



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 10:35 AM EDT

PDB ID : 7UKP  
Title : Integrin alaphIIBbeta3 complex with a gantofiban analog  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-04-01  
Resolution : 2.80 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 : 2.36  
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) : 2.36

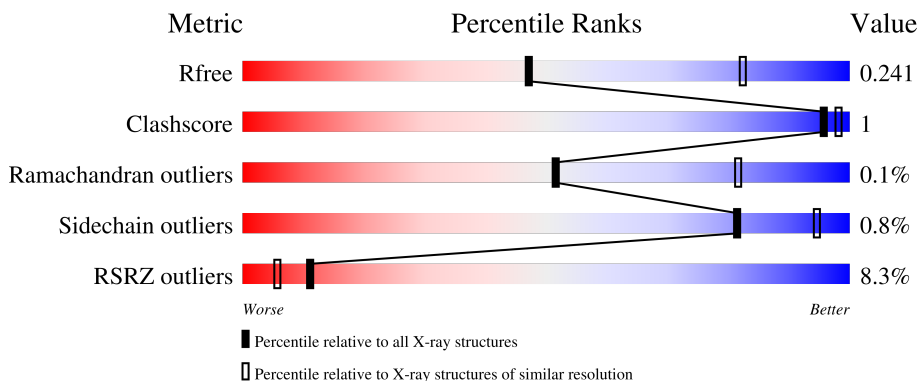
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



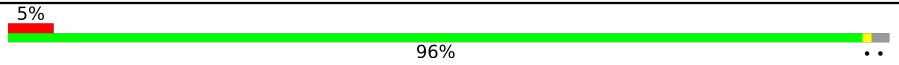
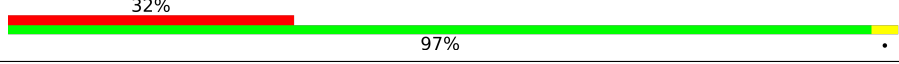
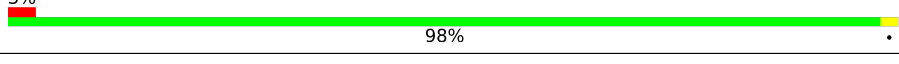
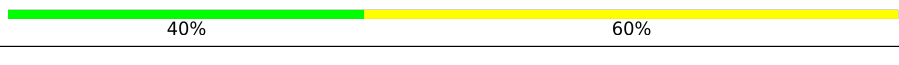
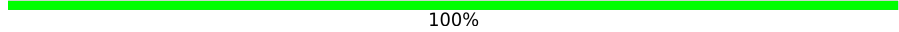

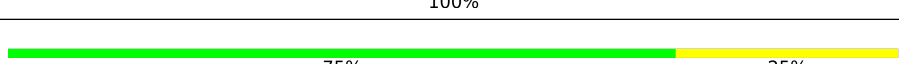
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">96%</p>
1	C	457	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">95%</p>
2	B	472	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93%</p>
2	D	472	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">95%</p>
3	E	221	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">95%</p>

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Mol	Chain	Length	Quality of chain
3	H	221	 5% 96% ..
4	F	214	 32% 97% .
4	L	214	 3% 98% .
5	G	5	 40% 60%
6	I	2	 100%
6	K	2	 100%
7	J	4	 75% 25%

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21371 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
			Total	C	N	O	S			
1	A	454	Total	C	N	O	S	0	2	0
			3489	2219	599	663	8			
1	C	453	Total	C	N	O	S	0	2	0
			3486	2214	600	664	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	466	Total	C	N	O	S	4	2	0
			3602	2243	615	711	33			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
5	G	5	61	34	2	25	0	0	0

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

- 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
			Total	C	N	O			
7	J	4	50	28	2	20	0	0	0

- 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	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		

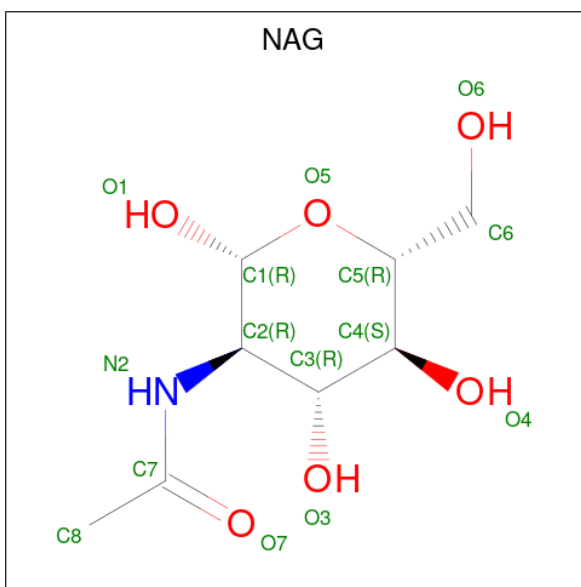
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

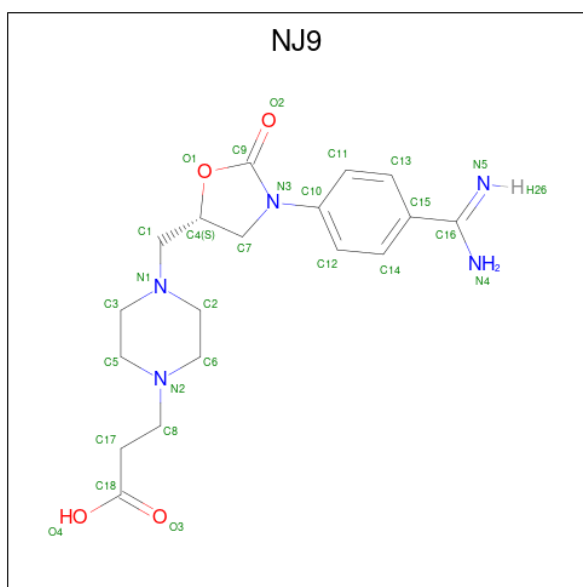
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total	Mn	0	0
			2	2		
10	D	2	Total	Mn	0	0
			2	2		

- 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 3-(4-{(5S)-3-(4-carbamimidoylphenyl)-2-oxo-1,3-oxazolidin-5-yl)methyl}piperazin-1-yl)propanoic acid (three-letter code: NJ9) (formula: C<sub>18</sub>H<sub>25</sub>N<sub>5</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	B	1	27	18	5	4	0	0
12	D	1	27	18	5	4	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
13	C	1	1	1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	152	152	152	0	0
14	B	67	67	67	0	0
14	C	55	55	55	0	0
14	D	25	25	25	0	0
14	E	4	4	4	0	0
14	F	4	4	4	0	0

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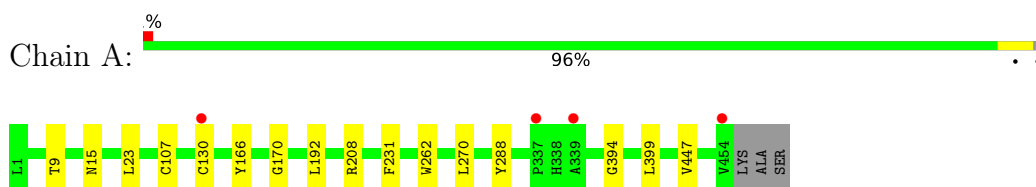
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
14	H	7	Total O 7 7	0	0
14	L	13	Total O 13 13	0	0

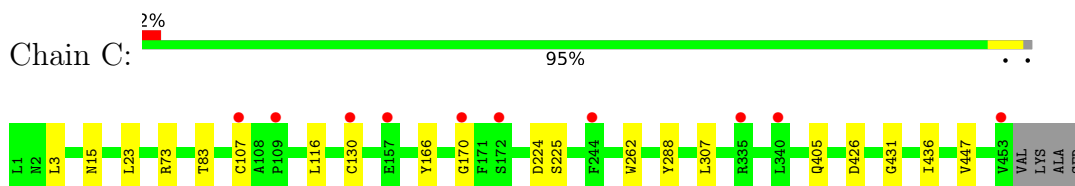
### 3 Residue-property plots [i](#)

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.

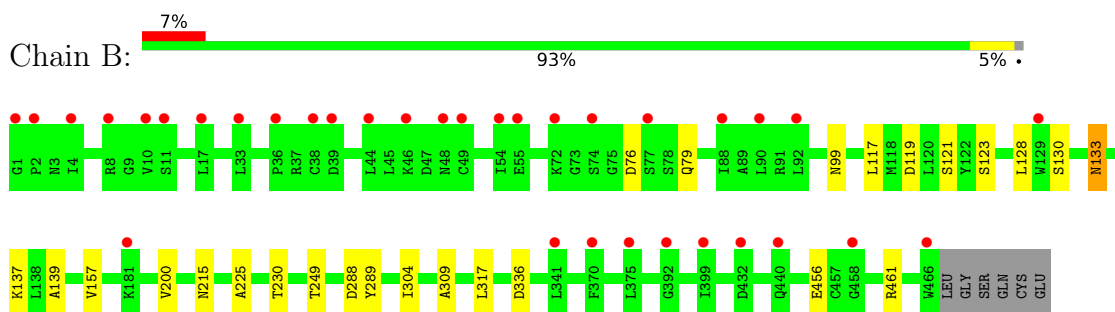
- Molecule 1: Integrin alpha-IIb heavy chain



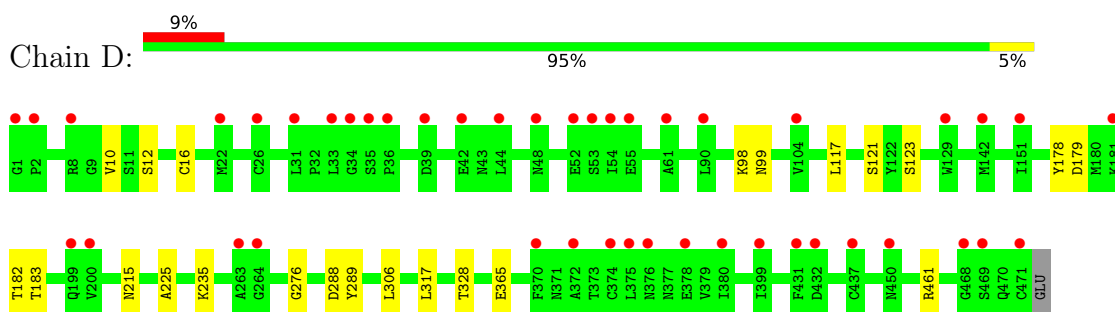
- Molecule 1: Integrin alpha-IIb heavy chain



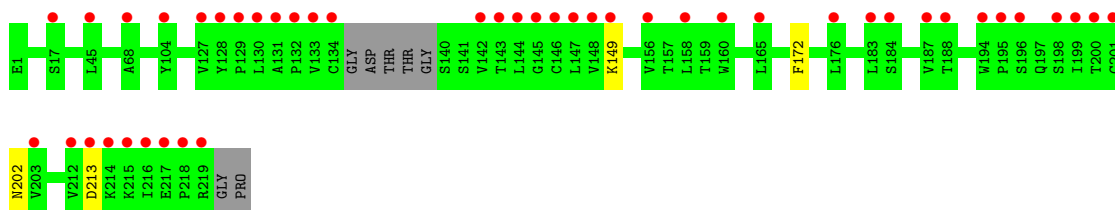
- Molecule 2: Isoform Beta-3C of Integrin beta-3



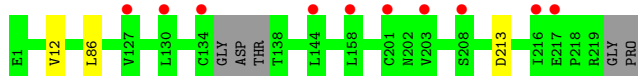
- Molecule 2: Isoform Beta-3C of Integrin beta-3



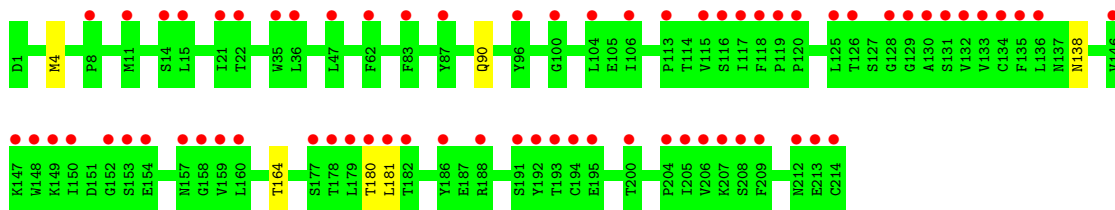
- Molecule 3: 10E5 Fab heavy chain



- Molecule 3: 10E5 Fab heavy chain



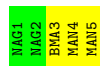
- Molecule 4: 10E5 Fab light chain



- 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

Chain K:  100%

MAG1  
MAG2

- 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  
MAN3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.32Å 144.50Å 104.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.80 48.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (48.25-2.80) 85.7 (48.25-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.219 , 0.241 0.219 , 0.241	Depositor DCC
$R_{free}$ test set	1983 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: NJ9, MN, BMA, SO4, CL, NAG, CA, 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	A	0.28	0/3591	0.48	0/4895
1	C	0.27	0/3585	0.46	0/4885
2	B	0.26	0/3672	0.46	0/4979
2	D	0.25	0/3690	0.45	0/5003
3	E	0.25	0/1673	0.45	0/2290
3	H	0.24	0/1684	0.46	0/2305
4	F	0.24	0/1673	0.44	0/2269
4	L	0.25	0/1673	0.45	0/2269
All	All	0.26	0/21241	0.46	0/28895

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	3489	0	3333	8	0
1	C	3486	0	3320	9	0
2	B	3602	0	3521	13	0
2	D	3623	0	3539	11	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	3	0
4	L	1637	0	1553	2	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	10	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	2	0	0	0	0
10	D	2	0	0	0	0
11	B	14	0	13	1	0
11	D	14	0	13	0	0
12	B	27	0	0	2	0
12	D	27	0	0	1	0
13	C	1	0	0	0	0
14	A	152	0	0	2	1
14	B	67	0	0	0	0
14	C	55	0	0	1	1
14	D	25	0	0	0	0
14	E	4	0	0	0	0
14	F	4	0	0	0	0
14	H	7	0	0	0	0
14	L	13	0	0	0	0
All	All	21371	0	20180	47	1

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 (47) 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:D:121:SER:HB2	12:D:2004:NJ9:C18	2.28	0.63
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.86	0.56
2:B:133:ASN:N	2:B:133:ASN:OD1	2.38	0.56
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.39	0.55
2:D:10:VAL:HG21	2:D:16:CYS:HB2	1.89	0.54
1:A:208:ARG:O	14:A:601:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:SER:HB2	12:B:2004:NJ9:O4	2.10	0.52
1:C:107:CYS:HA	1:C:130:CYS:HA	1.93	0.51
2:D:288:ASP:OD1	2:D:289:TYR:N	2.41	0.51
1:C:3:LEU:O	1:C:405:GLN:NE2	2.35	0.51
1:A:15:ASN:ND2	14:A:611:HOH:O	2.44	0.50
1:C:436:ILE:HG22	1:C:447:VAL:HG22	1.94	0.50
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.93	0.50
2:B:117:LEU:HD11	2:B:225:ALA:HB1	1.94	0.49
4:L:66:GLY:HA3	4:L:71:TYR:HA	1.95	0.48
1:C:224:ASP:OD1	1:C:225:SER:N	2.42	0.48
1:C:73:ARG:NH1	14:C:609:HOH:O	2.47	0.47
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.30	0.46
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.98	0.46
3:H:213:ASP:OD1	3:H:213:ASP:N	2.49	0.45
2:B:119:ASP:OD1	2:B:121:SER:OG	2.34	0.45
2:B:288:ASP:OD1	2:B:289:TYR:N	2.50	0.45
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.97	0.45
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.99	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.45
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.99	0.45
1:A:9:THR:HB	1:A:447:VAL:HB	1.98	0.44
1:A:192:LEU:HD11	1:A:231:PHE:CD1	2.53	0.44
1:A:262:TRP:HB3	2:B:317:LEU:HD13	2.00	0.43
2:B:230:THR:HG23	2:B:304:ILE:HG13	2.00	0.43
2:B:130:SER:OG	2:B:336:ASP:O	2.23	0.43
2:D:182:THR:OG1	2:D:183:THR:N	2.51	0.43
1:A:107:CYS:HB3	1:A:170:GLY:HA3	1.99	0.43
2:B:249:THR:HA	2:B:309:ALA:O	2.19	0.43
2:D:178:TYR:CG	2:D:179:ASP:N	2.86	0.43
1:A:107:CYS:HA	1:A:130:CYS:HA	2.00	0.42
2:B:121:SER:HB2	12:B:2004:NJ9:C18	2.50	0.42
1:C:107:CYS:HB3	1:C:170:GLY:HA3	2.02	0.42
1:A:394:GLY:HA2	1:A:399:LEU:HD23	2.02	0.42
2:D:117:LEU:HD11	2:D:225:ALA:HB1	2.00	0.42
3:H:12:VAL:HG21	3:H:86:LEU:HD13	2.02	0.41
4:F:4:MET:HE2	4:F:90:GLN:HB3	2.01	0.41
2:B:99:ASN:ND2	11:B:2003:NAG:O7	2.53	0.41
2:D:235:LYS:HE3	2:D:276:GLY:O	2.21	0.41
1:C:426:ASP:OD2	1:C:431:GLY:N	2.51	0.40
1:C:83:THR:HB	1:C:116:LEU:HB2	2.03	0.40
2:D:98:LYS:HD2	2:D:99:ASN:H	1.86	0.40



All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:712:HOH:O	14:C:648:HOH:O[1_554]	2.11	0.09

### 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	454/457 (99%)	438 (96%)	16 (4%)	0	100	100
1	C	453/457 (99%)	434 (96%)	19 (4%)	0	100	100
2	B	466/472 (99%)	448 (96%)	16 (3%)	2 (0%)	34	66
2	D	469/472 (99%)	444 (95%)	25 (5%)	0	100	100
3	E	210/221 (95%)	194 (92%)	16 (8%)	0	100	100
3	H	212/221 (96%)	199 (94%)	13 (6%)	0	100	100
4	F	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	29	61
4	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	61
All	All	2688/2728 (98%)	2563 (95%)	121 (4%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	76	ASP
4	F	138	ASN
4	L	77	SER
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	364/364 (100%)	360 (99%)	4 (1%)	73	92
1	C	363/364 (100%)	358 (99%)	5 (1%)	67	90
2	B	414/417 (99%)	408 (99%)	6 (1%)	67	90
2	D	416/417 (100%)	413 (99%)	3 (1%)	84	95
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	96
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2306/2318 (100%)	2287 (99%)	19 (1%)	81	94

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	270	LEU
1	A	288	TYR
2	B	79	GLN
2	B	123	SER
2	B	128	LEU
2	B	133	ASN
2	B	137	LYS
2	B	215	ASN
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	288	TYR
1	C	307	LEU
2	D	123	SER
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
1	A	333	GLN
2	B	438	GLN
2	D	15	GLN
2	D	280	HIS

### 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](#)

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	0.41	0	17,19,21	0.50	0
5	NAG	G	2	5	14,14,15	0.35	0	17,19,21	0.43	0
5	BMA	G	3	5	11,11,12	1.38	2 (18%)	15,15,17	0.96	1 (6%)
5	MAN	G	4	5	11,11,12	1.22	1 (9%)	15,15,17	1.40	1 (6%)
5	MAN	G	5	5	11,11,12	1.10	1 (9%)	15,15,17	1.15	1 (6%)
6	NAG	I	1	6,2	14,14,15	0.51	0	17,19,21	0.35	0
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.39	0
7	NAG	J	1	7,2	14,14,15	0.30	0	17,19,21	0.52	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.38	0
7	BMA	J	3	7	11,11,12	0.46	0	15,15,17	0.77	0
7	MAN	J	4	7	11,11,12	0.77	0	15,15,17	0.94	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	K	2	6	14,14,15	0.30	0	17,19,21	0.51	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	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
7	NAG	J	1	7,2	-	2/6/23/26	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	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	4	MAN	O5-C5	3.40	1.50	1.43
5	G	3	BMA	C4-C5	3.31	1.60	1.53
5	G	5	MAN	C1-C2	2.53	1.58	1.52
5	G	3	BMA	C4-C3	2.35	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	4.47	118.24	112.19
5	G	5	MAN	C1-O5-C5	3.26	116.61	112.19
5	G	3	BMA	O2-C2-C3	-2.24	105.65	110.14
7	J	4	MAN	O2-C2-C3	-2.20	105.74	110.14
7	J	4	MAN	C1-O5-C5	2.18	115.14	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	4	MAN	O5-C5-C6-O6

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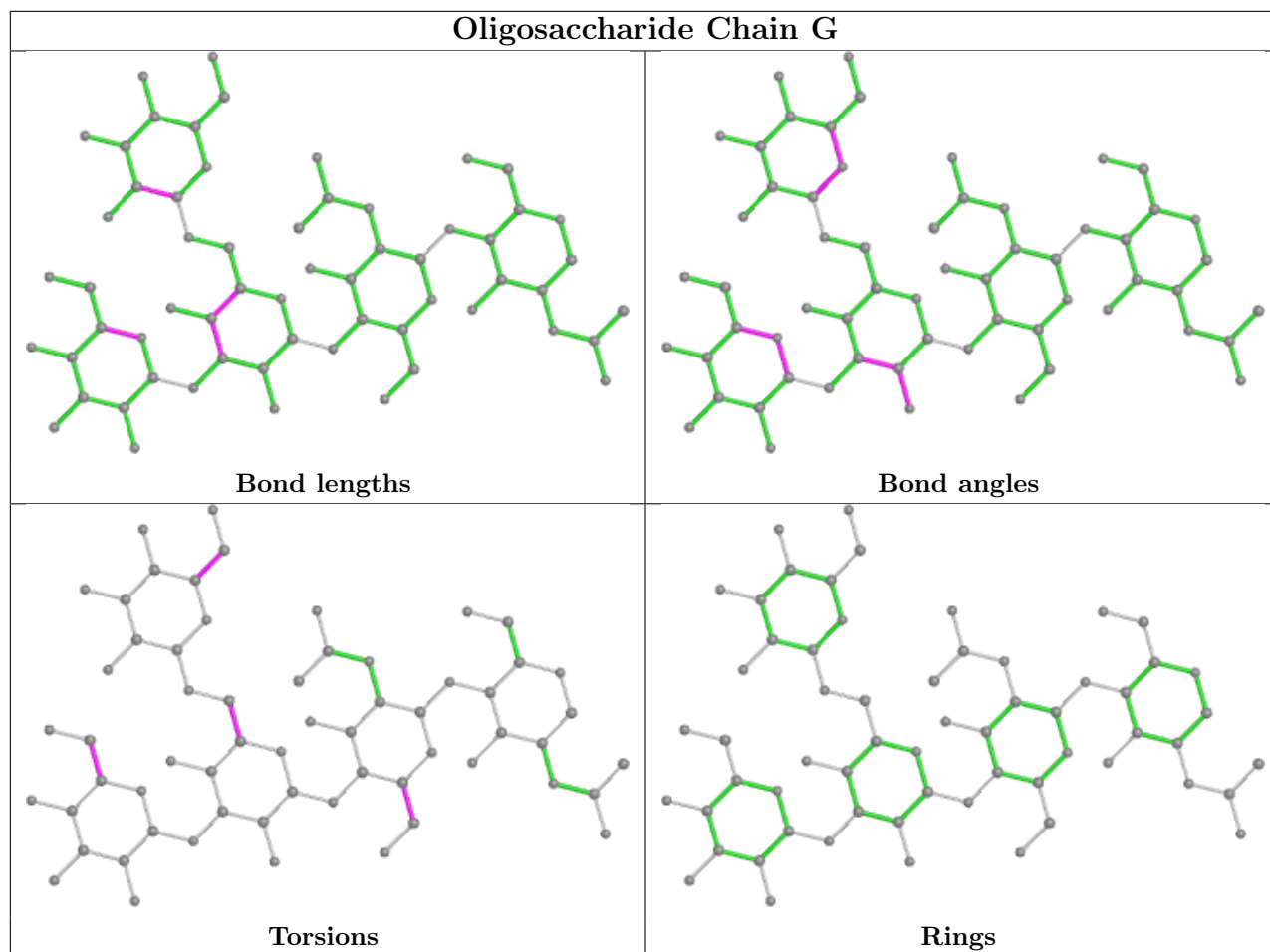
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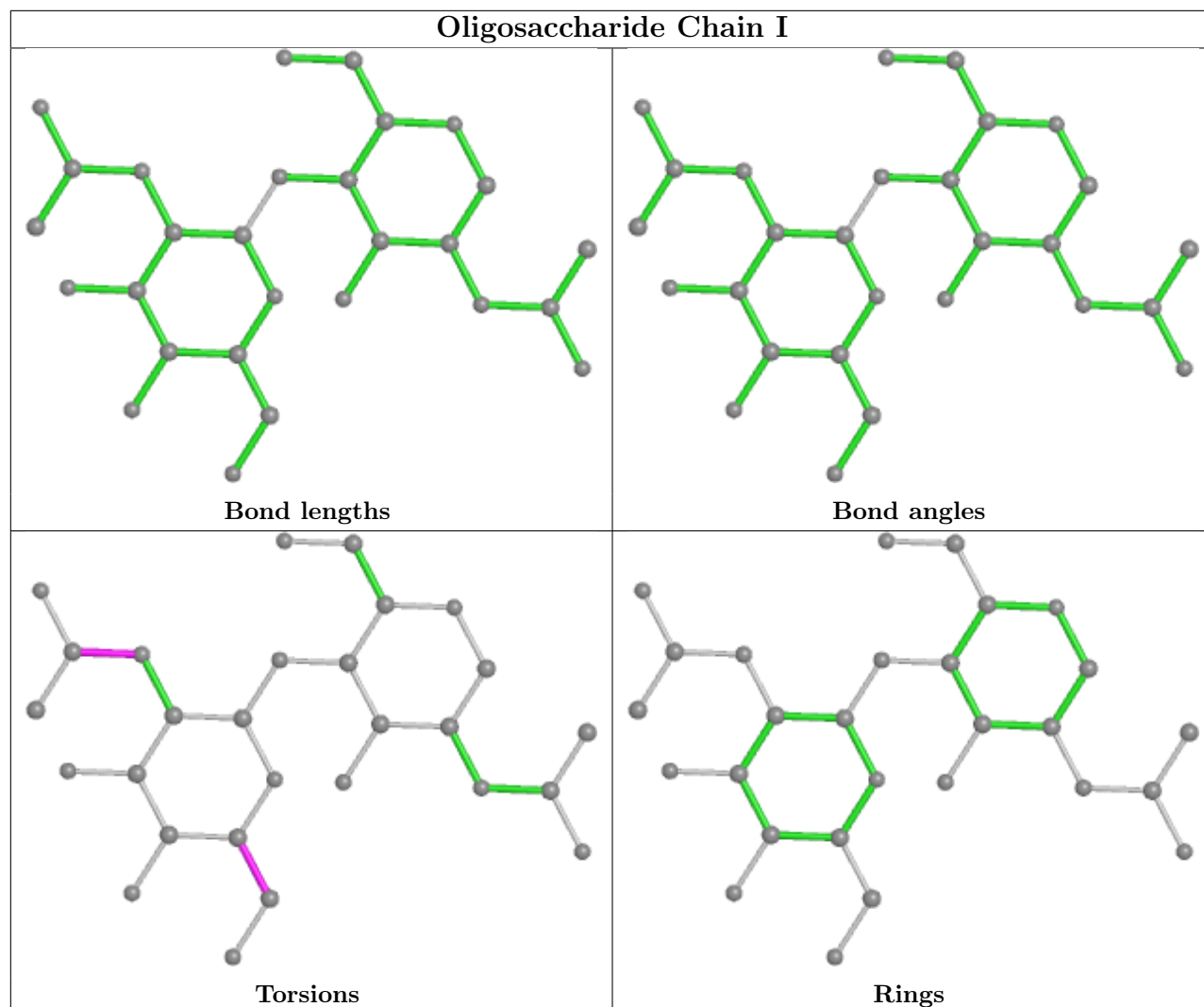
Mol	Chain	Res	Type	Atoms
5	G	5	MAN	O5-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	J	1	NAG	C1-C2-N2-C7
6	I	2	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
7	J	1	NAG	C3-C2-N2-C7

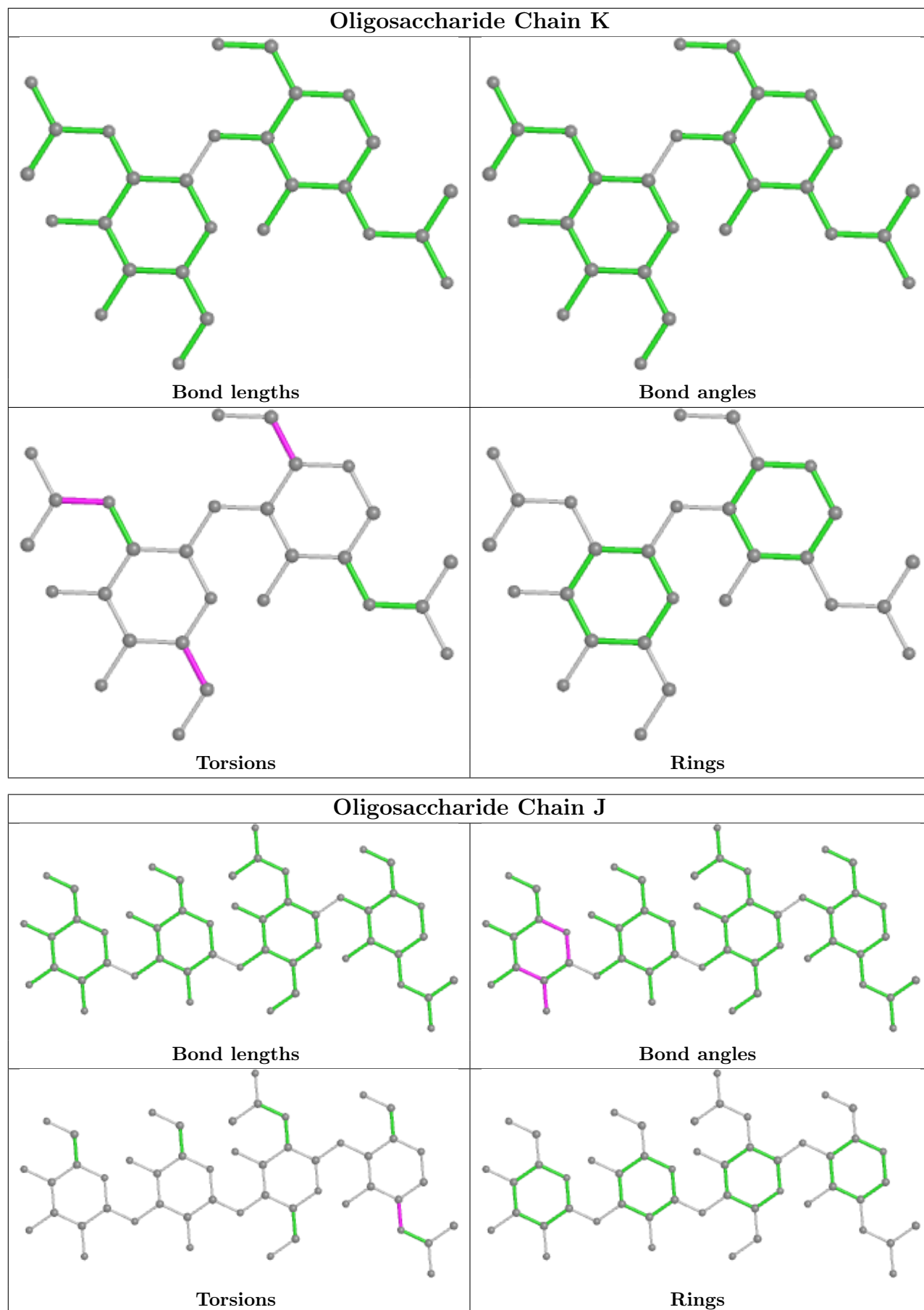
There are no ring outliers.

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.









## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 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	509	-	4,4,4	0.14	0	6,6,6	0.08	0
11	NAG	D	2003	2	14,14,15	0.42	0	17,19,21	0.54	0
12	NJ9	B	2004	10	29,29,29	1.25	2 (6%)	35,40,40	1.66	3 (8%)
8	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.07	0
8	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.07	0
12	NJ9	D	2004	10	29,29,29	1.20	2 (6%)	35,40,40	1.66	3 (8%)
11	NAG	B	2003	2	14,14,15	0.52	0	17,19,21	1.08	1 (5%)
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.09	0
8	SO4	L	301	-	4,4,4	0.13	0	6,6,6	0.07	0
8	SO4	A	501	-	4,4,4	0.13	0	6,6,6	0.24	0
8	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.08	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	NJ9	B	2004	10	-	7/17/39/39	0/3/3/3
12	NJ9	D	2004	10	-	5/17/39/39	0/3/3/3
11	NAG	D	2003	2	-	0/6/23/26	0/1/1/1
11	NAG	B	2003	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2004	NJ9	O1-C4	-3.04	1.42	1.46
12	B	2004	NJ9	C9-N3	2.95	1.39	1.36
12	D	2004	NJ9	O1-C4	-2.90	1.42	1.46
12	D	2004	NJ9	C9-N3	2.59	1.39	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2004	NJ9	C4-O1-C9	6.37	115.17	110.15
12	B	2004	NJ9	C4-O1-C9	5.83	114.74	110.15
12	B	2004	NJ9	O1-C9-N3	-5.49	106.05	109.83
12	D	2004	NJ9	O1-C9-N3	-4.95	106.42	109.83
11	B	2003	NAG	C1-O5-C5	3.84	117.39	112.19
12	D	2004	NJ9	O1-C4-C7	-2.68	101.87	104.57
12	B	2004	NJ9	O1-C4-C7	-2.43	102.12	104.57

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	2003	NAG	C3-C2-N2-C7
12	B	2004	NJ9	C13-C15-C16-N4
12	B	2004	NJ9	C14-C15-C16-N4
12	B	2004	NJ9	C17-C8-N2-C6
12	D	2004	NJ9	C17-C8-N2-C6
12	D	2004	NJ9	C18-C17-C8-N2
12	D	2004	NJ9	N1-C1-C4-C7
12	B	2004	NJ9	C11-C10-N3-C9
11	B	2003	NAG	C1-C2-N2-C7
12	B	2004	NJ9	C8-C17-C18-O3
12	B	2004	NJ9	C8-C17-C18-O4
12	B	2004	NJ9	C12-C10-N3-C9
12	D	2004	NJ9	C8-C17-C18-O3
12	D	2004	NJ9	C8-C17-C18-O4

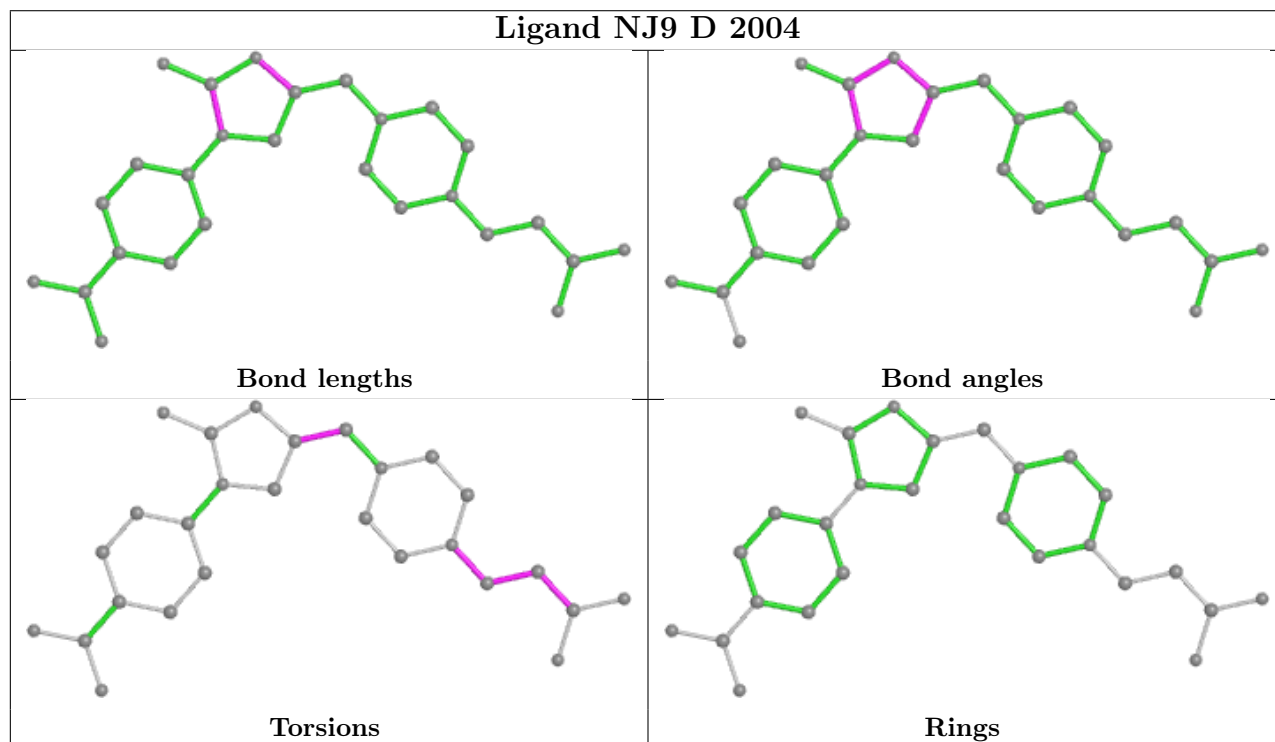
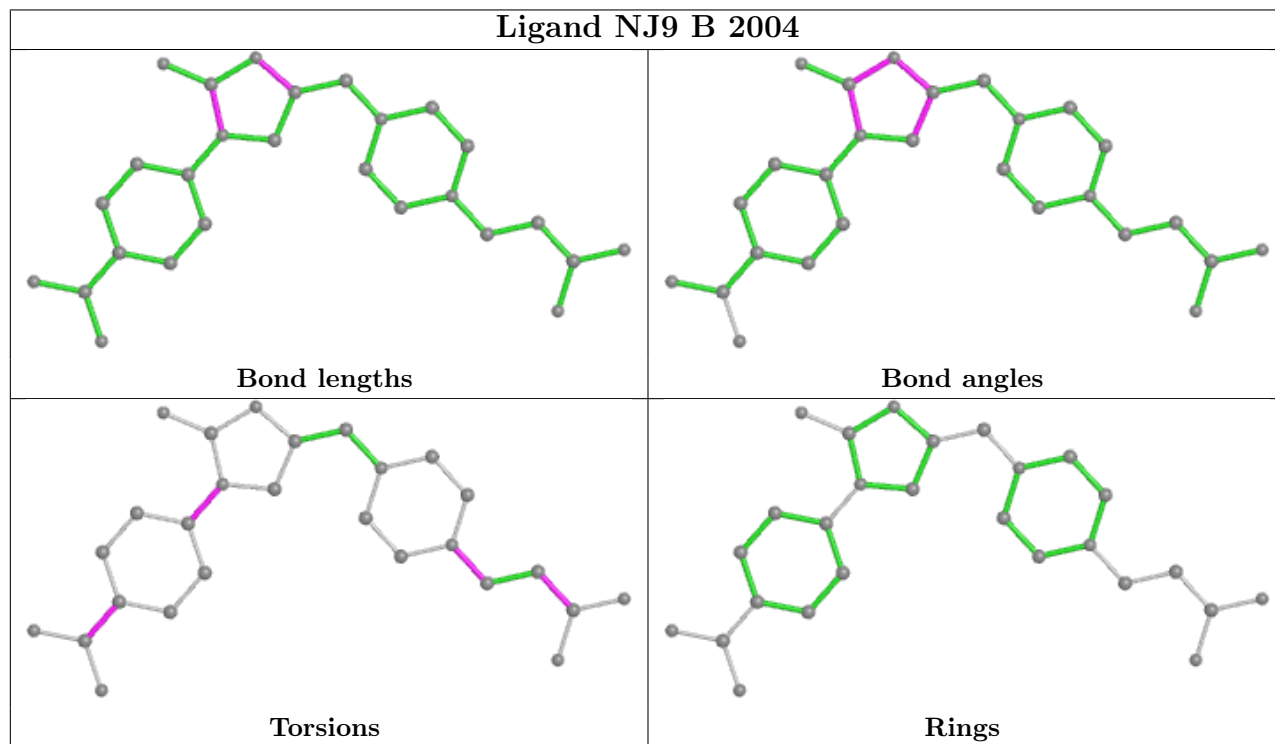
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	2004	NJ9	2	0
12	D	2004	NJ9	1	0
11	B	2003	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	A	454/457 (99%)	0.29	4 (0%) 84 80	56, 71, 94, 109	0
1	C	453/457 (99%)	0.31	10 (2%) 62 52	64, 92, 117, 144	0
2	B	466/472 (98%)	0.60	34 (7%) 15 8	57, 102, 169, 188	1 (0%)
2	D	471/472 (99%)	0.66	44 (9%) 8 4	74, 126, 161, 178	1 (0%)
3	E	214/221 (96%)	1.19	45 (21%) 1 0	109, 149, 218, 228	0
3	H	216/221 (97%)	0.32	10 (4%) 32 22	85, 119, 164, 172	0
4	F	214/214 (100%)	1.50	69 (32%) 0 0	113, 163, 223, 236	0
4	L	214/214 (100%)	0.30	7 (3%) 46 36	89, 115, 135, 158	0
All	All	2702/2728 (99%)	0.58	223 (8%) 11 6	56, 108, 191, 236	2 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	180	THR	8.7
4	F	130	ALA	8.7
3	E	194	TRP	7.9
4	F	115	VAL	7.8
3	E	219	ARG	7.8
4	F	179	LEU	7.6
3	E	134	CYS	7.4
4	F	181	LEU	7.3
3	E	195	PRO	7.3
4	F	193	THR	7.2
3	E	142	VAL	7.2
4	F	135	PHE	7.1
4	F	194	CYS	7.0
2	D	181	LYS	6.8
4	F	134	CYS	6.7
3	E	147	LEU	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	178	THR	6.6
3	E	131	ALA	6.5
3	E	129	PRO	6.4
2	D	469	SER	6.2
3	E	130	LEU	6.2
2	D	375	LEU	6.1
3	E	132	PRO	6.1
4	F	148	TRP	6.0
4	F	117	ILE	5.9
4	F	147	LYS	5.8
3	E	133	VAL	5.8
4	F	158	GLY	5.8
3	E	201	CYS	5.7
3	E	216	ILE	5.6
4	F	132	VAL	5.6
1	A	454	VAL	5.5
4	F	209	PHE	5.4
4	F	214	CYS	5.4
4	F	118	PHE	5.4
2	B	10	VAL	5.3
3	E	144	LEU	5.3
2	D	90	LEU	5.1
4	F	125	LEU	5.0
3	E	160	TRP	5.0
3	E	143	THR	4.9
3	E	148	VAL	4.7
2	D	22	MET	4.6
4	L	214	CYS	4.6
3	E	212	VAL	4.6
3	E	215	LYS	4.5
4	F	146	VAL	4.5
2	B	77	SER	4.4
2	B	36	PRO	4.4
2	B	458	GLY	4.3
2	D	471	CYS	4.3
2	B	1	GLY	4.1
4	F	150	ILE	4.1
4	F	113	PRO	4.1
3	E	127	VAL	4.1
2	D	1	GLY	4.0
3	E	156	VAL	4.0
4	F	195	GLU	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	2	PRO	4.0
4	F	159	VAL	4.0
4	L	212	ASN	4.0
4	F	133	VAL	3.9
4	F	120	PRO	3.9
4	F	21	ILE	3.8
2	B	466	TRP	3.8
4	F	208	SER	3.8
2	B	4	ILE	3.8
2	B	49	CYS	3.7
2	D	44	LEU	3.7
4	F	131	SER	3.7
1	C	453	VAL	3.7
3	H	217	GLU	3.6
2	D	8	ARG	3.6
3	E	184	SER	3.6
2	B	39	ASP	3.6
2	D	36	PRO	3.6
3	E	158	LEU	3.6
4	F	116	SER	3.5
4	F	207	LYS	3.5
3	E	199	ILE	3.5
4	F	119	PRO	3.5
2	B	33	LEU	3.5
2	B	181	LYS	3.5
2	D	55	GLU	3.5
2	D	54	ILE	3.4
3	E	128	TYR	3.4
4	F	212	ASN	3.4
2	D	35	SER	3.4
4	F	206	VAL	3.4
3	E	200	THR	3.4
3	E	217	GLU	3.3
3	E	17	SER	3.3
2	D	34	GLY	3.3
4	F	129	GLY	3.2
3	E	149	LYS	3.2
4	F	149	LYS	3.2
3	E	176	LEU	3.2
2	B	11	SER	3.1
3	E	165	LEU	3.1
2	B	38	CYS	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	160	LEU	3.1
1	C	340	LEU	3.1
4	F	191	SER	3.1
3	E	203	VAL	3.0
3	E	183	LEU	3.0
2	B	55	GLU	3.0
4	F	83	PHE	3.0
4	F	106	ILE	3.0
2	B	8	ARG	3.0
3	E	146	CYS	3.0
3	E	214	LYS	2.9
2	D	437	CYS	2.9
3	E	196	SER	2.9
4	F	205	ILE	2.9
4	F	204	PRO	2.9
2	B	17	LEU	2.9
3	E	218	PRO	2.8
4	F	11	MET	2.8
4	F	15	LEU	2.8
3	H	208	SER	2.8
4	F	35	TRP	2.8
2	B	92	LEU	2.8
4	F	192	TYR	2.8
2	D	42	GLU	2.8
2	B	440	GLN	2.8
2	D	199	GLN	2.8
2	B	90	LEU	2.8
2	B	392	GLY	2.8
3	H	216	ILE	2.8
2	D	376	ASN	2.7
2	D	33	LEU	2.7
1	C	130	CYS	2.7
3	E	68	ALA	2.7
2	D	374	CYS	2.7
3	H	203	VAL	2.7
4	L	136	LEU	2.7
4	F	126	THR	2.7
2	B	54	ILE	2.7
2	D	39	ASP	2.7
4	F	136	LEU	2.7
3	E	198	SER	2.6
2	D	450	ASN	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	88	ILE	2.6
4	F	8	PRO	2.6
2	D	378	GLU	2.6
3	H	134	CYS	2.5
2	D	380	ILE	2.5
4	F	100	GLY	2.5
4	F	104	LEU	2.5
4	F	182	THR	2.5
2	B	129	TRP	2.5
2	D	372	ALA	2.5
2	D	399	ILE	2.5
4	F	157	ASN	2.5
4	F	213	GLU	2.5
2	D	52	GLU	2.4
3	E	104	TYR	2.4
2	B	370	PHE	2.4
4	F	186	TYR	2.4
2	D	104	VAL	2.4
2	B	46	LYS	2.4
2	B	399	ILE	2.4
4	F	177	SER	2.4
2	D	61	ALA	2.4
2	B	375	LEU	2.4
2	D	468	GLY	2.4
4	F	128	GLY	2.3
1	A	337	PRO	2.3
3	E	213	ASP	2.3
3	H	144	LEU	2.3
3	H	201	CYS	2.3
4	F	47	LEU	2.3
2	B	48	ASN	2.3
4	L	33	ILE	2.3
1	A	130	CYS	2.3
4	F	154	GLU	2.3
2	D	129	TRP	2.3
2	B	72	LYS	2.3
2	D	53	SER	2.3
1	A	339	ALA	2.3
4	F	14	SER	2.3
4	F	22	THR	2.3
3	H	130	LEU	2.3
4	F	200	THR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	432	ASP	2.2
2	B	44	LEU	2.2
1	C	244	PHE	2.2
4	L	183	LYS	2.2
1	C	107	CYS	2.2
2	D	431	PHE	2.2
4	F	87	TYR	2.2
3	E	45	LEU	2.2
3	E	145	GLY	2.2
2	D	200	VAL	2.2
3	E	188	THR	2.2
3	H	127	VAL	2.2
2	D	142	MET	2.2
1	C	335	ARG	2.2
4	F	152	GLY	2.2
2	D	48	ASN	2.2
2	D	151	ILE	2.2
4	F	153	SER	2.1
2	D	264	GLY	2.1
1	C	157	GLU	2.1
4	L	205	ILE	2.1
4	F	36	LEU	2.1
4	L	135	PHE	2.1
2	D	26	CYS	2.1
1	C	172	SER	2.1
1	C	170	GLY	2.1
2	D	370	PHE	2.1
2	B	2	PRO	2.1
2	B	341	LEU	2.0
2	B	74	SER	2.0
2	B	432	ASP	2.0
2	D	263	ALA	2.0
4	F	188	ARG	2.0
3	E	187	VAL	2.0
1	C	109	PRO	2.0
4	F	96	TYR	2.0
4	F	62	PHE	2.0
2	D	31	LEU	2.0
3	H	158	LEU	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](#)

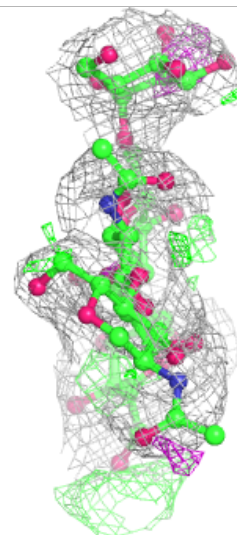
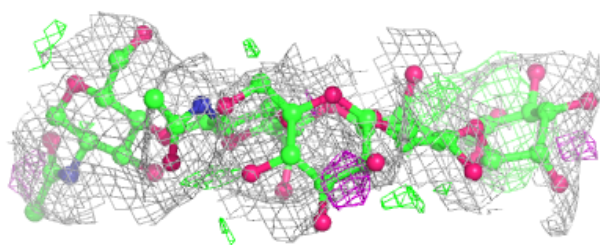
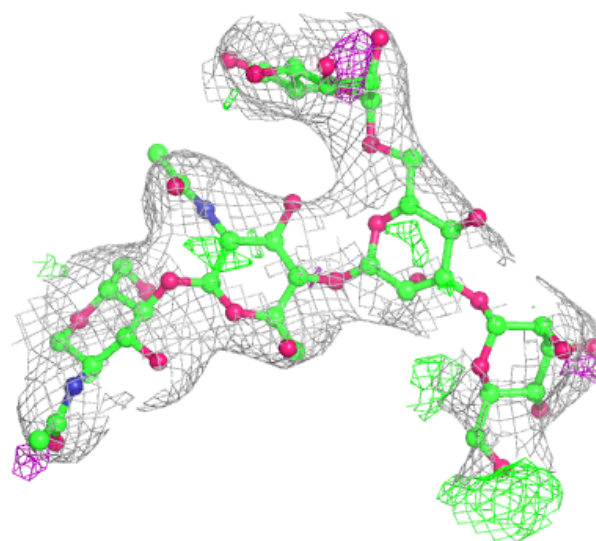
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	G	4	11/12	0.62	0.24	106,106,106,106	0
6	NAG	K	2	14/15	0.76	0.27	147,147,147,147	0
5	MAN	G	5	11/12	0.80	0.22	110,110,110,110	0
7	BMA	J	3	11/12	0.81	0.19	127,127,127,127	0
5	BMA	G	3	11/12	0.84	0.12	108,108,108,108	0
7	MAN	J	4	11/12	0.86	0.18	127,127,127,127	0
6	NAG	I	2	14/15	0.88	0.24	135,135,135,135	0
7	NAG	J	1	14/15	0.89	0.17	116,116,116,116	0
7	NAG	J	2	14/15	0.89	0.19	122,122,122,122	0
6	NAG	K	1	14/15	0.89	0.21	143,143,143,143	0
5	NAG	G	2	14/15	0.89	0.16	97,97,97,97	0
6	NAG	I	1	14/15	0.92	0.23	131,131,131,131	0
5	NAG	G	1	14/15	0.93	0.18	81,81,81,81	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.

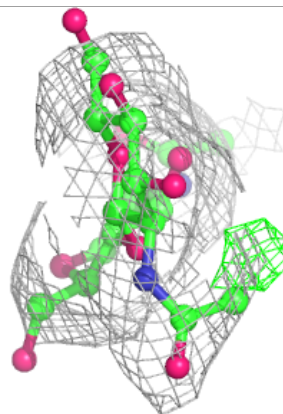
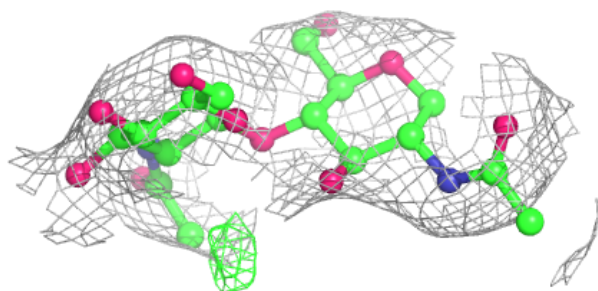
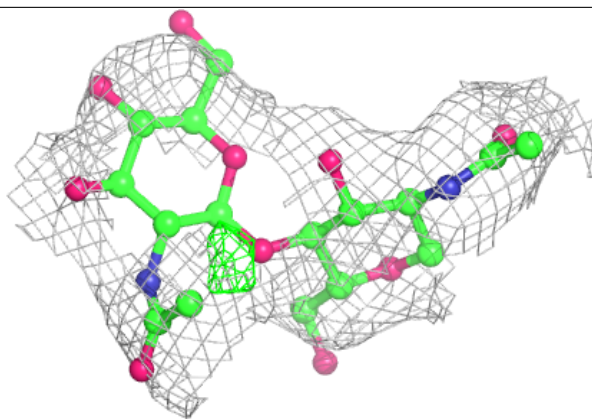
**Electron density around Chain G:**

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

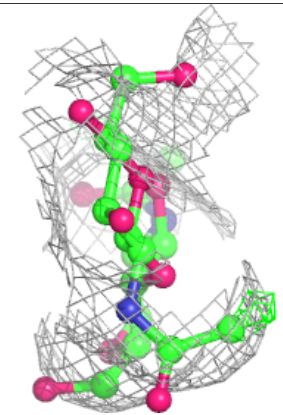
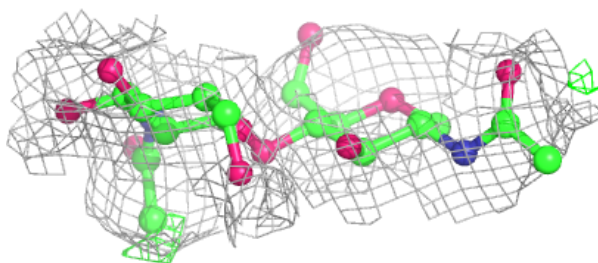
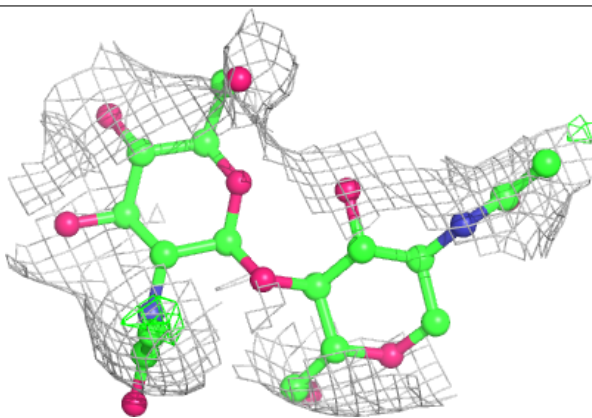


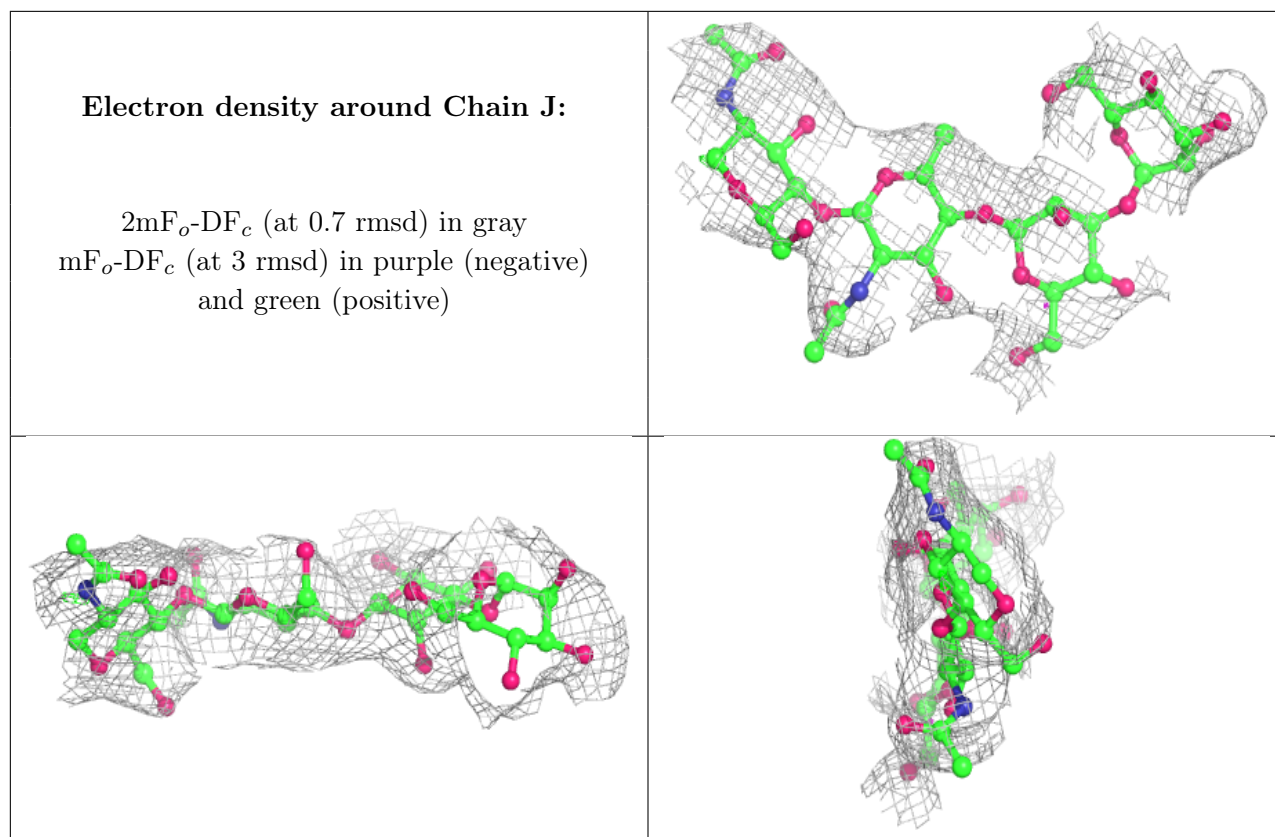
**Electron density around Chain I:**

$2mF_o-DF_c$  (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 [\(i\)](#)

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.

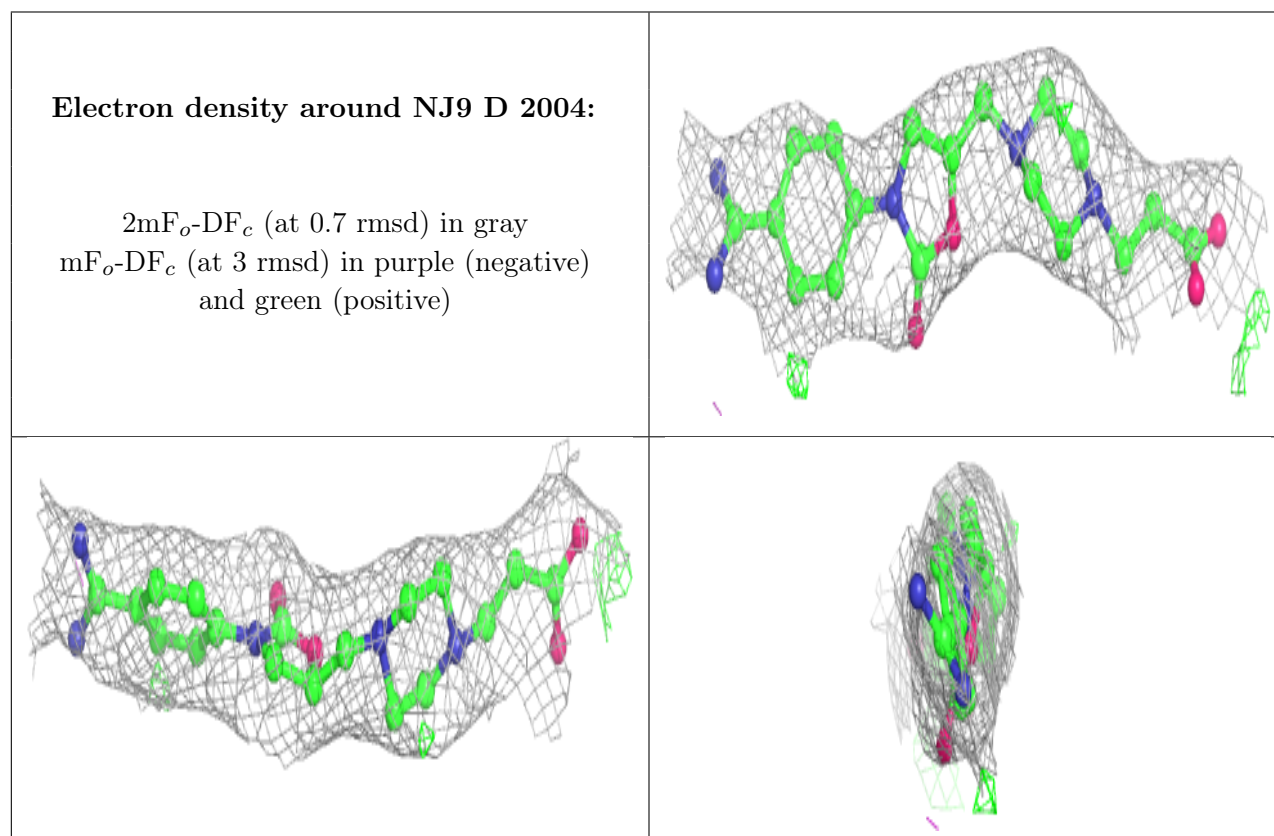
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	CA	C	505	1/1	0.79	0.09	122,122,122,122	0
8	SO4	C	503	5/5	0.83	0.25	129,129,129,129	0
8	SO4	A	506	5/5	0.88	0.15	103,103,103,103	0
8	SO4	C	509	5/5	0.88	0.12	124,124,124,124	0
8	SO4	C	501	5/5	0.88	0.25	103,103,103,103	0
11	NAG	B	2003	14/15	0.88	0.28	132,132,132,132	0
9	CA	C	506	1/1	0.89	0.07	104,104,104,104	0
11	NAG	D	2003	14/15	0.89	0.21	137,137,137,137	0
13	CL	C	504	1/1	0.89	0.15	85,85,85,85	0
8	SO4	L	301	5/5	0.91	0.22	114,114,114,114	0
9	CA	A	502	1/1	0.93	0.12	81,81,81,81	0
9	CA	C	508	1/1	0.93	0.19	81,81,81,81	0
12	NJ9	D	2004	27/27	0.93	0.20	100,100,100,100	0
10	MN	D	2001	1/1	0.93	0.17	98,98,98,98	0

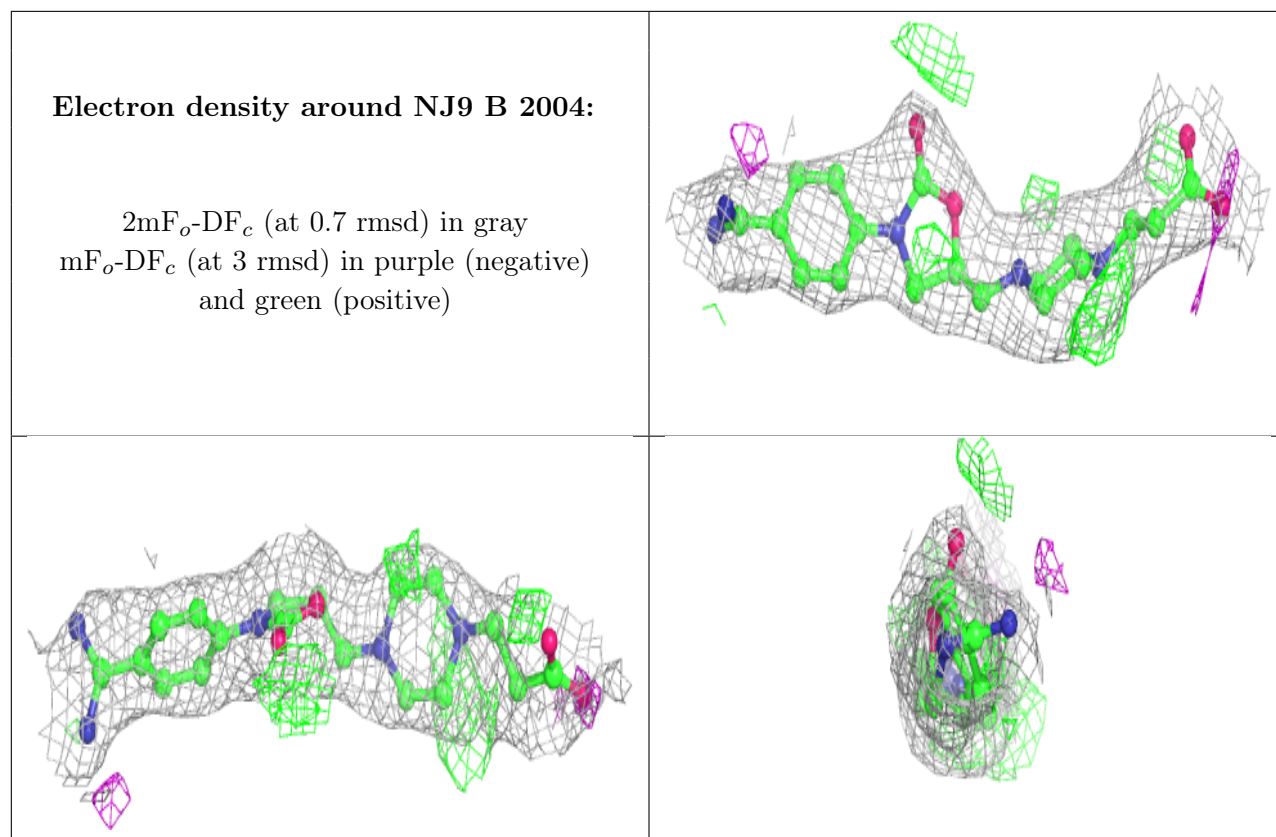
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CA	A	503	1/1	0.94	0.15	69,69,69,69	0
9	CA	A	504	1/1	0.94	0.21	62,62,62,62	0
12	NJ9	B	2004	27/27	0.94	0.20	73,73,73,73	0
8	SO4	C	502	5/5	0.94	0.14	117,117,117,117	0
10	MN	D	2002	1/1	0.94	0.18	98,98,98,98	0
9	CA	C	507	1/1	0.95	0.11	90,90,90,90	0
8	SO4	A	501	5/5	0.97	0.13	83,83,83,83	0
10	MN	B	2001	1/1	0.98	0.21	66,66,66,66	0
9	CA	A	505	1/1	0.98	0.16	63,63,63,63	0
10	MN	B	2002	1/1	1.00	0.21	65,65,65,65	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.