.21	0.34	116,142,167,186	0
8	NAG	F	570	14/15	0.90	0.25	0.25	144,174,187,199	0
6	NAG	L	570	14/15	0.92	0.17	-0.47	125,143,162,176	0
6	NAG	C	570	14/15	0.94	0.13	-0.93	102,112,125,146	0
6	MAN	C	573	11/12	0.79	0.27	-	188,198,216,216	0
6	MAN	C	574	11/12	0.80	0.15	-	202,209,216,216	0
6	NAG	L	571	14/15	0.88	0.17	-	158,179,191,206	0
6	BMA	L	572	11/12	0.52	0.33	-	211,219,224,230	0
6	NAG	C	571	14/15	0.87	0.23	-	125,168,183,204	0
6	MAN	K	574	11/12	0.79	0.27	-	216,236,238,239	0
6	MAN	L	574	11/12	0.58	0.44	-	209,235,239,239	0
6	BMA	K	572	11/12	0.24	0.23	-	230,237,239,242	0
6	NAG	K	571	14/15	0.70	0.30	-	118,182,200,219	0
8	NAG	F	571	14/15	0.89	0.27	-	190,206,214,217	0
6	MAN	L	573	11/12	0.75	0.29	-	159,191,200,207	0
6	MAN	K	573	11/12	0.78	0.38	-	217,221,232,232	0
6	BMA	C	572	11/12	0.65	0.22	-	211,218,224,225	0

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	TRS	K	405	8/8	0.59	0.42	34.75	164,183,188,188	0
4	NAG	A	948	14/15	0.91	0.29	8.03	152,166,176,182	0
5	BGC	A	506	12/12	0.63	0.49	6.20	179,199,203,205	0
5	BGC	D	505	12/12	0.61	0.35	4.32	162,179,185,185	0
5	BGC	A	508	12/12	0.85	0.34	3.61	141,162,172,177	0
5	BGC	I	401	12/12	0.77	0.27	2.88	136,156,176,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	588	14/15	0.69	0.46	2.51	193,207,215,219	0
5	BGC	G	503	12/12	0.75	0.27	2.27	92,146,155,156	0
5	BGC	B	406	12/12	0.80	0.25	1.90	140,182,188,189	0
7	TRS	D	500	8/8	0.83	0.28	1.49	108,137,143,151	0
5	BGC	A	494	12/12	0.66	0.28	1.40	161,182,188,188	0
4	NAG	A	776	14/15	0.84	0.27	1.37	98,128,144,144	0
4	NAG	G	886	14/15	0.91	0.24	0.94	94,111,128,136	0
7	TRS	J	501	8/8	0.89	0.22	0.79	125,145,154,155	0
4	NAG	I	948	14/15	0.90	0.21	0.64	152,171,176,185	0
4	NAG	I	892	14/15	0.93	0.21	0.63	149,165,177,179	0
4	NAG	D	892	14/15	0.90	0.22	0.53	134,145,164,165	0
4	NAG	I	795	14/15	0.92	0.22	0.41	98,133,154,155	0
4	NAG	A	795	14/15	0.91	0.16	0.39	109,120,136,142	0
4	NAG	D	776	14/15	0.88	0.23	0.33	126,154,166,168	0
4	NAG	A	734	14/15	0.96	0.25	0.26	79,103,109,113	0
7	TRS	D	402	8/8	0.94	0.17	0.12	84,102,120,123	0
7	TRS	A	403	8/8	0.95	0.18	0.02	98,108,120,124	0
4	NAG	I	741	14/15	0.81	0.19	-0.00	149,180,190,191	0
4	NAG	G	762	14/15	0.97	0.20	-0.13	80,91,111,118	0
4	NAG	I	762	14/15	0.96	0.22	-0.17	98,113,118,123	0
4	NAG	D	734	14/15	0.96	0.19	-0.19	108,119,137,140	0
4	NAG	I	776	14/15	0.89	0.19	-0.27	146,173,183,184	0
4	NAG	G	776	14/15	0.93	0.16	-0.28	120,140,150,156	0
4	NAG	A	892	14/15	0.89	0.17	-0.31	123,151,163,164	0
4	NAG	D	762	14/15	0.95	0.16	-0.37	79,88,99,100	0
4	NAG	G	892	14/15	0.96	0.14	-0.41	71,107,123,133	0
4	NAG	D	795	14/15	0.97	0.16	-0.48	86,107,115,121	0
4	NAG	A	834	14/15	0.92	0.14	-0.58	122,135,148,151	0
4	NAG	I	734	14/15	0.93	0.17	-0.59	116,136,144,147	0
5	BGC	C	504	12/12	0.60	0.20	-0.71	197,212,216,216	0
4	NAG	A	762	14/15	0.97	0.13	-0.74	80,90,107,107	0
4	NAG	I	789	14/15	0.93	0.18	-0.76	120,132,137,142	0
5	BGC	B	407	12/12	0.88	0.18	-0.79	114,145,150,152	0
4	NAG	G	834	14/15	0.95	0.12	-0.86	136,145,179,186	0
4	NAG	G	734	14/15	0.96	0.13	-0.88	91,106,120,120	0
4	NAG	G	588	14/15	0.86	0.28	-0.89	159,171,176,177	0
4	NAG	D	789	14/15	0.94	0.17	-0.93	105,121,137,138	0
4	NAG	G	789	14/15	0.93	0.16	-1.08	110,116,129,134	0
4	NAG	A	588	14/15	0.97	0.12	-1.11	63,79,89,90	0
7	TRS	I	502	8/8	0.94	0.13	-1.16	113,126,128,130	0
4	NAG	A	789	14/15	0.96	0.15	-1.24	79,90,111,126	0
4	NAG	G	795	14/15	0.91	0.13	-1.42	97,123,136,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BGC	E	511	12/12	0.68	0.30	-	162,194,197,198	0
4	NAG	D	855	14/15	0.85	0.22	-	170,185,192,193	0
4	NAG	D	948	14/15	0.90	0.15	-	129,149,163,168	0
4	NAG	A	855	14/15	0.77	0.43	-	191,212,221,221	0
4	NAG	D	741	14/15	0.79	0.47	-	176,190,202,207	0
4	NAG	D	886	14/15	0.93	0.17	-	82,103,121,122	0
4	NAG	I	886	14/15	0.95	0.14	-	102,127,140,149	0
5	BGC	J	507	12/12	0.38	0.29	-	197,218,223,223	0
5	BGC	A	495	12/12	0.85	0.13	-	113,153,160,160	0
4	NAG	I	834	14/15	0.89	0.17	-	124,151,159,166	0
4	NAG	A	886	14/15	0.93	0.18	-	72,86,111,112	0
4	NAG	D	834	14/15	0.89	0.23	-	116,132,139,144	0
5	BGC	I	400	12/12	0.83	0.33	-	208,216,220,220	0
7	TRS	A	493	8/8	0.66	0.21	-	156,167,171,172	0
4	NAG	G	948	14/15	0.86	0.22	-	153,173,179,179	0
4	NAG	G	741	14/15	0.88	0.18	-	143,160,167,171	0
4	NAG	A	741	14/15	0.90	0.12	-	105,126,137,138	0
4	NAG	I	588	14/15	0.78	0.33	-	167,178,186,187	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.