



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:53 PM GMT

PDB ID : 3D11  
Title : Crystal Structures of the Nipah G Attachment Glycoprotein  
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Deposited on : 2008-05-02  
Resolution : 2.31 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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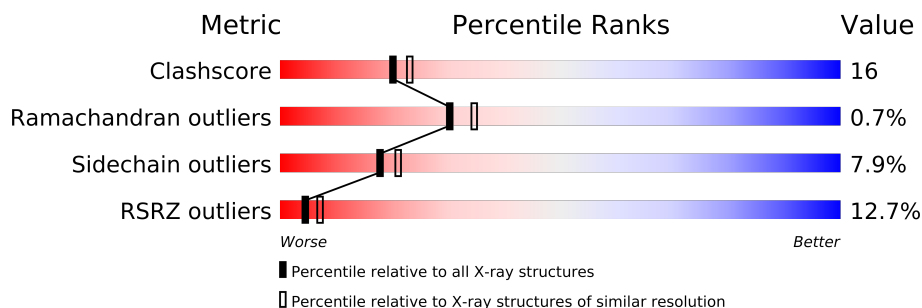
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.31 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	428	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	1210	-	X
5	IOD	A	14	-	X
5	IOD	A	16	-	X
5	IOD	A	17	-	X
5	IOD	A	18	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3721 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3361	2141	567	632	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	EXPRESSION TAG	UNP Q9IH62

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	EXPRESSION TAG	UNP Q9IH62
A	603	ALA	-	EXPRESSION TAG	UNP Q9IH62

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	EXPRESSION TAG	UNP Q9IH62

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	I	0	0
			19	19		

- Molecule 6 is water.

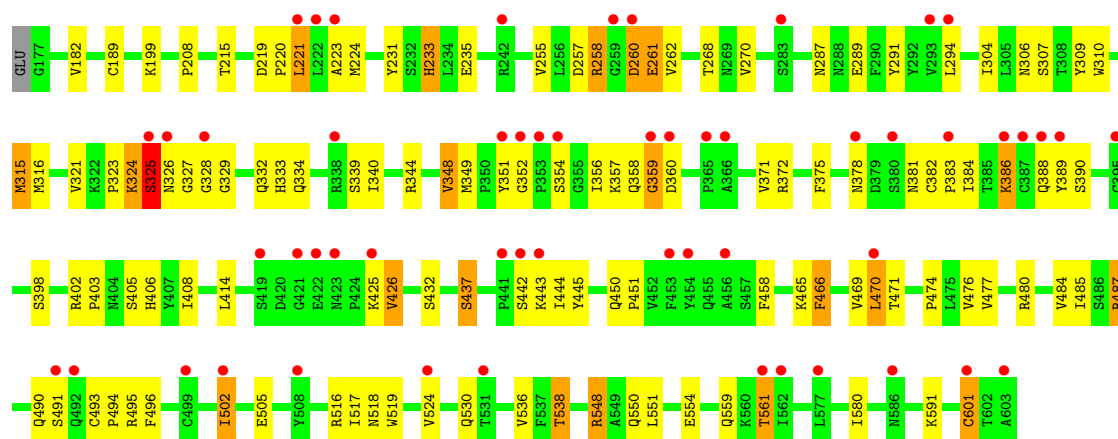
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		

### 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: Hemagglutinin-neuraminidase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.16Å 130.16Å 130.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.24 – 2.31 39.25 – 2.31	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.24-2.31) 90.7 (39.25-2.31)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.31Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.228 , 0.257 0.230 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.2	EDS
Estimated twinning fraction	0.031 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31070 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, BMA, NAG, NDG, 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	0.37	0/3442	0.55	0/4682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3361	0	3306	99	0
2	A	14	0	13	1	0
3	A	56	0	50	5	0
4	A	61	0	52	1	0
5	A	19	0	0	16	0
6	A	210	0	0	16	0
All	All	3721	0	3421	110	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:601:CYS:HB2	5:A:14:IOD:I	2.08	1.23
1:A:601:CYS:CB	5:A:14:IOD:I	2.75	1.03
1:A:601:CYS:SG	5:A:14:IOD:I	2.90	1.00
5:A:9:IOD:I	5:A:14:IOD:I	3.21	0.98
1:A:189:CYS:SG	5:A:14:IOD:I	2.97	0.93
5:A:2:IOD:I	6:A:1366:HOH:O	2.66	0.83
1:A:550:GLN:HE22	1:A:554:GLU:HG2	1.44	0.82
1:A:344:ARG:NH1	5:A:16:IOD:I	2.82	0.82
1:A:471:THR:HG22	1:A:476:VAL:HG22	1.63	0.80
1:A:548:ARG:HH11	1:A:548:ARG:HB3	1.47	0.78
1:A:386:LYS:HA	1:A:386:LYS:NZ	1.98	0.77
1:A:471:THR:HG23	1:A:474:PRO:O	1.86	0.75
1:A:359:GLY:HA2	1:A:360:ASP:OD1	1.87	0.75
1:A:306:ASN:OD1	1:A:309:TYR:HB2	1.90	0.71
3:A:1314:NAG:H61	6:A:1458:HOH:O	1.91	0.70
1:A:359:GLY:HA2	1:A:360:ASP:CG	2.13	0.69
1:A:382:CYS:O	1:A:384:ILE:HD13	1.92	0.68
1:A:182:VAL:CG2	5:A:13:IOD:I	3.12	0.67
5:A:15:IOD:I	6:A:1379:HOH:O	2.84	0.66
5:A:12:IOD:I	6:A:1441:HOH:O	2.85	0.65
1:A:182:VAL:HG22	5:A:13:IOD:I	2.66	0.65
3:A:1313:NAG:H3	3:A:1314:NAG:O5	1.98	0.64
1:A:524:VAL:O	1:A:561:THR:HG21	1.96	0.64
1:A:327:GLY:HA2	6:A:1512:HOH:O	1.97	0.63
1:A:348:VAL:HG11	1:A:414:LEU:HD21	1.80	0.62
1:A:257:ASP:OD1	1:A:258:ARG:O	2.18	0.62
1:A:548:ARG:CB	1:A:548:ARG:HH11	2.13	0.61
1:A:182:VAL:HG23	5:A:13:IOD:I	2.70	0.61
1:A:375:PHE:HD1	5:A:7:IOD:I	2.54	0.61
1:A:375:PHE:CD1	5:A:7:IOD:I	3.23	0.61
1:A:344:ARG:HD2	6:A:1397:HOH:O	2.00	0.61
1:A:386:LYS:HA	1:A:386:LYS:HZ2	1.66	0.59
1:A:494:PRO:HB3	1:A:530:GLN:HE21	1.67	0.59
1:A:580:ILE:HG13	1:A:591:LYS:HD2	1.84	0.59
1:A:332:GLN:O	1:A:333:HIS:HB3	2.02	0.58
1:A:561:THR:CG2	6:A:1364:HOH:O	2.52	0.57
1:A:208:PRO:HG3	5:A:6:IOD:I	2.75	0.56
3:A:1361:NAG:O3	3:A:1361:NAG:H83	2.06	0.56
1:A:371:VAL:HG23	6:A:1540:HOH:O	2.06	0.55
1:A:339:SER:OG	1:A:425:LYS:HG2	2.07	0.55
1:A:466:PHE:O	1:A:480:ARG:HG2	2.06	0.55
1:A:386:LYS:HZ3	1:A:386:LYS:HA	1.72	0.55
1:A:348:VAL:CG1	1:A:414:LEU:HD21	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:ARG:NH1	1:A:403:PRO:O	2.42	0.53
1:A:384:ILE:HG13	1:A:390:SER:O	2.08	0.53
1:A:516:ARG:HD2	6:A:1509:HOH:O	2.09	0.52
1:A:258:ARG:HG3	1:A:262:VAL:O	2.10	0.52
1:A:329:GLY:O	1:A:333:HIS:HD2	1.91	0.52
5:A:19:IOD:I	6:A:1366:HOH:O	2.89	0.51
1:A:445:TYR:O	1:A:451:PRO:HA	2.12	0.50
1:A:559:GLN:HG2	6:A:1536:HOH:O	2.12	0.50
1:A:487:ARG:NH2	1:A:493:CYS:O	2.44	0.50
1:A:233:HIS:HE1	1:A:235:GLU:OE2	1.95	0.50
1:A:378:ASN:OD1	2:A:1210:NAG:H5	2.12	0.50
1:A:233:HIS:CE1	1:A:235:GLU:HG3	2.46	0.49
1:A:360:ASP:HB2	6:A:1529:HOH:O	2.11	0.49
1:A:315:MET:HG3	1:A:334:GLN:HE22	1.78	0.48
1:A:324:LYS:NZ	1:A:324:LYS:HB2	2.29	0.48
1:A:536:VAL:HG12	1:A:538:THR:HG22	1.96	0.47
1:A:372:ARG:HH12	1:A:403:PRO:C	2.17	0.47
1:A:294:LEU:HD13	1:A:316:MET:HE2	1.95	0.47
1:A:258:ARG:HH21	1:A:260:ASP:CG	2.18	0.47
1:A:223:ALA:HB2	1:A:354:SER:HB3	1.97	0.46
1:A:325:SER:HB3	1:A:326:ASN:H	1.56	0.46
1:A:324:LYS:O	1:A:324:LYS:HG2	2.15	0.45
1:A:324:LYS:O	1:A:325:SER:C	2.54	0.45
1:A:231:TYR:OH	1:A:233:HIS:HD2	2.00	0.45
1:A:340:ILE:HG12	1:A:426:VAL:CG2	2.47	0.45
1:A:199:LYS:HD3	6:A:1494:HOH:O	2.15	0.45
1:A:268:THR:O	1:A:323:PRO:HG2	2.17	0.45
1:A:469:VAL:HG22	1:A:477:VAL:HG22	1.99	0.45
1:A:224:MET:HE3	1:A:255:VAL:HG21	1.98	0.45
1:A:495:ARG:O	1:A:496:PHE:HB2	2.17	0.45
3:A:1313:NAG:H5	3:A:1314:NAG:O5	2.17	0.44
1:A:372:ARG:HD2	1:A:405:SER:O	2.17	0.44
1:A:383:PRO:C	1:A:384:ILE:HD12	2.37	0.44
1:A:289:GLU:O	1:A:321:VAL:HG22	2.17	0.44
1:A:470:LEU:HD12	1:A:470:LEU:HA	1.71	0.44
1:A:261:GLU:O	1:A:261:GLU:OE1	2.35	0.44
1:A:443:LYS:HE3	6:A:1373:HOH:O	2.18	0.44
1:A:458:PHE:HA	1:A:505:GLU:O	2.17	0.43
1:A:548:ARG:CG	1:A:548:ARG:HH11	2.30	0.43
1:A:260:ASP:O	1:A:261:GLU:HB2	2.17	0.43
1:A:398:SER:OG	1:A:502:ILE:HA	2.18	0.43
1:A:219:ASP:N	1:A:220:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1313:NAG:C3	3:A:1314:NAG:O5	2.63	0.43
1:A:260:ASP:O	1:A:261:GLU:CB	2.67	0.43
1:A:406:HIS:HE1	6:A:1562:HOH:O	2.02	0.42
1:A:450:GLN:HG3	1:A:451:PRO:HD2	2.01	0.42
1:A:287:ASN:HD21	1:A:360:ASP:HB3	1.84	0.42
1:A:378:ASN:HB3	1:A:381:ASN:OD1	2.19	0.42
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.78	0.42
1:A:382:CYS:O	1:A:384:ILE:CD1	2.65	0.42
1:A:517:ILE:HG22	1:A:518:ASN:OD1	2.20	0.42
1:A:304:ILE:HG12	1:A:349:MET:HE1	2.01	0.42
1:A:384:ILE:CG1	1:A:390:SER:O	2.68	0.42
4:A:1142:MAN:C6	6:A:1406:HOH:O	2.68	0.42
1:A:310:TRP:CH2	1:A:349:MET:HB3	2.55	0.42
1:A:437:SER:HB2	1:A:465:LYS:NZ	2.34	0.41
1:A:352:GLY:HA3	1:A:442:SER:O	2.21	0.41
1:A:490:GLN:HB3	1:A:491:SER:H	1.73	0.41
1:A:384:ILE:O	1:A:384:ILE:CG2	2.68	0.41
1:A:356:ILE:HD13	1:A:444:ILE:HG12	2.02	0.41
1:A:403:PRO:HG3	1:A:502:ILE:HD11	2.03	0.41
1:A:221:LEU:C	1:A:221:LEU:HD23	2.40	0.41
1:A:357:LYS:O	1:A:357:LYS:HG2	2.21	0.41
1:A:484:VAL:HG23	1:A:485:ILE:HG12	2.03	0.40
1:A:408:ILE:HD12	1:A:408:ILE:C	2.41	0.40
1:A:402:ARG:HA	1:A:403:PRO:HD3	1.93	0.40
1:A:470:LEU:CB	1:A:476:VAL:HG23	2.52	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	A	425/428 (99%)	384 (90%)	38 (9%)	3 (1%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	A	359	GLY
1	A	328	GLY

### 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	381/382 (100%)	351 (92%)	30 (8%)	18 21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	221	LEU
1	A	233	HIS
1	A	258	ARG
1	A	260	ASP
1	A	261	GLU
1	A	270	VAL
1	A	291	TYR
1	A	307	SER
1	A	315	MET
1	A	324	LYS
1	A	325	SER
1	A	348	VAL
1	A	351	TYR
1	A	358	GLN
1	A	386	LYS
1	A	388	GLN
1	A	389	TYR
1	A	426	VAL
1	A	432	SER
1	A	437	SER
1	A	466	PHE
1	A	470	LEU
1	A	487	ARG
1	A	502	ILE

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Mol	Chain	Res	Type
1	A	519	TRP
1	A	538	THR
1	A	548	ARG
1	A	561	THR
1	A	601	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	233	HIS
1	A	287	ASN
1	A	333	HIS
1	A	334	GLN
1	A	434	GLN
1	A	492	GLN
1	A	497	ASN
1	A	530	GLN
1	A	550	GLN
1	A	586	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 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
4	NDG	A	1138	1,4	12,14,15	1.21	1 (8%)	15,19,21	2.52	6 (40%)
4	NAG	A	1139	4	12,14,15	1.14	1 (8%)	15,19,21	1.80	5 (33%)
4	BMA	A	1140	4	10,11,12	0.82	0	11,15,17	1.38	1 (9%)
4	BMA	A	1141	4	10,11,12	0.70	0	11,15,17	2.09	3 (27%)
4	MAN	A	1142	4	10,11,12	0.54	0	11,15,17	2.03	5 (45%)
3	NAG	A	1313	1,3	12,14,15	0.56	0	15,19,21	0.88	0
3	NAG	A	1314	3	12,14,15	0.55	0	15,19,21	1.14	1 (6%)
3	NAG	A	1361	1,3	12,14,15	0.60	0	15,19,21	1.36	2 (13%)
3	NAG	A	1362	3	12,14,15	0.68	1 (8%)	15,19,21	1.32	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	A	1138	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1139	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1140	4	-	0/2/19/22	0/1/1/1
4	BMA	A	1141	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1142	4	-	0/2/19/22	0/1/1/1
3	NAG	A	1313	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1314	3	-	1/6/23/26	0/1/1/1
3	NAG	A	1361	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1362	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1138	NDG	C7-N2	2.79	1.45	1.34
4	A	1139	NAG	C7-N2	2.77	1.45	1.34
3	A	1362	NAG	O5-C5	-2.04	1.41	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1138	NDG	O-C5-C4	6.71	119.16	110.65
4	A	1141	BMA	O5-C5-C4	5.32	117.40	110.65
3	A	1362	NAG	C2-N2-C7	-4.02	116.34	123.09
4	A	1138	NDG	C2-N2-C7	-3.98	116.40	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1139	NAG	O5-C5-C4	3.78	115.45	110.65
4	A	1142	MAN	O5-C5-C4	3.67	115.31	110.65
3	A	1314	NAG	O5-C5-C6	3.58	110.74	106.98
4	A	1140	BMA	O5-C5-C4	3.22	114.74	110.65
4	A	1139	NAG	C3-C2-N2	-2.87	107.39	111.76
4	A	1138	NDG	O-C5-C6	2.76	109.88	106.98
4	A	1142	MAN	O3-C3-C2	-2.70	104.99	109.94
3	A	1361	NAG	O4-C4-C3	-2.69	104.31	110.35
3	A	1362	NAG	O5-C5-C6	2.65	109.76	106.98
4	A	1141	BMA	O5-C5-C6	2.57	109.68	106.98
3	A	1361	NAG	C2-N2-C7	-2.49	118.91	123.09
4	A	1139	NAG	O4-C4-C3	-2.47	104.81	110.35
4	A	1142	MAN	O5-C5-C6	2.45	109.55	106.98
4	A	1142	MAN	O3-C3-C4	-2.44	104.87	110.35
4	A	1141	BMA	C6-C5-C4	-2.42	107.14	113.00
4	A	1138	NDG	C6-C5-C4	-2.40	107.21	113.00
4	A	1139	NAG	C2-N2-C7	-2.36	119.13	123.09
4	A	1139	NAG	C6-C5-C4	-2.29	107.47	113.00
4	A	1142	MAN	C6-C5-C4	-2.12	107.88	113.00
4	A	1138	NDG	C3-C2-N2	-2.07	108.60	111.76
4	A	1138	NDG	C8-C7-N2	2.04	120.09	116.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1314	NAG	O7-C7-N2-C2

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 19 are monoatomic - leaving 1 for Mogul analysis.

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	1210	1	12,14,15	0.54	0	15,19,21	1.30	2 (13%)

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	1210	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1210	NAG	O5-C5-C4	3.25	114.78	110.65
2	A	1210	NAG	C3-C4-C5	2.38	114.45	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1210	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	427/428 (99%)	0.67	54 (12%) 4 7	28, 40, 59, 72	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	TYR	5.7
1	A	338	ARG	5.3
1	A	259	GLY	4.7
1	A	603	ALA	4.3
1	A	442	SER	4.1
1	A	387	CYS	4.0
1	A	441	PRO	4.0
1	A	388	GLN	4.0
1	A	422	GLU	4.0
1	A	326	ASN	3.8
1	A	508	TYR	3.8
1	A	359	GLY	3.7
1	A	365	PRO	3.6
1	A	562	ILE	3.6
1	A	395	CYS	3.4
1	A	601	CYS	3.3
1	A	454	TYR	3.2
1	A	421	GLY	3.2
1	A	423	ASN	3.0
1	A	386	LYS	3.0
1	A	586	ASN	2.9
1	A	456	ALA	2.8
1	A	502	ILE	2.8
1	A	221	LEU	2.8
1	A	360	ASP	2.7
1	A	222	LEU	2.7
1	A	223	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	283	SER	2.6
1	A	354	SER	2.6
1	A	242	ARG	2.6
1	A	383	PRO	2.5
1	A	470	LEU	2.5
1	A	352	GLY	2.5
1	A	491	SER	2.5
1	A	561	THR	2.5
1	A	524	VAL	2.4
1	A	366	ALA	2.4
1	A	328	GLY	2.4
1	A	325	SER	2.4
1	A	577	LEU	2.3
1	A	380	SER	2.3
1	A	531	THR	2.3
1	A	443	LYS	2.2
1	A	260	ASP	2.2
1	A	453	PHE	2.2
1	A	492	GLN	2.1
1	A	425	LYS	2.1
1	A	499	CYS	2.1
1	A	351	TYR	2.1
1	A	378	ASN	2.1
1	A	293	VAL	2.1
1	A	419	SER	2.1
1	A	294	LEU	2.0
1	A	353	PRO	2.0

## 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1361	14/15	0.23	7.02	54,56,59,59	0
3	NAG	A	1314	14/15	0.53	5.45	51,63,65,65	0
4	MAN	A	1142	11/12	0.19	2.43	49,51,53,56	0
3	NAG	A	1313	14/15	0.20	2.00	49,56,60,60	0
4	BMA	A	1141	11/12	0.17	1.52	44,48,50,52	0
4	NDG	A	1138	14/15	0.12	0.55	38,39,41,42	0
4	NAG	A	1139	14/15	0.15	0.50	40,42,45,47	0
4	BMA	A	1140	11/12	0.08	-21.89	47,50,52,52	0
3	NAG	A	1362	14/15	0.29	-	58,59,61,61	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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1210	14/15	0.54	178.33	74,76,78,80	0
5	IOD	A	14	1/1	0.56	6.57	95,95,95,95	0
5	IOD	A	18	1/1	0.20	4.38	105,105,105,105	0
5	IOD	A	16	1/1	0.24	2.57	105,105,105,105	0
5	IOD	A	17	1/1	0.21	2.49	91,91,91,91	0
5	IOD	A	12	1/1	0.17	1.11	80,80,80,80	0
5	IOD	A	13	1/1	0.17	-0.45	92,92,92,92	0
5	IOD	A	11	1/1	0.18	-0.47	85,85,85,85	0
5	IOD	A	7	1/1	0.07	-2.14	78,78,78,78	0
5	IOD	A	19	1/1	0.16	-2.16	96,96,96,96	0
5	IOD	A	3	1/1	0.05	-2.18	47,47,47,47	0
5	IOD	A	10	1/1	0.07	-2.20	81,81,81,81	0
5	IOD	A	2	1/1	0.07	-2.71	43,43,43,43	0
5	IOD	A	5	1/1	0.04	-2.79	57,57,57,57	0
5	IOD	A	1	1/1	0.07	-2.92	44,44,44,44	0
5	IOD	A	9	1/1	0.16	-3.16	79,79,79,79	0
5	IOD	A	15	1/1	0.11	-3.17	82,82,82,82	0
5	IOD	A	8	1/1	0.06	-5.32	74,74,74,74	0
5	IOD	A	6	1/1	0.02	-6.20	61,61,61,61	0
5	IOD	A	4	1/1	0.01	-7.47	47,47,47,47	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.