



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2025 – 10:04 AM EDT

PDB ID : 9C0X / pdb\_00009c0x  
Title : Crystal structure of chimeric hemagglutinin cH11/1 in complex with broad protective antibody 31.b.09  
Authors : Nguyen, T.K.Y.; Zhu, X.; Wilson, I.A.  
Deposited on : 2024-05-28  
Resolution : 4.35 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

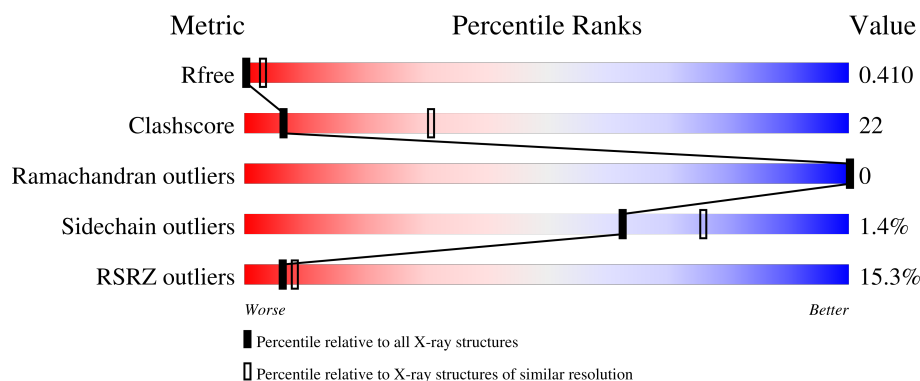
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.35 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))
$R_{free}$	164625	1019 (4.80-3.88)
Clashscore	180529	1038 (4.76-3.90)
Ramachandran outliers	177936	1011 (4.80-3.86)
Sidechain outliers	177891	1014 (4.84-3.84)
RSRZ outliers	164620	1016 (4.80-3.88)

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	B	166	<div> <div>13%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	L	114	<div> <div>11%</div> <div>48%</div> <div>49%</div> <div>.</div> </div>
3	H	121	<div> <div>13%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>
4	A	322	<div> <div>19%</div> <div>64%</div> <div>33%</div> <div>..</div> </div>
5	C	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5699 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 Hemagglutinin HA2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	166	Total	C	N	O	S	0	0	0
			1346	839	229	272	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6J3XB93

- Molecule 2 is a protein called Antibody 31.b.09 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	114	Total	C	N	O	S	0	0	0
			889	561	153	171	4			

- Molecule 3 is a protein called Antibody 31.b.09 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	121	Total	C	N	O	S	0	0	0
			937	589	161	182	5			

- Molecule 4 is a protein called Hemagglutinin HA1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	320	Total	C	N	O	S	0	0	0
			2485	1573	429	471	12			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).

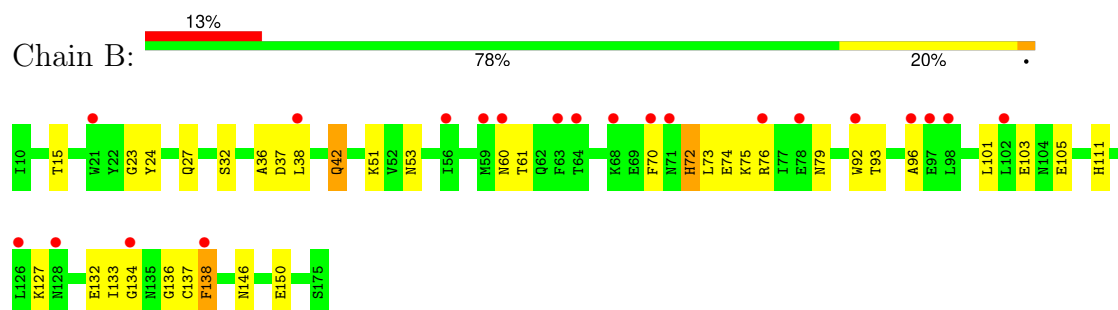


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

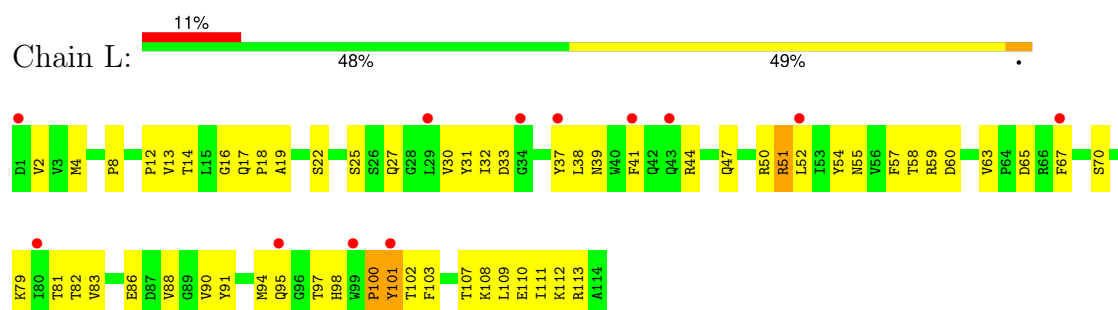
### 3 Residue-property plots [i](#)

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.

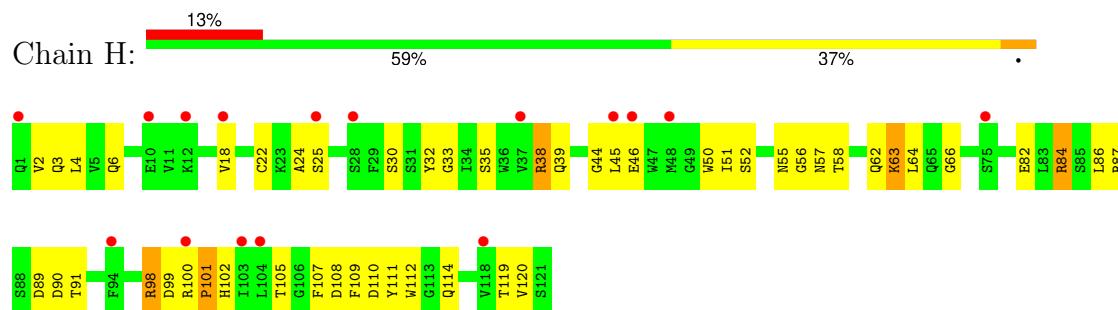
- Molecule 1: Hemagglutinin HA2 subunit



- Molecule 2: Antibody 31.b.09 Fab light chain

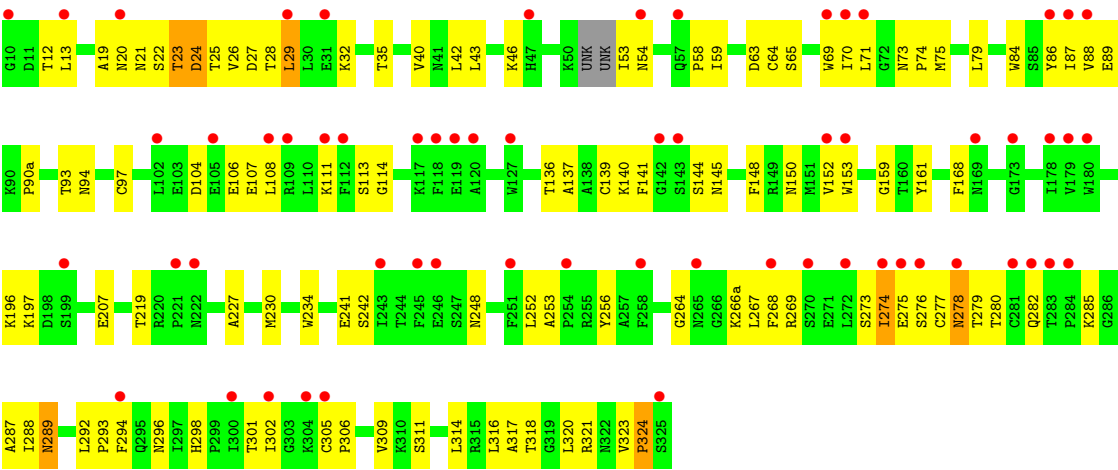


- Molecule 3: Antibody 31.b.09 Fab heavy chain



- Molecule 4: Hemagglutinin HA1 subunit





● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.04Å 169.04Å 169.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 4.35 48.80 – 4.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.80-4.35) 99.9 (48.80-4.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.335 , 0.382 0.350 , 0.410	Depositor DCC
$R_{free}$ test set	496 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	145.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 240.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.126 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	5699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: 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	B	0.47	0/1372	0.81	5/1849 (0.3%)
2	L	0.42	0/911	0.81	3/1239 (0.2%)
3	H	0.52	1/959 (0.1%)	1.09	4/1301 (0.3%)
4	A	0.46	1/2545 (0.0%)	0.74	5/3452 (0.1%)
All	All	0.47	2/5787 (0.0%)	0.83	17/7841 (0.2%)

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
2	L	0	2
3	H	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	324	PRO	N-CD	-7.67	1.37	1.47
3	H	101	PRO	N-CD	-5.94	1.39	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	64	LEU	N-CA-C	-22.34	86.60	114.75
3	H	63	LYS	CB-CA-C	-12.71	85.12	110.42
2	L	100	PRO	N-CA-C	-10.46	90.93	112.47
1	B	138	PHE	N-CA-C	-10.00	91.65	108.75
4	A	23	THR	O-C-N	9.09	132.93	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	GLN	CA-CB-CG	-8.33	97.44	114.10
1	B	74	GLU	N-CA-C	-7.91	102.60	111.14
4	A	23	THR	CA-C-N	-7.68	109.58	121.56
4	A	23	THR	C-N-CA	-7.68	109.58	121.56
2	L	101	TYR	N-CA-C	-7.42	97.78	109.50
3	H	64	LEU	N-CA-CB	6.23	120.24	111.15
1	B	127	LYS	CB-CA-C	-5.62	109.58	117.23
2	L	101	TYR	N-CA-CB	5.55	121.47	111.37
3	H	57	ASN	N-CA-CB	5.49	119.88	110.77
4	A	24	ASP	CB-CA-C	5.43	117.25	109.71
1	B	72	HIS	CA-C-O	-5.39	115.85	119.68
4	A	324	PRO	CA-N-CD	5.02	119.02	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	38	ARG	Sidechain
3	H	84	ARG	Sidechain
3	H	98	ARG	Sidechain
2	L	50	ARG	Sidechain
2	L	51	ARG	Sidechain

## 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	B	1346	0	1264	30	0
2	L	889	0	862	65	0
3	H	937	0	899	57	0
4	A	2485	0	2435	104	0
5	C	28	0	25	1	0
6	A	14	0	13	5	0
All	All	5699	0	5498	241	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 22.

All (241) 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:H:50:TRP:NE1	3:H:99:ASP:HB3	1.58	1.18
3:H:50:TRP:HE1	3:H:99:ASP:CB	1.68	1.04
4:A:75:MET:HB2	4:A:94:ASN:HD21	1.26	1.00
3:H:50:TRP:HE1	3:H:99:ASP:HB3	0.79	0.94
3:H:35:SER:HB2	3:H:50:TRP:HD1	1.33	0.93
2:L:54:TYR:HB2	2:L:58:THR:HB	1.50	0.91
2:L:95:GLN:HG2	2:L:101:TYR:CD1	2.08	0.88
2:L:88:VAL:HA	2:L:109:LEU:HD23	1.56	0.86
3:H:50:TRP:NE1	3:H:99:ASP:CB	2.33	0.85
4:A:289:ASN:HD21	6:A:401:NAG:H4	1.42	0.85
3:H:35:SER:HB2	3:H:50:TRP:CD1	2.13	0.82
4:A:23:THR:O	4:A:24:ASP:C	2.21	0.82
4:A:289:ASN:OD1	6:A:401:NAG:O6	1.97	0.82
4:A:23:THR:HA	4:A:35:THR:HG23	1.61	0.81
4:A:75:MET:HB2	4:A:94:ASN:ND2	1.95	0.80
4:A:289:ASN:ND2	6:A:401:NAG:H4	1.96	0.80
1:B:51:LYS:HE3	1:B:103:GLU:HB3	1.64	0.79
3:H:38:ARG:HD3	3:H:45:LEU:HD22	1.64	0.78
4:A:87:ILE:HB	4:A:267:LEU:CD2	2.12	0.78
4:A:59:ILE:HD11	4:A:87:ILE:HG12	1.66	0.78
2:L:32:ILE:HG23	4:A:318:THR:HB	1.65	0.77
4:A:87:ILE:HB	4:A:267:LEU:HD22	1.65	0.77
3:H:100:ARG:HE	3:H:105:THR:HG21	1.50	0.76
4:A:73:ASN:ND2	4:A:97:CYS:SG	2.57	0.75
3:H:87:ARG:HG3	3:H:89:ASP:H	1.50	0.75
4:A:276:SER:O	4:A:277:CYS:SG	2.45	0.74
4:A:54:ASN:HB3	4:A:277:CYS:HB3	1.70	0.73
4:A:46:LYS:HB2	4:A:288:ILE:HG21	1.71	0.73
2:L:16:GLY:HA2	2:L:82:THR:HA	1.70	0.73
2:L:52:LEU:HD13	2:L:67:PHE:CD2	2.24	0.72
3:H:107:PHE:O	3:H:108:ASP:OD1	2.07	0.72
2:L:12:PRO:HA	2:L:110:GLU:HB2	1.70	0.72
4:A:26:VAL:HG21	4:A:317:ALA:HB2	1.72	0.72
4:A:74:PRO:HB3	4:A:141:PHE:HB2	1.71	0.72
2:L:88:VAL:CA	2:L:109:LEU:HD23	2.19	0.71
1:B:23:GLY:HA3	1:B:36:ALA:HA	1.74	0.69
1:B:132:GLU:HG2	1:B:138:PHE:HE1	1.59	0.68
2:L:14:THR:HA	2:L:112:LYS:HA	1.75	0.67
2:L:54:TYR:N	2:L:58:THR:O	2.24	0.67
4:A:75:MET:CB	4:A:94:ASN:HD21	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:TRP:CH2	3:H:52:SER:HB2	2.31	0.66
4:A:278:ASN:HB2	4:A:282:GLN:HB2	1.77	0.66
4:A:152:VAL:HG13	4:A:253:ALA:HB3	1.78	0.66
1:B:136:GLY:O	1:B:137:CYS:SG	2.54	0.65
2:L:103:PHE:HD2	3:H:46:GLU:HA	1.61	0.65
4:A:53:ILE:HG22	4:A:54:ASN:N	2.12	0.65
3:H:38:ARG:HD3	3:H:45:LEU:CD2	2.26	0.65
4:A:43:LEU:HB2	4:A:314:LEU:HB2	1.78	0.65
4:A:219:THR:HG23	4:A:227:ALA:HB1	1.79	0.65
4:A:276:SER:OG	4:A:277:CYS:N	2.28	0.65
1:B:72:HIS:ND1	1:B:79:ASN:HB3	2.12	0.64
4:A:86:TYR:CE1	4:A:302:ILE:HG21	2.33	0.64
3:H:50:TRP:CD1	3:H:99:ASP:OD2	2.51	0.64
3:H:6:GLN:HB2	3:H:114:GLN:HG2	1.80	0.64
3:H:91:THR:HG23	3:H:119:THR:HA	1.79	0.64
3:H:35:SER:CB	3:H:50:TRP:HD1	2.10	0.63
2:L:39:ASN:H	2:L:94:MET:HB3	1.64	0.63
4:A:266(a):LYS:O	4:A:267:LEU:HD23	2.00	0.62
3:H:33:GLY:HA3	3:H:50:TRP:CZ2	2.35	0.61
3:H:18:VAL:O	3:H:82:GLU:HA	2.00	0.61
3:H:30:SER:HB2	3:H:32:TYR:CE2	2.35	0.61
1:B:38:LEU:O	1:B:42:GLN:HB2	2.00	0.60
4:A:309:VAL:HG12	4:A:311:SER:H	1.66	0.60
1:B:23:GLY:HA2	1:B:37:ASP:H	1.66	0.60
2:L:52:LEU:HD13	2:L:67:PHE:HD2	1.67	0.60
4:A:86:TYR:HE1	4:A:302:ILE:HG21	1.65	0.59
2:L:95:GLN:HA	2:L:101:TYR:HB2	1.83	0.59
2:L:94:MET:HG3	2:L:95:GLN:H	1.68	0.59
1:B:111:HIS:CB	4:A:320:LEU:HD13	2.34	0.58
2:L:95:GLN:HG2	2:L:101:TYR:CE1	2.38	0.58
4:A:64:CYS:HA	4:A:94:ASN:HB2	1.86	0.57
2:L:103:PHE:CD2	3:H:46:GLU:HA	2.39	0.57
4:A:136:THR:HG23	4:A:153:TRP:HZ3	1.69	0.57
4:A:152:VAL:CG1	4:A:253:ALA:HB3	2.35	0.56
4:A:87:ILE:HB	4:A:267:LEU:HD21	1.85	0.56
1:B:72:HIS:CE1	1:B:79:ASN:HB3	2.39	0.56
3:H:30:SER:HB2	3:H:32:TYR:CZ	2.40	0.56
1:B:73:LEU:O	1:B:73:LEU:HG	2.06	0.56
2:L:4:MET:HG2	2:L:102:THR:OG1	2.06	0.56
4:A:106:GLU:CD	4:A:106:GLU:H	2.13	0.56
4:A:97:CYS:HB2	4:A:139:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:86:LEU:HD13	3:H:120:VAL:HG22	1.88	0.56
4:A:53:ILE:CG2	4:A:54:ASN:N	2.69	0.56
2:L:39:ASN:H	2:L:94:MET:CB	2.18	0.55
4:A:59:ILE:CD1	4:A:87:ILE:HG12	2.35	0.55
4:A:74:PRO:HG2	4:A:139:CYS:O	2.06	0.55
1:B:24:TYR:HB3	4:A:13:LEU:HD11	1.87	0.55
1:B:111:HIS:HB2	4:A:320:LEU:HD13	1.89	0.55
4:A:90(a):PRO:HA	4:A:269:ARG:HB3	1.89	0.54
2:L:90:VAL:HG22	2:L:108:LYS:HG2	1.89	0.54
3:H:45:LEU:HG	3:H:46:GLU:H	1.73	0.54
2:L:88:VAL:HG21	2:L:111:ILE:HD13	1.90	0.54
1:B:51:LYS:CE	1:B:103:GLU:HB3	2.34	0.54
4:A:23:THR:HA	4:A:35:THR:CG2	2.35	0.54
2:L:13:VAL:HB	2:L:109:LEU:HD11	1.90	0.54
2:L:2:VAL:O	2:L:102:THR:HG21	2.08	0.53
2:L:39:ASN:HB2	2:L:94:MET:HG2	1.90	0.53
2:L:51:ARG:HD3	2:L:54:TYR:OH	2.08	0.53
2:L:98:HIS:O	2:L:100:PRO:O	2.26	0.53
2:L:94:MET:HG3	2:L:95:GLN:N	2.23	0.53
3:H:87:ARG:HB3	3:H:90:ASP:CG	2.34	0.53
2:L:41:PHE:CB	2:L:51:ARG:HA	2.39	0.52
4:A:114:GLY:HA2	4:A:264:GLY:O	2.09	0.52
2:L:44:ARG:NH1	2:L:86:GLU:O	2.40	0.52
3:H:2:VAL:HG22	3:H:111:TYR:CZ	2.45	0.52
3:H:32:TYR:HA	3:H:101:PRO:HG3	1.92	0.52
1:B:101:LEU:HB3	4:A:29:LEU:CA	2.40	0.52
3:H:6:GLN:HG2	3:H:22:CYS:SG	2.50	0.52
4:A:266(a):LYS:C	4:A:267:LEU:HD23	2.35	0.51
1:B:27:GLN:HG3	1:B:32:SER:HB3	1.93	0.51
4:A:58:PRO:HB2	4:A:86:TYR:O	2.10	0.51
4:A:42:LEU:HD22	4:A:293:PRO:HG2	1.91	0.51
4:A:301:THR:HB	4:A:305:CYS:SG	2.50	0.51
3:H:38:ARG:HH11	3:H:45:LEU:HD22	1.75	0.51
4:A:43:LEU:HD11	4:A:296:ASN:HB3	1.93	0.51
4:A:64:CYS:HB2	4:A:79:LEU:HD11	1.91	0.51
4:A:106:GLU:CD	4:A:106:GLU:N	2.69	0.51
4:A:136:THR:CG2	4:A:153:TRP:HZ3	2.24	0.51
2:L:91:TYR:HB2	2:L:107:THR:OG1	2.11	0.51
1:B:132:GLU:HG2	1:B:138:PHE:CE1	2.44	0.51
4:A:89:GLU:O	4:A:269:ARG:HA	2.11	0.50
2:L:88:VAL:HA	2:L:109:LEU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:ASN:H	2:L:94:MET:HG2	1.76	0.50
4:A:107:GLU:OE1	4:A:107:GLU:N	2.42	0.50
4:A:137:ALA:O	4:A:140:LYS:NZ	2.41	0.50
2:L:94:MET:CG	2:L:95:GLN:H	2.25	0.50
4:A:289:ASN:CG	6:A:401:NAG:HO6	2.07	0.50
3:H:3:GLN:OE1	3:H:25:SER:HB3	2.12	0.50
4:A:59:ILE:CG1	4:A:87:ILE:HG12	2.41	0.50
3:H:52:SER:HB3	3:H:55:ASN:O	2.12	0.50
1:B:101:LEU:HB3	4:A:29:LEU:HA	1.93	0.50
2:L:14:THR:HB	2:L:17:GLN:HG3	1.93	0.50
3:H:50:TRP:NE1	3:H:99:ASP:CG	2.69	0.50
1:B:51:LYS:NZ	1:B:103:GLU:OE1	2.44	0.49
1:B:53:ASN:OD1	2:L:30:VAL:HG22	2.12	0.49
4:A:84:TRP:CE2	4:A:87:ILE:HD11	2.47	0.49
4:A:289:ASN:CG	6:A:401:NAG:H4	2.37	0.49
4:A:276:SER:C	4:A:277:CYS:SG	2.95	0.49
2:L:37:TYR:HB3	3:H:107:PHE:HZ	1.78	0.49
2:L:31:TYR:HB3	2:L:33:ASP:OD1	2.13	0.49
3:H:62:GLN:HG2	3:H:63:LYS:HG3	1.95	0.49
2:L:44:ARG:HB2	2:L:47:GLN:HB2	1.94	0.49
4:A:104:ASP:C	4:A:234:TRP:HE1	2.21	0.49
4:A:159:GLY:HA2	4:A:196:LYS:HE3	1.93	0.49
2:L:39:ASN:H	2:L:94:MET:CG	2.26	0.49
2:L:60:ASP:HB3	2:L:63:VAL:HG23	1.94	0.49
2:L:95:GLN:HG2	2:L:101:TYR:CG	2.45	0.49
2:L:83:VAL:CG1	2:L:109:LEU:HD21	2.43	0.48
4:A:285:LYS:HE3	4:A:298:HIS:HD2	1.78	0.48
2:L:51:ARG:NE	3:H:109:PHE:O	2.47	0.48
4:A:140:LYS:CB	4:A:145:ASN:HA	2.43	0.48
2:L:54:TYR:CB	2:L:58:THR:HB	2.33	0.48
4:A:294:PHE:HA	4:A:306:PRO:HB3	1.94	0.48
2:L:52:LEU:CD2	2:L:63:VAL:HG22	2.43	0.48
2:L:83:VAL:HG11	2:L:109:LEU:HD21	1.95	0.48
3:H:2:VAL:HG22	3:H:111:TYR:CE1	2.48	0.48
3:H:50:TRP:CH2	3:H:101:PRO:HA	2.49	0.48
1:B:92:TRP:O	1:B:93:THR:C	2.54	0.48
4:A:84:TRP:CD1	4:A:87:ILE:HG13	2.48	0.48
3:H:3:GLN:O	3:H:24:ALA:HA	2.14	0.48
2:L:37:TYR:HB2	2:L:97:THR:HG23	1.96	0.47
4:A:108:LEU:HB2	4:A:234:TRP:CE2	2.49	0.47
4:A:230:MET:SD	4:A:252:LEU:HD11	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:TYR:CE2	1:B:37:ASP:HB2	2.49	0.47
3:H:87:ARG:HG3	3:H:89:ASP:N	2.26	0.47
3:H:98:ARG:HG2	3:H:99:ASP:N	2.30	0.47
4:A:320:LEU:HD12	4:A:321:ARG:H	1.79	0.47
4:A:53:ILE:CG2	4:A:54:ASN:H	2.28	0.47
3:H:66:GLY:O	3:H:84:ARG:NH2	2.49	0.46
4:A:108:LEU:HD22	4:A:234:TRP:CG	2.51	0.46
2:L:52:LEU:HD22	2:L:63:VAL:HG22	1.97	0.46
4:A:71:LEU:O	4:A:148:PHE:HB3	2.15	0.46
4:A:168:PHE:O	4:A:242:SER:HA	2.15	0.46
1:B:101:LEU:HB3	4:A:29:LEU:N	2.31	0.46
3:H:50:TRP:CZ3	3:H:52:SER:HB2	2.50	0.46
4:A:70:ILE:O	4:A:150:ASN:ND2	2.47	0.46
4:A:20:ASN:HB3	4:A:21:ASN:H	1.51	0.46
2:L:38:LEU:O	2:L:38:LEU:HD12	2.15	0.46
2:L:52:LEU:HA	2:L:63:VAL:HG21	1.97	0.46
2:L:88:VAL:N	2:L:109:LEU:HD23	2.31	0.46
4:A:40:VAL:CG2	4:A:316:LEU:HB3	2.46	0.46
2:L:41:PHE:HA	2:L:51:ARG:HA	1.98	0.45
3:H:51:ILE:HB	3:H:58:THR:HG22	1.98	0.45
3:H:109:PHE:N	3:H:109:PHE:CD1	2.83	0.45
4:A:113:SER:HB3	4:A:266(a):LYS:HG2	1.98	0.45
2:L:59:ARG:NH2	2:L:65:ASP:O	2.49	0.45
4:A:111:LYS:HA	4:A:111:LYS:HD3	1.75	0.45
3:H:33:GLY:HA3	3:H:50:TRP:HZ2	1.80	0.45
3:H:86:LEU:HD22	3:H:120:VAL:HG21	2.00	0.44
4:A:58:PRO:HG2	4:A:274:ILE:HG22	2.00	0.44
1:B:60:ASN:OD1	1:B:61:THR:N	2.51	0.44
4:A:65:SER:O	4:A:69:TRP:N	2.47	0.44
4:A:207:GLU:CB	4:A:241:GLU:HG2	2.47	0.44
2:L:25:SER:OG	2:L:27:GLN:O	2.30	0.44
4:A:23:THR:O	4:A:25:THR:HG23	2.17	0.44
4:A:140:LYS:HA	4:A:145:ASN:HA	2.00	0.44
4:A:140:LYS:HB2	4:A:145:ASN:HA	2.00	0.43
3:H:110:ASP:C	3:H:111:TYR:HD1	2.26	0.43
2:L:18:PRO:HG3	2:L:81:THR:HA	2.00	0.43
2:L:39:ASN:OD1	2:L:55:ASN:N	2.51	0.43
4:A:150:ASN:HA	4:A:256:TYR:HD2	1.84	0.43
3:H:102:HIS:H	3:H:102:HIS:CD2	2.36	0.43
1:B:105:GLU:HB2	4:A:28:THR:HB	2.00	0.43
3:H:4:LEU:HB2	3:H:112:TRP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASN:O	1:B:150:GLU:HG2	2.19	0.43
3:H:55:ASN:O	3:H:56:GLY:C	2.62	0.43
4:A:108:LEU:HD22	4:A:234:TRP:CD2	2.53	0.43
3:H:50:TRP:CD1	3:H:99:ASP:CB	3.00	0.43
4:A:268:PHE:CG	4:A:269:ARG:N	2.87	0.43
4:A:252:LEU:HD23	4:A:252:LEU:HA	1.89	0.42
3:H:110:ASP:O	3:H:111:TYR:HD1	2.02	0.42
4:A:292:LEU:O	4:A:293:PRO:C	2.63	0.42
4:A:197:LYS:HD2	4:A:248:ASN:O	2.19	0.42
4:A:71:LEU:HB3	4:A:148:PHE:CD1	2.54	0.42
4:A:323:VAL:HA	4:A:324:PRO:HD2	1.76	0.42
1:B:15:THR:HA	4:A:19:ALA:O	2.19	0.42
4:A:279:THR:H	4:A:287:ALA:HB1	1.84	0.42
1:B:27:GLN:HB3	4:A:12:THR:OG1	2.20	0.42
2:L:16:GLY:HA2	2:L:82:THR:CA	2.44	0.42
4:A:161:TYR:HE2	4:A:248:ASN:C	2.27	0.42
2:L:19:ALA:O	2:L:79:LYS:HA	2.20	0.41
3:H:50:TRP:HH2	3:H:101:PRO:HA	1.85	0.41
2:L:57:PHE:HE1	2:L:70:SER:HA	1.86	0.41
4:A:27:ASP:HB3	4:A:32:LYS:HD2	2.02	0.41
1:B:133:ILE:O	1:B:134:GLY:C	2.64	0.41
1:B:92:TRP:CD1	1:B:96:ALA:HB2	2.55	0.41
3:H:39:GLN:HA	3:H:44:GLY:HA2	2.01	0.41
2:L:14:THR:OG1	2:L:113:ARG:HG2	2.21	0.41
2:L:37:TYR:HB3	3:H:107:PHE:CZ	2.55	0.41
4:A:59:ILE:O	4:A:88:VAL:N	2.53	0.41
4:A:63:ASP:O	4:A:93:THR:N	2.54	0.41
2:L:41:PHE:HB3	2:L:51:ARG:HA	2.03	0.41
2:L:88:VAL:HG22	2:L:109:LEU:HG	2.02	0.41
4:A:278:ASN:H	4:A:278:ASN:HD22	1.69	0.41
5:C:1:NAG:H82	5:C:1:NAG:H2	1.87	0.41
3:H:6:GLN:O	3:H:114:GLN:NE2	2.54	0.40
3:H:50:TRP:NE1	3:H:99:ASP:OD2	2.54	0.40
4:A:140:LYS:HB2	4:A:144:SER:O	2.20	0.40
2:L:37:TYR:HB2	2:L:97:THR:CG2	2.51	0.40
1:B:75:LYS:HD3	1:B:76:ARG:N	2.36	0.40
2:L:8:PRO:HD3	2:L:22:SER:OG	2.22	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	B	164/166 (99%)	151 (92%)	13 (8%)	0	100	100
2	L	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
3	H	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
4	A	316/322 (98%)	286 (90%)	30 (10%)	0	100	100
All	All	711/723 (98%)	650 (91%)	61 (9%)	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	B	146/146 (100%)	145 (99%)	1 (1%)	81	87
2	L	99/99 (100%)	99 (100%)	0	100	100
3	H	100/100 (100%)	100 (100%)	0	100	100
4	A	276/276 (100%)	268 (97%)	8 (3%)	37	58
All	All	621/621 (100%)	612 (99%)	9 (1%)	62	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	PHE
4	A	22	SER

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Mol	Chain	Res	Type
4	A	29	LEU
4	A	273	SER
4	A	274	ILE
4	A	275	GLU
4	A	278	ASN
4	A	280	THR
4	A	289	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	81	ASN
3	H	102	HIS
4	A	38	HIS
4	A	73	ASN
4	A	94	ASN
4	A	278	ASN

### 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 ⓘ

2 monosaccharides 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	1	5	14,14,15	0.40	0	17,19,21	0.64	1 (5%)
5	NAG	C	2	5	14,14,15	0.38	0	17,19,21	0.90	1 (5%)

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	1	5	-	3/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	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(°)
5	C	2	NAG	O5-C1-C2	2.91	115.80	111.29
5	C	1	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

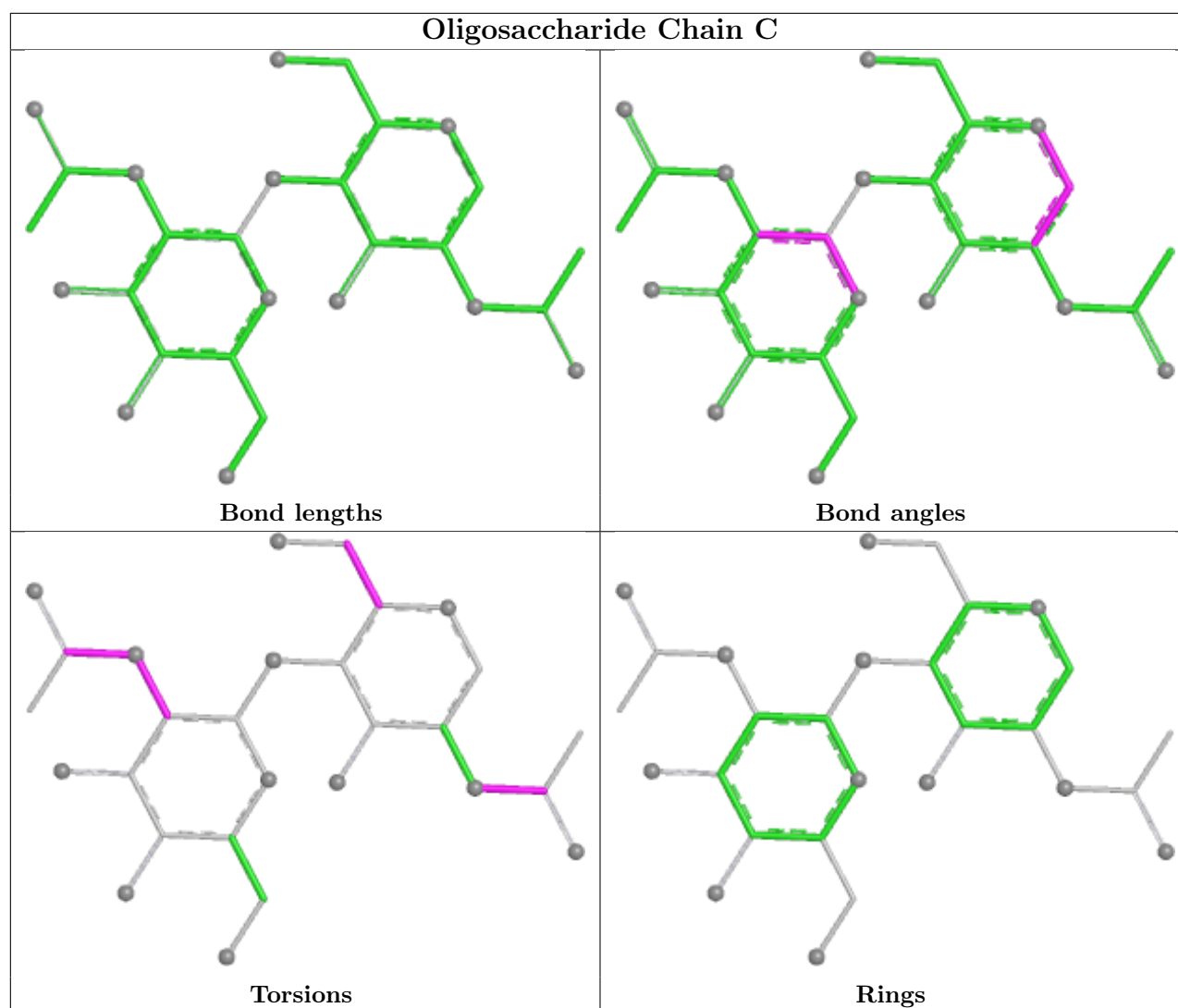
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
5	C	2	NAG	C1-C2-N2-C7
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
5	C	1	NAG	O5-C5-C6-O6
5	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 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	401	-	14,14,15	0.39	0	17,19,21	0.79	1 (5%)

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	401	-	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	NAG	C1-C2-N2	2.22	113.92	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

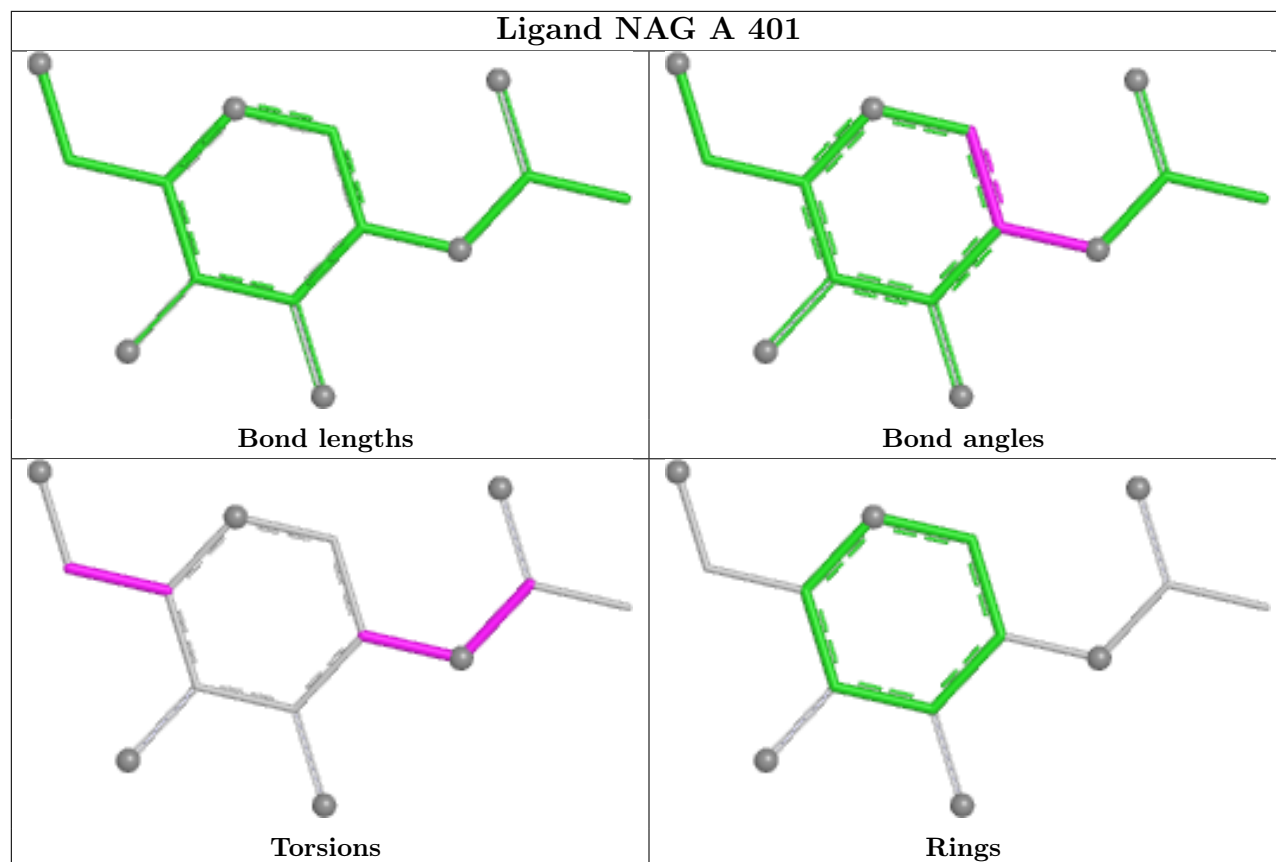
Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C1-C2-N2-C7
6	A	401	NAG	C8-C7-N2-C2
6	A	401	NAG	O7-C7-N2-C2
6	A	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	B	166/166 (100%)	0.83	21 (12%)	9 10	89, 142, 244, 309	0
2	L	114/114 (100%)	0.89	12 (10%)	13 13	138, 225, 278, 298	0
3	H	121/121 (100%)	0.98	16 (13%)	8 10	30, 184, 215, 230	0
4	A	320/322 (99%)	1.03	61 (19%)	4 6	30, 200, 254, 280	0
All	All	721/723 (99%)	0.95	110 (15%)	6 8	30, 190, 262, 309	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	ASN	9.9
4	A	268	PHE	6.6
2	L	99	TRP	6.5
4	A	305	CYS	6.4
4	A	251	PHE	6.2
4	A	112	PHE	6.1
4	A	274	ILE	6.1
3	H	37	VAL	5.8
4	A	245	PHE	5.8
4	A	278	ASN	5.6
1	B	78	GLU	4.8
1	B	70	PHE	4.6
1	B	63	PHE	4.5
4	A	304	LYS	4.5
4	A	69	TRP	4.4
3	H	94	PHE	4.4
2	L	41	PHE	4.3
3	H	118	VAL	4.3
4	A	108	LEU	4.2
4	A	265	ASN	4.2
4	A	281	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	4.2
2	L	67	PHE	4.2
3	H	48	MET	4.2
1	B	92	TRP	4.1
4	A	31	GLU	4.1
3	H	104	LEU	4.0
4	A	29	LEU	4.0
1	B	102	LEU	3.9
4	A	284	PRO	3.9
1	B	98	LEU	3.8
4	A	180	TRP	3.8
1	B	134	GLY	3.7
4	A	120	ALA	3.7
4	A	70	ILE	3.6
1	B	56	ILE	3.6
4	A	300	ILE	3.5
4	A	254	PRO	3.5
3	H	46	GLU	3.4
4	A	179	VAL	3.3
4	A	270	SER	3.3
4	A	20	ASN	3.3
4	A	102	LEU	3.3
1	B	126	LEU	3.2
4	A	127	TRP	3.2
4	A	152	VAL	3.1
4	A	153	TRP	3.0
1	B	38	LEU	3.0
1	B	64	THR	3.0
4	A	276	SER	3.0
3	H	103	ILE	3.0
4	A	178	ILE	2.9
2	L	1	ASP	2.9
4	A	54	ASN	2.9
3	H	1	GLN	2.9
3	H	18	VAL	2.9
1	B	76	ARG	2.8
1	B	21	TRP	2.8
4	A	143	SER	2.8
4	A	272	LEU	2.7
3	H	25	SER	2.7
4	A	111	LYS	2.7
2	L	80	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	H	12	LYS	2.7
3	H	10	GLU	2.6
4	A	57	GLN	2.6
4	A	258	PHE	2.6
3	H	75	SER	2.6
4	A	282	GLN	2.6
4	A	169	ASN	2.5
4	A	88	VAL	2.5
4	A	71	LEU	2.5
4	A	105	GLU	2.5
4	A	10	GLY	2.5
4	A	302	ILE	2.5
4	A	117	LYS	2.5
3	H	45	LEU	2.5
4	A	119	GLU	2.5
4	A	275	GLU	2.5
2	L	37	TYR	2.5
3	H	28	SER	2.4
4	A	325	SER	2.4
4	A	246	GLU	2.4
1	B	138	PHE	2.4
4	A	86	TYR	2.4
1	B	128	ASN	2.4
4	A	142	GLY	2.4
4	A	294	PHE	2.4
4	A	109	ARG	2.3
2	L	101	TYR	2.3
4	A	222	ASN	2.3
4	A	199	SER	2.3
2	L	52	LEU	2.3
2	L	34	GLY	2.2
4	A	118	PHE	2.2
4	A	47	HIS	2.2
4	A	243	ILE	2.2
2	L	43	GLN	2.2
4	A	87	ILE	2.2
1	B	68	LYS	2.2
4	A	221	PRO	2.2
2	L	29	LEU	2.2
1	B	97	GLU	2.2
3	H	100	ARG	2.1
1	B	60	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	283	THR	2.1
4	A	13	LEU	2.0
2	L	95	GLN	2.0
1	B	59	MET	2.0
4	A	173	GLY	2.0

## 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](#)

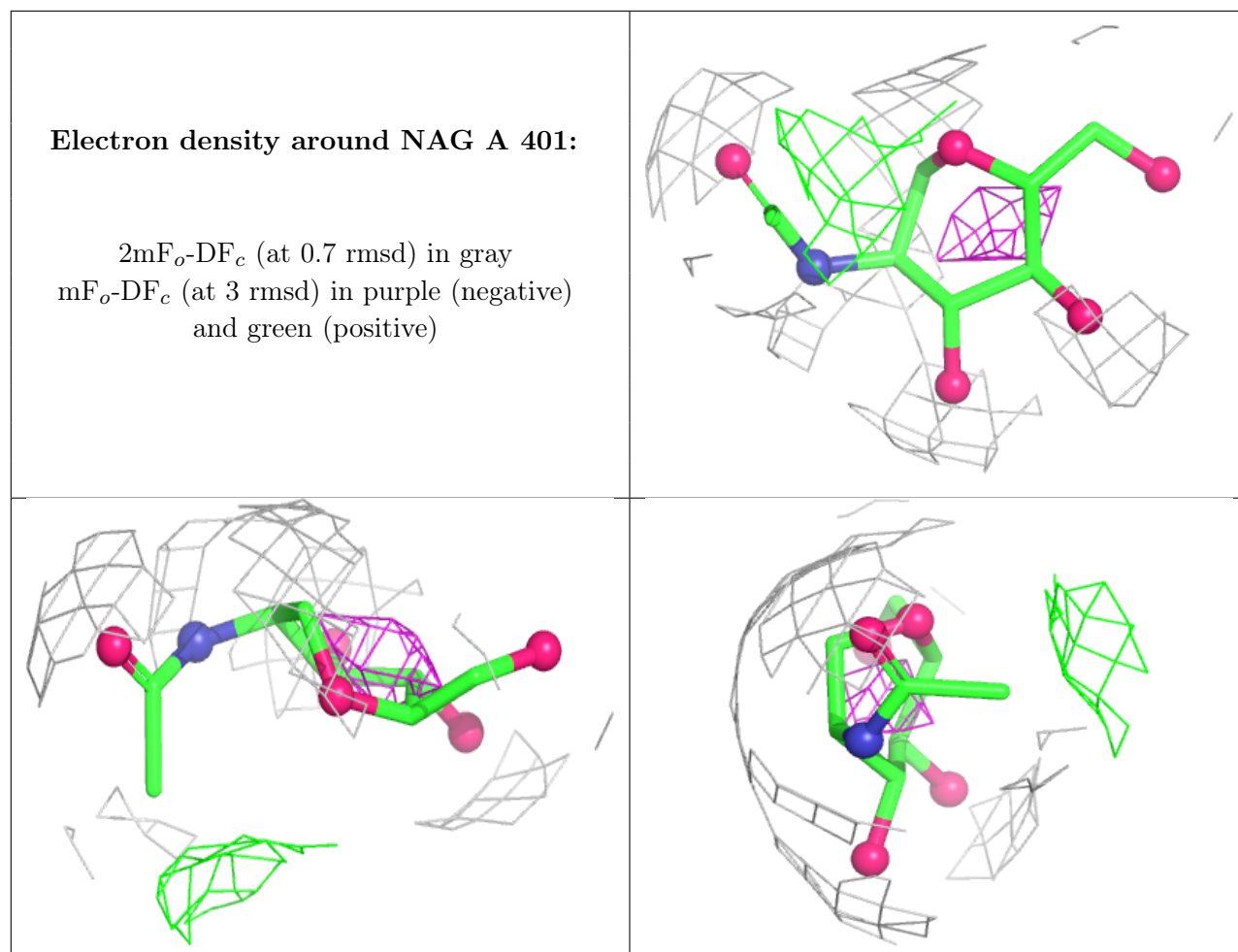
SUGAR-RSR INFOmissingINFO

## 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
6	NAG	A	401	14/15	0.86	0.12	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.