



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:37 AM UTC

PDB ID : 6LSA / pdb_00006lsa
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

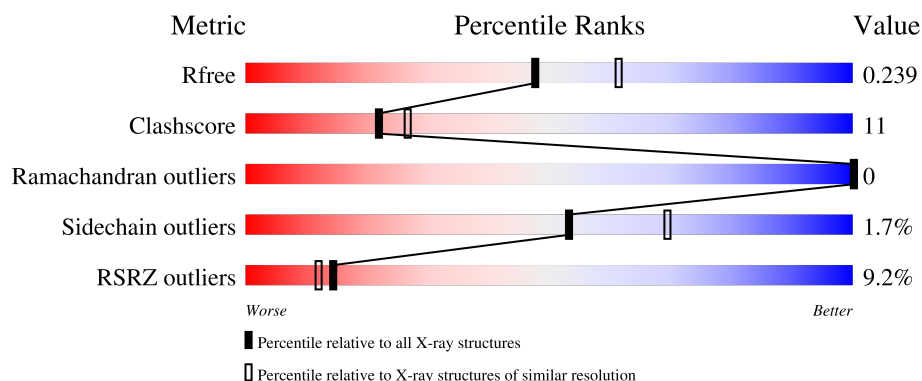
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 ≥ 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	13% 78% 21% .
1	B	109	15% 72% 26% ..
2	C	311	6% 66% 11% . 22%
2	F	311	5% 65% 12% . 22%

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Mol	Chain	Length	Quality of chain
3	D	2	

2 Entry composition

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
1	A	109	Total	C	N	O	S	0	0	0
			849	540	144	160	5			
1	B	109	Total	C	N	O	S	0	0	0
			849	540	144	160	5			

- Molecule 2 is a protein called Envelope glycoprotein D.

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

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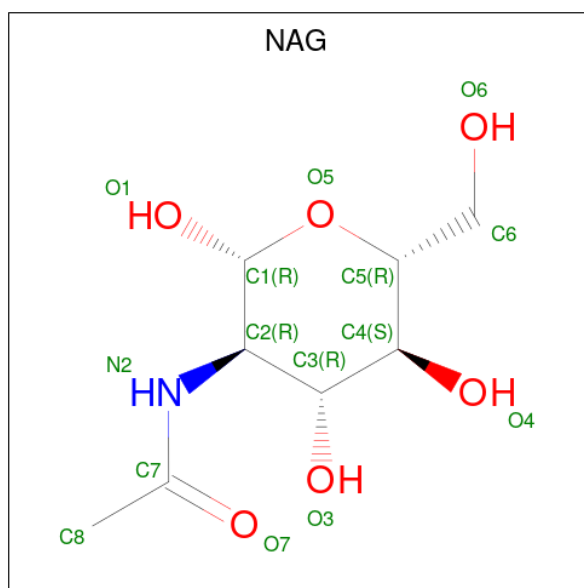
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP Q76PF1
C	305	HIS	-	expression tag	UNP Q76PF1
C	306	HIS	-	expression tag	UNP Q76PF1
C	307	HIS	-	expression tag	UNP Q76PF1

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

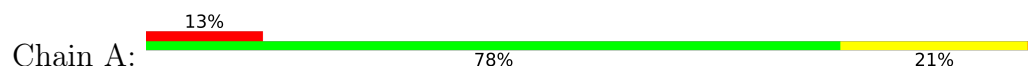
- Molecule 5 is water.

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

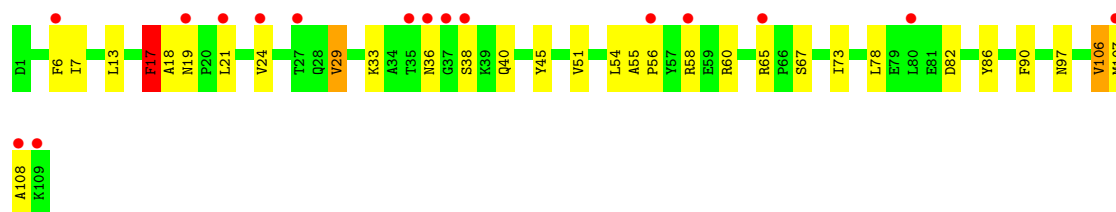
3 Residue-property plots

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.

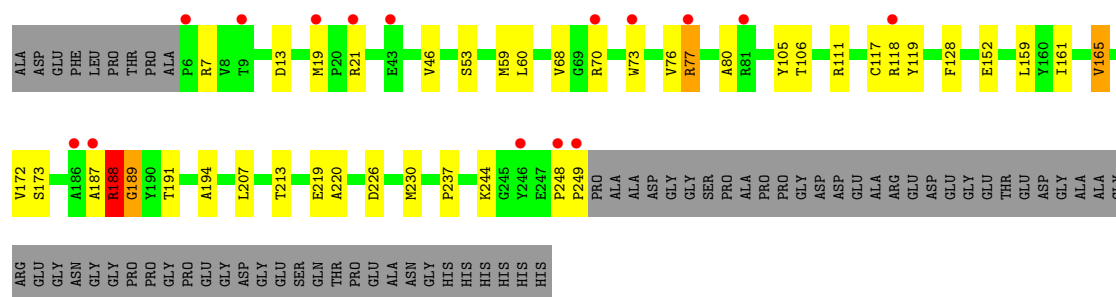
- Molecule 1: Nectin cell adhesion molecule 1



- Molecule 1: Nectin cell adhesion molecule 1

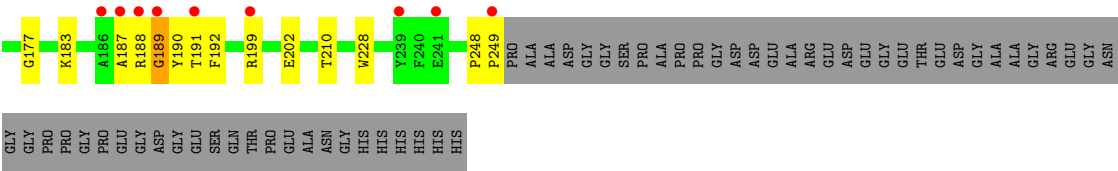


- Molecule 2: Envelope glycoprotein D

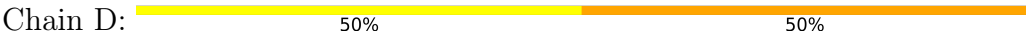


- Molecule 2: Envelope glycoprotein D





● Molecule 3: 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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.200 , 0.236 0.203 , 0.239	Depositor DCC
R_{free} test set	2906 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5935	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	A	0.45	0/867	0.78	1/1177 (0.1%)
1	B	0.56	2/867 (0.2%)	0.89	5/1177 (0.4%)
2	C	0.47	2/2065 (0.1%)	0.73	9/2820 (0.3%)
2	F	0.63	6/2065 (0.3%)	0.69	6/2820 (0.2%)
All	All	0.54	10/5864 (0.2%)	0.75	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	F	21	ARG	NE-CZ	-10.34	1.21	1.33
2	F	21	ARG	CZ-NH2	-10.09	1.20	1.33
2	F	21	ARG	CD-NE	-9.61	1.32	1.46
2	C	43	GLU	CG-CD	8.46	1.73	1.52
1	B	17	PHE	C-N	-7.67	1.24	1.33
2	F	77	ARG	CZ-NH1	-6.98	1.23	1.32
2	F	77	ARG	CB-CG	-6.04	1.34	1.52
1	B	56	PRO	N-CD	5.66	1.55	1.47
2	C	42	ARG	CA-C	5.53	1.59	1.52
2	F	21	ARG	CZ-NH1	-5.07	1.25	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	MET	CG-SD-CE	-9.69	79.57	100.90
2	C	43	GLU	CB-CG-CD	8.81	127.58	112.60
2	C	42	ARG	N-CA-C	8.77	120.76	111.03
2	F	77	ARG	CB-CG-CD	-8.40	91.98	111.30
1	B	17	PHE	CA-C-N	-8.34	106.56	121.81
1	B	17	PHE	C-N-CA	-8.34	106.56	121.81
2	C	42	ARG	NE-CZ-NH1	7.20	128.70	121.50
2	C	42	ARG	CG-CD-NE	-6.91	96.81	112.00
2	F	188	ARG	CA-C-N	6.00	132.50	121.70
2	F	188	ARG	C-N-CA	6.00	132.50	121.70
2	F	189	GLY	N-CA-C	5.91	130.43	113.30
2	F	188	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	C	43	GLU	CG-CD-OE2	5.71	131.52	118.40
1	B	55	ALA	C-N-CD	-5.58	108.31	120.60
2	F	77	ARG	NE-CZ-NH1	-5.47	116.03	121.50
2	C	42	ARG	NH1-CZ-NH2	-5.40	112.28	119.30
1	B	55	ALA	CA-C-N	5.37	139.88	127.00
1	B	55	ALA	C-N-CA	5.37	139.88	127.00
2	C	189	GLY	N-CA-C	5.26	128.56	113.30
2	C	43	GLU	CA-C-N	5.19	131.05	121.70
2	C	43	GLU	C-N-CA	5.19	131.05	121.70

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 ⓘ

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	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	849	0	841	21	0
2	C	1991	0	1885	40	3
2	F	1991	0	1886	37	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	120	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 11.

All (120) 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
2:C:43:GLU:HA	2:C:44:GLN:CD	1.97	0.90
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: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:42:ARG:HD3	2:C:42:ARG:C	2.18	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: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
2:F:187:ALA:HA	2:F:188:ARG:C	2.25	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:F:19:MET:HA	2:F:19:MET:HE2	1.82	0.59
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
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:C:187:ALA:HA	2:C:188:ARG:C	2.34	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:43:GLU:C	2:C:44:GLN:OE1	2.54	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:C:42:ARG:N	2:C:43:GLU:C	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:65:ASP:CG	2:C:67:GLN:HE22	2.22	0.46
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
2:C:190:TYR:C	2:C:190:TYR:CD1	2.94	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
2:C:65:ASP:CG	2:C:67:GLN:NE2	2.76	0.44
1:B:29:VAL:HG13	1:B:90:PHE:CE1	2.53	0.44
2:C:42:ARG:C	2:C:42:ARG:CD	2.90	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:104:LEU:C	2.44	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:106:VAL:C	1:B:107:MET:CG	2.94	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
1:A:81:GLU:CD	1:A:81:GLU:H	2.30	0.40
2:C:108:CYS:HA	2:C:117:CYS:HA	2.04	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	90 (97%)	3 (3%)	34	47
1	B	93/93 (100%)	91 (98%)	2 (2%)	45	61
2	C	201/246 (82%)	200 (100%)	1 (0%)	81	90
2	F	201/246 (82%)	197 (98%)	4 (2%)	48	64
All	All	588/678 (87%)	578 (98%)	10 (2%)	53	69

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	40	GLN
1	A	75	LEU
2	F	13	ASP
2	F	46	VAL
2	F	165	VAL
2	F	207	LEU
1	B	29	VAL
1	B	40	GLN
2	C	159	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	44	GLN

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Mol	Chain	Res	Type
2	F	203	GLN
1	B	14	HIS
1	B	28	GLN
2	C	67	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 ⓘ

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	3,2	14,14,15	0.87	1 (7%)	17,19,21	0.92	1 (5%)
3	NAG	D	2	3	14,14,15	1.12	1 (7%)	17,19,21	1.67	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	3,2	-	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	3.78	1.50	1.43
3	D	1	NAG	O5-C1	-3.07	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	4.88	118.72	112.19
3	D	2	NAG	C2-N2-C7	4.51	128.94	122.90
3	D	1	NAG	O4-C4-C5	-2.49	103.18	109.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

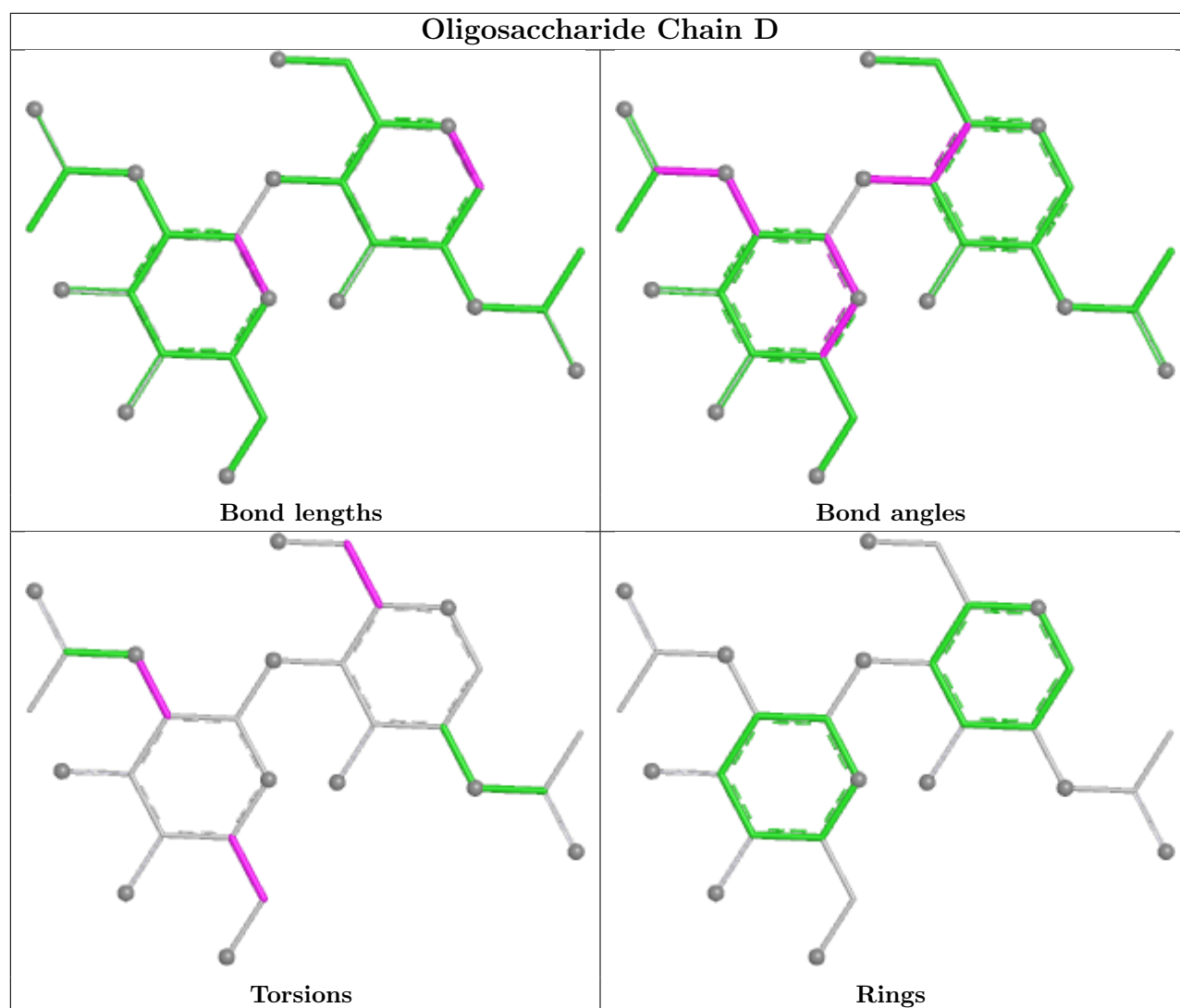
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C3-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

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	C	1001	2	14,14,15	0.41	0	17,19,21	1.08	1 (5%)
4	NAG	F	1001	2	14,14,15	0.59	0	17,19,21	0.76	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	C	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1001	2	-	1/6/23/26	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(°)
4	C	1001	NAG	C1-O5-C5	3.36	116.69	112.19
4	F	1001	NAG	C1-O5-C5	2.62	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, 95th 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 ²)	Q<0.9
1	A	109/109 (100%)	0.80	14 (12%) 7 5	45, 71, 101, 119	0
1	B	109/109 (100%)	0.92	16 (14%) 6 4	44, 68, 104, 127	0
2	C	244/311 (78%)	0.41	20 (8%) 17 15	38, 54, 98, 131	0
2	F	244/311 (78%)	0.19	15 (6%) 27 24	37, 50, 85, 121	0
All	All	706/840 (84%)	0.47	65 (9%) 14 12	37, 57, 99, 131	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	249	PRO	4.9
1	B	108	ALA	4.8
2	C	45	PRO	4.8
2	C	41	GLY	4.8
1	B	109	LYS	4.7
2	C	8	VAL	4.7
2	C	6	PRO	4.5
2	C	44	GLN	4.4
2	C	39	ALA	4.3
2	C	40	ASP	4.3
1	B	21	LEU	4.3
1	A	96	GLY	4.0
2	F	6	PRO	3.9
1	B	35	THR	3.9
2	F	186	ALA	3.9
2	C	42	ARG	3.7
2	C	9	THR	3.6
2	F	246	TYR	3.6
2	F	187	ALA	3.6
2	F	249	PRO	3.6
2	C	186	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	21	ARG	3.6
2	C	188	ARG	3.5
1	B	36	ASN	3.4
1	A	6	PHE	3.3
1	A	18	ALA	3.3
1	A	109	LYS	3.2
2	C	43	GLU	3.0
1	A	21	LEU	2.9
2	F	73	TRP	2.9
1	A	108	ALA	2.8
2	F	248	PRO	2.8
2	C	187	ALA	2.8
1	B	65	ARG	2.8
2	F	118	ARG	2.8
1	A	35	THR	2.7
1	B	107	MET	2.7
2	F	77	ARG	2.7
1	B	56	PRO	2.7
1	A	80	LEU	2.7
2	F	19	MET	2.6
2	F	43	GLU	2.6
1	A	97	ASN	2.6
1	B	27	THR	2.5
1	B	19	ASN	2.5
1	A	58	ARG	2.5
1	B	80	LEU	2.4
2	F	9	THR	2.4
2	F	81	ARG	2.4
1	B	58	ARG	2.4
2	C	189	GLY	2.4
1	B	37	GLY	2.3
1	B	6	PHE	2.3
2	C	239	TYR	2.3
1	A	107	MET	2.3
1	B	24	VAL	2.3
2	C	199	ARG	2.2
2	C	21	ARG	2.2
2	C	191	THR	2.2
1	A	81	GLU	2.2
2	F	70	ARG	2.1
2	C	241	GLU	2.1
1	A	56	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	13	LEU	2.1
1	B	38	SER	2.0

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

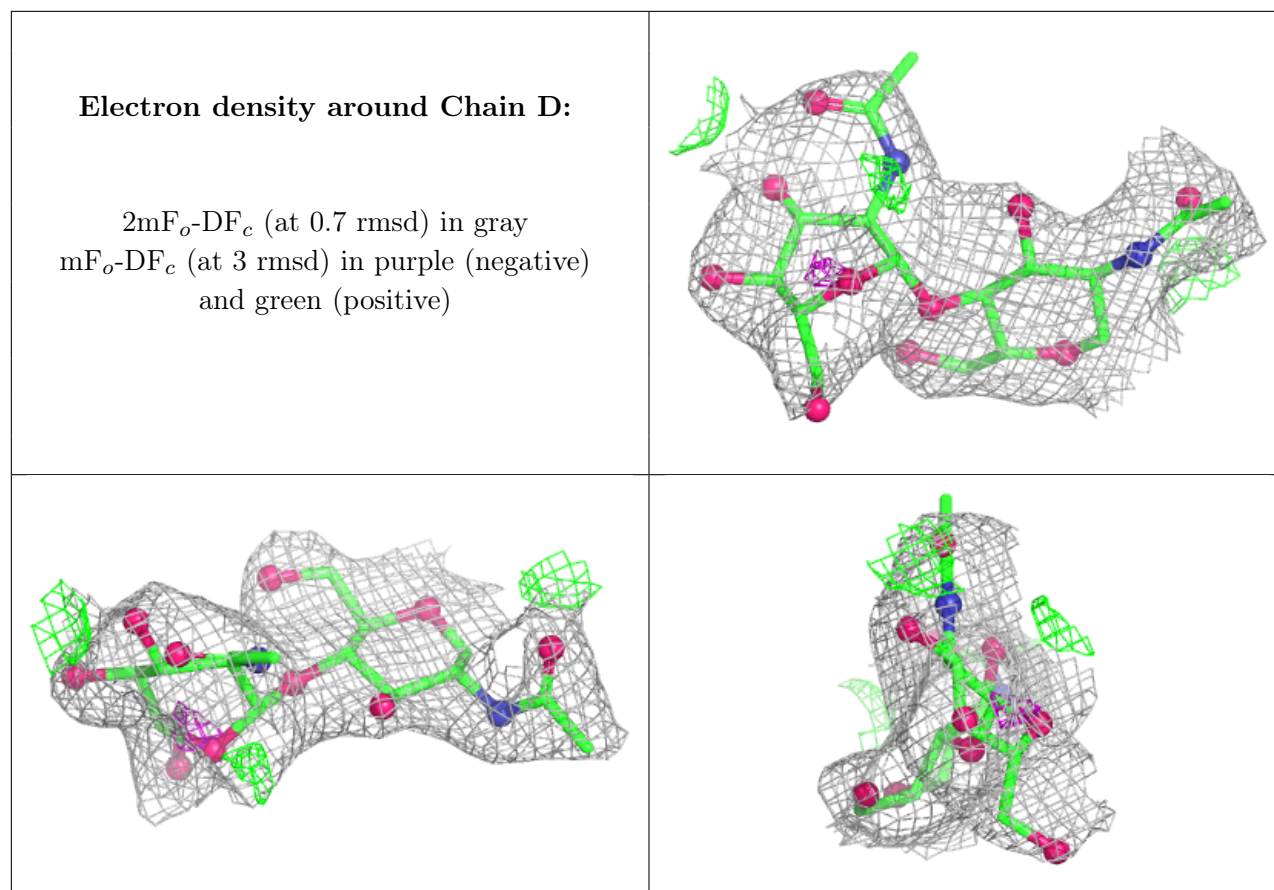
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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
3	NAG	D	1	14/15	-	-	63,80,86,90	0
3	NAG	D	2	14/15	-	-	81,94,96,96	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, 95th 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	0.58	0.22	89,96,104,111	0
4	NAG	F	1001	14/15	0.89	0.13	55,71,81,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.