



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 PM GMT

PDB ID : 4FQP  
Title : Crystal structure of human Nectin-like 5 full ectodomain (D1-D3)  
Authors : Harrison, O.J.; Jin, X.; Brasch, J.; Shapiro, L.  
Deposited on : 2012-06-25  
Resolution : 3.60 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  
<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

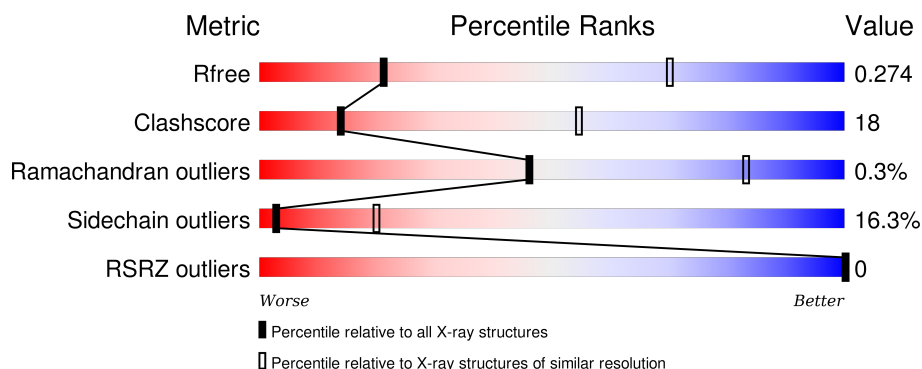
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	313	

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	A	416	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2599 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 Poliovirus receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2342	1478	403	449	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	EXPRESSION TAG	UNP P15151
A	336	HIS	-	EXPRESSION TAG	UNP P15151
A	337	HIS	-	EXPRESSION TAG	UNP P15151
A	338	HIS	-	EXPRESSION TAG	UNP P15151
A	339	HIS	-	EXPRESSION TAG	UNP P15151
A	340	HIS	-	EXPRESSION TAG	UNP P15151

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

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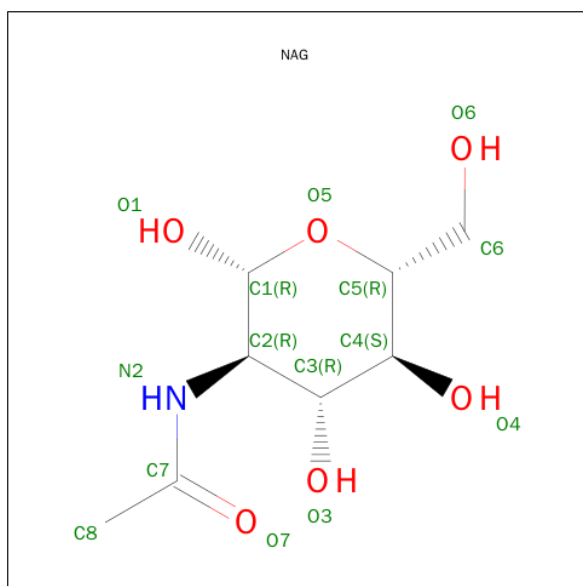
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

**i**

- Molecule 1: Poliovirus receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.92Å 138.92Å 273.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.60 29.99 – 3.56	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.60) 99.1 (29.99-3.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.56Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.248 , 0.272 0.247 , 0.274	Depositor DCC
$R_{free}$ test set	959 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.3	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	3 of 19158 reflections (0.016%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	0.65	0/2400	0.57	0/3286

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	A	2342	0	2294	86	0
2	A	78	0	68	3	0
3	A	60	0	52	2	0
4	A	56	0	50	3	0
5	A	49	0	43	8	0
6	A	14	0	13	1	0
All	All	2599	0	2520	94	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 18.

All (94) 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:283:MET:CE	1:A:308:THR:HG22	1.82	1.09
1:A:140:ARG:HH11	1:A:140:ARG:HG3	1.21	1.04
3:A:404:NAG:H4	3:A:406:FUC:H5	1.39	1.00
1:A:283:MET:HE2	1:A:308:THR:HG22	1.48	0.94
1:A:183:LEU:HD12	1:A:183:LEU:H	1.33	0.92
1:A:68:ARG:HB3	1:A:71:GLU:HG3	1.52	0.91
1:A:147:ASN:ND2	1:A:223:VAL:HG11	1.88	0.86
1:A:162:PRO:HB3	1:A:205:LEU:HD12	1.60	0.81
1:A:305:PRO:HB2	5:A:416:NAG:H82	1.63	0.80
1:A:216:GLY:O	2:A:413:NAG:H82	1.81	0.79
1:A:170:GLY:H	1:A:201:THR:HG22	1.49	0.78
1:A:140:ARG:HG3	1:A:140:ARG:NH1	1.95	0.77
1:A:68:ARG:CB	1:A:71:GLU:HG3	2.18	0.74
1:A:90:LYS:H	1:A:90:LYS:HD2	1.55	0.72
1:A:183:LEU:HD12	1:A:183:LEU:N	2.06	0.71
1:A:68:ARG:HB3	1:A:71:GLU:CG	2.21	0.70
5:A:416:NAG:H62	5:A:418:NAG:C1	2.22	0.69
1:A:61:VAL:HG11	1:A:103:LEU:O	1.94	0.68
1:A:124:LEU:CB	1:A:134:SER:HB3	2.25	0.67
5:A:416:NAG:H61	5:A:417:FUC:O2	1.97	0.65
1:A:167:VAL:HB	1:A:203:THR:HG23	1.79	0.65
1:A:44:SER:HB3	1:A:111:PHE:HA	1.78	0.65
1:A:169:THR:HA	1:A:201:THR:HB	1.79	0.65
1:A:218:ASN:ND2	4:A:411:NAG:O7	2.29	0.65
5:A:416:NAG:C6	5:A:418:NAG:C1	2.75	0.64
1:A:124:LEU:HB3	1:A:134:SER:HB3	1.78	0.64
5:A:416:NAG:C6	5:A:417:FUC:O2	2.46	0.63
1:A:189:THR:HG23	1:A:204:SER:HB2	1.80	0.62
1:A:92:LEU:HD23	1:A:110:MET:HB3	1.81	0.62
1:A:39:GLY:H	1:A:45:VAL:HG11	1.65	0.62
1:A:251:TYR:CE1	1:A:327:VAL:HG23	2.35	0.61
1:A:322:GLN:HE22	6:A:420:NAG:H82	1.66	0.61
1:A:283:MET:CE	1:A:308:THR:CG2	2.71	0.60
1:A:142:LEU:HA	1:A:172:ARG:HG3	1.82	0.60
1:A:154:VAL:HG21	1:A:163:MET:HG2	1.85	0.59
1:A:147:ASN:OD1	1:A:232:GLN:NE2	2.30	0.59
1:A:118:GLU:HB2	1:A:141:VAL:CG1	2.32	0.59
1:A:274:PRO:HA	1:A:316:ASN:HB2	1.87	0.57
1:A:306:ILE:H	1:A:329:VAL:HG23	1.69	0.57
1:A:120:ASN:ND2	3:A:406:FUC:H61	2.19	0.57
1:A:170:GLY:N	1:A:201:THR:HG22	2.20	0.56
1:A:283:MET:HE1	1:A:308:THR:HG22	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLY:O	2:A:413:NAG:C8	2.54	0.56
1:A:114:ARG:NH1	1:A:117:ASP:OD1	2.39	0.56
1:A:309:THR:OG1	1:A:326:THR:HG22	2.07	0.55
1:A:140:ARG:CG	1:A:140:ARG:NH1	2.69	0.54
1:A:63:GLN:HB3	1:A:79:HIS:HD2	1.72	0.54
5:A:416:NAG:H62	5:A:418:NAG:HN2	1.72	0.53
1:A:142:LEU:HA	1:A:172:ARG:CG	2.38	0.53
1:A:90:LYS:CD	1:A:90:LYS:H	2.22	0.53
1:A:218:ASN:ND2	4:A:411:NAG:C7	2.72	0.53
1:A:39:GLY:N	1:A:45:VAL:HG11	2.24	0.52
1:A:64:LEU:CD1	1:A:106:ALA:HA	2.39	0.52
1:A:154:VAL:HG12	1:A:155:GLN:O	2.09	0.52
1:A:32:GLN:HG2	1:A:52:GLN:HE21	1.75	0.52
1:A:124:LEU:HB3	1:A:134:SER:CB	2.40	0.51
1:A:211:SER:O	1:A:214:VAL:HG22	2.11	0.50
1:A:287:PRO:HG2	1:A:308:THR:HG21	1.94	0.50
1:A:64:LEU:HD12	1:A:106:ALA:CB	2.42	0.50
1:A:135:VAL:HG22	1:A:136:ASP:N	2.27	0.50
1:A:143:ALA:HB3	1:A:172:ARG:HB3	1.95	0.49
1:A:287:PRO:CG	1:A:308:THR:HG21	2.42	0.48
1:A:252:ASP:O	1:A:254:ASN:N	2.46	0.48
1:A:124:LEU:HB2	1:A:134:SER:HB3	1.92	0.48
1:A:95:VAL:CG1	2:A:401:NAG:H62	2.43	0.48
1:A:244:PRO:HG3	1:A:316:ASN:HB3	1.95	0.48
1:A:39:GLY:HA3	1:A:140:ARG:O	2.13	0.48
1:A:30:VAL:HG13	1:A:52:GLN:HB2	1.95	0.48
1:A:218:ASN:HD22	4:A:411:NAG:C7	2.24	0.47
1:A:114:ARG:O	1:A:117:ASP:HB2	2.15	0.47
1:A:300:ARG:HB3	1:A:301:PRO:HD2	1.97	0.46
1:A:29:VAL:O	1:A:29:VAL:CG1	2.64	0.46
5:A:416:NAG:H62	5:A:418:NAG:N2	2.31	0.46
1:A:254:ASN:OD1	1:A:254:ASN:N	2.48	0.46
1:A:245:GLU:OE1	1:A:269:ARG:NH1	2.48	0.45
1:A:255:TRP:CZ3	1:A:299:ILE:HG21	2.51	0.45
1:A:63:GLN:HB3	1:A:79:HIS:CD2	2.50	0.45
1:A:205:LEU:N	1:A:205:LEU:HD23	2.32	0.45
1:A:64:LEU:N	1:A:64:LEU:HD23	2.32	0.45
1:A:163:MET:HB3	1:A:163:MET:HE2	1.77	0.45
5:A:416:NAG:H61	5:A:417:FUC:H3	1.98	0.45
1:A:38:PRO:HA	1:A:140:ARG:O	2.18	0.43
1:A:47:LEU:HB3	1:A:66:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLY:HA2	1:A:201:THR:HG23	2.00	0.43
1:A:271:ASN:HA	1:A:272:PRO:HA	1.86	0.42
1:A:206:TRP:CH2	1:A:208:LEU:HD22	2.55	0.42
1:A:61:VAL:HA	1:A:127:THR:HA	2.00	0.42
1:A:128:PHE:C	1:A:128:PHE:CD1	2.93	0.41
1:A:160:PRO:HG3	1:A:209:VAL:HG22	2.01	0.41
1:A:68:ARG:HG2	1:A:121:TYR:CE2	2.55	0.41
1:A:118:GLU:HG3	1:A:139:LEU:O	2.20	0.41
1:A:177:ILE:HG21	1:A:204:SER:HB3	2.02	0.41
1:A:283:MET:HE1	1:A:308:THR:CG2	2.48	0.40
1:A:142:LEU:HB2	1:A:172:ARG:O	2.21	0.40

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	304/313 (97%)	284 (93%)	19 (6%)	1 (0%)	46 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	263/270 (97%)	220 (84%)	43 (16%)	3 20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	47	LEU
1	A	57	GLU
1	A	62	SER
1	A	64	LEU
1	A	68	ARG
1	A	69	HIS
1	A	72	SER
1	A	82	GLN
1	A	90	LYS
1	A	103	LEU
1	A	114	ARG
1	A	122	THR
1	A	124	LEU
1	A	132	SER
1	A	139	LEU
1	A	140	ARG
1	A	141	VAL
1	A	142	LEU
1	A	147	ASN
1	A	148	THR
1	A	150	GLU
1	A	159	GLU
1	A	165	ARG
1	A	167	VAL
1	A	169	THR
1	A	183	LEU
1	A	196	LEU
1	A	202	VAL
1	A	203	THR
1	A	205	LEU
1	A	209	VAL
1	A	232	GLN
1	A	254	ASN
1	A	264	LEU
1	A	267	ASP
1	A	269	ARG
1	A	297	LEU

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Mol	Chain	Res	Type
1	A	302	VAL
1	A	316	ASN
1	A	327	VAL
1	A	329	VAL
1	A	330	LYS

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

Mol	Chain	Res	Type
1	A	52	GLN
1	A	180	HIS
1	A	322	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 ⓘ

19 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	$\# Z  > 2$
2	NAG	A	401	1,2	14,14,15	0.94	0	15,19,21	1.01	1 (6%)
2	NAG	A	402	2	14,14,15	0.53	0	15,19,21	0.93	0
2	BMA	A	403	2	11,11,12	0.62	0	14,15,17	1.08	0
3	NAG	A	404	1,3	14,14,15	1.04	1 (7%)	15,19,21	1.82	4 (26%)
3	NAG	A	405	3	14,14,15	0.73	0	15,19,21	1.11	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	A	406	3	10,10,11	0.90	0	14,14,16	1.63	4 (28%)
3	BMA	A	407	3	11,11,12	0.26	0	14,15,17	0.60	0
3	MAN	A	408	3	11,11,12	0.64	0	14,15,17	0.59	0
4	NAG	A	409	1,4	14,14,15	0.79	0	15,19,21	1.43	2 (13%)
4	NAG	A	410	4	14,14,15	0.69	0	15,19,21	0.74	0
4	NAG	A	411	1,4	14,14,15	0.72	0	15,19,21	0.73	0
4	NAG	A	412	4	14,14,15	0.66	0	15,19,21	1.00	0
2	NAG	A	413	1,2	14,14,15	0.72	0	15,19,21	1.17	3 (20%)
2	NAG	A	414	2	14,14,15	0.45	0	15,19,21	1.25	1 (6%)
2	BMA	A	415	2	11,11,12	0.26	0	14,15,17	0.60	0
5	NAG	A	416	1,5	14,14,15	0.54	0	15,19,21	0.59	0
5	FUC	A	417	5	10,10,11	0.76	0	14,14,16	1.27	1 (7%)
5	NAG	A	418	5	14,14,15	0.53	0	15,19,21	1.20	2 (13%)
5	BMA	A	419	5	11,11,12	0.26	0	14,15,17	0.61	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
2	NAG	A	401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	402	2	-	0/6/23/26	0/1/1/1
2	BMA	A	403	2	-	0/2/19/22	1/1/1/1
3	NAG	A	404	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	405	3	-	0/6/23/26	0/1/1/1
3	FUC	A	406	3	-	0/0/17/20	0/1/1/1
3	BMA	A	407	3	-	0/2/19/22	0/1/1/1
3	MAN	A	408	3	-	0/2/19/22	0/1/1/1
4	NAG	A	409	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	410	4	-	0/6/23/26	0/1/1/1
4	NAG	A	411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	412	4	-	0/6/23/26	0/1/1/1
2	NAG	A	413	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	414	2	-	0/6/23/26	0/1/1/1
2	BMA	A	415	2	-	0/2/19/22	0/1/1/1
5	NAG	A	416	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	417	5	-	0/0/17/20	0/1/1/1
5	NAG	A	418	5	-	0/6/23/26	0/1/1/1
5	BMA	A	419	5	-	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	404	NAG	C1-C2	-2.18	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	FUC	O5-C1-C2	-3.59	105.03	110.86
3	A	404	NAG	O4-C4-C3	-3.57	102.30	110.34
5	A	418	NAG	C4-C3-C2	-2.35	107.57	111.23
2	A	413	NAG	C6-C5-C4	-2.09	107.87	113.02
3	A	406	FUC	C2-C3-C4	-2.09	107.50	111.04
3	A	406	FUC	O5-C5-C6	2.04	109.51	106.13
3	A	404	NAG	C3-C4-C5	2.11	113.88	110.20
5	A	418	NAG	C1-O5-C5	2.14	114.97	112.25
2	A	413	NAG	O5-C5-C6	2.30	112.32	107.35
3	A	406	FUC	O3-C3-C2	2.51	114.54	110.00
2	A	413	NAG	C1-O5-C5	2.53	115.46	112.25
2	A	401	NAG	C1-O5-C5	2.55	115.48	112.25
2	A	414	NAG	O5-C5-C6	2.58	112.92	107.35
5	A	417	FUC	O5-C5-C6	2.63	110.48	106.13
4	A	409	NAG	C1-O5-C5	2.90	115.93	112.25
3	A	405	NAG	C4-C3-C2	2.94	115.80	111.23
3	A	404	NAG	C6-C5-C4	3.44	121.50	113.02
3	A	404	NAG	O6-C6-C5	3.59	123.19	111.33
4	A	409	NAG	C4-C3-C2	3.63	116.87	111.23

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAG	1	0
3	A	404	NAG	1	0
3	A	406	FUC	2	0
4	A	411	NAG	3	0
2	A	413	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	416	NAG	8	0
5	A	417	FUC	3	0
5	A	418	NAG	4	0

## 5.6 Ligand geometry [i](#)

1 ligand is 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	A	420	1	14,14,15	1.33	1 (7%)	15,19,21	1.58	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
6	NAG	A	420	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	420	NAG	C1-C2	3.72	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	420	NAG	C1-O5-C5	4.64	118.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	420	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	306/313 (97%)	-0.31	0 100 100	88, 109, 148, 180	0

There are no RSRZ outliers to report.

### 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](#)

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
5	FUC	A	417	10/11	0.75	0.51	-	163,164,167,168	0
4	NAG	A	409	14/15	0.84	0.24	-	132,143,147,149	0
2	NAG	A	402	14/15	0.85	0.39	-	139,145,153,160	0
5	BMA	A	419	11/12	0.50	0.42	-	181,183,184,184	0
3	FUC	A	406	10/11	0.85	0.37	-	122,126,127,129	0
2	BMA	A	403	11/12	0.76	0.46	-	164,167,169,170	0
3	BMA	A	407	11/12	0.71	0.34	-	158,161,165,170	0
4	NAG	A	412	14/15	0.86	0.37	-	155,164,169,176	0
2	NAG	A	401	14/15	0.87	0.28	-	103,108,113,118	0
4	NAG	A	411	14/15	0.88	0.27	-	125,130,138,143	0
2	NAG	A	413	14/15	0.87	0.40	-	117,127,138,141	0
3	NAG	A	405	14/15	0.89	0.41	-	127,136,142,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	418	14/15	0.87	0.49	-	162,170,175,180	0
2	BMA	A	415	11/12	0.71	0.46	-	177,180,181,184	0
2	NAG	A	414	14/15	0.85	0.64	-	163,168,172,176	0
4	NAG	A	410	14/15	0.77	0.50	-	159,165,167,168	0
3	NAG	A	404	14/15	0.94	0.26	-	98,106,116,121	0
5	NAG	A	416	14/15	0.84	0.49	-	131,142,151,160	0
3	MAN	A	408	11/12	0.81	0.36	-	171,175,176,176	0

## 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
6	NAG	A	420	14/15	0.81	0.28	-	108,111,113,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.