



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 05:54 PM JST

PDB ID : 6LSA  
Title : Complex structure of bovine herpesvirus 1 glycoprotein D and bovine nectin-1 IgV  
Authors : Yue, D.; Chen, Z.J.; Yang, F.L.; Ye, F.; Lin, S.; Cheng, Y.W.; Wang, J.C.; Chen, Z.M.; Lin, X.; Yang, J.; Chen, H.; Zhang, Z.L.; You, Y.; Sun, H.L.; Wen, A.; Wang, L.L.; Zheng, Y.; Cao, Y.; Li, Y.H.; Lu, G.W.  
Deposited on : 2020-01-17  
Resolution : 2.20 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

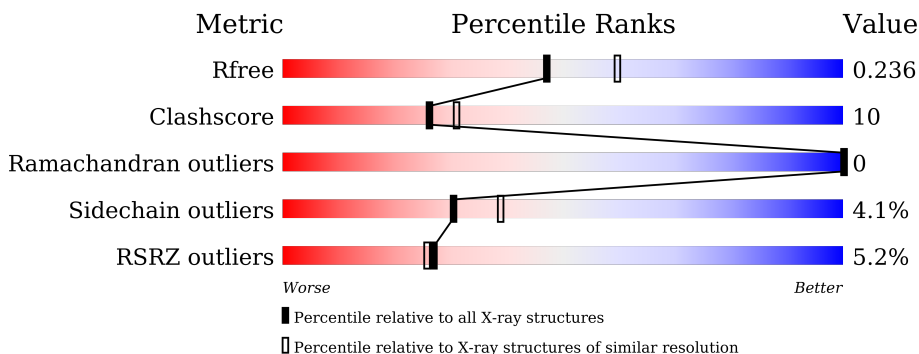
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	109	
1	B	109	
2	C	311	
2	F	311	
3	D	2	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5935 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 Nectin cell adhesion molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	109	849	540	144	160	5	0	0	0
1	B	109	849	540	144	160	5	0	0	0

- Molecule 2 is a protein called Envelope glycoprotein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	244	1991	1292	335	352	12	0	0	0
2	C	244	1991	1292	335	352	12	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	ALA	-	expression tag	UNP Q76PF1
F	-2	ASP	-	expression tag	UNP Q76PF1
F	-1	GLU	-	expression tag	UNP Q76PF1
F	0	PHE	-	expression tag	UNP Q76PF1
F	302	HIS	-	expression tag	UNP Q76PF1
F	303	HIS	-	expression tag	UNP Q76PF1
F	304	HIS	-	expression tag	UNP Q76PF1
F	305	HIS	-	expression tag	UNP Q76PF1
F	306	HIS	-	expression tag	UNP Q76PF1
F	307	HIS	-	expression tag	UNP Q76PF1
C	-3	ALA	-	expression tag	UNP Q76PF1
C	-2	ASP	-	expression tag	UNP Q76PF1
C	-1	GLU	-	expression tag	UNP Q76PF1
C	0	PHE	-	expression tag	UNP Q76PF1
C	302	HIS	-	expression tag	UNP Q76PF1
C	303	HIS	-	expression tag	UNP Q76PF1

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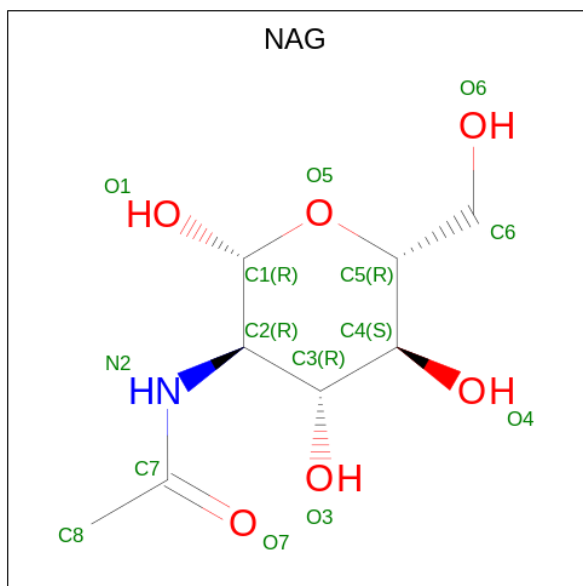
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP Q76PF1
C	305	HIS	-	expression tag	UNP Q76PF1
C	306	HIS	-	expression tag	UNP Q76PF1
C	307	HIS	-	expression tag	UNP Q76PF1

- Molecule 3 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
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	F	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0

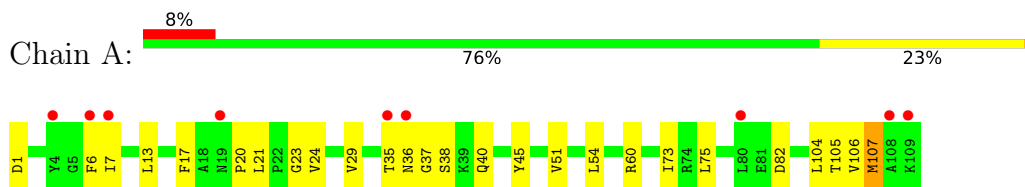
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	F	99	Total O 99 99	0	0
5	B	9	Total O 9 9	0	0
5	C	79	Total O 79 79	0	0

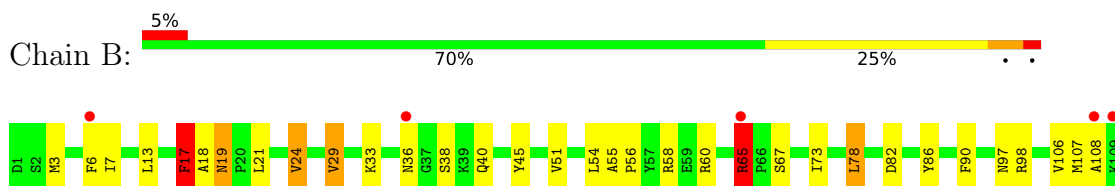
### 3 Residue-property plots [i](#)

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.

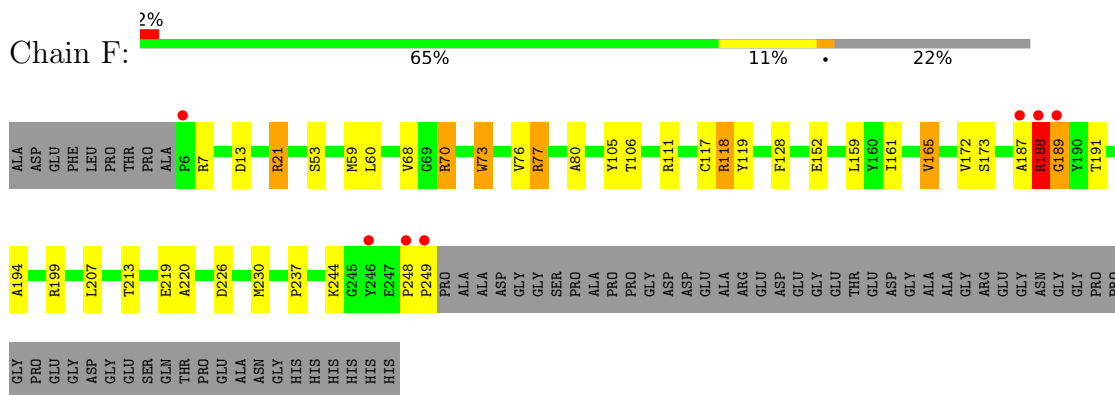
- Molecule 1: Nectin cell adhesion molecule 1



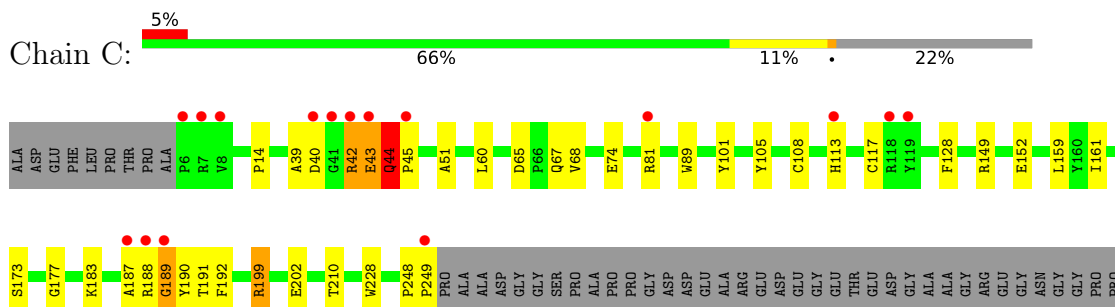
- Molecule 1: Nectin cell adhesion molecule 1



- Molecule 2: Envelope glycoprotein D



- Molecule 2: Envelope glycoprotein D



GLY  
PRO  
GLU  
GLY  
ASP  
GLY  
GLU  
SER  
GLN  
THR  
PRO  
GLU  
ALA  
ASN  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.87Å 64.23Å 102.93Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	45.20 – 2.20 45.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.20-2.20) 97.5 (45.20-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.16-3549	Depositor
R, $R_{free}$	0.200 , 0.236 0.200 , 0.236	Depositor DCC
$R_{free}$ test set	2905 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtrriage
Anisotropy	0.627	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: 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	A	0.46	0/867	0.81	1/1177 (0.1%)
1	B	0.53	1/867 (0.1%)	0.90	6/1177 (0.5%)
2	C	0.58	2/2065 (0.1%)	0.78	8/2820 (0.3%)
2	F	0.67	7/2065 (0.3%)	0.73	6/2820 (0.2%)
All	All	0.59	10/5864 (0.2%)	0.79	21/7994 (0.3%)

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	B	0	2
2	C	0	1
2	F	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	43	GLU	CG-CD	14.16	1.73	1.51
2	F	21	ARG	CZ-NH2	-9.78	1.20	1.33
2	F	21	ARG	NE-CZ	-8.75	1.21	1.33
2	F	21	ARG	CD-NE	-8.03	1.32	1.46
2	F	77	ARG	CZ-NH1	-7.75	1.23	1.33
2	C	43	GLU	CB-CG	7.34	1.66	1.52
2	F	77	ARG	CB-CG	-6.75	1.34	1.52
2	F	73	TRP	CE3-CZ3	-6.62	1.27	1.38
2	F	21	ARG	CZ-NH1	-5.69	1.25	1.33
1	B	56	PRO	N-CD	5.66	1.55	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	42	ARG	NE-CZ-NH1	16.80	128.70	120.30
1	A	107	MET	CG-SD-CE	-12.89	79.57	100.20
1	B	65	ARG	NE-CZ-NH2	-10.02	115.29	120.30
2	F	77	ARG	NE-CZ-NH1	-8.54	116.03	120.30
2	F	188	ARG	NE-CZ-NH2	8.12	124.36	120.30
2	F	77	ARG	CB-CG-CD	-7.55	91.98	111.60
1	B	65	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	C	42	ARG	CG-CD-NE	-7.14	96.81	111.80
2	F	189	GLY	N-CA-C	6.93	130.43	113.10
2	C	43	GLU	CG-CD-OE2	6.61	131.52	118.30
2	C	42	ARG	NH1-CZ-NH2	-6.47	112.28	119.40
2	C	43	GLU	OE1-CD-OE2	-6.19	115.88	123.30
2	C	189	GLY	N-CA-C	6.18	128.56	113.10
2	F	188	ARG	CA-C-N	6.14	128.48	116.20
1	B	78	LEU	CB-CG-CD1	-6.14	100.57	111.00
2	C	199	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	17	PHE	C-N-CA	-6.06	106.56	121.70
1	B	24	VAL	CG1-CB-CG2	-5.82	101.59	110.90
2	F	21	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	55	ALA	C-N-CD	-5.58	108.31	120.60
2	C	43	GLU	N-CA-C	5.17	124.97	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	VAL	Peptide
1	B	17	PHE	Mainchain
2	C	44	GLN	Peptide
2	F	188	ARG	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	849	0	841	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	849	0	841	23	0
2	C	1991	0	1885	38	3
2	F	1991	0	1886	36	1
3	D	28	0	25	1	0
4	C	14	0	13	0	0
4	F	14	0	13	0	0
5	A	12	0	0	1	0
5	B	9	0	0	1	0
5	C	79	0	0	3	0
5	F	99	0	0	4	0
All	All	5935	0	5504	117	3

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.

All (117) 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)
2:C:43:GLU:HA	2:C:44:GLN:OE1	1.24	1.37
2:C:43:GLU:CA	2:C:44:GLN:OE1	1.93	1.16
2:C:199:ARG:NH2	2:C:202:GLU:OE2	1.92	1.02
1:A:35:THR:HG23	1:A:36:ASN:H	1.38	0.88
2:C:191:THR:HG23	2:C:192:PHE:H	1.40	0.86
1:A:38:SER:HB3	2:F:194:ALA:HB2	1.58	0.85
2:C:43:GLU:HA	2:C:44:GLN:CD	1.97	0.85
2:F:53:SER:O	5:F:1101:HOH:O	1.97	0.81
1:B:36:ASN:OD1	1:B:38:SER:OG	1.98	0.81
2:C:188:ARG:HB2	2:C:189:GLY:HA3	1.61	0.81
2:F:213:THR:OG1	5:F:1102:HOH:O	1.99	0.78
2:C:42:ARG:HB3	2:C:43:GLU:HB2	1.66	0.77
2:C:74:GLU:OE2	5:C:1101:HOH:O	2.03	0.76
1:B:21:LEU:O	1:B:24:VAL:HG12	1.85	0.76
1:B:60:ARG:NH2	1:B:82:ASP:OD2	2.16	0.76
1:B:19:ASN:O	1:B:19:ASN:ND2	2.20	0.75
1:A:35:THR:HG23	1:A:36:ASN:N	2.02	0.72
2:F:73:TRP:CH2	2:F:77:ARG:NH1	2.57	0.72
1:A:36:ASN:N	1:A:37:GLY:HA2	2.05	0.72
1:B:97:ASN:OD1	5:B:201:HOH:O	2.08	0.71
1:B:65:ARG:NH2	1:B:67:SER:OG	2.23	0.71
2:F:188:ARG:NH2	2:F:189:GLY:HA3	2.05	0.71
1:A:6:PHE:CD1	1:A:107:MET:HB3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:HD1	1:A:51:VAL:HG22	1.55	0.70
2:F:128:PHE:CB	2:F:191:THR:O	2.41	0.69
2:C:43:GLU:CB	2:C:44:GLN:OE1	2.42	0.67
2:C:39:ALA:HB3	2:C:40:ASP:HA	1.75	0.66
2:C:42:ARG:HD3	2:C:42:ARG:C	2.18	0.64
2:C:42:ARG:HD3	2:C:42:ARG:O	1.99	0.62
1:A:21:LEU:O	1:A:24:VAL:HG12	2.00	0.61
2:F:226:ASP:O	2:F:230:MET:HG3	2.01	0.61
2:F:188:ARG:HG2	2:F:188:ARG:HH21	1.66	0.60
1:A:20:PRO:O	5:A:201:HOH:O	2.17	0.60
2:C:51:ALA:HB1	2:C:60:LEU:HD11	1.84	0.60
2:C:191:THR:HG23	2:C:192:PHE:N	2.15	0.59
1:B:65:ARG:O	1:B:65:ARG:HD2	2.04	0.57
2:C:113:HIS:O	5:C:1102:HOH:O	2.18	0.57
2:F:59:MET:SD	2:F:237:PRO:HD2	2.46	0.56
1:A:6:PHE:HD1	1:A:107:MET:HB3	1.71	0.56
2:F:244:LYS:NZ	5:F:1110:HOH:O	2.40	0.55
2:F:73:TRP:HH2	2:F:77:ARG:NH1	2.04	0.55
2:F:187:ALA:HA	2:F:188:ARG:C	2.25	0.55
1:A:7:ILE:HG13	1:A:107:MET:O	2.07	0.54
2:F:188:ARG:HH21	2:F:189:GLY:HA3	1.72	0.53
2:F:105:TYR:HB3	2:F:117:CYS:SG	2.48	0.53
1:A:36:ASN:H	1:A:37:GLY:HA2	1.73	0.53
1:B:24:VAL:HG13	1:B:24:VAL:O	2.09	0.52
2:F:128:PHE:HB2	2:F:191:THR:O	2.09	0.52
2:C:43:GLU:HA	2:C:44:GLN:CG	2.39	0.52
2:F:106:THR:OG1	2:F:119:TYR:HB2	2.09	0.52
2:C:152:GLU:HG2	2:C:173:SER:HA	1.92	0.51
2:C:191:THR:CG2	2:C:192:PHE:H	2.18	0.50
2:C:248:PRO:N	2:C:249:PRO:HD2	2.27	0.50
1:A:60:ARG:NH2	1:A:82:ASP:OD2	2.35	0.50
1:B:17:PHE:HD1	1:B:18:ALA:N	2.11	0.49
1:B:33:LYS:HD2	1:B:86:TYR:CZ	2.48	0.48
2:F:60:LEU:HD21	2:F:172:VAL:HG13	1.95	0.48
2:F:152:GLU:HG2	2:F:173:SER:HA	1.95	0.48
1:B:78:LEU:HD12	1:B:78:LEU:H	1.78	0.48
2:C:183:LYS:HE2	2:C:228:TRP:CE2	2.49	0.47
2:C:187:ALA:HA	2:C:188:ARG:C	2.34	0.47
1:A:35:THR:CG2	1:A:36:ASN:H	2.20	0.47
1:A:13:LEU:HD12	1:A:73:ILE:HD11	1.96	0.47
2:F:188:ARG:HD3	2:F:188:ARG:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ARG:CB	2:C:189:GLY:HA3	2.32	0.47
2:F:219:GLU:HG2	2:F:220:ALA:N	2.29	0.47
1:A:104:LEU:HD21	1:A:106:VAL:HG23	1.96	0.47
1:B:65:ARG:HH22	1:B:67:SER:HG	1.61	0.47
1:A:23:GLY:HA2	2:C:14:PRO:HB3	1.97	0.46
2:C:44:GLN:HB3	2:C:45:PRO:HD2	1.98	0.46
2:F:188:ARG:CZ	2:F:189:GLY:HA3	2.46	0.45
1:A:6:PHE:HE1	1:A:107:MET:HG2	1.81	0.45
1:A:104:LEU:CD2	1:A:106:VAL:HG23	2.47	0.45
1:B:54:LEU:HD22	2:C:210:THR:HA	1.98	0.45
2:C:89:TRP:HB2	2:C:101:TYR:HB3	1.99	0.45
2:F:188:ARG:HD3	2:F:189:GLY:HA3	1.98	0.45
2:F:76:VAL:HG22	2:F:111:ARG:HG3	1.99	0.44
2:F:128:PHE:HB3	2:F:191:THR:O	2.17	0.44
1:B:33:LYS:HZ2	1:B:82:ASP:HA	1.82	0.44
1:B:29:VAL:HG13	1:B:90:PHE:CE1	2.53	0.44
2:C:42:ARG:N	2:C:43:GLU:C	2.71	0.44
1:B:45:TYR:HD1	1:B:51:VAL:CG2	2.31	0.44
1:B:7:ILE:CD1	1:B:108:ALA:HA	2.48	0.43
1:A:104:LEU:HD23	1:A:105:THR:N	2.33	0.43
2:C:44:GLN:HB2	5:C:1104:HOH:O	2.18	0.43
2:F:80:ALA:O	2:F:111:ARG:NH1	2.49	0.43
2:F:159:LEU:O	2:F:165:VAL:HA	2.19	0.42
1:B:6:PHE:CE2	1:B:107:MET:HE3	2.53	0.42
1:B:13:LEU:HD12	1:B:73:ILE:HD11	2.01	0.42
1:B:58:ARG:HG3	1:B:58:ARG:HH21	1.83	0.42
2:F:68:VAL:HG23	2:F:161:ILE:HD13	2.01	0.42
3:D:2:NAG:O7	3:D:2:NAG:C3	2.68	0.42
1:A:6:PHE:CE1	1:A:107:MET:HG2	2.55	0.42
2:F:118:ARG:N	2:F:118:ARG:HD3	2.32	0.42
2:C:65:ASP:CG	2:C:67:GLN:HE22	2.22	0.42
2:F:73:TRP:CZ3	2:F:77:ARG:NH1	2.88	0.42
1:A:6:PHE:CD1	1:A:107:MET:CB	2.99	0.42
2:F:188:ARG:NH2	2:F:189:GLY:CA	2.78	0.42
2:C:43:GLU:C	2:C:44:GLN:OE1	2.54	0.42
2:C:128:PHE:CB	2:C:191:THR:O	2.67	0.42
2:F:76:VAL:CG2	2:F:111:ARG:HG3	2.50	0.41
2:C:149:ARG:HD3	2:C:177:GLY:HA2	2.01	0.41
1:B:6:PHE:CE2	1:B:107:MET:CE	3.04	0.41
2:C:188:ARG:HG2	2:C:188:ARG:HH21	1.84	0.41
2:F:7:ARG:NH2	5:F:1103:HOH:O	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:ARG:NH2	2:F:188:ARG:HG2	2.29	0.41
1:B:65:ARG:NH2	1:B:67:SER:CB	2.83	0.41
1:A:6:PHE:HD1	1:A:107:MET:CB	2.34	0.41
2:C:128:PHE:HB2	2:C:191:THR:O	2.21	0.41
2:C:68:VAL:CG2	2:C:161:ILE:HD11	2.51	0.41
2:F:128:PHE:CG	2:F:191:THR:O	2.75	0.40
2:F:248:PRO:HA	2:F:249:PRO:HD3	1.84	0.40
2:C:108:CYS:HA	2:C:117:CYS:HA	2.04	0.40
2:C:190:TYR:CD1	2:C:190:TYR:C	2.94	0.40
1:B:65:ARG:HH22	1:B:67:SER:CB	2.34	0.40
2:F:188:ARG:CD	2:F:189:GLY:HA3	2.51	0.40
2:C:105:TYR:HB3	2:C:117:CYS:SG	2.61	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ARG:NH2	2:C:42:ARG:NH2[2_456]	1.66	0.54
2:F:70:ARG:NH2	2:C:42:ARG:O[4_446]	1.87	0.33
2:C:42:ARG:NH1	2:C:42:ARG:NH2[2_456]	2.08	0.12

## 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	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
1	B	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
2	C	242/311 (78%)	233 (96%)	9 (4%)	0	100	100
2	F	242/311 (78%)	234 (97%)	8 (3%)	0	100	100
All	All	698/840 (83%)	674 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	93/93 (100%)	87 (94%)	6 (6%)	17	19
1	B	93/93 (100%)	86 (92%)	7 (8%)	13	14
2	C	201/246 (82%)	198 (98%)	3 (2%)	65	78
2	F	201/246 (82%)	193 (96%)	8 (4%)	31	40
All	All	588/678 (87%)	564 (96%)	24 (4%)	30	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	17	PHE
1	A	29	VAL
1	A	40	GLN
1	A	54	LEU
1	A	75	LEU
2	F	13	ASP
2	F	21	ARG
2	F	70	ARG
2	F	118	ARG
2	F	165	VAL
2	F	188	ARG
2	F	199	ARG
2	F	207	LEU
1	B	3	MET
1	B	17	PHE
1	B	19	ASN
1	B	29	VAL
1	B	40	GLN
1	B	65	ARG
1	B	98	ARG
2	C	44	GLN

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Mol	Chain	Res	Type
2	C	81	ARG
2	C	159	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	203	GLN
2	C	67	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

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
3	NAG	D	1	2,3	14,14,15	0.91	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	D	2	3	14,14,15	1.15	1 (7%)	17,19,21	1.61	2 (11%)

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
3	NAG	D	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	3.96	1.50	1.43
3	D	1	NAG	O5-C1	-3.24	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	4.82	118.72	112.19
3	D	2	NAG	C2-N2-C7	4.24	128.94	122.90
3	D	1	NAG	O4-C4-C5	-2.46	103.18	109.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

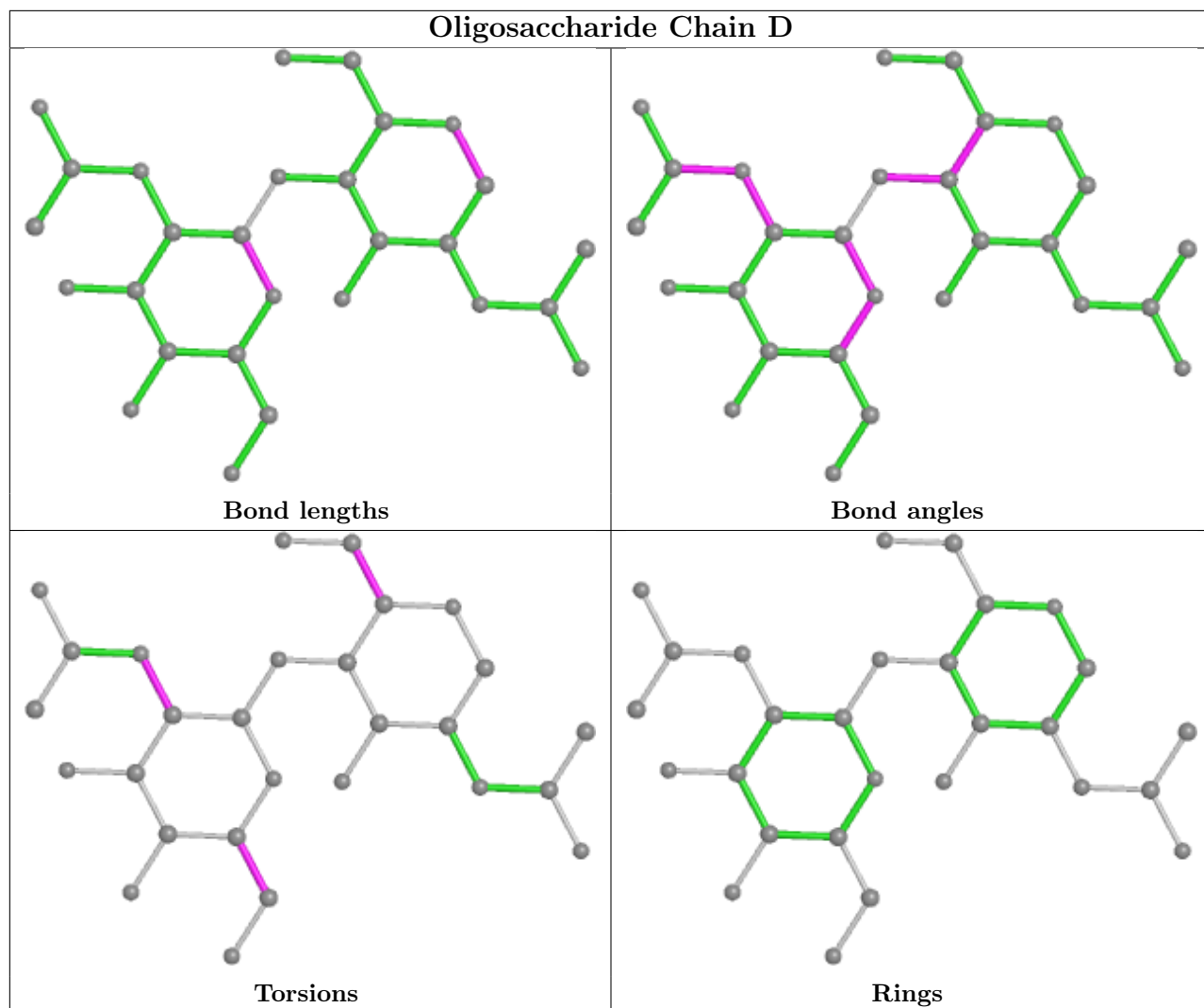
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C3-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	F	1001	2	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
4	NAG	C	1001	2	14,14,15	0.40	0	17,19,21	1.06	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
4	NAG	F	1001	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1001	2	-	2/6/23/26	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	C	1001	NAG	C1-O5-C5	3.32	116.69	112.19
4	F	1001	NAG	C1-O5-C5	2.58	115.69	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1001	NAG	C4-C5-C6-O6
4	C	1001	NAG	O5-C5-C6-O6
4	F	1001	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	109/109 (100%)	0.37	9 (8%) 11 10	45, 71, 101, 119	0
1	B	109/109 (100%)	0.31	5 (4%) 32 31	44, 68, 104, 127	0
2	C	244/311 (78%)	0.18	16 (6%) 18 17	38, 54, 98, 131	0
2	F	244/311 (78%)	0.18	7 (2%) 51 49	37, 50, 85, 121	0
All	All	706/840 (84%)	0.23	37 (5%) 27 26	37, 57, 99, 131	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	189	GLY	7.0
2	C	188	ARG	6.9
2	C	42	ARG	6.5
2	C	6	PRO	6.0
2	C	249	PRO	5.4
2	C	8	VAL	5.3
1	B	108	ALA	5.0
1	A	36	ASN	4.7
2	F	249	PRO	4.5
2	F	188	ARG	4.5
2	C	40	ASP	4.4
2	F	189	GLY	4.0
1	B	36	ASN	3.8
2	F	248	PRO	3.7
2	F	246	TYR	3.6
1	A	6	PHE	3.5
2	F	187	ALA	3.4
2	C	187	ALA	3.3
2	F	6	PRO	3.2
2	C	43	GLU	3.2
1	A	109	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	109	LYS	3.1
1	A	35	THR	2.8
1	A	108	ALA	2.6
1	A	19	ASN	2.4
1	A	7	ILE	2.4
1	B	65	ARG	2.3
2	C	81	ARG	2.3
2	C	45	PRO	2.3
1	B	6	PHE	2.3
2	C	118	ARG	2.3
2	C	119	TYR	2.3
1	A	4	TYR	2.2
2	C	41	GLY	2.1
2	C	7	ARG	2.1
2	C	113	HIS	2.0
1	A	80	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

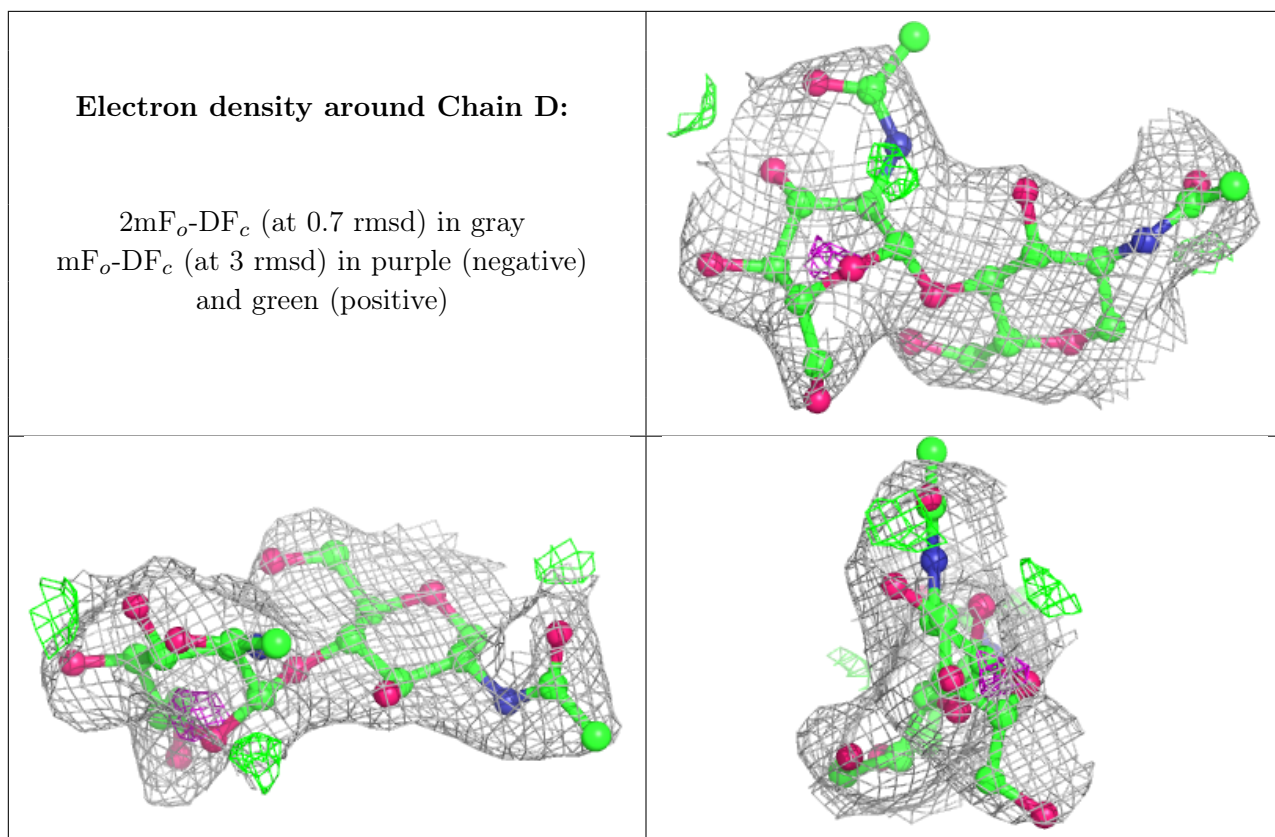
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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(Å <sup>2</sup> )	Q<0.9
3	NAG	D	2	14/15	0.87	0.35	81,94,96,96	0
3	NAG	D	1	14/15	0.92	0.28	63,80,86,90	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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
4	NAG	C	1001	14/15	0.70	0.32	89,96,104,111	0
4	NAG	F	1001	14/15	0.95	0.11	55,71,81,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.