



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 12:57 pm GMT

PDB ID : 7NKS  
Title : Structure of the Hantaan virus Gn glycoprotein ectodomain in complex with Fab HTN-Gn1  
Authors : Rissanen, I.; Bowden, T.A.; Huiskonen, J.T.; Stass, R.  
Deposited on : 2021-02-18  
Resolution : 3.50 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 : 1.8.4, CSD as541be (2020)  
Xtriage (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

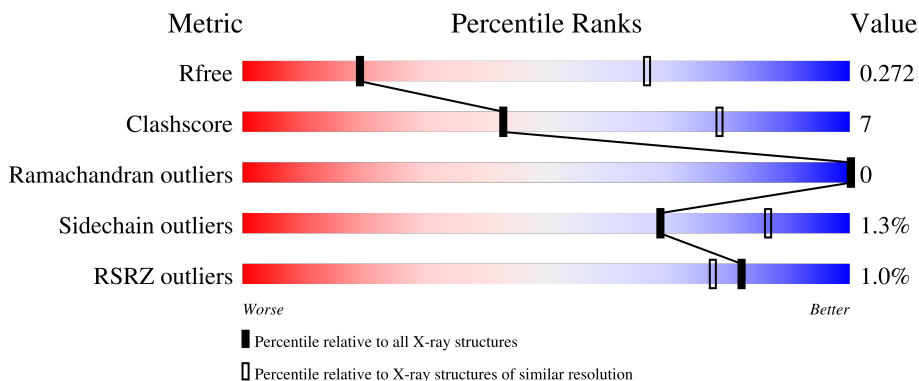
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	365	 2% 76% 17% • 6%
1	B	365	 2% 81% 10% • 8%
2	C	231	 73% 23% •
2	H	231	 76% 19% 5%
3	D	217	 88% 12%

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Mol	Chain	Length	Quality of chain
3	L	217	 % 81% 18%
4	G	7	 29% 71%
5	F	7	 43% 29% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	401	-	-	-	X
6	GOL	C	301	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11860 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 Envelope polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	336	2597	1647	423	502	25	0	0	0
1	A	342	2635	1677	425	509	24	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	THR	-	cloning artifact	UNP A0A077D153
B	17	GLY	-	cloning artifact	UNP A0A077D153
B	372	GLY	-	expression tag	UNP A0A077D153
B	373	THR	-	expression tag	UNP A0A077D153
B	374	LYS	-	expression tag	UNP A0A077D153
B	375	HIS	-	expression tag	UNP A0A077D153
B	376	HIS	-	expression tag	UNP A0A077D153
B	377	HIS	-	expression tag	UNP A0A077D153
B	378	HIS	-	expression tag	UNP A0A077D153
B	379	HIS	-	expression tag	UNP A0A077D153
B	380	HIS	-	expression tag	UNP A0A077D153
A	16	THR	-	cloning artifact	UNP A0A077D153
A	17	GLY	-	cloning artifact	UNP A0A077D153
A	372	GLY	-	expression tag	UNP A0A077D153
A	373	THR	-	expression tag	UNP A0A077D153
A	374	LYS	-	expression tag	UNP A0A077D153
A	375	HIS	-	expression tag	UNP A0A077D153
A	376	HIS	-	expression tag	UNP A0A077D153
A	377	HIS	-	expression tag	UNP A0A077D153
A	378	HIS	-	expression tag	UNP A0A077D153
A	379	HIS	-	expression tag	UNP A0A077D153
A	380	HIS	-	expression tag	UNP A0A077D153

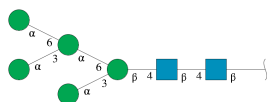
- Molecule 2 is a protein called Fab HTN-Gn1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	221	Total 1618	C 1021	N 266	O 321	S 10	0	0	0
2	H	220	Total 1613	C 1018	N 265	O 320	S 10	0	0	0

- Molecule 3 is a protein called Fab HTN-Gn1 light chain.

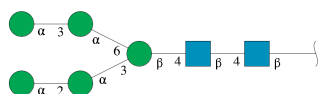
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	216	Total 1603	C 995	N 263	O 339	S 6	0	0	0
3	L	215	Total 1596	C 991	N 262	O 337	S 6	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-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			
4	G	7	Total 83	C 46	N 2	O 35	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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			
5	F	7	Total 83	C 46	N 2	O 35	0	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			6	3 3		
6	C	1	Total	C O	0	0
			6	3 3		
6	C	1	Total	C O	0	0
			6	3 3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

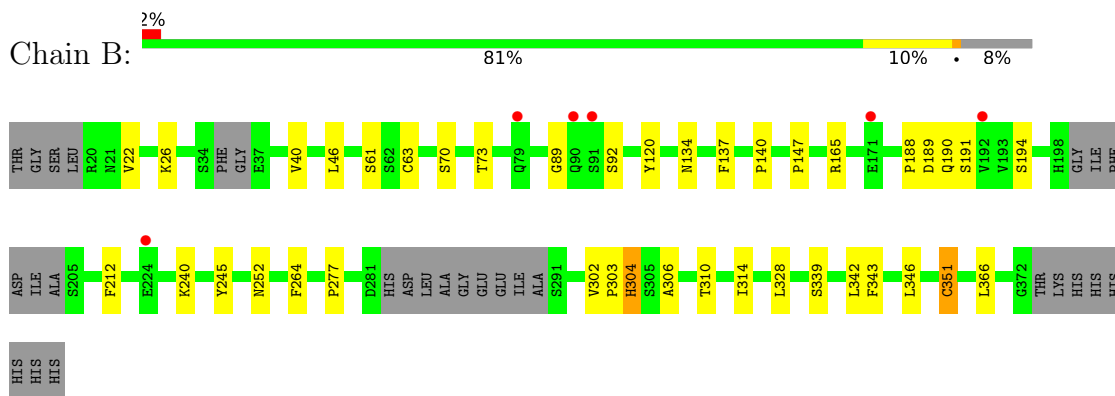


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	14	8	1	5	0	0

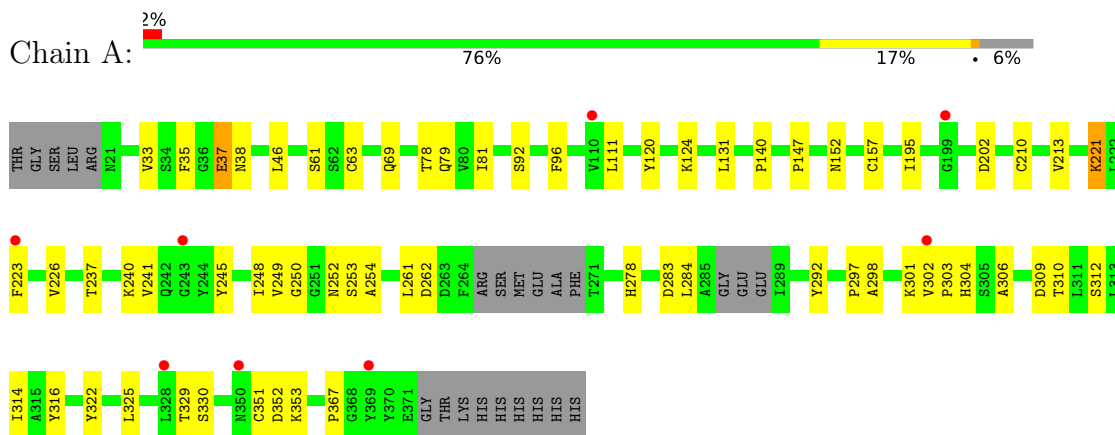
### 3 Residue-property plots [i](#)

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.

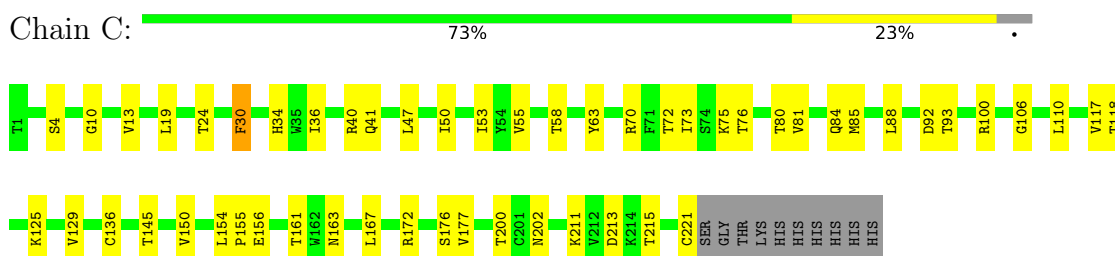
- Molecule 1: Envelope polyprotein



- Molecule 1: Envelope polyprotein




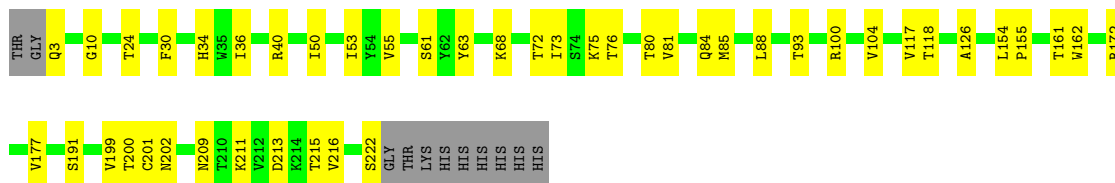
- Molecule 2: Fab HTN-Gn1 heavy chain






- Molecule 2: Fab HTN-Gn1 heavy chain

Chain H:  76% 19% 5%




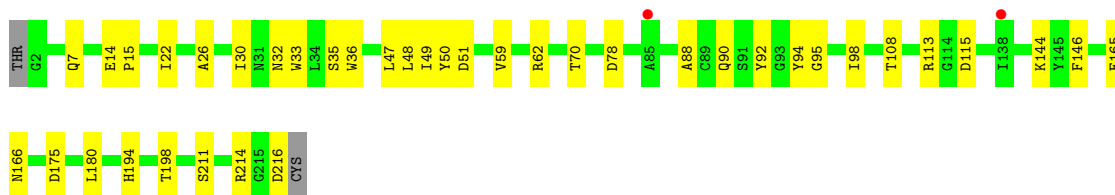
- Molecule 3: Fab HTN-Gn1 light chain

Chain D:  88% 12%



- Molecule 3: Fab HTN-Gn1 light chain

Chain L:  81% 18% .



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  29% 71%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  43% 29% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.02Å 158.63Å 70.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.01 – 3.50 62.26 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.01-3.50) 99.9 (62.26-3.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, $R_{free}$	0.224 , 0.274 0.222 , 0.272	Depositor DCC
$R_{free}$ test set	1681 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.3	Xtrriage
Anisotropy	0.880	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 67.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: MAN, BMA, GOL, 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	0.25	0/2698	0.47	0/3667
1	B	0.25	0/2657	0.47	0/3606
2	C	0.25	0/1659	0.49	0/2278
2	H	0.24	0/1654	0.49	0/2271
3	D	0.24	0/1635	0.46	0/2241
3	L	0.24	0/1628	0.46	0/2231
All	All	0.25	0/11931	0.47	0/16294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2635	0	2573	41	0
1	B	2597	0	2536	25	0
2	C	1618	0	1588	35	0
2	H	1613	0	1580	31	0
3	D	1603	0	1536	15	0
3	L	1596	0	1526	24	0
4	G	83	0	70	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	83	0	70	1	0
6	B	6	0	8	0	0
6	C	12	0	16	1	0
7	B	14	0	13	0	0
All	All	11860	0	11516	160	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 7.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG11	1:A:152:ASN:HD22	1.50	0.76
1:B:189:ASP:HB3	1:B:194:SER:HB3	1.66	0.76
2:H:53:ILE:HG22	2:H:55:VAL:H	1.50	0.75
1:A:35:PHE:HB3	1:A:252:ASN:HD21	1.52	0.73
2:C:58:THR:HG21	4:G:1:NAG:H82	1.73	0.71
3:L:35:SER:HB2	3:L:90:GLN:HG2	1.73	0.70
2:H:40:ARG:HB3	2:H:50:ILE:HD11	1.73	0.69
2:C:36:ILE:HG12	2:C:55:VAL:HG21	1.75	0.69
2:H:72:THR:HB	2:H:84:GLN:HB2	1.75	0.69
2:H:100:ARG:HH22	1:A:92:SER:HA	1.57	0.68
1:B:188:PRO:HB3	1:B:366:LEU:HD13	1.76	0.68
1:B:302:VAL:HG11	1:B:328:LEU:HD22	1.74	0.68
2:C:40:ARG:HB3	2:C:50:ILE:HD11	1.75	0.67
2:C:215:THR:HG22	2:H:209:ASN:HB3	1.77	0.67
2:C:13:VAL:HG11	2:C:19:LEU:HB2	1.77	0.67
3:L:7:GLN:HE22	3:L:88:ALA:HA	1.62	0.65
1:A:96:PHE:HE1	1:A:298:ALA:HB2	1.61	0.64
2:C:72:THR:HB	2:C:84:GLN:HB2	1.80	0.63
1:A:303:PRO:O	1:A:304:HIS:ND1	2.31	0.62
2:H:36:ILE:HG21	2:H:81:VAL:HG11	1.82	0.61
2:H:154:LEU:HD12	2:H:155:PRO:HA	1.82	0.61
1:A:69:GLN:OE1	1:A:124:LYS:NZ	2.34	0.60
3:D:194:HIS:O	3:D:214:ARG:NH1	2.35	0.59
1:A:312:SER:H	1:A:353:LYS:HB3	1.67	0.59
2:H:24:THR:HG22	2:H:80:THR:HG22	1.85	0.58
1:A:241:VAL:N	1:A:329:THR:O	2.34	0.57
1:A:221:LYS:HD3	1:A:221:LYS:H	1.70	0.57
2:C:145:THR:HG21	3:D:122:LEU:HD13	1.86	0.56
1:A:292:TYR:HE1	1:A:316:TYR:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:SER:OG	1:B:63:CYS:SG	2.64	0.56
2:C:211:LYS:HB3	2:H:213:ASP:HB2	1.87	0.55
2:C:213:ASP:HB2	2:H:211:LYS:HB3	1.86	0.55
2:H:222:SER:O	2:H:222:SER:OG	2.24	0.55
2:H:34:HIS:HD2	2:H:100:ARG:HE	1.53	0.55
2:C:200:THR:HA	2:C:215:THR:HA	1.88	0.55
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.88	0.54
1:A:248:ILE:HG23	1:A:254:ALA:HB1	1.89	0.54
2:C:163:ASN:HB2	2:C:167:LEU:HD22	1.90	0.54
6:C:301:GOL:H12	2:H:126:ALA:HB3	1.88	0.54
2:C:53:ILE:HG23	2:C:55:VAL:HG13	1.88	0.54
3:L:194:HIS:O	3:L:214:ARG:NH1	2.41	0.54
1:B:303:PRO:O	1:B:304:HIS:ND1	2.34	0.54
1:A:63:CYS:N	1:A:157:CYS:SG	2.81	0.53
3:D:115:ASP:N	3:D:115:ASP:OD1	2.40	0.53
3:L:198:THR:HG23	3:L:211:SER:HB2	1.91	0.53
2:C:30:PHE:HE2	2:C:55:VAL:HB	1.74	0.52
1:A:352:ASP:HB2	1:A:353:LYS:HD2	1.90	0.52
3:D:36:TRP:HB2	3:D:49:ILE:HB	1.91	0.52
2:H:63:TYR:CZ	2:H:73:ILE:HG22	2.44	0.52
3:L:30:ILE:HG22	3:L:33:TRP:HB2	1.92	0.52
1:B:303:PRO:HG2	1:B:306:ALA:HB2	1.92	0.52
2:C:161:THR:HG23	2:C:202:ASN:HB2	1.92	0.52
2:C:76:THR:OG1	2:C:80:THR:OG1	2.26	0.51
2:C:24:THR:HG22	2:C:80:THR:HG22	1.92	0.51
2:C:85:MET:HB3	2:C:88:LEU:HD21	1.93	0.51
3:D:47:LEU:HD11	3:D:50:TYR:HB3	1.93	0.51
2:C:63:TYR:CZ	2:C:73:ILE:HG22	2.46	0.51
3:D:32:ASN:O	3:D:32:ASN:ND2	2.44	0.51
1:B:314:ILE:HB	1:B:343:PHE:HB2	1.92	0.50
2:H:199:VAL:HG23	2:H:216:VAL:HG23	1.92	0.50
3:L:115:ASP:N	3:L:115:ASP:OD1	2.45	0.50
1:A:46:LEU:HB2	1:A:140:PRO:HG2	1.94	0.50
1:A:240:LYS:HG2	1:A:330:SER:HA	1.94	0.50
2:C:70:ARG:NH2	2:C:92:ASP:OD1	2.44	0.50
2:H:53:ILE:HD11	2:H:73:ILE:HG23	1.93	0.49
1:A:301:LYS:NZ	1:A:306:ALA:O	2.41	0.49
3:D:198:THR:HG23	3:D:211:SER:HB2	1.93	0.49
1:A:248:ILE:HG22	1:A:250:GLY:H	1.77	0.49
2:C:10:GLY:HA2	2:C:117:VAL:HG22	1.95	0.49
2:C:177:VAL:HG21	3:D:165:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:ARG:NH1	3:D:78:ASP:O	2.46	0.48
1:B:120:TYR:HA	1:B:147:PRO:HG3	1.95	0.48
3:D:22:ILE:HD13	3:D:108:THR:HG21	1.95	0.48
2:H:104:VAL:HG13	3:L:98:ILE:HD12	1.93	0.48
1:A:302:VAL:HG13	1:A:303:PRO:HD3	1.95	0.48
1:B:302:VAL:HG12	1:B:310:THR:OG1	2.14	0.48
1:A:37:GLU:HA	1:A:120:TYR:CZ	2.48	0.48
2:C:129:VAL:HG22	2:C:150:VAL:HG22	1.94	0.48
3:L:62:ARG:NH1	3:L:78:ASP:O	2.47	0.48
2:C:41:GLN:HB2	2:C:47:LEU:HD23	1.96	0.47
2:C:156:GLU:OE2	2:C:176:SER:OG	2.32	0.47
3:L:48:LEU:HA	3:L:59:VAL:HG21	1.96	0.47
2:H:72:THR:O	2:H:84:GLN:N	2.43	0.47
1:A:131:LEU:HG	1:A:325:LEU:HD11	1.95	0.47
3:L:51:ASP:OD1	3:L:92:TYR:OH	2.32	0.47
1:B:190:GLN:HG3	1:B:264:PHE:CE1	2.50	0.47
1:A:195:ILE:HD11	1:A:367:PRO:HB2	1.96	0.47
3:L:47:LEU:HD11	3:L:50:TYR:HB3	1.96	0.47
1:A:284:LEU:HD22	1:A:292:TYR:HB2	1.96	0.47
2:C:36:ILE:HG21	2:C:81:VAL:HG21	1.98	0.46
2:C:172:ARG:NE	3:D:143:ASN:OD1	2.49	0.46
2:H:85:MET:HB3	2:H:88:LEU:HD21	1.98	0.46
1:A:120:TYR:CD1	1:A:147:PRO:HB3	2.50	0.46
1:B:188:PRO:HB3	1:B:366:LEU:CD1	2.44	0.46
2:H:200:THR:HG23	2:H:215:THR:HG22	1.97	0.46
1:B:339:SER:HB2	1:B:342:LEU:HB2	1.98	0.46
2:H:177:VAL:HG21	3:L:165:GLU:HB3	1.97	0.46
2:H:34:HIS:CD2	2:H:100:ARG:HE	2.32	0.46
1:A:312:SER:N	1:A:353:LYS:HB3	2.30	0.45
2:C:53:ILE:HG12	2:C:55:VAL:H	1.82	0.45
1:B:89:GLY:O	1:B:92:SER:OG	2.29	0.45
2:C:154:LEU:HD12	2:C:155:PRO:HA	1.99	0.45
2:H:55:VAL:HG23	2:H:75:LYS:HG3	1.97	0.45
2:H:93:THR:HG23	2:H:118:THR:HA	1.99	0.45
2:C:93:THR:HG23	2:C:118:THR:HA	1.99	0.45
1:A:223:PHE:CE2	1:A:329:THR:HB	2.52	0.45
1:A:261:LEU:O	1:A:262:ASP:HB2	2.17	0.44
1:B:190:GLN:HG3	1:B:264:PHE:CZ	2.53	0.44
2:H:10:GLY:HA2	2:H:117:VAL:HG22	2.00	0.44
1:A:61:SER:OG	1:A:63:CYS:SG	2.75	0.44
1:B:314:ILE:O	1:B:343:PHE:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:ARG:HA	3:D:146:PHE:CZ	2.52	0.44
1:B:40:VAL:HG12	1:B:252:ASN:HB2	2.00	0.44
3:L:26:ALA:O	3:L:70:THR:OG1	2.33	0.44
1:A:210:CYS:SG	1:A:245:TYR:HD2	2.41	0.44
2:H:161:THR:HG23	2:H:202:ASN:HB2	1.99	0.44
3:L:7:GLN:HE21	3:L:108:THR:HG23	1.82	0.44
3:L:7:GLN:NE2	3:L:108:THR:HG23	2.33	0.43
1:A:223:PHE:HA	1:A:226:VAL:HB	2.00	0.43
1:B:46:LEU:HB2	1:B:140:PRO:HG2	2.00	0.43
1:A:278:HIS:HB3	1:A:322:TYR:CE2	2.53	0.43
2:H:172:ARG:HH22	2:H:191:SER:HG	1.57	0.43
1:A:249:VAL:HG22	1:A:254:ALA:HA	1.99	0.43
1:B:277:PRO:HB2	1:B:346:LEU:HD13	2.00	0.43
1:B:212:PHE:HB2	1:B:245:TYR:CE1	2.53	0.43
1:B:134:ASN:HD22	4:G:1:NAG:H83	1.84	0.42
2:C:34:HIS:HD2	2:C:100:ARG:HD2	1.84	0.42
3:L:32:ASN:O	3:L:32:ASN:ND2	2.52	0.42
2:H:76:THR:OG1	2:H:80:THR:OG1	2.32	0.42
1:A:111:LEU:O	1:A:213:VAL:HG12	2.20	0.42
3:D:137:THR:HB	3:D:185:THR:HG23	2.01	0.42
3:L:95:GLY:HA3	1:A:79:GLN:OE1	2.18	0.42
3:L:113:ARG:HA	3:L:146:PHE:CZ	2.54	0.42
1:A:302:VAL:CG1	1:A:303:PRO:HD3	2.50	0.42
3:L:14:GLU:HA	3:L:15:PRO:HD3	1.92	0.42
2:C:4:SER:HA	2:C:110:LEU:HD21	2.00	0.42
3:L:166:ASN:HB3	3:L:180:LEU:HD11	2.00	0.42
1:B:189:ASP:C	1:B:191:SER:H	2.23	0.42
2:C:30:PHE:CE2	2:C:55:VAL:HB	2.54	0.42
2:H:162:TRP:CZ3	2:H:201:CYS:HB3	2.55	0.42
1:A:237:THR:HA	1:A:240:LYS:HD2	2.01	0.42
1:A:78:THR:HG21	1:A:302:VAL:O	2.20	0.41
5:F:4:MAN:H2	5:F:5:MAN:H2	1.72	0.41
1:B:22:VAL:HG13	1:B:165:ARG:HB2	2.02	0.41
2:C:125:LYS:HE2	2:C:125:LYS:HB2	1.90	0.41
2:C:154:LEU:HD12	2:C:154:LEU:HA	1.86	0.41
3:D:40:ARG:HD3	3:D:85:ALA:HB2	2.01	0.41
1:A:302:VAL:HG12	1:A:310:THR:OG1	2.20	0.41
1:B:70:SER:O	1:B:73:THR:OG1	2.31	0.41
3:L:144:LYS:HE2	3:L:175:ASP:OD2	2.19	0.41
2:H:53:ILE:HD13	2:H:61:SER:HB3	2.02	0.41
2:H:202:ASN:ND2	2:H:213:ASP:OD1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLY:HA2	3:D:92:TYR:HB2	2.03	0.41
3:L:22:ILE:HG23	3:L:108:THR:HG21	2.03	0.41
3:L:94:TYR:HB3	1:A:81:ILE:HD13	2.02	0.41
1:A:38:ASN:CG	1:A:253:SER:H	2.25	0.41
1:A:301:LYS:HG3	1:A:309:ASP:HA	2.03	0.40
1:B:137:PHE:CD2	4:G:1:NAG:H5	2.57	0.40
1:B:240:LYS:NZ	1:B:351:CYS:HB3	2.36	0.40
1:A:297:PRO:HA	1:A:314:ILE:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/365 (92%)	320 (95%)	16 (5%)	0	100	100
1	B	328/365 (90%)	314 (96%)	14 (4%)	0	100	100
2	C	219/231 (95%)	211 (96%)	8 (4%)	0	100	100
2	H	218/231 (94%)	211 (97%)	7 (3%)	0	100	100
3	D	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
3	L	213/217 (98%)	207 (97%)	6 (3%)	0	100	100
All	All	1528/1626 (94%)	1471 (96%)	57 (4%)	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	306/325 (94%)	301 (98%)	5 (2%)	62	83
1	B	303/325 (93%)	300 (99%)	3 (1%)	76	88
2	C	187/196 (95%)	183 (98%)	4 (2%)	53	79
2	H	187/196 (95%)	184 (98%)	3 (2%)	62	83
3	D	183/184 (100%)	182 (100%)	1 (0%)	88	94
3	L	182/184 (99%)	181 (100%)	1 (0%)	88	94
All	All	1348/1410 (96%)	1331 (99%)	17 (1%)	69	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	LYS
1	B	304	HIS
1	B	351	CYS
2	C	30	PHE
2	C	75	LYS
2	C	136	CYS
2	C	221	CYS
3	D	216	ASP
2	H	3	GLN
2	H	30	PHE
2	H	68	LYS
3	L	216	ASP
1	A	37	GLU
1	A	202	ASP
1	A	221	LYS
1	A	283	ASP
1	A	351	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN

### 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](#)

14 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	F	1	5,1	14,14,15	0.32	0	17,19,21	0.46	0
5	NAG	F	2	5	14,14,15	0.27	0	17,19,21	0.39	0
5	BMA	F	3	5	11,11,12	0.55	0	15,15,17	0.77	0
5	MAN	F	4	5	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
5	MAN	F	5	5	11,11,12	0.73	0	15,15,17	0.95	1 (6%)
5	MAN	F	6	5	11,11,12	0.62	0	15,15,17	1.19	2 (13%)
5	MAN	F	7	5	11,11,12	0.65	0	15,15,17	0.98	2 (13%)
4	NAG	G	1	4,1	14,14,15	0.35	0	17,19,21	0.61	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.50	0
4	BMA	G	3	4	11,11,12	0.63	0	15,15,17	0.75	0
4	MAN	G	4	4	11,11,12	0.74	0	15,15,17	0.99	2 (13%)
4	MAN	G	5	4	11,11,12	0.66	0	15,15,17	0.97	2 (13%)
4	MAN	G	6	4	11,11,12	0.64	0	15,15,17	1.15	2 (13%)
4	MAN	G	7	4	11,11,12	0.63	0	15,15,17	1.00	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
5	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	2/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	6	MAN	C1-O5-C5	3.29	116.65	112.19
5	F	6	MAN	C1-O5-C5	3.21	116.54	112.19
5	F	4	MAN	O2-C2-C3	-2.92	104.29	110.14
4	G	7	MAN	C1-O5-C5	2.66	115.79	112.19
5	F	4	MAN	C1-O5-C5	2.61	115.72	112.19
5	F	7	MAN	C1-O5-C5	2.42	115.47	112.19
4	G	5	MAN	C1-O5-C5	2.29	115.30	112.19
5	F	5	MAN	O2-C2-C3	-2.27	105.60	110.14
4	G	4	MAN	O2-C2-C3	-2.16	105.80	110.14
4	G	4	MAN	C1-O5-C5	2.15	115.11	112.19
5	F	7	MAN	O2-C2-C3	-2.15	105.82	110.14
4	G	5	MAN	O2-C2-C3	-2.15	105.83	110.14
5	F	6	MAN	O2-C2-C3	-2.15	105.84	110.14
4	G	6	MAN	O2-C2-C3	-2.09	105.95	110.14
4	G	7	MAN	O2-C2-C3	-2.06	106.00	110.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2

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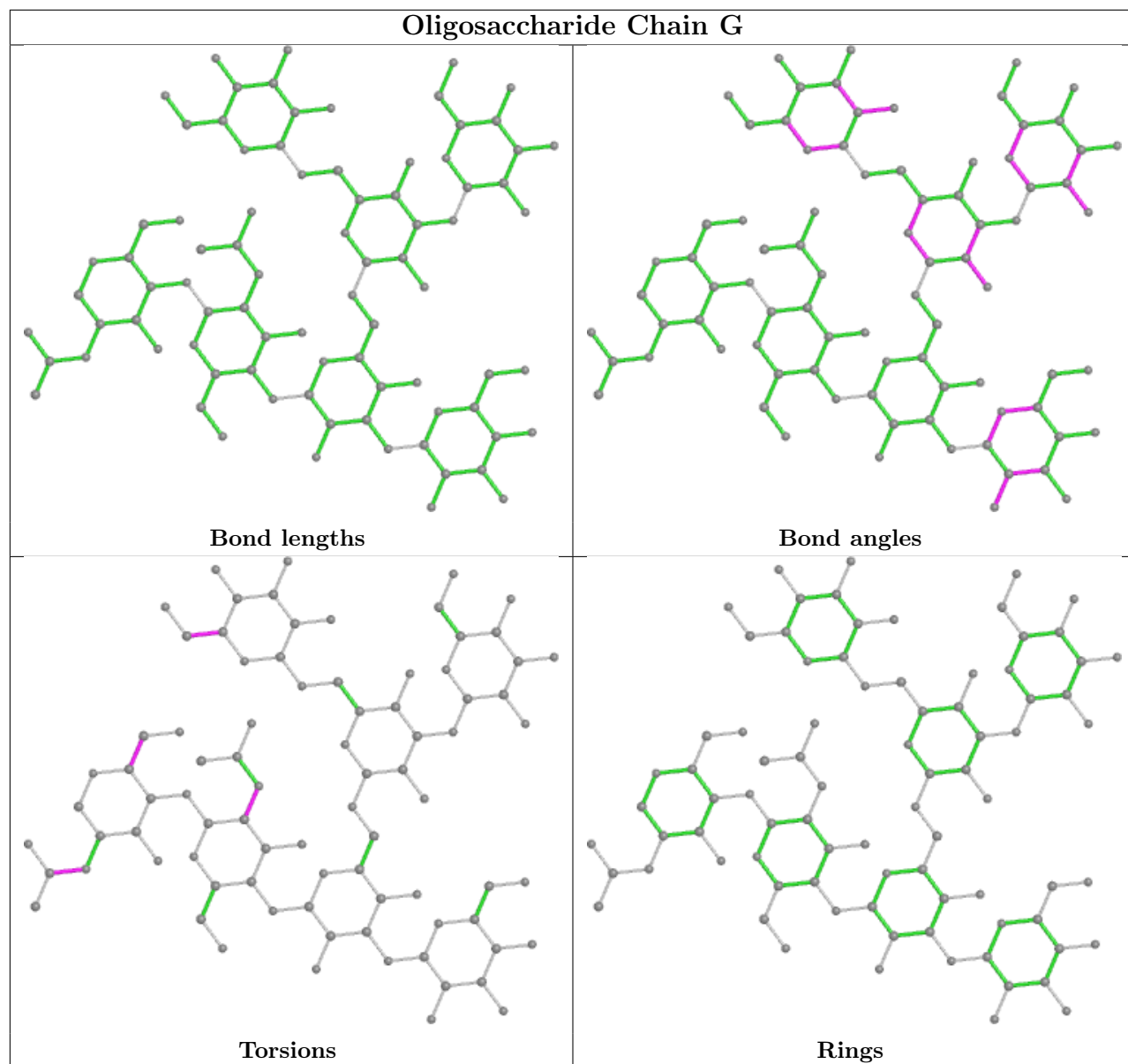
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	G	6	MAN	C4-C5-C6-O6
5	F	6	MAN	C4-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6
5	F	6	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7

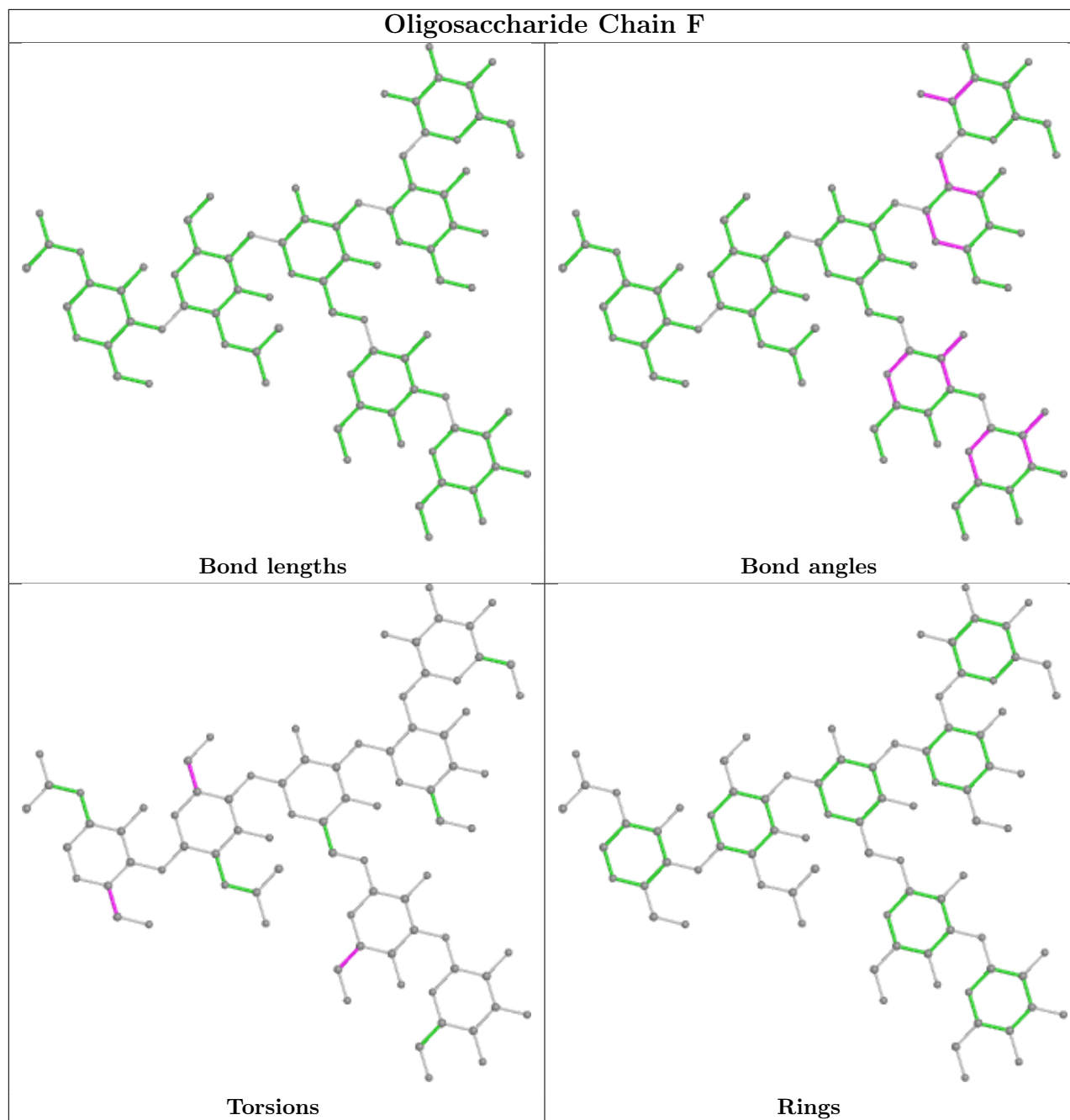
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	4	MAN	1	0
5	F	5	MAN	1	0
4	G	1	NAG	3	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](#)

4 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
6	GOL	C	302	-	5,5,5	0.92	0	5,5,5	0.97	0
7	NAG	B	402	1	14,14,15	0.16	0	17,19,21	0.49	0
6	GOL	B	401	-	5,5,5	0.91	0	5,5,5	0.98	0
6	GOL	C	301	-	5,5,5	0.93	0	5,5,5	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	302	-	-	0/4/4/4	-
7	NAG	B	402	1	-	3/6/23/26	0/1/1/1
6	GOL	B	401	-	-	0/4/4/4	-
6	GOL	C	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	402	NAG	O5-C5-C6-O6
7	B	402	NAG	C1-C2-N2-C7
7	B	402	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
6	C	301	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	342/365 (93%)	0.23	8 (2%) 60 54	84, 136, 212, 310	0
1	B	336/365 (92%)	0.22	6 (1%) 68 62	70, 137, 209, 234	0
2	C	221/231 (95%)	-0.14	0 100 100	65, 106, 153, 202	0
2	H	220/231 (95%)	-0.07	0 100 100	77, 112, 156, 214	0
3	D	216/217 (99%)	0.01	0 100 100	68, 93, 147, 186	0
3	L	215/217 (99%)	0.24	2 (0%) 84 79	68, 106, 152, 220	0
All	All	1550/1626 (95%)	0.10	16 (1%) 82 77	65, 117, 194, 310	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	VAL	4.3
1	A	350	ASN	3.6
1	A	243	GLY	3.1
1	A	302	VAL	2.8
1	B	90	GLN	2.8
1	A	223	PHE	2.7
1	A	328	LEU	2.5
1	A	199	GLY	2.5
1	B	224	GLU	2.5
1	A	110	VAL	2.4
1	A	369	TYR	2.4
1	B	91	SER	2.4
1	B	79	GLN	2.4
3	L	85	ALA	2.3
1	B	171	GLU	2.2
3	L	138	ILE	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](#)

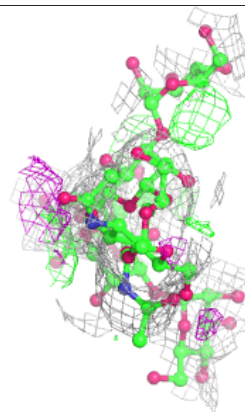
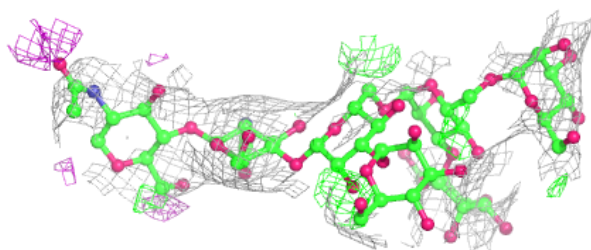
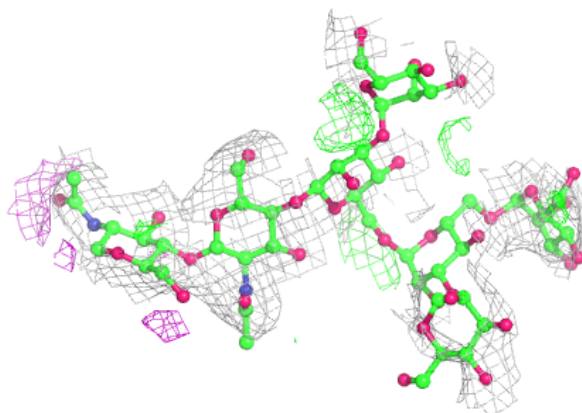
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

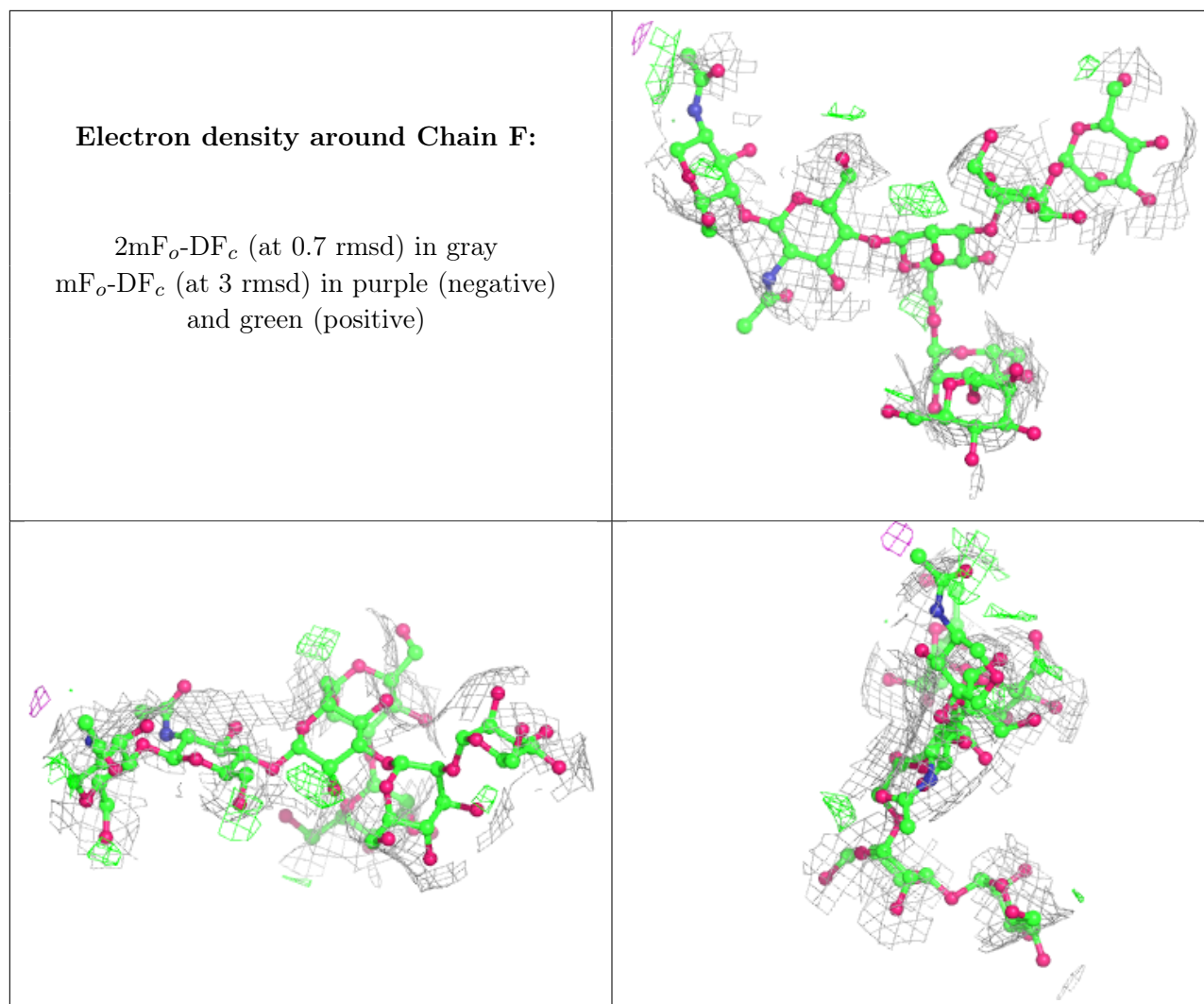
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	G	5	11/12	0.60	0.34	169,197,207,211	0
4	MAN	G	4	11/12	0.69	0.15	182,194,208,209	0
4	MAN	G	6	11/12	0.72	0.33	204,215,220,223	0
5	MAN	F	7	11/12	0.72	0.29	181,210,221,223	0
5	MAN	F	6	11/12	0.81	0.22	199,204,214,216	0
4	BMA	G	3	11/12	0.82	0.15	116,153,158,169	0
4	MAN	G	7	11/12	0.83	0.21	139,164,180,183	0
5	BMA	F	3	11/12	0.87	0.15	125,163,177,180	0
4	NAG	G	1	14/15	0.91	0.29	95,106,115,122	0
5	MAN	F	4	11/12	0.91	0.10	144,163,168,169	0
5	NAG	F	2	14/15	0.92	0.21	90,100,122,146	0
5	MAN	F	5	11/12	0.92	0.10	123,152,162,166	0
5	NAG	F	1	14/15	0.94	0.22	90,117,132,141	0
4	NAG	G	2	14/15	0.95	0.14	78,91,123,129	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.

**Electron density around Chain G:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 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(Å <sup>2</sup> )	Q<0.9
6	GOL	B	401	6/6	0.62	0.45	78,103,104,107	0
6	GOL	C	301	6/6	0.77	0.53	69,117,120,121	0
6	GOL	C	302	6/6	0.87	0.52	72,83,103,111	0
7	NAG	B	402	14/15	0.94	0.23	125,142,154,164	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.