



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:13 PM EDT

PDB ID : 7UKT  
Title : Integrin  $\alpha$ IIb $\beta$ 3 complex with BMS4.2  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-04-01  
Resolution : 2.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

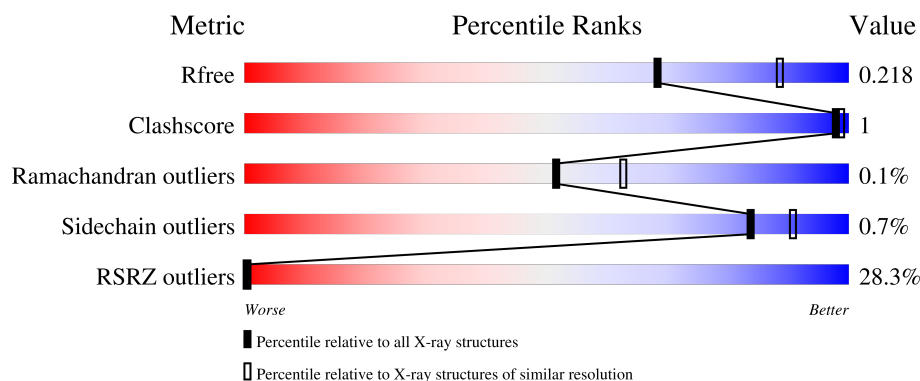
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	457	<div> <div>31%</div> <div>96%</div> </div>
1	C	457	<div> <div>20%</div> <div>96%</div> </div>
2	B	472	<div> <div>26%</div> <div>95%</div> </div>
2	D	472	<div> <div>21%</div> <div>97%</div> </div>
3	E	221	<div> <div>54%</div> <div>95%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

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
13	CL	C	505	-	-	-	X
7	BMA	J	3	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22157 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 Integrin alpha-IIb heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	4	0
			3499	2226	601	664	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	4	0
			3618	2252	617	715	34			
2	D	471	Total	C	N	O	S	3	0	0
			3623	2255	619	715	34			

- Molecule 3 is a protein called 10E5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called 10E5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called 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
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called 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
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	C	4	Total	Ca	0	0
			4	4		

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

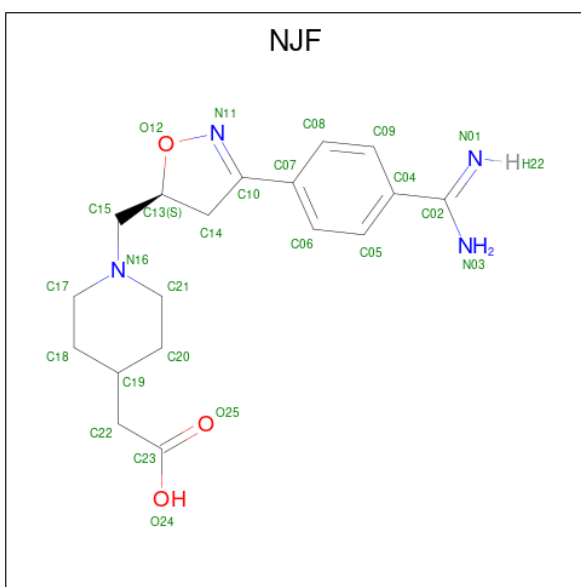
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- 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
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is (1-{[(5S)-3-(4-carbamimidoylphenyl)-4,5-dihydro-1,2-oxazol-5-yl]methyl}piperidin-4-yl)acetic acid (three-letter code: NJF) (formula: C<sub>18</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			25	18	4	3		
12	D	1	Total	C	N	O	0	0
			25	18	4	3		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	2	Total	Cl	0	0
			2	2		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	408	Total	O	0	0
			408	408		
14	B	246	Total	O	0	0
			246	246		
14	C	161	Total	O	0	0
			161	161		
14	D	128	Total	O	0	0
			128	128		
14	E	15	Total	O	0	0
			15	15		
14	F	9	Total	O	0	0
			9	9		

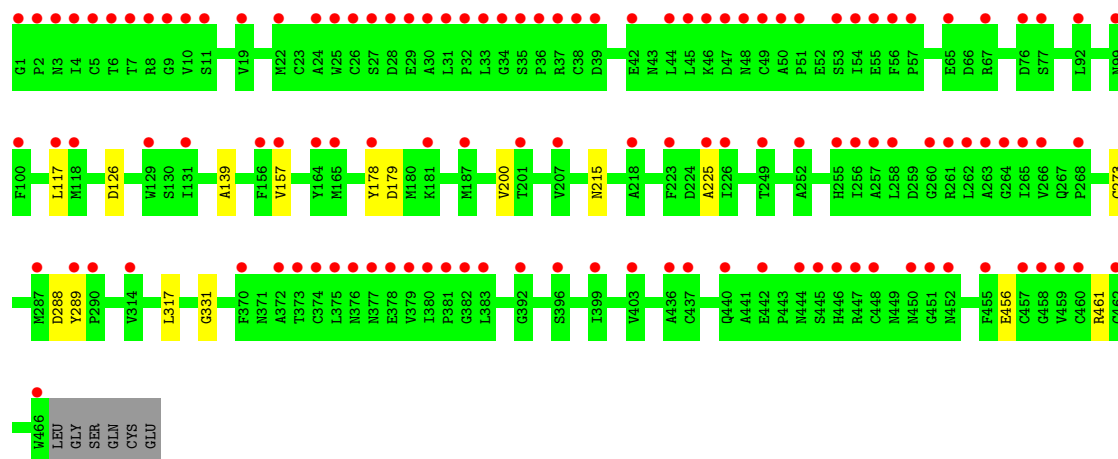
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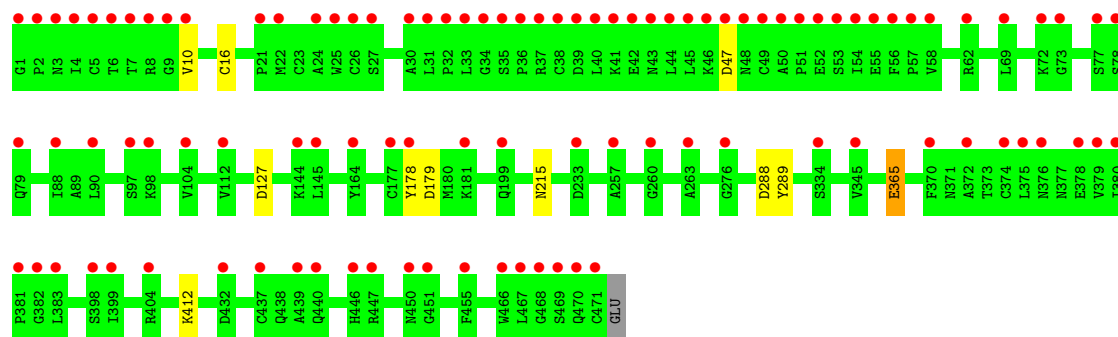
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	39	Total	O	0	0
			39	39		
14	L	56	Total	O	0	0
			56	56		

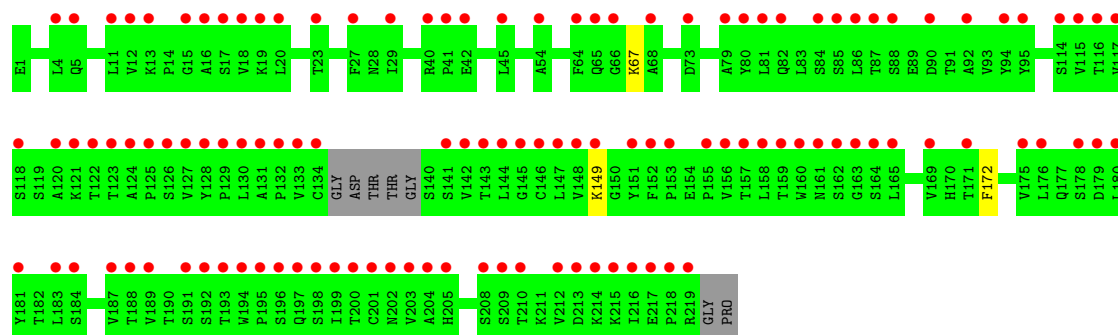




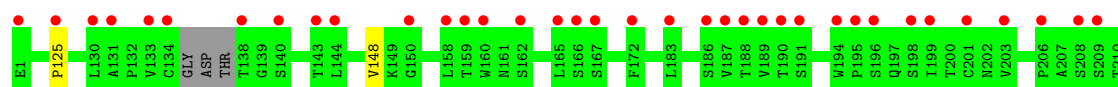
• Molecule 2: Isoform Beta-3C of Integrin beta-3

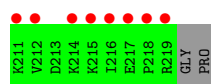


• Molecule 3: 10E5 Fab heavy chain

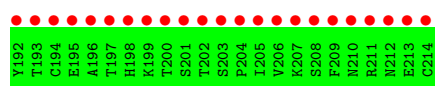
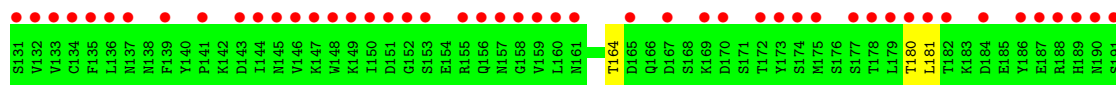
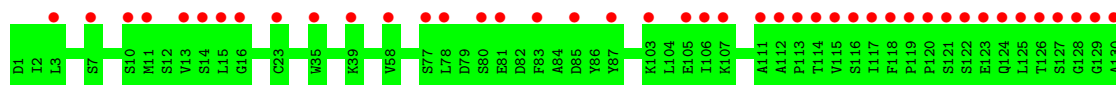


• Molecule 3: 10E5 Fab heavy chain

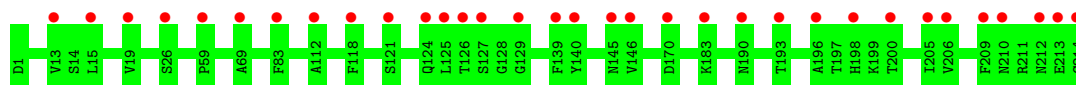




- Molecule 4: 10E5 Fab light chain



- Molecule 4: 10E5 Fab light chain



- Molecule 5: 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



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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

Chain J:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.82Å 144.37Å 105.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.37 49.04 – 2.37	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.04-2.37) 96.7 (49.04-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.194 , 0.218 0.194 , 0.218	Depositor DCC
$R_{free}$ test set	1933 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NJF, BMA, MN, CL, NAG, CA, SO4

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	0.25	0/3608	0.45	0/4918
1	C	0.25	0/3605	0.44	0/4912
2	B	0.24	0/3688	0.43	0/5000
2	D	0.24	0/3690	0.42	0/5003
3	E	0.24	0/1673	0.44	0/2290
3	H	0.24	0/1684	0.44	0/2305
4	F	0.24	0/1673	0.43	0/2269
4	L	0.24	0/1673	0.44	0/2269
All	All	0.24	0/21294	0.44	0/28966

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3499	0	3345	6	0
1	C	3502	0	3334	5	0
2	B	3618	0	3533	9	0
2	D	3623	0	3540	4	0
3	E	1631	0	1590	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	2	0
4	F	1637	0	1553	2	0
4	L	1637	0	1553	0	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	20	0	0	0	0
8	C	20	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	25	0	0	1	0
12	D	25	0	0	1	0
13	C	2	0	0	0	0
14	A	408	0	0	1	0
14	B	246	0	0	2	0
14	C	161	0	0	1	0
14	D	128	0	0	0	0
14	E	15	0	0	0	0
14	F	9	0	0	0	0
14	H	39	0	0	2	0
14	L	56	0	0	0	0
All	All	22157	0	20219	28	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 (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:CYS:SG	14:B:2262:HOH:O	2.57	0.59
2:B:331:GLY:N	14:B:2103:HOH:O	2.34	0.58
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.37	0.58
3:H:125:PRO:HB2	14:H:314:HOH:O	2.06	0.55
2:B:126[A]:ASP:OD1	2:B:126[A]:ASP:N	2.40	0.55
1:C:1:LEU:N	14:C:605:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.95	0.49
1:C:107:CYS:HA	1:C:130:CYS:HA	1.94	0.49
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.46	0.49
1:A:225:SER:O	12:B:2005:NJF:N03	2.47	0.47
2:D:288:ASP:OD1	2:D:289:TYR:N	2.45	0.47
2:B:288:ASP:OD1	2:B:289:TYR:N	2.50	0.45
1:A:107:CYS:HA	1:A:130:CYS:HA	1.97	0.45
1:C:225:SER:O	12:D:2005:NJF:N03	2.49	0.45
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.00	0.44
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.32	0.44
2:D:10:VAL:HG21	2:D:16:CYS:HB2	1.99	0.44
2:D:178:TYR:CG	2:D:179:ASP:N	2.86	0.43
1:C:224:ASP:OD1	1:C:225:SER:N	2.46	0.42
3:H:148:VAL:HA	14:H:314:HOH:O	2.19	0.42
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.55	0.42
1:A:9:THR:HB	1:A:447:VAL:HB	2.00	0.42
2:B:178:TYR:CG	2:B:179:ASP:N	2.88	0.42
3:E:67:LYS:HE3	3:E:67:LYS:HB2	1.95	0.41
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.03	0.41
1:C:377:ALA:HB2	1:C:421:LEU:HD11	2.03	0.40
1:A:41:ARG:NH2	14:A:626:HOH:O	2.53	0.40
1:A:230:TYR:OH	1:A:279:ARG:NH2	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/457 (100%)	442 (97%)	14 (3%)	0	100	100
1	C	455/457 (100%)	438 (96%)	16 (4%)	1 (0%)	47	56
2	B	468/472 (99%)	455 (97%)	12 (3%)	1 (0%)	47	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	469/472 (99%)	449 (96%)	20 (4%)	0	100	100
3	E	210/221 (95%)	194 (92%)	16 (8%)	0	100	100
3	H	212/221 (96%)	201 (95%)	11 (5%)	0	100	100
4	F	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	2694/2728 (99%)	2583 (96%)	109 (4%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	GLU
2	B	157	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/364 (100%)	361 (99%)	5 (1%)	67	78
1	C	365/364 (100%)	359 (98%)	6 (2%)	62	75
2	B	416/417 (100%)	415 (100%)	1 (0%)	93	97
2	D	416/417 (100%)	412 (99%)	4 (1%)	76	85
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	94
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2312/2318 (100%)	2295 (99%)	17 (1%)	84	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU

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Mol	Chain	Res	Type
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
1	C	1	LEU
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	270	LEU
1	C	288	TYR
2	D	47	ASP
2	D	127	ASP
2	D	215	ASN
2	D	365	GLU
4	F	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
2	B	301	GLN
2	D	15	GLN
2	D	301	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

13 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
5	NAG	G	1	5,2	14,14,15	0.36	0	17,19,21	0.54	0
5	NAG	G	2	5	14,14,15	0.18	0	17,19,21	0.44	0
5	BMA	G	3	5	11,11,12	0.71	0	15,15,17	0.81	0
5	MAN	G	4	5	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
5	MAN	G	5	5	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.38	0	17,19,21	0.43	0
6	NAG	I	2	6	14,14,15	0.28	0	17,19,21	0.39	0
7	NAG	J	1	7,2	14,14,15	0.29	0	17,19,21	0.48	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.41	0
7	BMA	J	3	7	11,11,12	0.59	0	15,15,17	0.87	0
7	MAN	J	4	7	11,11,12	0.69	0	15,15,17	1.08	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.16	0	17,19,21	0.48	0
6	NAG	K	2	6	14,14,15	0.23	0	17,19,21	0.40	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
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
7	NAG	J	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	4	MAN	C1-O5-C5	2.79	115.97	112.19
5	G	5	MAN	C1-O5-C5	2.70	115.85	112.19
7	J	4	MAN	O2-C2-C3	-2.37	105.39	110.14
5	G	4	MAN	C1-O5-C5	2.36	115.38	112.19
5	G	4	MAN	O2-C2-C3	-2.24	105.66	110.14
5	G	5	MAN	O2-C2-C3	-2.17	105.78	110.14

There are no chirality outliers.

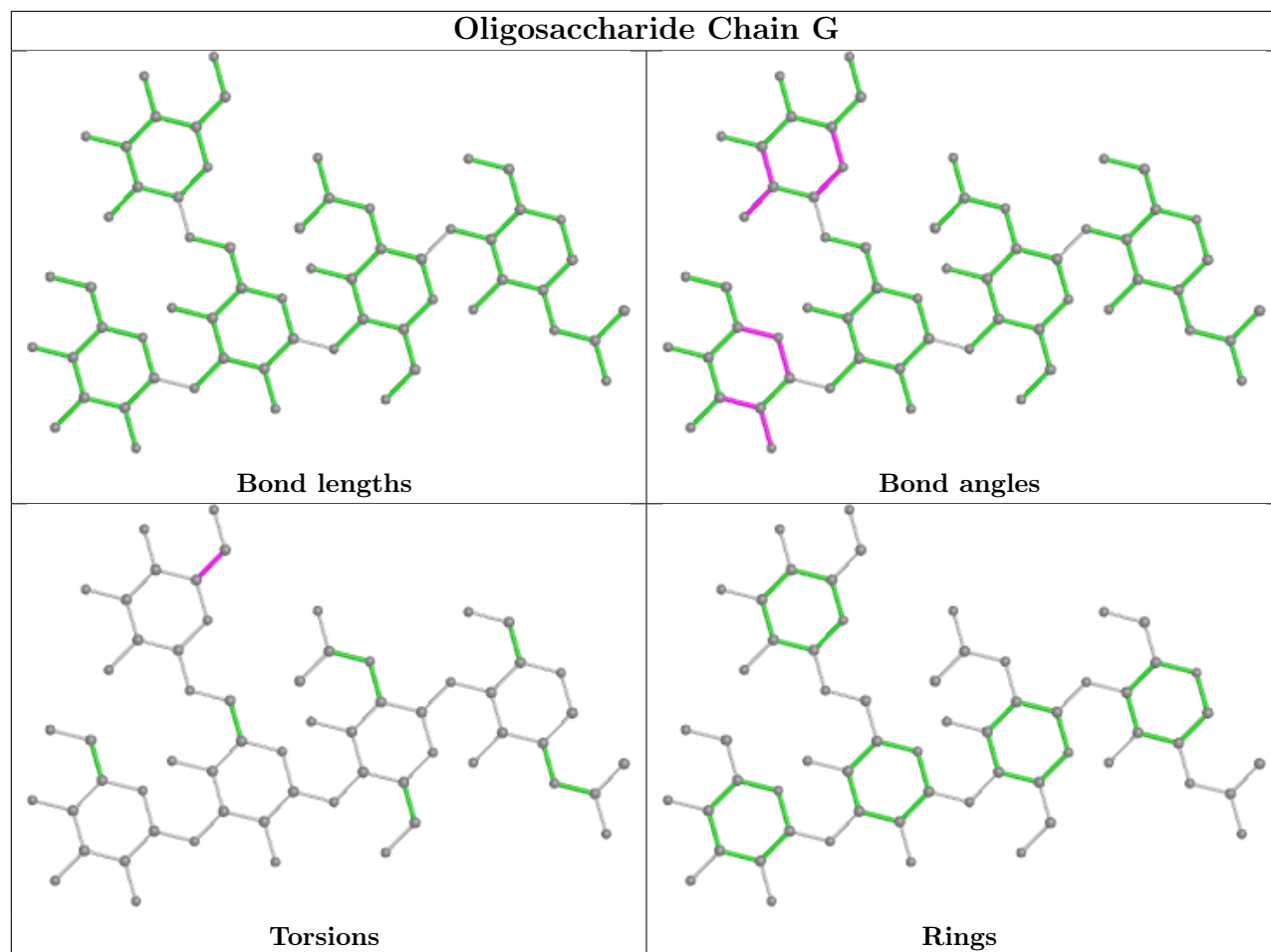
All (11) torsion outliers are listed below:

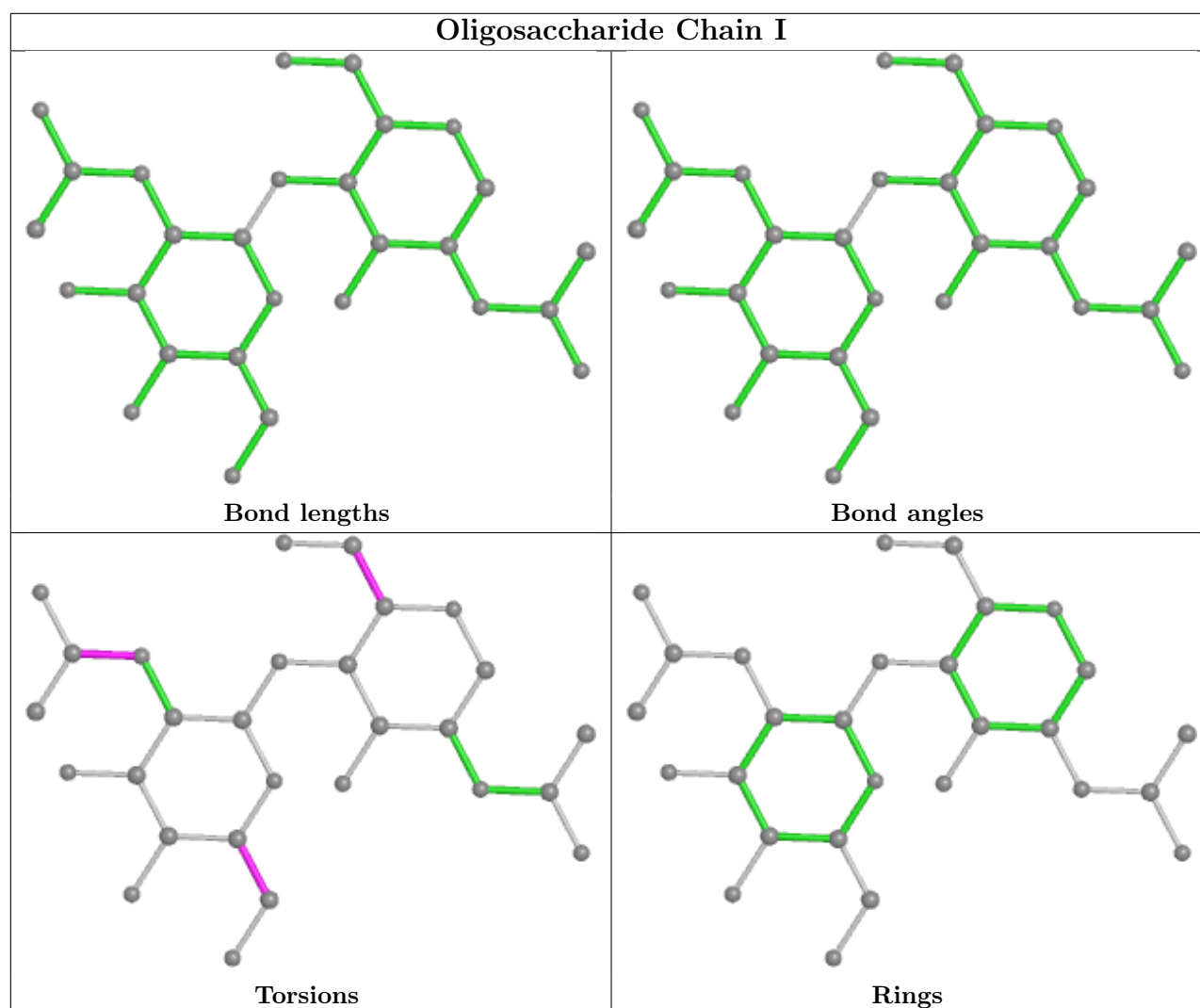
Mol	Chain	Res	Type	Atoms
7	J	4	MAN	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

There are no ring outliers.

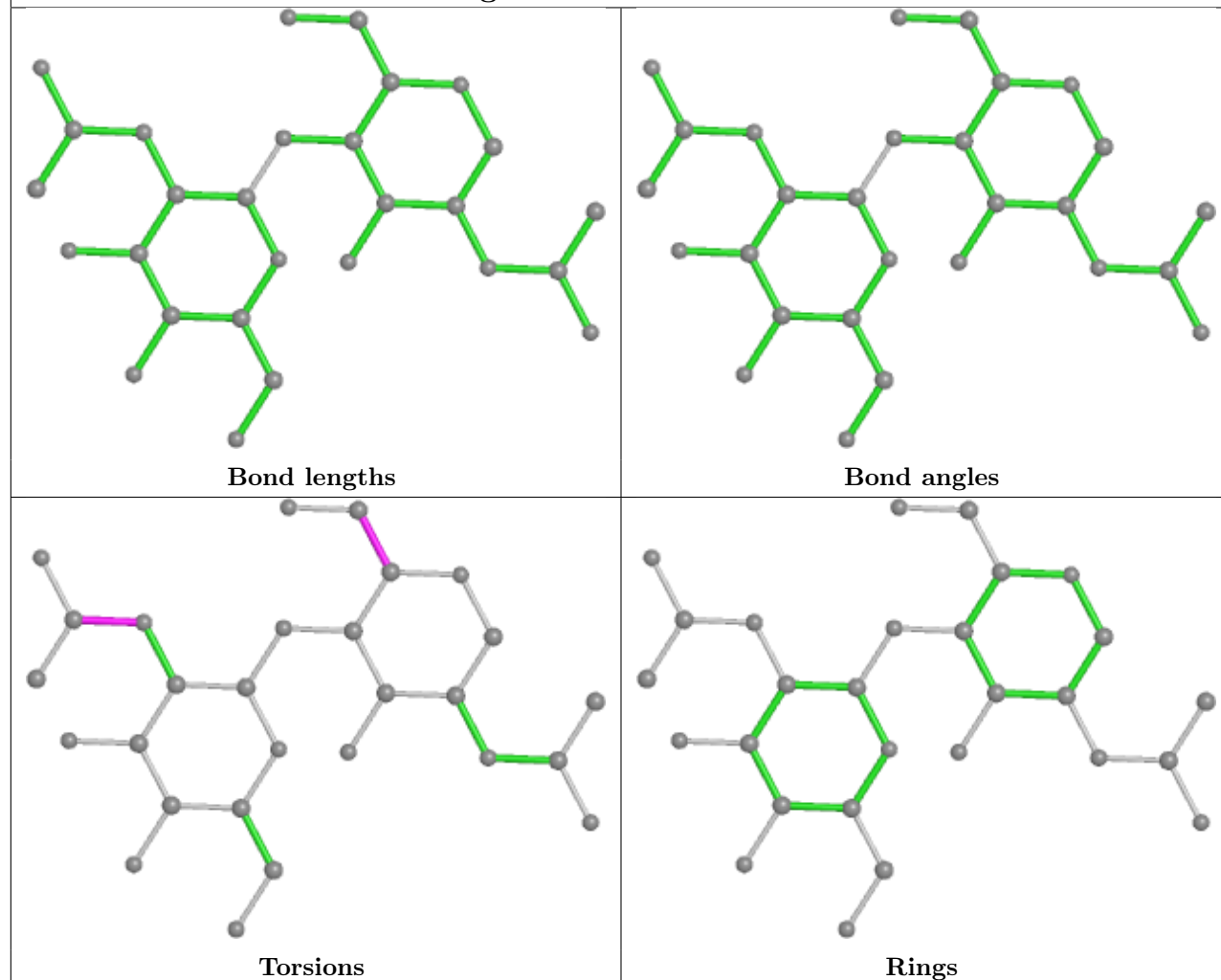
No monomer is involved in short contacts.

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

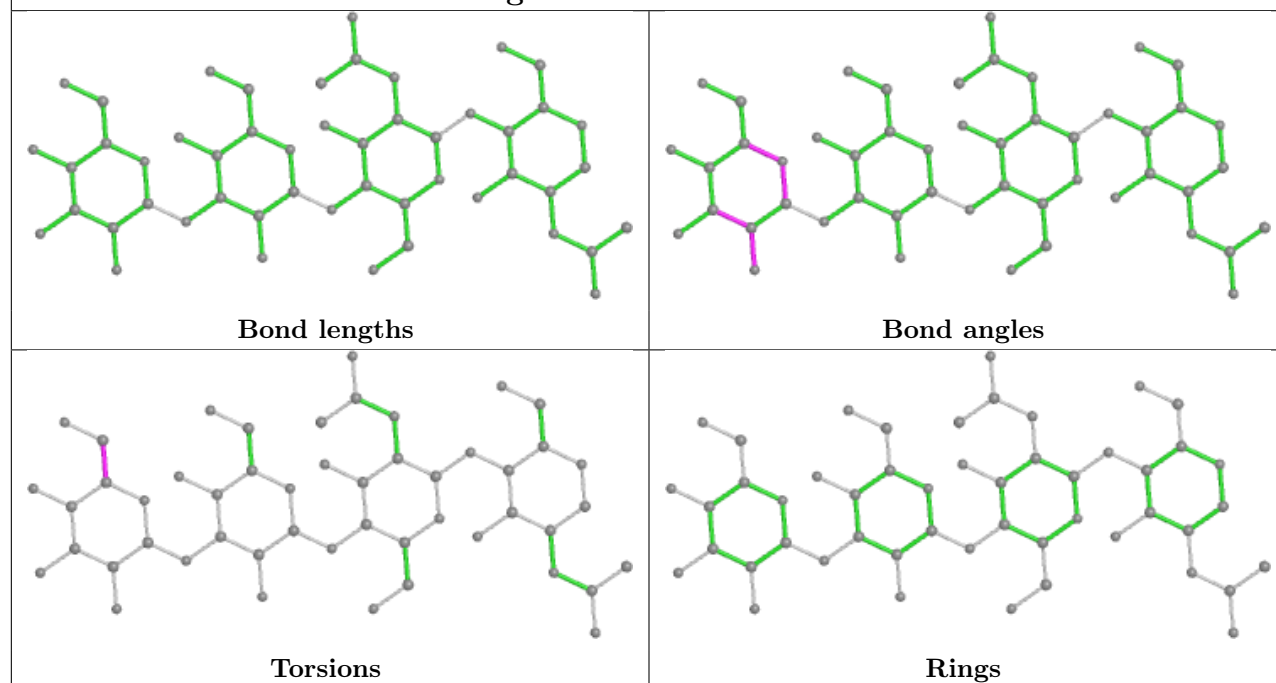




## Oligosaccharide Chain K



## Oligosaccharide Chain J





## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
12	NJF	B	2005	10	27,27,27	1.02	1 (3%)	30,37,37	0.97	1 (3%)
11	NAG	D	2004	2	14,14,15	0.35	0	17,19,21	0.50	0
11	NAG	B	2004	2	14,14,15	0.53	0	17,19,21	0.53	0
12	NJF	D	2005	10	27,27,27	1.02	1 (3%)	30,37,37	0.91	0
8	SO4	C	510	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	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
12	NJF	D	2005	10	-	6/16/35/35	0/3/3/3
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	NJF	B	2005	10	-	4/16/35/35	0/3/3/3
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	NJF	O12-C13	-2.36	1.43	1.46
12	D	2005	NJF	O12-C13	-2.28	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2005	NJF	O12-C13-C14	-2.06	102.41	104.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

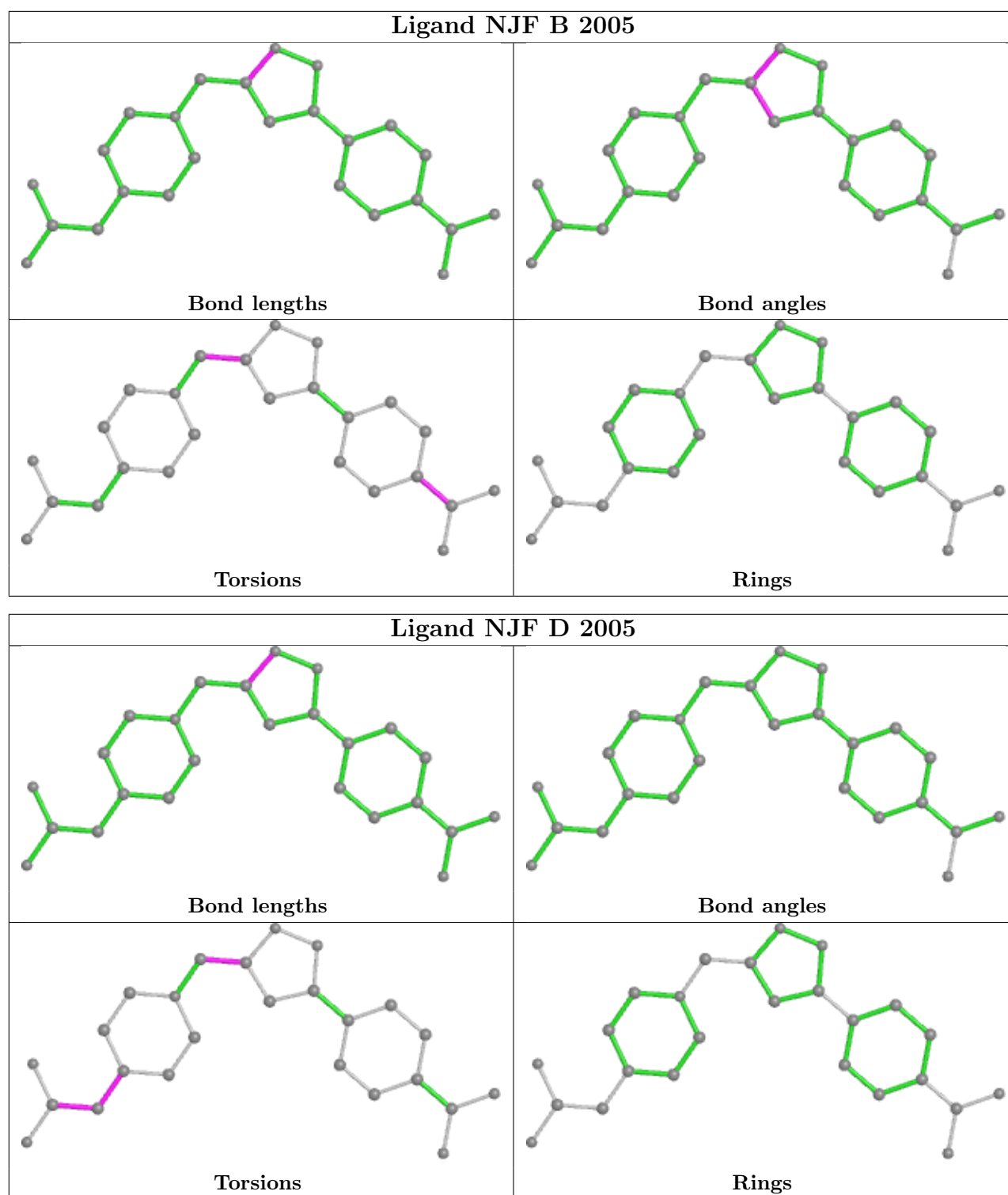
Mol	Chain	Res	Type	Atoms
12	B	2005	NJF	N03-C02-C04-C05
12	B	2005	NJF	N03-C02-C04-C09
12	B	2005	NJF	C14-C13-C15-N16
12	B	2005	NJF	O12-C13-C15-N16
12	D	2005	NJF	O12-C13-C15-N16
12	D	2005	NJF	C18-C19-C22-C23
12	D	2005	NJF	C20-C19-C22-C23
11	D	2004	NAG	O5-C5-C6-O6
11	D	2004	NAG	C4-C5-C6-O6
12	D	2005	NJF	C14-C13-C15-N16
12	D	2005	NJF	C19-C22-C23-O24
12	D	2005	NJF	C19-C22-C23-O25

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	2005	NJF	1	0
12	D	2005	NJF	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	454/457 (99%)	1.49	142 (31%) <b>0</b> <b>0</b>	46, 61, 98, 134	0
1	C	453/457 (99%)	1.20	91 (20%) <b>1</b> <b>2</b>	55, 83, 122, 159	0
2	B	466/472 (98%)	1.61	121 (25%) <b>0</b> <b>0</b>	45, 93, 176, 215	1 (0%)
2	D	471/472 (99%)	1.37	101 (21%) <b>0</b> <b>1</b>	61, 108, 160, 193	1 (0%)
3	E	214/221 (96%)	3.15	119 (55%) <b>0</b> <b>0</b>	97, 151, 221, 242	0
3	H	216/221 (97%)	1.15	44 (20%) <b>1</b> <b>1</b>	71, 116, 173, 187	0
4	F	214/214 (100%)	3.13	114 (53%) <b>0</b> <b>0</b>	94, 151, 224, 245	0
4	L	214/214 (100%)	0.96	33 (15%) <b>2</b> <b>3</b>	71, 106, 136, 185	0
All	All	2702/2728 (99%)	1.63	765 (28%) <b>0</b> <b>0</b>	45, 99, 189, 245	2 (0%)

All (765) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	14.0
3	E	216	ILE	13.7
4	F	125	LEU	12.7
4	F	181	LEU	12.2
3	E	199	ILE	12.0
4	F	115	VAL	11.7
2	B	77	SER	11.6
4	F	132	VAL	11.1
4	F	193	THR	11.0
2	B	33	LEU	11.0
3	E	160	TRP	10.8
3	E	131	ALA	10.4
2	D	8	ARG	10.2
3	E	219	ARG	10.2
3	E	194	TRP	10.0
4	F	150	ILE	10.0

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Mol	Chain	Res	Type	RSRZ
4	F	148	TRP	9.9
3	E	134	CYS	9.8
4	F	126	THR	9.7
3	E	142	VAL	9.5
3	E	215	LYS	9.4
4	F	209	PHE	9.2
4	F	214	CYS	9.2
2	D	469	SER	8.9
4	F	118	PHE	8.8
2	B	4	ILE	8.8
3	E	200	THR	8.7
4	F	206	VAL	8.7
3	E	133	VAL	8.4
4	F	136	LEU	8.4
4	F	117	ILE	8.3
2	B	49	CYS	8.3
2	B	34	GLY	8.2
4	L	214	CYS	8.1
3	E	128	TYR	8.0
2	D	471	CYS	8.0
4	F	180	THR	8.0
2	B	51	PRO	7.9
3	E	201	CYS	7.9
3	E	217	GLU	7.9
3	E	132	PRO	7.8
3	E	144	LEU	7.8
2	B	10	VAL	7.7
4	F	194	CYS	7.7
4	F	147	LYS	7.6
3	E	143	THR	7.6
4	F	192	TYR	7.6
4	F	179	LEU	7.5
4	F	160	LEU	7.5
3	H	216	ILE	7.5
4	F	119	PRO	7.5
3	E	183	LEU	7.4
2	B	36	PRO	7.3
4	F	120	PRO	7.1
4	F	130	ALA	7.0
4	F	122	SER	7.0
4	F	190	ASN	7.0
4	F	186	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
4	F	182	THR	6.9
2	B	50	ALA	6.9
2	D	33	LEU	6.9
2	D	44	LEU	6.9
2	B	26	CYS	6.8
2	D	32	PRO	6.8
4	F	135	PHE	6.8
4	F	202	THR	6.8
3	E	195	PRO	6.8
2	D	2	PRO	6.8
2	D	375	LEU	6.7
3	E	20	LEU	6.7
3	E	169	VAL	6.7
3	E	129	PRO	6.7
4	F	144	ILE	6.6
2	B	445	SER	6.6
4	F	205	ILE	6.6
3	E	123	THR	6.6
4	F	204	PRO	6.5
3	E	196	SER	6.5
3	E	17	SER	6.4
2	B	44	LEU	6.4
2	B	1	GLY	6.4
3	E	130	LEU	6.4
2	B	466	TRP	6.3
3	E	127	VAL	6.3
3	E	156	VAL	6.3
4	F	197	THR	6.3
2	B	375	LEU	6.3
4	F	191	SER	6.3
3	E	12	VAL	6.3
3	E	165	LEU	6.3
4	F	152	GLY	6.3
2	B	450	ASN	6.2
2	B	54	ILE	6.2
4	F	127	SER	6.2
4	F	208	SER	6.2
2	D	376	ASN	6.1
3	E	198	SER	6.1
3	E	189	VAL	6.1
4	F	159	VAL	6.1
2	D	380	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
4	F	14	SER	5.9
3	E	180	LEU	5.9
3	H	217	GLU	5.9
1	A	337	PRO	5.8
2	D	378	GLU	5.8
2	B	8	ARG	5.8
2	B	31	LEU	5.8
3	E	11	LEU	5.8
2	D	52	GLU	5.8
4	F	174	SER	5.8
4	F	134	CYS	5.7
3	H	203	VAL	5.7
3	E	191	SER	5.7
2	D	36	PRO	5.6
4	F	145	ASN	5.6
2	B	2	PRO	5.6
3	E	116	THR	5.6
3	E	161	ASN	5.5
4	F	195	GLU	5.5
2	D	35	SER	5.5
2	D	48	ASN	5.5
4	F	156	GLN	5.5
4	F	133	VAL	5.4
4	F	155	ARG	5.4
4	F	178	THR	5.4
4	F	158	GLY	5.4
3	E	203	VAL	5.4
2	D	178	TYR	5.3
4	F	129	GLY	5.3
3	E	117	VAL	5.3
3	H	189	VAL	5.3
3	E	124	ALA	5.3
2	B	38	CYS	5.3
3	H	134	CYS	5.3
3	E	218	PRO	5.3
2	D	1	GLY	5.2
4	F	113	PRO	5.2
3	E	86	LEU	5.2
3	H	211	LYS	5.2
2	B	48	ASN	5.2
3	E	176	LEU	5.2
2	D	181	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
4	F	213	GLU	5.2
2	B	30	ALA	5.2
2	D	54	ILE	5.2
3	E	122	THR	5.1
2	B	451	GLY	5.1
2	D	382	GLY	5.1
2	B	381	PRO	5.1
2	D	46	LYS	5.1
4	F	201	SER	5.0
3	E	126	SER	5.0
4	F	116	SER	5.0
1	A	454	VAL	4.9
2	D	398	SER	4.9
3	E	204	ALA	4.9
4	F	173	TYR	4.9
2	B	380	ILE	4.9
3	H	133	VAL	4.9
3	E	147	LEU	4.9
4	F	210	ASN	4.9
1	C	337	PRO	4.8
3	H	201	CYS	4.8
3	E	181	TYR	4.8
2	B	27	SER	4.8
3	E	214	LYS	4.8
4	F	149	LYS	4.8
2	D	73	GLY	4.8
3	E	193	THR	4.7
3	E	179	ASP	4.7
2	B	45	LEU	4.7
2	B	372	ALA	4.7
2	B	28	ASP	4.7
4	F	83	PHE	4.7
2	B	37	ARG	4.7
2	B	458	GLY	4.7
2	B	39	ASP	4.6
3	E	175	VAL	4.6
2	D	4	ILE	4.6
4	F	212	ASN	4.6
4	F	207	LYS	4.6
2	D	399	ILE	4.5
2	D	9	GLY	4.5
4	F	146	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	51	PRO	4.5
4	F	200	THR	4.5
2	D	10	VAL	4.5
2	B	29	GLU	4.5
3	E	16	ALA	4.4
4	F	157	ASN	4.4
2	B	460	CYS	4.4
2	B	76	ASP	4.4
4	F	124	GLN	4.4
4	F	187	GLU	4.4
2	B	382	GLY	4.4
4	F	151	ASP	4.4
3	E	202	ASN	4.4
2	B	57	PRO	4.4
4	F	203	SER	4.4
3	E	115	VAL	4.3
2	B	455	PHE	4.3
3	E	145	GLY	4.3
2	D	42	GLU	4.3
2	D	468	GLY	4.3
2	D	404	ARG	4.3
3	H	219	ARG	4.2
4	F	121	SER	4.2
3	E	148	VAL	4.2
2	B	22	MET	4.2
2	B	46	LYS	4.2
2	B	35	SER	4.2
4	F	153	SER	4.2
4	F	13	VAL	4.2
3	E	68	ALA	4.2
4	F	189	HIS	4.2
3	E	213	ASP	4.2
3	E	149	LYS	4.1
3	E	88	SER	4.1
2	D	58	VAL	4.1
3	E	18	VAL	4.1
2	D	55	GLU	4.1
2	D	3	ASN	4.1
3	E	4	LEU	4.1
2	B	459	VAL	4.1
2	D	22	MET	4.1
4	F	15	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
3	H	160	TRP	4.1
3	H	166	SER	4.1
3	E	162	SER	4.1
3	E	205	HIS	4.0
4	F	77	SER	4.0
3	E	151	TYR	4.0
1	A	421	LEU	4.0
2	D	372	ALA	3.9
2	D	39	ASP	3.9
1	A	407	LEU	3.9
2	B	373	THR	3.9
2	D	383	LEU	3.9
3	E	80	TYR	3.9
2	D	49	CYS	3.9
4	F	78	LEU	3.9
1	A	436	ILE	3.9
4	F	106	ILE	3.9
3	E	5	GLN	3.9
2	B	370	PHE	3.9
2	D	450	ASN	3.9
3	E	192	SER	3.9
2	B	32	PRO	3.8
2	D	437	CYS	3.8
1	A	358	SER	3.8
1	C	340	LEU	3.8
2	B	377	ASN	3.8
2	D	27	SER	3.8
3	H	131	ALA	3.8
2	B	55	GLU	3.8
2	D	466	TRP	3.8
3	E	94	TYR	3.8
3	E	164	SER	3.8
1	A	171	PHE	3.8
4	F	211	ARG	3.8
2	D	26	CYS	3.8
4	F	196	ALA	3.8
2	B	446	HIS	3.8
4	L	205	ILE	3.7
2	D	451	GLY	3.7
1	C	303	ARG	3.7
1	C	320	ARG	3.7
4	L	125	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	42	GLU	3.7
4	F	111	ALA	3.7
2	B	379	VAL	3.7
1	A	319	ASP	3.7
2	B	25	TRP	3.7
4	L	212	ASN	3.6
3	E	114	SER	3.6
2	B	378	GLU	3.6
1	A	183	LEU	3.6
2	B	383	LEU	3.6
2	D	38	CYS	3.6
3	E	82	GLN	3.6
1	C	244	PHE	3.6
3	E	152	PHE	3.6
2	B	376	ASN	3.6
3	E	19	LYS	3.6
1	A	338	HIS	3.6
2	B	24	ALA	3.6
2	B	374	CYS	3.6
2	D	470	GLN	3.6
2	D	40	LEU	3.6
1	A	235	TRP	3.6
1	A	339	ALA	3.6
3	H	195	PRO	3.6
3	E	13	LYS	3.6
4	F	131	SER	3.6
3	E	79	ALA	3.5
3	E	157	THR	3.6
3	H	188	THR	3.6
4	F	10	SER	3.5
3	H	140	SER	3.5
1	A	23	LEU	3.5
2	B	462	CYS	3.5
2	B	436	ALA	3.5
3	H	130	LEU	3.5
1	A	377	ALA	3.5
1	C	130	CYS	3.5
2	B	53	SER	3.5
3	E	66	GLY	3.4
4	F	161	ASN	3.4
4	L	127	SER	3.4
2	B	457	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	146	CYS	3.4
2	D	53	SER	3.4
3	E	118	SER	3.4
1	A	169	ALA	3.4
3	H	194	TRP	3.4
3	E	163	GLY	3.4
2	B	262	LEU	3.4
3	H	158	LEU	3.4
2	B	9	GLY	3.4
4	L	129	GLY	3.4
3	H	167	SER	3.4
4	L	13	VAL	3.3
1	C	129	SER	3.3
1	A	185	ALA	3.3
4	F	85	ASP	3.3
1	A	258	PRO	3.3
1	C	109	PRO	3.3
4	F	177	SER	3.3
1	C	196	ALA	3.3
1	C	338	HIS	3.3
3	H	165	LEU	3.3
2	B	437	CYS	3.3
4	F	103	LYS	3.3
4	F	184	ASP	3.3
1	A	389	VAL	3.3
4	F	128	GLY	3.2
1	C	183	LEU	3.2
2	D	79	GLN	3.2
3	H	209	SER	3.2
3	H	190	THR	3.2
1	C	453	VAL	3.2
1	A	186	PRO	3.2
3	H	199	ILE	3.2
3	E	81	LEU	3.2
1	A	130	CYS	3.2
3	E	84	SER	3.2
3	H	212	VAL	3.1
4	F	170	ASP	3.1
2	D	90	LEU	3.1
3	E	158	LEU	3.1
3	E	197	GLN	3.1
1	A	21	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	131	PHE	3.1
2	D	57	PRO	3.1
2	B	5	CYS	3.1
2	B	265	ILE	3.1
2	B	178	TYR	3.1
1	A	193	GLY	3.1
1	A	167	CYS	3.1
1	A	192	LEU	3.1
2	D	21	PRO	3.1
1	A	146	CYS	3.1
1	A	336	GLY	3.1
2	B	56	PHE	3.1
2	D	276	GLY	3.1
2	B	448	CYS	3.1
1	C	171	PHE	3.1
1	A	109	PRO	3.0
1	A	95	ALA	3.0
2	B	257	ALA	3.0
3	H	187	VAL	3.0
4	F	137	ASN	3.0
1	A	184	GLY	3.0
1	A	194	LEU	3.0
4	F	175	MET	3.0
3	E	65	GLN	3.0
1	A	419	PHE	3.0
2	D	56	PHE	3.0
3	E	85	SER	3.0
1	A	237	TYR	3.0
3	H	206	PRO	3.0
1	A	359	ALA	3.0
4	F	107	LYS	3.0
1	A	410	PRO	3.0
3	E	153	PRO	3.0
2	D	69	LEU	3.0
4	L	210	ASN	3.0
1	A	35	ILE	3.0
1	A	20	GLY	3.0
1	A	387	GLY	3.0
1	C	186	PRO	3.0
1	C	107	CYS	3.0
2	D	374	CYS	3.0
2	B	287	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	31	LEU	2.9
1	C	167	CYS	2.9
4	F	139	PHE	2.9
1	A	129	SER	2.9
2	B	47	ASP	2.9
1	A	170	GLY	2.9
2	B	444	ASN	2.9
2	B	11	SER	2.9
2	D	97	SER	2.9
3	E	45	LEU	2.9
3	E	209	SER	2.9
1	C	213	LEU	2.9
2	D	45	LEU	2.9
1	C	360	ILE	2.9
2	B	7	THR	2.9
3	E	210	THR	2.9
4	L	206	VAL	2.9
1	A	3	LEU	2.9
1	C	359	ALA	2.9
4	F	188	ARG	2.9
1	C	249	ASN	2.8
1	C	336	GLY	2.8
1	C	108	ALA	2.8
1	C	421	LEU	2.8
1	A	379	PRO	2.8
1	A	110	TRP	2.8
1	C	319	ASP	2.8
2	B	19	VAL	2.8
2	B	67	ARG	2.8
2	B	447	ARG	2.8
1	A	172	SER	2.8
4	F	114	THR	2.8
2	B	266	VAL	2.8
3	H	1	GLU	2.8
4	L	213	GLU	2.8
1	A	195	LEU	2.8
1	C	132	LEU	2.8
3	H	144	LEU	2.8
3	H	183	LEU	2.8
1	A	188	GLY	2.8
1	A	439	ALA	2.8
1	C	95	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	407	LEU	2.8
1	C	143	TYR	2.8
4	F	112	ALA	2.8
1	A	8	LEU	2.8
1	C	194	LEU	2.8
4	F	39	LYS	2.8
3	E	171	THR	2.8
4	L	200	THR	2.8
1	A	234	TYR	2.8
1	C	335	ARG	2.8
1	A	127	VAL	2.7
3	E	54	ALA	2.7
1	C	358[A]	SER	2.7
1	C	195	LEU	2.7
2	B	258	LEU	2.7
3	H	143	THR	2.7
2	D	177	CYS	2.7
1	A	418	GLY	2.7
2	D	439	ALA	2.7
1	A	417	PHE	2.7
1	A	187	GLY	2.7
1	A	40	PRO	2.7
3	H	214	LYS	2.7
2	B	164	TYR	2.7
1	A	248	LEU	2.7
2	B	99	ASN	2.7
3	H	215	LYS	2.7
3	H	208	SER	2.7
4	F	80	SER	2.7
3	E	120	ALA	2.7
4	F	11	MET	2.7
1	A	106	ALA	2.7
1	A	435	LEU	2.7
3	H	159	THR	2.7
2	D	447	ARG	2.6
3	E	40	ARG	2.6
1	A	288	TYR	2.6
1	C	184	GLY	2.6
2	B	223	PHE	2.6
3	H	198	SER	2.6
1	A	145	PRO	2.6
1	C	211	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	446	ALA	2.6
1	A	236	GLY	2.6
3	E	42	GLU	2.6
4	F	3	LEU	2.6
1	A	360	ILE	2.6
2	D	5	CYS	2.6
2	D	257	ALA	2.6
1	A	381	GLY	2.6
1	A	390	LEU	2.6
1	A	447	VAL	2.6
1	C	191	PHE	2.6
1	C	147	ARG	2.6
1	A	357	GLY	2.6
4	F	143	ASP	2.6
2	D	7	THR	2.6
1	A	173	SER	2.6
1	A	420	SER	2.6
2	B	452	ASN	2.6
1	A	293	VAL	2.6
2	D	104	VAL	2.6
4	L	209	PHE	2.6
4	F	123	GLU	2.6
2	B	399	ILE	2.6
2	D	25	TRP	2.6
3	H	162	SER	2.6
1	A	107	CYS	2.6
3	E	155	PRO	2.6
2	B	289	TYR	2.6
1	A	93	LEU	2.5
1	A	36	VAL	2.5
1	A	175	VAL	2.5
1	A	182	VAL	2.5
1	A	437	VAL	2.5
2	B	157	VAL	2.5
2	D	379	VAL	2.5
2	D	78	SER	2.5
1	A	162	TRP	2.5
3	E	73	ASP	2.5
2	D	41	LYS	2.5
1	C	302	GLY	2.5
1	C	377	ALA	2.5
2	B	6	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	188	THR	2.5
2	D	72	LYS	2.5
1	C	93	LEU	2.5
1	A	37	VAL	2.5
1	C	6	VAL	2.5
1	A	190	TYR	2.5
1	A	448	TYR	2.5
3	E	178	SER	2.5
4	F	7	SER	2.5
1	A	9	THR	2.5
1	A	94	GLY	2.5
3	H	150	GLY	2.5
1	C	1	LEU	2.5
2	B	118	MET	2.5
2	B	442	GLU	2.5
4	L	146	VAL	2.5
1	C	169	ALA	2.5
2	D	440	GLN	2.5
3	E	208	SER	2.5
3	H	186	SER	2.5
2	B	256	ILE	2.5
4	F	16	GLY	2.5
3	E	184	SER	2.5
1	A	108	ALA	2.5
1	A	378	ALA	2.5
2	D	381	PRO	2.5
4	F	199	LYS	2.5
1	C	192	LEU	2.5
2	D	432	ASP	2.5
1	C	106	ALA	2.4
3	E	92	ALA	2.4
4	L	118	PHE	2.4
1	A	233	GLY	2.4
1	A	380	TYR	2.4
1	A	181	LEU	2.4
4	L	15	LEU	2.4
1	A	311	PRO	2.4
1	C	214	TRP	2.4
4	F	23	CYS	2.4
1	A	266	ALA	2.4
4	L	69	ALA	2.4
1	C	105	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	406	VAL	2.4
4	L	19	VAL	2.4
3	E	90	ASP	2.4
1	C	436	ILE	2.4
1	C	435	LEU	2.4
1	C	38	GLY	2.4
1	C	21	PHE	2.4
3	E	64	PHE	2.4
1	C	234	TYR	2.4
3	E	141	SER	2.4
2	B	3	ASN	2.4
4	L	124	GLN	2.4
1	C	23	LEU	2.4
1	C	94	GLY	2.4
2	B	263	ALA	2.4
2	D	446	HIS	2.4
1	A	25	PHE	2.4
1	A	262	TRP	2.4
1	A	312	LEU	2.4
1	A	310	ALA	2.4
2	B	201	THR	2.4
1	A	131	PHE	2.4
3	H	191	SER	2.4
1	C	126	PRO	2.3
4	F	141	PRO	2.3
1	A	191	PHE	2.3
1	A	200	VAL	2.3
1	C	376	VAL	2.3
1	C	419	PHE	2.3
3	E	187	VAL	2.3
1	A	440	TYR	2.3
1	C	311	PRO	2.3
1	C	410	PRO	2.3
2	D	164	TYR	2.3
2	B	181	LYS	2.3
1	A	375	ALA	2.3
2	D	30	ALA	2.3
1	A	19	PHE	2.3
2	D	370	PHE	2.3
1	C	170	GLY	2.3
2	B	392	GLY	2.3
2	B	268	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1	LEU	2.3
2	D	43	ASN	2.3
3	E	159	THR	2.3
4	L	126	THR	2.3
1	C	110	TRP	2.3
2	D	34	GLY	2.3
2	D	199	GLN	2.3
2	D	263	ALA	2.3
1	C	187	GLY	2.3
1	C	370	GLY	2.3
1	A	445	VAL	2.3
2	D	455	PHE	2.3
2	D	47	ASP	2.3
1	A	104	ILE	2.3
2	D	88	ILE	2.3
3	E	121	LYS	2.3
2	D	24	ALA	2.3
4	L	112	ALA	2.3
1	C	8	LEU	2.3
2	D	467	LEU	2.3
1	A	196	ALA	2.3
1	A	446	ALA	2.3
1	A	309	GLY	2.2
1	A	353	TYR	2.2
4	F	87	TYR	2.2
4	L	145	ASN	2.2
1	A	411	PHE	2.2
1	C	182	VAL	2.2
1	C	389	VAL	2.2
1	A	433	PRO	2.2
3	E	125	PRO	2.2
1	C	339	ALA	2.2
2	B	187[A]	MET	2.2
4	L	190	ASN	2.2
2	B	100	PHE	2.2
3	E	27	PHE	2.2
3	H	172	PHE	2.2
1	A	189	TYR	2.2
4	L	59	PRO	2.2
1	A	103	VAL	2.2
1	A	239[A]	VAL	2.2
1	A	376	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	96	SER	2.2
2	D	334	SER	2.2
4	L	26	SER	2.2
2	B	260	GLY	2.2
1	A	141	ALA	2.2
1	A	450	ALA	2.2
2	D	50	ALA	2.2
2	B	255	HIS	2.2
4	F	105	GLU	2.2
4	F	169	LYS	2.2
1	A	256	GLY	2.2
4	F	81	GLU	2.2
1	A	388	GLN	2.2
2	B	117	LEU	2.2
1	C	172	SER	2.2
1	A	38	GLY	2.2
1	C	97	VAL	2.2
1	C	418	GLY	2.2
2	D	233	ASP	2.2
1	C	437	VAL	2.2
2	B	156	PHE	2.2
1	A	291	HIS	2.2
4	L	196	ALA	2.2
4	L	198	HIS	2.2
1	C	146	CYS	2.2
1	A	260	TRP	2.2
1	C	142	GLU	2.2
1	C	300	GLY	2.2
2	D	144	LYS	2.1
1	C	237	TYR	2.1
3	E	95	TYR	2.1
1	A	406	VAL	2.1
2	B	207	VAL	2.1
3	E	23	THR	2.1
3	E	87	THR	2.1
4	L	193	THR	2.1
1	A	55	LEU	2.1
1	C	212	LEU	2.1
4	L	170	ASP	2.1
1	A	362	PRO	2.1
2	B	129	TRP	2.1
1	A	290	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	423	GLY	2.1
2	D	62	ARG	2.1
1	A	143	TYR	2.1
2	B	403	VAL	2.1
1	A	361	ALA	2.1
2	D	6	THR	2.1
1	C	248	LEU	2.1
4	L	121	SER	2.1
1	A	6	VAL	2.1
1	A	12	ALA	2.1
1	A	166	TYR	2.1
2	B	252	ALA	2.1
1	A	385	GLY	2.1
2	D	77	SER	2.1
3	E	15	GLY	2.1
3	H	125	PRO	2.1
2	B	165	MET	2.1
4	F	165	ASP	2.1
1	A	416	ALA	2.1
1	C	37	VAL	2.1
2	D	112	VAL	2.1
2	B	261	ARG	2.1
1	A	238	SER	2.1
3	H	196	SER	2.1
4	F	198	HIS	2.1
1	A	50	THR	2.1
1	A	113	TRP	2.1
2	D	37	ARG	2.1
1	A	257	ALA	2.1
1	C	185	ALA	2.1
2	D	345	VAL	2.1
1	A	164	LYS	2.1
1	C	242	GLY	2.1
1	C	440	TYR	2.1
4	L	83	PHE	2.1
3	H	218	PRO	2.1
1	A	340	LEU	2.1
2	B	92	LEU	2.1
4	F	167	ASP	2.1
1	A	22	SER	2.1
1	A	97	VAL	2.1
1	A	354	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	314	VAL	2.1
4	F	35	TRP	2.1
1	C	417	PHE	2.1
2	B	290	PRO	2.1
3	E	41	PRO	2.1
4	L	139	PHE	2.1
2	B	65	GLU	2.0
1	A	363	LEU	2.0
2	B	226	ILE	2.0
3	E	29	ILE	2.0
4	L	183	LYS	2.0
3	H	138	THR	2.0
2	B	218	ALA	2.0
2	B	225	ALA	2.0
2	D	260	GLY	2.0
1	A	105	VAL	2.0
1	C	445	VAL	2.0
4	F	58	VAL	2.0
1	C	189	TYR	2.0
4	L	140	TYR	2.0
2	D	98	LYS	2.0
2	B	131	ILE	2.0
2	D	145	LEU	2.0
2	B	249	THR	2.0
4	F	172	THR	2.0
1	C	145	PRO	2.0
1	C	53	VAL	2.0
1	A	356	PHE	2.0
1	C	19	PHE	2.0
1	A	221	LEU	2.0
1	C	177[A]	GLN	2.0
2	B	264	GLY	2.0
2	B	440	GLN	2.0
2	B	396	SER	2.0
1	C	198	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates

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

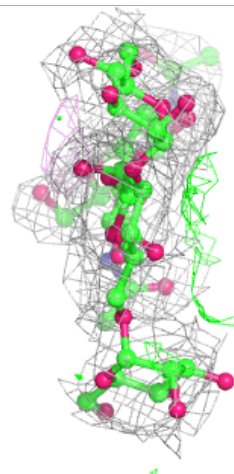
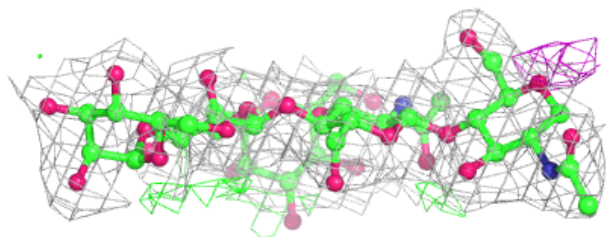
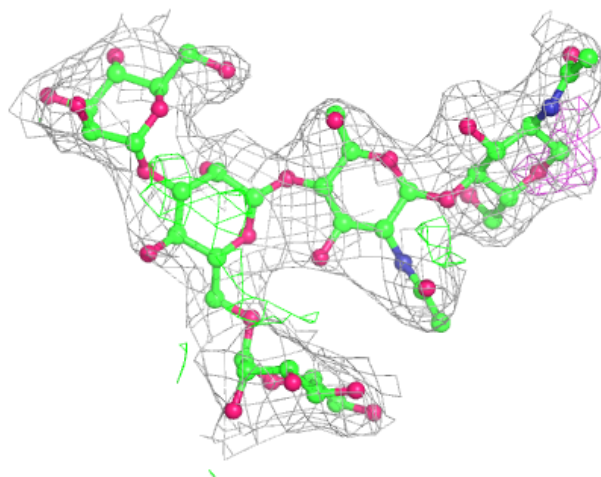
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	BMA	J	3	11/12	0.78	0.45	141,153,161,162	0
5	BMA	G	3	11/12	0.81	0.16	129,143,149,151	0
5	MAN	G	5	11/12	0.82	0.18	140,148,161,165	0
6	NAG	K	2	14/15	0.83	0.40	148,164,169,170	0
6	NAG	K	1	14/15	0.83	0.26	134,143,159,159	0
7	NAG	J	2	14/15	0.85	0.26	121,128,133,145	0
5	MAN	G	4	11/12	0.85	0.14	117,123,142,144	0
6	NAG	I	2	14/15	0.86	0.33	140,149,155,157	0
7	MAN	J	4	11/12	0.86	0.45	139,151,157,159	0
6	NAG	I	1	14/15	0.88	0.35	125,140,149,150	0
5	NAG	G	2	14/15	0.90	0.15	91,108,124,127	0
5	NAG	G	1	14/15	0.92	0.16	60,75,96,97	0
7	NAG	J	1	14/15	0.93	0.16	90,115,132,132	0

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



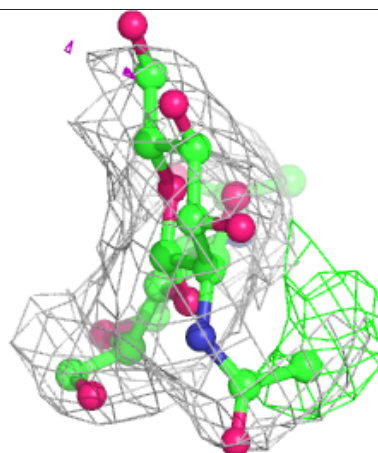
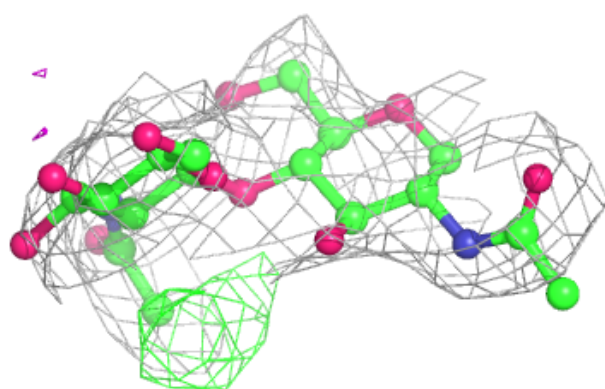
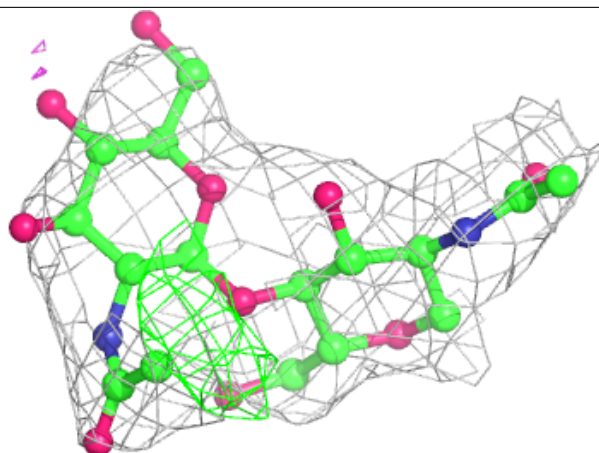
**Electron density around Chain G:**

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

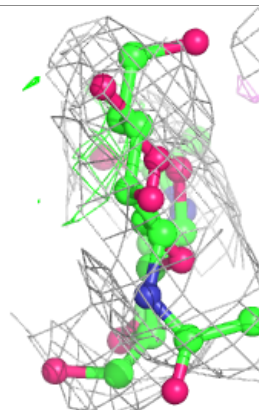
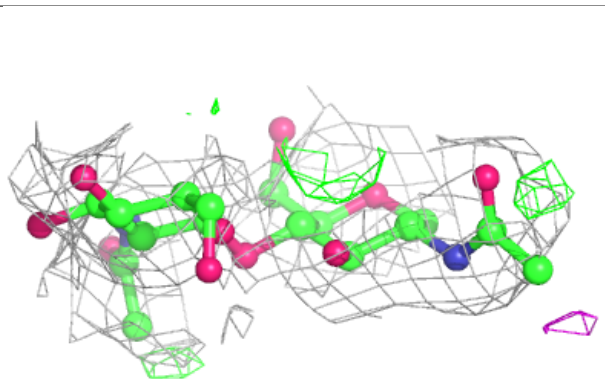
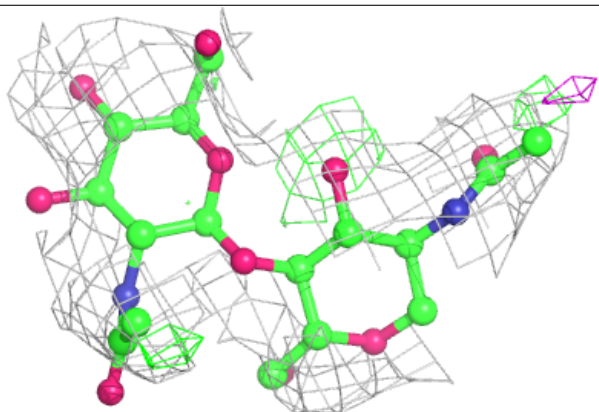


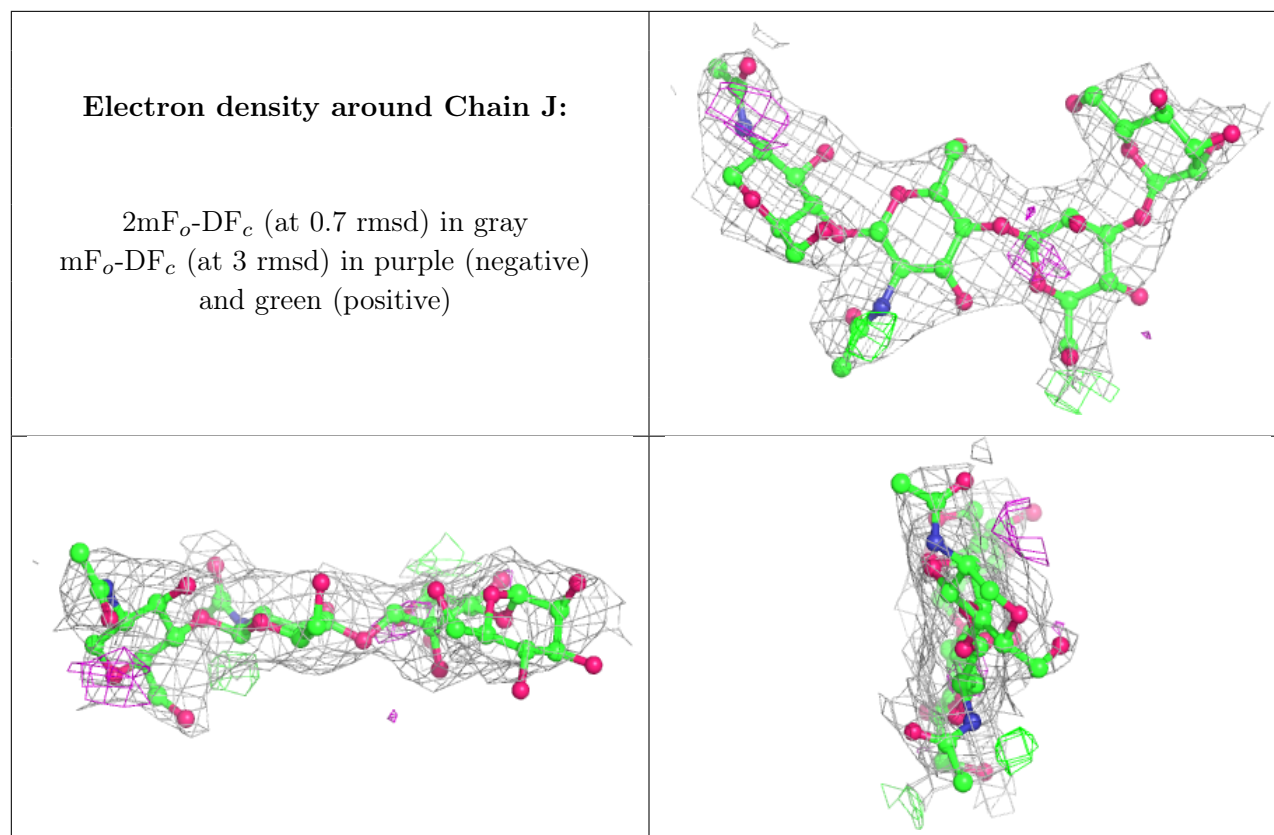
**Electron density around Chain I:**

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

**Electron density around Chain K:**

$2mF_o - DF_c$  (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.

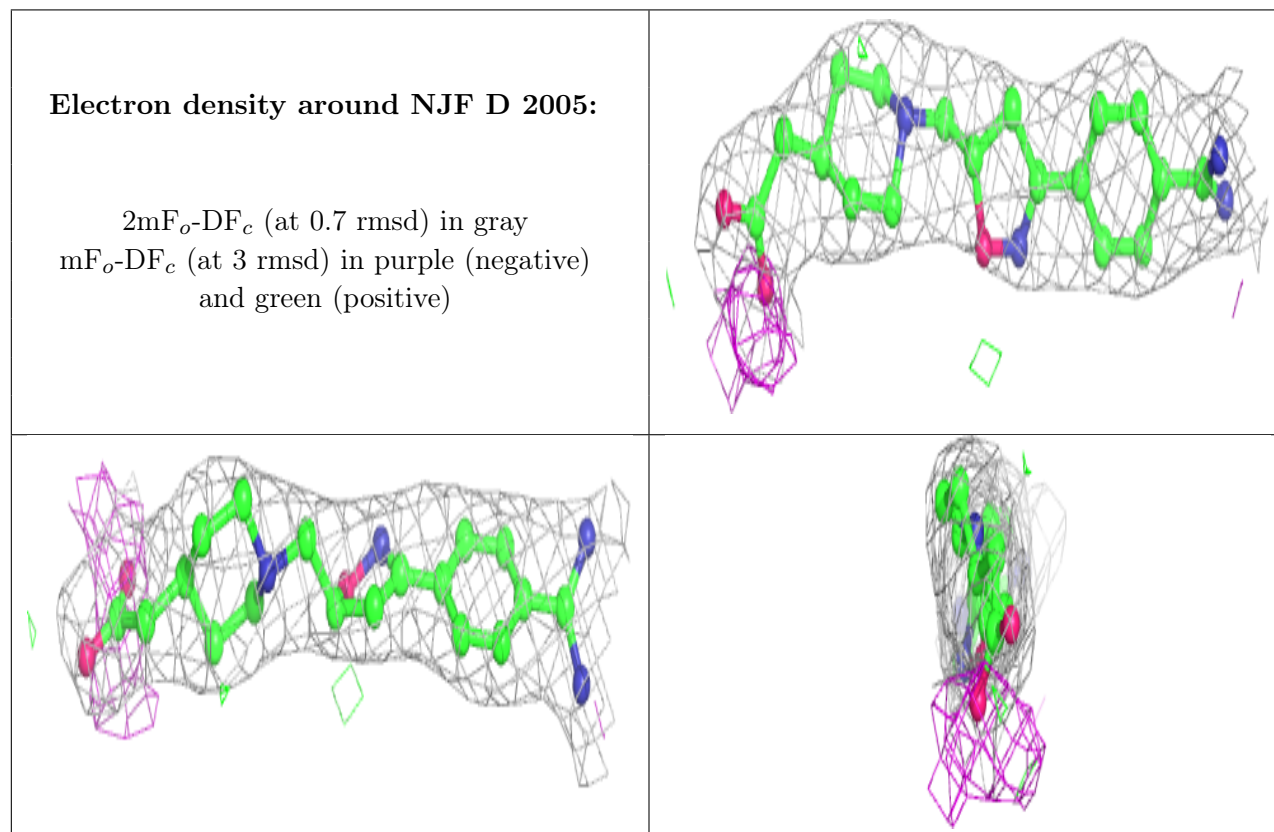
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MN	B	2002	1/1	0.44	0.25	144,144,144,144	0
13	CL	C	505	1/1	0.46	0.56	131,131,131,131	0
11	NAG	D	2004	14/15	0.70	0.29	130,142,147,149	0
8	SO4	A	508	5/5	0.73	0.26	126,136,142,145	0
10	MN	D	2002	1/1	0.80	0.13	129,129,129,129	0
8	SO4	C	503	5/5	0.80	0.36	156,156,159,161	0
8	SO4	A	507	5/5	0.80	0.16	124,128,139,141	0
9	CA	C	506	1/1	0.81	0.13	134,134,134,134	0
8	SO4	C	502	5/5	0.83	0.28	135,138,140,152	0
8	SO4	L	301	5/5	0.86	0.20	127,127,133,137	0
11	NAG	B	2004	14/15	0.87	0.33	138,144,148,148	0
12	NJF	D	2005	25/25	0.88	0.22	65,85,103,107	0
8	SO4	C	510	5/5	0.88	0.26	147,148,152,156	0
8	SO4	C	501	5/5	0.90	0.20	122,123,129,131	0

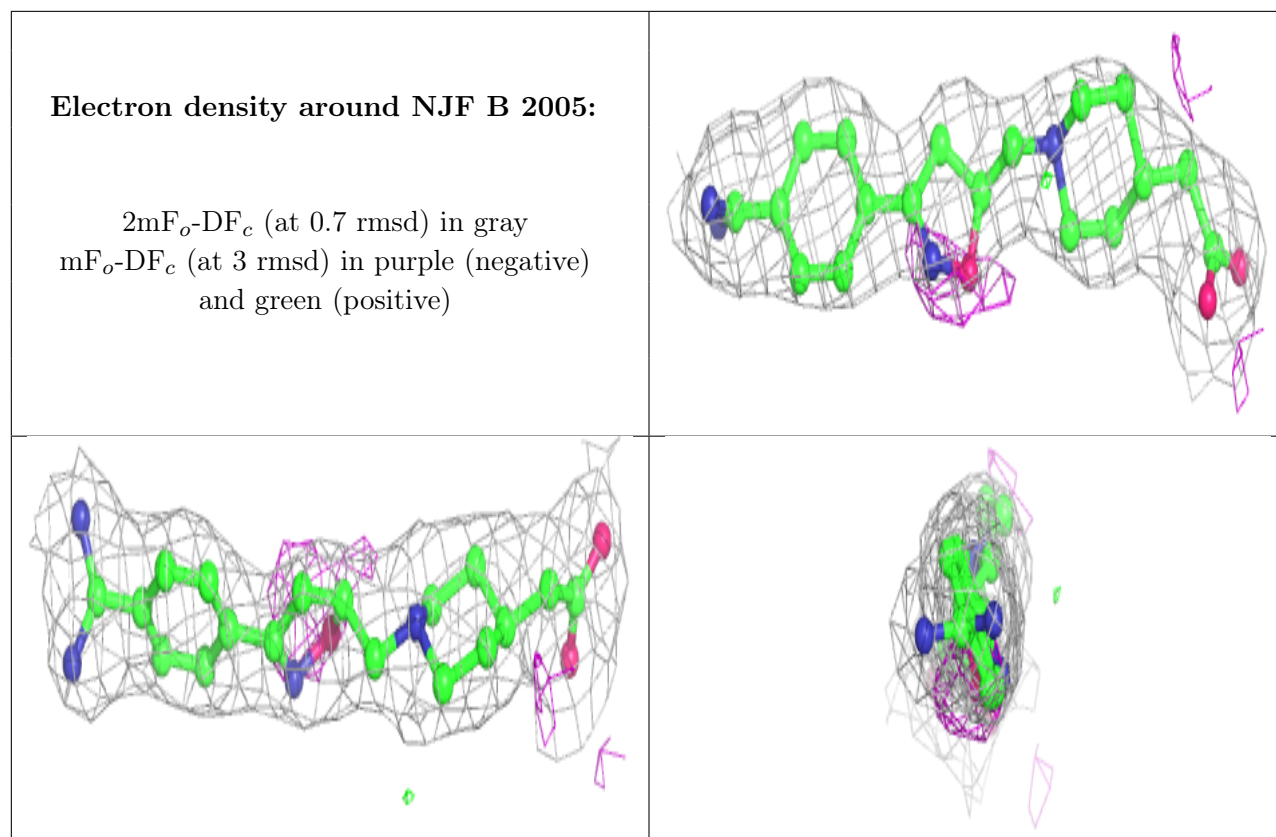
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	A	501	5/5	0.90	0.21	102,102,107,111	0
12	NJF	B	2005	25/25	0.92	0.28	44,81,96,102	0
9	CA	C	509	1/1	0.93	0.11	75,75,75,75	0
13	CL	C	504	1/1	0.93	0.46	92,92,92,92	0
10	MN	D	2001	1/1	0.93	0.14	85,85,85,85	0
9	CA	C	507	1/1	0.94	0.05	96,96,96,96	0
10	MN	B	2003	1/1	0.95	0.16	63,63,63,63	0
9	CA	C	508	1/1	0.96	0.10	83,83,83,83	0
9	CA	A	503	1/1	0.96	0.07	70,70,70,70	0
9	CA	A	505	1/1	0.97	0.17	55,55,55,55	0
10	MN	D	2003	1/1	0.97	0.11	79,79,79,79	0
9	CA	A	504	1/1	0.98	0.11	57,57,57,57	0
8	SO4	A	502	5/5	0.98	0.17	90,94,97,108	0
9	CA	A	506	1/1	0.98	0.16	53,53,53,53	0
10	MN	B	2001	1/1	0.99	0.18	56,56,56,56	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.