



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2021 – 10:04 AM EDT

PDB ID : 7N0U  
Title : Complex of recombinant Bet v 1 with Fab fragment of REGN5713  
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Deposited on : 2021-05-26  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

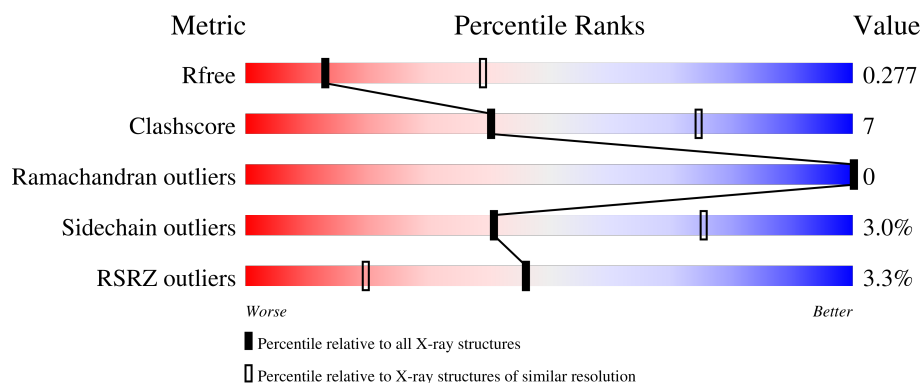
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	221	<div> <div>76%</div> <div>16%</div> <div>6%</div> </div>
2	L	214	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
3	C	187	<div> <div>7%</div> <div>69%</div> <div>16%</div> <div>15%</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
5	NAG	C	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4466 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 REGN5713 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	207	Total	C	N	O	S	0	0	0
			1550	985	250	309	6			

- Molecule 2 is a protein called REGN5713 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1657	1039	284	329	5			

- Molecule 3 is a protein called Recombinant Bet v 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	159	Total	C	N	O	S	0	0	0
			1229	783	202	243	1			

There are 29 discrepancies between the modelled and reference sequences:

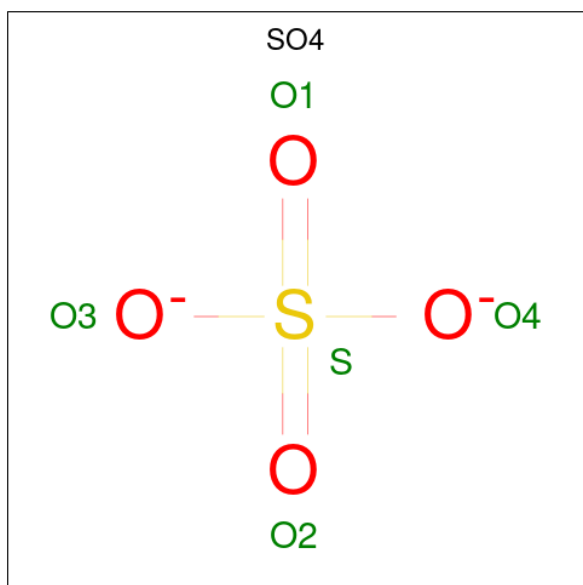
Chain	Residue	Modelled	Actual	Comment	Reference
C	62	LEU	PHE	engineered mutation	UNP P15494
C	160	GLU	-	expression tag	UNP P15494
C	161	GLN	-	expression tag	UNP P15494
C	162	LYS	-	expression tag	UNP P15494
C	163	LEU	-	expression tag	UNP P15494
C	164	ILE	-	expression tag	UNP P15494
C	165	SER	-	expression tag	UNP P15494
C	166	GLU	-	expression tag	UNP P15494
C	167	GLU	-	expression tag	UNP P15494
C	168	ASP	-	expression tag	UNP P15494
C	169	LEU	-	expression tag	UNP P15494
C	170	GLY	-	expression tag	UNP P15494
C	171	GLY	-	expression tag	UNP P15494
C	172	GLU	-	expression tag	UNP P15494

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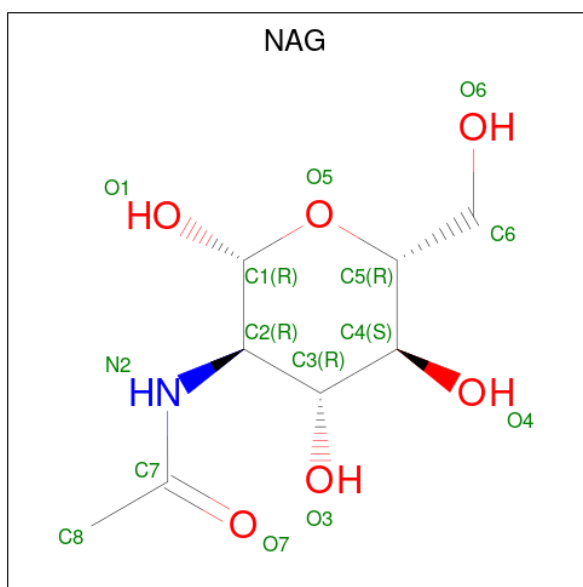
Chain	Residue	Modelled	Actual	Comment	Reference
C	173	GLN	-	expression tag	UNP P15494
C	174	LYS	-	expression tag	UNP P15494
C	175	LEU	-	expression tag	UNP P15494
C	176	ILE	-	expression tag	UNP P15494
C	177	SER	-	expression tag	UNP P15494
C	178	GLU	-	expression tag	UNP P15494
C	179	GLU	-	expression tag	UNP P15494
C	180	ASP	-	expression tag	UNP P15494
C	181	LEU	-	expression tag	UNP P15494
C	182	HIS	-	expression tag	UNP P15494
C	183	HIS	-	expression tag	UNP P15494
C	184	HIS	-	expression tag	UNP P15494
C	185	HIS	-	expression tag	UNP P15494
C	186	HIS	-	expression tag	UNP P15494
C	187	HIS	-	expression tag	UNP P15494

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



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

- Molecule 5 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
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

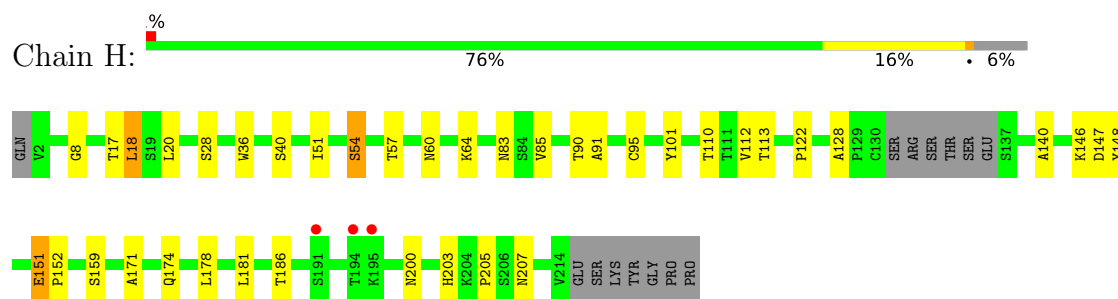
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	4	Total	O	0	0
			4	4		
6	L	6	Total	O	0	0
			6	6		
6	C	1	Total	O	0	0
			1	1		

### 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: REGN5713 Fab fragment heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.77Å 140.77Å 94.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.08 – 3.00 46.08 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.08-3.00) 98.7 (46.08-2.99)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.240 , 0.280 0.237 , 0.277	Depositor DCC
$R_{free}$ test set	1039 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: SO4, 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	0.26	0/1590	0.51	0/2176
2	L	0.26	0/1695	0.53	0/2301
3	C	0.27	0/1254	0.49	0/1696
All	All	0.26	0/4539	0.51	0/6173

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

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	1550	0	1506	25	0
2	L	1657	0	1613	25	0
3	C	1229	0	1220	17	0
4	L	5	0	0	0	0
5	C	14	0	11	1	0
6	C	1	0	0	0	0
6	H	4	0	0	0	0
6	L	6	0	0	0	0
All	All	4466	0	4350	63	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 7.

All (63) 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:C:80:LYS:HG2	3:C:103:LYS:HG3	1.71	0.72
3:C:20:LYS:HE3	3:C:158:TYR:HD1	1.56	0.71
2:L:132:VAL:HG23	2:L:179:LEU:HB3	1.73	0.70
1:H:54:SER:HG	3:C:145:ARG:HE	1.43	0.66
1:H:90:THR:HG23	1:H:113:THR:HA	1.76	0.66
1:H:54:SER:OG	3:C:145:ARG:NE	2.27	0.61
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.84	0.58
2:L:120:PRO:HD3	2:L:132:VAL:HG12	1.85	0.58
3:C:105:VAL:HG22	3:C:113:ILE:HB	1.86	0.57
2:L:94:TRP:CD2	2:L:95:PRO:HA	2.40	0.56
2:L:149:LYS:HA	2:L:153:ALA:O	2.06	0.56
3:C:7:THR:HG23	3:C:116:ILE:HB	1.88	0.55
2:L:192:TYR:HB2	2:L:209:PHE:CE1	2.42	0.55
1:H:40:SER:HB3	1:H:91:ALA:HB2	1.89	0.54
1:H:54:SER:HB2	3:C:141:GLU:OE2	2.08	0.54
2:L:32:PHE:HB3	2:L:91:ARG:HG2	1.91	0.53
2:L:136:LEU:HD11	2:L:146:VAL:HG22	1.90	0.53
1:H:17:THR:HA	1:H:83:ASN:HA	1.90	0.52
1:H:171:ALA:HA	1:H:181:LEU:HB3	1.94	0.50
1:H:151:GLU:HG2	1:H:152:PRO:HA	1.93	0.49
1:H:18:LEU:CD1	1:H:112:VAL:HG11	2.42	0.49
1:H:146:LYS:NZ	1:H:174:GLN:OE1	2.46	0.48
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.49	0.48
2:L:83:PHE:HB2	2:L:106:ILE:HG12	1.96	0.47
3:C:5:TYR:HB2	3:C:118:ASN:HB2	1.97	0.47
1:H:203:HIS:CD2	1:H:205:PRO:HD2	2.50	0.46
2:L:110:VAL:HG23	2:L:141:PRO:HD3	1.97	0.46
1:H:36:TRP:CZ3	1:H:95:CYS:HB3	2.51	0.46
2:L:186:TYR:O	2:L:192:TYR:OH	2.33	0.46
2:L:30:LYS:HB3	2:L:30:LYS:HE3	1.54	0.46
3:C:70:ARG:NH1	3:C:72:ASP:OD1	2.49	0.45
2:L:182:SER:OG	2:L:185:ASP:OD2	2.34	0.45
2:L:120:PRO:HD3	2:L:132:VAL:CG1	2.46	0.45
3:C:41:VAL:HG22	3:C:56:ILE:HG23	1.98	0.45
2:L:21:LEU:HD23	2:L:102:THR:HB	1.98	0.45
3:C:148:GLU:O	3:C:152:LEU:HG	2.17	0.44
2:L:29:ILE:HG21	2:L:90:GLN:HB2	1.98	0.44
2:L:158:ASN:OD1	2:L:158:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:ASP:OD1	1:H:174:GLN:NE2	2.51	0.44
1:H:171:ALA:HB2	1:H:181:LEU:HD23	2.00	0.44
2:L:158:ASN:HD22	2:L:181:LEU:HD21	1.83	0.43
3:C:37:ALA:O	3:C:38:ILE:HD13	2.18	0.43
1:H:159:SER:HA	1:H:200:ASN:ND2	2.34	0.43
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.99	0.43
3:C:44:ILE:HD11	3:C:55:LYS:HB2	2.01	0.43
1:H:18:LEU:HB2	1:H:85:VAL:HG11	2.00	0.42
1:H:60:ASN:O	1:H:64:LYS:N	2.51	0.42
2:L:29:ILE:O	2:L:29:ILE:HG13	2.19	0.42
3:C:44:ILE:CD1	3:C:55:LYS:HB2	2.49	0.42
2:L:37:ARG:HB2	2:L:47:LEU:HD11	2.01	0.42
3:C:99:SER:OG	5:C:201:NAG:H5	2.20	0.42
3:C:1:GLY:N	3:C:122:THR:O	2.52	0.42
1:H:18:LEU:HD12	1:H:112:VAL:HG11	2.02	0.42
1:H:174:GLN:HG3	1:H:178:LEU:O	2.20	0.42
1:H:51:ILE:HD12	1:H:57:THR:HG22	2.02	0.41
1:H:128:ALA:O	2:L:119:PRO:HD2	2.20	0.41
1:H:20:LEU:HD22	1:H:110:THR:HG21	2.03	0.41
3:C:29:LEU:O	3:C:33:VAL:HG22	2.21	0.41
2:L:11:LEU:HD11	2:L:104:VAL:HG22	2.02	0.40
1:H:140:ALA:HB2	1:H:186:THR:HG22	2.03	0.40
1:H:122:PRO:HB3	1:H:148:TYR:HB3	2.03	0.40
2:L:7:SER:HA	2:L:8:PRO:HA	1.94	0.40
2:L:116:PHE:CD1	2:L:116:PHE:N	2.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	203/221 (92%)	199 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
3	C	157/187 (84%)	154 (98%)	3 (2%)	0	100	100
All	All	572/622 (92%)	559 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	H	178/191 (93%)	172 (97%)	6 (3%)	37	72
2	L	187/187 (100%)	182 (97%)	5 (3%)	44	77
3	C	134/160 (84%)	130 (97%)	4 (3%)	41	75
All	All	499/538 (93%)	484 (97%)	15 (3%)	41	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	18	LEU
1	H	28	SER
1	H	54	SER
1	H	101	TYR
1	H	151	GLU
1	H	207	ASN
2	L	7	SER
2	L	116	PHE
2	L	185	ASP
2	L	207	LYS
2	L	209	PHE
3	C	99	SER
3	C	117	SER
3	C	121	HIS
3	C	132	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	31	ASN
1	H	77	GLN
3	C	4	ASN
3	C	132	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](#)

2 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	$\# Z  > 2$
5	NAG	C	201	3	14,14,15	0.32	0	17,19,21	0.41	0
4	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.07	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
5	NAG	C	201	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 (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	NAG	C4-C5-C6-O6
5	C	201	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
5	C	201	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	H	207/221 (93%)	-0.06	3 (1%) 75 49	41, 59, 97, 124	0
2	L	214/214 (100%)	-0.04	3 (1%) 75 49	42, 61, 110, 138	0
3	C	159/187 (85%)	0.21	13 (8%) 11 3	44, 78, 132, 152	0
All	All	580/622 (93%)	0.02	19 (3%) 46 20	41, 62, 116, 152	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	154	LEU	3.8
3	C	127	GLU	3.6
3	C	126	HIS	3.3
2	L	210	ASN	3.1
1	H	191	SER	3.0
3	C	123	LYS	3.0
3	C	128	VAL	3.0
3	C	93	ASP	2.9
1	H	194	THR	2.7
3	C	1	GLY	2.7
3	C	125	ASP	2.6
3	C	96	GLU	2.6
3	C	92	GLY	2.5
3	C	2	VAL	2.4
1	H	195	LYS	2.3
3	C	120	TYR	2.2
2	L	212	GLY	2.2
3	C	124	GLY	2.2
3	C	63	PRO	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
5	NAG	C	201	14/15	0.52	0.43	100,105,110,111	0
4	SO4	L	301	5/5	0.91	0.14	68,68,73,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.