



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:42 PM BST

PDB ID : 5M5E  
Title : Crystal structure of a interleukin-2 variant in complex with interleukin-2 receptor  
Authors : Klein, C.; Freimoser-Grundschober, A.; Waldhauer, I.; Stihle, M.; Birk, M.; Benz, J.  
Deposited on : 2016-10-21  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

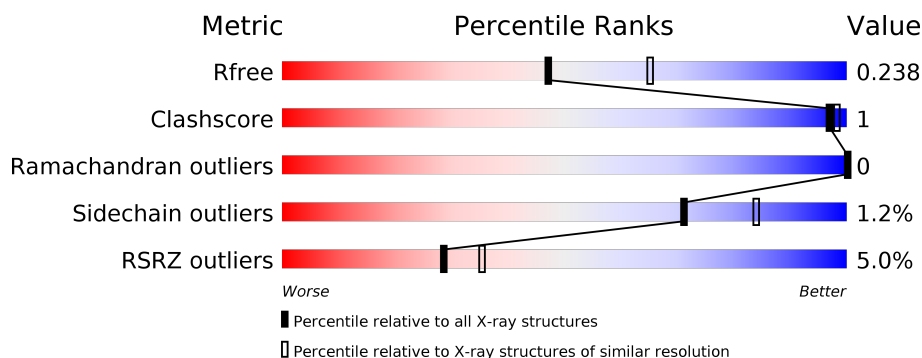
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



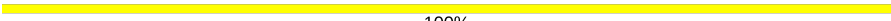
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	233	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>13%</div> </div> </div>
2	C	259	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>•</div> <div>25%</div> </div> </div>
3	D	160	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>•</div> <div>24%</div> </div> </div>
4	A	3	<div> <div></div> <div>100%</div> </div>
4	E	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
5	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	G	2	 100%

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
4	FUC	A	3	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4636 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 Interleukin-2 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	203	Total	C	N	O	S	0	0	0
			1667	1061	295	301	10			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	215	GLY	-	expression tag	UNP P14784
B	216	ALA	-	expression tag	UNP P14784
B	217	GLN	-	expression tag	UNP P14784
B	218	ASP	-	expression tag	UNP P14784
B	219	LYS	-	expression tag	UNP P14784
B	220	THR	-	expression tag	UNP P14784
B	221	HIS	-	expression tag	UNP P14784
B	222	THR	-	expression tag	UNP P14784
B	223	CYS	-	expression tag	UNP P14784
B	224	PRO	-	expression tag	UNP P14784
B	225	PRO	-	expression tag	UNP P14784
B	226	CYS	-	expression tag	UNP P14784
B	227	PRO	-	expression tag	UNP P14784
B	228	ALA	-	expression tag	UNP P14784
B	229	PRO	-	expression tag	UNP P14784
B	230	GLU	-	expression tag	UNP P14784
B	231	LEU	-	expression tag	UNP P14784
B	232	LEU	-	expression tag	UNP P14784
B	233	GLY	-	expression tag	UNP P14784

- Molecule 2 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	193	Total	C	N	O	S	0	0	0
			1641	1044	292	297	8			

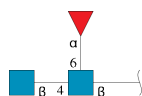
There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	241	GLY	-	expression tag	UNP P31785
C	242	ALA	-	expression tag	UNP P31785
C	243	GLN	-	expression tag	UNP P31785
C	244	ASP	-	expression tag	UNP P31785
C	245	LYS	-	expression tag	UNP P31785
C	246	THR	-	expression tag	UNP P31785
C	247	HIS	-	expression tag	UNP P31785
C	248	THR	-	expression tag	UNP P31785
C	249	CYS	-	expression tag	UNP P31785
C	250	PRO	-	expression tag	UNP P31785
C	251	PRO	-	expression tag	UNP P31785
C	252	CYS	-	expression tag	UNP P31785
C	253	PRO	-	expression tag	UNP P31785
C	254	ALA	-	expression tag	UNP P31785
C	255	PRO	-	expression tag	UNP P31785
C	256	GLU	-	expression tag	UNP P31785
C	257	LEU	-	expression tag	UNP P31785
C	258	LEU	-	expression tag	UNP P31785
C	259	GLY	-	expression tag	UNP P31785

- Molecule 3 is a protein called Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	121	Total	C	N	O	S	0	0	0
			962	610	161	185	6			

- Molecule 4 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
4	A	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



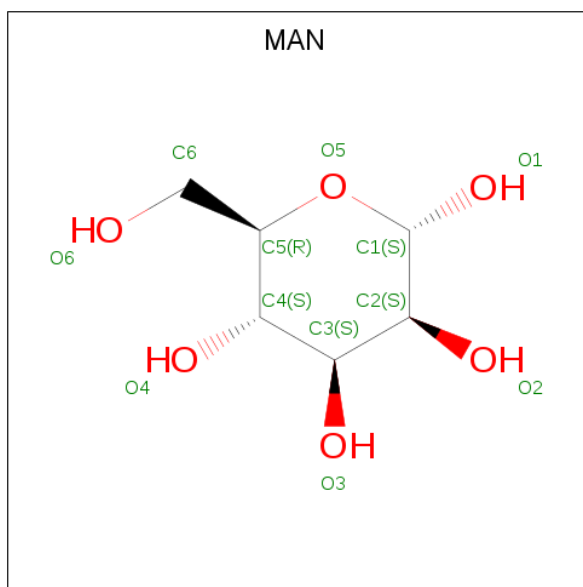
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



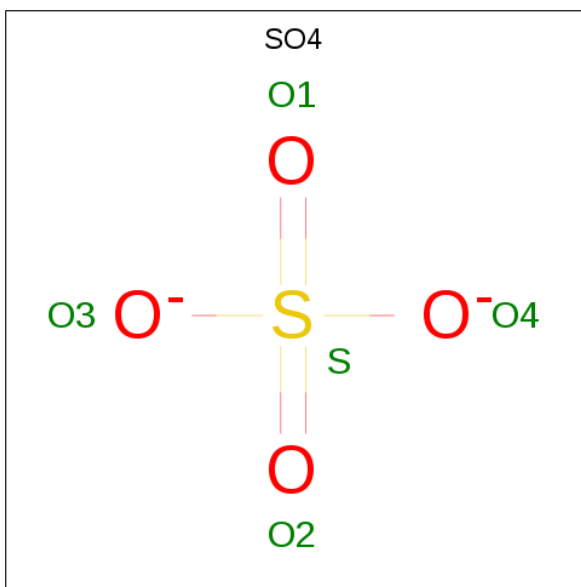
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



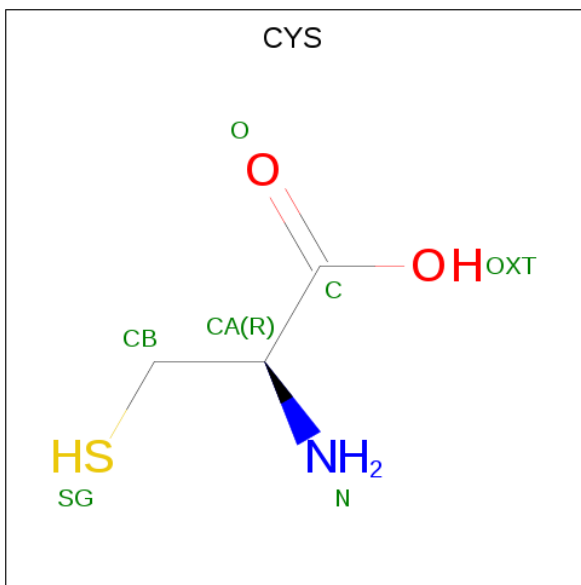
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



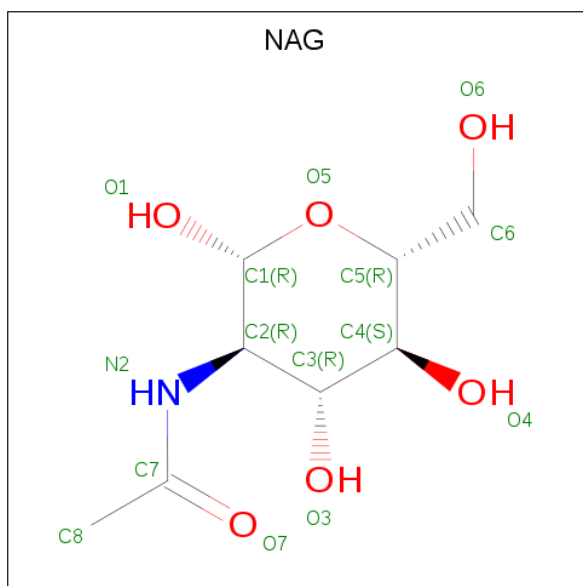
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

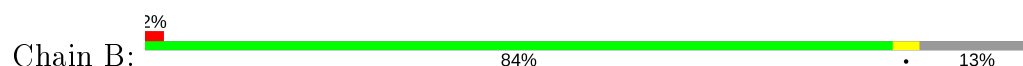
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	88	Total	O	0	0
			88	88		
11	C	50	Total	O	0	0
			50	50		
11	D	34	Total	O	0	0
			34	34		

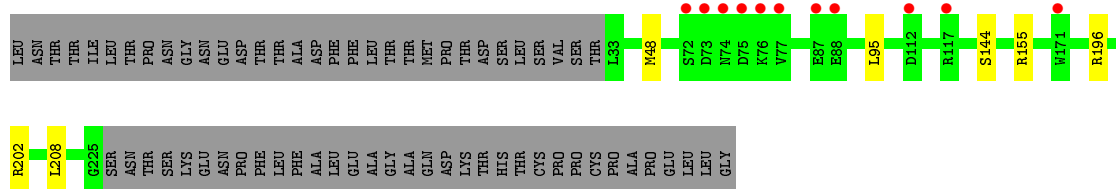
### 3 Residue-property plots [i](#)

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.

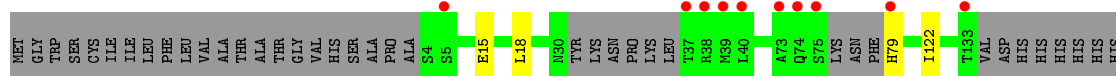
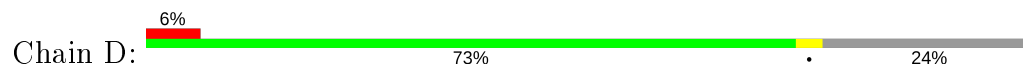
- Molecule 1: Interleukin-2 receptor subunit beta



- Molecule 2: Cytokine receptor common subunit gamma



- Molecule 3: Interleukin-2



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



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






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

Chain F: 



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

Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.97Å 127.97Å 135.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	111.07 – 2.30 46.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (111.07-2.30) 99.7 (46.45-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.199 , 0.235 0.204 , 0.238	Depositor DCC
$R_{free}$ test set	2812 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: FUC, NAG, SO4, MAN

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	B	0.55	0/1716	0.72	0/2342
2	C	0.54	0/1696	0.73	2/2310 (0.1%)
3	D	0.56	0/972	0.68	0/1310
All	All	0.55	0/4384	0.72	2/5962 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	196	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	C	196	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1667	0	1609	4	0
2	C	1641	0	1541	2	0
3	D	962	0	991	2	0
4	A	38	0	34	1	0
4	E	38	0	34	0	0
5	F	28	0	25	0	0
6	G	24	0	22	0	0
7	B	11	0	10	0	0
8	B	10	0	0	1	0
8	C	5	0	0	0	0
8	D	5	0	0	0	0
9	B	7	0	3	0	0
10	C	28	0	26	0	0
11	B	88	0	0	2	0
11	C	50	0	0	0	0
11	D	34	0	0	0	0
All	All	4636	0	4295	8	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 1.

All (8) 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)
1:B:66:ALA:N	8:B:311:SO4:O3	2.37	0.56
1:B:137:ARG:NH2	11:B:401:HOH:O	2.42	0.52
1:B:54:SER:OG	1:B:55:GLN:N	2.48	0.47
2:C:48:MET:CE	2:C:95:LEU:HD12	2.48	0.44
3:D:18:LEU:HD11	3:D:122:ILE:HG23	2.02	0.42
11:B:445:HOH:O	4:A:3:FUC:H3	2.20	0.41
2:C:208:LEU:HD22	3:D:15:GLU:HG2	2.02	0.40
1:B:12:TYR:CE2	1:B:14:SER:HA	2.56	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	B	201/233 (86%)	190 (94%)	11 (6%)	0	100	100
2	C	191/259 (74%)	182 (95%)	9 (5%)	0	100	100
3	D	115/160 (72%)	114 (99%)	1 (1%)	0	100	100
All	All	507/652 (78%)	486 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	185/207 (89%)	184 (100%)	1 (0%)	88	95
2	C	186/244 (76%)	183 (98%)	3 (2%)	62	78
3	D	111/144 (77%)	110 (99%)	1 (1%)	78	89
All	All	482/595 (81%)	477 (99%)	5 (1%)	71	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	SER
2	C	144	SER
2	C	155	ARG
2	C	202	ARG
3	D	79	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	GLN
2	C	53	ASN
2	C	94	GLN

### 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](#)

10 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	A	1	1,4	14,14,15	0.53	0	17,19,21	1.25	2 (11%)
4	NAG	A	2	4	14,14,15	0.57	0	17,19,21	2.14	3 (17%)
4	FUC	A	3	4	10,10,11	0.58	0	14,14,16	1.02	0
4	NAG	E	1	1,4	14,14,15	0.54	0	17,19,21	1.47	3 (17%)
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	0.88	0
4	FUC	E	3	4	10,10,11	0.28	0	14,14,16	0.61	0
5	NAG	F	1	1,5	14,14,15	0.69	0	17,19,21	2.78	4 (23%)
5	NAG	F	2	5	14,14,15	0.44	0	17,19,21	0.75	0
6	NAG	G	1	2,6	14,14,15	0.70	0	17,19,21	1.61	2 (11%)
6	FUC	G	2	6	10,10,11	0.64	0	14,14,16	2.25	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1
4	FUC	A	3	4	1/1/4/5	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1
6	FUC	G	2	6	-	-	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	9.52	125.09	112.19
4	A	2	NAG	C1-O5-C5	6.48	120.97	112.19
6	G	1	NAG	C1-O5-C5	5.17	119.20	112.19
6	G	2	FUC	O5-C1-C2	5.06	118.58	110.77
6	G	2	FUC	C1-C2-C3	4.41	115.08	109.67
5	F	1	NAG	C3-C4-C5	3.95	117.28	110.24
4	A	2	NAG	C6-C5-C4	-3.32	105.23	113.00
4	E	1	NAG	C1-C2-N2	3.10	115.79	110.49
4	A	2	NAG	O5-C5-C4	2.88	117.82	110.83
4	E	1	NAG	O5-C1-C2	-2.75	106.94	111.29
5	F	1	NAG	C2-N2-C7	2.74	126.81	122.90
4	A	1	NAG	O5-C5-C6	2.68	111.41	107.20
6	G	2	FUC	O2-C2-C3	-2.64	104.85	110.14
4	E	1	NAG	O3-C3-C2	-2.35	104.61	109.47
6	G	2	FUC	C1-O5-C5	2.25	117.88	112.78
5	F	1	NAG	O4-C4-C3	-2.23	105.19	110.35
6	G	1	NAG	O5-C5-C6	2.08	110.46	107.20
4	A	1	NAG	O6-C6-C5	-2.07	104.19	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3	FUC	C1

All (9) torsion outliers are listed below:

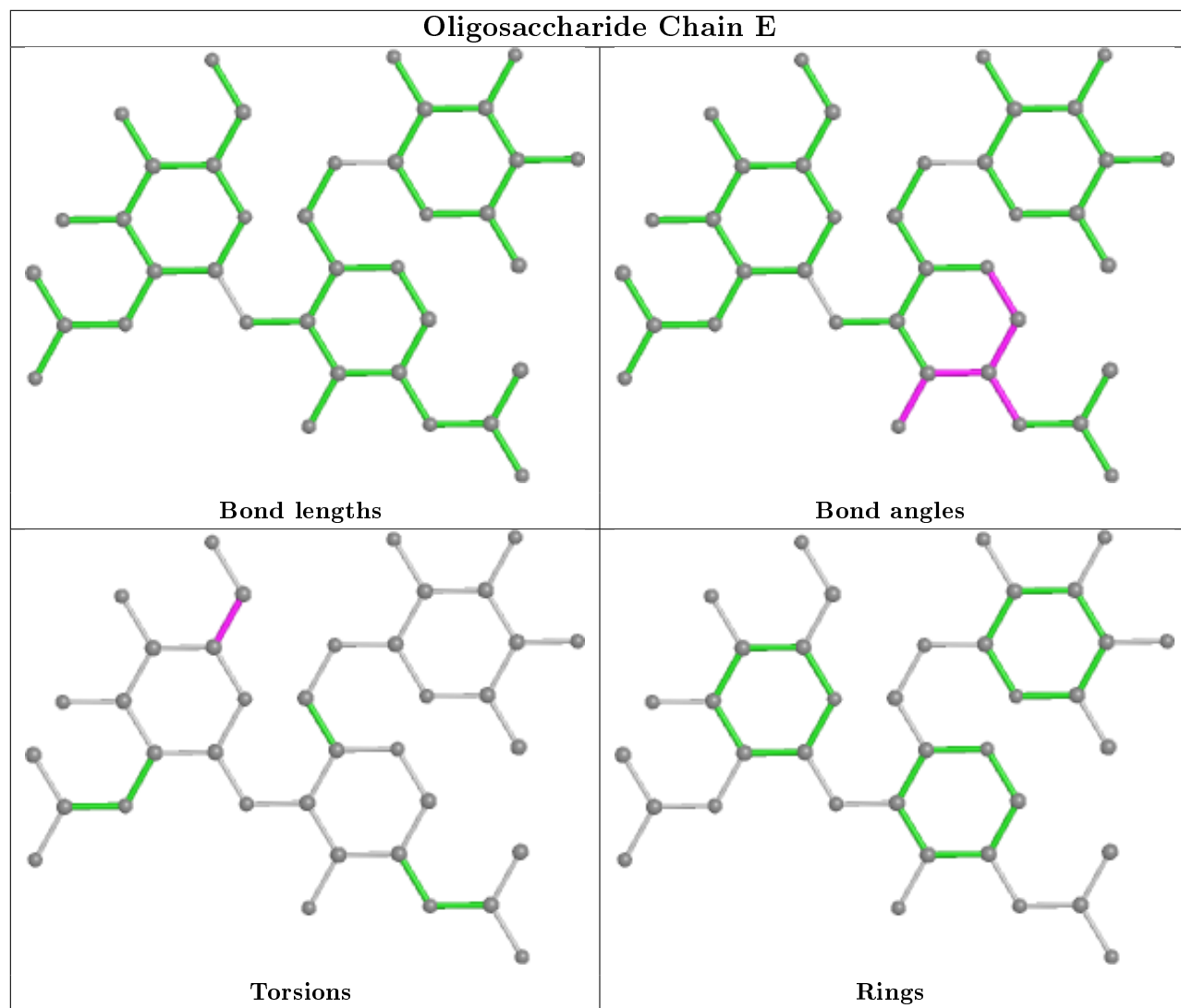
Mol	Chain	Res	Type	Atoms
6	G	1	NAG	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

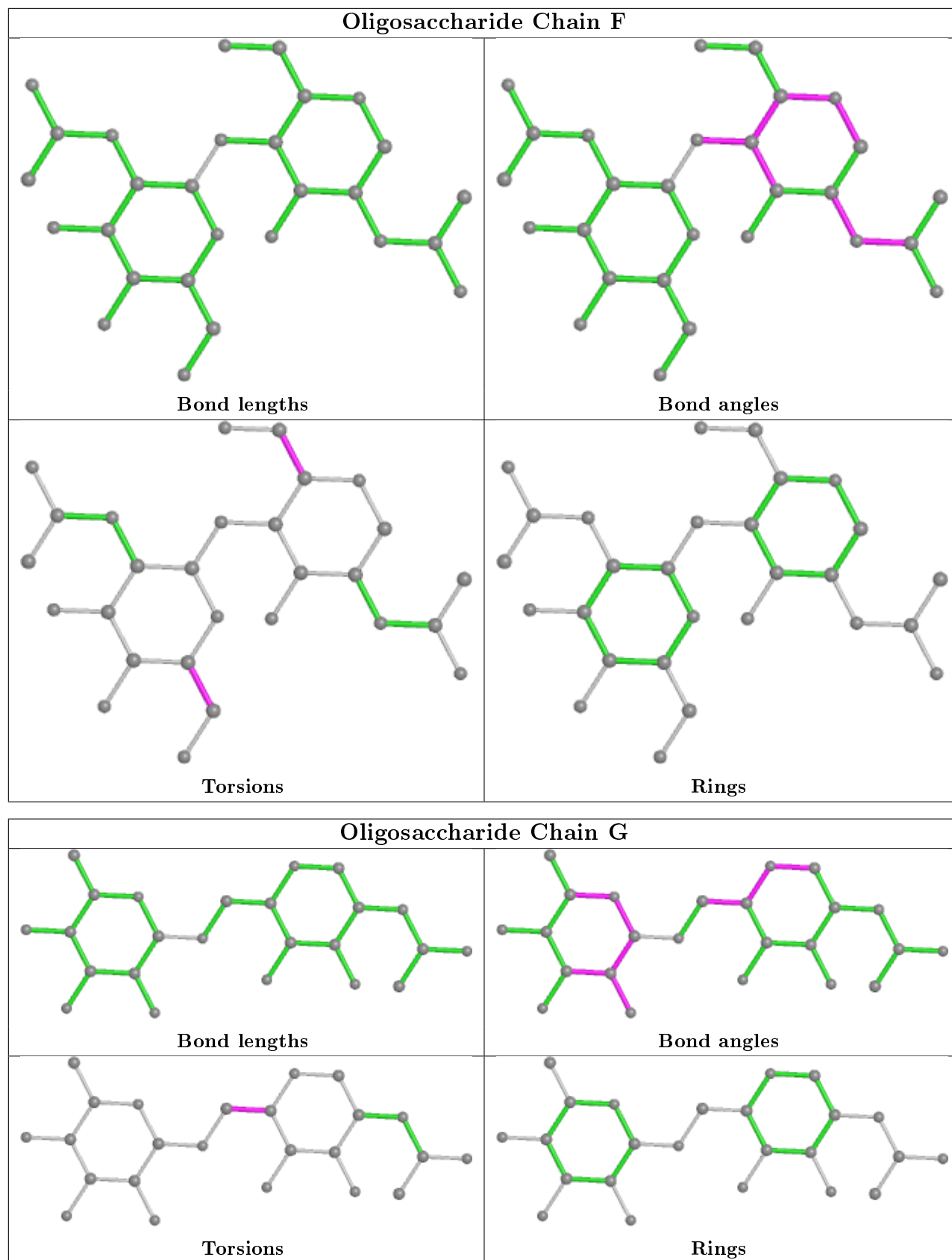
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3	FUC	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

8 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	$\# Z  > 2$
8	SO4	D	201	-	4,4,4	0.38	0	6,6,6	0.14	0
8	SO4	C	305	-	4,4,4	0.30	0	6,6,6	0.31	0
10	NAG	C	303	2	14,14,15	0.85	0	17,19,21	1.82	4 (23%)
10	NAG	C	304	2	14,14,15	0.75	0	17,19,21	1.19	1 (5%)
8	SO4	B	311	-	4,4,4	0.42	0	6,6,6	0.39	0
7	MAN	B	309	1	11,11,12	0.56	0	15,15,17	3.02	3 (20%)
8	SO4	B	310	-	4,4,4	0.34	0	6,6,6	0.37	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	MAN	B	309	1	-	1/2/19/22	0/1/1/1
10	NAG	C	303	2	-	1/6/23/26	0/1/1/1
10	NAG	C	304	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	309	MAN	C1-O5-C5	10.77	126.79	112.19
10	C	303	NAG	O5-C1-C2	-3.64	105.54	111.29
10	C	303	NAG	C2-N2-C7	3.60	128.03	122.90
10	C	304	NAG	O5-C5-C6	3.14	112.12	107.20
7	B	309	MAN	C3-C4-C5	3.06	115.70	110.24
10	C	303	NAG	C1-O5-C5	3.01	116.27	112.19
7	B	309	MAN	O5-C5-C4	2.35	116.54	110.83
10	C	303	NAG	O5-C5-C4	2.03	115.77	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	304	NAG	C4-C5-C6-O6
7	B	309	MAN	C4-C5-C6-O6
10	C	303	NAG	C3-C2-N2-C7
10	C	304	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	311	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	203/233 (87%)	0.07	5 (2%) 57 64	33, 43, 80, 99	0
2	C	193/259 (74%)	0.45	11 (5%) 23 30	36, 57, 97, 146	0
3	D	121/160 (75%)	0.31	10 (8%) 11 15	34, 46, 96, 127	0
All	All	517/652 (79%)	0.27	26 (5%) 28 35	33, 49, 95, 146	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	73	ASP	6.9
2	C	76	LYS	6.6
3	D	75	SER	6.3
3	D	74	GLN	5.5
2	C	74	ASN	5.3
3	D	37	THR	4.4
2	C	75	ASP	4.4
3	D	79	HIS	4.3
2	C	72	SER	3.9
3	D	73	ALA	3.7
3	D	39	MET	3.1
2	C	117	ARG	3.1
1	B	150	HIS	3.0
1	B	25	ASP	2.7
3	D	133	THR	2.7
1	B	27	ALA	2.6
3	D	5	SER	2.6
2	C	171	TRP	2.5
3	D	38	ARG	2.4
2	C	87	GLU	2.2
2	C	77	VAL	2.1
1	B	175	ASP	2.1
3	D	40	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	88	GLU	2.1
2	C	112	ASP	2.1
1	B	207	PRO	2.0

## 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](#)

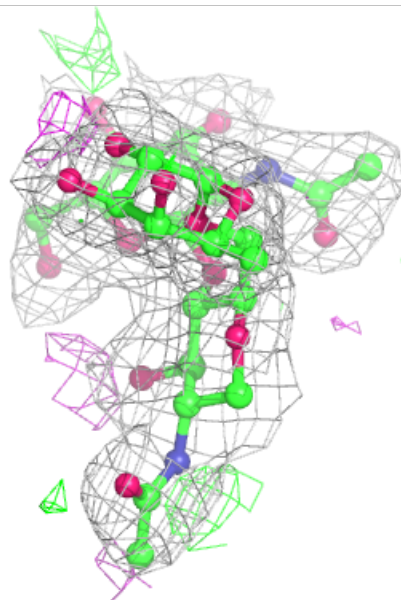
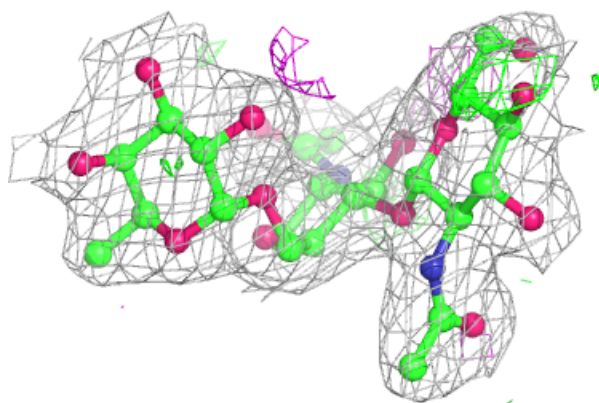
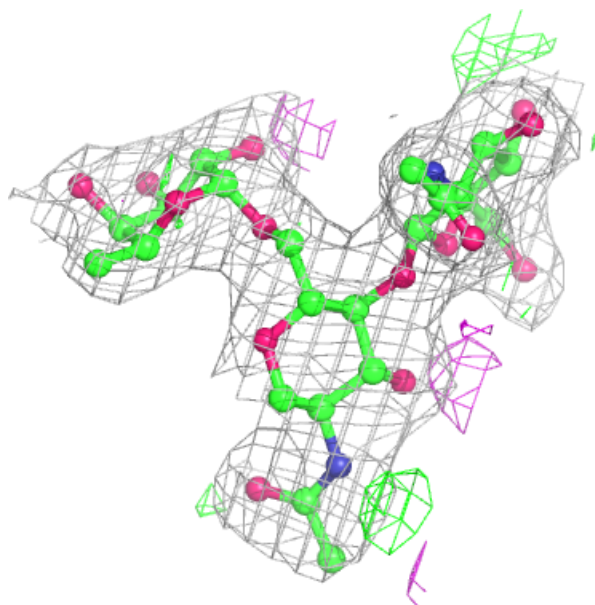
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	FUC	A	3	10/11	0.91	0.17	52,60,64,68	0
5	NAG	F	1	14/15	0.92	0.15	58,61,67,70	0
4	NAG	A	2	14/15	0.92	0.18	54,65,72,75	0
6	NAG	G	1	14/15	0.92	0.16	67,71,76,76	0
6	FUC	G	2	10/11	0.92	0.20	77,81,85,86	0
4	NAG	E	2	14/15	0.93	0.11	44,55,63,67	0
5	NAG	F	2	14/15	0.94	0.11	64,69,76,77	0
4	NAG	A	1	14/15	0.96	0.11	46,49,54,55	0
4	FUC	E	3	10/11	0.98	0.12	35,36,37,38	0
4	NAG	E	1	14/15	0.98	0.09	38,41,46,47	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.

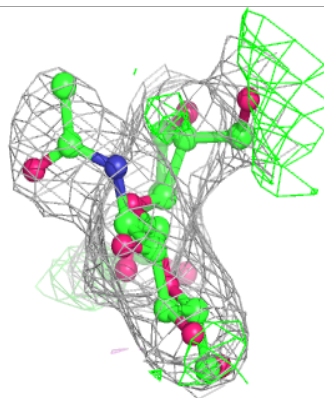
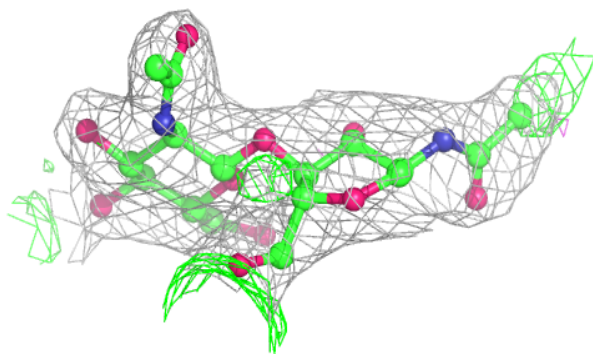
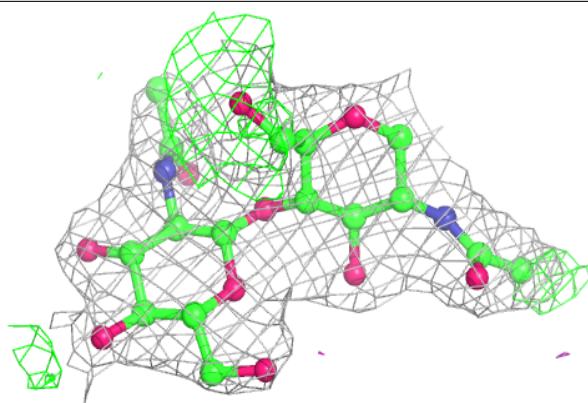
**Electron density around Chain E:**

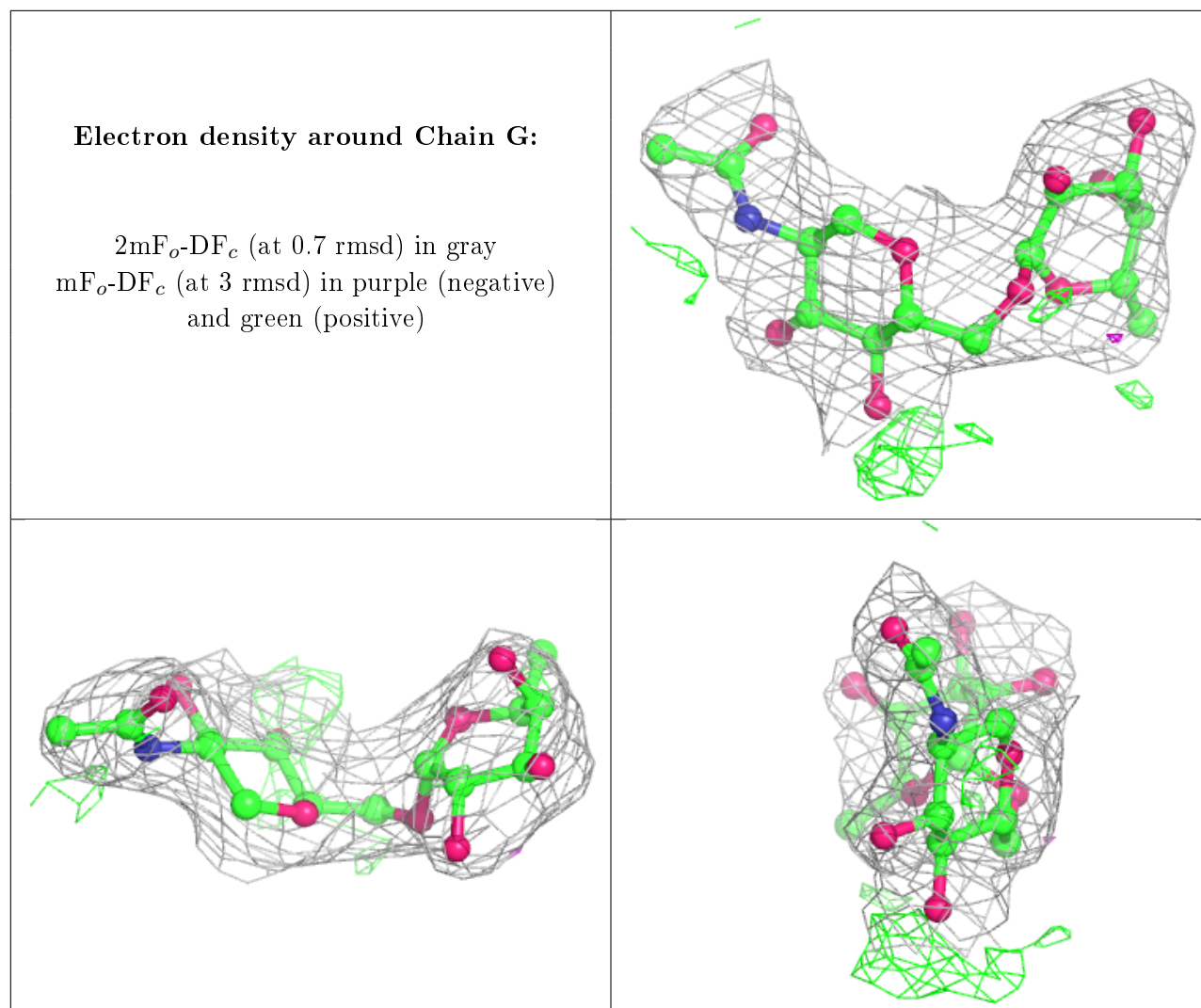
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands ⓘ

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
10	NAG	C	303	14/15	0.80	0.24	73,80,84,85	0
10	NAG	C	304	14/15	0.80	0.20	66,79,85,88	0
9	CYS	B	312	7/7	0.87	0.25	88,92,96,99	0
8	SO4	B	311	5/5	0.89	0.25	80,84,86,88	0
8	SO4	D	201	5/5	0.93	0.24	87,89,95,97	0
7	MAN	B	309	11/12	0.97	0.11	50,52,53,54	0
8	SO4	B	310	5/5	0.97	0.20	60,62,67,73	0
8	SO4	C	305	5/5	0.99	0.11	65,67,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.