



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 04:13 AM EDT

PDB ID : 4F2M  
Title : Crystal structure of a TGEV coronavirus Spike fragment in complex with the TGEV neutralizing monoclonal antibody 1AF10  
Authors : Reguera, J.; Santiago, C.; Mudgal, G.; Ordone, D.; Enjuanes, L.; Casasnovas, J.M.  
Deposited on : 2012-05-08  
Resolution : 3.00 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)

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

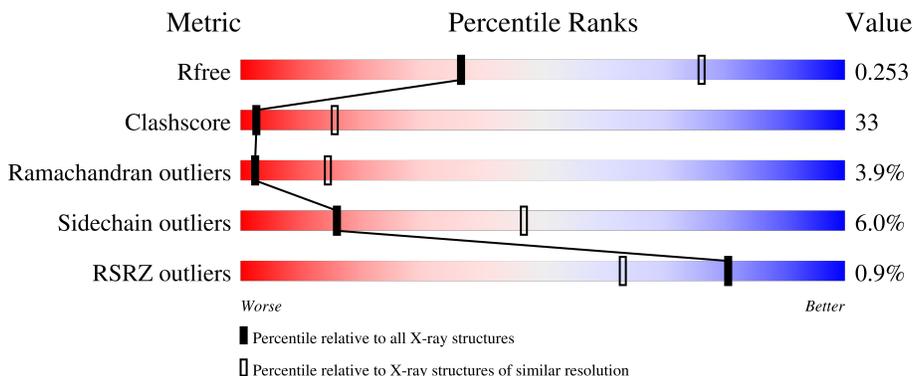
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	221	
1	C	221	
2	B	214	
2	D	214	
3	E	209	

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Mol	Chain	Length	Quality of chain
3	F	209	
4	G	2	
4	H	2	
4	I	2	
4	J	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	F	705	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8998 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 monoclonal antibody 1AF10, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	Total 1614	C 1024	N 264	O 319	S 7	0	0	0
1	C	220	Total 1655	C 1047	N 270	O 330	S 8	1	0	0

- Molecule 2 is a protein called monoclonal antibody 1AF10, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total 1643	C 1017	N 280	O 341	S 5	1	0	0
2	D	211	Total 1626	C 1008	N 277	O 336	S 5	0	0	0

- Molecule 3 is a protein called Spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	148	Total 1162	C 736	N 194	O 224	S 8	0	0	0
3	F	148	Total 1162	C 736	N 194	O 224	S 8	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	456	TYR	-	expression tag	UNP Q0PKZ5
E	457	PRO	-	expression tag	UNP Q0PKZ5
E	458	TYR	-	expression tag	UNP Q0PKZ5
E	459	ASP	-	expression tag	UNP Q0PKZ5
E	460	VAL	-	expression tag	UNP Q0PKZ5
E	461	PRO	-	expression tag	UNP Q0PKZ5
E	462	ASP	-	expression tag	UNP Q0PKZ5
E	463	TYR	-	expression tag	UNP Q0PKZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	464	ALA	-	expression tag	UNP Q0PKZ5
E	465	GLY	-	expression tag	UNP Q0PKZ5
E	466	ALA	-	expression tag	UNP Q0PKZ5
E	467	GLN	-	expression tag	UNP Q0PKZ5
E	468	PRO	-	expression tag	UNP Q0PKZ5
E	469	ALA	-	expression tag	UNP Q0PKZ5
E	470	ARG	-	expression tag	UNP Q0PKZ5
E	471	SER	-	expression tag	UNP Q0PKZ5
E	472	PRO	-	expression tag	UNP Q0PKZ5
E	473	GLY	-	expression tag	UNP Q0PKZ5
E	474	LEU	-	expression tag	UNP Q0PKZ5
E	475	VAL	-	expression tag	UNP Q0PKZ5
E	476	PRO	-	expression tag	UNP Q0PKZ5
E	477	ARG	-	expression tag	UNP Q0PKZ5
E	478	GLY	-	expression tag	UNP Q0PKZ5
E	479	SER	-	expression tag	UNP Q0PKZ5
E	480	ARG	-	expression tag	UNP Q0PKZ5
E	651	LEU	-	expression tag	UNP Q0PKZ5
E	652	VAL	-	expression tag	UNP Q0PKZ5
E	653	PRO	-	expression tag	UNP Q0PKZ5
E	654	ARG	-	expression tag	UNP Q0PKZ5
E	655	GLY	-	expression tag	UNP Q0PKZ5
E	656	SER	-	expression tag	UNP Q0PKZ5
E	657	ASP	-	expression tag	UNP Q0PKZ5
E	658	TYR	-	expression tag	UNP Q0PKZ5
E	659	LYS	-	expression tag	UNP Q0PKZ5
E	660	ASP	-	expression tag	UNP Q0PKZ5
E	661	ASP	-	expression tag	UNP Q0PKZ5
E	662	ASP	-	expression tag	UNP Q0PKZ5
E	663	ASP	-	expression tag	UNP Q0PKZ5
E	664	LYS	-	expression tag	UNP Q0PKZ5
F	456	TYR	-	expression tag	UNP Q0PKZ5
F	457	PRO	-	expression tag	UNP Q0PKZ5
F	458	TYR	-	expression tag	UNP Q0PKZ5
F	459	ASP	-	expression tag	UNP Q0PKZ5
F	460	VAL	-	expression tag	UNP Q0PKZ5
F	461	PRO	-	expression tag	UNP Q0PKZ5
F	462	ASP	-	expression tag	UNP Q0PKZ5
F	463	TYR	-	expression tag	UNP Q0PKZ5
F	464	ALA	-	expression tag	UNP Q0PKZ5
F	465	GLY	-	expression tag	UNP Q0PKZ5
F	466	ALA	-	expression tag	UNP Q0PKZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	467	GLN	-	expression tag	UNP Q0PKZ5
F	468	PRO	-	expression tag	UNP Q0PKZ5
F	469	ALA	-	expression tag	UNP Q0PKZ5
F	470	ARG	-	expression tag	UNP Q0PKZ5
F	471	SER	-	expression tag	UNP Q0PKZ5
F	472	PRO	-	expression tag	UNP Q0PKZ5
F	473	GLY	-	expression tag	UNP Q0PKZ5
F	474	LEU	-	expression tag	UNP Q0PKZ5
F	475	VAL	-	expression tag	UNP Q0PKZ5
F	476	PRO	-	expression tag	UNP Q0PKZ5
F	477	ARG	-	expression tag	UNP Q0PKZ5
F	478	GLY	-	expression tag	UNP Q0PKZ5
F	479	SER	-	expression tag	UNP Q0PKZ5
F	480	ARG	-	expression tag	UNP Q0PKZ5
F	651	LEU	-	expression tag	UNP Q0PKZ5
F	652	VAL	-	expression tag	UNP Q0PKZ5
F	653	PRO	-	expression tag	UNP Q0PKZ5
F	654	ARG	-	expression tag	UNP Q0PKZ5
F	655	GLY	-	expression tag	UNP Q0PKZ5
F	656	SER	-	expression tag	UNP Q0PKZ5
F	657	ASP	-	expression tag	UNP Q0PKZ5
F	658	TYR	-	expression tag	UNP Q0PKZ5
F	659	LYS	-	expression tag	UNP Q0PKZ5
F	660	ASP	-	expression tag	UNP Q0PKZ5
F	661	ASP	-	expression tag	UNP Q0PKZ5
F	662	ASP	-	expression tag	UNP Q0PKZ5
F	663	ASP	-	expression tag	UNP Q0PKZ5
F	664	LYS	-	expression tag	UNP Q0PKZ5

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



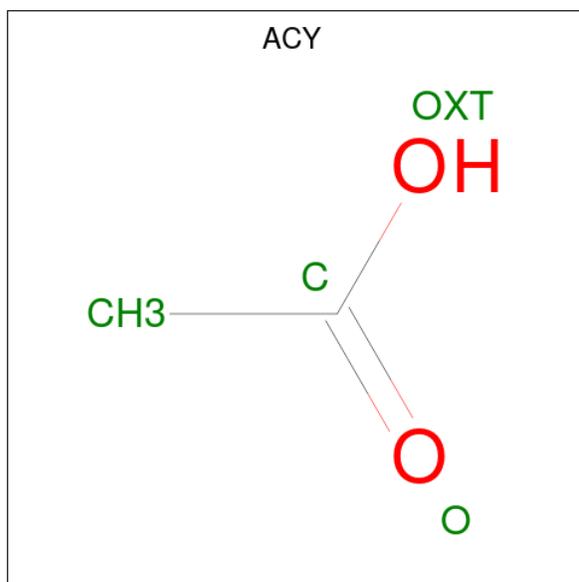
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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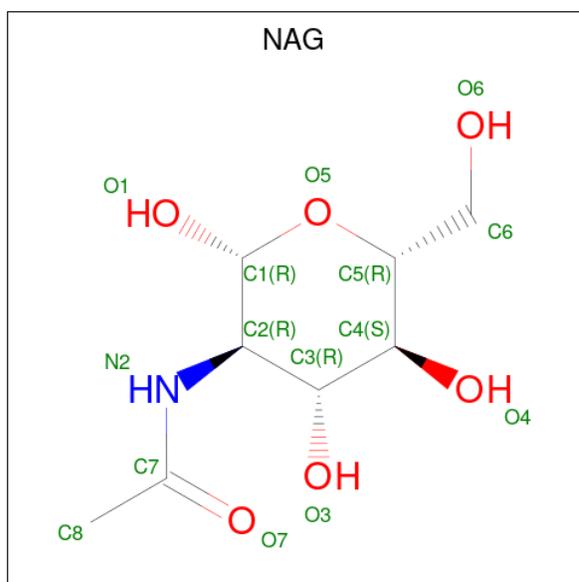
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

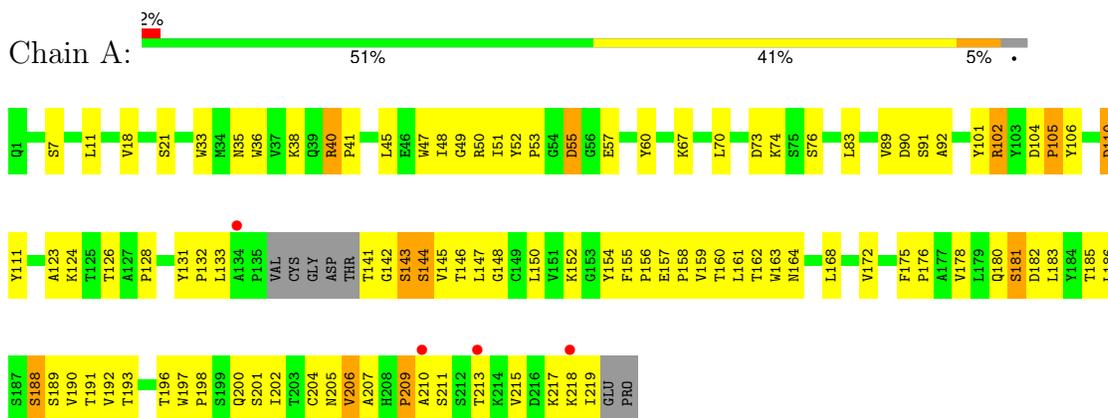
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	D	1	Total	O	0	0
			1	1		

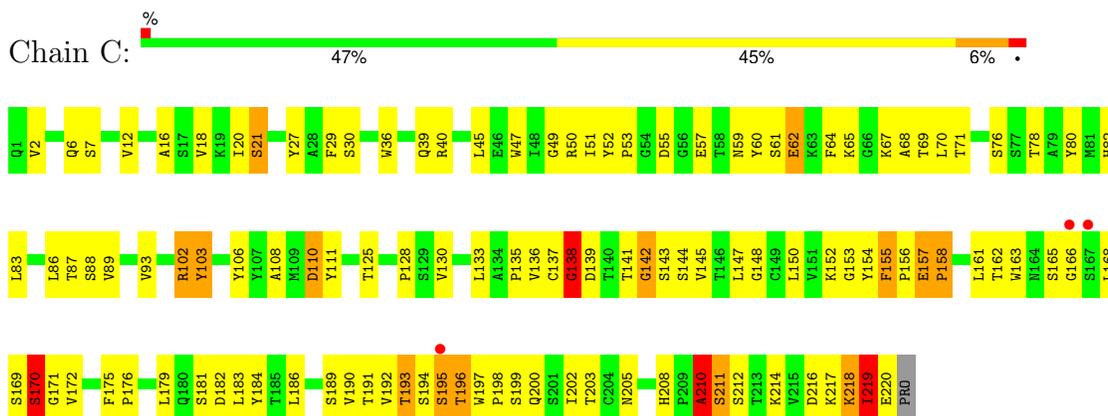
### 3 Residue-property plots [i](#)

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.

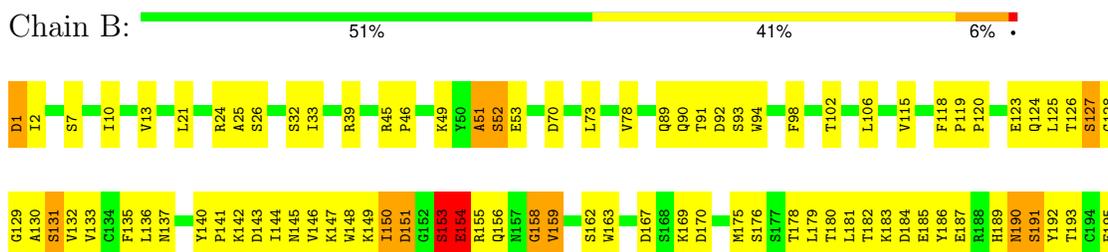
- Molecule 1: monoclonal antibody 1AF10, heavy chain



- Molecule 1: monoclonal antibody 1AF10, heavy chain

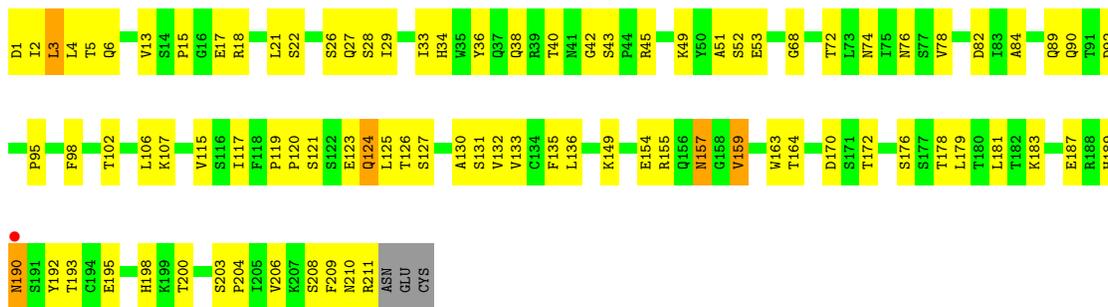


- Molecule 2: monoclonal antibody 1AF10, light chain

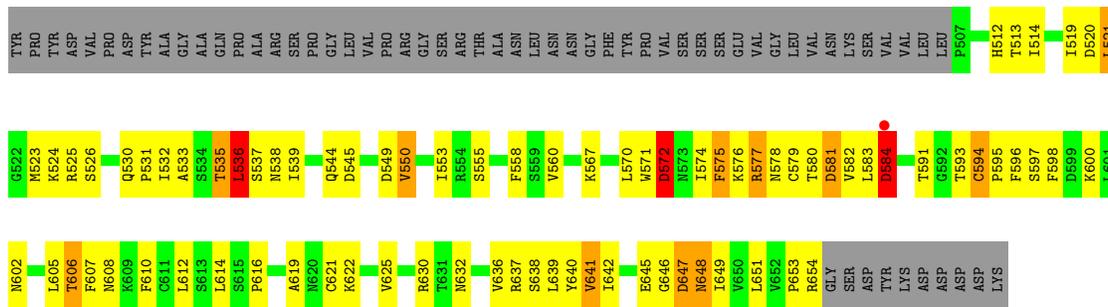




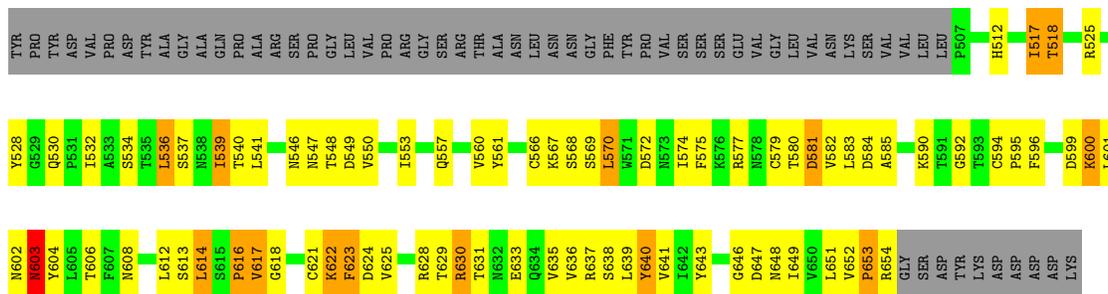
• Molecule 2: monoclonal antibody 1AF10, light chain



• Molecule 3: Spike protein



• Molecule 3: Spike protein



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



MAG1  
MAG2

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

Chain H:  100%MAG1  
MAG2

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

Chain I:  50% 50%MAG1  
MAG2

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

Chain J:  100%MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.77Å 106.05Å 103.52Å 90.00° 95.13° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (25.00-3.00) 94.6 (25.00-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 2.99Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.216 , 0.251 0.217 , 0.253	Depositor DCC
$R_{free}$ test set	1704 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtrriage
Anisotropy	0.324	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ACY

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	0.28	0/1658	0.52	0/2261
1	C	0.32	0/1700	0.63	1/2320 (0.0%)
2	B	0.33	0/1679	0.63	1/2282 (0.0%)
2	D	0.29	0/1662	0.49	0/2259
3	E	0.32	0/1186	0.58	0/1614
3	F	0.36	0/1186	0.63	0/1614
All	All	0.31	0/9071	0.58	2/12350 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
2	B	0	3
3	E	0	3
3	F	0	2
All	All	0	12

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	GLY	N-CA-C	-6.79	96.12	113.10
2	B	212	ASN	N-CA-C	5.45	125.72	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	150	ILE	Peptide
2	B	158	GLY	Peptide
2	B	211	ARG	Peptide
1	C	138	GLY	Peptide
1	C	157	GLU	Peptide

## 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	1614	0	1568	97	0
1	C	1655	0	1603	130	0
2	B	1643	0	1570	120	0
2	D	1626	0	1558	67	0
3	E	1162	0	1133	79	0
3	F	1162	0	1132	120	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	3	0
4	J	28	0	25	0	0
5	B	4	0	3	1	0
5	D	4	0	3	0	0
6	F	14	0	13	0	0
7	B	1	0	0	0	0
7	D	1	0	0	1	0
All	All	8998	0	8683	586	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 33.

The worst 5 of 586 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:E:521:LEU:HA	3:E:537:SER:HB3	1.22	1.18
3:F:590:LYS:O	3:F:623:PHE:HB2	1.52	1.09
3:F:616:PRO:HG2	3:F:640:TYR:CD2	1.89	1.06
3:F:549:ASP:HA	3:F:614:LEU:HB2	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASP:CG	2:B:190:ASN:HB2	1.82	0.99

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	210/221 (95%)	186 (89%)	17 (8%)	7 (3%)	<b>3</b> <b>18</b>
1	C	218/221 (99%)	186 (85%)	18 (8%)	14 (6%)	<b>1</b> <b>6</b>
2	B	211/214 (99%)	177 (84%)	22 (10%)	12 (6%)	<b>1</b> <b>8</b>
2	D	209/214 (98%)	193 (92%)	14 (7%)	2 (1%)	<b>13</b> <b>46</b>
3	E	146/209 (70%)	121 (83%)	18 (12%)	7 (5%)	<b>2</b> <b>11</b>
3	F	146/209 (70%)	119 (82%)	24 (16%)	3 (2%)	<b>5</b> <b>28</b>
All	All	1140/1288 (88%)	982 (86%)	113 (10%)	45 (4%)	<b>2</b> <b>14</b>

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	52	SER
2	B	131	SER
2	B	153	SER
2	B	154	GLU
2	B	212	ASN

### 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	181/187 (97%)	174 (96%)	7 (4%)	27	61
1	C	186/187 (100%)	173 (93%)	13 (7%)	12	41
2	B	190/191 (100%)	183 (96%)	7 (4%)	29	63
2	D	188/191 (98%)	181 (96%)	7 (4%)	29	63
3	E	135/187 (72%)	122 (90%)	13 (10%)	7	27
3	F	135/187 (72%)	121 (90%)	14 (10%)	5	23
All	All	1015/1130 (90%)	954 (94%)	61 (6%)	16	47

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	43	SER
3	F	603	ASN
3	E	535	THR
3	F	581	ASP
3	F	630	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	27	GLN
2	D	37	GLN
3	F	557	GLN
2	D	210	ASN
3	E	648	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	4,3	14,14,15	0.82	0	17,19,21	1.54	2 (11%)
4	NAG	G	2	4	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
4	NAG	H	1	4,3	14,14,15	0.63	0	17,19,21	1.80	3 (17%)
4	NAG	H	2	4	14,14,15	0.56	0	17,19,21	1.40	1 (5%)
4	NAG	I	1	4,3	14,14,15	0.83	0	17,19,21	1.58	2 (11%)
4	NAG	I	2	4	14,14,15	0.64	0	17,19,21	0.76	0
4	NAG	J	1	4,3	14,14,15	0.69	0	17,19,21	1.10	1 (5%)
4	NAG	J	2	4	14,14,15	0.46	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
4	NAG	G	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,3	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	O5-C1-C2	-4.90	103.71	111.29

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	4.55	118.28	112.19
4	H	2	NAG	C1-O5-C5	4.43	118.13	112.19
4	G	1	NAG	O5-C1-C2	-4.34	104.58	111.29
4	H	1	NAG	C3-C4-C5	4.12	117.70	110.23

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

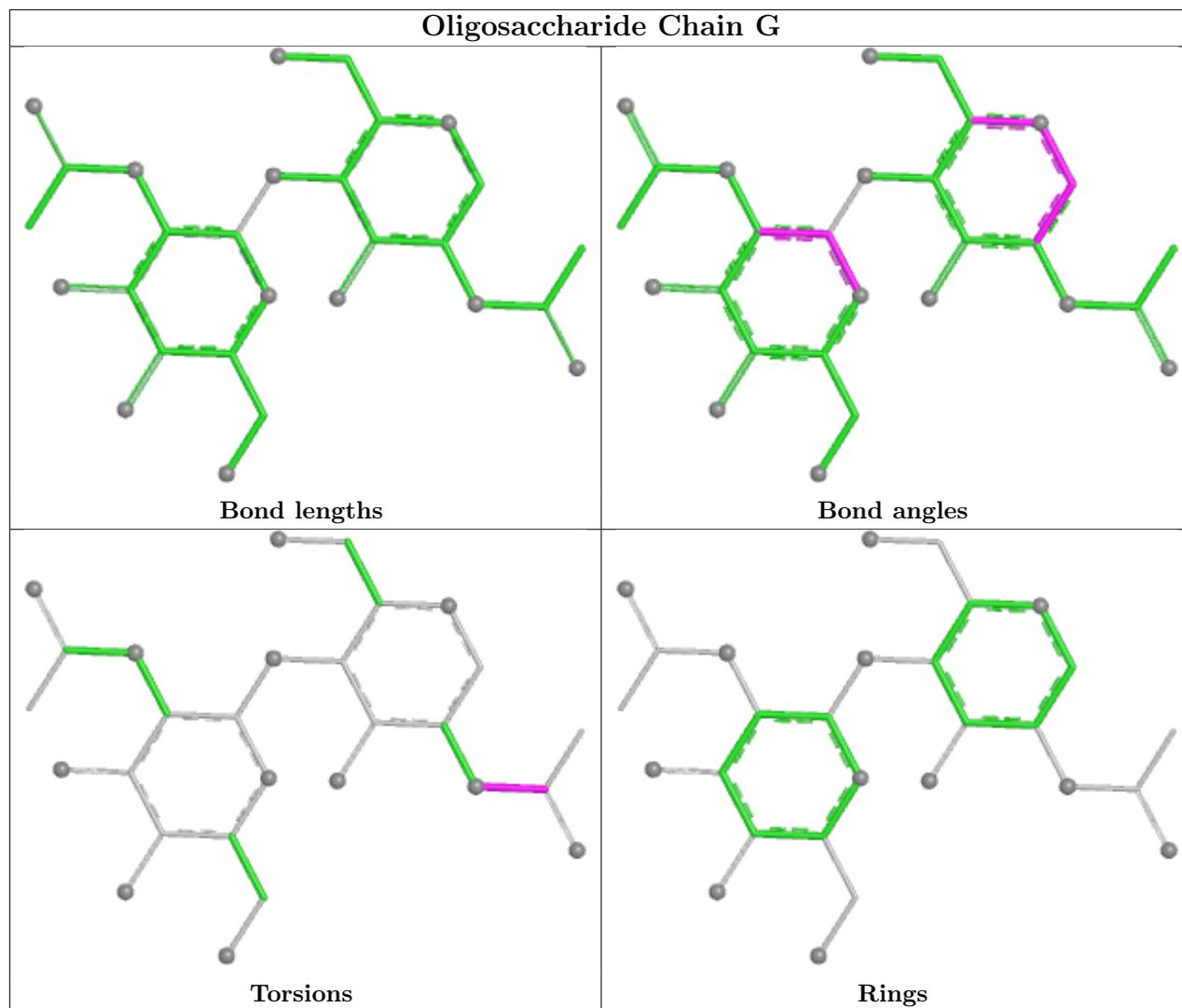
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2

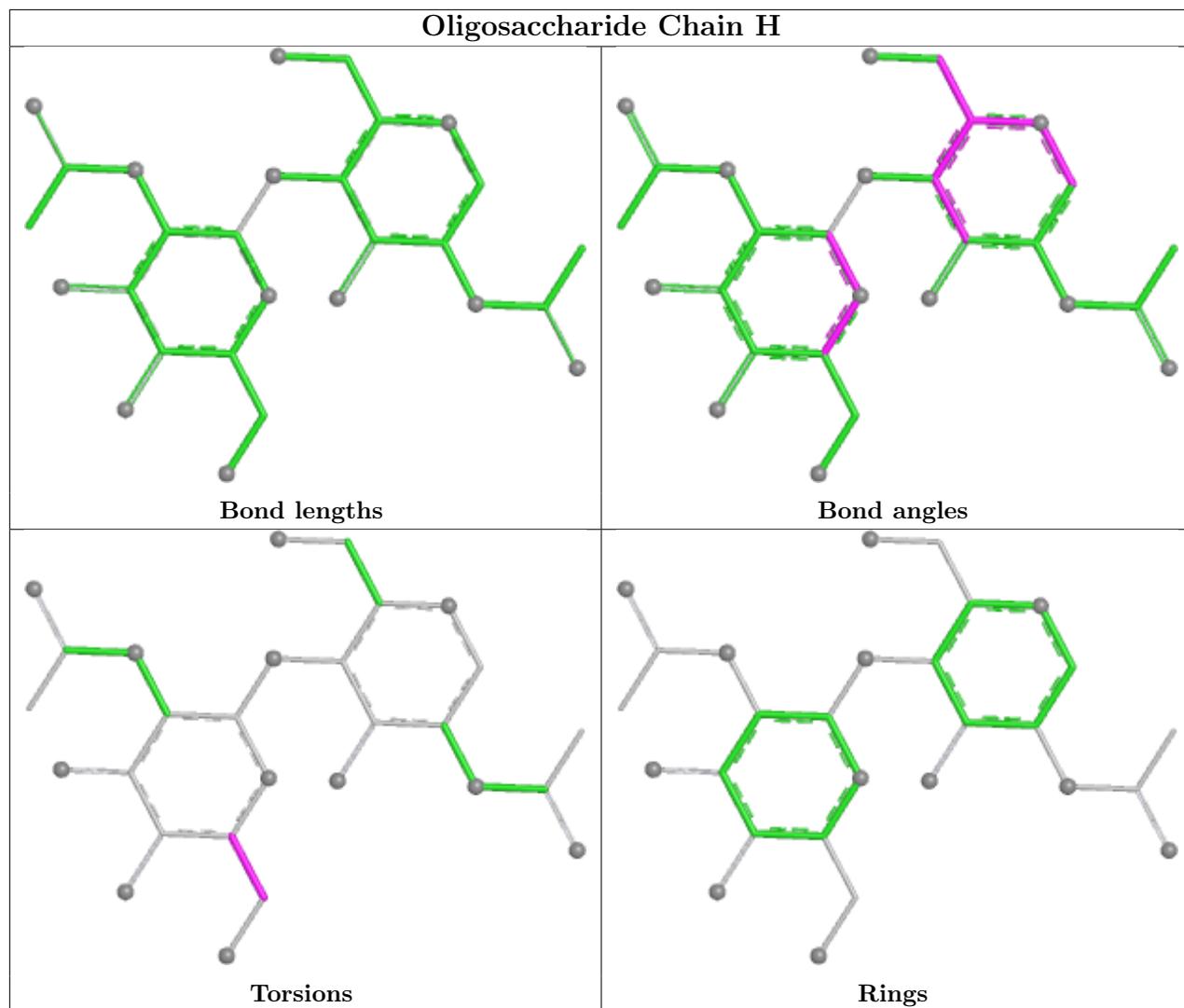
There are no ring outliers.

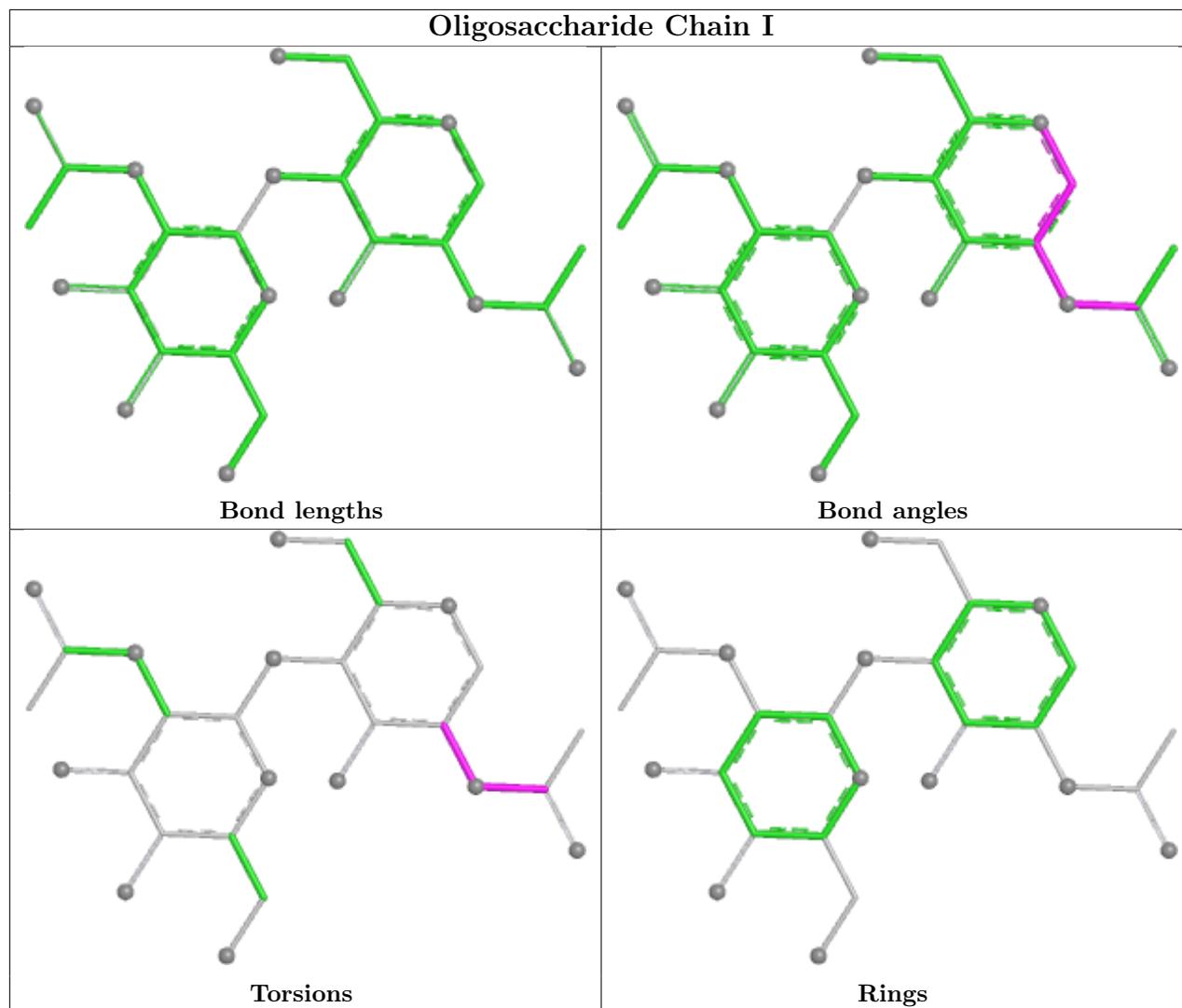
2 monomers are involved in 3 short contacts:

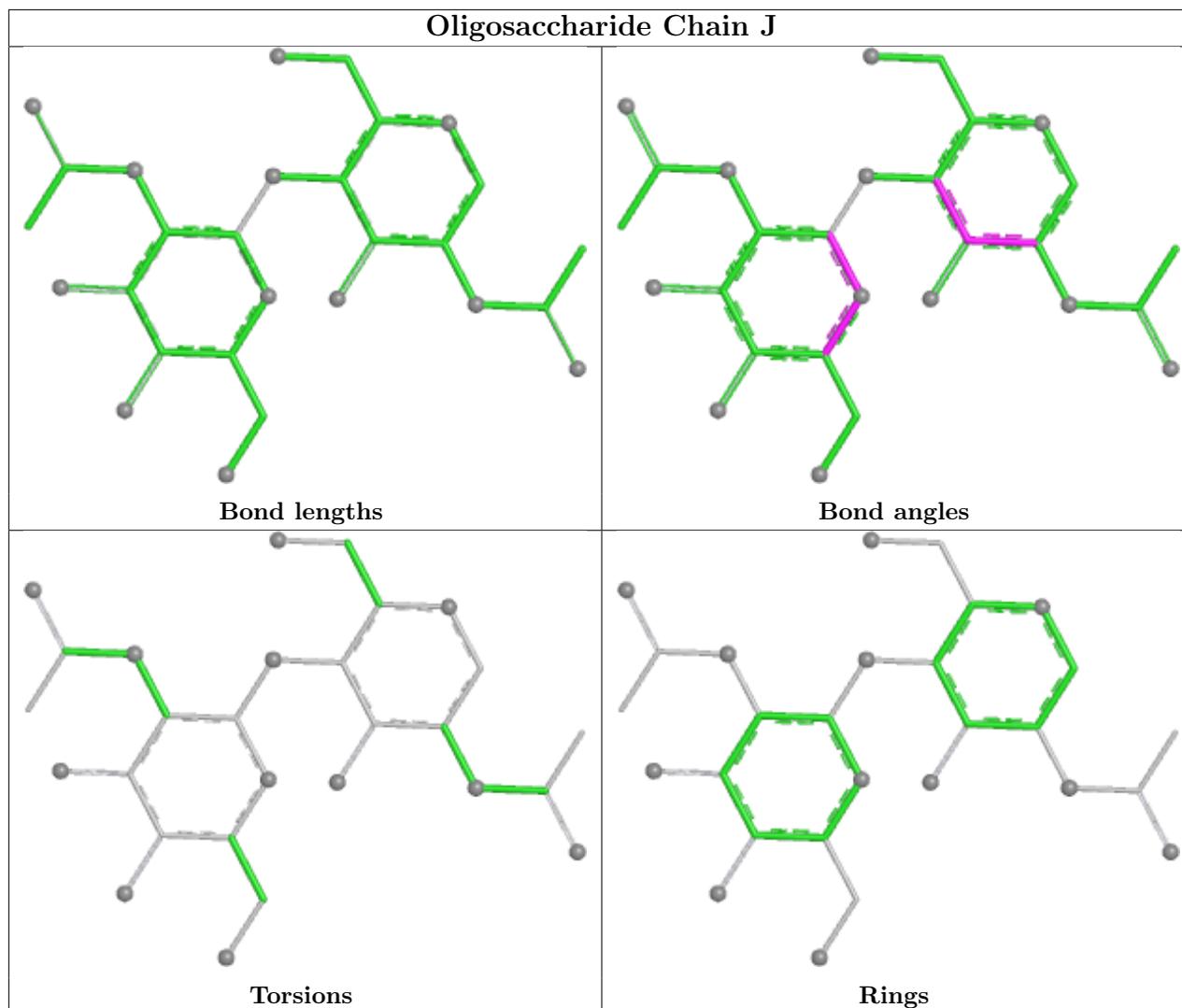
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	3	0
4	I	2	NAG	1	0

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](#)

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	ACY	B	301	-	3,3,3	0.81	0	3,3,3	0.69	0
6	NAG	F	705	3	14,14,15	0.53	0	17,19,21	0.79	1 (5%)
5	ACY	D	301	-	3,3,3	0.74	0	3,3,3	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	705	3	1/1/5/7	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	705	NAG	C2-N2-C7	-2.05	120.16	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	705	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	705	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	ACY	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	214/221 (96%)	-0.34	4 (1%) 66 44	34, 67, 121, 166	1 (0%)
1	C	220/221 (99%)	-0.12	3 (1%) 73 52	43, 83, 117, 156	3 (1%)
2	B	213/214 (99%)	-0.28	1 (0%) 87 75	39, 77, 156, 170	4 (1%)
2	D	211/214 (98%)	-0.52	1 (0%) 87 75	32, 62, 114, 127	0
3	E	148/209 (70%)	-0.10	1 (0%) 84 68	54, 83, 146, 185	0
3	F	148/209 (70%)	-0.13	0 100 100	50, 87, 136, 187	0
All	All	1154/1288 (89%)	-0.26	10 (0%) 81 63	32, 77, 135, 187	8 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	584	ASP	2.9
1	C	167	SER	2.8
2	D	190	ASN	2.7
2	B	210	ASN	2.7
1	A	134	ALA	2.6

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

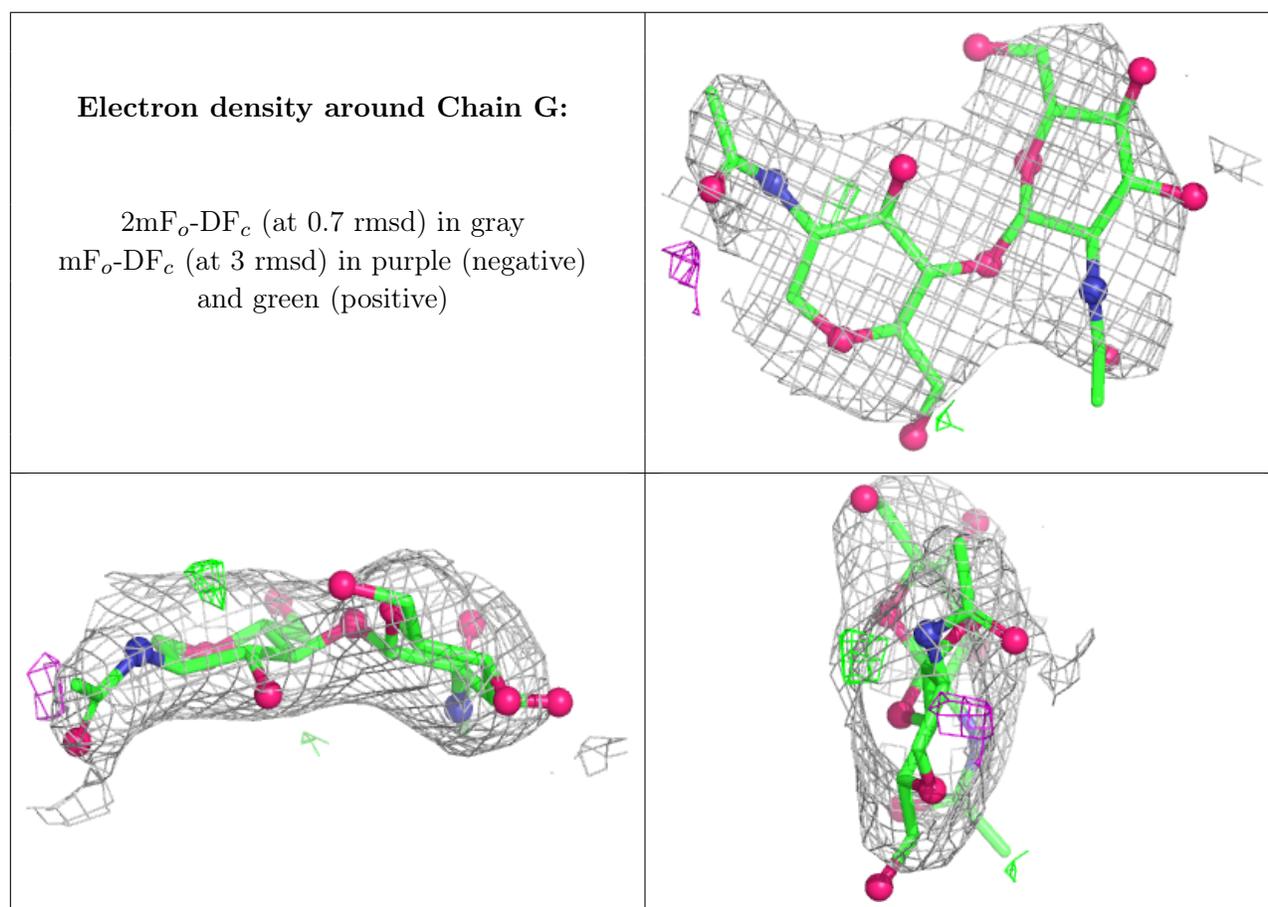
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

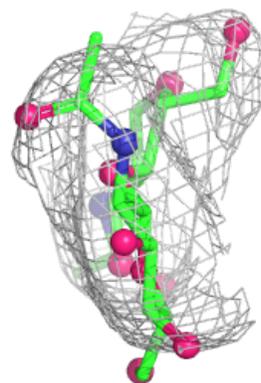
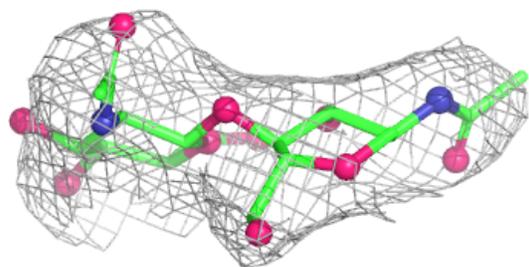
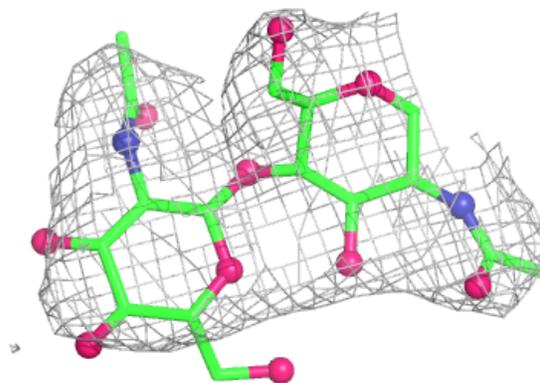
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	I	2	14/15	0.65	0.12	123,126,134,135	0
4	NAG	H	2	14/15	0.72	0.12	137,147,152,152	0
4	NAG	G	2	14/15	0.79	0.12	130,137,143,145	0
4	NAG	J	2	14/15	0.81	0.10	117,119,121,122	0
4	NAG	G	1	14/15	0.87	0.14	85,94,106,118	0
4	NAG	I	1	14/15	0.90	0.13	96,102,106,114	0
4	NAG	J	1	14/15	0.91	0.11	91,96,106,111	0
4	NAG	H	1	14/15	0.91	0.08	74,116,123,134	0

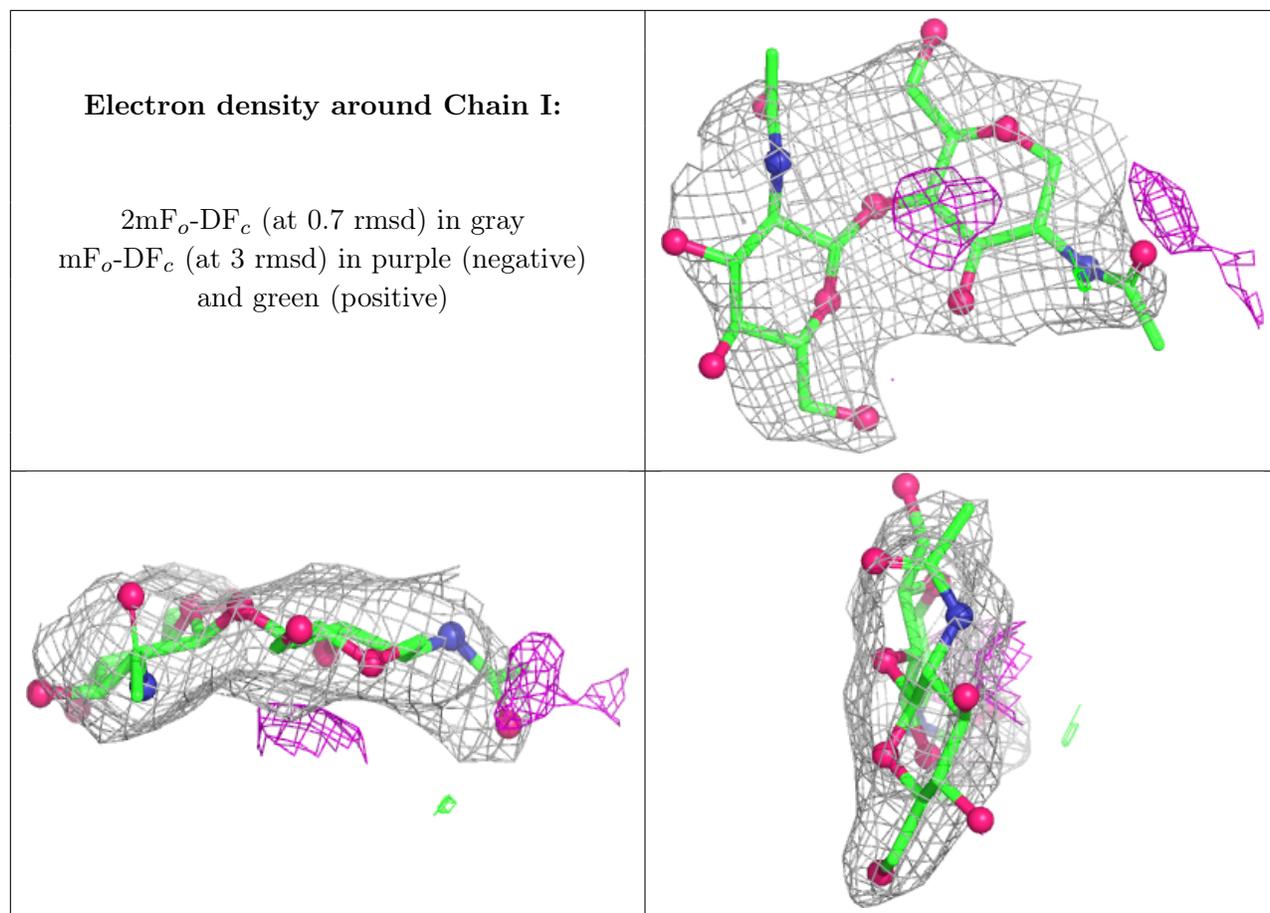
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

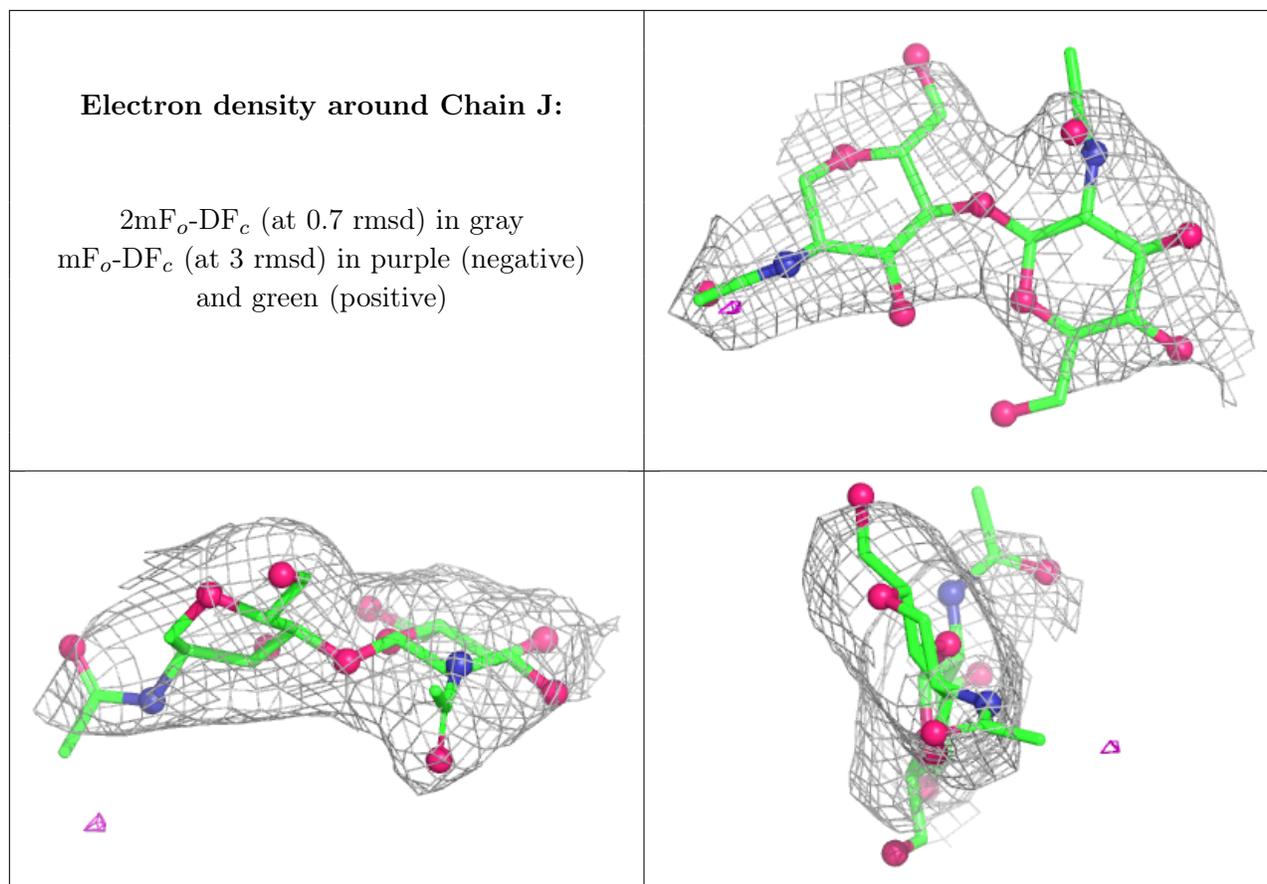


**Electron density around Chain H:**

$2mF_o-DF_c$  (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
6	NAG	F	705	14/15	0.41	0.13	150,154,156,157	0
5	ACY	B	301	4/4	0.94	0.12	55,69,73,78	0
5	ACY	D	301	4/4	0.95	0.08	51,59,59,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.