



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2016 – 05:17 PM EDT

PDB ID : 5L56  
Title : Plexin A1 full extracellular region, domains 1 to 10, to 4 angstrom  
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.  
Deposited on : 2016-05-28  
Resolution : 4.00 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.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

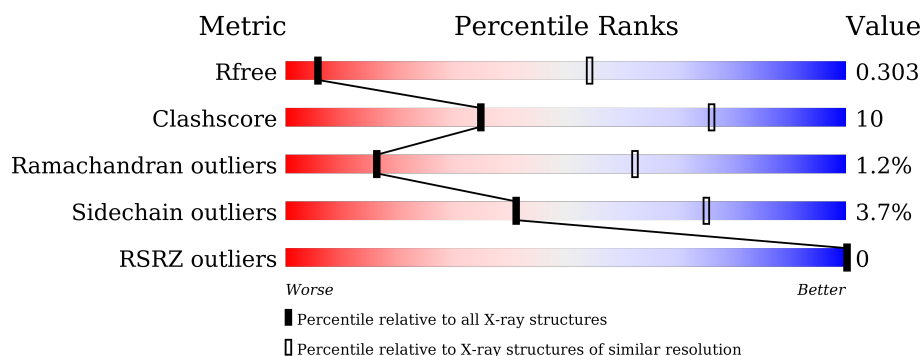
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	1212	73% 22% ..

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
2	NAG	A	1344	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9692 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.

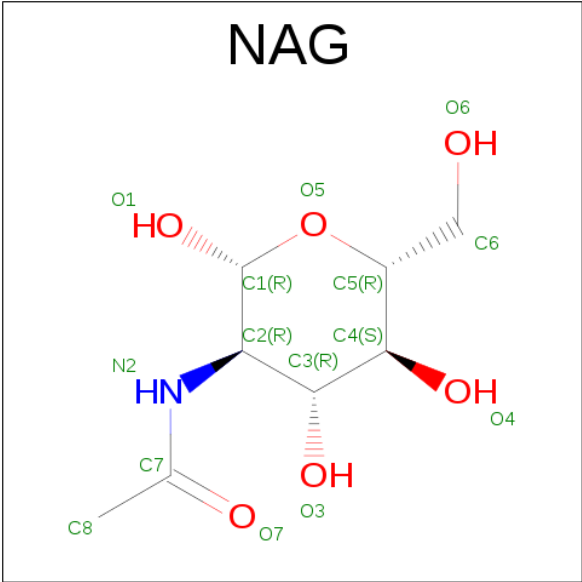
- Molecule 1 is a protein called Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1171	Total	C	N	O	S	0	0	0
			9085	5719	1593	1715	58			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	-	expression tag	UNP P70206
A	35	THR	-	expression tag	UNP P70206
A	36	GLY	-	expression tag	UNP P70206
A	1237	ARG	-	expression tag	UNP P70206
A	1238	THR	-	expression tag	UNP P70206
A	1239	LYS	-	expression tag	UNP P70206
A	1240	HIS	-	expression tag	UNP P70206
A	1241	HIS	-	expression tag	UNP P70206
A	1242	HIS	-	expression tag	UNP P70206
A	1243	HIS	-	expression tag	UNP P70206
A	1244	HIS	-	expression tag	UNP P70206
A	1245	HIS	-	expression tag	UNP P70206

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



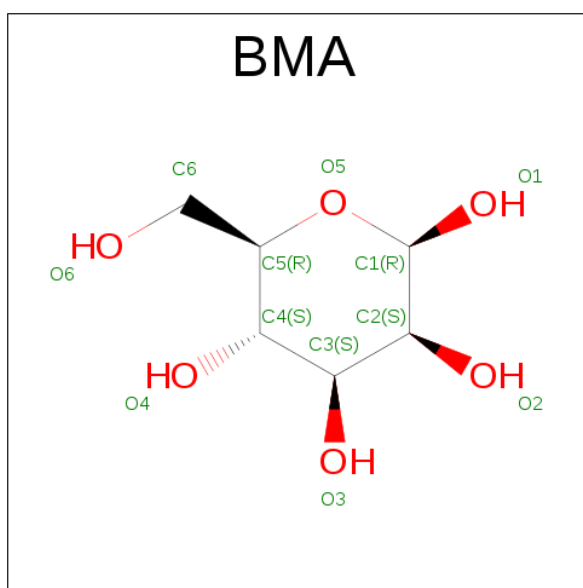
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

Continued on next page...

*Continued from previous page...*

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



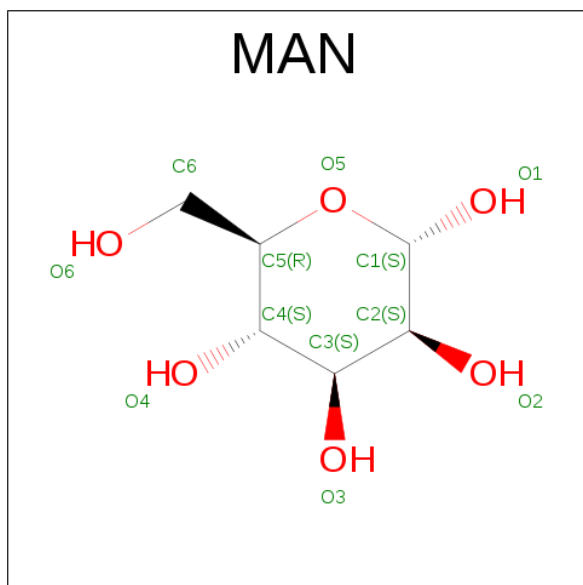
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

*Continued on next page...*

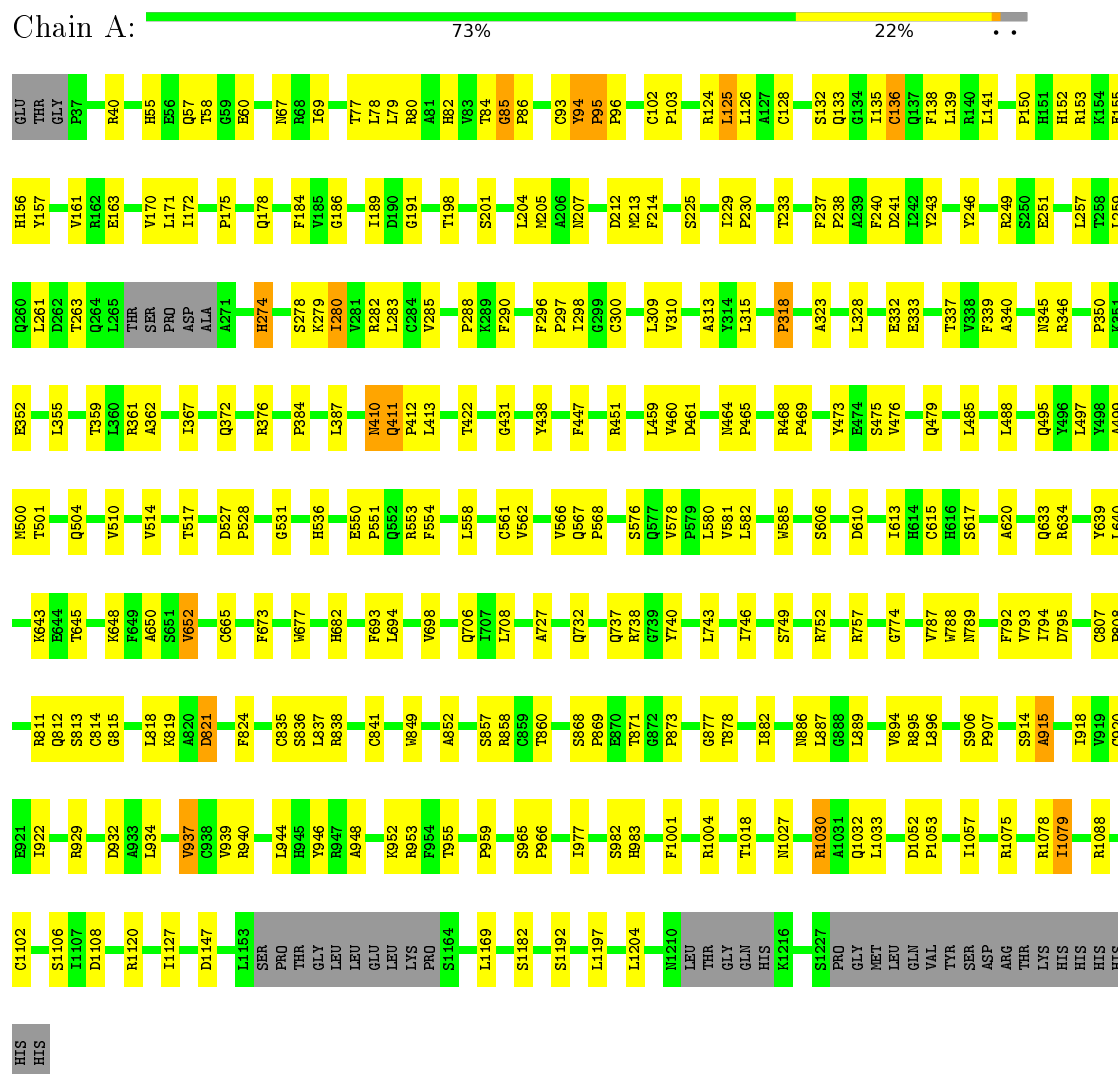
*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

### 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: Plexin-A1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.34Å 195.34Å 176.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.51 – 4.00 87.36 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.51-4.00) 98.6 (87.36-4.00)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.257 , 0.308 0.253 , 0.303	Depositor DCC
$R_{free}$ test set	1471 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	117.4	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: 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	0.33	0/9297	0.59	0/12642

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	ASN	Peptide
1	A	527	ASP	Peptide
1	A	807	CYS	Peptide
1	A	85	GLY	Peptide
1	A	94	TYR	Peptide

### 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	9085	0	8879	187	0
2	A	266	0	228	3	0
3	A	99	0	76	0	0
4	A	242	0	212	0	0
All	All	9692	0	9395	189	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 189 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:A:411:GLN:HG2	1:A:412:PRO:HD2	1.35	1.06
1:A:860:THR:HA	1:A:946:TYR:CE1	1.93	1.01
1:A:860:THR:HA	1:A:946:TYR:HE1	1.29	0.91
1:A:468:ARG:HG2	1:A:469:PRO:HD2	1.51	0.89
1:A:94:TYR:CD2	1:A:95:PRO:HD3	2.08	0.89

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	1163/1212 (96%)	1056 (91%)	93 (8%)	14 (1%)	16 62

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	95	PRO
1	A	411	GLN
1	A	869	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	915	ALA

### 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	1015/1051 (97%)	977 (96%)	38 (4%)	41 75

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	562	VAL
1	A	652	VAL
1	A	1075	ARG
1	A	610	ASP
1	A	693	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	706	GLN
1	A	899	HIS
1	A	729	ASN
1	A	345	ASN
1	A	764	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

41 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	NAG	A	1301	1,2	14,14,15	0.76	0	15,19,21	1.74	3 (20%)
2	NAG	A	1302	3,2	14,14,15	0.56	0	15,19,21	1.43	1 (6%)
4	MAN	A	1304	3	11,11,12	0.64	0	15,15,17	1.01	1 (6%)
2	NAG	A	1305	1,2	14,14,15	0.63	0	15,19,21	1.22	1 (6%)
2	NAG	A	1306	3,2	14,14,15	0.48	0	15,19,21	1.19	1 (6%)
4	MAN	A	1308	3	11,11,12	0.57	0	15,15,17	1.07	2 (13%)
4	MAN	A	1309	3,4	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
4	MAN	A	1310	4	11,11,12	0.58	0	15,15,17	1.23	2 (13%)
2	NAG	A	1311	1,2	14,14,15	0.62	0	15,19,21	1.14	1 (6%)
2	NAG	A	1312	3,2	14,14,15	0.53	0	15,19,21	1.20	2 (13%)
4	MAN	A	1314	3	11,11,12	0.58	0	15,15,17	1.03	2 (13%)
2	NAG	A	1315	1,2	14,14,15	0.64	0	15,19,21	1.17	1 (6%)
2	NAG	A	1316	3,2	14,14,15	0.52	0	15,19,21	1.09	1 (6%)
4	MAN	A	1318	3	11,11,12	0.58	0	15,15,17	0.87	1 (6%)
4	MAN	A	1319	3,4	11,11,12	0.61	0	15,15,17	0.91	0
4	MAN	A	1320	4	11,11,12	0.53	0	15,15,17	1.22	1 (6%)
4	MAN	A	1321	4	11,11,12	0.56	0	15,15,17	1.32	2 (13%)
2	NAG	A	1322	1,2	14,14,15	0.59	0	15,19,21	1.21	1 (6%)
2	NAG	A	1323	3,2	14,14,15	0.51	0	15,19,21	1.05	1 (6%)
4	MAN	A	1325	3	11,11,12	0.54	0	15,15,17	1.08	1 (6%)
4	MAN	A	1326	3,4	11,11,12	0.64	0	15,15,17	0.83	0
4	MAN	A	1327	4	11,11,12	0.62	0	15,15,17	1.21	3 (20%)
4	MAN	A	1328	4	11,11,12	0.59	0	15,15,17	0.94	1 (6%)
2	NAG	A	1329	1,2	14,14,15	0.62	0	15,19,21	0.94	1 (6%)
2	NAG	A	1330	3,2	14,14,15	0.64	0	15,19,21	1.07	1 (6%)
4	MAN	A	1332	3	11,11,12	0.54	0	15,15,17	0.89	1 (6%)
4	MAN	A	1333	3	11,11,12	0.53	0	15,15,17	1.46	2 (13%)
2	NAG	A	1334	1	14,14,15	0.51	0	15,19,21	0.97	0
2	NAG	A	1335	1,2	14,14,15	0.56	0	15,19,21	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1336	3,2	14,14,15	0.54	0	15,19,21	1.06	1 (6%)
2	NAG	A	1338	1,2	14,14,15	0.57	0	15,19,21	1.05	1 (6%)
2	NAG	A	1339	3,2	14,14,15	0.54	0	15,19,21	1.20	1 (6%)
4	MAN	A	1341	3	11,11,12	0.64	0	15,15,17	0.87	1 (6%)
4	MAN	A	1342	3,4	11,11,12	0.75	0	15,15,17	1.34	1 (6%)
4	MAN	A	1343	4	11,11,12	0.60	0	15,15,17	1.06	2 (13%)
2	NAG	A	1344	1,2	14,14,15	0.40	0	15,19,21	1.56	2 (13%)
2	NAG	A	1345	3,2	14,14,15	0.52	0	15,19,21	1.39	2 (13%)
4	MAN	A	1347	3	11,11,12	0.61	0	15,15,17	1.11	2 (13%)
4	MAN	A	1348	3,4	11,11,12	0.62	0	15,15,17	0.92	0
4	MAN	A	1349	4	11,11,12	0.62	0	15,15,17	1.27	1 (6%)
4	MAN	A	1350	4	11,11,12	0.63	0	15,15,17	1.05	1 (6%)

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
2	NAG	A	1301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1304	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1305	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1308	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1309	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1310	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1311	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1312	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1314	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1315	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1316	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1318	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1319	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1320	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1321	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1322	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1323	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1325	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1326	3,4	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	1327	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1328	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1329	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1330	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1332	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1333	3	-	0/2/19/22	1/1/1/1
2	NAG	A	1334	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1335	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1336	3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1338	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1339	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1341	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1342	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1343	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1344	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1345	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	1347	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1348	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1349	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1350	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1339	NAG	O5-C5-C4	-2.41	106.14	110.13
4	A	1327	MAN	C1-C2-C3	2.01	111.99	109.55
4	A	1318	MAN	C1-O5-C5	2.03	115.13	112.14
4	A	1347	MAN	C1-O5-C5	2.11	115.25	112.14
4	A	1314	MAN	C1-O5-C5	2.12	115.26	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1344	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1333	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0
2	A	1315	NAG	1	0
2	A	1316	NAG	1	0
2	A	1344	NAG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

50 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	$\# Z  > 2$
2	NAG	A	1301	1,2	14,14,15	0.76	0	15,19,21	1.74	3 (20%)
2	NAG	A	1302	3,2	14,14,15	0.56	0	15,19,21	1.43	1 (6%)
3	BMA	A	1303	2,4	11,11,12	0.65	0	15,15,17	0.83	0
4	MAN	A	1304	3	11,11,12	0.64	0	15,15,17	1.01	1 (6%)
2	NAG	A	1305	1,2	14,14,15	0.63	0	15,19,21	1.22	1 (6%)
2	NAG	A	1306	3,2	14,14,15	0.48	0	15,19,21	1.19	1 (6%)
3	BMA	A	1307	2,4	11,11,12	0.54	0	15,15,17	0.66	0
4	MAN	A	1308	3	11,11,12	0.57	0	15,15,17	1.07	2 (13%)
4	MAN	A	1309	3,4	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
4	MAN	A	1310	4	11,11,12	0.58	0	15,15,17	1.23	2 (13%)
2	NAG	A	1311	1,2	14,14,15	0.62	0	15,19,21	1.14	1 (6%)
2	NAG	A	1312	3,2	14,14,15	0.53	0	15,19,21	1.20	2 (13%)
3	BMA	A	1313	2,4	11,11,12	0.86	1 (9%)	15,15,17	2.24	4 (26%)
4	MAN	A	1314	3	11,11,12	0.58	0	15,15,17	1.03	2 (13%)
2	NAG	A	1315	1,2	14,14,15	0.64	0	15,19,21	1.17	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1316	3,2	14,14,15	0.52	0	15,19,21	1.09	1 (6%)
3	BMA	A	1317	2,4	11,11,12	0.61	0	15,15,17	1.65	3 (20%)
4	MAN	A	1318	3	11,11,12	0.58	0	15,15,17	0.87	1 (6%)
4	MAN	A	1319	3,4	11,11,12	0.61	0	15,15,17	0.91	0
4	MAN	A	1320	4	11,11,12	0.53	0	15,15,17	1.22	1 (6%)
4	MAN	A	1321	4	11,11,12	0.56	0	15,15,17	1.32	2 (13%)
2	NAG	A	1322	1,2	14,14,15	0.59	0	15,19,21	1.21	1 (6%)
2	NAG	A	1323	3,2	14,14,15	0.51	0	15,19,21	1.05	1 (6%)
3	BMA	A	1324	2,4	11,11,12	0.54	0	15,15,17	0.82	0
4	MAN	A	1325	3	11,11,12	0.54	0	15,15,17	1.08	1 (6%)
4	MAN	A	1326	3,4	11,11,12	0.64	0	15,15,17	0.83	0
4	MAN	A	1327	4	11,11,12	0.62	0	15,15,17	1.21	3 (20%)
4	MAN	A	1328	4	11,11,12	0.59	0	15,15,17	0.94	1 (6%)
2	NAG	A	1329	1,2	14,14,15	0.62	0	15,19,21	0.94	1 (6%)
2	NAG	A	1330	3,2	14,14,15	0.64	0	15,19,21	1.07	1 (6%)
3	BMA	A	1331	2,4	11,11,12	0.43	0	15,15,17	1.70	2 (13%)
4	MAN	A	1332	3	11,11,12	0.54	0	15,15,17	0.89	1 (6%)
4	MAN	A	1333	3	11,11,12	0.53	0	15,15,17	1.46	2 (13%)
2	NAG	A	1334	1	14,14,15	0.51	0	15,19,21	0.97	0
2	NAG	A	1335	1,2	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
2	NAG	A	1336	3,2	14,14,15	0.54	0	15,19,21	1.06	1 (6%)
3	BMA	A	1337	2	11,11,12	0.49	0	15,15,17	1.16	2 (13%)
2	NAG	A	1338	1,2	14,14,15	0.57	0	15,19,21	1.05	1 (6%)
2	NAG	A	1339	3,2	14,14,15	0.54	0	15,19,21	1.20	1 (6%)
3	BMA	A	1340	2,4	11,11,12	0.54	0	15,15,17	1.25	2 (13%)
4	MAN	A	1341	3	11,11,12	0.64	0	15,15,17	0.87	1 (6%)
4	MAN	A	1342	3,4	11,11,12	0.75	0	15,15,17	1.34	1 (6%)
4	MAN	A	1343	4	11,11,12	0.60	0	15,15,17	1.06	2 (13%)
2	NAG	A	1344	1,2	14,14,15	0.40	0	15,19,21	1.56	2 (13%)
2	NAG	A	1345	3,2	14,14,15	0.52	0	15,19,21	1.39	2 (13%)
3	BMA	A	1346	2,4	11,11,12	0.37	0	15,15,17	0.76	0
4	MAN	A	1347	3	11,11,12	0.61	0	15,15,17	1.11	2 (13%)
4	MAN	A	1348	3,4	11,11,12	0.62	0	15,15,17	0.92	0
4	MAN	A	1349	4	11,11,12	0.62	0	15,15,17	1.27	1 (6%)
4	MAN	A	1350	4	11,11,12	0.63	0	15,15,17	1.05	1 (6%)

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
2	NAG	A	1301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1303	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1304	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1305	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1307	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1308	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1309	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1310	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1311	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1312	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1313	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1314	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1315	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1316	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1317	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1318	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1319	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1320	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1321	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1322	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1323	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1324	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1325	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1326	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1327	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1328	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1329	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1330	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1331	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1332	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1333	3	-	0/2/19/22	1/1/1/1
2	NAG	A	1334	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1335	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1336	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1337	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1338	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1339	3,2	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	1340	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1341	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1342	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1343	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1344	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1345	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1346	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1347	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1348	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1349	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1350	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1313	BMA	C2-C3	2.32	1.55	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1339	NAG	O5-C5-C4	-2.41	106.14	110.13
4	A	1327	MAN	C1-C2-C3	2.01	111.99	109.55
3	A	1313	BMA	C1-O5-C5	2.02	115.11	112.14
4	A	1318	MAN	C1-O5-C5	2.03	115.13	112.14
3	A	1340	BMA	C2-C3-C4	2.06	114.64	111.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1344	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1333	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1315	NAG	1	0
2	A	1316	NAG	1	0
2	A	1344	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1171/1212 (96%)	-0.54	0 100 100	43, 122, 212, 302	0

There are no RSRZ outliers to report.

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

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
2	NAG	A	1338	14/15	0.80	0.20	1.13	230,258,278,292	0
2	NAG	A	1315	14/15	0.96	0.17	-0.30	171,181,191,194	0
2	NAG	A	1301	14/15	0.91	0.14	-0.91	143,163,173,182	0
2	NAG	A	1305	14/15	0.97	0.13	-1.64	130,149,159,165	0
2	NAG	A	1330	14/15	0.88	0.27	-	148,161,174,195	0
4	MAN	A	1304	11/12	0.58	0.31	-	262,282,287,288	0
2	NAG	A	1322	14/15	0.90	0.21	-	166,190,206,218	0
4	MAN	A	1321	11/12	0.64	0.20	-	246,255,269,271	0
4	MAN	A	1310	11/12	0.64	0.24	-	227,255,259,262	0
2	NAG	A	1316	14/15	0.93	0.13	-	182,208,219,230	0
4	MAN	A	1309	11/12	0.86	0.15	-	230,242,254,256	0
4	MAN	A	1348	11/12	0.78	0.13	-	282,295,299,300	0
4	MAN	A	1350	11/12	0.68	0.14	-	264,275,278,279	0
4	MAN	A	1326	11/12	0.84	0.11	-	235,258,264,269	0
4	MAN	A	1318	11/12	0.86	0.19	-	232,245,257,259	0
2	NAG	A	1329	14/15	0.94	0.18	-	112,127,138,142	0
2	NAG	A	1306	14/15	0.91	0.17	-	184,202,222,233	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	A	1319	11/12	0.93	0.08	-	208,222,237,250	0
2	NAG	A	1302	14/15	0.93	0.12	-	192,203,221,240	0
4	MAN	A	1320	11/12	0.91	0.17	-	197,204,207,215	0
4	MAN	A	1349	11/12	0.82	0.15	-	263,278,284,287	0
4	MAN	A	1327	11/12	0.85	0.19	-	250,253,259,261	0
2	NAG	A	1345	14/15	0.72	0.15	-	253,275,297,308	0
2	NAG	A	1344	14/15	0.88	0.12	-	186,212,241,250	0
4	MAN	A	1342	11/12	0.90	0.21	-	229,248,250,253	0
4	MAN	A	1314	11/12	0.93	0.18	-	210,234,236,238	0
2	NAG	A	1312	14/15	0.89	0.30	-	206,233,247,257	0
4	MAN	A	1325	11/12	0.88	0.26	-	230,245,248,256	0
4	MAN	A	1341	11/12	0.92	0.19	-	236,244,249,250	0
2	NAG	A	1323	14/15	0.92	0.18	-	206,226,233,240	0
4	MAN	A	1332	11/12	0.86	0.22	-	189,227,234,237	0
2	NAG	A	1334	14/15	0.69	0.30	-	203,226,240,242	0
2	NAG	A	1339	14/15	0.73	0.21	-	227,255,266,272	0
4	MAN	A	1308	11/12	0.79	0.27	-	247,257,267,268	0
4	MAN	A	1343	11/12	0.79	0.15	-	225,241,245,246	0
4	MAN	A	1347	11/12	0.71	0.27	-	244,272,282,284	0
4	MAN	A	1333	11/12	0.69	0.30	-	229,246,253,254	0
2	NAG	A	1336	14/15	0.86	0.17	-	224,240,248,256	0
4	MAN	A	1328	11/12	0.88	0.12	-	246,253,256,257	0
2	NAG	A	1335	14/15	0.92	0.14	-	192,213,227,237	0
2	NAG	A	1311	14/15	0.94	0.39	-	170,185,213,214	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1338	14/15	0.80	0.20	1.13	230,258,278,292	0
2	NAG	A	1315	14/15	0.96	0.17	-0.30	171,181,191,194	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1301	14/15	0.91	0.14	-0.91	143,163,173,182	0
2	NAG	A	1305	14/15	0.97	0.13	-1.64	130,149,159,165	0
2	NAG	A	1334	14/15	0.69	0.30	-	203,226,240,242	0
3	BMA	A	1340	11/12	0.82	0.19	-	253,262,269,272	0
4	MAN	A	1342	11/12	0.90	0.21	-	229,248,250,253	0
2	NAG	A	1330	14/15	0.88	0.27	-	148,161,174,195	0
4	MAN	A	1348	11/12	0.78	0.13	-	282,295,299,300	0
2	NAG	A	1322	14/15	0.90	0.21	-	166,190,206,218	0
4	MAN	A	1321	11/12	0.64	0.20	-	246,255,269,271	0
4	MAN	A	1310	11/12	0.64	0.24	-	227,255,259,262	0
3	BMA	A	1313	11/12	0.84	0.10	-	202,234,254,265	0
2	NAG	A	1316	14/15	0.93	0.13	-	182,208,219,230	0
3	BMA	A	1303	11/12	0.69	0.23	-	218,254,267,281	0
4	MAN	A	1304	11/12	0.58	0.31	-	262,282,287,288	0
4	MAN	A	1350	11/12	0.68	0.14	-	264,275,278,279	0
4	MAN	A	1326	11/12	0.84	0.11	-	235,258,264,269	0
4	MAN	A	1318	11/12	0.86	0.19	-	232,245,257,259	0
2	NAG	A	1329	14/15	0.94	0.18	-	112,127,138,142	0
2	NAG	A	1306	14/15	0.91	0.17	-	184,202,222,233	0
4	MAN	A	1319	11/12	0.93	0.08	-	208,222,237,250	0
2	NAG	A	1302	14/15	0.93	0.12	-	192,203,221,240	0
4	MAN	A	1320	11/12	0.91	0.17	-	197,204,207,215	0
2	NAG	A	1323	14/15	0.92	0.18	-	206,226,233,240	0
3	BMA	A	1307	11/12	0.82	0.17	-	235,240,250,265	0
3	BMA	A	1324	11/12	0.74	0.19	-	244,248,254,254	0
4	MAN	A	1327	11/12	0.85	0.19	-	250,253,259,261	0
2	NAG	A	1345	14/15	0.72	0.15	-	253,275,297,308	0
2	NAG	A	1344	14/15	0.88	0.12	-	186,212,241,250	0
4	MAN	A	1328	11/12	0.88	0.12	-	246,253,256,257	0
4	MAN	A	1314	11/12	0.93	0.18	-	210,234,236,238	0
4	MAN	A	1309	11/12	0.86	0.15	-	230,242,254,256	0
4	MAN	A	1325	11/12	0.88	0.26	-	230,245,248,256	0
4	MAN	A	1341	11/12	0.92	0.19	-	236,244,249,250	0
3	BMA	A	1331	11/12	0.86	0.19	-	217,237,244,251	0
3	BMA	A	1317	11/12	0.85	0.10	-	232,248,259,265	0
4	MAN	A	1332	11/12	0.86	0.22	-	189,227,234,237	0
2	NAG	A	1312	14/15	0.89	0.30	-	206,233,247,257	0
2	NAG	A	1339	14/15	0.73	0.21	-	227,255,266,272	0
4	MAN	A	1308	11/12	0.79	0.27	-	247,257,267,268	0
3	BMA	A	1346	11/12	0.75	0.14	-	276,290,297,300	0
4	MAN	A	1343	11/12	0.79	0.15	-	225,241,245,246	0
3	BMA	A	1337	11/12	0.80	0.19	-	218,235,247,251	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	A	1347	11/12	0.71	0.27	-	244,272,282,284	0
4	MAN	A	1333	11/12	0.69	0.30	-	229,246,253,254	0
2	NAG	A	1336	14/15	0.86	0.17	-	224,240,248,256	0
4	MAN	A	1349	11/12	0.82	0.15	-	263,278,284,287	0
2	NAG	A	1335	14/15	0.92	0.14	-	192,213,227,237	0
2	NAG	A	1311	14/15	0.94	0.39	-	170,185,213,214	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.