



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:47 AM BST

PDB ID : 5UG0  
Title : Human antibody H2897 in complex with influenza hemagglutinin H1 Solomon Islands/03/2006  
Authors : Raymond, D.D.; Caradonna, T.; Schmidt, A.G.; Harrison, S.C.  
Deposited on : 2017-01-06  
Resolution : 3.40 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

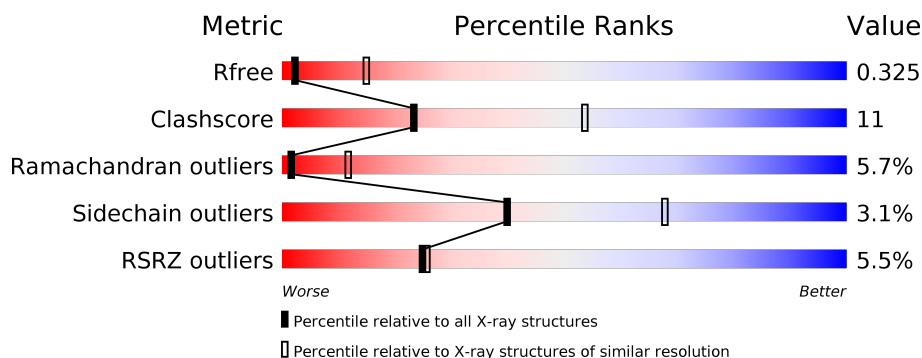
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.



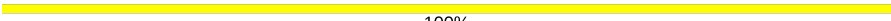
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	327	<div> <div>100%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>•</div> </div> </div>
2	B	182	<div> <div>100%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>7%</div> </div> </div>
3	C	216	<div> <div>10%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>••</div> </div> </div>
4	D	232	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>••</div> </div> </div>
5	E	3	<div> <div>100%</div> </div>
5	G	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	2	 100%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7416 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2558	1611	445	491	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1371	857	235	272	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP A7UPX0
B	178	SER	-	expression tag	UNP A7UPX0
B	179	LEU	-	expression tag	UNP A7UPX0
B	180	VAL	-	expression tag	UNP A7UPX0
B	181	PRO	-	expression tag	UNP A7UPX0
B	182	ARG	-	expression tag	UNP A7UPX0

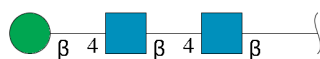
- Molecule 3 is a protein called 2897 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1625	1023	270	328	4			

- Molecule 4 is a protein called 2897 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	0	0	0
			1686	1061	285	333	7			

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



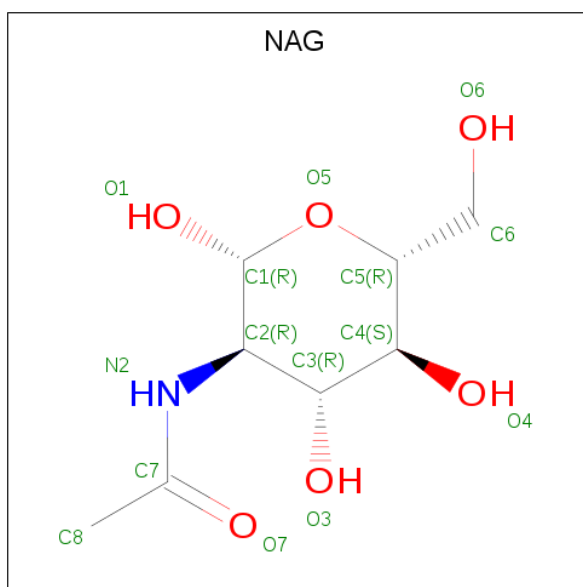
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

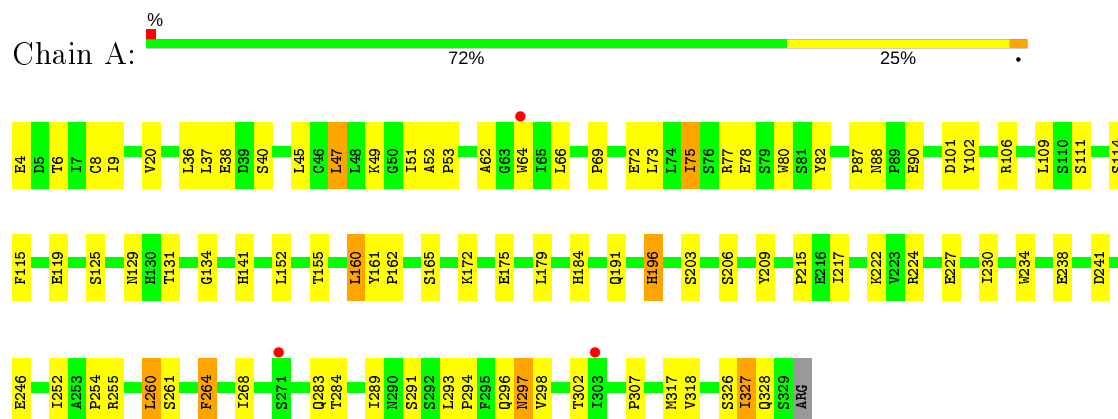


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

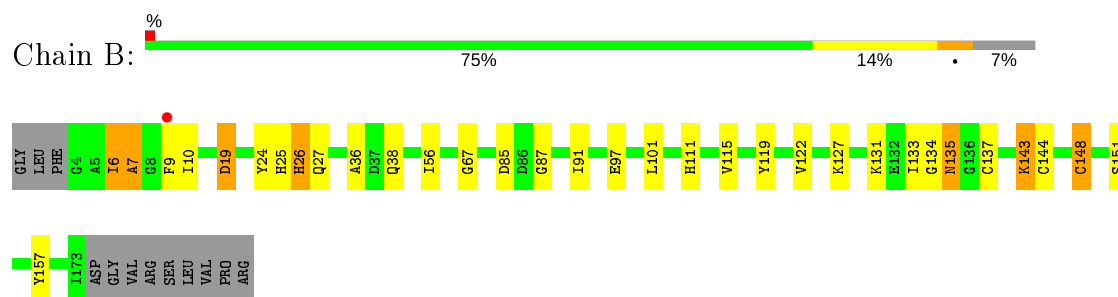
### 3 Residue-property plots [i](#)

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.

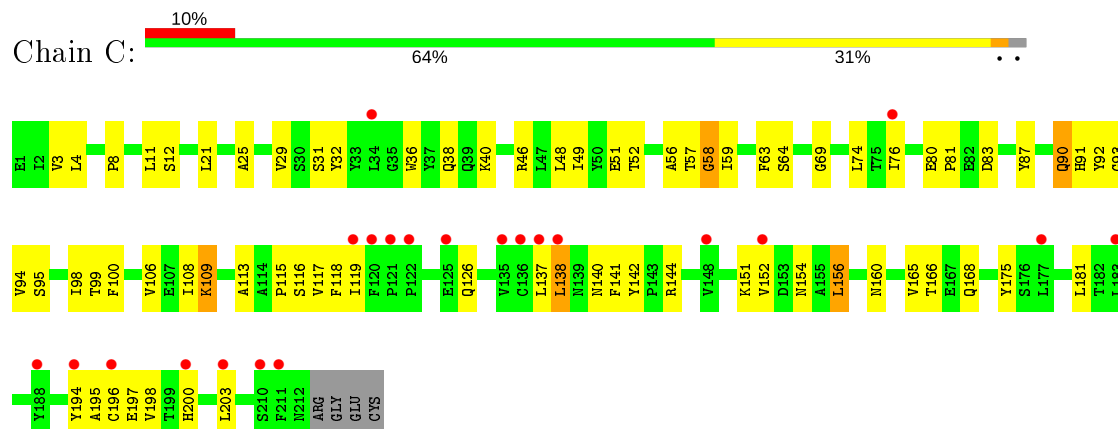
#### • Molecule 1: Hemagglutinin HA1



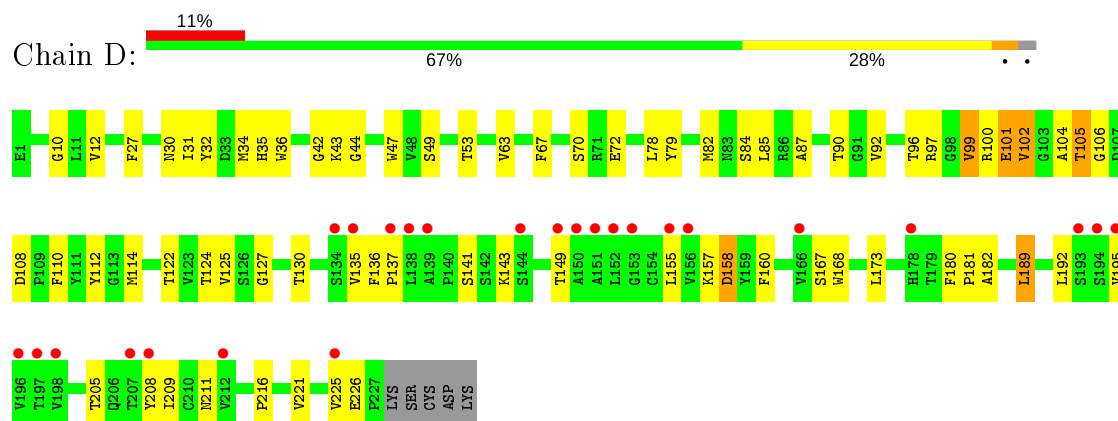
#### • Molecule 2: Hemagglutinin HA2



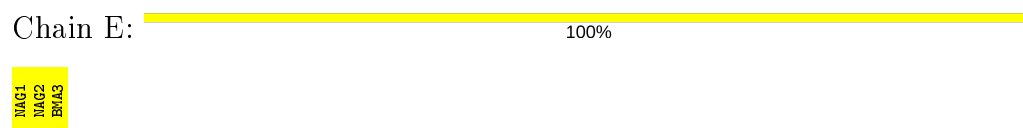
#### • Molecule 3: 2897 light chain



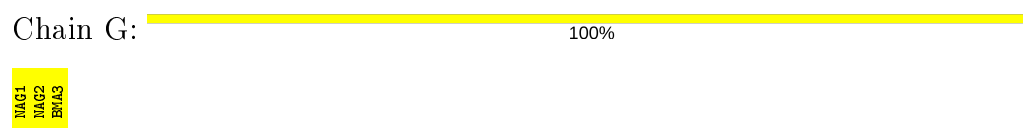
- Molecule 4: 2897 heavy chain



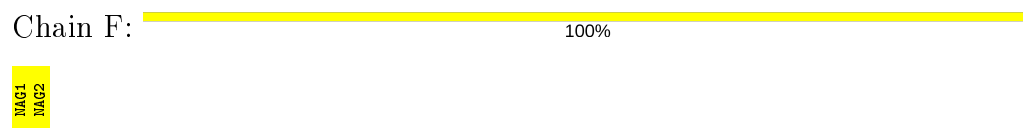
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 6: 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 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.20Å 142.20Å 200.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.41 – 3.40 46.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.41-3.40) 98.9 (46.41-3.40)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.240 , 0.278 0.287 , 0.325	Depositor DCC
$R_{free}$ test set	1621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.4	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 121.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.096 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: BMA, 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	0.49	0/2624	0.77	2/3571 (0.1%)
2	B	0.47	0/1397	0.72	0/1877
3	C	0.51	0/1662	0.81	2/2259 (0.1%)
4	D	0.48	0/1728	0.75	0/2356
All	All	0.49	0/7411	0.77	4/10063 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	51	GLU	C-N-CA	6.00	136.71	121.70
3	C	138	LEU	CD1-CG-CD2	-5.74	93.27	110.50
1	A	160	LEU	CD1-CG-CD2	-5.66	93.52	110.50
1	A	160	LEU	C-N-CA	5.09	134.43	121.70

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	2558	0	2463	57	0
2	B	1371	0	1299	18	0
3	C	1625	0	1583	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1686	0	1636	52	0
5	E	39	0	34	1	0
5	G	39	0	34	0	0
6	F	28	0	25	0	0
7	A	56	0	52	0	0
7	B	14	0	13	0	0
All	All	7416	0	7139	165	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 11.

All (165) 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)
4:D:92:VAL:HG22	4:D:122:THR:HG22	1.28	1.12
1:A:37:LEU:HD11	1:A:297:ASN:HB3	1.39	1.03
1:A:80:TRP:CH2	1:A:115:PHE:HE2	1.80	1.00
1:A:80:TRP:HH2	1:A:115:PHE:HE2	1.05	0.92
1:A:80:TRP:CH2	1:A:115:PHE:CE2	2.64	0.86
1:A:64:TRP:CD1	1:A:73:LEU:HD11	2.15	0.82
4:D:96:THR:CG2	4:D:114:MET:HB3	2.11	0.81
3:C:152:VAL:HG21	3:C:156:LEU:HD12	1.63	0.81
3:C:46:ARG:HH21	3:C:59:ILE:CD1	1.93	0.80
2:B:10:ILE:HB	2:B:135:ASN:HB3	1.65	0.79
4:D:96:THR:HG21	4:D:114:MET:HB3	1.62	0.79
4:D:160:PHE:HB2	4:D:189:LEU:HD23	1.68	0.76
4:D:92:VAL:HG22	4:D:122:THR:CG2	2.16	0.73
4:D:72:GLU:HG2	4:D:79:TYR:HE2	1.53	0.72
4:D:12:VAL:HG21	4:D:85:LEU:HD13	1.73	0.70
4:D:53:THR:HG21	4:D:101:GLU:HG2	1.73	0.70
4:D:34:MET:HB3	4:D:78:LEU:HD22	1.74	0.70
1:A:80:TRP:HH2	1:A:115:PHE:CE2	1.97	0.69
3:C:56:ALA:HB3	3:C:59:ILE:CG1	2.23	0.68
4:D:155:LEU:CD2	4:D:157:LYS:HB2	2.25	0.67
3:C:46:ARG:HH21	3:C:59:ILE:HD12	1.61	0.65
3:C:151:LYS:HB2	3:C:195:ALA:HB3	1.79	0.65
3:C:90:GLN:NE2	3:C:92:TYR:HB2	2.12	0.64
3:C:21:LEU:CD1	3:C:36:TRP:CZ3	2.81	0.64
3:C:3:VAL:O	3:C:25:ALA:HA	1.99	0.63
3:C:36:TRP:HB2	3:C:49:ILE:HD13	1.79	0.63
2:B:6:ILE:HG22	2:B:7:ALA:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:GLU:HB3	3:C:81:PRO:HD2	1.80	0.62
4:D:31:ILE:HA	4:D:101:GLU:HG3	1.82	0.62
3:C:56:ALA:HB3	3:C:59:ILE:HG12	1.81	0.62
1:A:106:ARG:HH21	1:A:268:ILE:HG21	1.65	0.62
3:C:160:ASN:HA	3:C:181:LEU:HD12	1.82	0.61
1:A:294:PRO:HG3	2:B:56:ILE:HG12	1.82	0.61
1:A:62:ALA:HB2	1:A:102:TYR:CE1	2.36	0.61
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.83	0.61
3:C:48:LEU:HB2	3:C:49:ILE:HD12	1.83	0.61
1:A:160:LEU:HG	1:A:196:HIS:HB2	1.83	0.61
1:A:191:GLN:HB2	1:A:217:ILE:HD11	1.83	0.60
1:A:9:ILE:HD13	2:B:119:TYR:HA	1.83	0.60
4:D:180:PHE:HE1	4:D:195:VAL:HG12	1.67	0.59
1:A:38:GLU:OE2	1:A:40:SER:HB3	2.01	0.59
3:C:38:GLN:OE1	3:C:46:ARG:HD3	2.02	0.59
2:B:6:ILE:HG22	2:B:7:ALA:H	1.68	0.59
4:D:99:VAL:HG21	4:D:112:TYR:CE1	2.38	0.59
1:A:4:GLU:HA	2:B:143:LYS:HE2	1.85	0.58
3:C:113:ALA:HB3	3:C:142:TYR:H	1.67	0.58
4:D:34:MET:CB	4:D:78:LEU:HD22	2.34	0.58
1:A:6:THR:OG1	2:B:27:GLN:HB3	2.05	0.56
4:D:63:VAL:HG12	4:D:67:PHE:HB2	1.86	0.56
3:C:12:SER:HB2	3:C:109:LYS:HB2	1.88	0.56
4:D:167:SER:HB3	4:D:211:ASN:HB2	1.88	0.56
3:C:126:GLN:HB3	4:D:136:PHE:CZ	2.42	0.55
2:B:7:ALA:HA	2:B:137:CYS:SG	2.46	0.55
3:C:21:LEU:HD12	3:C:36:TRP:CZ3	2.42	0.55
3:C:93:GLY:HA2	4:D:112:TYR:CE1	2.42	0.55
1:A:296:GLN:HE21	1:A:298:VAL:HB	1.72	0.55
4:D:90:THR:HG22	4:D:124:THR:HA	1.88	0.55
4:D:182:ALA:HA	4:D:192:LEU:HB3	1.89	0.55
3:C:144:ARG:HE	3:C:165:VAL:HG11	1.72	0.54
4:D:136:PHE:CZ	4:D:155:LEU:HD22	2.43	0.54
4:D:101:GLU:O	4:D:102:VAL:HG23	2.08	0.53
2:B:111:HIS:O	2:B:115:VAL:HG23	2.08	0.53
3:C:152:VAL:HG13	3:C:194:TYR:HE2	1.73	0.53
4:D:31:ILE:HD12	4:D:100:ARG:HG3	1.90	0.53
1:A:8:CYS:O	2:B:24:TYR:HA	2.09	0.53
1:A:224:ARG:HH12	5:E:1:NAG:C7	2.22	0.53
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.91	0.52
3:C:166:THR:HG22	4:D:181:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:O	1:A:114:SER:HA	2.10	0.52
1:A:230:ILE:HG21	1:A:252:ILE:HG13	1.91	0.52
3:C:8:PRO:HG3	3:C:11:LEU:HD13	1.91	0.52
3:C:152:VAL:HG22	3:C:194:TYR:HD2	1.75	0.51
1:A:20:VAL:HG21	1:A:318:VAL:HB	1.93	0.51
1:A:64:TRP:HD1	1:A:73:LEU:HD11	1.68	0.51
1:A:69:PRO:HB2	1:A:141:HIS:HB2	1.93	0.51
1:A:179:LEU:O	1:A:254:PRO:HB3	2.10	0.50
3:C:117:VAL:HG22	3:C:198:VAL:HG21	1.92	0.50
1:A:62:ALA:HB2	1:A:102:TYR:HE1	1.76	0.50
4:D:63:VAL:O	4:D:63:VAL:HG12	2.11	0.50
3:C:49:ILE:N	3:C:49:ILE:HD12	2.26	0.50
4:D:168:TRP:CB	4:D:173:LEU:HD12	2.42	0.50
1:A:160:LEU:HD23	1:A:161:TYR:O	2.11	0.50
4:D:70:SER:O	4:D:78:LEU:HD12	2.11	0.49
3:C:92:TYR:HE2	4:D:99:VAL:HG23	1.77	0.49
4:D:158:ASP:HB3	4:D:189:LEU:HD13	1.94	0.49
1:A:9:ILE:CD1	2:B:119:TYR:HA	2.43	0.49
3:C:118:PHE:HB2	3:C:137:LEU:HB2	1.95	0.48
1:A:75:ILE:C	1:A:77:ARG:H	2.16	0.48
3:C:11:LEU:HB3	3:C:106:VAL:HG22	1.94	0.48
4:D:168:TRP:HB3	4:D:173:LEU:HD12	1.96	0.48
4:D:97:ARG:HG2	4:D:97:ARG:HH11	1.78	0.48
1:A:8:CYS:HB2	2:B:25:HIS:HB3	1.96	0.48
1:A:36:LEU:HD11	1:A:317:MET:HB2	1.96	0.48
4:D:63:VAL:HG11	4:D:67:PHE:CD1	2.49	0.48
3:C:138:LEU:HD12	3:C:141:PHE:CE1	2.49	0.47
1:A:227:GLU:H	4:D:105:THR:HG23	1.79	0.47
1:A:179:LEU:HD23	1:A:234:TRP:CB	2.44	0.47
4:D:32:TYR:CG	4:D:97:ARG:HD2	2.49	0.47
3:C:144:ARG:HH21	3:C:165:VAL:HG12	1.80	0.47
4:D:135:VAL:HB	4:D:221:VAL:HG11	1.97	0.46
1:A:179:LEU:CD2	1:A:234:TRP:HB3	2.45	0.46
4:D:209:ILE:HD12	4:D:211:ASN:HD21	1.80	0.46
1:A:38:GLU:HG2	1:A:289:ILE:HG23	1.98	0.46
1:A:9:ILE:HD11	2:B:122:VAL:HG21	1.95	0.46
3:C:116:SER:O	3:C:138:LEU:HA	2.14	0.46
1:A:184:HIS:CD2	1:A:215:PRO:HA	2.51	0.46
1:A:203:SER:HB3	1:A:246:GLU:HB2	1.97	0.46
3:C:152:VAL:HG13	3:C:194:TYR:CE2	2.49	0.46
3:C:48:LEU:HD22	3:C:59:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HB2	1:A:255:ARG:HB2	1.98	0.46
3:C:115:PRO:HD3	3:C:200:HIS:ND1	2.32	0.45
1:A:293:LEU:O	1:A:307:PRO:HB3	2.16	0.45
1:A:131:THR:HG23	1:A:155:THR:OG1	2.17	0.45
1:A:45:LEU:HD23	1:A:283:GLN:NE2	2.32	0.45
4:D:100:ARG:HE	4:D:104:ALA:HB3	1.82	0.45
4:D:96:THR:HG22	4:D:97:ARG:N	2.31	0.45
1:A:327:ILE:HG22	1:A:328:GLN:N	2.32	0.45
3:C:64:SER:O	3:C:74:LEU:HD12	2.16	0.45
1:A:238:GLU:HG2	1:A:241:ASP:HB2	1.97	0.45
4:D:155:LEU:HD23	4:D:157:LYS:HB2	1.98	0.44
3:C:119:ILE:HD12	3:C:196:CYS:HB2	1.98	0.44
1:A:206:SER:HB2	1:A:209:TYR:HB3	1.99	0.44
3:C:92:TYR:CD1	3:C:98:ILE:HD12	2.51	0.44
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.52	0.44
3:C:29:VAL:HG13	3:C:91:HIS:CD2	2.52	0.44
2:B:131:LYS:HG3	2:B:133:ILE:HG23	1.98	0.44
3:C:63:PHE:CD1	3:C:76:ILE:HG12	2.53	0.44
4:D:100:ARG:NH2	4:D:110:PHE:HB2	2.32	0.44
4:D:82:MET:HB3	4:D:85:LEU:HD21	2.00	0.43
4:D:182:ALA:HB2	4:D:192:LEU:HD23	2.00	0.43
4:D:43:LYS:HG2	4:D:44:GLY:H	1.82	0.43
4:D:27:PHE:CE1	4:D:97:ARG:HD3	2.54	0.43
1:A:49:LYS:HB2	1:A:51:ILE:HD12	2.00	0.43
2:B:87:GLY:O	2:B:91:ILE:HG12	2.18	0.43
4:D:63:VAL:CG1	4:D:67:PHE:HB2	2.48	0.43
4:D:32:TYR:OH	4:D:108:ASP:HB3	2.19	0.42
1:A:111:SER:HB3	1:A:264:PHE:CE2	2.54	0.42
1:A:222:LYS:HG3	1:A:227:GLU:HG3	2.01	0.42
2:B:148:CYS:O	2:B:151:SER:HB2	2.19	0.42
3:C:151:LYS:HE2	3:C:197:GLU:HB2	2.01	0.42
1:A:66:LEU:HD23	1:A:179:LEU:HD13	2.00	0.42
1:A:73:LEU:O	1:A:77:ARG:HB2	2.19	0.42
4:D:63:VAL:CG1	4:D:67:PHE:CG	3.03	0.42
3:C:92:TYR:HD1	3:C:98:ILE:HD12	1.83	0.42
3:C:4:LEU:HD12	3:C:25:ALA:HB2	2.02	0.42
1:A:160:LEU:O	1:A:162:PRO:HD3	2.20	0.41
1:A:36:LEU:HA	1:A:293:LEU:HD22	2.00	0.41
3:C:115:PRO:HD2	3:C:203:LEU:HG	2.02	0.41
4:D:208:TYR:CE1	4:D:225:VAL:HB	2.54	0.41
3:C:40:LYS:HE3	3:C:46:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:ILE:HD11	3:C:74:LEU:HD13	2.03	0.41
3:C:56:ALA:C	3:C:58:GLY:H	2.24	0.41
1:A:260:LEU:HD23	1:A:260:LEU:H	1.86	0.41
1:A:134:GLY:HA2	4:D:102:VAL:HG21	2.02	0.41
3:C:11:LEU:O	3:C:106:VAL:HA	2.21	0.41
4:D:87:ALA:HA	4:D:125:VAL:HG21	2.03	0.41
1:A:47:LEU:HB3	1:A:52:ALA:HA	2.02	0.41
3:C:168:GLN:HG3	3:C:175:TYR:CZ	2.56	0.41
4:D:143:LYS:NZ	4:D:149:THR:HG21	2.35	0.40
3:C:56:ALA:HB3	3:C:59:ILE:HB	2.03	0.40
4:D:36:TRP:HD1	4:D:49:SER:OG	2.04	0.40
3:C:138:LEU:CD1	3:C:141:PHE:CE1	3.05	0.40
1:A:222:LYS:HE3	1:A:227:GLU:HG3	2.02	0.40
2:B:97:GLU:O	2:B:101:LEU:HD13	2.21	0.40
3:C:38:GLN:HB2	3:C:48:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/327 (99%)	278 (86%)	37 (11%)	9 (3%)	5	24
2	B	168/182 (92%)	144 (86%)	14 (8%)	10 (6%)	1	10
3	C	210/216 (97%)	168 (80%)	26 (12%)	16 (8%)	1	6
4	D	225/232 (97%)	184 (82%)	23 (10%)	18 (8%)	1	6
All	All	927/957 (97%)	774 (84%)	100 (11%)	53 (6%)	1	12

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ILE
2	B	135	ASN
3	C	31	SER
3	C	32	TYR
3	C	140	ASN
4	D	99	VAL
4	D	102	VAL
4	D	205	THR
1	A	75	ILE
1	A	172	LYS
1	A	196	HIS
1	A	291	SER
2	B	67	GLY
2	B	134	GLY
3	C	87	TYR
3	C	108	ILE
4	D	101	GLU
4	D	127	GLY
4	D	130	THR
1	A	119	GLU
1	A	125	SER
2	B	7	ALA
2	B	9	PHE
3	C	58	GLY
3	C	94	VAL
3	C	95	SER
3	C	109	LYS
4	D	84	SER
4	D	137	PRO
4	D	189	LEU
4	D	226	GLU
1	A	87	PRO
2	B	6	ILE
2	B	26	HIS
2	B	127	LYS
2	B	143	LYS
2	B	157	TYR
3	C	57	THR
3	C	156	LEU
4	D	105	THR
4	D	106	GLY
3	C	83	ASP
3	C	99	THR

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Mol	Chain	Res	Type
3	C	154	ASN
4	D	141	SER
4	D	158	ASP
1	A	326	SER
3	C	52	THR
4	D	30	ASN
4	D	10	GLY
4	D	42	GLY
4	D	216	PRO
3	C	69	GLY

### 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	286/287 (100%)	271 (95%)	15 (5%)	23	53
2	B	147/157 (94%)	141 (96%)	6 (4%)	30	59
3	C	184/187 (98%)	182 (99%)	2 (1%)	73	86
4	D	186/191 (97%)	184 (99%)	2 (1%)	73	86
All	All	803/822 (98%)	778 (97%)	25 (3%)	40	68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	72	GLU
1	A	88	ASN
1	A	90	GLU
1	A	101	ASP
1	A	109	LEU
1	A	129	ASN
1	A	165	SER
1	A	175	GLU
1	A	260	LEU
1	A	261	SER

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Mol	Chain	Res	Type
1	A	264	PHE
1	A	284	THR
1	A	297	ASN
1	A	302	THR
2	B	19	ASP
2	B	26	HIS
2	B	38	GLN
2	B	85	ASP
2	B	144	CYS
2	B	148	CYS
3	C	90	GLN
3	C	100	PHE
4	D	35	HIS
4	D	47	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	HIS
1	A	296	GLN
2	B	43	ASN
3	C	90	GLN
3	C	91	HIS
4	D	211	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](#)

8 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	E	1	1,5	14,14,15	0.32	0	17,19,21	0.72	0
5	NAG	E	2	5	14,14,15	0.33	0	17,19,21	1.27	2 (11%)
5	BMA	E	3	5	11,11,12	0.37	0	15,15,17	0.84	1 (6%)
6	NAG	F	1	1,6	14,14,15	0.37	0	17,19,21	0.87	1 (5%)
6	NAG	F	2	6	14,14,15	0.35	0	17,19,21	0.86	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.35	0	17,19,21	1.02	2 (11%)
5	NAG	G	2	5	14,14,15	0.33	0	17,19,21	0.94	2 (11%)
5	BMA	G	3	5	11,11,12	0.41	0	15,15,17	0.94	1 (6%)

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	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	O5-C1-C2	-3.73	105.39	111.29
6	F	2	NAG	C1-O5-C5	3.10	116.39	112.19
5	G	3	BMA	C1-O5-C5	3.06	116.34	112.19
5	G	1	NAG	C1-O5-C5	2.81	116.00	112.19
5	G	2	NAG	O5-C1-C2	-2.80	106.87	111.29
5	E	3	BMA	C1-O5-C5	2.71	115.87	112.19
5	G	1	NAG	O5-C1-C2	-2.43	107.44	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	C1-C2-N2	2.37	114.53	110.49
5	G	2	NAG	C1-O5-C5	2.33	115.35	112.19
6	F	1	NAG	O5-C1-C2	-2.24	107.75	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

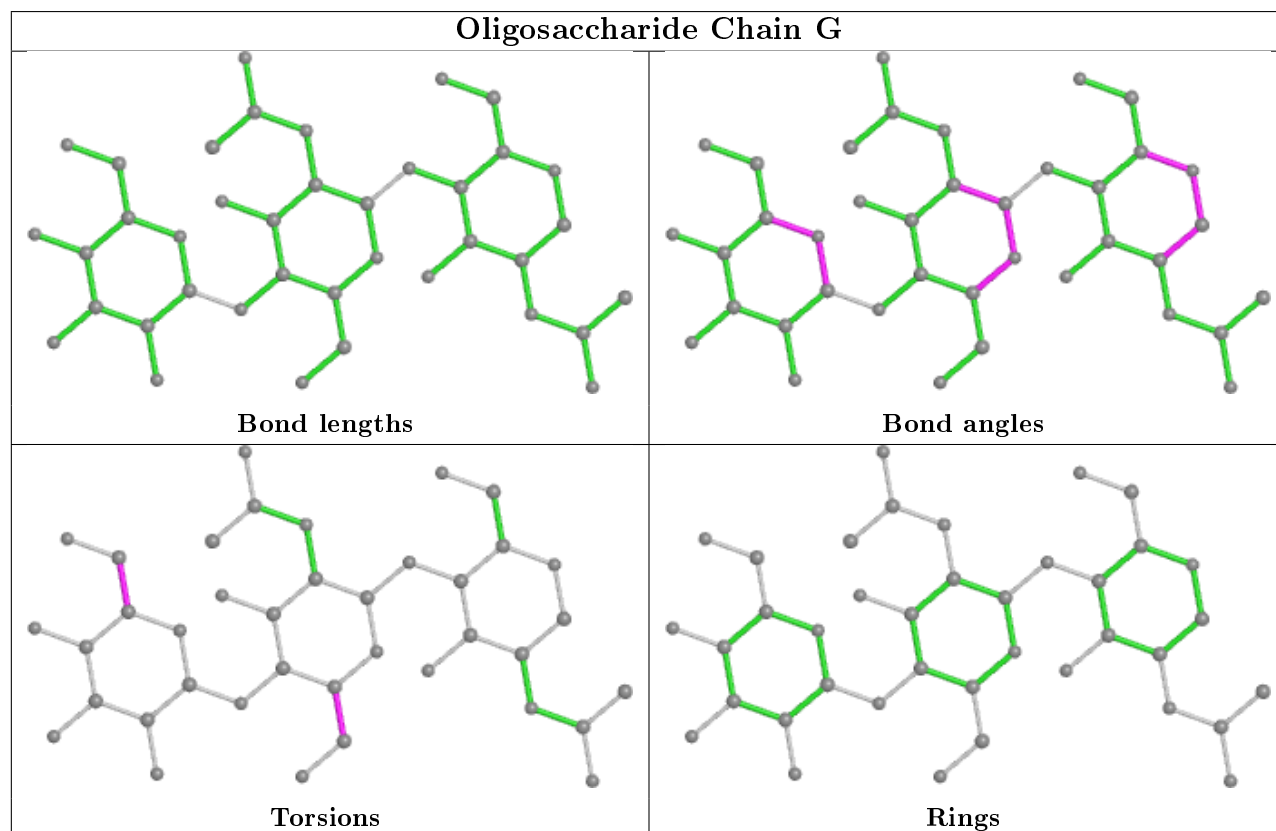
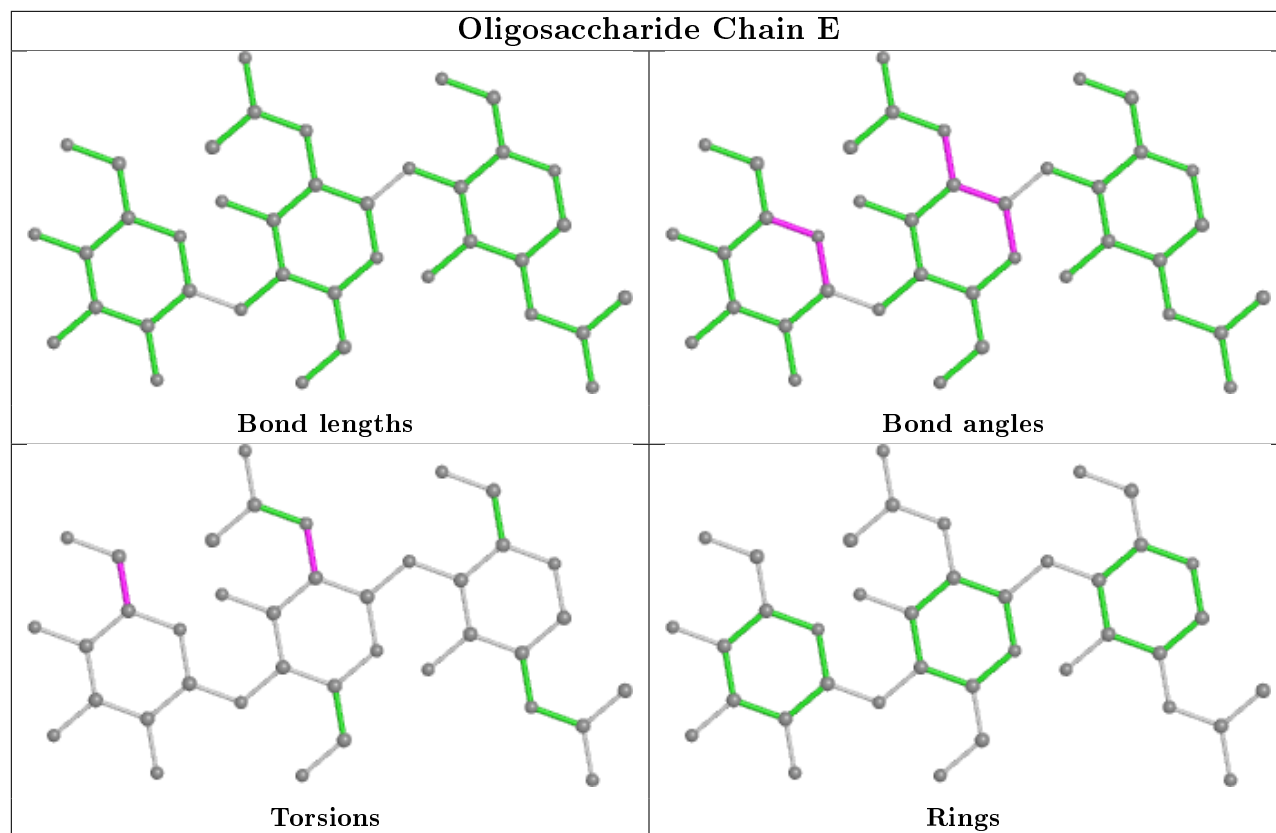
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
5	G	2	NAG	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6

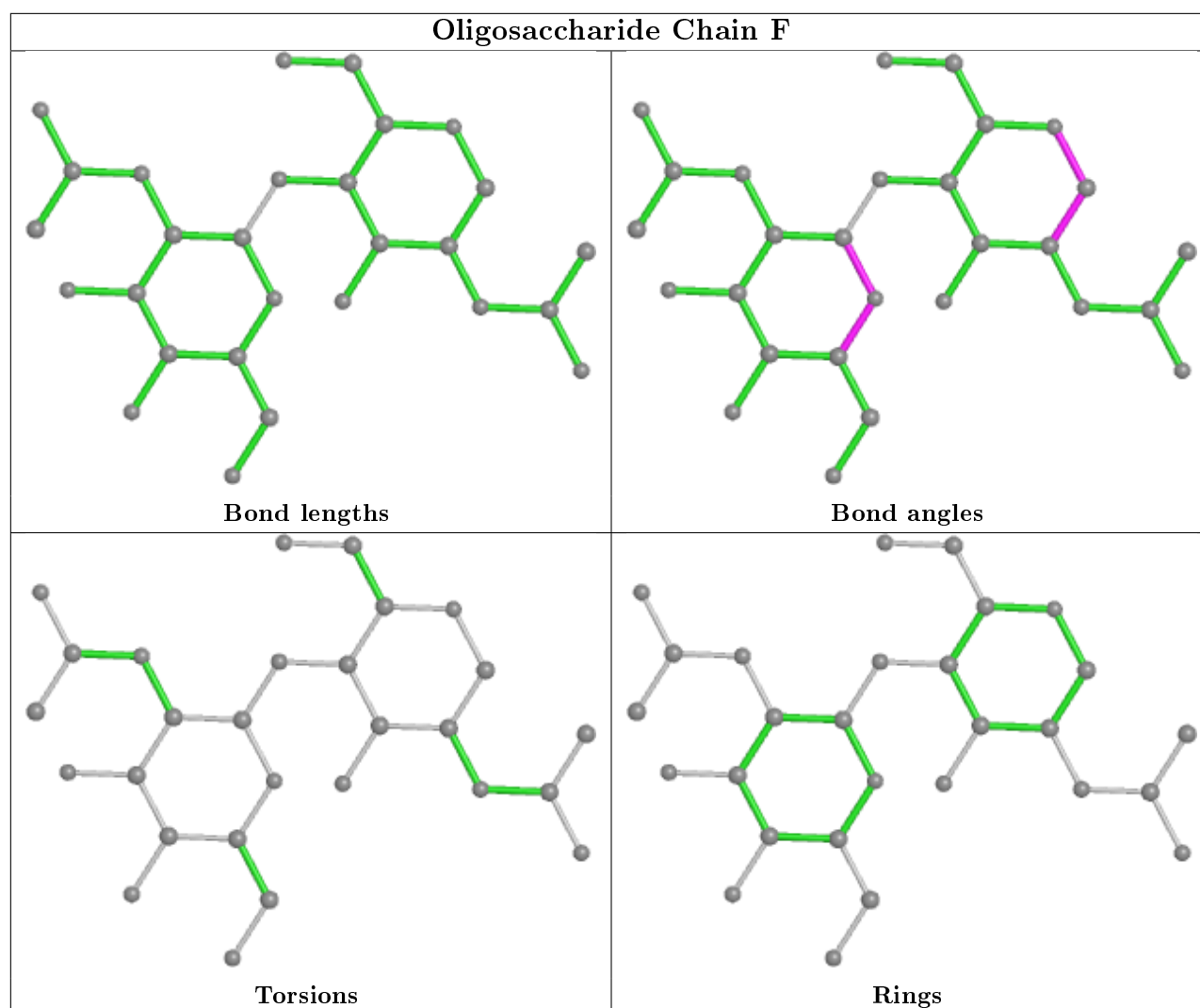
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	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](#)

5 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	$\# Z  > 2$
7	NAG	A	402	1	14,14,15	0.40	0	17,19,21	1.78	2 (11%)
7	NAG	A	407	-	14,14,15	0.33	0	19,19,21	0.89	1 (5%)
7	NAG	B	201	2	14,14,15	0.34	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	401	1	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
7	NAG	A	406	1	14,14,15	0.36	0	17,19,21	0.40	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
7	NAG	A	402	1	-	2/6/23/26	0/1/1/1
7	NAG	A	407	-	-	1/6/22/26	0/1/1/1
7	NAG	B	201	2	-	1/6/23/26	0/1/1/1
7	NAG	A	401	1	-	1/6/23/26	0/1/1/1
7	NAG	A	406	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	NAG	O5-C1-C2	5.08	119.31	111.29
7	A	402	NAG	C1-O5-C5	4.60	118.43	112.19
7	A	407	NAG	O1-C1-C2	2.43	114.26	109.22
7	A	401	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	NAG	O5-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	B	201	NAG	O5-C5-C6-O6
7	A	402	NAG	C4-C5-C6-O6
7	A	402	NAG	O5-C5-C6-O6
7	A	406	NAG	C4-C5-C6-O6
7	A	407	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	326/327 (99%)	-0.00	3 (0%) 84 83	112, 136, 159, 178	0
2	B	170/182 (93%)	0.08	1 (0%) 89 89	102, 142, 175, 188	0
3	C	212/216 (98%)	0.49	22 (10%) 6 8	128, 171, 231, 243	0
4	D	227/232 (97%)	0.69	25 (11%) 5 6	121, 153, 250, 257	0
All	All	935/957 (97%)	0.29	51 (5%) 25 25	102, 146, 235, 257	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	195	VAL	11.1
4	D	196	VAL	10.0
4	D	194	SER	8.9
4	D	152	LEU	7.2
3	C	119	ILE	6.8
4	D	138	LEU	6.7
3	C	120	PHE	6.6
4	D	208	TYR	6.5
4	D	139	ALA	6.2
3	C	121	PRO	5.9
4	D	197	THR	5.4
3	C	137	LEU	5.1
4	D	155	LEU	5.0
3	C	138	LEU	4.5
4	D	193	SER	4.4
4	D	198	VAL	4.2
4	D	151	ALA	4.1
4	D	225	VAL	4.1
4	D	135	VAL	4.0
3	C	196	CYS	4.0
4	D	166	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
4	D	137	PRO	3.8
3	C	211	PHE	3.8
1	A	303	ILE	3.5
3	C	188	TYR	3.3
3	C	194	TYR	3.2
4	D	156	VAL	3.2
3	C	183	LEU	3.1
4	D	212	VAL	2.9
3	C	122	PRO	2.8
3	C	200	HIS	2.8
4	D	153	GLY	2.7
4	D	144	SER	2.6
3	C	203	LEU	2.6
3	C	76	ILE	2.5
1	A	271	SER	2.5
4	D	149	THR	2.4
3	C	34	LEU	2.3
3	C	135	VAL	2.3
2	B	9	PHE	2.3
3	C	136	CYS	2.2
4	D	150	ALA	2.2
4	D	178	HIS	2.2
3	C	177	LEU	2.1
4	D	134	SER	2.1
3	C	125	GLU	2.1
4	D	207	THR	2.1
3	C	210	SER	2.1
3	C	152	VAL	2.1
1	A	64	TRP	2.0
3	C	148	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

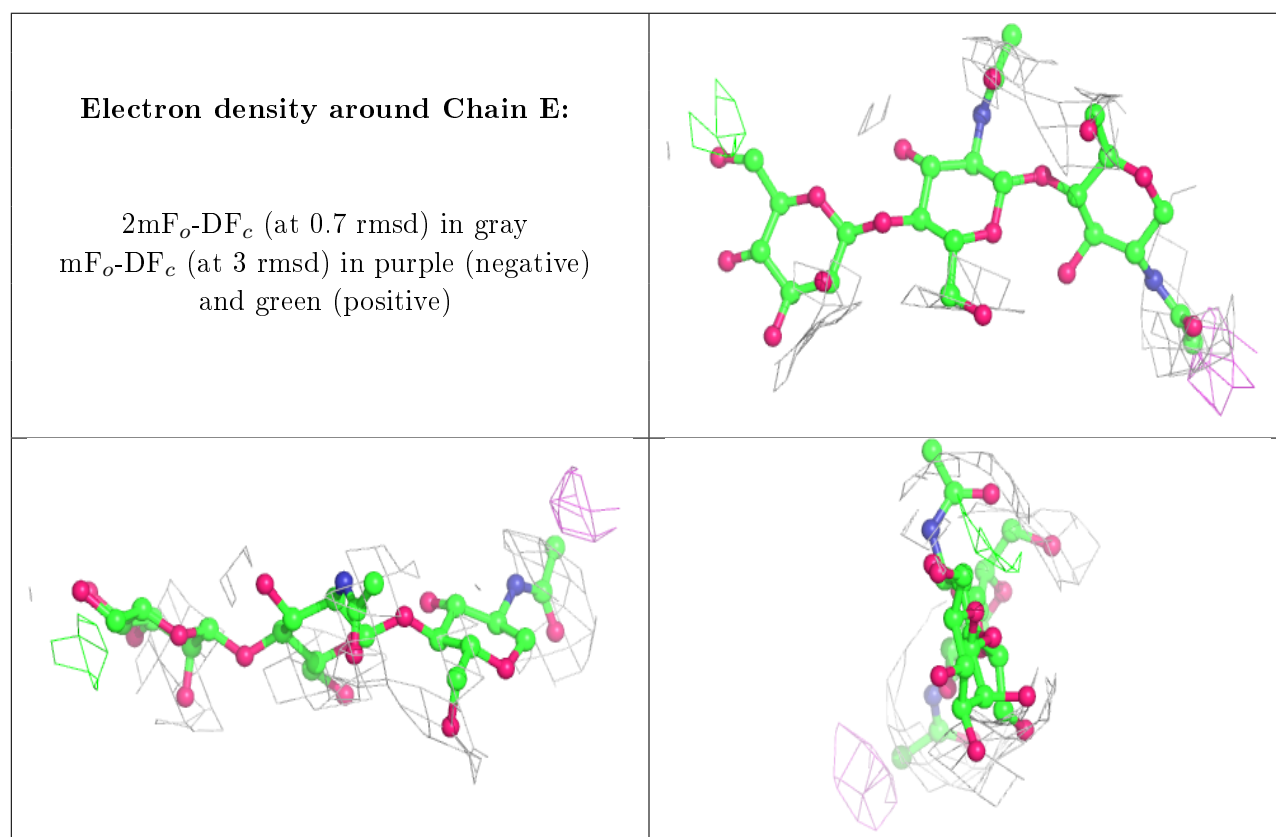
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

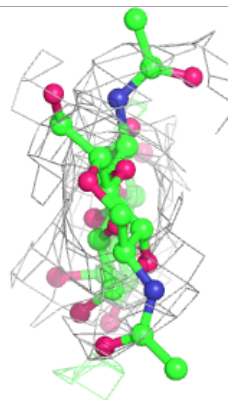
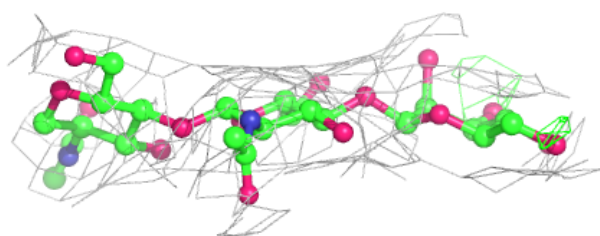
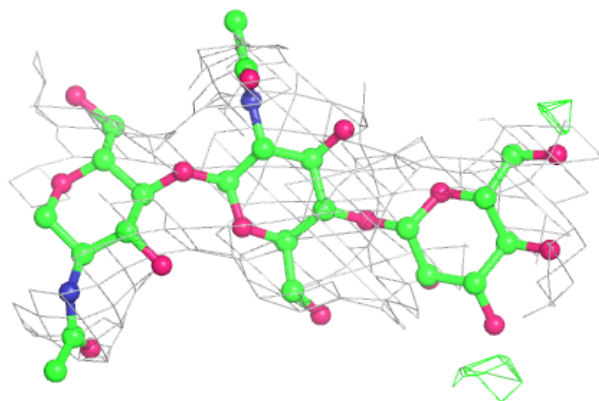
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	G	3	11/12	0.71	0.17	224,227,227,228	0
6	NAG	F	2	14/15	0.79	0.19	213,219,220,220	0
5	NAG	G	1	14/15	0.83	0.22	208,211,216,219	0
6	NAG	F	1	14/15	0.83	0.15	209,213,215,217	0
5	NAG	G	2	14/15	0.84	0.24	222,225,226,227	0
5	BMA	E	3	11/12	0.85	0.13	209,214,215,215	0
5	NAG	E	1	14/15	0.93	0.23	156,165,172,180	0
5	NAG	E	2	14/15	0.94	0.14	188,192,198,204	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.

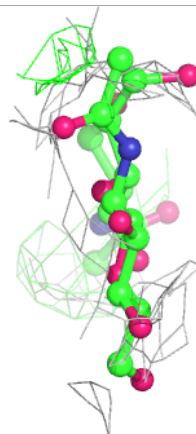
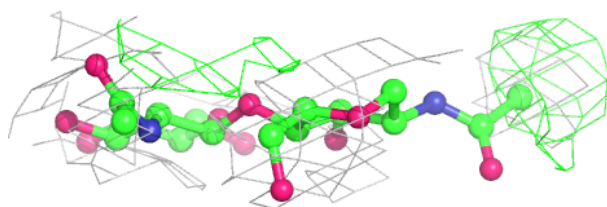
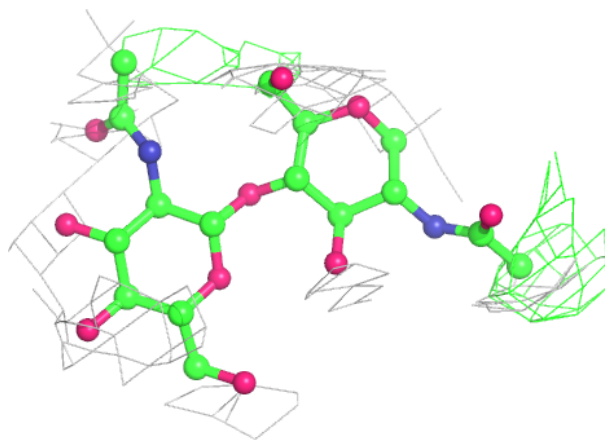


**Electron density around Chain G:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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
7	NAG	B	201	14/15	0.52	0.31	241,244,247,247	0
7	NAG	A	407	14/15	0.78	0.15	199,208,209,209	0
7	NAG	A	406	14/15	0.79	0.15	212,214,217,218	0
7	NAG	A	401	14/15	0.93	0.11	181,185,188,188	0
7	NAG	A	402	14/15	0.93	0.09	190,193,195,196	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.