



# wwPDB X-ray Structure Validation Summary Report

Aug 7, 2020 – 10:37 AM BST

PDB ID : 6MU8  
Title : Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-386150 in Complex with Human Antibodies 3H109L and 35O22 at 3.5 Angstrom  
Authors : Lai, Y.-T.; Kwong, P.D.  
Deposited on : 2018-10-22  
Resolution : 2.99 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.

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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  
buster-report : 1.1.7 (2018)  
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

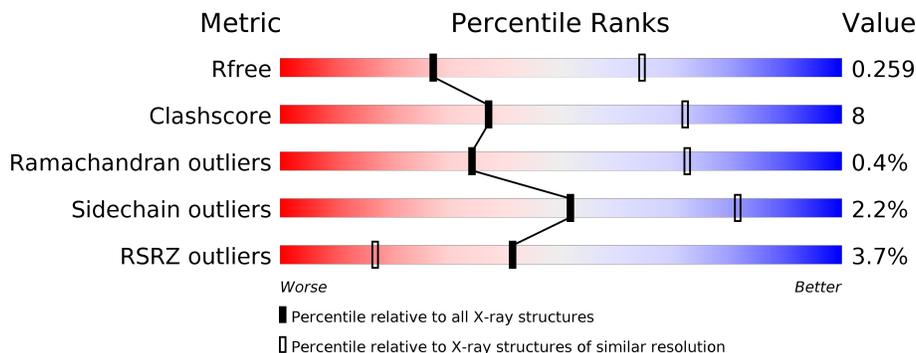
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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.



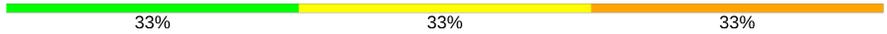
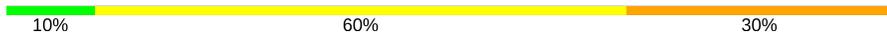
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	153	
2	D	134	
3	E	114	
4	G	481	
5	H	244	
6	L	217	

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Mol	Chain	Length	Quality of chain
7	A	6	 33% 33% 33%
8	C	3	 100%
8	F	3	 33% 67%
9	I	2	 100%
9	J	2	 100%
9	M	2	 50% 50%
10	K	10	 10% 60% 30%

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
11	NAG	B	702	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 10171 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	133	1056	673	182	195	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 scFv heavy chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	128	994	628	169	192	5	0	0	0

- Molecule 3 is a protein called 35O22 scFv light chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	105	805	506	133	160	6	0	0	0

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	439	3461	2177	613	643	28	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

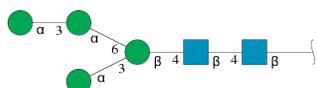
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	226	1715	1093	278	338	6	0	0	0

- Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	211	1604	1009	276	312	7	0	0	0

- Molecule 7 is an oligosaccharide called 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
			Total	C	N	O			
7	A	6	72	40	2	30	0	0	0

- Molecule 8 is an oligosaccharide called 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
			Total	C	N	O			
8	C	3	39	22	2	15	0	0	0

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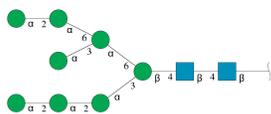
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	F	3	39	22	2	15	0	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



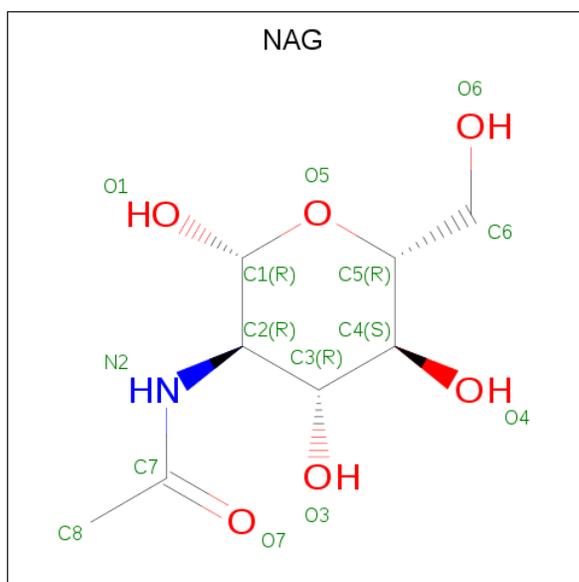
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	2	28	16	2	10	0	0	0
9	J	2	28	16	2	10	0	0	0
9	M	2	28	16	2	10	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



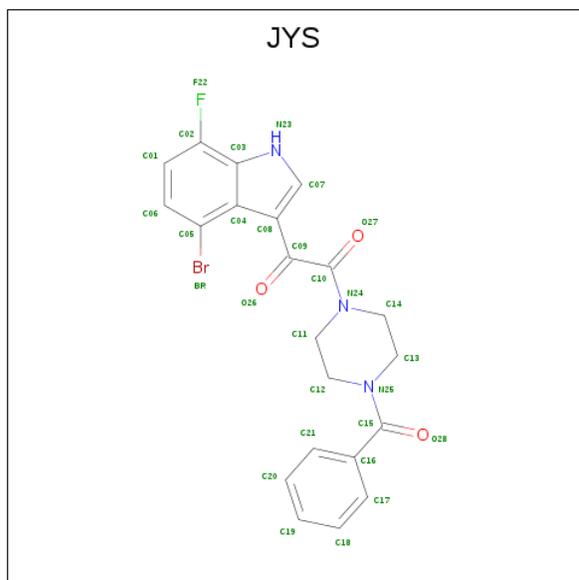
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	K	10	116	64	2	50	0	0	0

- Molecule 11 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		
11	B	1	14	8	1	5	0	0
11	B	1	14	8	1	5	0	0
11	D	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0
11	G	1	14	8	1	5	0	0

- Molecule 12 is 1-[4-(benzenecarbonyl)piperazin-1-yl]-2-(4-bromo-7-fluoro-1H-indol-3-yl)ethane-1,2-dione (three-letter code: JYS) (formula:  $C_{21}H_{17}BrFN_3O_3$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	F	N			O
12	G	1	29	1	21	1	3	3	0	0

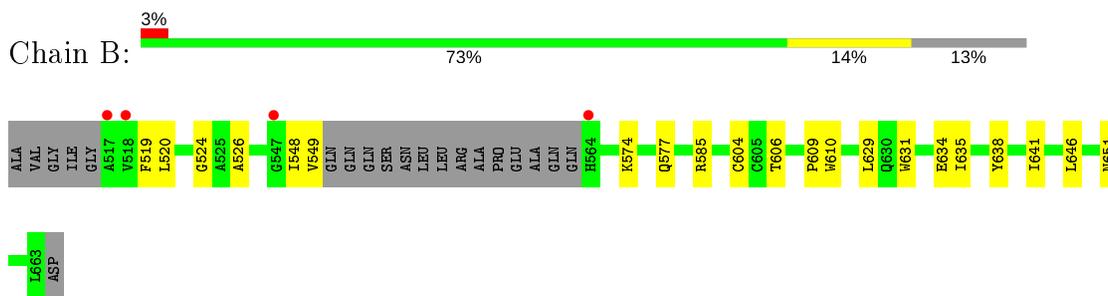
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total O 1 1	0	0
13	G	1	Total O 1 1	0	0
13	L	1	Total O 1 1	0	0

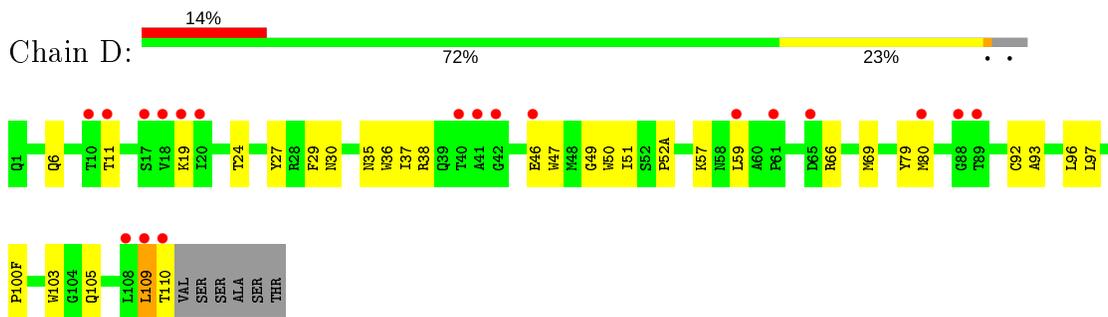
### 3 Residue-property plots [i](#)

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.

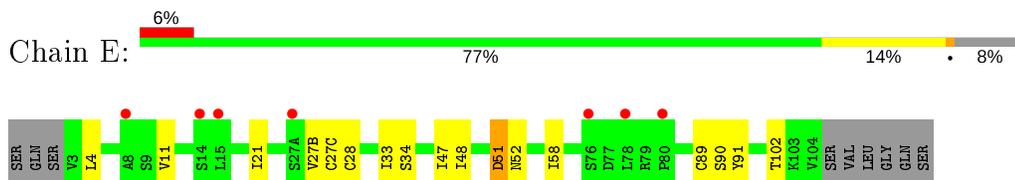
- Molecule 1: Envelope glycoprotein gp160



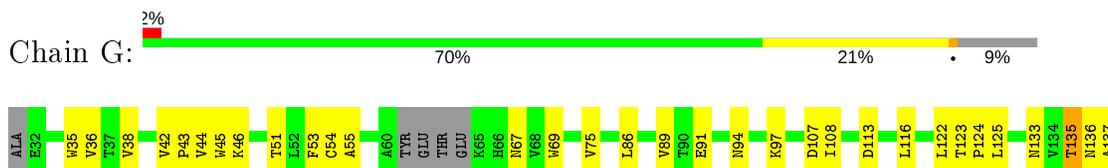
- Molecule 2: 35O22 scFv heavy chain portion

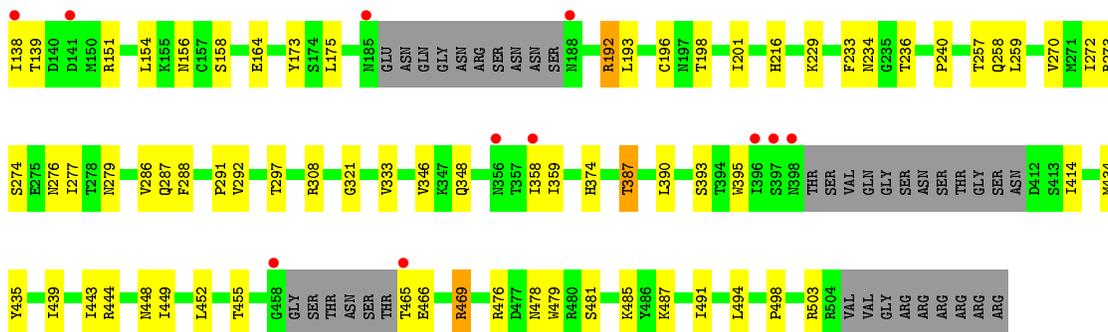


- Molecule 3: 35O22 scFv light chain portion

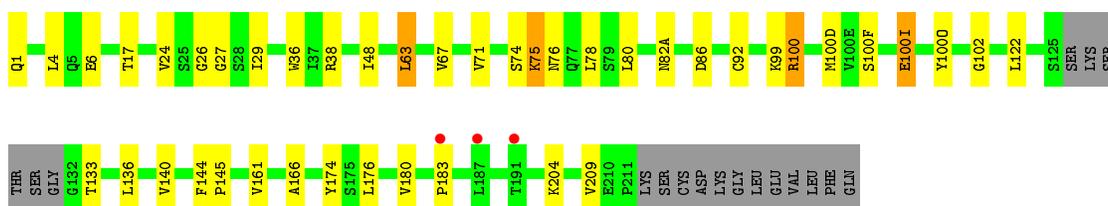


- Molecule 4: Envelope glycoprotein gp160

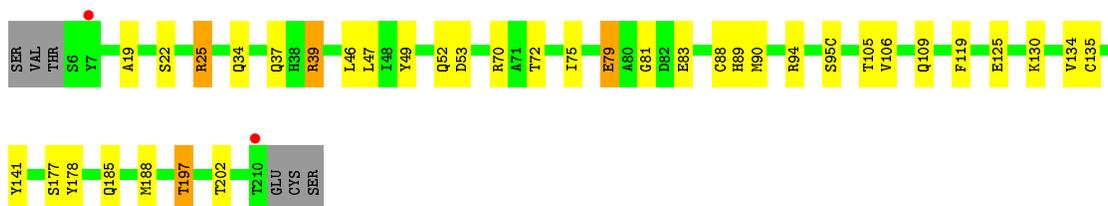
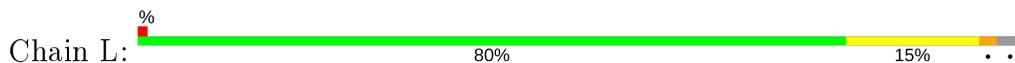




- Molecule 5: 3H109L Fab heavy chain



- Molecule 6: 3H109L Fab light chain



- Molecule 7: 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



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%

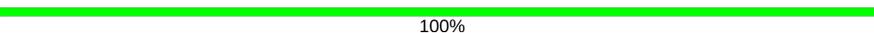
MAG1  
MAG2  
B01A3

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1  
MAG2

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  10% 60% 30%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.41Å 131.41Å 315.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.15 – 2.99 46.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	45.4 (46.15-2.99) 44.9 (46.15-2.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.219 , 0.259 0.219 , 0.259	Depositor DCC
$R_{free}$ test set	1411 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 25.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	10171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: JYS, BMA, NAG, 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	0.23	0/1075	0.39	0/1458
2	D	0.24	0/1021	0.47	0/1390
3	E	0.25	0/829	0.46	0/1133
4	G	0.24	0/3532	0.45	0/4791
5	H	0.24	0/1758	0.47	0/2397
6	L	0.25	0/1647	0.45	0/2247
All	All	0.24	0/9862	0.45	0/13416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1056	0	1050	16	0
2	D	994	0	952	22	0
3	E	805	0	752	8	0
4	G	3461	0	3409	69	0
5	H	1715	0	1685	26	0
6	L	1604	0	1553	26	0
7	A	72	0	61	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	39	0	34	0	0
8	F	39	0	34	1	0
9	I	28	0	25	0	0
9	J	28	0	25	0	0
9	M	28	0	25	0	0
10	K	116	0	97	3	0
11	B	28	0	26	0	0
11	D	14	0	13	0	0
11	G	112	0	104	3	0
12	G	29	0	0	2	0
13	D	1	0	0	0	0
13	G	1	0	0	0	0
13	L	1	0	0	0	0
All	All	10171	0	9845	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 156 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)
4:G:137:ALA:H	4:G:151:ARG:HH21	1.35	0.74
2:D:49:GLY:HA3	2:D:59:LEU:HD23	1.68	0.73
2:D:109:LEU:HD23	2:D:110:THR:HG22	1.73	0.71
5:H:136:LEU:HD13	5:H:209:VAL:HG21	1.72	0.70
4:G:270:VAL:HG23	4:G:348:GLN:HG3	1.76	0.68

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	129/153 (84%)	120 (93%)	9 (7%)	0	100	100
2	D	126/134 (94%)	108 (86%)	18 (14%)	0	100	100
3	E	103/114 (90%)	88 (85%)	13 (13%)	2 (2%)	8	36
4	G	429/481 (89%)	398 (93%)	28 (6%)	3 (1%)	22	60
5	H	222/244 (91%)	203 (91%)	19 (9%)	0	100	100
6	L	209/217 (96%)	197 (94%)	12 (6%)	0	100	100
All	All	1218/1343 (91%)	1114 (92%)	99 (8%)	5 (0%)	34	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	52	ASN
3	E	11	VAL
4	G	321	GLY
4	G	135	THR
4	G	240	PRO

### 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	114/129 (88%)	111 (97%)	3 (3%)	46	78
2	D	107/112 (96%)	105 (98%)	2 (2%)	57	84
3	E	92/100 (92%)	90 (98%)	2 (2%)	52	81
4	G	391/427 (92%)	384 (98%)	7 (2%)	59	85
5	H	196/212 (92%)	190 (97%)	6 (3%)	40	75
6	L	175/181 (97%)	171 (98%)	4 (2%)	50	80
All	All	1075/1161 (93%)	1051 (98%)	24 (2%)	52	81

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	229	LYS
4	G	485	LYS
6	L	79	GLU
4	G	387	THR
4	G	469	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	287	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](#)

28 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	$\# Z  > 2$
7	NAG	A	1	4,7	14,14,15	0.26	0	17,19,21	0.43	0
7	NAG	A	2	7	14,14,15	0.41	0	17,19,21	1.28	1 (5%)
7	BMA	A	3	7	11,11,12	0.72	0	15,15,17	0.72	0
7	MAN	A	4	7	11,11,12	1.37	2 (18%)	15,15,17	2.02	4 (26%)
7	MAN	A	5	7	11,11,12	1.63	2 (18%)	15,15,17	2.26	4 (26%)
7	MAN	A	6	7	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.31	0	17,19,21	0.42	0
8	NAG	C	2	8	14,14,15	0.24	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	C	3	8	11,11,12	0.61	0	15,15,17	0.74	0
8	NAG	F	1	8,4	14,14,15	0.25	0	17,19,21	0.56	0
8	NAG	F	2	8	14,14,15	0.24	0	17,19,21	0.54	0
8	BMA	F	3	8	11,11,12	0.67	0	15,15,17	0.76	0
9	NAG	I	1	9,4	14,14,15	0.32	0	17,19,21	0.39	0
9	NAG	I	2	9	14,14,15	0.25	0	17,19,21	0.37	0
9	NAG	J	1	9,4	14,14,15	0.24	0	17,19,21	0.43	0
9	NAG	J	2	9	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	K	1	10,4	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
10	MAN	K	10	10	11,11,12	1.06	0	15,15,17	1.13	1 (6%)
10	NAG	K	2	10	14,14,15	0.22	0	17,19,21	0.42	0
10	BMA	K	3	10	11,11,12	1.09	1 (9%)	15,15,17	1.00	0
10	MAN	K	4	10	11,11,12	0.72	1 (9%)	15,15,17	1.32	2 (13%)
10	MAN	K	5	10	11,11,12	0.70	0	15,15,17	0.96	2 (13%)
10	MAN	K	6	10	11,11,12	0.74	0	15,15,17	0.87	1 (6%)
10	MAN	K	7	10	11,11,12	0.80	0	15,15,17	1.00	1 (6%)
10	MAN	K	8	10	11,11,12	0.68	0	15,15,17	1.09	1 (6%)
10	MAN	K	9	10	11,11,12	0.69	0	15,15,17	1.36	2 (13%)
9	NAG	M	1	9,4	14,14,15	2.24	2 (14%)	17,19,21	1.76	4 (23%)
9	NAG	M	2	9	14,14,15	0.47	0	17,19,21	0.39	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	NAG	A	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	NAG	F	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	I	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
9	NAG	J	1	9,4	-	1/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
10	NAG	K	1	10,4	-	3/6/23/26	0/1/1/1
10	MAN	K	10	10	-	0/2/19/22	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	2/2/19/22	0/1/1/1
10	MAN	K	5	10	-	2/2/19/22	0/1/1/1
10	MAN	K	6	10	-	2/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1
10	MAN	K	8	10	-	0/2/19/22	0/1/1/1
10	MAN	K	9	10	-	2/2/19/22	0/1/1/1
9	NAG	M	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1	NAG	O5-C1	7.78	1.56	1.43
7	A	5	MAN	C1-C2	4.09	1.61	1.52
7	A	4	MAN	C1-C2	3.67	1.60	1.52
7	A	5	MAN	O5-C1	3.11	1.48	1.43
9	M	1	NAG	C1-C2	2.94	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5	MAN	C1-O5-C5	6.62	121.16	112.19
9	M	1	NAG	C1-O5-C5	5.27	119.33	112.19
7	A	4	MAN	C1-C2-C3	5.23	116.09	109.67
10	K	1	NAG	C2-N2-C7	4.48	129.28	122.90
10	K	9	MAN	C1-O5-C5	4.34	118.07	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

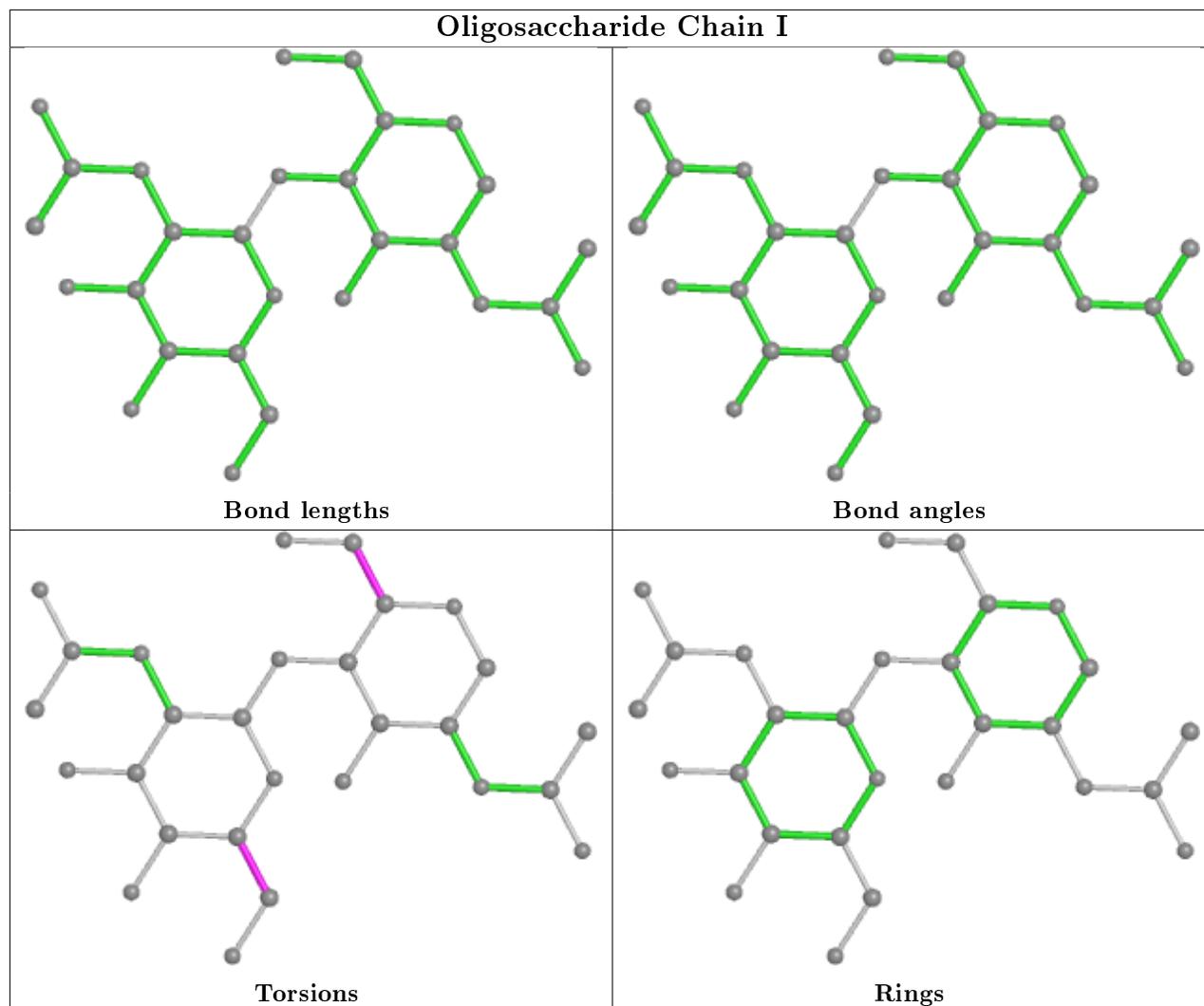
Mol	Chain	Res	Type	Atoms
10	K	4	MAN	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6

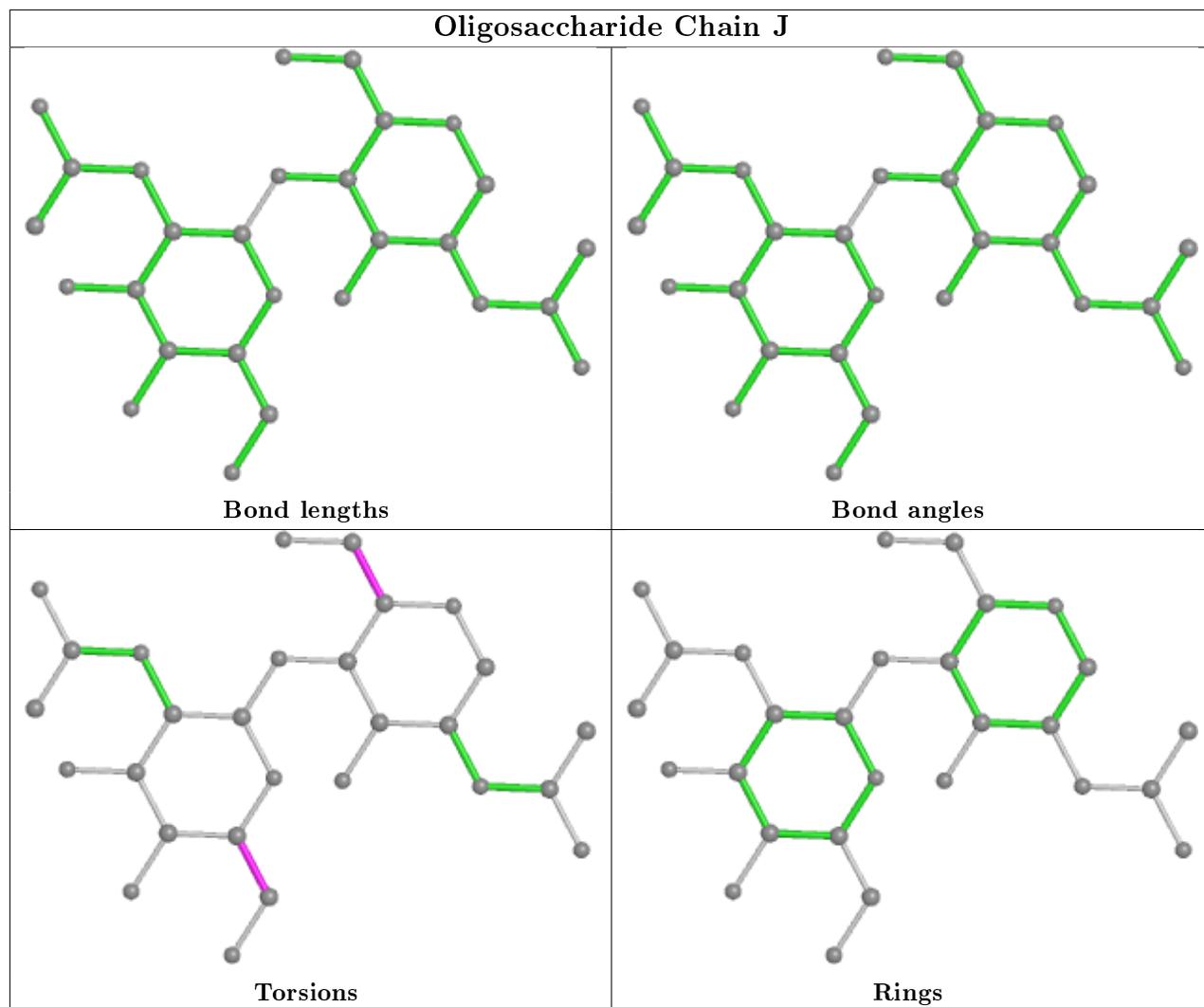
There are no ring outliers.

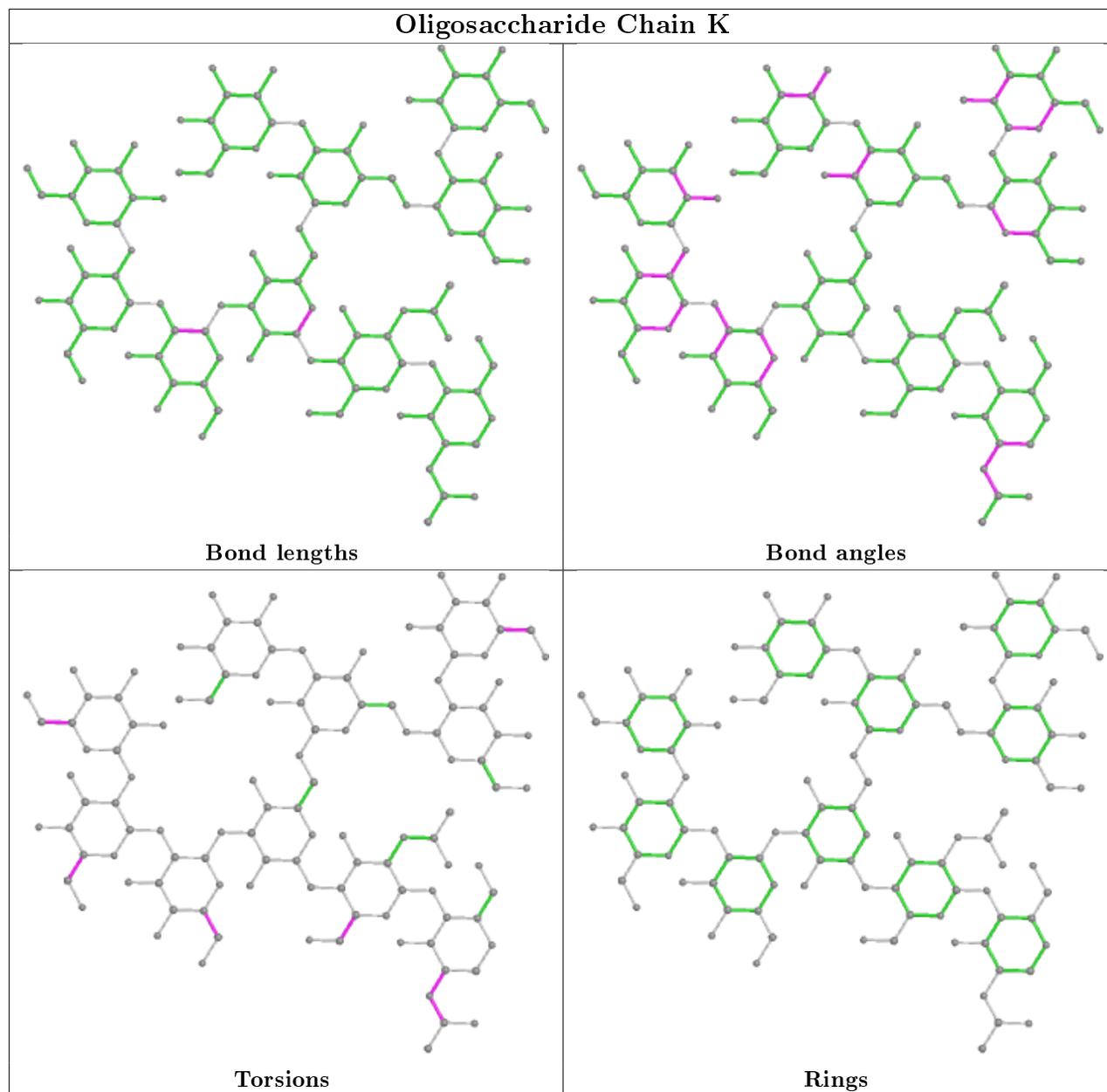
7 monomers are involved in 6 short contacts:

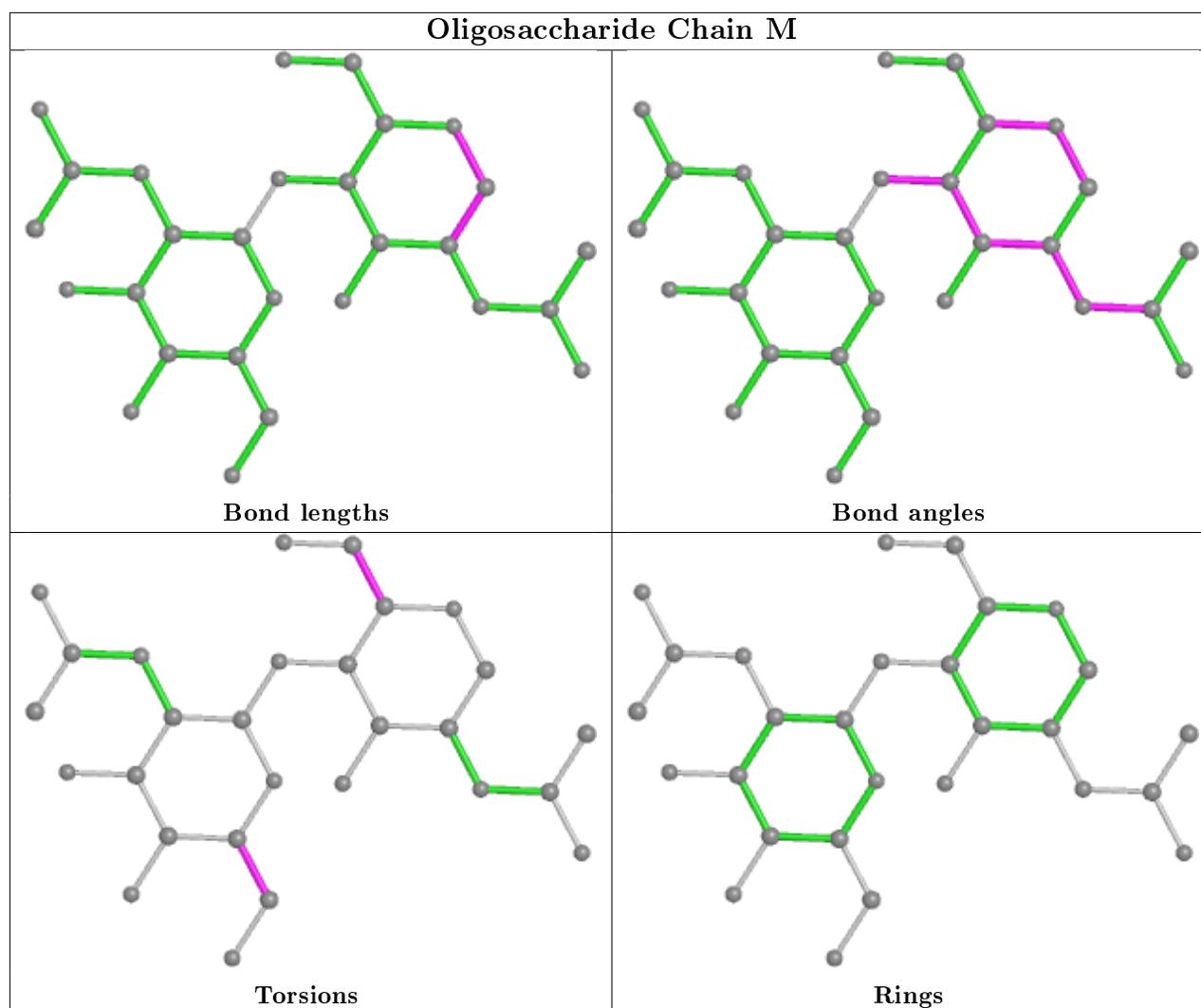
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4	MAN	1	0
10	K	4	MAN	1	0
8	F	1	NAG	1	0
10	K	9	MAN	1	0
7	A	2	NAG	1	0
10	K	1	NAG	1	0
8	F	2	NAG	1	0

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](#)

12 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	$\# Z  > 2$
11	NAG	D	201	2	14,14,15	0.34	0	17,19,21	0.53	0
12	JYS	G	637	-	30,32,32	5.65	16 (53%)	38,46,46	1.79	8 (21%)
11	NAG	G	633	4	14,14,15	0.25	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	G	634	4	14,14,15	0.23	0	17,19,21	0.60	1 (5%)
11	NAG	G	611	4	14,14,15	0.37	0	17,19,21	0.49	0
11	NAG	B	701	1	14,14,15	0.33	0	17,19,21	0.54	0
11	NAG	G	617	4	14,14,15	0.30	0	17,19,21	0.44	0
11	NAG	G	613	4	14,14,15	0.31	0	17,19,21	0.44	0
11	NAG	G	607	4	14,14,15	0.21	0	17,19,21	0.57	0
11	NAG	G	612	4	14,14,15	0.23	0	17,19,21	0.53	0
11	NAG	B	702	1	14,14,15	0.23	0	17,19,21	0.47	0
11	NAG	G	632	4	14,14,15	0.29	0	17,19,21	0.48	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
11	NAG	D	201	2	-	2/6/23/26	0/1/1/1
12	JYS	G	637	-	-	3/16/30/30	0/4/4/4
11	NAG	G	633	4	-	2/6/23/26	0/1/1/1
11	NAG	G	634	4	-	2/6/23/26	0/1/1/1
11	NAG	G	611	4	-	2/6/23/26	0/1/1/1
11	NAG	B	701	1	-	1/6/23/26	0/1/1/1
11	NAG	G	617	4	-	2/6/23/26	0/1/1/1
11	NAG	G	613	4	-	1/6/23/26	0/1/1/1
11	NAG	G	607	4	-	2/6/23/26	0/1/1/1
11	NAG	G	612	4	-	2/6/23/26	0/1/1/1
11	NAG	B	702	1	-	1/6/23/26	0/1/1/1
11	NAG	G	632	4	-	0/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	637	JYS	C02-C03	16.83	1.57	1.41
12	G	637	JYS	C01-C02	11.93	1.50	1.36
12	G	637	JYS	C05-C04	8.29	1.59	1.43
12	G	637	JYS	C21-C16	8.27	1.53	1.39
12	G	637	JYS	C17-C16	7.97	1.53	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	637	JYS	C01-C02-C03	-5.21	120.43	123.09
12	G	637	JYS	F22-C02-C03	4.75	119.32	117.40
12	G	637	JYS	C07-C08-C09	-3.94	120.36	127.45
12	G	637	JYS	C09-C10-N24	3.05	121.52	118.52
12	G	637	JYS	C11-C12-N25	2.85	116.54	110.44

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

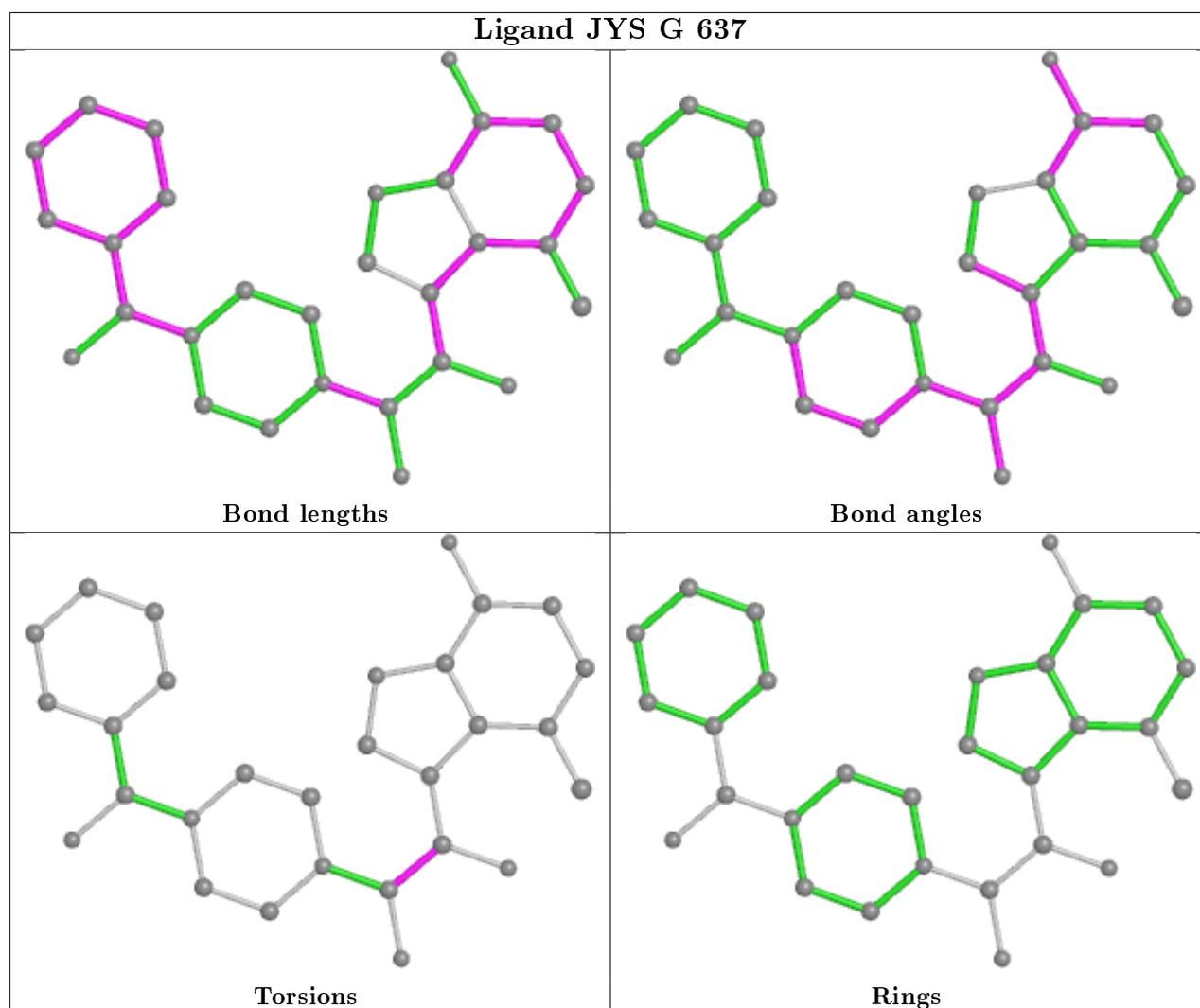
Mol	Chain	Res	Type	Atoms
11	G	634	NAG	O5-C5-C6-O6
11	G	633	NAG	C4-C5-C6-O6
11	G	633	NAG	O5-C5-C6-O6
11	G	611	NAG	C4-C5-C6-O6
11	G	611	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	637	JYS	2	0
11	G	613	NAG	2	0
11	G	612	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	B	133/153 (86%)	-0.19	4 (3%) 50 22	17, 47, 90, 121	0
2	D	128/134 (95%)	0.78	19 (14%) 2 1	46, 91, 133, 146	0
3	E	105/114 (92%)	0.48	7 (6%) 17 5	44, 80, 113, 127	0
4	G	439/481 (91%)	-0.38	11 (2%) 57 29	8, 35, 96, 145	0
5	H	226/244 (92%)	-0.20	3 (1%) 77 51	15, 56, 89, 121	0
6	L	211/217 (97%)	-0.49	2 (0%) 84 63	14, 39, 65, 116	0
All	All	1242/1343 (92%)	-0.15	46 (3%) 41 17	8, 49, 113, 146	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	ALA	7.2
4	G	188	ASN	7.2
2	D	18	VAL	6.5
2	D	65	ASP	5.4
4	G	141	ASP	5.0

### 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](#)

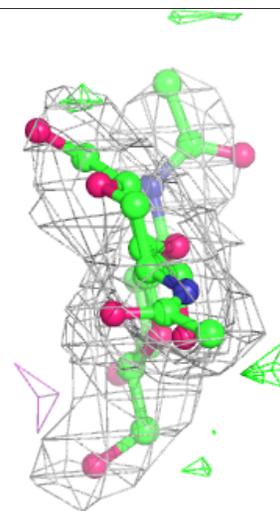
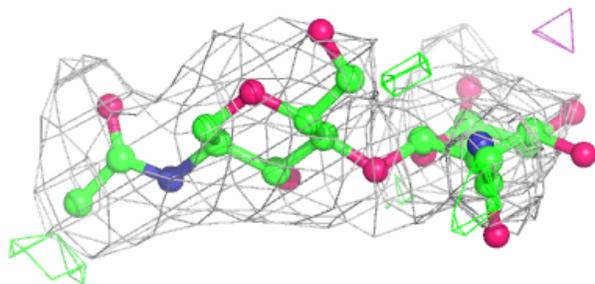
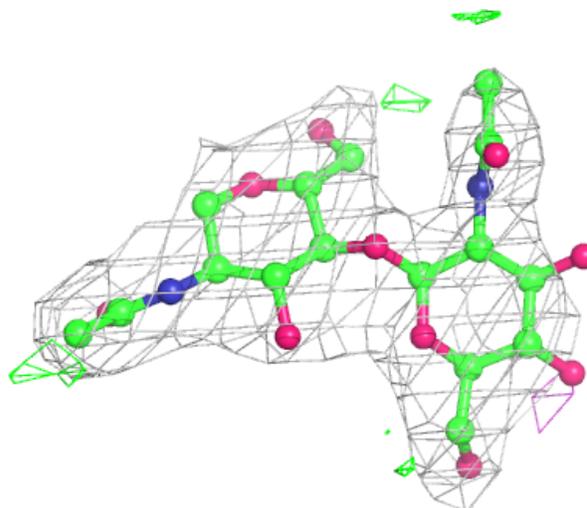
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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
8	BMA	C	3	11/12	0.80	0.34	83,115,135,144	0
9	NAG	I	2	14/15	0.86	0.29	64,89,110,112	0
8	NAG	C	2	14/15	0.88	0.24	83,98,117,125	0
7	MAN	A	5	11/12	0.88	0.28	77,102,109,118	0
10	MAN	K	10	11/12	0.89	0.20	62,71,76,100	0
7	MAN	A	4	11/12	0.89	0.24	78,100,109,109	0
9	NAG	M	2	14/15	0.90	0.28	85,120,146,151	0
8	BMA	F	3	11/12	0.91	0.25	79,98,104,104	0
9	NAG	J	2	14/15	0.91	0.32	73,88,102,110	0
10	MAN	K	9	11/12	0.93	0.32	70,91,101,120	0
10	NAG	K	1	14/15	0.94	0.15	39,58,70,72	0
9	NAG	I	1	14/15	0.94	0.14	35,48,82,83	0
8	NAG	F	2	14/15	0.94	0.12	54,64,79,90	0
10	MAN	K	6	11/12	0.94	0.17	40,46,68,77	0
10	MAN	K	8	11/12	0.95	0.14	38,51,62,89	0
7	MAN	A	6	11/12	0.95	0.12	40,47,65,73	0
9	NAG	M	1	14/15	0.95	0.18	63,85,110,116	0
10	BMA	K	3	11/12	0.96	0.10	28,41,47,55	0
8	NAG	C	1	14/15	0.96	0.12	41,58,76,91	0
7	NAG	A	2	14/15	0.97	0.12	38,51,59,64	0
9	NAG	J	1	14/15	0.97	0.14	19,43,57,71	0
10	MAN	K	7	11/12	0.97	0.13	33,57,66,67	0
10	NAG	K	2	14/15	0.97	0.14	34,46,58,67	0
7	NAG	A	1	14/15	0.97	0.14	22,40,59,61	0
8	NAG	F	1	14/15	0.97	0.13	13,25,40,49	0
10	MAN	K	4	11/12	0.98	0.14	22,37,50,68	0
7	BMA	A	3	11/12	0.98	0.13	41,54,60,78	0
10	MAN	K	5	11/12	0.99	0.12	23,37,49,51	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.

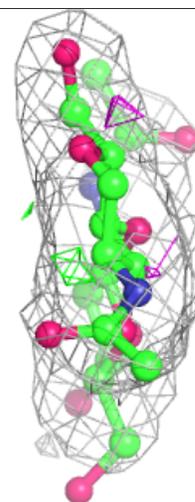
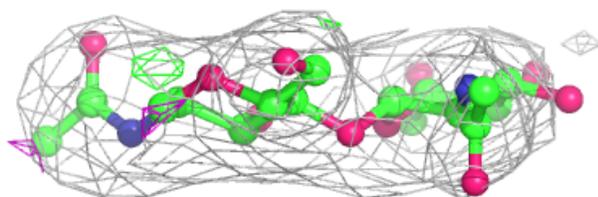
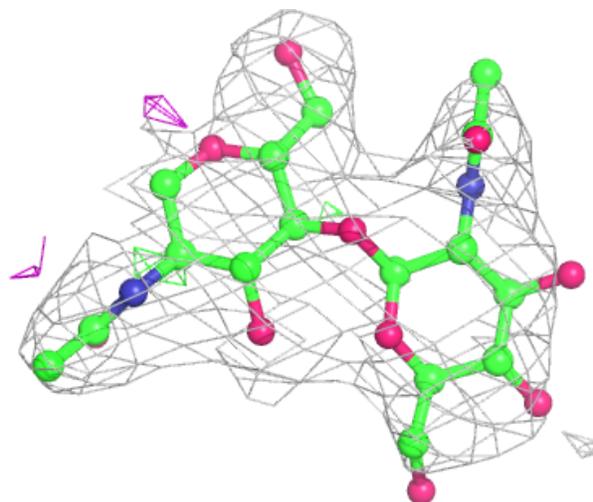
**Electron density around Chain I:**

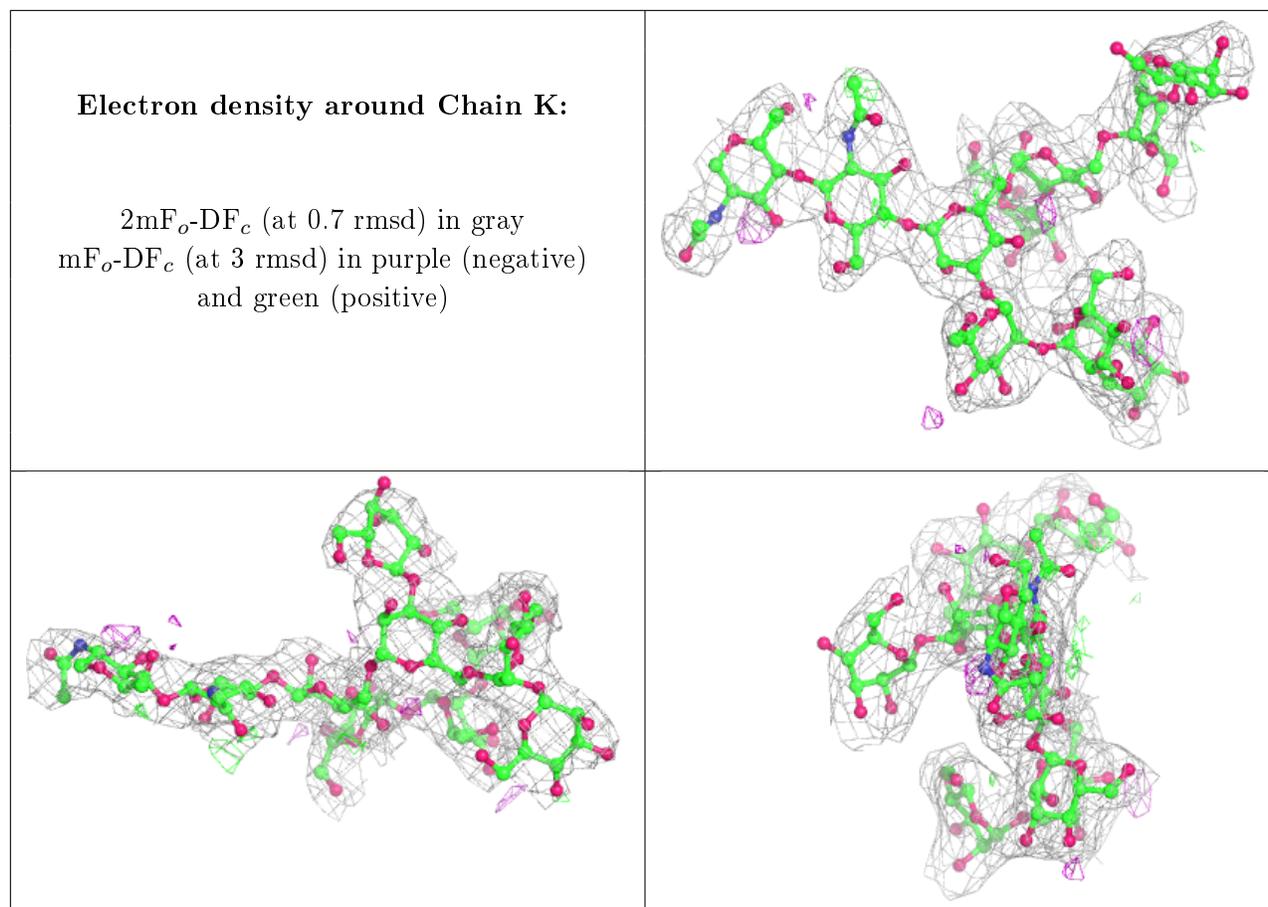
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

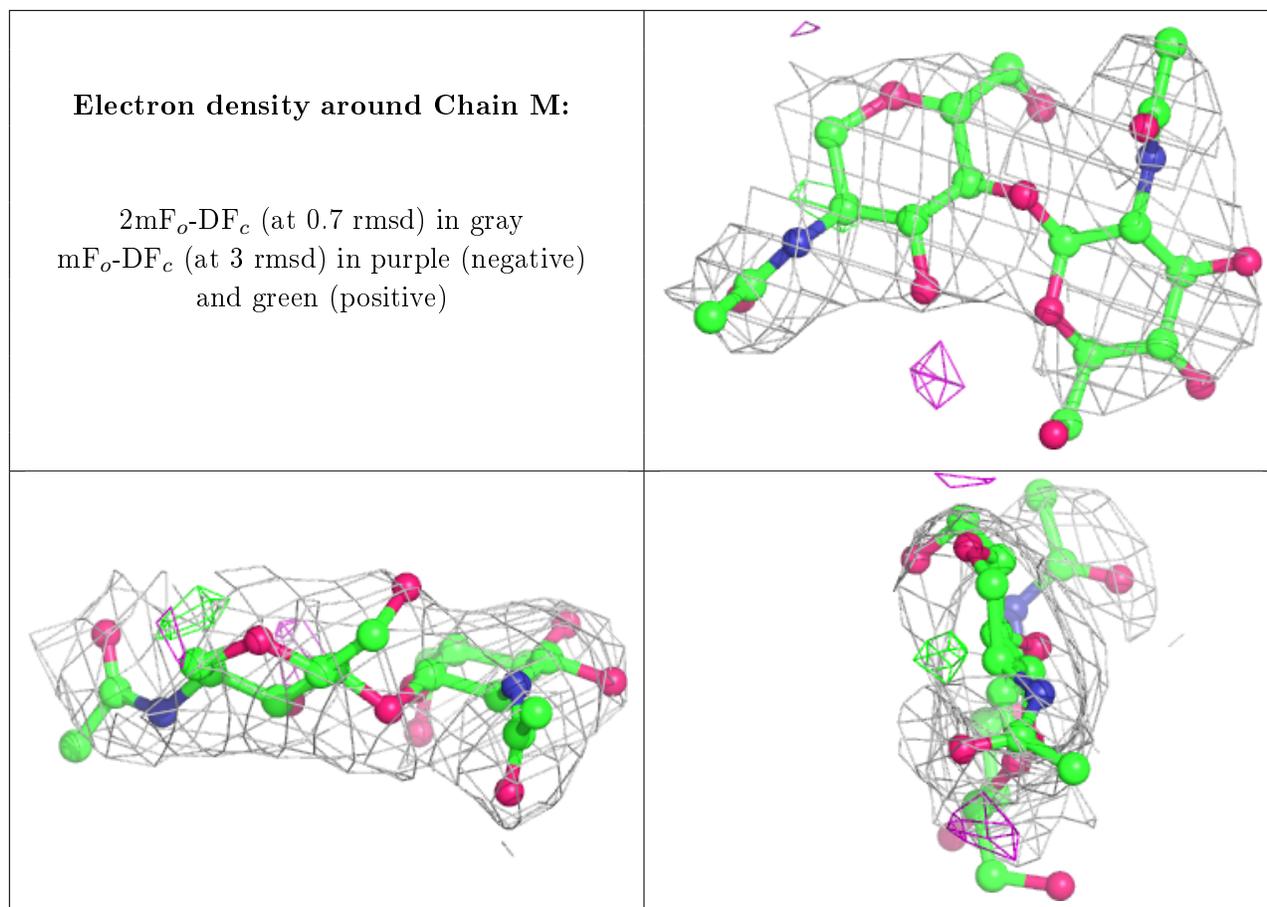


**Electron density around Chain J:**

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





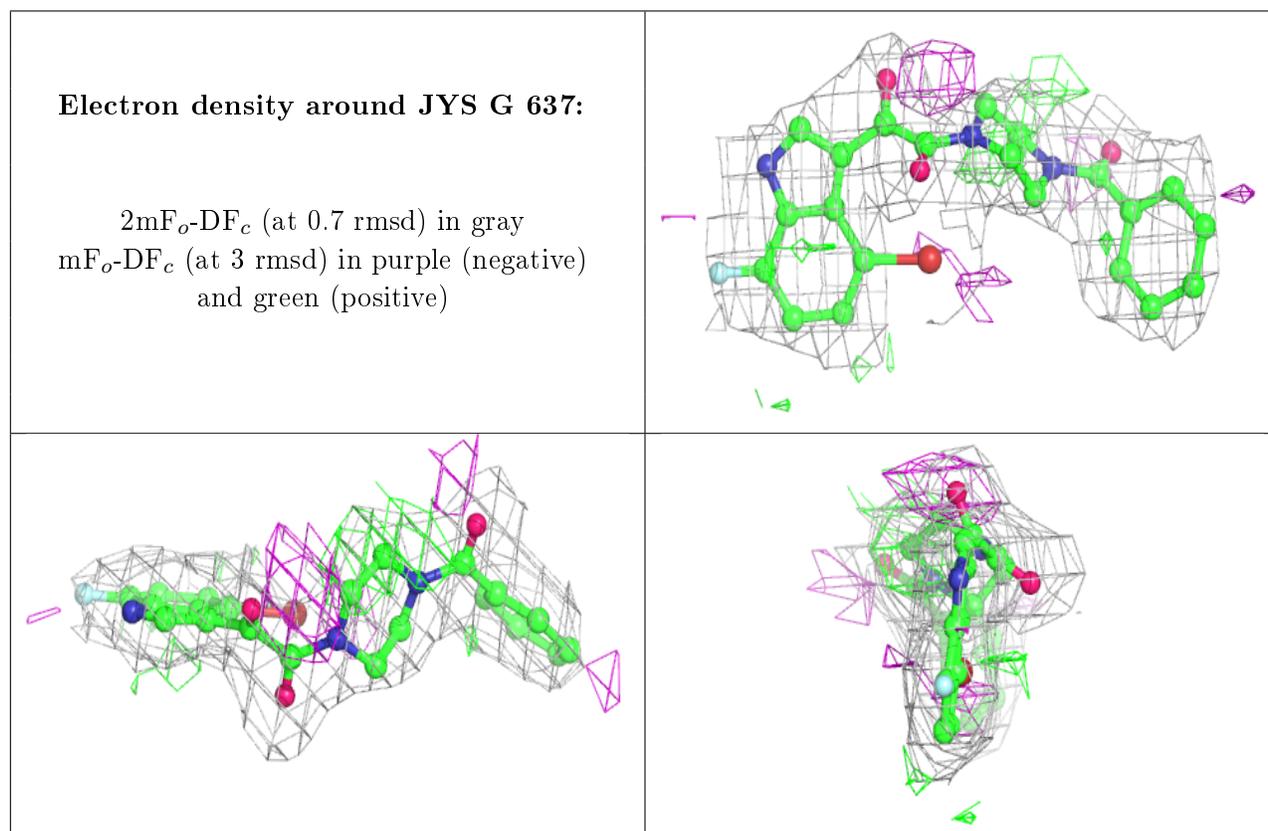


## 6.4 Ligands [i](#)

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
11	NAG	B	702	14/15	0.77	0.46	103,124,132,141	0
11	NAG	G	607	14/15	0.82	0.34	84,118,130,132	0
11	NAG	B	701	14/15	0.85	0.45	78,110,121,122	0
11	NAG	D	201	14/15	0.89	0.34	79,100,116,121	0
11	NAG	G	633	14/15	0.91	0.22	45,64,79,84	0
11	NAG	G	613	14/15	0.91	0.24	55,84,94,96	0
11	NAG	G	612	14/15	0.92	0.18	43,58,76,77	0
11	NAG	G	617	14/15	0.92	0.34	55,85,103,107	0
11	NAG	G	632	14/15	0.93	0.28	62,88,94,98	0
11	NAG	G	611	14/15	0.94	0.17	54,70,81,90	0
11	NAG	G	634	14/15	0.96	0.15	43,51,59,65	0
12	JYS	G	637	29/29	0.97	0.16	11,32,42,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.