



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 07:43 AM EDT

PDB ID : 1YKB  
Title : Crystal Structure of Insect Cell Expressed IL-22  
Authors : Xu, T.; Logsdon, N.J.; Walter, M.R.  
Deposited on : 2005-01-17  
Resolution : 2.60 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

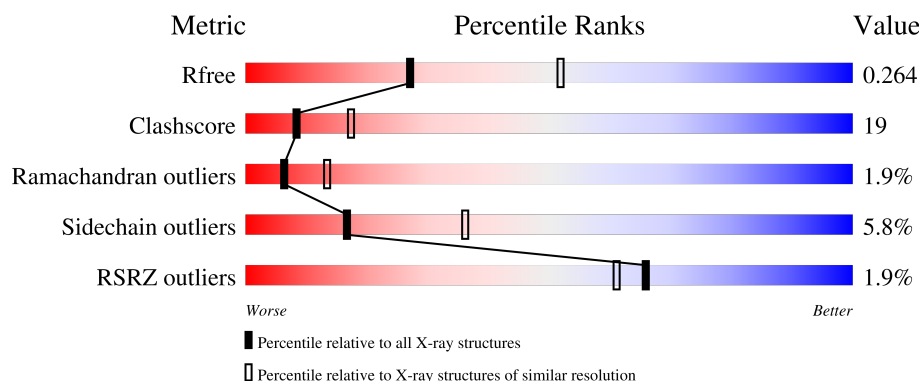
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.




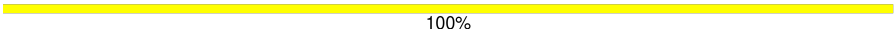
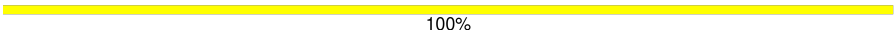



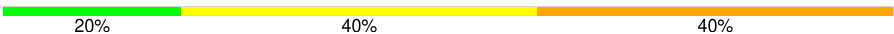
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	142	<div> <div>3%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	B	142	<div> <div>2%</div> <div>57%</div> <div>35%</div> <div>8%</div> <div>.</div> </div>
1	C	142	<div> <div>67%</div> <div>28%</div> <div>..</div> </div>
1	D	142	<div> <div>%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
1	E	142	<div> <div>62%</div> <div>31%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	142	
2	G	3	
3	H	2	
3	J	2	
3	K	2	
3	L	2	
4	I	5	

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
2	FUC	G	3	-	-	X	-
3	NAG	H	2	X	-	-	-
4	MAN	I	3	X	-	-	-

## 2 Entry composition [i](#)

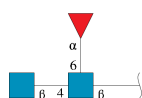
There are 6 unique types of molecules in this entry. The entry contains 7197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (Interleukin-22).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1144	721	201	212	10			
1	B	142	Total	C	N	O	S	0	1	0
			1150	724	202	214	10			
1	C	142	Total	C	N	O	S	0	1	0
			1150	725	202	214	9			
1	D	142	Total	C	N	O	S	0	2	0
			1153	725	204	214	10			
1	E	142	Total	C	N	O	S	0	0	0
			1147	722	202	214	9			
1	F	142	Total	C	N	O	S	0	1	0
			1150	723	204	214	9			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



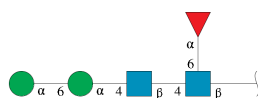
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



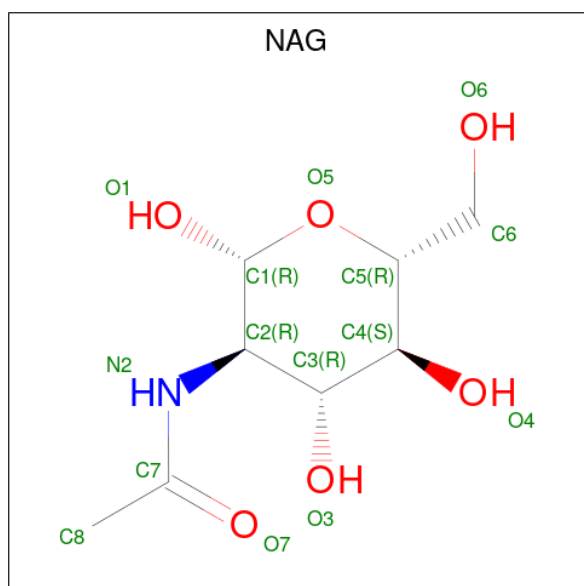
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

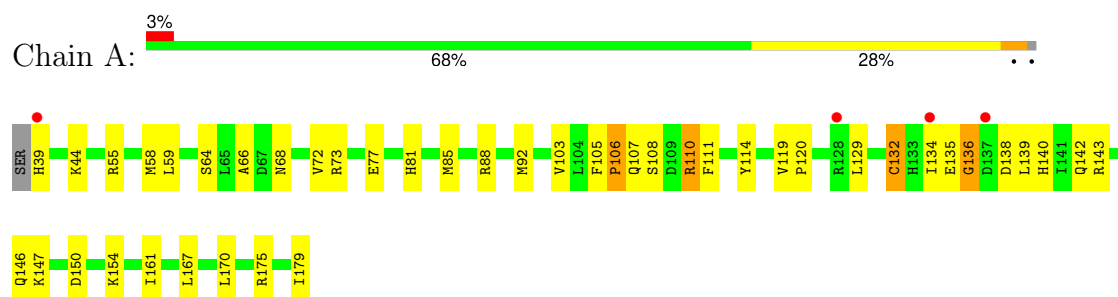
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	8	Total	O	0	0
			8	8		
6	C	11	Total	O	0	0
			11	11		
6	D	15	Total	O	0	0
			15	15		
6	E	5	Total	O	0	0
			5	5		
6	F	4	Total	O	0	0
			4	4		

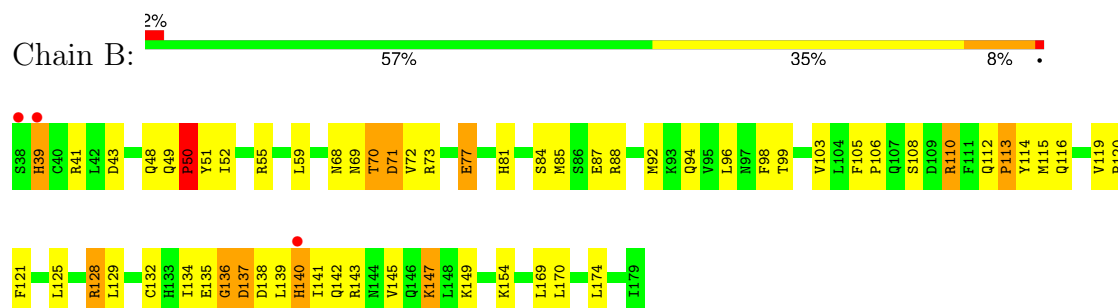
### 3 Residue-property plots [i](#)

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.

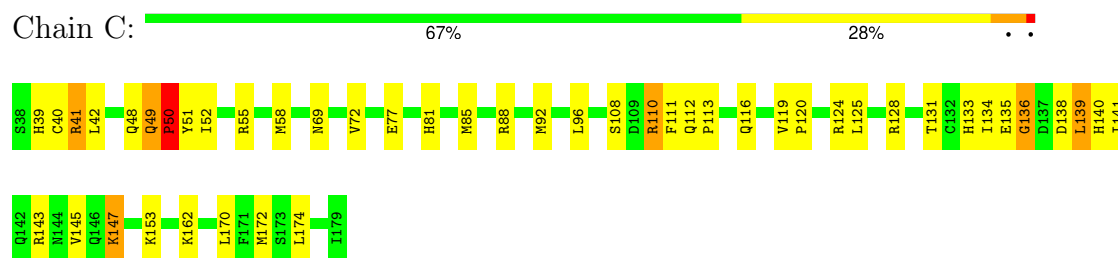
#### • Molecule 1: PROTEIN (Interleukin-22)



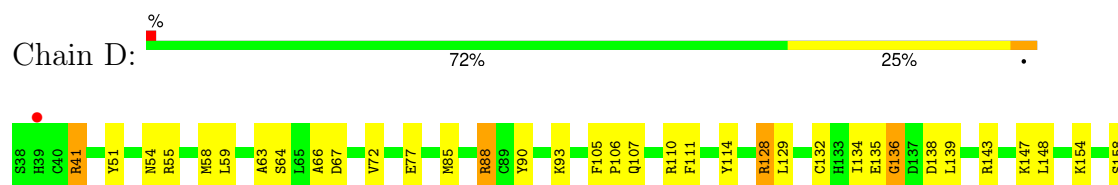
#### • Molecule 1: PROTEIN (Interleukin-22)



#### • Molecule 1: PROTEIN (Interleukin-22)



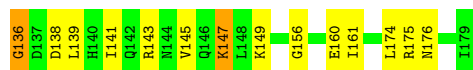
#### • Molecule 1: PROTEIN (Interleukin-22)





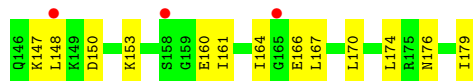
- Molecule 1: PROTEIN (Interleukin-22)

Chain E: 62% 31% 7%



- Molecule 1: PROTEIN (Interleukin-22)

Chain F: 6% 67% 30%



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

Chain G: 100%



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

Chain H: 100%



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

Chain J: 100%



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



Chain K:  50% 50%


MAG1  
MAG2

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

Chain L:  100%

MAG1  
MAG2

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

Chain I:  20% 40% 40%

MAG1  
MAG2  
MAN3  
MAN4  
FUC5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.88Å 62.23Å 139.52Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.93-2.60) 94.7 (19.93-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.265 0.239 , 0.264	Depositor DCC
$R_{free}$ test set	1651 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l 0.012 for -k,-h,-l 0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: MAN, NAG, FUC

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	0/1167	0.65	0/1566
1	B	0.49	0/1173	0.65	0/1574
1	C	0.50	0/1173	0.66	0/1575
1	D	0.49	0/1184	0.63	0/1588
1	E	0.45	0/1165	0.63	0/1564
1	F	0.41	0/1176	0.65	0/1578
All	All	0.47	0/7038	0.65	0/9445

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 [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	1144	0	1149	40	0
1	B	1150	0	1155	64	0
1	C	1150	0	1157	53	0
1	D	1153	0	1151	34	0
1	E	1147	0	1150	50	0
1	F	1150	0	1146	36	0
2	G	38	0	34	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	J	28	0	25	2	0
3	K	28	0	25	1	0
3	L	28	0	25	3	0
4	I	60	0	52	6	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	E	14	0	13	0	0
6	A	8	0	0	2	0
6	B	8	0	0	0	0
6	C	11	0	0	0	0
6	D	15	0	0	4	0
6	E	5	0	0	2	0
6	F	4	0	0	2	0
All	All	7197	0	7133	269	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 19.

All (269) 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)
3:L:1:NAG:H62	3:L:2:NAG:H82	1.41	1.03
1:A:55:ARG:NH2	2:G:3:FUC:H5	1.77	0.99
1:B:48:GLN:HE22	2:G:2:NAG:H83	1.31	0.95
1:B:134:ILE:HD11	1:B:138:ASP:HB3	1.50	0.94
1:D:134:ILE:HD11	1:D:138:ASP:HB3	1.52	0.92
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.39	0.87
1:F:110:ARG:HH22	1:F:161:ILE:HD11	1.43	0.82
1:F:134:ILE:HD11	1:F:138:ASP:HB3	1.61	0.81
1:C:40:CYS:O	1:C:41:ARG:HG2	1.81	0.81
1:A:110:ARG:HG3	1:A:111:PHE:H	1.43	0.81
1:D:110:ARG:NH1	1:D:161:ILE:HD11	1.98	0.79
1:D:158:SER:HB2	6:D:1437:HOH:O	1.82	0.79
1:E:69:ASN:N	1:E:69:ASN:HD22	1.78	0.79
3:L:1:NAG:C6	3:L:2:NAG:H82	2.14	0.78
1:A:134:ILE:HD11	1:A:138:ASP:HB3	1.69	0.74
1:D:59:LEU:HD13	1:D:114:TYR:HB2	1.69	0.74
1:C:147:LYS:HE2	1:C:147:LYS:HA	1.71	0.72
1:A:150:ASP:OD1	6:A:325:HOH:O	2.08	0.71
3:L:1:NAG:H62	3:L:2:NAG:C8	2.17	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ARG:HG3	1:C:111:PHE:N	2.06	0.70
1:A:55:ARG:HH22	2:G:3:FUC:H5	1.57	0.70
1:E:112:GLN:HE22	1:E:116:GLN:H	1.40	0.69
1:F:67:ASP:HA	6:F:1634:HOH:O	1.91	0.69
1:C:49:GLN:O	1:C:52:ILE:HG22	1.93	0.69
1:A:179:ILE:HD11	1:B:73:ARG:CZ	2.23	0.69
1:E:51:TYR:H	1:E:51:TYR:HD2	1.41	0.69
1:C:72:VAL:HG23	1:C:162:LYS:HE3	1.75	0.68
1:F:59:LEU:HD13	1:F:114:TYR:HB2	1.75	0.68
1:C:42:LEU:HD13	1:C:125[B]:LEU:HD11	1.73	0.68
1:B:96:LEU:HD22	1:B:174:LEU:HD11	1.74	0.68
1:E:134:ILE:HD11	1:E:138:ASP:HB3	1.75	0.68
1:A:55:ARG:NH2	2:G:3:FUC:C5	2.55	0.68
1:E:73:ARG:HD2	1:F:176:ASN:OD1	1.93	0.67
1:A:110:ARG:HG3	1:A:111:PHE:N	2.10	0.67
1:C:39:HIS:HB2	1:C:131:THR:O	1.94	0.67
1:C:55:ARG:HA	1:C:58:MET:HE3	1.77	0.66
1:B:128:ARG:HD2	1:B:128:ARG:O	1.95	0.66
1:C:135:GLU:HG2	1:C:136:GLY:H	1.60	0.66
1:E:147:LYS:HE2	1:E:147:LYS:HA	1.78	0.66
1:B:48:GLN:NE2	2:G:2:NAG:H2	2.12	0.65
1:C:134:ILE:HD11	1:C:138:ASP:HB3	1.79	0.65
1:B:128:ARG:O	1:B:128:ARG:CD	2.45	0.65
1:F:71:ASP:O	1:F:72:VAL:HG23	1.97	0.65
1:F:105:PHE:HB2	1:F:106:PRO:HD3	1.79	0.64
1:B:105:PHE:HB2	1:B:106:PRO:HD3	1.78	0.64
1:C:49:GLN:O	1:C:51:TYR:N	2.30	0.64
1:B:135:GLU:HG2	1:B:136:GLY:H	1.62	0.64
1:A:103:VAL:C	1:A:106:PRO:HD2	2.20	0.63
1:E:107:GLN:HG2	1:E:160:GLU:OE1	1.98	0.63
1:C:48:GLN:C	1:C:50:PRO:HD3	2.20	0.62
4:I:2:NAG:O3	4:I:4:MAN:H5	2.00	0.62
1:C:96:LEU:HD22	1:C:174:LEU:HD11	1.82	0.62
1:C:124:ARG:CZ	1:E:156:GLY:HA2	2.30	0.61
1:F:150:ASP:HA	1:F:153:LYS:HE2	1.82	0.61
1:C:125[B]:LEU:HD23	1:C:174:LEU:HD13	1.82	0.61
1:E:112:GLN:NE2	1:E:116:GLN:H	1.98	0.61
1:F:129:LEU:O	1:F:132:CYS:HB3	2.00	0.61
1:C:172:MET:HE1	1:D:54:ASN:HA	1.83	0.61
1:C:110:ARG:HG2	1:C:110:ARG:NH1	2.06	0.61
1:E:69:ASN:N	1:E:69:ASN:ND2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:OE1	1:B:116:GLN:HG3	2.01	0.60
1:A:85:MET:HE2	1:A:88:ARG:NE	2.15	0.60
1:F:110:ARG:NH2	1:F:161:ILE:HD11	2.13	0.60
1:C:69:ASN:OD1	1:C:72:VAL:HG22	2.01	0.60
1:B:147:LYS:HE2	1:B:147:LYS:HA	1.83	0.59
1:A:129:LEU:O	1:A:132:CYS:HB3	2.02	0.59
1:F:58:MET:HE1	3:K:1:NAG:C1	2.32	0.59
1:C:135:GLU:HG2	1:C:136:GLY:N	2.17	0.59
1:E:73:ARG:HG3	1:F:176:ASN:HB3	1.83	0.59
1:E:110:ARG:NH2	1:E:161:ILE:HD11	2.18	0.59
1:B:154:LYS:HZ2	1:B:154:LYS:HB2	1.68	0.59
1:E:119:VAL:HB	1:E:120:PRO:HD3	1.85	0.58
1:B:70:THR:HG23	1:B:73:ARG:NH2	2.19	0.58
1:B:112:GLN:NE2	1:B:115:MET:HB3	2.18	0.58
1:D:135:GLU:HG2	1:D:136:GLY:N	2.18	0.58
1:F:54:ASN:OD1	1:F:58:MET:HE2	2.03	0.58
1:E:135:GLU:HG2	1:E:136:GLY:H	1.68	0.57
1:C:125[B]:LEU:CD2	1:C:174:LEU:HD13	2.34	0.57
1:D:107:GLN:OE1	1:D:110:ARG:HD2	2.03	0.57
1:B:154:LYS:CB	1:B:154:LYS:NZ	2.68	0.57
1:C:42:LEU:CD1	1:C:125[B]:LEU:HD11	2.35	0.57
1:E:45:SER:O	1:E:49:GLN:NE2	2.38	0.56
1:B:112:GLN:HE22	1:B:115:MET:HB3	1.70	0.56
1:C:50:PRO:HB3	6:D:1439:HOH:O	2.05	0.56
1:B:112:GLN:OE1	1:B:113:PRO:HA	2.05	0.56
1:F:85:MET:HE2	1:F:85:MET:HA	1.88	0.56
1:E:39:HIS:HB2	1:E:131:THR:O	2.06	0.56
1:B:135:GLU:HG2	1:B:136:GLY:N	2.21	0.56
1:D:85:MET:HE2	1:D:85:MET:HA	1.87	0.55
1:D:135:GLU:HG2	1:D:136:GLY:H	1.72	0.55
1:A:135:GLU:HG2	1:A:136:GLY:N	2.22	0.55
1:C:81:HIS:CE1	1:D:77:GLU:HB2	2.41	0.55
1:C:41:ARG:HG3	1:C:41:ARG:HH11	1.72	0.55
1:B:69:ASN:OD1	1:B:72:VAL:HG23	2.07	0.55
1:C:55:ARG:HD3	1:C:58:MET:HE1	1.89	0.55
1:E:112:GLN:HE22	1:E:116:GLN:N	2.05	0.55
1:D:129:LEU:O	1:D:132:CYS:HB3	2.06	0.54
1:E:73:ARG:HG3	1:F:176:ASN:CB	2.38	0.54
1:A:55:ARG:HH22	2:G:3:FUC:C6	2.21	0.54
1:B:39:HIS:HE1	1:B:128:ARG:HH22	1.55	0.54
1:B:85:MET:CE	1:B:88:ARG:CZ	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ASP:HA	1:F:153:LYS:CE	2.38	0.54
1:E:69:ASN:C	1:E:71:ASP:H	2.11	0.53
1:C:55:ARG:HD3	1:C:58:MET:CE	2.39	0.53
3:J:1:NAG:C6	3:J:2:NAG:H82	2.39	0.53
1:F:90:TYR:O	1:F:93:LYS:HB3	2.08	0.53
1:D:105:PHE:HB2	1:D:106:PRO:HD3	1.92	0.52
1:C:41:ARG:HG3	1:C:41:ARG:NH1	2.25	0.52
1:F:135:GLU:HG2	1:F:136:GLY:N	2.24	0.52
1:C:85:MET:HE2	1:C:88:ARG:NE	2.25	0.52
1:D:55:ARG:HH21	4:I:5:FUC:H5	1.74	0.52
1:B:139:LEU:HD21	1:B:143:ARG:HH22	1.74	0.52
1:C:110:ARG:HG3	1:C:111:PHE:CG	2.44	0.52
1:D:107:GLN:NE2	1:D:160:GLU:OE1	2.39	0.52
1:E:135:GLU:HG2	1:E:136:GLY:N	2.24	0.52
1:C:85:MET:HE1	1:C:88:ARG:NH2	2.25	0.52
1:E:103:VAL:C	1:E:106:PRO:HD2	2.31	0.51
1:C:119:VAL:HB	1:C:120:PRO:HD3	1.92	0.51
1:A:81:HIS:O	1:A:140:HIS:HE1	1.93	0.51
1:E:106:PRO:C	1:E:108:SER:H	2.13	0.51
1:B:49:GLN:CG	1:B:50:PRO:HD2	2.42	0.51
3:J:1:NAG:H61	3:J:2:NAG:H82	1.92	0.50
1:C:77:GLU:OE2	1:C:81:HIS:NE2	2.44	0.50
1:C:141:ILE:O	1:C:145:VAL:HG23	2.11	0.50
1:A:135:GLU:HG2	1:A:136:GLY:H	1.76	0.50
1:B:128:ARG:O	1:B:128:ARG:HD3	2.11	0.50
1:A:179:ILE:HD11	1:B:73:ARG:NH2	2.27	0.50
1:E:70:THR:O	1:E:73:ARG:NH2	2.45	0.50
1:E:73:ARG:NH2	1:F:179:ILE:HD11	2.27	0.50
1:B:110:ARG:HH11	1:B:110:ARG:CG	2.25	0.50
1:A:110:ARG:NH2	1:A:161:ILE:HD11	2.27	0.49
1:D:55:ARG:NH2	4:I:5:FUC:H5	2.27	0.49
1:B:92:MET:CE	1:B:170:LEU:HD12	2.42	0.49
1:B:98:PHE:CE1	1:B:149:LYS:HG2	2.46	0.49
1:A:55:ARG:HH22	2:G:3:FUC:C5	2.20	0.49
1:F:107:GLN:O	1:F:109:ASP:N	2.46	0.49
1:B:98:PHE:CD1	1:B:149:LYS:HG2	2.47	0.49
1:E:96:LEU:HD22	1:E:174:LEU:HD11	1.93	0.49
1:E:77:GLU:OE2	1:E:81:HIS:CE1	2.66	0.48
1:A:44:LYS:HE3	1:A:179:ILE:CD1	2.43	0.48
1:B:85:MET:HE1	1:B:88:ARG:CZ	2.43	0.48
1:B:154:LYS:HB2	1:B:154:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ARG:NH1	1:D:114:TYR:CE1	2.82	0.48
1:D:139:LEU:HD23	1:D:143:ARG:NH2	2.28	0.48
1:A:146:GLN:NE2	6:A:325:HOH:O	2.47	0.48
1:C:124:ARG:NH2	1:E:156:GLY:HA2	2.29	0.48
1:A:175:ARG:CZ	1:B:169:LEU:HD11	2.44	0.47
1:C:110:ARG:CG	1:C:111:PHE:N	2.77	0.47
1:E:110:ARG:HH21	1:E:161:ILE:HD11	1.78	0.47
1:F:109:ASP:OD1	1:F:110:ARG:N	2.45	0.47
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.79	0.47
1:B:119:VAL:HB	1:B:120:PRO:HD3	1.96	0.47
1:D:128:ARG:HD3	6:D:1433:HOH:O	2.13	0.47
1:A:110:ARG:CG	1:A:111:PHE:N	2.77	0.47
1:B:51:TYR:HE1	1:B:55:ARG:HE	1.59	0.47
1:A:105:PHE:HD2	1:F:128:ARG:HH12	1.63	0.47
1:D:64:SER:C	1:D:66:ALA:H	2.18	0.47
1:A:59:LEU:HD23	1:A:167:LEU:CD1	2.45	0.47
1:B:70:THR:HG23	1:B:70:THR:O	2.15	0.47
1:C:42:LEU:HD22	1:C:128:ARG:HG3	1.97	0.47
1:F:143:ARG:CB	1:F:143:ARG:HH11	2.28	0.47
1:B:121:PHE:CE2	1:B:125:LEU:HD11	2.50	0.46
1:B:128:ARG:HD2	1:B:128:ARG:C	2.34	0.46
1:E:175:ARG:C	1:E:175:ARG:HD2	2.36	0.46
1:A:139:LEU:HD23	1:A:143:ARG:HH22	1.81	0.46
1:F:135:GLU:HG2	1:F:136:GLY:H	1.79	0.46
1:B:85:MET:HE2	1:B:88:ARG:NE	2.29	0.46
1:B:99:THR:O	1:B:103:VAL:HB	2.16	0.46
1:C:128:ARG:O	1:C:128:ARG:NH1	2.47	0.46
1:A:59:LEU:HD13	1:A:114:TYR:HB2	1.97	0.46
1:A:106:PRO:O	1:A:108:SER:N	2.43	0.46
1:C:92:MET:CE	1:C:170:LEU:HD12	2.46	0.46
1:C:139:LEU:HD21	1:C:143:ARG:HH22	1.79	0.46
1:A:55:ARG:NH1	1:A:114:TYR:CE1	2.83	0.46
1:B:105:PHE:N	1:B:106:PRO:CD	2.79	0.46
1:B:141:ILE:O	1:B:145:VAL:HG23	2.15	0.46
1:F:131:THR:HA	6:F:1635:HOH:O	2.15	0.46
1:B:112:GLN:CD	1:B:116:GLN:HG3	2.36	0.46
1:D:67:ASP:OD1	6:D:1437:HOH:O	2.21	0.46
1:E:42:LEU:HD13	1:E:125:LEU:HD22	1.98	0.46
1:D:58[A]:MET:HE1	4:I:1:NAG:C1	2.47	0.45
1:F:73:ARG:HD3	1:F:166:GLU:OE2	2.17	0.45
1:C:110:ARG:O	1:C:112:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:MET:HE2	1:D:88:ARG:NE	2.31	0.45
1:E:134:ILE:HD11	1:E:138:ASP:CB	2.46	0.45
1:F:59:LEU:HD23	1:F:167:LEU:CD1	2.46	0.45
1:D:41:ARG:HG3	1:D:41:ARG:NH1	2.30	0.45
1:C:49:GLN:N	1:C:50:PRO:HD3	2.32	0.45
1:F:143:ARG:NH1	1:F:143:ARG:HB2	2.32	0.44
1:B:128:ARG:CD	1:B:128:ARG:C	2.85	0.44
1:B:129:LEU:O	1:B:132:CYS:HB3	2.17	0.44
1:B:112:GLN:OE1	1:B:112:GLN:HA	2.17	0.44
1:C:134:ILE:HD11	1:C:138:ASP:CB	2.46	0.44
1:D:72:VAL:HB	1:D:162:LYS:HE3	1.99	0.44
1:D:85:MET:HE1	1:D:88:ARG:CZ	2.47	0.44
1:E:46:ASN:C	1:E:49:GLN:HE21	2.21	0.44
1:E:105:PHE:N	1:E:106:PRO:CD	2.81	0.44
1:F:96:LEU:HD22	1:F:174:LEU:HD11	2.00	0.44
1:B:108:SER:HA	1:B:115:MET:HG2	1.98	0.44
1:A:55:ARG:HD3	1:A:58[A]:MET:CE	2.48	0.44
1:E:51:TYR:O	1:E:55:ARG:HG2	2.18	0.44
1:E:54:ASN:HB3	1:E:58:MET:HE2	2.00	0.44
1:E:69:ASN:C	1:E:71:ASP:N	2.71	0.44
1:E:98:PHE:CE1	1:E:149:LYS:HG2	2.53	0.44
1:B:49:GLN:HG3	1:B:50:PRO:HD2	2.00	0.44
1:C:85:MET:CE	1:C:88:ARG:CZ	2.96	0.44
1:E:141:ILE:O	1:E:145:VAL:HG23	2.18	0.44
1:B:41:ARG:NH2	1:B:43:ASP:HA	2.32	0.43
1:E:78:LYS:HA	1:E:81:HIS:CD2	2.53	0.43
1:B:71:ASP:OD1	1:B:71:ASP:N	2.51	0.43
1:B:85:MET:HE1	1:B:88:ARG:NH2	2.33	0.43
1:E:54:ASN:O	1:E:58:MET:HG3	2.17	0.43
1:E:139:LEU:HD21	1:E:143:ARG:HH22	1.83	0.43
1:E:38:SER:HB3	6:E:403:HOH:O	2.17	0.43
1:A:59:LEU:HD23	1:A:167:LEU:HD12	2.01	0.43
1:F:55:ARG:NH1	1:F:114:TYR:CE1	2.87	0.43
1:A:44:LYS:HE3	1:A:179:ILE:HD12	1.99	0.43
1:B:77:GLU:OE2	1:B:81:HIS:NE2	2.48	0.43
1:F:64:SER:C	1:F:66:ALA:H	2.20	0.43
1:F:148:LEU:C	1:F:148:LEU:HD23	2.39	0.43
1:A:39:HIS:N	1:A:39:HIS:HD1	2.17	0.43
1:D:154:LYS:O	1:D:154:LYS:HG2	2.18	0.43
1:F:52:ILE:HD12	1:F:52:ILE:HA	1.91	0.43
1:E:98:PHE:CD1	1:E:149:LYS:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD13	1:B:114:TYR:HB2	2.00	0.42
1:C:42:LEU:HD22	1:C:128:ARG:CG	2.48	0.42
1:E:54:ASN:HB3	1:E:58:MET:CE	2.48	0.42
1:D:63:ALA:HA	1:D:111:PHE:CE1	2.53	0.42
1:E:175:ARG:NH2	1:E:176:ASN:OD1	2.41	0.42
1:F:92:MET:CE	1:F:170:LEU:HD12	2.49	0.42
1:B:48:GLN:NE2	2:G:2:NAG:H83	2.14	0.42
1:A:77:GLU:HG3	1:B:81:HIS:CE1	2.55	0.42
1:E:112:GLN:NE2	1:E:116:GLN:HB2	2.34	0.42
1:A:55:ARG:NH2	2:G:3:FUC:C6	2.83	0.42
1:B:94:GLN:HE21	1:B:142:GLN:HE22	1.66	0.42
1:C:85:MET:HE1	1:C:88:ARG:CZ	2.49	0.42
1:D:175[B]:ARG:NH1	1:D:176:ASN:OD1	2.53	0.42
1:C:42:LEU:CD2	1:C:128:ARG:HG3	2.49	0.42
1:F:140:HIS:HA	1:F:143:ARG:HH11	1.85	0.42
1:D:51:TYR:HE1	4:I:5:FUC:H3	1.85	0.41
1:B:51:TYR:O	1:B:55:ARG:HG2	2.20	0.41
1:F:160:GLU:O	1:F:164:ILE:HG13	2.19	0.41
1:A:64:SER:C	1:A:66:ALA:H	2.24	0.41
1:E:92:MET:HB3	1:E:174:LEU:HD23	2.03	0.41
1:A:39:HIS:N	1:A:39:HIS:ND1	2.68	0.41
1:C:153:LYS:HA	1:C:153:LYS:HD3	1.91	0.41
1:D:55:ARG:NH2	4:I:5:FUC:C6	2.84	0.41
1:B:85:MET:HE2	1:B:88:ARG:CZ	2.50	0.41
1:D:90:TYR:O	1:D:93:LYS:HB3	2.21	0.41
1:B:39:HIS:CE1	1:B:128:ARG:HH22	2.36	0.41
1:C:172:MET:CE	1:D:54:ASN:HA	2.48	0.41
1:E:40:CYS:O	1:E:41:ARG:HG2	2.20	0.41
1:A:85:MET:HE2	1:A:88:ARG:CD	2.51	0.41
1:D:148:LEU:HD23	1:D:148:LEU:C	2.40	0.41
1:E:93:LYS:HE3	1:E:129:LEU:O	2.21	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.21	0.41
1:B:137:ASP:O	1:B:140:HIS:CE1	2.74	0.41
1:C:139:LEU:HD21	1:C:143:ARG:NH2	2.36	0.41
1:A:119:VAL:HB	1:A:120:PRO:HD3	2.03	0.40
1:B:73:ARG:HA	1:B:73:ARG:HD3	1.94	0.40
1:C:125[B]:LEU:HD23	1:C:174:LEU:CD1	2.50	0.40
1:A:138:ASP:O	1:A:142:GLN:HG2	2.21	0.40
1:B:70:THR:O	1:B:73:ARG:NH2	2.54	0.40
1:C:124:ARG:HG2	6:E:388:HOH:O	2.20	0.40
1:D:41:ARG:HG3	1:D:41:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:CE	1:A:170:LEU:HD12	2.51	0.40
1:E:110:ARG:HG2	1:E:111:PHE:CD2	2.57	0.40
1:B:110:ARG:CG	1:B:110:ARG:NH1	2.84	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	140/142 (99%)	134 (96%)	3 (2%)	3 (2%)	5	11
1	B	141/142 (99%)	134 (95%)	5 (4%)	2 (1%)	9	19
1	C	141/142 (99%)	133 (94%)	5 (4%)	3 (2%)	5	11
1	D	142/142 (100%)	136 (96%)	5 (4%)	1 (1%)	19	38
1	E	140/142 (99%)	126 (90%)	10 (7%)	4 (3%)	3	6
1	F	141/142 (99%)	133 (94%)	5 (4%)	3 (2%)	5	11
All	All	845/852 (99%)	796 (94%)	33 (4%)	16 (2%)	6	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	B	50	PRO
1	C	50	PRO
1	E	50	PRO
1	E	106	PRO
1	A	106	PRO
1	A	136	GLY
1	B	136	GLY
1	C	136	GLY

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Mol	Chain	Res	Type
1	D	136	GLY
1	E	107	GLN
1	E	136	GLY
1	F	108	SER
1	F	136	GLY
1	C	108	SER
1	F	72	VAL

### 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	130/130 (100%)	123 (95%)	7 (5%)	18	39
1	B	131/130 (101%)	118 (90%)	13 (10%)	6	13
1	C	131/130 (101%)	121 (92%)	10 (8%)	11	23
1	D	132/130 (102%)	128 (97%)	4 (3%)	36	63
1	E	130/130 (100%)	123 (95%)	7 (5%)	18	39
1	F	131/130 (101%)	127 (97%)	4 (3%)	35	62
All	All	785/780 (101%)	740 (94%)	45 (6%)	17	37

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	72	VAL
1	A	73	ARG
1	A	110	ARG
1	A	132	CYS
1	A	147	LYS
1	A	154	LYS
1	B	39	HIS
1	B	50	PRO
1	B	52	ILE
1	B	68	ASN

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Mol	Chain	Res	Type
1	B	70	THR
1	B	71	ASP
1	B	77	GLU
1	B	110	ARG
1	B	113	PRO
1	B	128	ARG
1	B	137	ASP
1	B	140	HIS
1	B	147	LYS
1	C	41	ARG
1	C	49	GLN
1	C	50	PRO
1	C	110	ARG
1	C	113	PRO
1	C	116	GLN
1	C	133	HIS
1	C	139	LEU
1	C	140	HIS
1	C	147	LYS
1	D	41	ARG
1	D	88	ARG
1	D	128	ARG
1	D	147	LYS
1	E	51	TYR
1	E	69	ASN
1	E	71	ASP
1	E	77	GLU
1	E	112	GLN
1	E	116	GLN
1	E	147	LYS
1	F	68	ASN
1	F	71	ASP
1	F	110	ARG
1	F	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	B	48	GLN
1	B	94	GLN
1	C	48	GLN

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Mol	Chain	Res	Type
1	C	94	GLN
1	C	112	GLN
1	C	116	GLN
1	C	140	HIS
1	D	69	ASN
1	D	133	HIS
1	E	49	GLN
1	E	69	ASN
1	E	112	GLN
1	E	140	HIS
1	E	142	GLN
1	F	140	HIS

### 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](#)

16 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	$\# Z  > 2$
2	NAG	G	1	1,2	14,14,15	0.81	1 (7%)	17,19,21	0.73	0
2	NAG	G	2	2	14,14,15	0.69	0	17,19,21	0.70	0
2	FUC	G	3	2	10,10,11	0.73	0	14,14,16	0.53	0
3	NAG	H	1	1,3	14,14,15	0.71	0	17,19,21	1.29	2 (11%)
3	NAG	H	2	3	14,14,15	0.77	0	17,19,21	0.93	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.57	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	I	2	4	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
4	MAN	I	3	4	11,11,12	0.71	0	15,15,17	0.27	0
4	MAN	I	4	4	11,11,12	0.58	0	15,15,17	0.82	1 (6%)
4	FUC	I	5	4	10,10,11	0.76	0	14,14,16	0.65	0
3	NAG	J	1	1,3	14,14,15	0.61	0	17,19,21	0.81	1 (5%)
3	NAG	J	2	3	14,14,15	0.75	0	17,19,21	0.72	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.62	0	17,19,21	0.88	1 (5%)
3	NAG	K	2	3	14,14,15	0.71	0	17,19,21	0.77	0
3	NAG	L	1	1,3	14,14,15	0.67	0	17,19,21	0.73	1 (5%)
3	NAG	L	2	3	14,14,15	0.76	0	17,19,21	0.82	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
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	5/6/23/26	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1
3	NAG	H	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	MAN	I	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	0/1/1/1
4	FUC	I	5	4	-	-	0/1/1/1
3	NAG	J	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	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)
2	G	1	NAG	C1-C2	2.03	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C4-C3-C2	-3.08	106.51	111.02
3	H	1	NAG	C2-N2-C7	-2.97	118.92	122.90
3	H	2	NAG	C2-N2-C7	-2.69	119.30	122.90
3	J	1	NAG	C2-N2-C7	-2.42	119.66	122.90
3	L	1	NAG	C2-N2-C7	-2.35	119.76	122.90
3	L	2	NAG	C2-N2-C7	-2.21	119.94	122.90
4	I	2	NAG	C2-N2-C7	-2.20	119.95	122.90
4	I	4	MAN	C1-O5-C5	2.16	115.08	112.19
3	J	2	NAG	C2-N2-C7	-2.08	120.12	122.90
3	K	1	NAG	C4-C3-C2	2.04	114.01	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	2	NAG	C1
4	I	3	MAN	C1

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
4	I	4	MAN	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2

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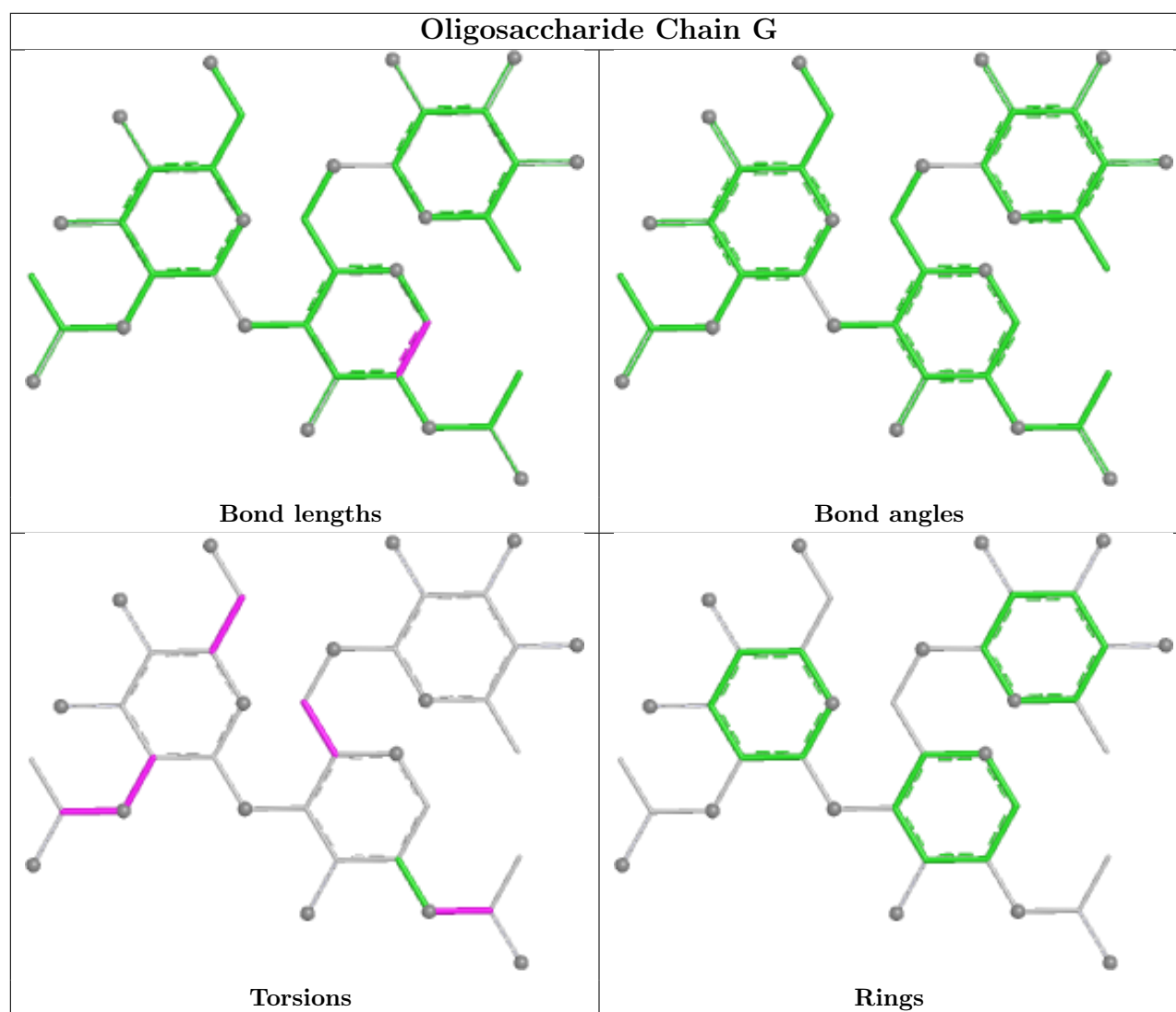
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
2	G	2	NAG	C1-C2-N2-C7
3	H	1	NAG	O7-C7-N2-C2

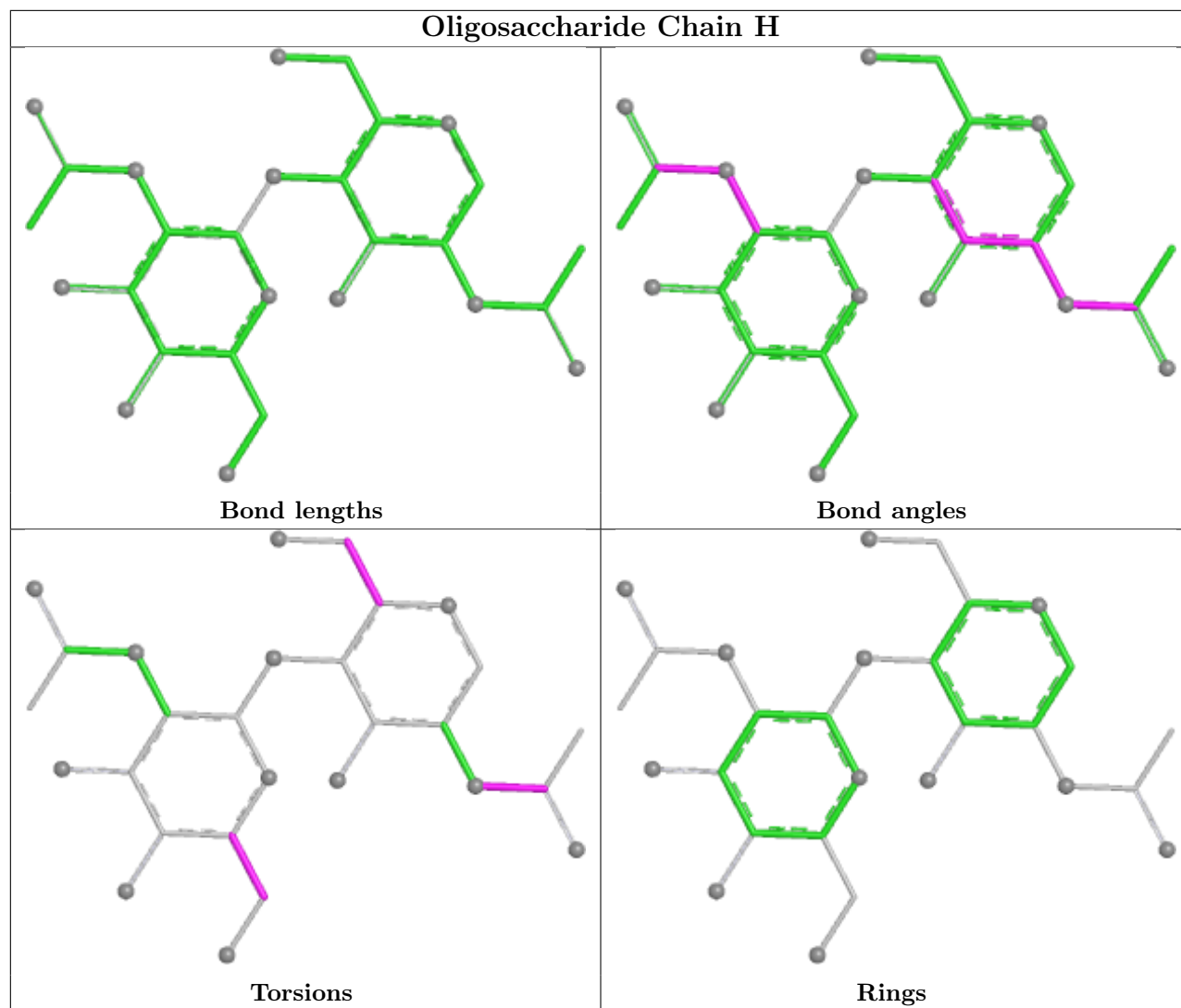
There are no ring outliers.

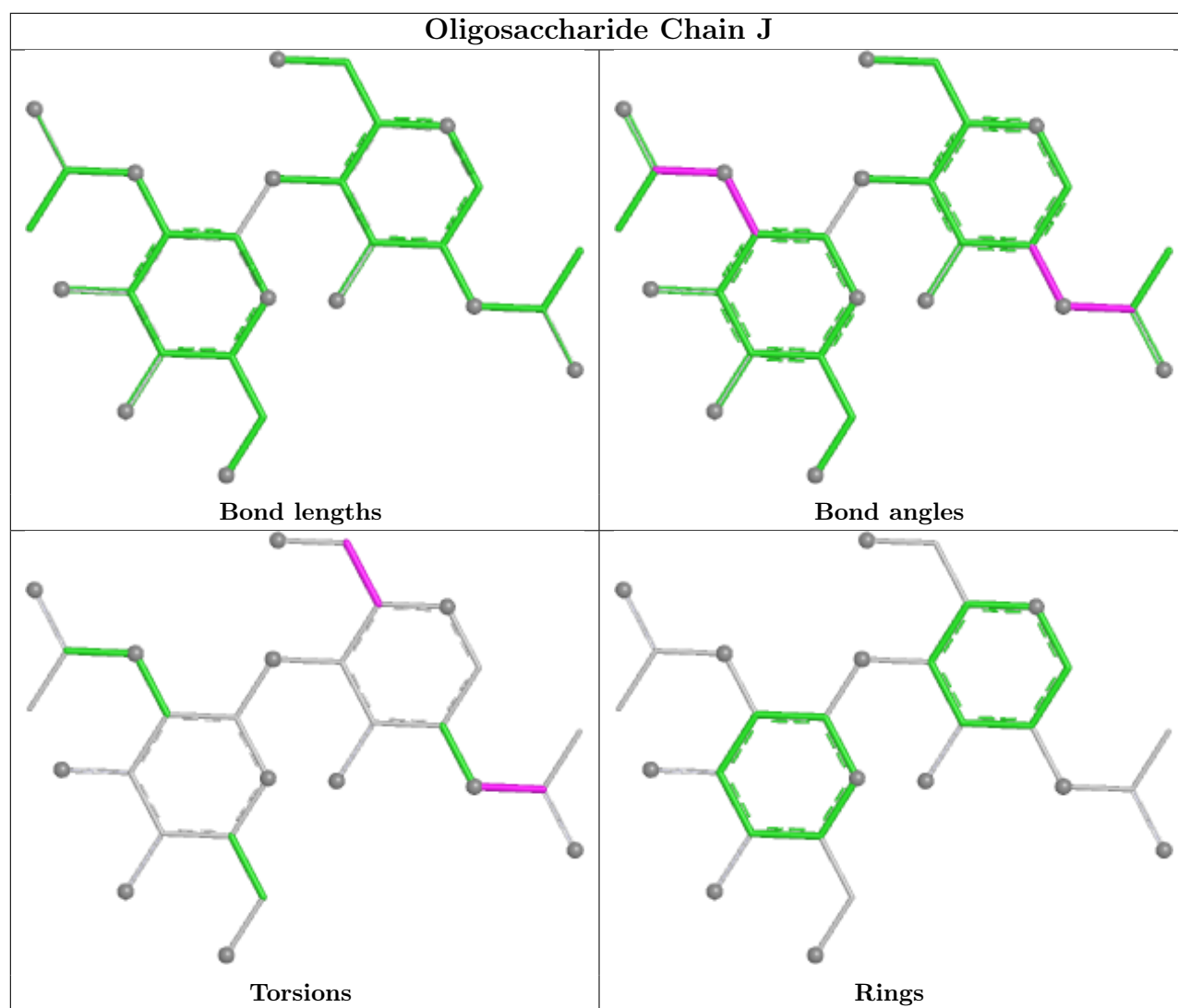
11 monomers are involved in 21 short contacts:

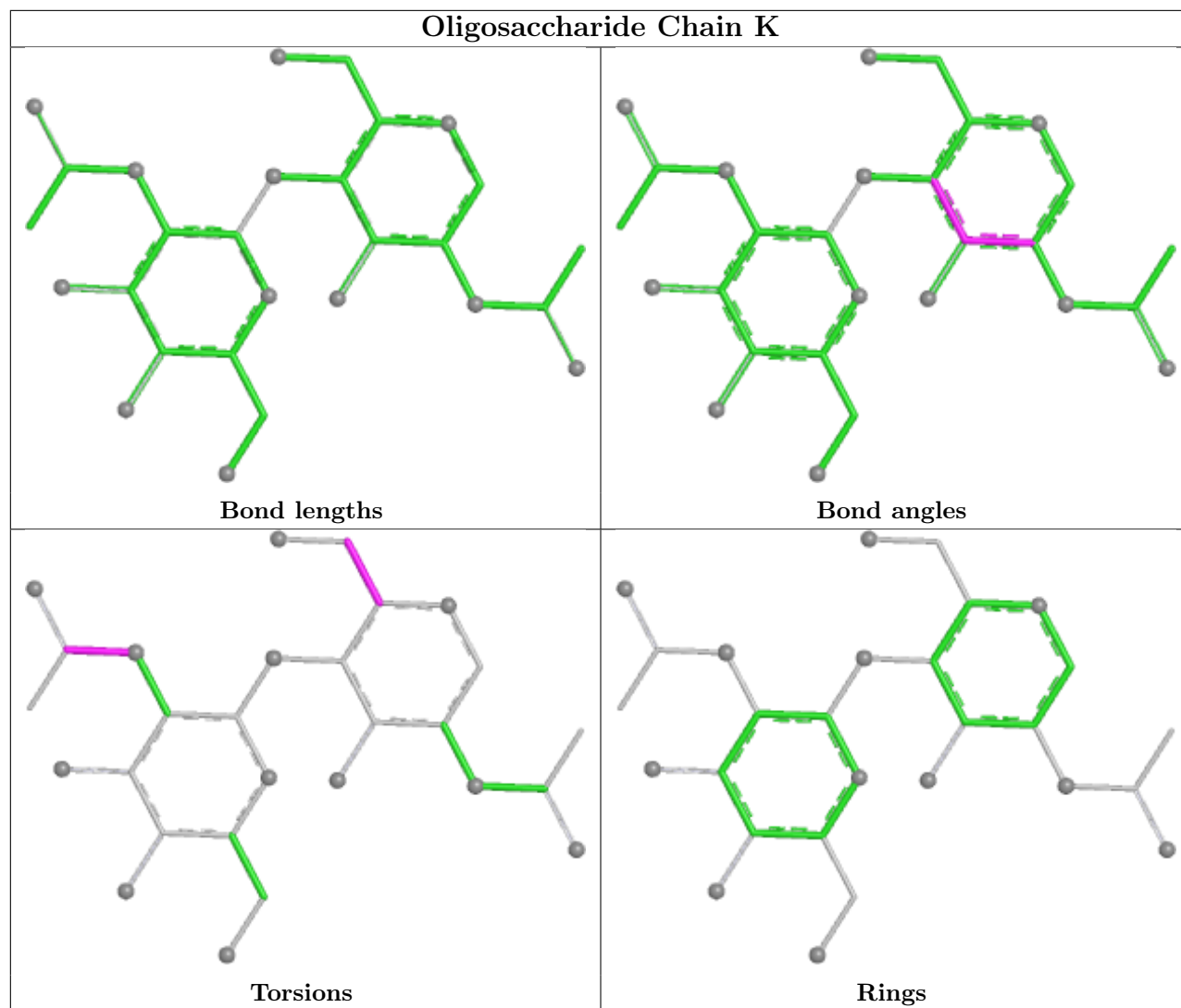
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0
2	G	3	FUC	6	0
4	I	5	FUC	4	0
3	K	1	NAG	1	0
2	G	2	NAG	3	0
3	L	1	NAG	3	0
3	J	2	NAG	2	0
4	I	1	NAG	1	0
4	I	4	MAN	1	0
3	J	1	NAG	2	0
3	L	2	NAG	3	0

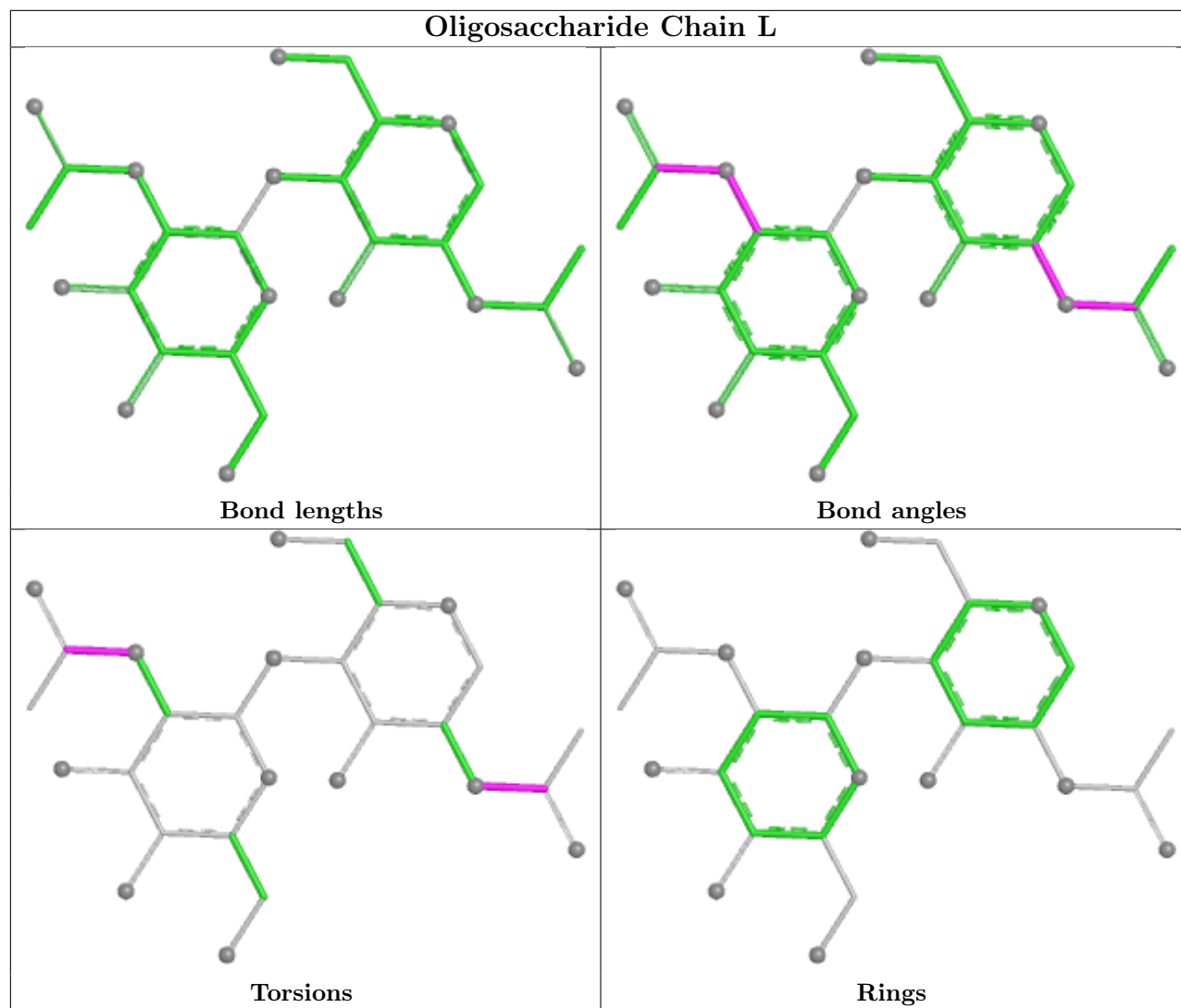
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

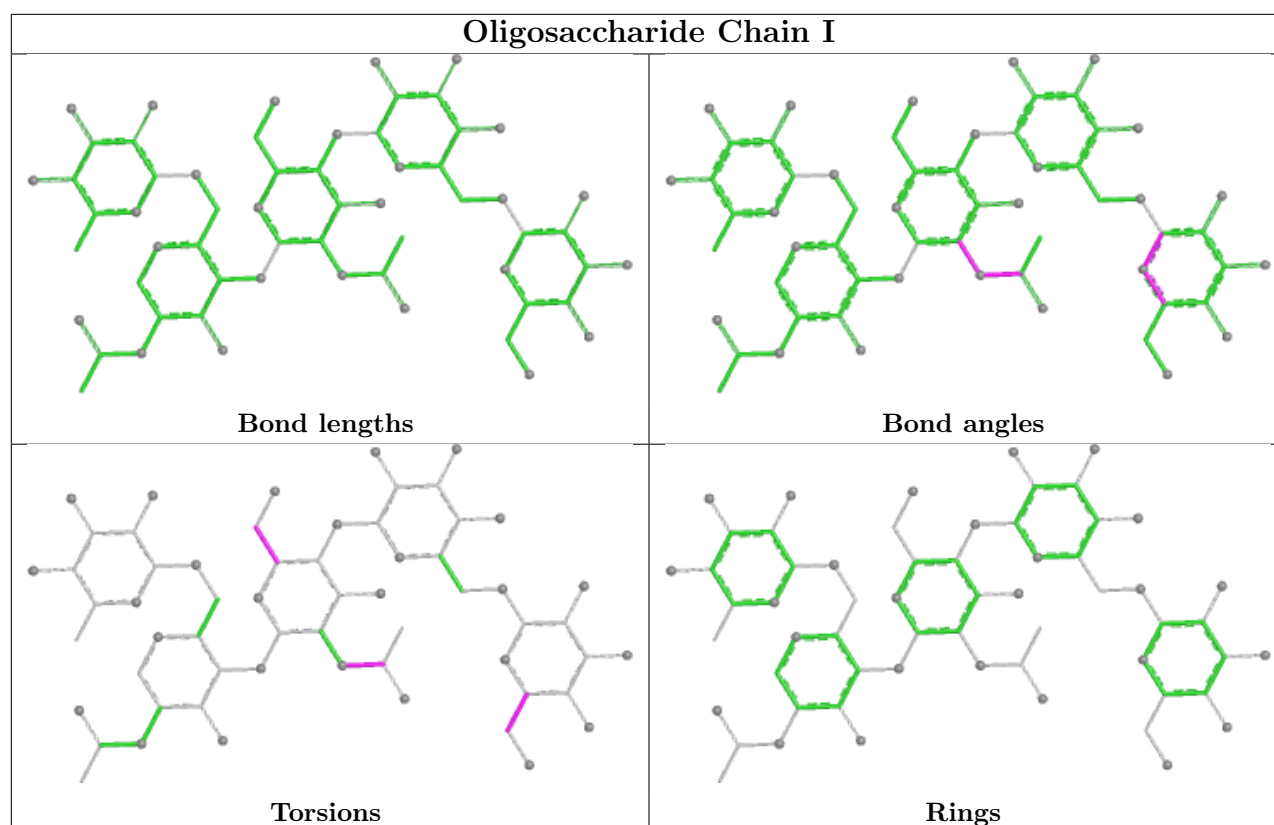












## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
5	NAG	E	1531	1	14,14,15	0.68	0	17,19,21	0.69	0
5	NAG	A	1131	1	14,14,15	0.46	0	17,19,21	1.03	2 (11%)
5	NAG	B	1231	1	14,14,15	0.83	0	17,19,21	0.98	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
5	NAG	E	1531	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1131	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1231	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1231	NAG	C2-N2-C7	-2.73	119.24	122.90
5	A	1131	NAG	C2-N2-C7	-2.24	119.90	122.90
5	A	1131	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1131	NAG	C8-C7-N2-C2
5	A	1131	NAG	O7-C7-N2-C2
5	B	1231	NAG	C8-C7-N2-C2
5	A	1131	NAG	O5-C5-C6-O6
5	B	1231	NAG	O7-C7-N2-C2
5	A	1131	NAG	C4-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	141/142 (99%)	-0.03	4 (2%) 55 49	25, 53, 82, 97	1 (0%)
1	B	142/142 (100%)	-0.10	3 (2%) 63 58	30, 52, 86, 103	1 (0%)
1	C	142/142 (100%)	-0.15	0 100 100	28, 47, 79, 100	1 (0%)
1	D	142/142 (100%)	-0.16	1 (0%) 84 81	24, 54, 88, 100	2 (1%)
1	E	142/142 (100%)	0.17	0 100 100	39, 60, 89, 102	0
1	F	142/142 (100%)	0.56	8 (5%) 31 25	33, 73, 111, 121	1 (0%)
All	All	851/852 (99%)	0.05	16 (1%) 66 61	24, 56, 95, 121	6 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	HIS	5.1
1	B	38	SER	3.0
1	A	134	ILE	3.0
1	F	145	VAL	2.7
1	F	90	TYR	2.7
1	F	82	GLY	2.4
1	F	165	GLY	2.4
1	F	148	LEU	2.3
1	A	128	ARG	2.3
1	A	137	ASP	2.2
1	F	141	ILE	2.2
1	B	140	HIS	2.1
1	F	158	SER	2.1
1	A	39	HIS	2.0
1	D	39	HIS	2.0
1	F	101	GLU	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 ⓘ

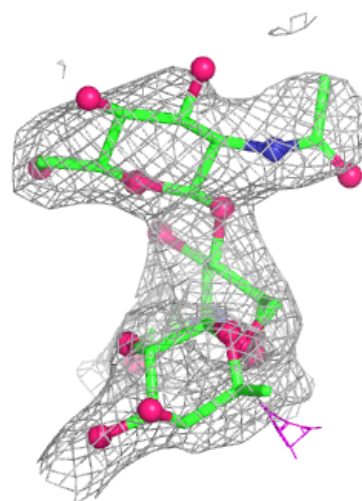
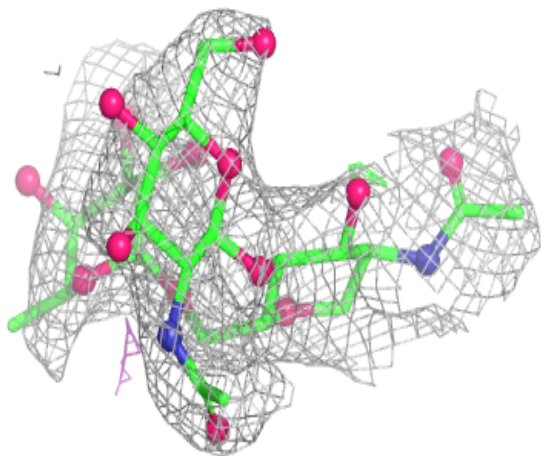
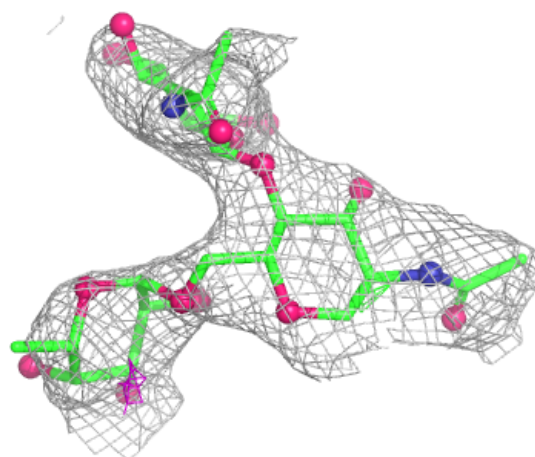
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	G	2	14/15	0.57	0.13	87,89,90,90	0
2	FUC	G	3	10/11	0.60	0.14	89,91,92,93	0
3	NAG	H	2	14/15	0.61	0.15	86,88,92,93	0
4	MAN	I	4	11/12	0.67	0.10	98,100,101,101	0
3	NAG	L	2	14/15	0.68	0.14	89,90,92,92	0
3	NAG	J	2	14/15	0.70	0.11	75,76,81,81	0
4	FUC	I	5	10/11	0.72	0.16	85,87,88,89	0
3	NAG	L	1	14/15	0.76	0.11	78,81,83,86	0
4	MAN	I	3	11/12	0.77	0.12	94,96,98,99	0
4	NAG	I	2	14/15	0.79	0.12	79,81,85,91	0
3	NAG	K	2	14/15	0.79	0.12	97,98,101,101	0
2	NAG	G	1	14/15	0.80	0.11	69,73,83,86	0
3	NAG	K	1	14/15	0.82	0.10	82,86,91,94	0
3	NAG	H	1	14/15	0.85	0.09	65,71,78,83	0
4	NAG	I	1	14/15	0.87	0.08	51,65,75,81	0
3	NAG	J	1	14/15	0.89	0.07	59,61,67,71	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.

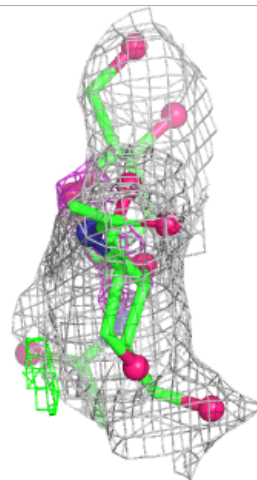
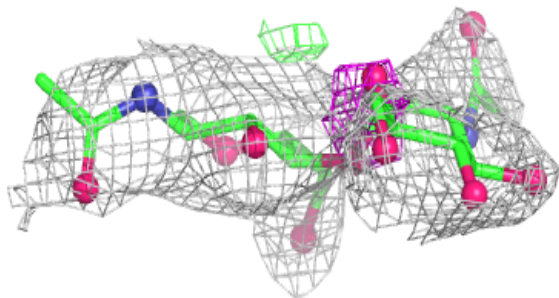
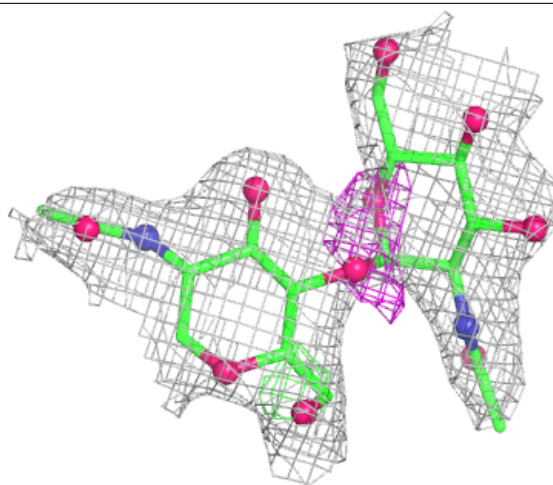
**Electron density around Chain G:**

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



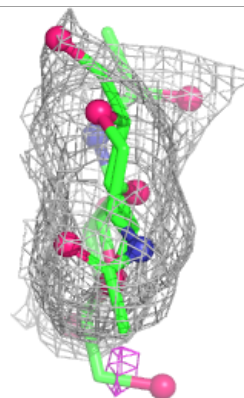
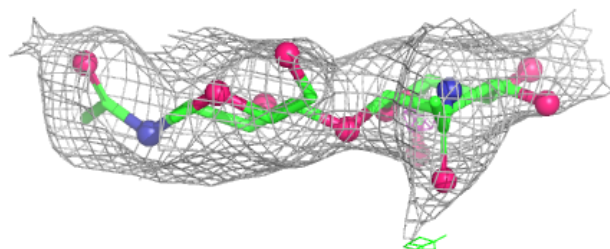
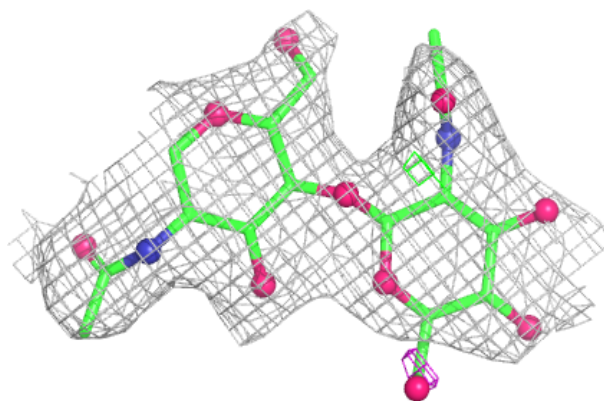
**Electron density around Chain H:**

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

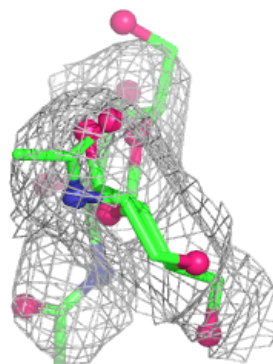
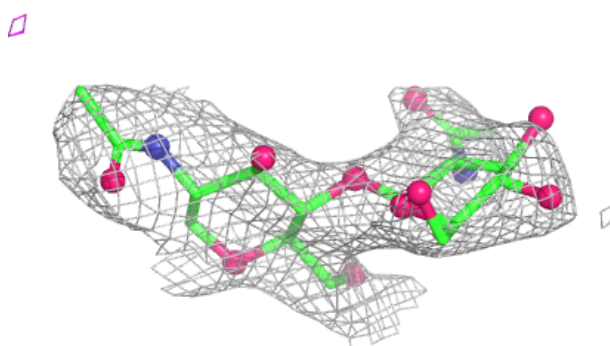
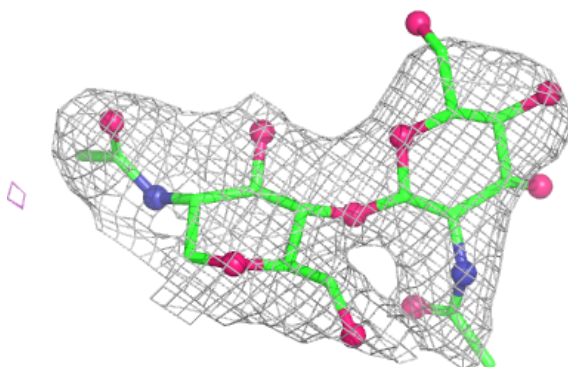


**Electron density around Chain J:**

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

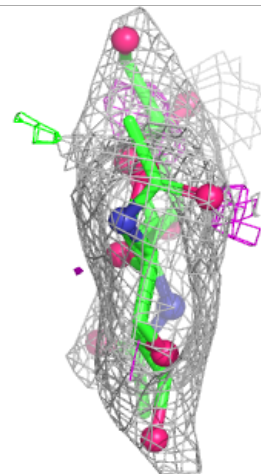
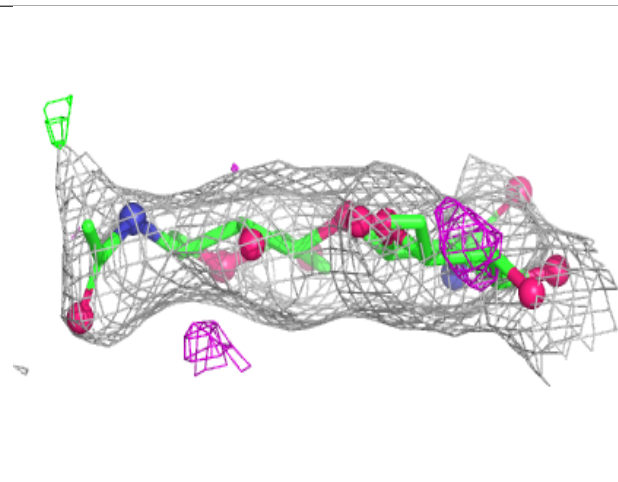
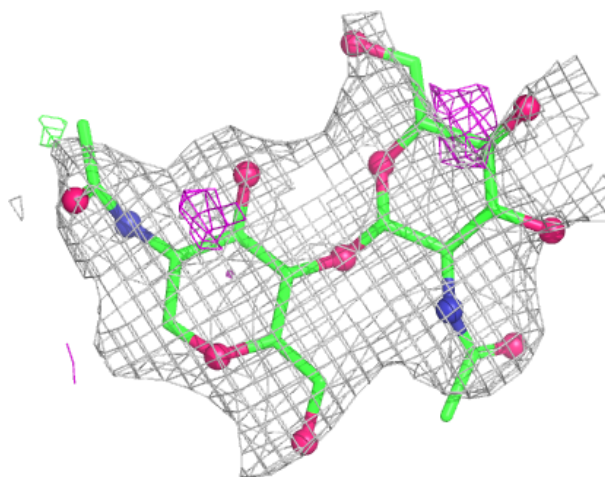
**Electron density around Chain K:**

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

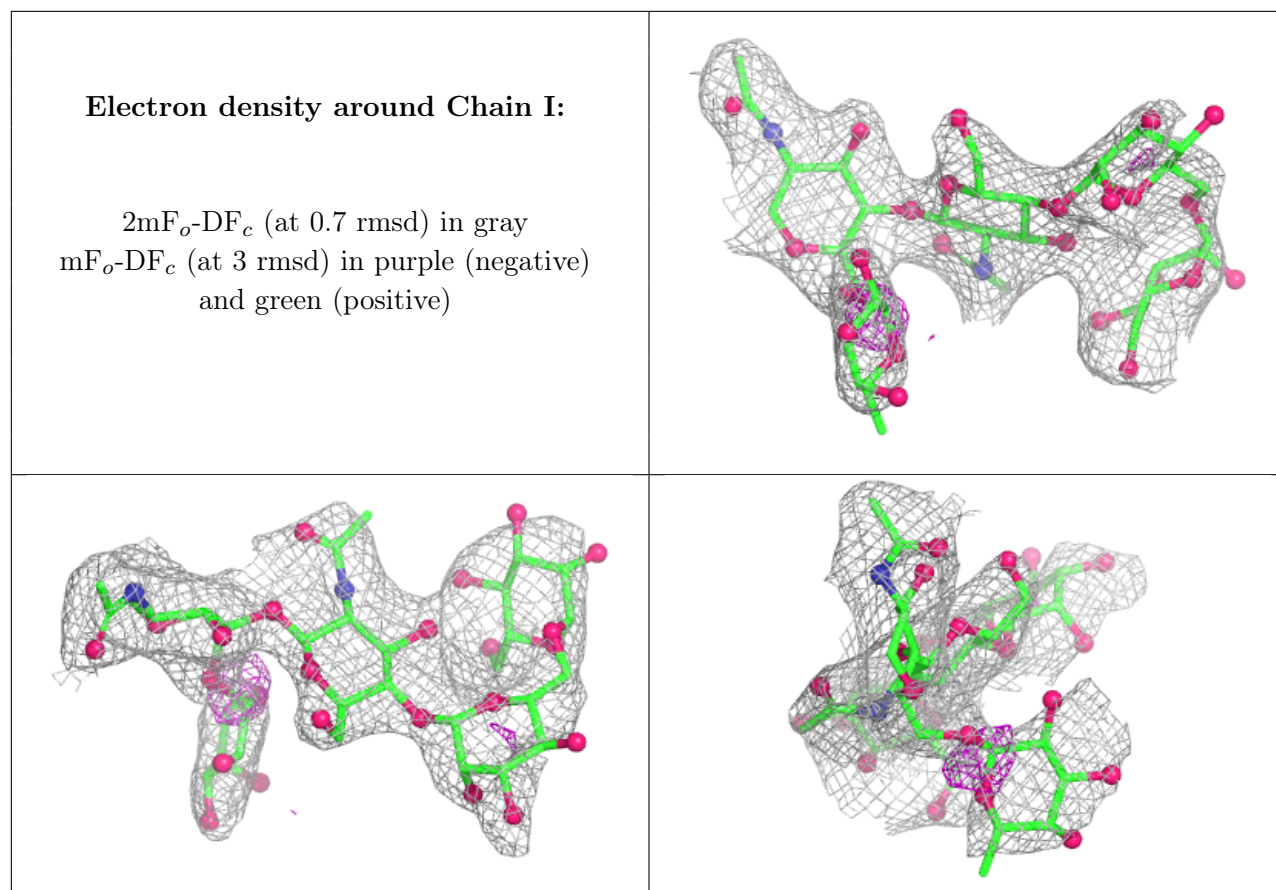


**Electron density around Chain L:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	1531	14/15	0.81	0.09	55,59,61,63	0
5	NAG	B	1231	14/15	0.82	0.09	67,70,71,73	0
5	NAG	A	1131	14/15	0.82	0.10	68,71,74,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.