



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:14 AM BST

PDB ID : 4JUN  
Title : Crystal structure of H5N1 influenza virus hemagglutinin, clade 5  
Authors : DuBois, R.M.; Zaraket, H.; Reddivari, M.; Coop, T.; Heath, R.J.; White, S.W.; Russell, C.J.  
Deposited on : 2013-03-25  
Resolution : 2.34 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

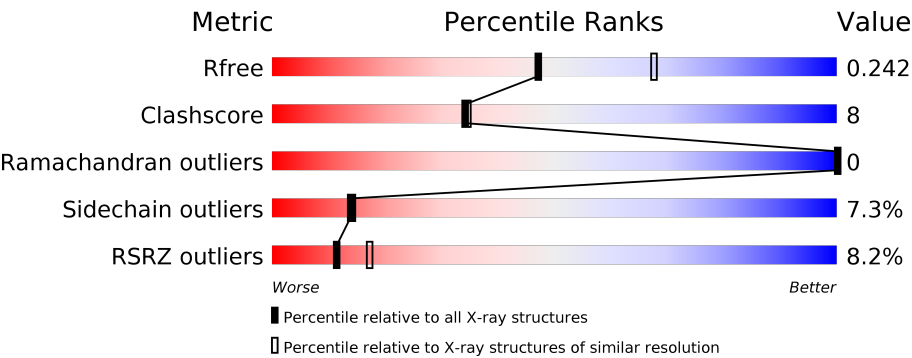
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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.



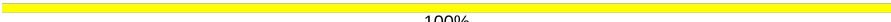
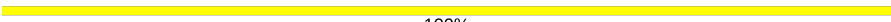
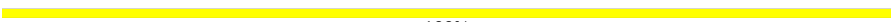
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	329	<div><div></div><div>84%12%••</div></div>
1	C	329	<div><div>3%</div><div>79%17%••</div></div>
1	E	329	<div><div>2%</div><div>79%17%••</div></div>
2	B	182	<div><div>4%</div><div>76%15%•7%</div></div>
2	D	182	<div><div>25%</div><div>66%19%5%10%</div></div>
2	F	182	<div><div>26%</div><div>63%25%•9%</div></div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 100%
3	I	2	 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12083 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	321	Total	C	N	O	S	0	1	0
			2543	1605	442	482	14			
1	C	321	Total	C	N	O	S	0	1	0
			2543	1605	442	482	14			
1	E	321	Total	C	N	O	S	0	1	0
			2543	1605	442	482	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP Q2F4V6
A	6	SER	-	expression tag	UNP Q2F4V6
A	7	ALA	-	expression tag	UNP Q2F4V6
A	8	ASP	-	expression tag	UNP Q2F4V6
A	9	PRO	-	expression tag	UNP Q2F4V6
A	10	GLY	-	expression tag	UNP Q2F4V6
C	5	GLY	-	expression tag	UNP Q2F4V6
C	6	SER	-	expression tag	UNP Q2F4V6
C	7	ALA	-	expression tag	UNP Q2F4V6
C	8	ASP	-	expression tag	UNP Q2F4V6
C	9	PRO	-	expression tag	UNP Q2F4V6
C	10	GLY	-	expression tag	UNP Q2F4V6
E	5	GLY	-	expression tag	UNP Q2F4V6
E	6	SER	-	expression tag	UNP Q2F4V6
E	7	ALA	-	expression tag	UNP Q2F4V6
E	8	ASP	-	expression tag	UNP Q2F4V6
E	9	PRO	-	expression tag	UNP Q2F4V6
E	10	GLY	-	expression tag	UNP Q2F4V6

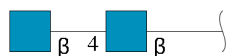
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1382	859	243	272	8			
2	D	164	Total	C	N	O	S	0	0	0
			1329	827	230	264	8			
2	F	166	Total	C	N	O	S	0	0	0
			1343	835	232	268	8			

There are 18 discrepancies between the modelled and reference sequences:

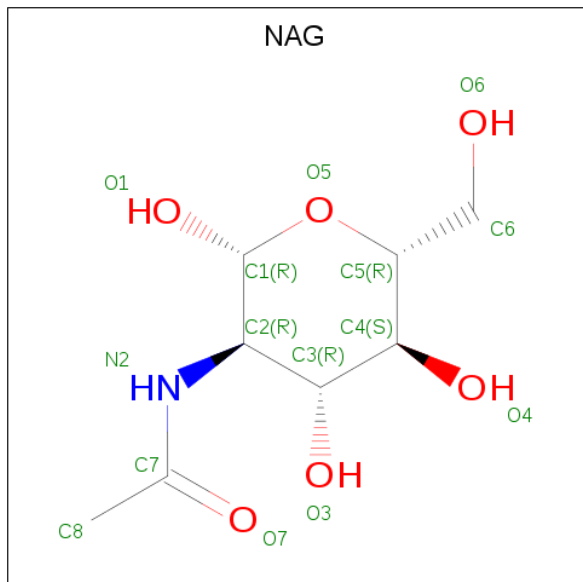
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP Q2F4V6
B	178	SER	-	expression tag	UNP Q2F4V6
B	179	LEU	-	expression tag	UNP Q2F4V6
B	180	VAL	-	expression tag	UNP Q2F4V6
B	181	PRO	-	expression tag	UNP Q2F4V6
B	182	ARG	-	expression tag	UNP Q2F4V6
D	177	ARG	-	expression tag	UNP Q2F4V6
D	178	SER	-	expression tag	UNP Q2F4V6
D	179	LEU	-	expression tag	UNP Q2F4V6
D	180	VAL	-	expression tag	UNP Q2F4V6
D	181	PRO	-	expression tag	UNP Q2F4V6
D	182	ARG	-	expression tag	UNP Q2F4V6
F	177	ARG	-	expression tag	UNP Q2F4V6
F	178	SER	-	expression tag	UNP Q2F4V6
F	179	LEU	-	expression tag	UNP Q2F4V6
F	180	VAL	-	expression tag	UNP Q2F4V6
F	181	PRO	-	expression tag	UNP Q2F4V6
F	182	ARG	-	expression tag	UNP Q2F4V6

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



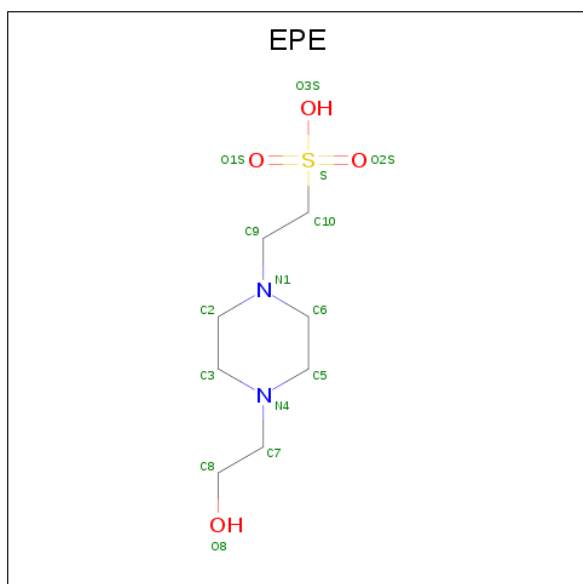
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		


- Molecule 6 is water.

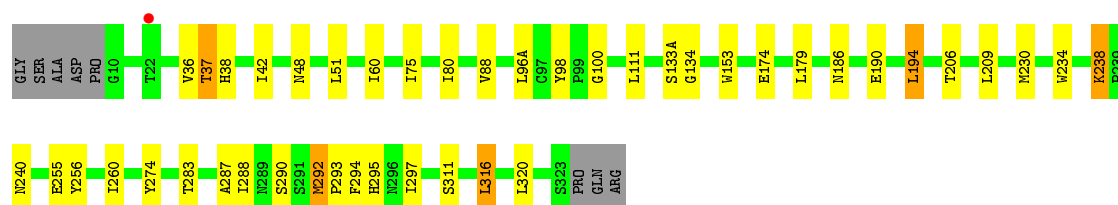
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	B	14	Total	O	0	0
			14	14		
6	C	68	Total	O	0	0
			68	68		
6	D	14	Total	O	0	0
			14	14		
6	E	66	Total	O	0	0
			66	66		
6	F	20	Total	O	0	0
			20	20		

### 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.

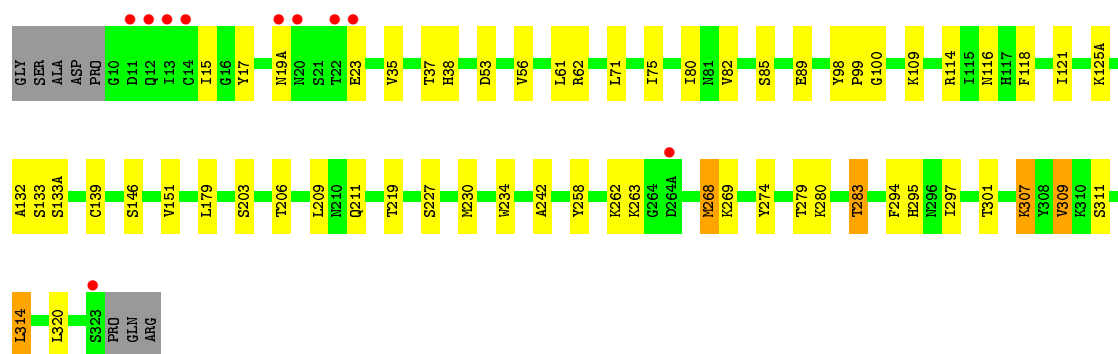
#### • Molecule 1: Hemagglutinin HA1

Chain A: 




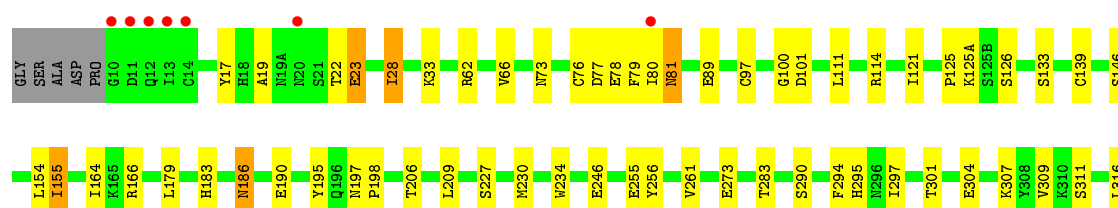
#### • Molecule 1: Hemagglutinin HA1

Chain C: 

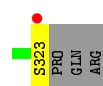


#### • Molecule 1: Hemagglutinin HA1

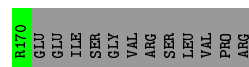
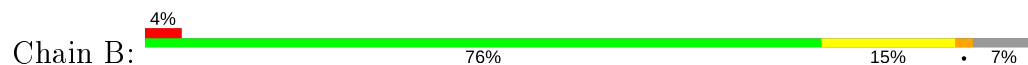
Chain E: 



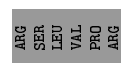
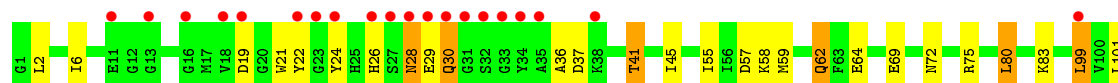




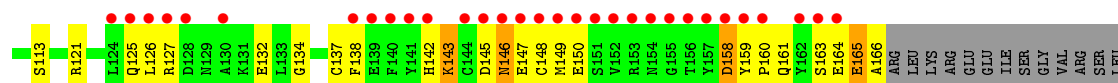
- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2




- Molecule 2: Hemagglutinin HA2



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




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

Chain H:  100%

HA01  
HA02

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

Chain I:  100%

HA01  
HA02

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.04Å 237.06Å 72.86Å 90.00° 119.18° 90.00°	Depositor
Resolution (Å)	49.62 – 2.34 49.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	81.7 (49.62-2.34) 86.3 (49.62-2.34)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.201 , 0.245 0.196 , 0.242	Depositor DCC
$R_{free}$ test set	3939 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,k,-h-l 0.008 for -h-l,k,h 0.027 for -h-l,-k,l 0.023 for h,-k,-h-l 0.028 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 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	0.48	0/2608	0.62	0/3542
1	C	0.46	0/2608	0.62	0/3542
1	E	0.45	0/2608	0.60	0/3542
2	B	0.39	0/1409	0.51	0/1894
2	D	0.37	0/1356	0.54	1/1825 (0.1%)
2	F	0.39	0/1370	0.55	0/1844
All	All	0.44	0/11959	0.59	1/16189 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	80	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2543	0	2486	25	0
1	C	2543	0	2486	37	0
1	E	2543	0	2484	41	0
2	B	1382	0	1291	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1329	0	1230	40	0
2	F	1343	0	1241	45	0
3	G	28	0	25	2	0
3	H	28	0	25	2	0
3	I	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
5	E	15	0	17	1	0
6	A	77	0	0	0	0
6	B	14	0	0	0	0
6	C	68	0	0	1	0
6	D	14	0	0	0	0
6	E	66	0	0	1	0
6	F	20	0	0	0	0
All	All	12083	0	11349	191	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 8.

All (191) 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:F:30:GLN:NE2	2:F:145:ASP:HB2	1.56	1.16
2:F:30:GLN:HE21	2:F:145:ASP:HB2	0.96	1.08
2:D:29:GLU:HB3	2:D:30:GLN:NE2	1.73	1.02
2:D:30:GLN:H	2:D:30:GLN:NE2	1.60	0.99
2:B:80:LEU:O	2:B:80:LEU:HD12	1.63	0.98
2:D:29:GLU:HB3	2:D:30:GLN:HE21	1.27	0.92
2:D:30:GLN:N	2:D:30:GLN:HE21	1.69	0.91
1:A:295:HIS:HD2	1:A:297:ILE:H	1.18	0.91
2:B:80:LEU:HD12	2:B:80:LEU:C	1.94	0.87
2:F:146:ASN:N	2:F:146:ASN:HD22	1.72	0.87
2:F:30:GLN:HE21	2:F:145:ASP:CB	1.86	0.86
1:E:295:HIS:HD2	1:E:297:ILE:H	1.25	0.82
2:B:28:ASN:HD22	2:B:28:ASN:C	1.82	0.80
2:F:26:HIS:HD2	2:F:149:MET:HG3	1.48	0.78
2:D:150:GLU:O	2:D:154:ASN:HB2	1.85	0.77
1:A:240:ASN:HD22	3:G:1:NAG:H5	1.50	0.77
2:D:30:GLN:H	2:D:30:GLN:HE21	1.23	0.77
2:D:150:GLU:OE1	2:D:150:GLU:HA	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:ASP:HB3	2:F:161:GLN:HB2	1.69	0.74
2:D:30:GLN:N	2:D:30:GLN:NE2	2.30	0.74
2:D:24:TYR:CE2	2:D:153:ARG:HG3	2.22	0.74
2:F:146:ASN:N	2:F:146:ASN:ND2	2.36	0.73
1:E:126:SER:OG	1:E:166:ARG:NH2	2.23	0.72
2:D:19:ASP:HB2	2:D:36:ALA:HB2	1.72	0.70
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.73	0.70
2:D:124:LEU:HD12	2:F:134:GLY:HA2	1.74	0.69
1:E:97:CYS:CB	1:E:139:CYS:SG	2.81	0.69
1:E:62:ARG:NH2	1:E:78:GLU:OE1	2.26	0.68
1:E:81:ASN:N	1:E:81:ASN:OD1	2.26	0.66
1:E:295:HIS:CD2	1:E:297:ILE:H	2.12	0.64
2:D:28:ASN:C	2:D:28:ASN:HD22	2.02	0.63
2:B:28:ASN:ND2	2:B:28:ASN:C	2.50	0.62
2:F:142:HIS:HB3	2:F:165:GLU:HG2	1.81	0.61
2:B:80:LEU:CD1	2:B:80:LEU:C	2.69	0.61
1:E:206:THR:OG1	1:E:209:LEU:N	2.29	0.61
2:D:146:ASN:HD22	2:D:146:ASN:N	1.98	0.61
2:D:26:HIS:HB2	2:D:149:MET:HE3	1.83	0.61
1:E:97:CYS:HB2	1:E:139:CYS:SG	2.40	0.61
1:A:295:HIS:CD2	1:A:297:ILE:H	2.09	0.60
2:D:28:ASN:C	2:D:28:ASN:ND2	2.53	0.60
1:C:294:PHE:HZ	2:D:59:MET:HG3	1.66	0.60
1:C:295:HIS:HD2	1:C:297:ILE:H	1.50	0.60
1:C:242:ALA:H	3:H:1:NAG:H82	1.66	0.60
1:E:307:LYS:HD2	2:F:62:GLN:HG2	1.84	0.59
2:D:29:GLU:CB	2:D:30:GLN:HE21	2.06	0.59
2:D:19:ASP:HB2	2:D:36:ALA:CB	2.32	0.59
2:F:165:GLU:O	2:F:166:ALA:C	2.40	0.59
1:C:19(A):ASN:ND2	1:C:37:THR:HB	2.17	0.59
1:E:77:ASP:O	1:E:79:PHE:N	2.36	0.58
2:F:30:GLN:NE2	2:F:145:ASP:CB	2.50	0.58
2:F:21:TRP:HB2	2:F:41:THR:HG23	1.86	0.58
2:F:165:GLU:OE2	2:F:165:GLU:CA	2.52	0.57
1:C:242:ALA:N	3:H:1:NAG:H82	2.20	0.57
2:F:146:ASN:H	2:F:146:ASN:ND2	2.03	0.56
2:B:30:GLN:HE21	2:B:30:GLN:H	1.54	0.56
1:C:19(A):ASN:HD21	1:C:37:THR:HB	1.70	0.56
2:F:165:GLU:OE2	2:F:165:GLU:N	2.37	0.56
2:B:68:ARG:NH1	2:B:81:ASN:OD1	2.38	0.55
1:E:154:LEU:O	1:E:155:ILE:HD13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:PHE:HZ	2:F:59:MET:HG3	1.71	0.55
2:F:145:ASP:O	2:F:148:CYS:HB3	2.07	0.55
2:B:30:GLN:HE21	2:B:30:GLN:N	2.05	0.54
2:D:72:ASN:HB2	2:D:75:ARG:HH21	1.73	0.54
1:E:206:THR:OG1	1:E:209:LEU:CB	2.57	0.53
1:A:75:ILE:O	1:A:75:ILE:HG22	2.09	0.53
1:E:166:ARG:NH1	6:E:556:HOH:O	2.42	0.53
2:F:17:MET:SD	2:F:23:GLY:HA3	2.49	0.52
2:F:28:ASN:C	2:F:28:ASN:ND2	2.62	0.52
2:D:29:GLU:CB	2:D:30:GLN:NE2	2.61	0.52
1:C:309:VAL:HG13	1:C:311:SER:H	1.73	0.52
1:A:288:ILE:HD11	1:A:297:ILE:HG13	1.91	0.52
2:F:125:GLN:O	2:F:126:LEU:HD23	2.10	0.52
1:A:100:GLY:HA3	1:A:230:MET:O	2.10	0.51
1:C:116:ASN:HB2	1:C:262:LYS:HG3	1.90	0.51
2:F:28:ASN:OD1	2:F:145:ASP:HA	2.11	0.51
2:F:142:HIS:ND1	2:F:143:LYS:O	2.38	0.51
1:C:219:THR:HG23	6:C:530:HOH:O	2.10	0.51
1:E:139:CYS:HB2	1:E:146:SER:O	2.11	0.50
2:D:150:GLU:OE1	2:D:150:GLU:CA	2.57	0.50
1:A:60:ILE:HD12	1:A:274:TYR:HB2	1.93	0.50
2:D:28:ASN:OD1	2:D:146:ASN:ND2	2.45	0.50
1:E:100:GLY:HA3	1:E:230:MET:O	2.11	0.50
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.94	0.49
2:F:26:HIS:CD2	2:F:149:MET:HG3	2.39	0.49
1:E:186:ASN:HB3	1:E:190:GLU:OE1	2.13	0.48
1:C:125(A):LYS:HE3	1:C:132:ALA:O	2.13	0.48
1:A:174:GLU:HG2	1:A:260:ILE:O	2.13	0.48
1:E:206:THR:OG1	1:E:209:LEU:HB3	2.14	0.48
2:F:84:MET:HG3	2:F:85:GLU:N	2.26	0.48
1:C:114:ARG:O	1:C:263:LYS:HG2	2.14	0.48
1:C:35:VAL:HG11	2:D:108:LEU:HD21	1.96	0.48
1:A:290:SER:OG	1:A:292:MET:HB2	2.14	0.48
1:C:206:THR:OG1	1:C:209:LEU:N	2.47	0.47
1:C:100:GLY:HA3	1:C:230:MET:O	2.15	0.47
1:C:75:ILE:H	1:C:75:ILE:HD12	1.78	0.47
1:A:206:THR:HG23	1:A:209:LEU:HB3	1.96	0.47
1:C:109:LYS:NZ	2:D:69:GLU:OE2	2.42	0.47
1:A:51:LEU:HD13	1:A:88:VAL:HG21	1.97	0.47
1:C:89:GLU:O	1:C:269:LYS:HA	2.14	0.47
1:C:206:THR:OG1	1:C:209:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:GLU:OE2	2:F:165:GLU:HA	2.15	0.46
2:F:142:HIS:CB	2:F:165:GLU:HG2	2.45	0.46
1:A:190:GLU:HG2	1:A:194:LEU:HD22	1.98	0.46
1:A:37:THR:HG22	1:A:38:HIS:ND1	2.29	0.46
1:E:77:ASP:C	1:E:79:PHE:H	2.18	0.46
2:F:150:GLU:OE2	2:F:150:GLU:HA	2.15	0.46
2:F:19:ASP:HB3	2:F:36:ALA:CB	2.45	0.46
1:A:255:GLU:HG2	1:A:256:TYR:CD2	2.51	0.46
2:B:30:GLN:H	2:B:30:GLN:NE2	2.14	0.46
1:C:283:THR:HG22	1:C:301:THR:HG22	1.98	0.45
2:F:26:HIS:O	2:F:26:HIS:ND1	2.49	0.45
1:E:164:ILE:O	1:E:246:GLU:HA	2.15	0.45
1:E:309:VAL:HG13	1:E:311:SER:H	1.82	0.45
2:F:160:PRO:HA	2:F:163:SER:HB2	1.98	0.45
2:B:150:GLU:HG2	2:B:153:ARG:HH21	1.81	0.45
2:B:2:LEU:HG	2:F:3:PHE:HZ	1.82	0.45
2:B:73:LEU:CD2	5:E:404:EPE:H31	2.46	0.45
1:E:125(A):LYS:HB2	1:E:125(A):LYS:HE2	1.70	0.45
1:E:19:ALA:HB2	2:F:13:GLY:HA3	1.99	0.45
1:E:28:ILE:HD11	2:F:102:MET:HG2	1.99	0.44
2:F:132:GLU:HG2	2:F:138:PHE:HE1	1.83	0.44
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.52	0.44
1:C:53:ASP:OD2	1:C:274:TYR:OH	2.28	0.44
2:B:133:LEU:HD21	2:B:139:GLU:HB2	1.99	0.44
2:F:51:LYS:HD2	2:F:103:GLU:HB3	2.00	0.44
1:A:295:HIS:HD2	1:A:297:ILE:N	2.00	0.43
2:F:58:LYS:HA	2:F:58:LYS:HD2	1.75	0.43
1:C:61:LEU:O	1:C:62:ARG:HB2	2.18	0.43
1:E:77:ASP:C	1:E:79:PHE:N	2.70	0.43
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.01	0.43
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.83	0.43
2:B:17:MET:HE3	2:B:17:MET:HB2	1.87	0.43
1:E:283:THR:HG22	1:E:301:THR:HG22	2.00	0.43
1:C:139:CYS:HB2	1:C:146:SER:O	2.18	0.43
2:F:132:GLU:HG2	2:F:138:PHE:CE1	2.54	0.43
2:F:15:GLN:HG3	2:F:15:GLN:O	2.18	0.43
1:A:48:ASN:HD21	1:A:287:ALA:HB3	1.84	0.43
1:C:80:ILE:HD13	1:C:80:ILE:HA	1.79	0.43
2:D:2:LEU:HA	2:D:2:LEU:HD12	1.89	0.43
1:E:23:GLU:H	1:E:23:GLU:HG2	1.52	0.43
2:D:118:LEU:HA	2:D:118:LEU:HD12	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ASN:HB2	2:D:75:ARG:NH2	2.33	0.43
1:C:56:VAL:HB	1:C:85:SER:HB3	2.00	0.43
2:D:58:LYS:HE3	2:F:97:GLU:HB3	2.00	0.42
2:B:150:GLU:HG2	2:B:153:ARG:NH2	2.35	0.42
2:B:160:PRO:HA	2:B:163:SER:OG	2.20	0.42
1:C:17:TYR:CZ	2:D:6:ILE:HG23	2.54	0.42
1:C:206:THR:OG1	1:C:209:LEU:CB	2.67	0.42
1:E:28:ILE:HG12	1:E:28:ILE:H	1.54	0.42
1:C:203:SER:HA	1:C:211:GLN:O	2.20	0.42
1:E:66:VAL:HG23	1:E:89:GLU:OE1	2.20	0.42
1:E:255:GLU:HG2	1:E:256:TYR:CD1	2.54	0.42
2:D:153:ARG:NH1	2:D:153:ARG:HG2	2.34	0.42
2:D:37:ASP:O	2:D:41:THR:HB	2.19	0.42
1:E:80:ILE:HA	1:E:80:ILE:HD13	1.93	0.42
2:B:144:CYS:SG	2:B:149:MET:HE3	2.60	0.42
1:C:307:LYS:HG3	2:D:62:GLN:HB2	2.02	0.42
1:C:98:TYR:CD2	1:C:99:PRO:HD2	2.55	0.42
1:E:179:LEU:HD23	1:E:234:TRP:HB3	2.02	0.42
2:F:28:ASN:C	2:F:28:ASN:HD22	2.23	0.42
1:E:73:ASN:O	1:E:76:CYS:N	2.44	0.42
1:C:15:ILE:HD11	2:D:122:VAL:HG21	2.02	0.41
1:C:268:MET:HE3	1:C:268:MET:HB3	1.90	0.41
2:F:19:ASP:HB3	2:F:36:ALA:HB2	2.00	0.41
1:C:320:LEU:HB3	2:D:111:HIS:CD2	2.55	0.41
1:E:77:ASP:O	1:E:78:GLU:C	2.59	0.41
1:C:38:HIS:CE1	2:D:21:TRP:HE1	2.37	0.41
1:E:166:ARG:HD2	1:E:166:ARG:HA	1.80	0.41
1:A:240:ASN:ND2	3:G:1:NAG:H5	2.28	0.41
2:B:131:LYS:O	2:B:138:PHE:HA	2.21	0.41
2:D:133:LEU:HD13	2:D:139:GLU:HB2	2.02	0.41
1:A:42:ILE:HD13	1:A:316:LEU:HD22	2.02	0.41
2:D:28:ASN:ND2	2:D:30:GLN:O	2.45	0.41
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.43	0.41
2:D:55:ILE:HG12	2:D:99:LEU:HD13	2.03	0.41
2:F:159:TYR:HB3	2:F:160:PRO:HD3	2.01	0.41
1:C:279:THR:OG1	1:C:280:LYS:N	2.54	0.41
2:D:41:THR:O	2:D:45:ILE:HG13	2.21	0.41
1:E:316:LEU:HA	1:E:316:LEU:HD12	1.93	0.41
1:A:42:ILE:HB	1:A:293:PRO:HG2	2.03	0.41
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.94	0.40
2:D:148:CYS:O	2:D:152:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:TYR:CZ	2:F:6:ILE:HG23	2.56	0.40
1:A:238:LYS:HD2	1:A:238:LYS:HA	1.80	0.40
1:E:62:ARG:CZ	1:E:78:GLU:OE1	2.68	0.40
1:A:98:TYR:CD2	1:A:230:MET:HG2	2.57	0.40
1:C:118:PHE:CD1	1:C:258:TYR:HB3	2.57	0.40
1:A:294:PHE:CZ	2:B:59:MET:HG3	2.56	0.40
2:B:123:ARG:HD2	2:B:132:GLU:OE1	2.22	0.40
1:E:125:PRO:O	1:E:126:SER:HB3	2.21	0.40
1:E:197:ASN:HA	1:E:198:PRO:HD3	1.98	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	320/329 (97%)	314 (98%)	6 (2%)	0	100	100
1	C	320/329 (97%)	314 (98%)	6 (2%)	0	100	100
1	E	320/329 (97%)	314 (98%)	6 (2%)	0	100	100
2	B	168/182 (92%)	166 (99%)	2 (1%)	0	100	100
2	D	162/182 (89%)	157 (97%)	5 (3%)	0	100	100
2	F	164/182 (90%)	156 (95%)	8 (5%)	0	100	100
All	All	1454/1533 (95%)	1421 (98%)	33 (2%)	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	286/291 (98%)	272 (95%)	14 (5%)	25	31
1	C	286/291 (98%)	273 (96%)	13 (4%)	27	34
1	E	286/291 (98%)	268 (94%)	18 (6%)	18	20
2	B	145/156 (93%)	131 (90%)	14 (10%)	8	7
2	D	140/156 (90%)	124 (89%)	16 (11%)	5	4
2	F	141/156 (90%)	123 (87%)	18 (13%)	4	3
All	All	1284/1341 (96%)	1191 (93%)	93 (7%)	14	14

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	37	THR
1	A	80	ILE
1	A	96(A)	LEU
1	A	111	LEU
1	A	133(A)	SER
1	A	186	ASN
1	A	194	LEU
1	A	238	LYS
1	A	283	THR
1	A	292	MET
1	A	311	SER
1	A	316	LEU
1	A	320	LEU
2	B	22	TYR
2	B	28	ASN
2	B	30	GLN
2	B	60	ASN
2	B	77	ILE
2	B	80	LEU
2	B	82	LYS
2	B	89	LEU
2	B	108	LEU
2	B	113	SER
2	B	124	LEU
2	B	149	MET
2	B	151	SER

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Mol	Chain	Res	Type
2	B	169	LYS
1	C	23	GLU
1	C	71	LEU
1	C	82	VAL
1	C	121	ILE
1	C	133	SER
1	C	133(A)	SER
1	C	151	VAL
1	C	227	SER
1	C	268	MET
1	C	283	THR
1	C	307	LYS
1	C	309	VAL
1	C	314	LEU
2	D	22	TYR
2	D	28	ASN
2	D	30	GLN
2	D	41	THR
2	D	57	ASP
2	D	62	GLN
2	D	64	GLU
2	D	80	LEU
2	D	83	LYS
2	D	99	LEU
2	D	101	LEU
2	D	108	LEU
2	D	124	LEU
2	D	128	ASP
2	D	144	CYS
2	D	153	ARG
1	E	22	THR
1	E	23	GLU
1	E	28	ILE
1	E	33	LYS
1	E	81	ASN
1	E	101	ASP
1	E	111	LEU
1	E	114	ARG
1	E	121	ILE
1	E	133	SER
1	E	155	ILE
1	E	186	ASN

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Mol	Chain	Res	Type
1	E	227	SER
1	E	261	VAL
1	E	273	GLU
1	E	290	SER
1	E	304	GLU
1	E	323	SER
2	F	26	HIS
2	F	28	ASN
2	F	39	GLU
2	F	56	ILE
2	F	69	GLU
2	F	84	MET
2	F	89	LEU
2	F	108	LEU
2	F	113	SER
2	F	121	ARG
2	F	127	ARG
2	F	137	CYS
2	F	143	LYS
2	F	146	ASN
2	F	147	GLU
2	F	158	ASP
2	F	164	GLU
2	F	165	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	20	ASN
1	A	240	ASN
1	A	295	HIS
2	B	28	ASN
2	B	60	ASN
2	B	95	ASN
2	B	114	ASN
2	B	129	ASN
2	B	146	ASN
2	B	161	GLN
1	C	240	ASN
1	C	295	HIS
2	D	26	HIS

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Mol	Chain	Res	Type
2	D	28	ASN
2	D	30	GLN
2	D	62	GLN
2	D	95	ASN
2	D	114	ASN
2	D	129	ASN
2	D	146	ASN
1	E	20	ASN
1	E	129	ASN
1	E	295	HIS
2	F	28	ASN
2	F	30	GLN
2	F	95	ASN
2	F	114	ASN
2	F	125	GLN
2	F	129	ASN
2	F	146	ASN
2	F	161	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 ⓘ

6 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	G	1	1,3	14,14,15	0.73	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	G	2	3	14,14,15	0.62	0	17,19,21	1.30	2 (11%)
3	NAG	H	1	1,3	14,14,15	0.70	0	17,19,21	0.95	0
3	NAG	H	2	3	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.70	0	17,19,21	1.64	4 (23%)
3	NAG	I	2	3	14,14,15	0.69	0	17,19,21	1.11	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	O5-C1-C2	-3.92	105.09	111.29
3	I	1	NAG	O5-C5-C6	3.22	112.25	107.20
3	I	1	NAG	C2-N2-C7	2.65	126.67	122.90
3	I	2	NAG	C1-O5-C5	2.57	115.68	112.19
3	H	2	NAG	C1-O5-C5	2.56	115.67	112.19
3	I	1	NAG	C1-O5-C5	-2.39	108.95	112.19
3	I	1	NAG	O5-C1-C2	-2.27	107.70	111.29
3	G	2	NAG	C3-C4-C5	2.19	114.15	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

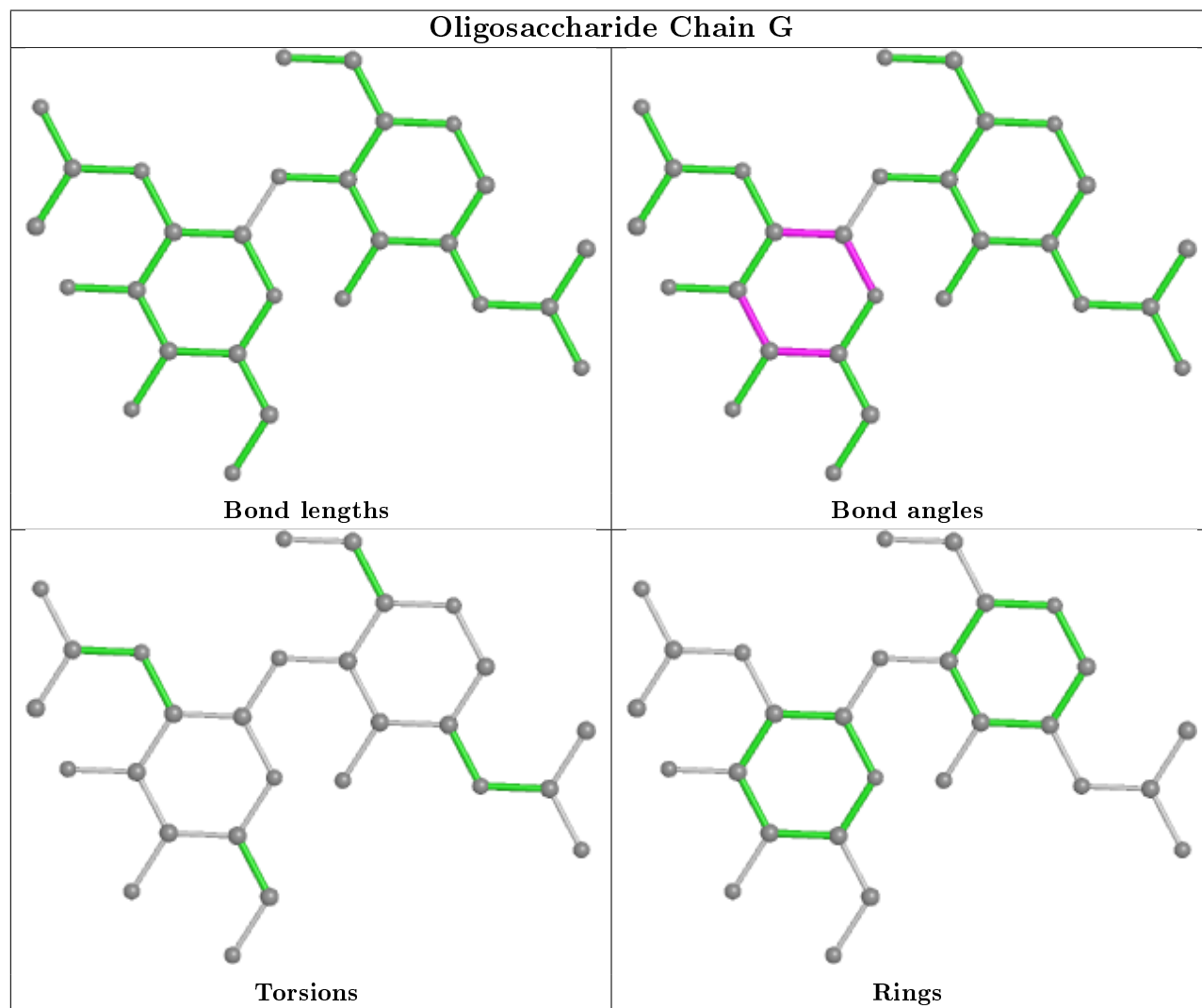
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6

There are no ring outliers.

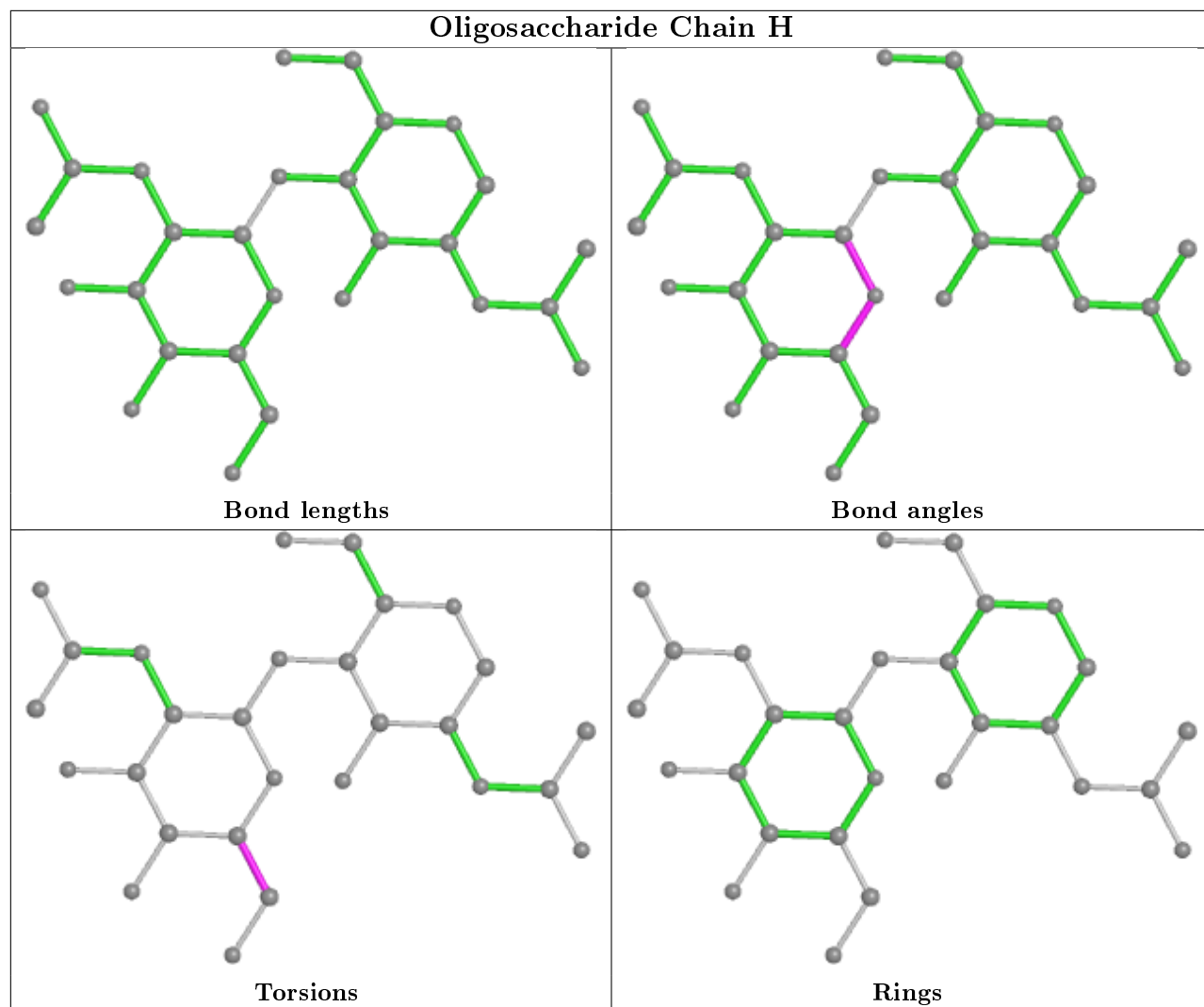
2 monomers are involved in 4 short contacts:

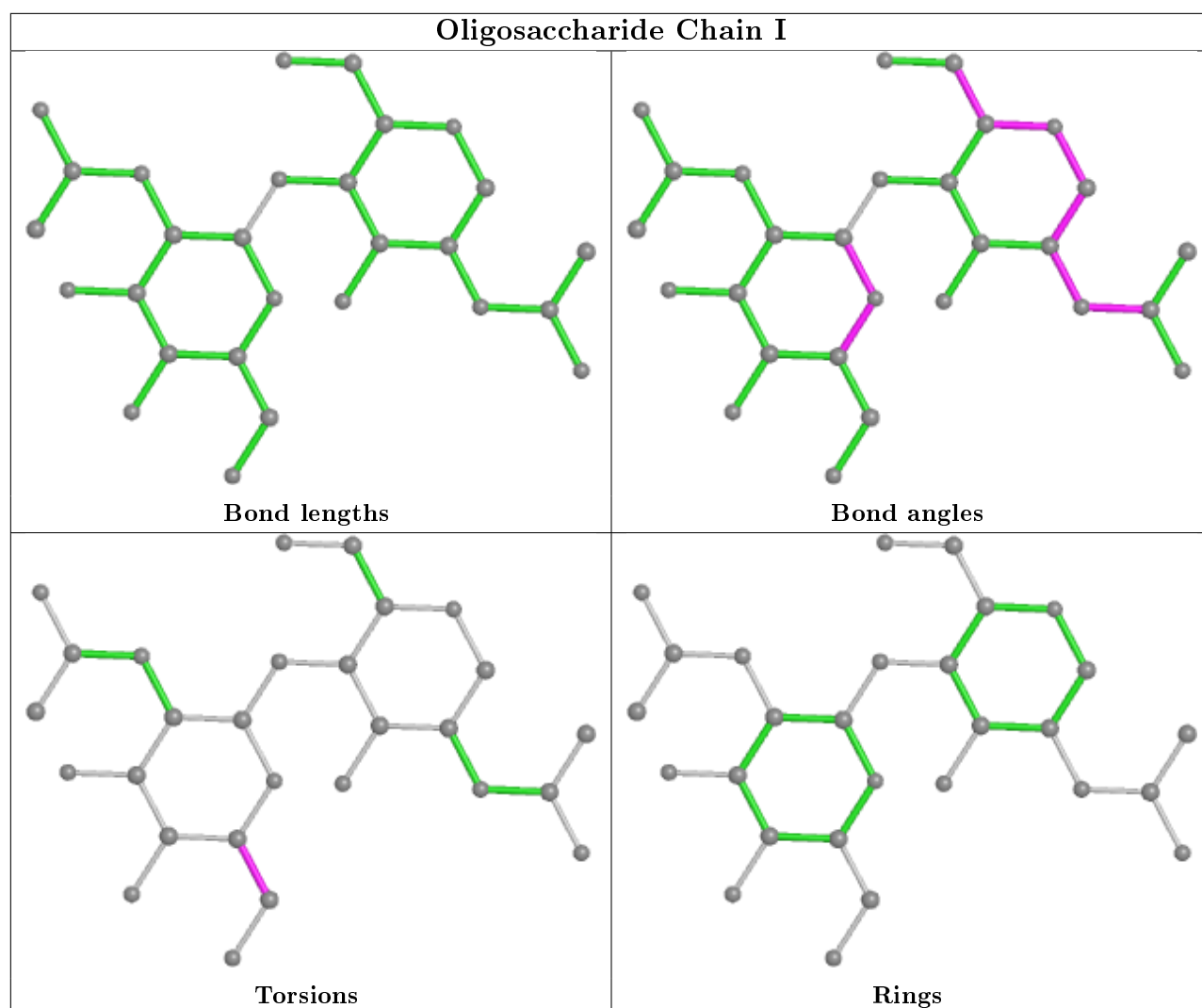
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	2	0
3	H	1	NAG	2	0

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
4	NAG	A	403	1	14,14,15	0.60	0	17,19,21	1.20	3 (17%)
5	EPE	E	404	-	15,15,15	1.27	1 (6%)	18,20,20	2.35	6 (33%)
4	NAG	E	403	1	14,14,15	0.60	0	17,19,21	1.42	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	403	1	14,14,15	0.56	0	17,19,21	1.23	3 (17%)

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	A	403	1	-	0/6/23/26	0/1/1/1
5	EPE	E	404	-	-	5/9/19/19	0/1/1/1
4	NAG	E	403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	403	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	404	EPE	C10-S	4.46	1.83	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	404	EPE	O2S-S-C10	5.63	113.69	106.92
5	E	404	EPE	C7-N4-C3	5.18	124.49	111.23
4	E	403	NAG	O5-C1-C2	-3.39	105.93	111.29
4	E	403	NAG	C3-C4-C5	3.22	115.98	110.24
5	E	404	EPE	C5-N4-C3	2.76	115.04	108.83
5	E	404	EPE	C7-N4-C5	2.70	118.14	111.23
4	C	403	NAG	O5-C5-C6	2.67	111.39	107.20
4	C	403	NAG	C3-C4-C5	2.62	114.91	110.24
5	E	404	EPE	C2-C3-N4	2.55	115.87	110.64
4	A	403	NAG	O5-C1-C2	-2.44	107.44	111.29
4	A	403	NAG	C4-C3-C2	-2.31	107.63	111.02
4	C	403	NAG	O5-C1-C2	-2.19	107.83	111.29
4	A	403	NAG	C2-N2-C7	-2.18	119.80	122.90
4	E	403	NAG	O5-C5-C6	2.07	110.44	107.20
5	E	404	EPE	C9-N1-C6	-2.06	105.96	111.23

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	404	EPE	N4-C7-C8-O8
4	E	403	NAG	O5-C5-C6-O6
4	C	403	NAG	O5-C5-C6-O6
5	E	404	EPE	C8-C7-N4-C5
4	C	403	NAG	C4-C5-C6-O6
4	E	403	NAG	C4-C5-C6-O6
5	E	404	EPE	C9-C10-S-O1S
5	E	404	EPE	C9-C10-S-O2S
5	E	404	EPE	C9-C10-S-O3S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	404	EPE	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 ⓘ

### 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	321/329 (97%)	-0.10	1 (0%) 94 97	15, 33, 55, 71	0
1	C	321/329 (97%)	-0.04	10 (3%) 49 59	12, 33, 61, 112	0
1	E	321/329 (97%)	0.02	8 (2%) 57 66	16, 32, 62, 104	0
2	B	170/182 (93%)	0.49	8 (4%) 31 42	15, 52, 71, 91	0
2	D	164/182 (90%)	1.35	46 (28%) 0 0	17, 64, 109, 117	0
2	F	166/182 (91%)	1.42	47 (28%) 0 0	18, 65, 117, 125	0
All	All	1463/1533 (95%)	0.34	120 (8%) 11 17	12, 38, 99, 125	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	160	PRO	7.3
2	F	27	SER	7.1
2	F	162	TYR	6.2
2	F	157	TYR	6.0
2	F	147	GLU	6.0
2	D	144	CYS	6.0
2	D	159	TYR	5.9
2	D	141	TYR	5.7
2	F	141	TYR	5.6
2	F	29	GLU	5.5
2	F	33	GLY	5.2
2	D	35	ALA	5.1
2	D	32	SER	5.1
2	D	138	PHE	4.9
1	E	10	GLY	4.9
2	D	31	GLY	4.9
2	F	159	TYR	4.8
2	F	148	CYS	4.8
1	C	20	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
2	F	31	GLY	4.8
2	D	140	PHE	4.7
2	F	156	THR	4.7
2	F	32	SER	4.6
2	F	146	ASN	4.6
2	D	148	CYS	4.5
1	C	12	GLN	4.5
1	E	13	ILE	4.5
2	D	133	LEU	4.4
1	C	11	ASP	4.3
2	D	146	ASN	4.3
2	D	27	SER	4.3
2	F	138	PHE	4.1
2	D	26	HIS	4.1
2	F	154	ASN	4.1
2	D	23	GLY	4.0
2	D	139	GLU	3.9
2	F	142	HIS	3.9
2	F	150	GLU	3.8
2	F	124	LEU	3.8
1	E	323	SER	3.8
1	E	14	CYS	3.8
2	B	31	GLY	3.8
2	D	19	ASP	3.7
2	F	155	GLY	3.7
2	F	18	VAL	3.7
2	F	19	ASP	3.6
2	F	144	CYS	3.6
2	F	149	MET	3.5
2	D	147	GLU	3.5
2	B	33	GLY	3.4
2	F	25	HIS	3.4
1	E	12	GLN	3.4
2	B	19	ASP	3.3
2	D	162	TYR	3.3
1	C	323	SER	3.3
2	B	32	SER	3.3
2	F	164	GLU	3.3
2	F	26	HIS	3.2
2	F	152	VAL	3.2
2	F	140	PHE	3.2
1	C	13	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	34	TYR	3.1
2	D	124	LEU	3.1
2	F	145	ASP	3.1
1	C	14	CYS	3.1
2	D	29	GLU	3.1
1	C	22	THR	3.1
2	F	151	SER	3.0
1	E	11	ASP	3.0
2	D	156	THR	3.0
2	D	149	MET	3.0
1	C	23	GLU	2.9
2	F	163	SER	2.8
2	D	135	ASN	2.8
2	D	152	VAL	2.8
2	B	168	LEU	2.8
2	F	30	GLN	2.8
2	F	130	ALA	2.7
2	D	132	GLU	2.7
2	F	127	ARG	2.7
2	D	16	GLY	2.7
2	F	139	GLU	2.7
1	E	80	ILE	2.7
2	F	34	TYR	2.7
2	B	18	VAL	2.7
2	D	11	GLU	2.7
2	D	30	GLN	2.7
2	F	35	ALA	2.6
2	D	38	LYS	2.6
2	D	145	ASP	2.6
2	F	128	ASP	2.6
2	F	153	ARG	2.5
2	F	9	PHE	2.5
2	F	126	LEU	2.5
2	F	28	ASN	2.5
2	D	121	ARG	2.5
2	B	29	GLU	2.4
2	D	160	PRO	2.4
2	F	16	GLY	2.4
1	E	20	ASN	2.4
2	D	28	ASN	2.4
2	D	131	LYS	2.3
2	F	158	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	157	TYR	2.3
2	D	18	VAL	2.3
2	D	137	CYS	2.3
2	D	143	LYS	2.3
2	D	22	TYR	2.2
2	D	24	TYR	2.2
2	F	125	GLN	2.1
2	F	38	LYS	2.1
1	C	264(A)	ASP	2.1
2	D	33	GLY	2.1
1	A	22	THR	2.1
2	B	164	GLU	2.1
2	D	99	LEU	2.0
1	C	19(A)	ASN	2.0
2	D	150	GLU	2.0
2	D	13	GLY	2.0
2	D	163	SER	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.

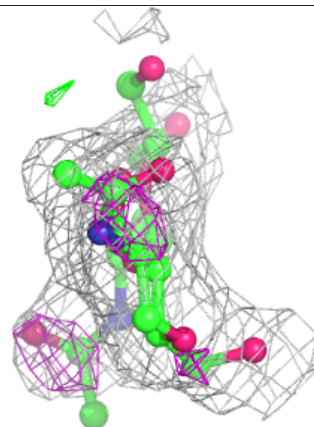
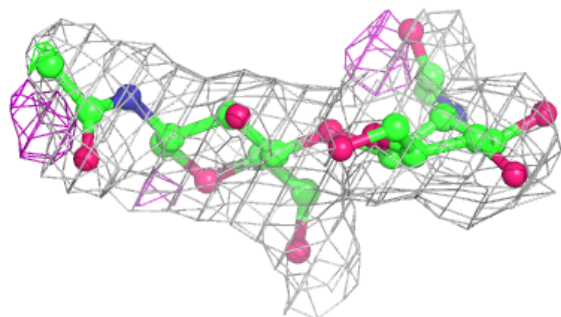
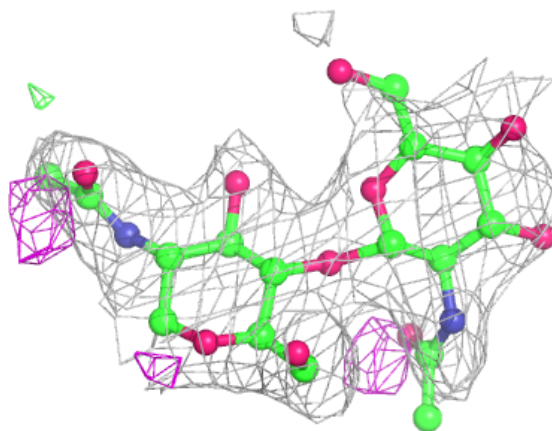
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	H	2	14/15	0.80	0.32	61,74,79,79	0
3	NAG	G	2	14/15	0.80	0.34	58,77,84,86	0
3	NAG	I	1	14/15	0.85	0.16	31,45,61,69	0
3	NAG	I	2	14/15	0.85	0.36	61,74,79,79	0
3	NAG	H	1	14/15	0.88	0.12	25,44,52,53	0
3	NAG	G	1	14/15	0.91	0.17	32,44,52,64	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.



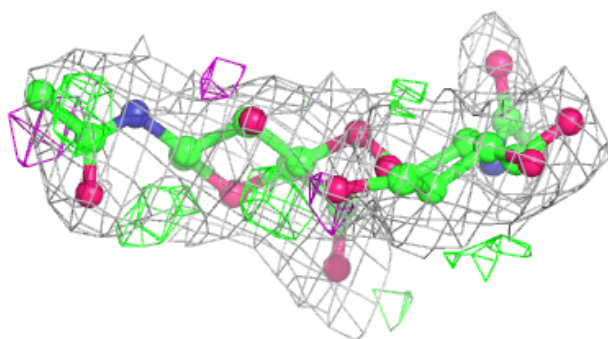
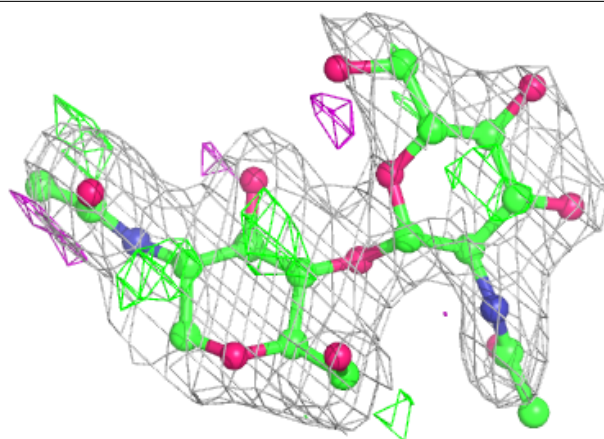
**Electron density around Chain G:**

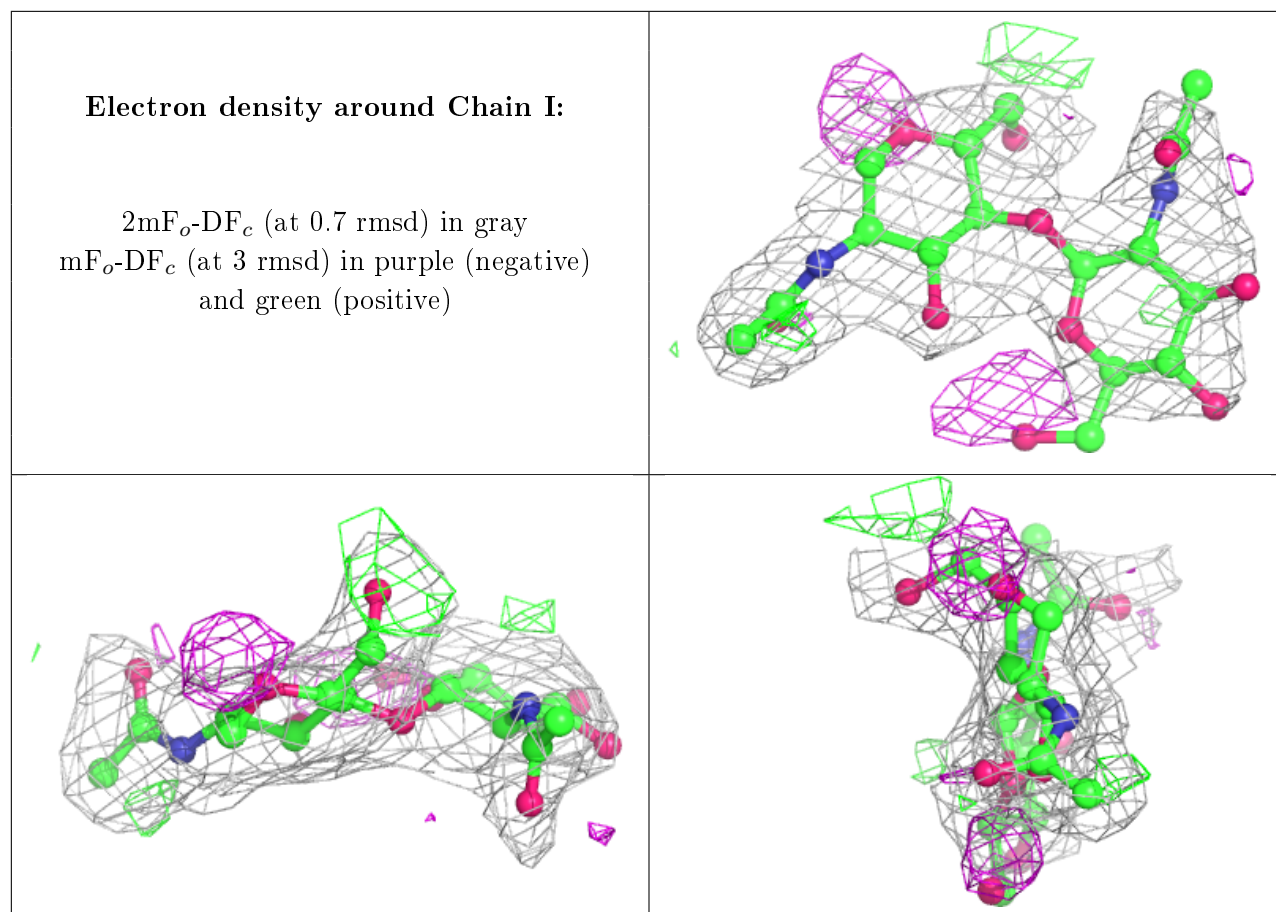
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain H:**

$2mF_o-DF_c$  (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
4	NAG	A	403	14/15	0.83	0.29	77,81,89,89	0
4	NAG	C	403	14/15	0.84	0.33	75,78,85,92	0
4	NAG	E	403	14/15	0.88	0.30	76,84,89,90	0
5	EPE	E	404	15/15	0.89	0.16	26,37,62,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.