



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 10, 2024 – 10:10 AM EST

PDB ID : 3T6Q  
Title : Crystal structure of mouse RP105/MD-1 complex  
Authors : Ohto, U.; Shimizu, T.  
Deposited on : 2011-07-28  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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

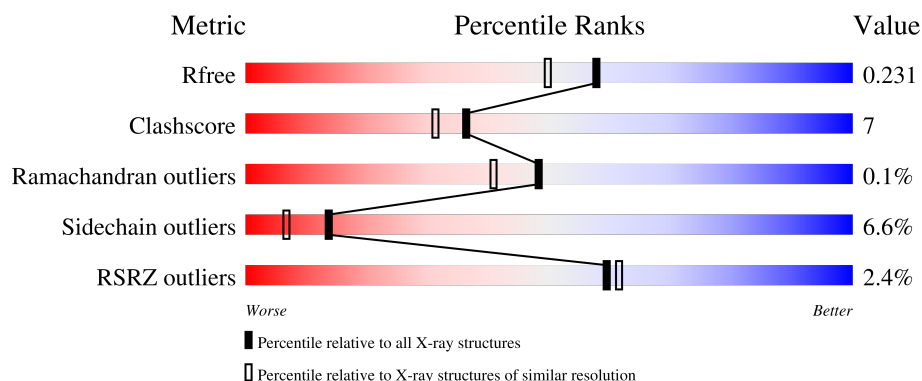
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.






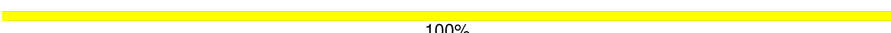
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	606	<div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	606	<div> <div>3%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
2	C	145	<div> <div>3%</div> <div>83%</div> <div>10%</div> <div>..</div> </div>
2	D	145	<div> <div>4%</div> <div>78%</div> <div>14%</div> <div>..</div> </div>
3	E	9	<div> <div>11%</div> <div>89%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	2	 50%50%
4	G	2	 50%50%
4	I	2	 50%50%
5	H	8	 100%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13571 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 CD180 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	19	0
			4887	3082	821	957	27			
1	B	601	Total	C	N	O	S	0	7	0
			4789	3030	803	931	25			

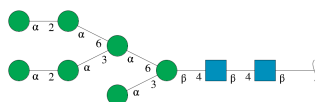
- Molecule 2 is a protein called Lymphocyte antigen 86.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	139	Total	C	N	O	S	0	1	0
			1099	692	186	214	7			
2	D	139	Total	C	N	O	S	0	0	0
			1091	688	185	211	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	163	GLU	-	expression tag	UNP O88188
C	164	PHE	-	expression tag	UNP O88188
D	163	GLU	-	expression tag	UNP O88188
D	164	PHE	-	expression tag	UNP O88188

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



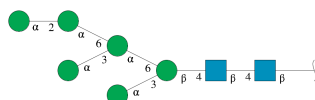
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 9 is water.

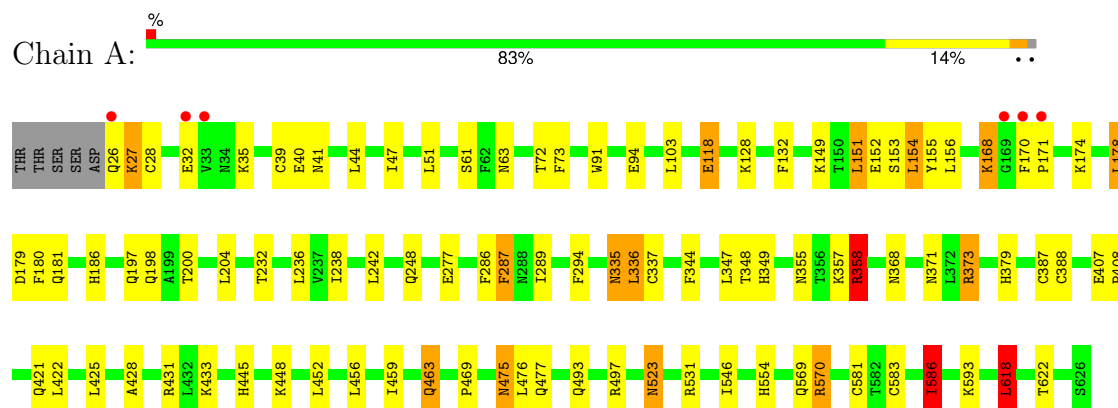
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	556	Total	O	0	0
			556	556		
9	C	97	Total	O	0	0
			97	97		
9	B	419	Total	O	0	0
			419	419		
9	D	77	Total	O	0	0
			77	77		



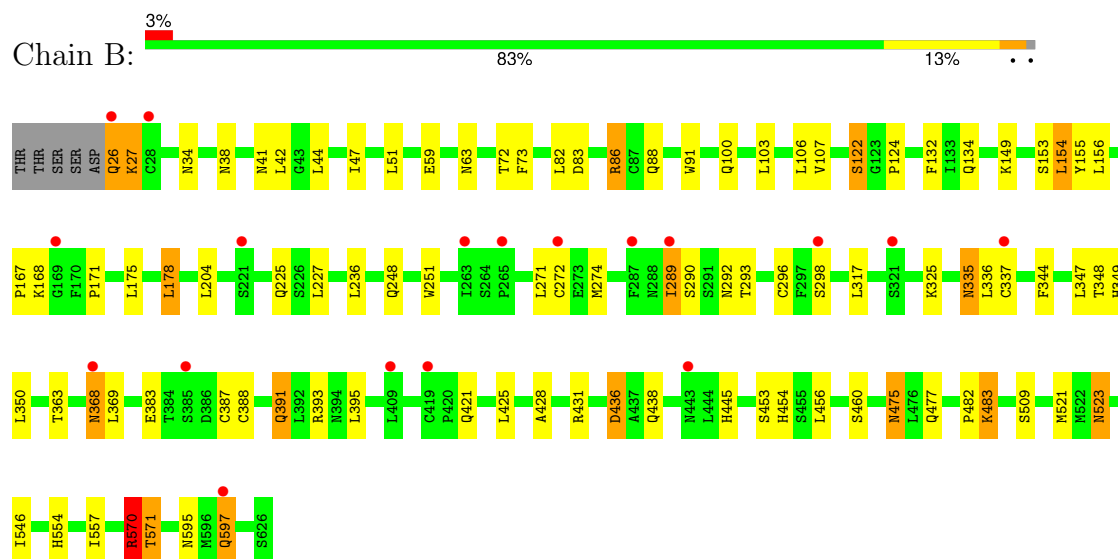
### 3 Residue-property plots [i](#)

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.

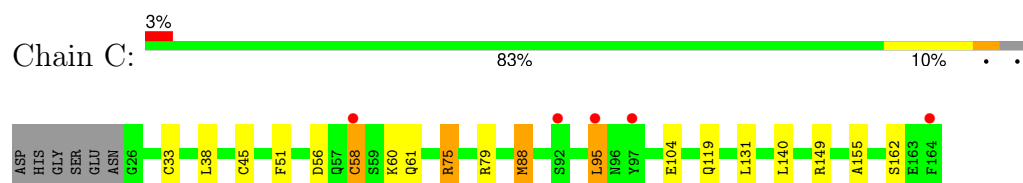
#### • Molecule 1: CD180 antigen



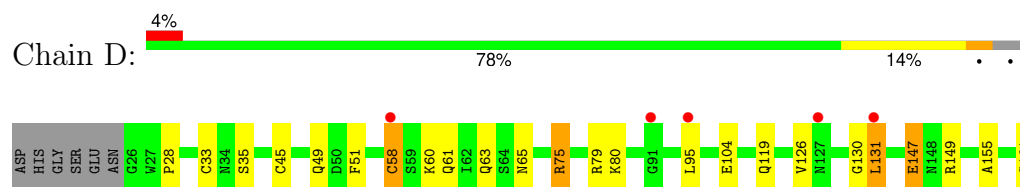
#### • Molecule 1: CD180 antigen



#### • Molecule 2: Lymphocyte antigen 86



- Molecule 2: Lymphocyte antigen 86



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



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



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.75Å 192.79Å 75.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.02-1.90) 98.4 (49.02-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.186 , 0.231 0.186 , 0.231	Depositor DCC
$R_{free}$ test set	8204 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: CU, MAN, GOL, 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	0.72	1/4975 (0.0%)	0.79	8/6743 (0.1%)
1	B	0.61	2/4877 (0.0%)	0.73	4/6612 (0.1%)
2	C	0.69	0/1121	0.84	3/1518 (0.2%)
2	D	0.59	0/1113	0.82	2/1507 (0.1%)
All	All	0.66	3/12086 (0.0%)	0.78	17/16380 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TRP	CD2-CE2	5.72	1.48	1.41
1	B	251	TRP	CD2-CE2	5.41	1.47	1.41
1	B	91	TRP	CD2-CE2	5.03	1.47	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	75	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	570	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	570	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	C	75	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	B	86	ARG	NE-CZ-NH2	-7.38	116.61	120.30

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	4887	0	4823	82	0
1	B	4789	0	4757	61	0
2	C	1099	0	1058	13	0
2	D	1091	0	1055	20	0
3	E	105	0	88	0	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	I	28	0	25	1	0
5	H	94	0	79	0	0
6	A	1	0	0	0	0
7	A	30	0	40	3	0
7	B	24	0	32	4	0
7	C	18	0	24	2	0
7	D	18	0	24	2	0
8	A	70	0	65	0	0
8	B	56	0	52	2	0
8	C	28	0	26	0	0
8	D	28	0	26	0	0
9	A	556	0	0	19	0
9	B	419	0	0	10	0
9	C	97	0	0	4	0
9	D	77	0	0	2	0
All	All	13571	0	12224	175	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 175 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ARG:NH1	2:C:104:GLU:HG2	1.64	1.11
2:C:79:ARG:HH12	2:C:104:GLU:HG2	1.20	0.99
1:B:391:GLN:HE21	1:B:391:GLN:H	1.15	0.90
1:A:431[B]:ARG:HH21	1:A:431[B]:ARG:HG3	1.37	0.89
1:A:431[B]:ARG:HH21	1:A:431[B]:ARG:CG	1.85	0.89

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	618/606 (102%)	592 (96%)	25 (4%)	1 (0%)	44	36
1	B	606/606 (100%)	579 (96%)	26 (4%)	1 (0%)	44	36
2	C	138/145 (95%)	131 (95%)	7 (5%)	0	100	100
2	D	137/145 (94%)	129 (94%)	8 (6%)	0	100	100
All	All	1499/1502 (100%)	1431 (96%)	66 (4%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	PHE
1	B	436	ASP

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	574/560 (102%)	540 (94%)	34 (6%)	16	9
1	B	562/560 (100%)	522 (93%)	40 (7%)	12	5
2	C	122/126 (97%)	112 (92%)	10 (8%)	9	4
2	D	121/126 (96%)	112 (93%)	9 (7%)	11	5
All	All	1379/1372 (100%)	1286 (93%)	93 (7%)	14	6

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	LEU
1	B	421	GLN
1	B	289	ILE
1	B	350	LEU
1	B	475	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
2	D	119	GLN
1	B	335	ASN
1	B	475	ASN
1	B	197	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 ⓘ

23 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	E	1	1,3	14,14,15	0.96	2 (14%)	17,19,21	0.77	0
3	NAG	E	2	3	14,14,15	0.79	0	17,19,21	1.90	4 (23%)
3	BMA	E	3	3	11,11,12	0.61	0	15,15,17	1.16	1 (6%)
3	MAN	E	4	3	11,11,12	1.02	1 (9%)	15,15,17	1.28	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	E	5	3	11,11,12	0.59	0	15,15,17	1.36	2 (13%)
3	MAN	E	6	3	11,11,12	0.61	0	15,15,17	0.85	0
3	MAN	E	7	3	11,11,12	0.60	0	15,15,17	1.29	2 (13%)
3	MAN	E	8	3	11,11,12	1.02	1 (9%)	15,15,17	0.82	0
3	MAN	E	9	3	11,11,12	0.49	0	15,15,17	1.78	5 (33%)
4	NAG	F	1	4,1	14,14,15	0.80	0	17,19,21	0.93	2 (11%)
4	NAG	F	2	4	14,14,15	0.85	0	17,19,21	1.40	2 (11%)
4	NAG	G	1	4,1	14,14,15	0.69	0	17,19,21	1.01	0
4	NAG	G	2	4	14,14,15	0.65	0	17,19,21	1.22	1 (5%)
5	NAG	H	1	5,1	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
5	NAG	H	2	5	14,14,15	0.60	0	17,19,21	1.12	1 (5%)
5	BMA	H	3	5	11,11,12	0.45	0	15,15,17	1.30	2 (13%)
5	MAN	H	4	5	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
5	MAN	H	5	5	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
5	MAN	H	6	5	11,11,12	0.70	0	15,15,17	1.41	3 (20%)
5	MAN	H	7	5	11,11,12	0.56	0	15,15,17	1.30	2 (13%)
5	MAN	H	8	5	11,11,12	0.58	0	15,15,17	1.18	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.68	0	17,19,21	1.31	2 (11%)
4	NAG	I	2	4	14,14,15	0.63	0	17,19,21	1.20	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
3	MAN	E	8	3	-	0/2/19/22	0/1/1/1
3	MAN	E	9	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
5	MAN	H	8	5	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	MAN	O5-C1	-2.58	1.39	1.43
3	E	1	NAG	O5-C1	-2.16	1.40	1.43
3	E	1	NAG	C1-C2	2.12	1.55	1.52
3	E	8	MAN	C2-C3	2.01	1.55	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	4.28	117.93	112.19
3	E	7	MAN	C1-O5-C5	3.86	117.36	112.19
5	H	6	MAN	C1-O5-C5	3.54	116.94	112.19
3	E	2	NAG	O6-C6-C5	-3.28	100.16	111.33
3	E	9	MAN	C3-C4-C5	3.22	116.06	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

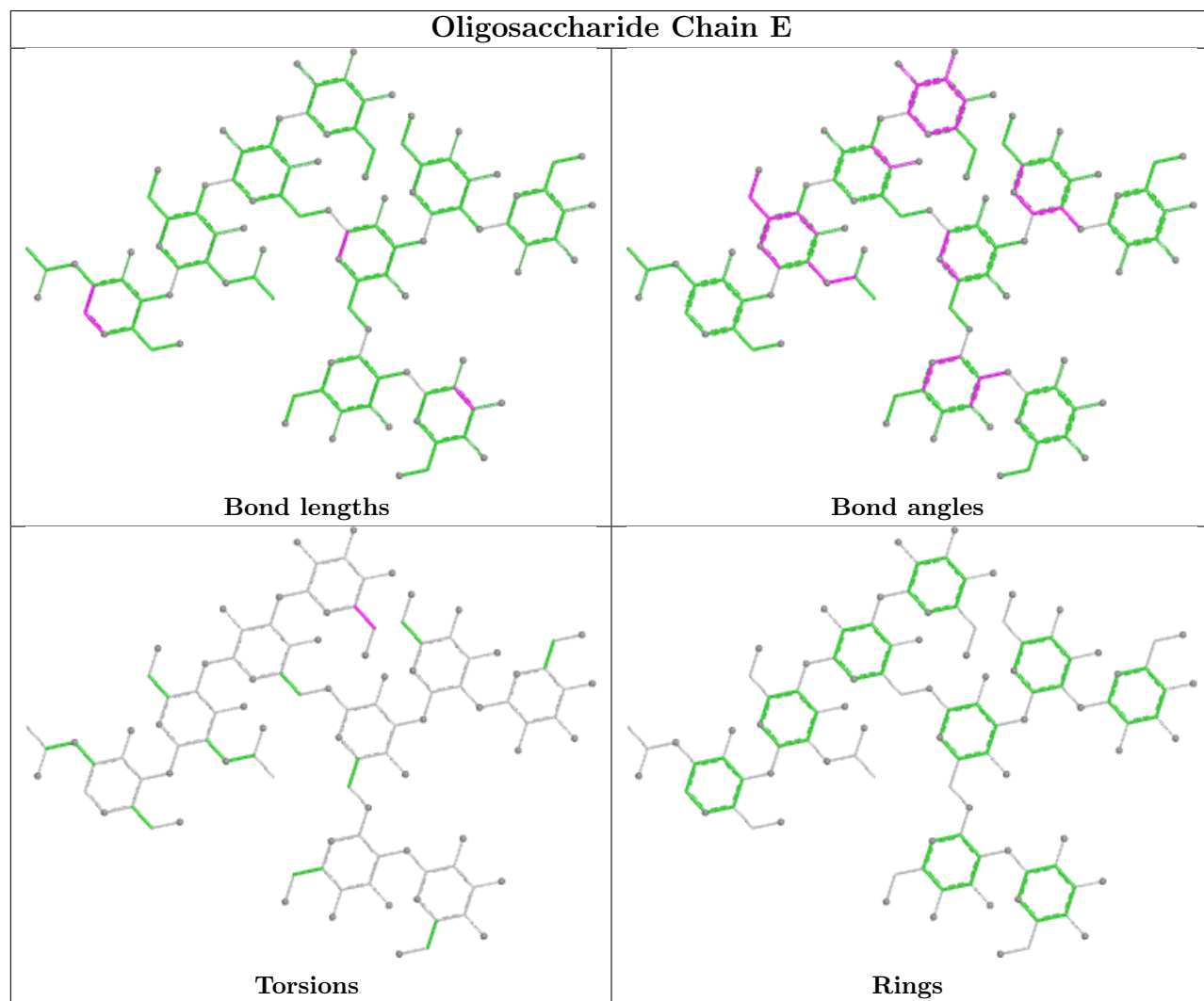
Mol	Chain	Res	Type	Atoms
3	E	9	MAN	O5-C5-C6-O6
5	H	8	MAN	O5-C5-C6-O6
3	E	9	MAN	C4-C5-C6-O6
5	H	8	MAN	C4-C5-C6-O6

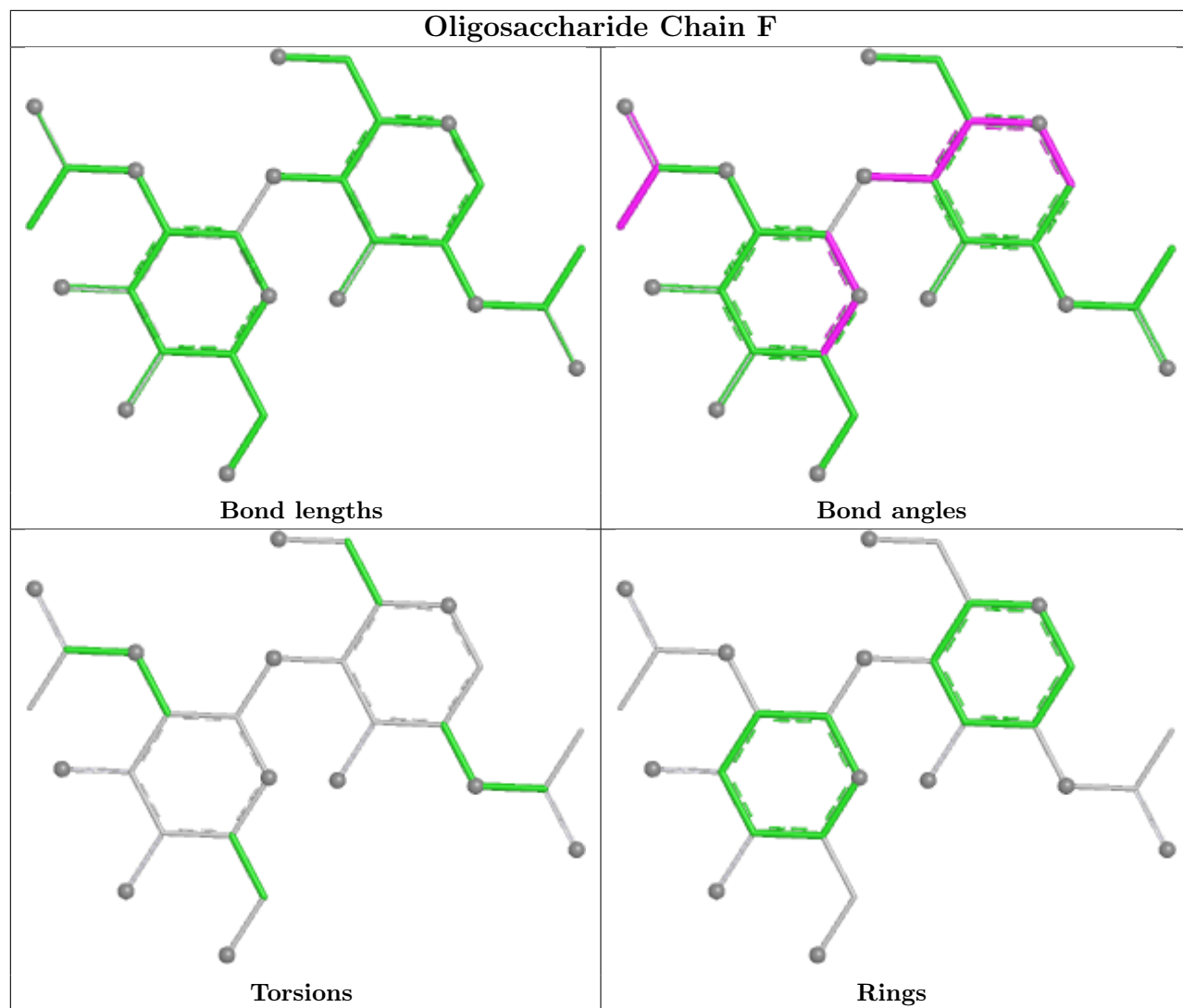
There are no ring outliers.

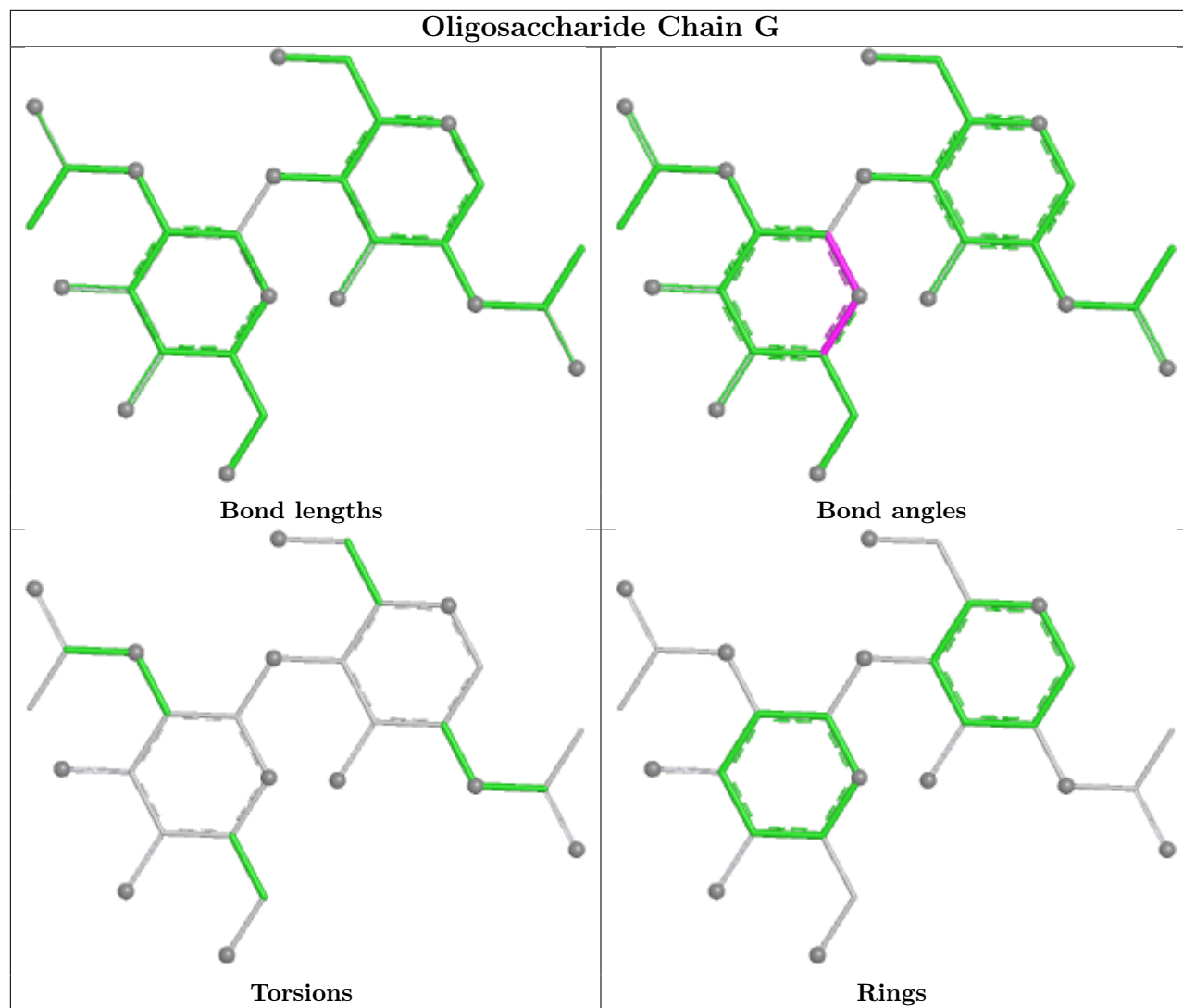
2 monomers are involved in 2 short contacts:

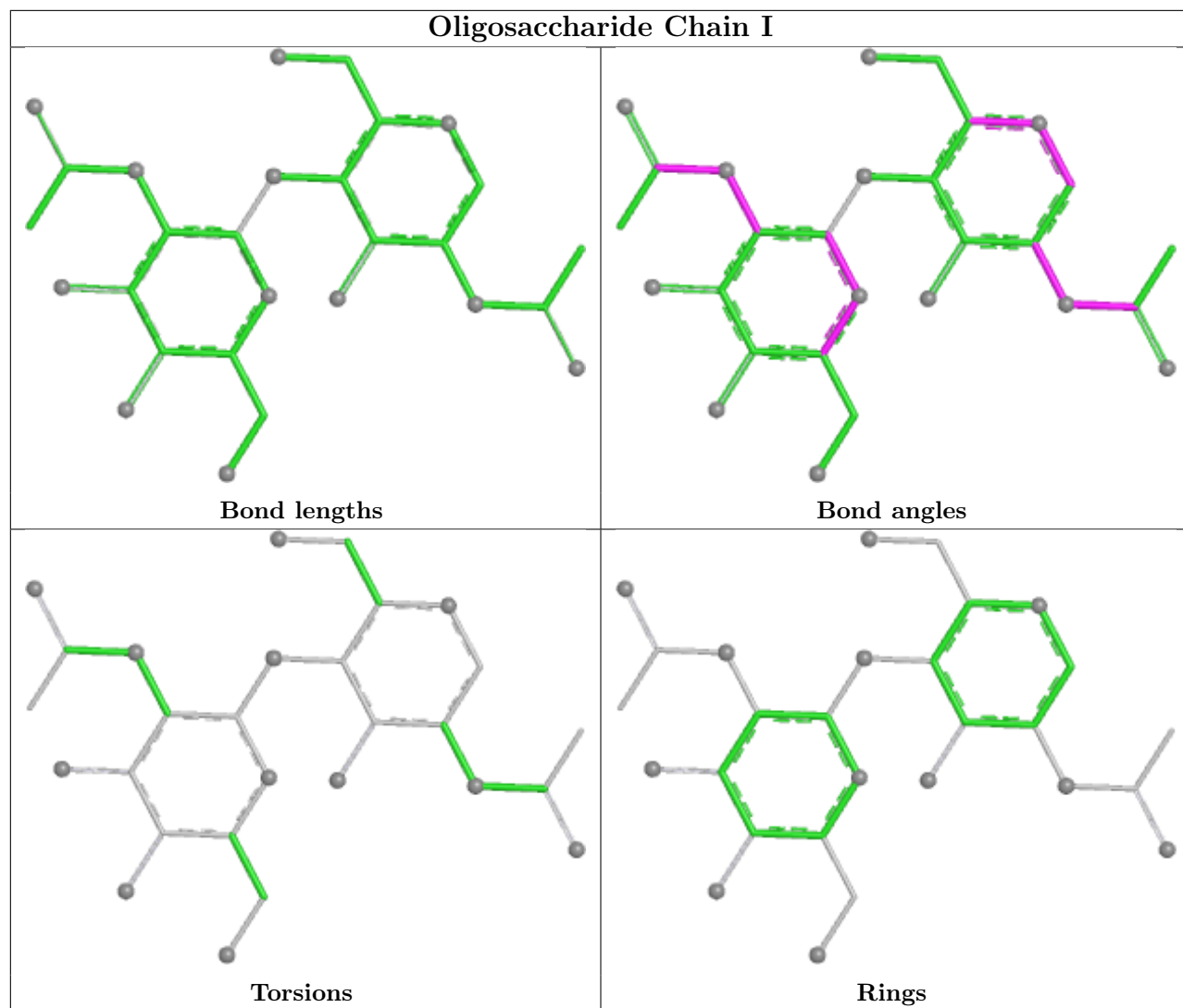
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	F	1	NAG	1	0

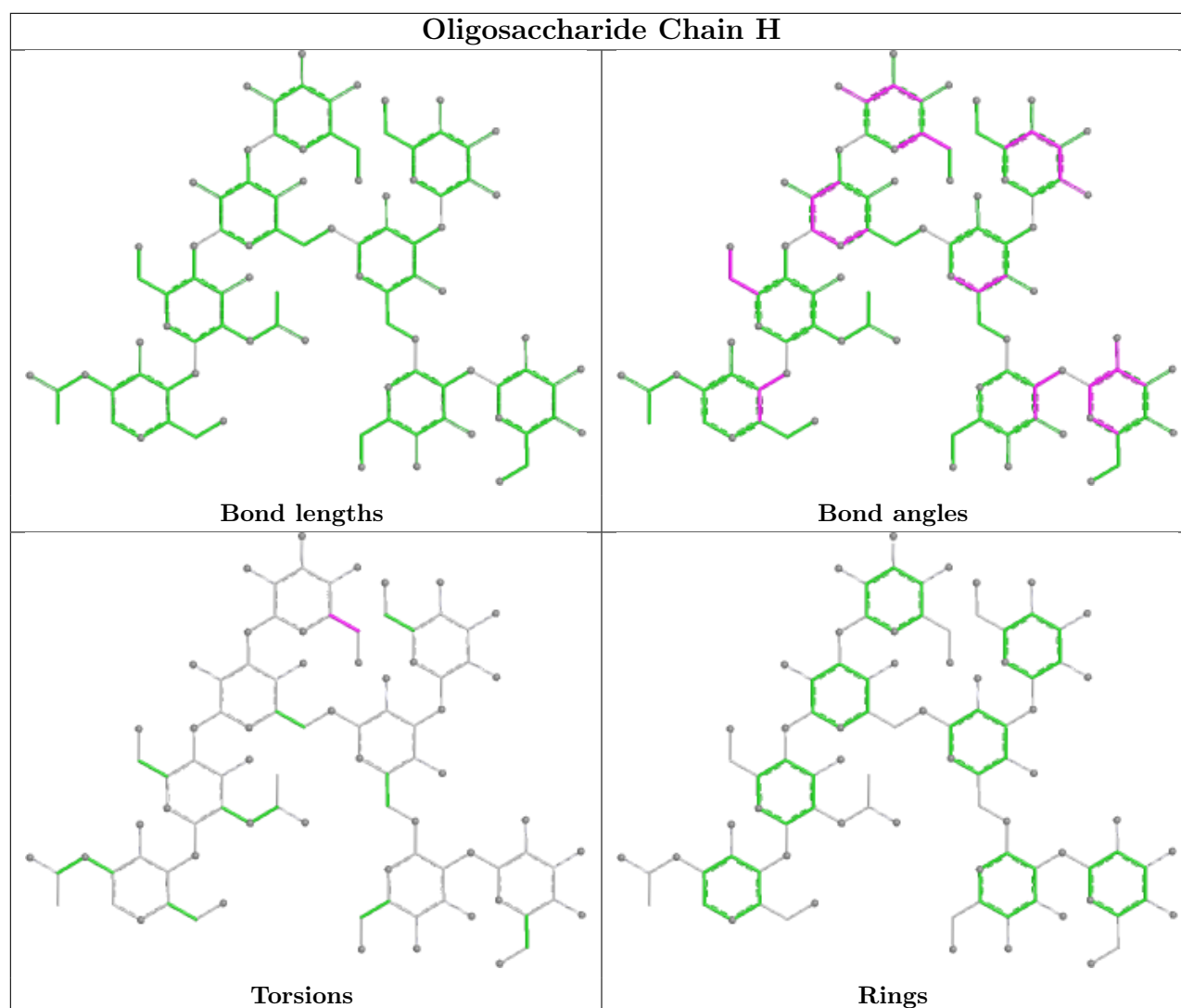
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 for Mogul analysis.

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	GOL	C	13	-	5,5,5	0.27	0	5,5,5	0.57	0
7	GOL	A	15	-	5,5,5	0.32	0	5,5,5	0.61	0
8	NAG	A	701	1	14,14,15	0.71	0	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	B	8	-	5,5,5	0.21	0	5,5,5	0.46	0
7	GOL	D	7	-	5,5,5	0.58	0	5,5,5	0.71	0
8	NAG	C	201	2	14,14,15	0.51	0	17,19,21	1.34	2 (11%)
8	NAG	A	703	1	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
7	GOL	C	12	-	5,5,5	0.34	0	5,5,5	0.43	0
7	GOL	A	9	-	5,5,5	0.70	0	5,5,5	0.65	0
8	NAG	B	700	1	14,14,15	0.58	0	17,19,21	1.86	5 (29%)
8	NAG	A	702	1	14,14,15	0.73	0	17,19,21	1.35	2 (11%)
8	NAG	B	703	1	14,14,15	0.56	0	17,19,21	0.92	0
7	GOL	B	5	-	5,5,5	0.13	0	5,5,5	1.16	1 (20%)
7	GOL	A	6	-	5,5,5	0.58	0	5,5,5	0.53	0
8	NAG	D	202	2	14,14,15	0.76	0	17,19,21	1.78	5 (29%)
7	GOL	C	4	-	5,5,5	0.28	0	5,5,5	0.44	0
7	GOL	A	10	-	5,5,5	0.40	0	5,5,5	0.38	0
8	NAG	B	704	1	14,14,15	0.52	0	17,19,21	0.78	0
8	NAG	D	201	2	14,14,15	0.63	0	17,19,21	1.37	2 (11%)
7	GOL	A	3	-	5,5,5	0.33	0	5,5,5	0.85	0
8	NAG	B	701	1	14,14,15	0.90	0	17,19,21	2.12	5 (29%)
7	GOL	B	11	-	5,5,5	0.32	0	5,5,5	0.30	0
8	NAG	A	700	1	14,14,15	0.54	0	17,19,21	1.11	1 (5%)
7	GOL	D	1	-	5,5,5	0.54	0	5,5,5	0.65	0
8	NAG	A	704	1	14,14,15	0.50	0	17,19,21	1.15	1 (5%)
8	NAG	C	202	2	14,14,15	0.60	0	17,19,21	2.16	4 (23%)
7	GOL	B	2	-	5,5,5	0.36	0	5,5,5	0.07	0
7	GOL	D	14	-	5,5,5	0.36	0	5,5,5	0.77	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	GOL	C	13	-	-	0/4/4/4	-
7	GOL	A	15	-	-	4/4/4/4	-
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1
7	GOL	B	8	-	-	1/4/4/4	-
7	GOL	D	7	-	-	2/4/4/4	-
8	NAG	C	201	2	-	1/6/23/26	0/1/1/1
8	NAG	A	703	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	C	12	-	-	2/4/4/4	-
7	GOL	A	9	-	-	4/4/4/4	-
8	NAG	B	700	1	-	3/6/23/26	0/1/1/1
8	NAG	A	702	1	-	0/6/23/26	0/1/1/1
8	NAG	B	703	1	-	2/6/23/26	0/1/1/1
7	GOL	B	5	-	-	0/4/4/4	-
7	GOL	A	6	-	-	0/4/4/4	-
8	NAG	D	202	2	-	1/6/23/26	0/1/1/1
7	GOL	C	4	-	-	0/4/4/4	-
7	GOL	A	10	-	-	2/4/4/4	-
8	NAG	B	704	1	-	2/6/23/26	0/1/1/1
8	NAG	D	201	2	-	0/6/23/26	0/1/1/1
7	GOL	A	3	-	-	4/4/4/4	-
8	NAG	B	701	1	-	0/6/23/26	0/1/1/1
7	GOL	B	11	-	-	2/4/4/4	-
8	NAG	A	700	1	-	2/6/23/26	0/1/1/1
7	GOL	D	1	-	-	0/4/4/4	-
8	NAG	A	704	1	-	0/6/23/26	0/1/1/1
8	NAG	C	202	2	-	1/6/23/26	0/1/1/1
7	GOL	B	2	-	-	4/4/4/4	-
7	GOL	D	14	-	-	0/4/4/4	-

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	202	NAG	C1-O5-C5	6.10	120.36	112.19
8	B	701	NAG	O5-C1-C2	4.62	118.44	111.29
8	C	202	NAG	C1-C2-N2	4.05	116.81	110.43
8	D	202	NAG	C1-O5-C5	3.96	117.49	112.19
8	B	701	NAG	C4-C3-C2	3.91	116.75	111.02

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3	GOL	C1-C2-C3-O3
7	A	3	GOL	O2-C2-C3-O3
7	A	9	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	A	9	GOL	O2-C2-C3-O3
7	A	10	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	12	GOL	2	0
8	B	700	NAG	1	0
7	B	5	GOL	2	0
7	A	6	GOL	3	0
8	B	701	NAG	1	0
7	B	11	GOL	2	0
7	D	14	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	601/606 (99%)	-0.28	6 (0%) 79 81	10, 25, 46, 76	19 (3%)
1	B	601/606 (99%)	0.21	18 (2%) 52 55	12, 35, 61, 88	7 (1%)
2	C	139/145 (95%)	0.03	5 (3%) 46 48	17, 30, 56, 75	1 (0%)
2	D	139/145 (95%)	0.35	6 (4%) 40 42	21, 36, 67, 94	0
All	All	1480/1502 (98%)	0.01	35 (2%) 59 61	10, 30, 58, 94	27 (1%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	4.5
1	A	170	PHE	4.0
1	B	289	ILE	3.8
2	D	164	PHE	3.6
1	B	337	CYS	3.2

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	G	2	14/15	0.70	0.15	51,61,76,81	0
3	MAN	E	9	11/12	0.80	0.15	40,49,66,71	0

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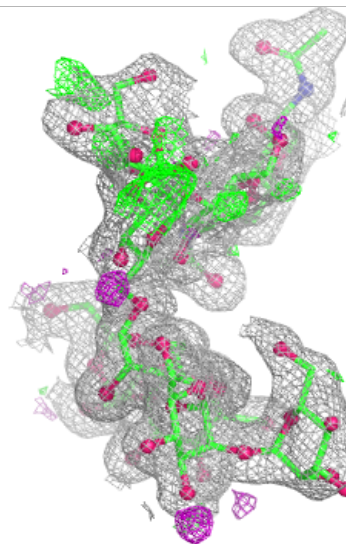
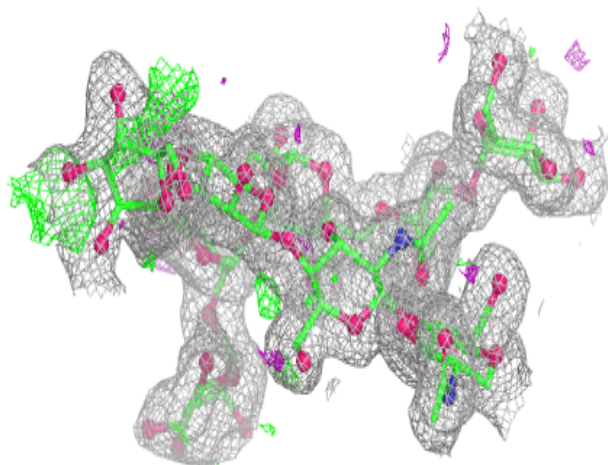
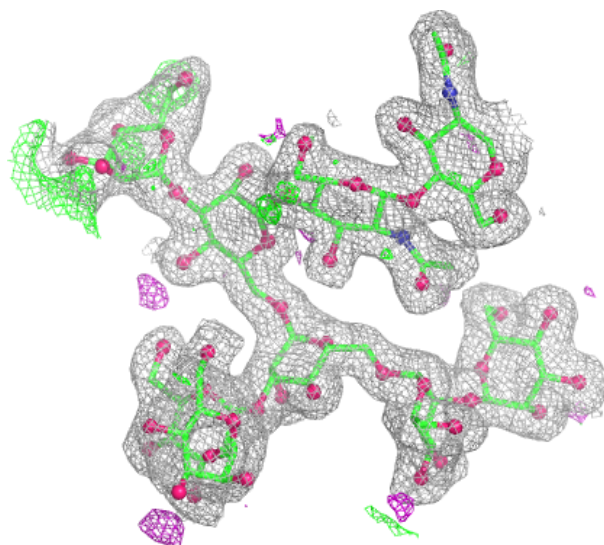
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	H	8	11/12	0.84	0.13	39,44,57,67	0
3	MAN	E	6	11/12	0.85	0.14	40,56,69,78	0
4	NAG	G	1	14/15	0.90	0.09	28,40,53,54	0
5	MAN	H	7	11/12	0.92	0.10	27,35,43,49	0
4	NAG	F	2	14/15	0.93	0.08	22,26,31,34	0
4	NAG	I	2	14/15	0.94	0.08	28,37,42,42	0
3	NAG	E	2	14/15	0.95	0.07	17,20,23,36	0
5	NAG	H	2	14/15	0.95	0.07	25,29,33,34	0
3	BMA	E	3	11/12	0.96	0.06	19,23,29,30	0
3	MAN	E	5	11/12	0.96	0.07	25,27,37,45	0
5	NAG	H	1	14/15	0.96	0.06	25,27,30,30	0
5	BMA	H	3	11/12	0.97	0.06	26,31,34,34	0
5	MAN	H	4	11/12	0.97	0.06	25,29,30,33	0
5	MAN	H	5	11/12	0.97	0.05	26,30,36,37	0
5	MAN	H	6	11/12	0.97	0.05	26,28,33,34	0
4	NAG	I	1	14/15	0.97	0.06	25,27,30,33	0
3	MAN	E	7	11/12	0.97	0.05	17,20,23,24	0
3	MAN	E	8	11/12	0.98	0.04	17,18,20,20	0
3	MAN	E	4	11/12	0.98	0.04	17,20,22,26	0
4	NAG	F	1	14/15	0.98	0.04	16,19,21,21	0
3	NAG	E	1	14/15	0.98	0.05	16,19,20,22	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.

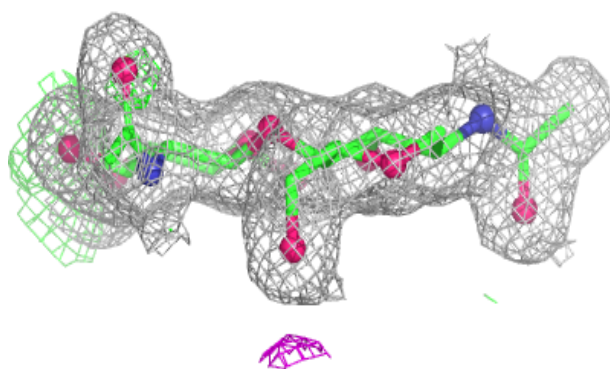
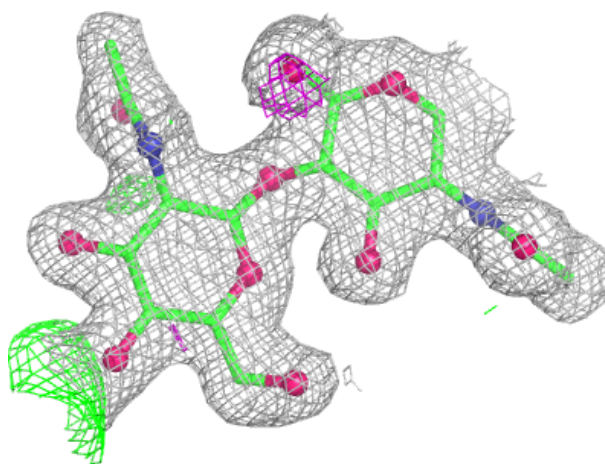
**Electron density around Chain E:**

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



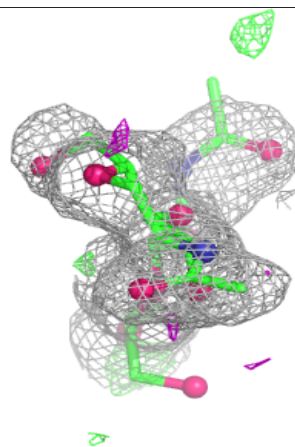
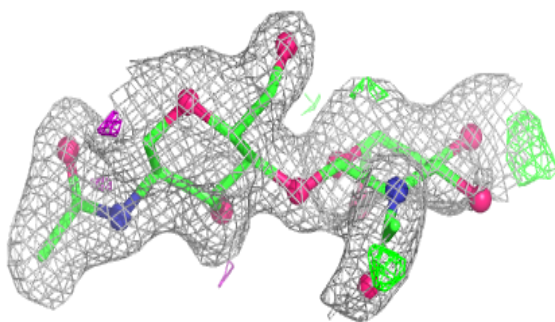
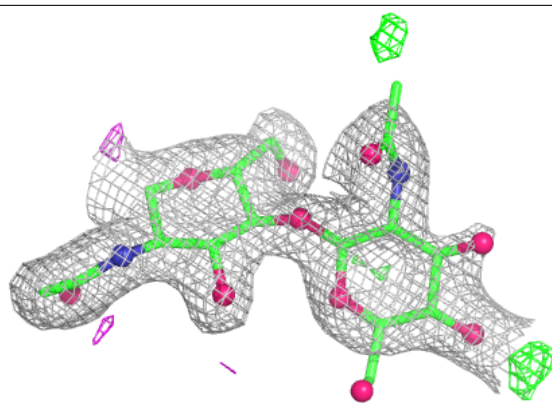
**Electron density around Chain F:**

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



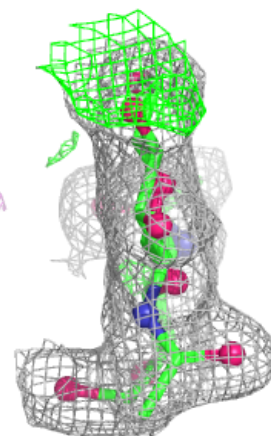
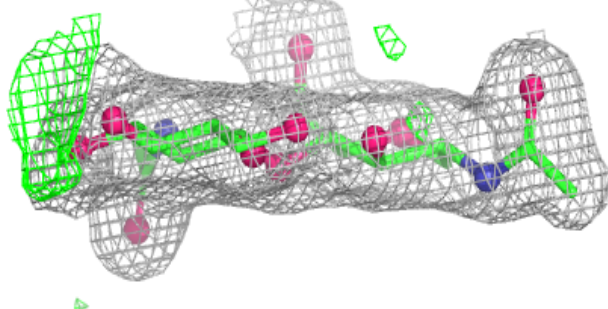
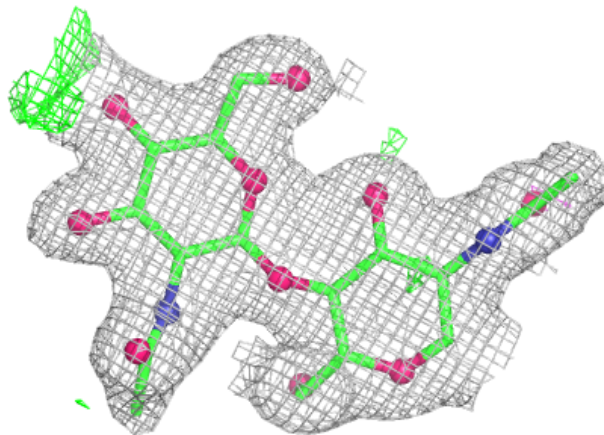
**Electron density around Chain G:**

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

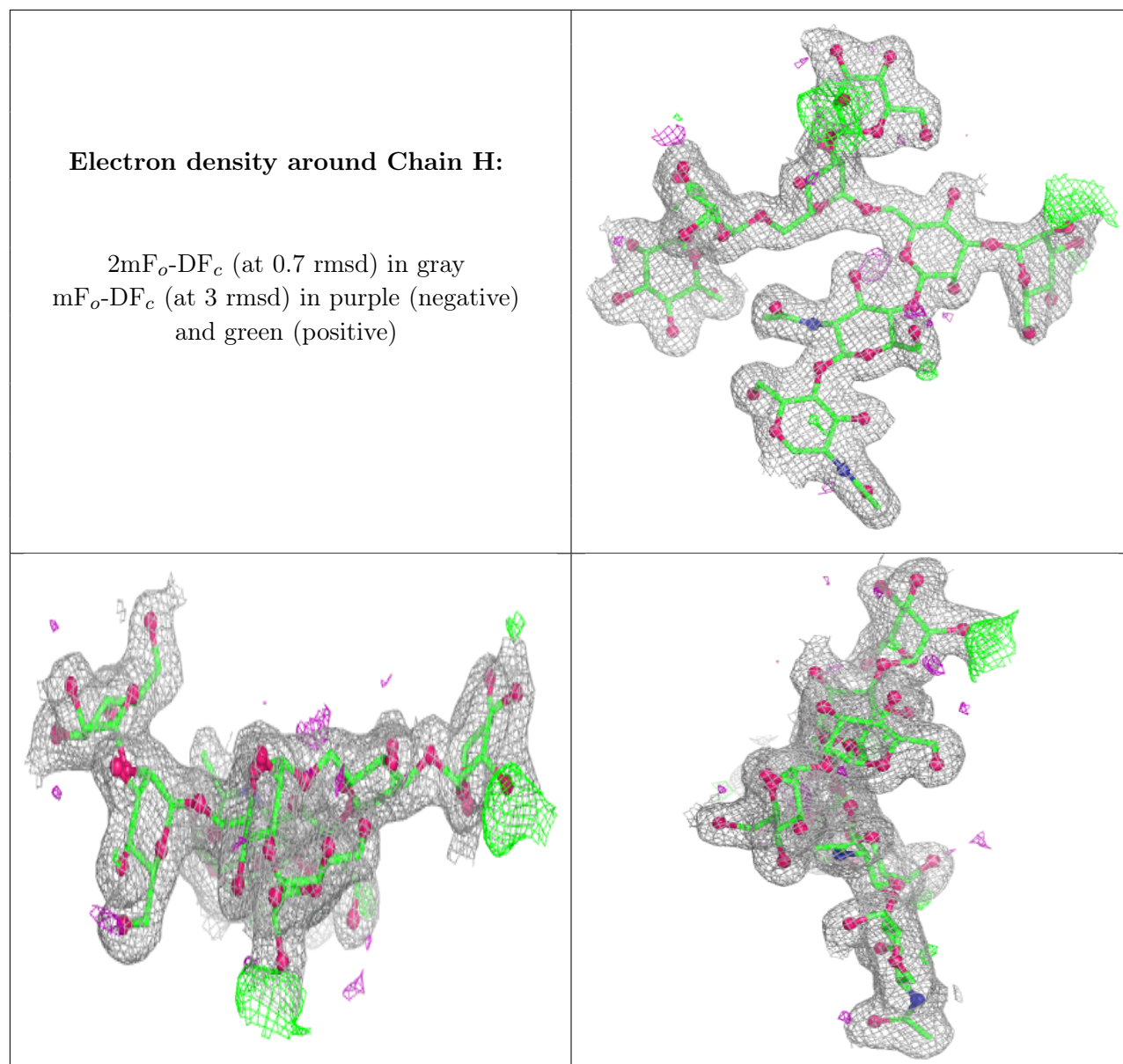


**Electron density around Chain I:**

$2mF_o-DF_c$  (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
8	NAG	B	700	14/15	0.53	0.17	65,85,96,98	0
8	NAG	D	201	14/15	0.67	0.17	88,98,104,120	0
8	NAG	A	700	14/15	0.68	0.18	81,89,96,111	0
8	NAG	D	202	14/15	0.71	0.17	68,81,94,102	0
8	NAG	C	202	14/15	0.74	0.13	57,68,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	701	14/15	0.75	0.16	64,74,80,83	0
8	NAG	B	701	14/15	0.77	0.17	57,69,83,89	0
8	NAG	C	201	14/15	0.78	0.14	53,67,70,73	0
8	NAG	B	704	14/15	0.82	0.13	58,74,87,88	0
7	GOL	A	3	6/6	0.82	0.22	39,48,54,69	0
7	GOL	A	6	6/6	0.82	0.16	35,45,52,58	0
7	GOL	A	9	6/6	0.83	0.19	42,50,61,62	0
8	NAG	A	702	14/15	0.85	0.13	37,46,57,58	0
7	GOL	D	7	6/6	0.86	0.13	41,51,53,58	0
7	GOL	D	14	6/6	0.86	0.14	47,54,63,67	0
7	GOL	C	13	6/6	0.86	0.14	58,63,65,65	0
7	GOL	B	8	6/6	0.86	0.15	51,56,60,73	0
7	GOL	B	5	6/6	0.87	0.12	35,41,49,61	0
7	GOL	B	11	6/6	0.87	0.15	31,44,64,65	0
7	GOL	A	15	6/6	0.88	0.12	51,60,65,67	0
7	GOL	B	2	6/6	0.88	0.13	50,53,57,63	0
8	NAG	B	703	14/15	0.89	0.10	47,60,74,88	0
7	GOL	C	12	6/6	0.90	0.14	42,52,55,56	0
7	GOL	A	10	6/6	0.92	0.12	47,51,60,66	0
7	GOL	D	1	6/6	0.93	0.09	26,33,34,35	0
8	NAG	A	704	14/15	0.93	0.07	28,37,43,50	0
8	NAG	A	703	14/15	0.94	0.08	25,32,40,41	0
7	GOL	C	4	6/6	0.97	0.06	21,30,32,35	0
6	CU	A	1	1/1	1.00	0.02	22,22,22,22	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.