



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:01 PM EDT

PDB ID : 7UK9  
Title : Integrin  $\alpha$ IIb $\beta$ 3 complex with lamifiban (Mn)  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-03-31  
Resolution : 2.60 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

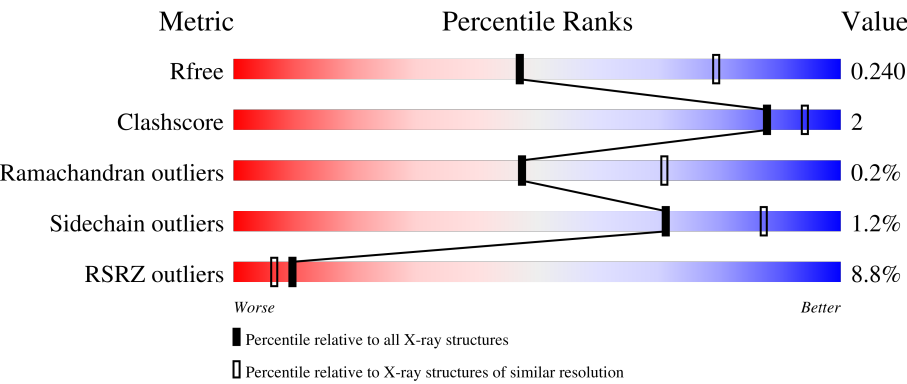
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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 <sub>free</sub>	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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></div><div><div></div><div>93%</div><div>6%</div><div></div></div><div></div></div>
1	C	457	<div><div></div><div><div></div><div>90%</div><div>9%</div><div></div></div><div></div></div>
2	B	472	<div><div>8%</div><div><div></div><div>92%</div><div>7%</div><div></div></div><div></div></div>
2	D	472	<div><div>7%</div><div><div></div><div>93%</div><div>7%</div><div></div></div><div></div></div>
3	E	221	<div><div>31%</div><div><div></div><div>90%</div><div>6%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	H	221	<div><div></div><div>6%</div><div>93%</div><div>5%</div><div></div></div>
4	F	214	<div><div></div><div>33%</div><div>96%</div><div></div><div></div></div>
4	L	214	<div><div></div><div>2%</div><div>94%</div><div>6%</div><div></div></div>
5	G	5	<div><div></div><div>40%</div><div>60%</div><div></div></div>
6	I	2	<div><div></div><div>100%</div><div></div></div>
6	K	2	<div><div></div><div>100%</div><div></div></div>
7	J	4	<div><div></div><div>50%</div><div>50%</div><div></div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21430 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
			3504	2228	603	665	8			
1	C	453	Total	C	N	O	S	0	3	0
			3495	2219	602	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	2	0
			3603	2245	615	710	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
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).

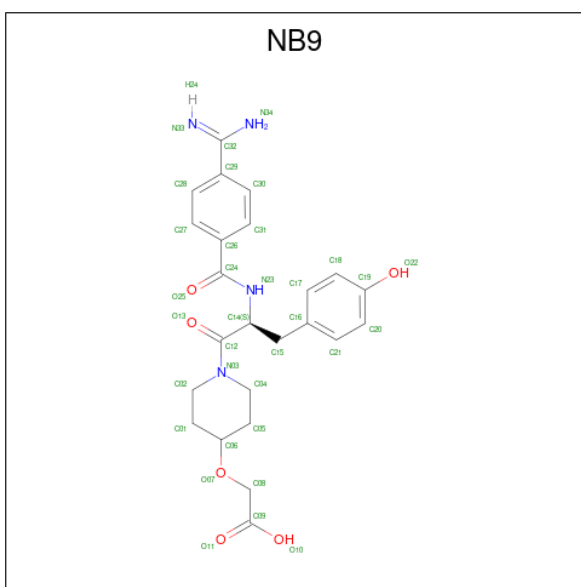
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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 Lamifiban (three-letter code: NB9) (formula:  $C_{24}H_{28}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			34	24	4	6		
12	D	1	Total	C	N	O	0	0
			34	24	4	6		

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

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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	150	Total	O	0	0
			150	150		
14	B	73	Total	O	0	0
			73	73		
14	C	42	Total	O	0	0
			42	42		
14	D	37	Total	O	0	0
			37	37		
14	E	6	Total	O	0	0
			6	6		
14	F	4	Total	O	0	0
			4	4		

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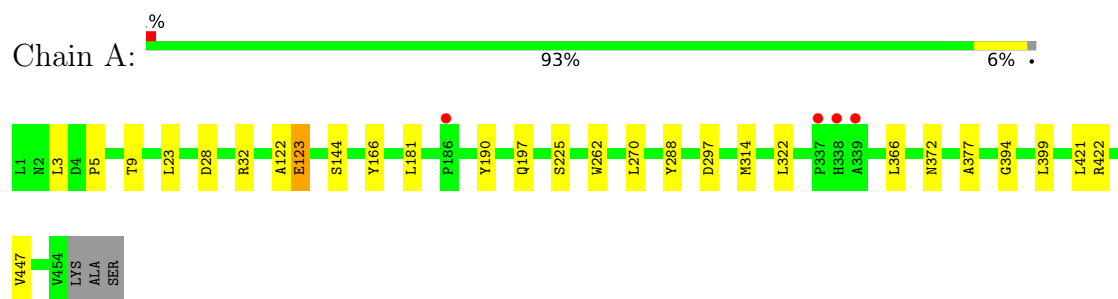
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	8	Total 8	O 8	0	0
14	L	20	Total 20	O 20	0	0

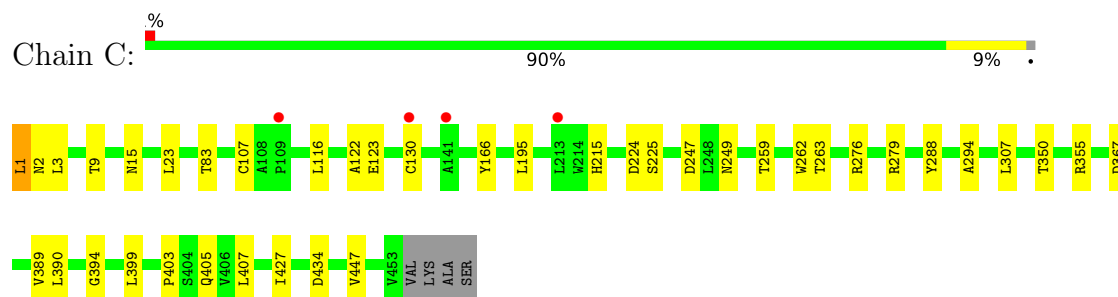
### 3 Residue-property plots [i](#)

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.

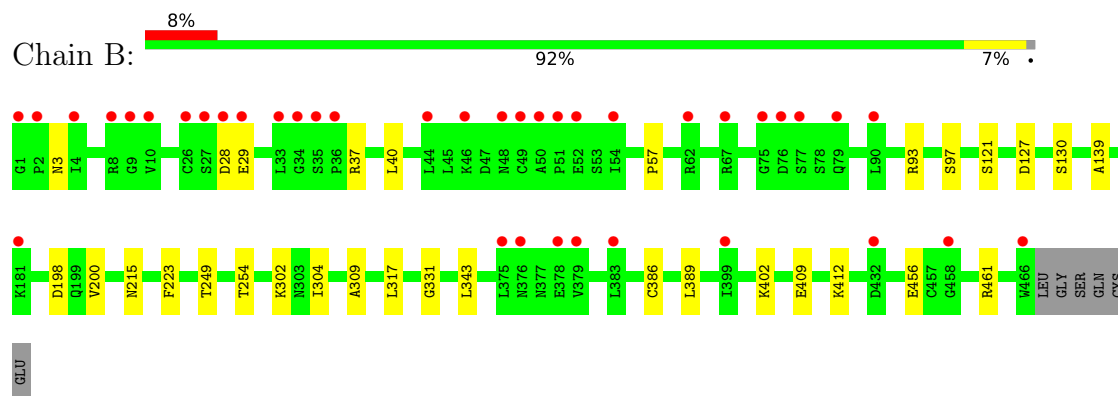
- Molecule 1: Integrin alpha-IIb heavy chain



- Molecule 1: Integrin alpha-IIb heavy chain

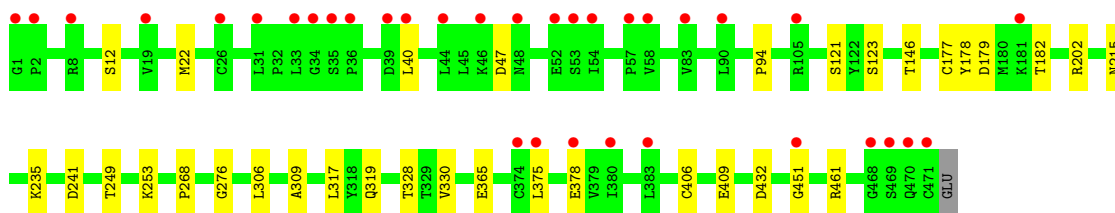


- Molecule 2: Isoform Beta-3C of Integrin beta-3

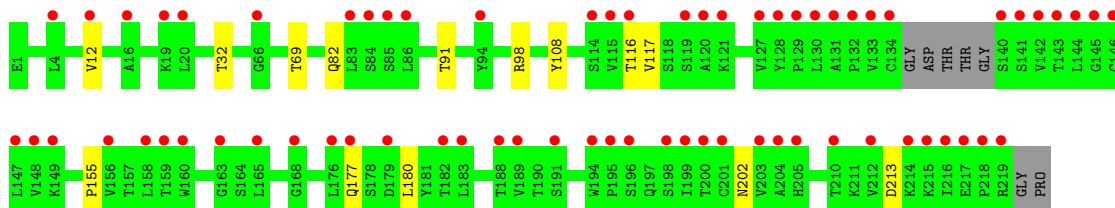
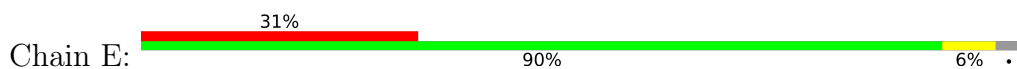


- Molecule 2: Isoform Beta-3C of Integrin beta-3

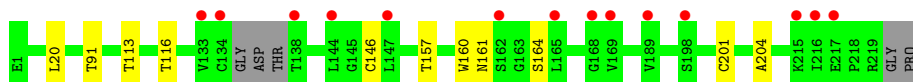




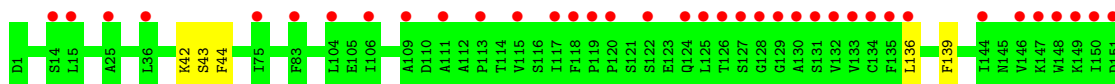
• Molecule 3: 10E5 Fab heavy chain



• 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

Chain I:  100%



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

Chain K:  100%



- 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:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.92Å 144.62Å 105.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.60 48.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.8 (48.97-2.60) 95.6 (48.97-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.223 , 0.242 0.223 , 0.240	Depositor DCC
$R_{free}$ test set	1948 reflections (1.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: CA, NB9, BMA, NAG, CL, MN, MAN, 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	0.27	0/3610	0.48	0/4920
1	C	0.26	0/3594	0.48	0/4897
2	B	0.26	0/3673	0.46	0/4981
2	D	0.25	0/3690	0.45	0/5003
3	E	0.26	0/1673	0.47	0/2290
3	H	0.26	0/1684	0.47	0/2305
4	F	0.26	0/1673	0.47	0/2269
4	L	0.26	0/1673	0.48	0/2269
All	All	0.26	0/21270	0.47	0/28934

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	3504	0	3345	12	0
1	C	3495	0	3327	19	0
2	B	3603	0	3525	17	0
2	D	3623	0	3539	16	0
3	E	1631	0	1590	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	6	0
4	F	1637	0	1553	5	0
4	L	1637	0	1553	5	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	15	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	34	0	0	2	0
12	D	34	0	0	1	0
13	C	1	0	0	0	0
14	A	150	0	0	0	0
14	B	73	0	0	0	0
14	C	42	0	0	0	0
14	D	37	0	0	0	0
14	E	6	0	0	0	0
14	F	4	0	0	1	0
14	H	8	0	0	0	0
14	L	20	0	0	0	0
All	All	21430	0	20203	82	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 2.

All (82) 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:57:PRO:HD2	2:B:93:ARG:NH1	2.19	0.58
2:B:386:CYS:HB3	2:B:389:LEU:HD11	1.86	0.57
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.87	0.55
3:H:91:THR:HG23	3:H:116:THR:HA	1.87	0.54
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.90	0.54
3:E:91:THR:HG23	3:E:116:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:66:GLY:HA3	4:L:71:TYR:HA	1.91	0.52
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.91	0.52
1:C:276:ARG:HD2	1:C:279:ARG:HB2	1.93	0.51
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.92	0.50
3:H:20:LEU:HD22	3:H:113:THR:HG21	1.94	0.50
4:F:210:ASN:OD1	14:F:301:HOH:O	2.20	0.49
2:B:121:SER:HB2	12:B:2005:NB9:O10	2.12	0.49
1:C:3:LEU:O	1:C:405:GLN:NE2	2.41	0.49
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.94	0.49
1:C:107:CYS:HA	1:C:130:CYS:HA	1.94	0.49
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.94	0.49
2:B:3:ASN:ND2	2:B:40:LEU:HG	2.28	0.48
2:D:177:CYS:HB3	2:D:182:THR:HG23	1.96	0.48
2:D:319:GLN:HA	2:D:330:VAL:HG21	1.95	0.48
4:F:43:SER:OG	4:F:44:PHE:N	2.45	0.48
1:C:1:LEU:H1	1:C:367:ASP:HB3	1.78	0.48
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.96	0.47
1:C:224:ASP:OD1	1:C:225:SER:N	2.43	0.47
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.50	0.46
2:B:198:ASP:OD1	2:B:198:ASP:N	2.49	0.46
1:A:225:SER:O	12:B:2005:NB9:N34	2.48	0.46
2:B:249:THR:HA	2:B:309:ALA:O	2.16	0.46
1:A:9:THR:HB	1:A:447:VAL:HB	1.98	0.46
3:H:161:ASN:HB2	3:H:164:SER:HB3	1.97	0.46
2:D:375:LEU:O	2:D:378:GLU:HG2	2.14	0.45
3:E:12:VAL:O	3:E:117:VAL:HA	2.17	0.45
1:C:294:ALA:HB3	1:C:307:LEU:HB2	1.99	0.45
2:B:409:GLU:HB2	2:B:412:LYS:HE2	1.98	0.45
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.52	0.44
3:E:177:GLN:N	3:E:180:LEU:O	2.49	0.44
1:A:377:ALA:HB2	1:A:421:LEU:HD11	1.99	0.44
2:D:178:TYR:CG	2:D:179:ASP:N	2.85	0.44
2:B:28:ASP:OD1	2:B:29:GLU:N	2.50	0.44
3:H:157:THR:OG1	3:H:204:ALA:HB3	2.18	0.44
4:F:136:LEU:HB2	4:F:175:MET:HB3	1.99	0.44
3:H:146:CYS:HB2	3:H:160:TRP:CH2	2.53	0.44
3:H:160:TRP:CZ3	3:H:201:CYS:HB2	2.53	0.44
2:B:331:GLY:HA3	2:B:343:LEU:HD21	1.99	0.43
2:B:97:SER:HB3	2:B:402:LYS:HG2	1.99	0.43
1:A:122:ALA:O	1:A:123:GLU:HB2	2.18	0.43
2:D:249:THR:HA	2:D:309:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLY:HA2	1:A:399:LEU:HD23	2.00	0.43
3:E:202:ASN:HA	3:E:213:ASP:HB3	2.00	0.43
3:E:98:ARG:HG3	3:E:108:TYR:HB2	2.01	0.43
4:F:139:PHE:HD2	4:F:198:HIS:HE2	1.66	0.43
2:D:121:SER:HB2	12:D:2005:NB9:O10	2.18	0.43
2:D:22:MET:HG2	2:D:40:LEU:HD22	2.01	0.42
1:C:427:ILE:HG22	1:C:434:ASP:OD2	2.19	0.42
4:F:42:LYS:N	4:F:42:LYS:HD2	2.34	0.42
1:C:259:THR:HA	1:C:263:THR:HA	2.02	0.42
1:C:389:VAL:HB	1:C:407:LEU:HB2	2.01	0.42
2:D:235:LYS:HE3	2:D:276:GLY:O	2.20	0.42
1:A:28:ASP:OD2	1:A:32:ARG:HB3	2.19	0.42
1:A:297:ASP:O	1:A:372:ASN:HB2	2.19	0.42
2:B:249:THR:HG22	2:B:309:ALA:HB3	2.01	0.42
1:C:83:THR:HB	1:C:116:LEU:HB2	2.01	0.42
1:A:3:LEU:HG	1:A:366:LEU:HD21	2.01	0.42
2:D:179:ASP:N	2:D:179:ASP:OD1	2.53	0.42
1:A:314:MET:HB3	1:A:322:LEU:HB3	2.02	0.42
1:C:122:ALA:O	1:C:123:GLU:HB2	2.21	0.41
1:C:262:TRP:CD1	2:D:253:LYS:HE2	2.55	0.41
2:D:365:GLU:CD	2:D:365:GLU:H	2.23	0.41
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.53	0.41
4:L:13:VAL:HG11	4:L:19:VAL:HG11	2.02	0.41
3:E:69:THR:HB	3:E:82:GLN:HB3	2.01	0.41
2:B:302:LYS:HB2	2:B:304:ILE:HG12	2.03	0.41
2:B:97:SER:HB3	2:B:402:LYS:HA	2.03	0.41
1:C:9:THR:HB	1:C:447:VAL:HB	2.03	0.41
1:C:355:ARG:NH2	2:D:268:PRO:HB3	2.35	0.41
4:L:103:LYS:HD2	4:L:105:GLU:OE2	2.20	0.41
1:C:394:GLY:HA2	1:C:399:LEU:HD23	2.03	0.40
2:D:94:PRO:HG3	2:D:406:CYS:HB2	2.02	0.40
1:A:3:LEU:O	1:A:5:PRO:HD3	2.21	0.40
1:A:181:LEU:O	1:A:197:GLN:HA	2.22	0.40
1:C:247:ASP:OD1	1:C:249:ASN:HB2	2.20	0.40
1:C:390:LEU:HD23	1:C:403:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	439 (96%)	16 (4%)	1 (0%)	47	71
1	C	454/457 (99%)	436 (96%)	18 (4%)	0	100	100
2	B	466/472 (99%)	442 (95%)	24 (5%)	0	100	100
2	D	469/472 (99%)	440 (94%)	28 (6%)	1 (0%)	47	71
3	E	210/221 (95%)	197 (94%)	12 (6%)	1 (0%)	29	52
3	H	212/221 (96%)	201 (95%)	11 (5%)	0	100	100
4	F	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
4	L	212/214 (99%)	203 (96%)	7 (3%)	2 (1%)	17	35
All	All	2691/2728 (99%)	2555 (95%)	131 (5%)	5 (0%)	47	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	451	GLY
4	L	77	SER
1	A	123	GLU
4	L	68	GLY
3	E	155	PRO

### 5.3.2 Protein sidechains

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%)	359 (98%)	7 (2%)	57	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	364/364 (100%)	356 (98%)	8 (2%)	52	76
2	B	414/417 (99%)	410 (99%)	4 (1%)	76	90
2	D	416/417 (100%)	408 (98%)	8 (2%)	57	79
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%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2309/2318 (100%)	2282 (99%)	27 (1%)	71	87

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	144	SER
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
1	A	422	ARG
2	B	37	ARG
2	B	127	ASP
2	B	130	SER
2	B	215	ASN
1	C	1	LEU
1	C	2	ASN
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	195	LEU
1	C	288	TYR
1	C	350	THR
2	D	47	ASP
2	D	123	SER
2	D	146	THR
2	D	202	ARG
2	D	215	ASN
2	D	241	ASP
2	D	409	GLU
2	D	432	ASP

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

Mol	Chain	Res	Type
1	A	395	GLN
2	D	280	HIS
2	D	446	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	0.34	0	17,19,21	0.51	0
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.44	0
5	BMA	G	3	5	11,11,12	1.26	2 (18%)	15,15,17	1.05	1 (6%)
5	MAN	G	4	5	11,11,12	0.81	0	15,15,17	1.26	2 (13%)
5	MAN	G	5	5	11,11,12	1.41	1 (9%)	15,15,17	2.08	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.32	0	17,19,21	0.41	0
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.44	0
7	NAG	J	1	7,2	14,14,15	0.39	0	17,19,21	0.53	0
7	NAG	J	2	7	14,14,15	0.24	0	17,19,21	0.56	0
7	BMA	J	3	7	11,11,12	0.96	0	15,15,17	1.24	3 (20%)
7	MAN	J	4	7	11,11,12	0.90	1 (9%)	15,15,17	1.07	1 (6%)
6	NAG	K	1	6,2	14,14,15	0.30	0	17,19,21	0.42	0
6	NAG	K	2	6	14,14,15	0.17	0	17,19,21	0.45	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	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	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	-	1/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	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	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	O5-C5	3.90	1.51	1.43
5	G	3	BMA	C4-C5	2.35	1.58	1.53
7	J	4	MAN	C1-C2	2.23	1.57	1.52
5	G	3	BMA	C4-C3	2.12	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-O5-C5	6.76	121.35	112.19
5	G	4	MAN	C1-O5-C5	3.40	116.80	112.19
7	J	3	BMA	C1-C2-C3	2.85	113.17	109.67
7	J	4	MAN	O2-C2-C3	-2.70	104.73	110.14
5	G	4	MAN	O2-C2-C3	-2.43	105.27	110.14
7	J	3	BMA	C1-O5-C5	2.43	115.48	112.19
5	G	3	BMA	O2-C2-C3	-2.29	105.55	110.14
5	G	5	MAN	O5-C1-C2	2.22	114.20	110.77
7	J	3	BMA	O2-C2-C3	-2.15	105.83	110.14

There are no chirality outliers.

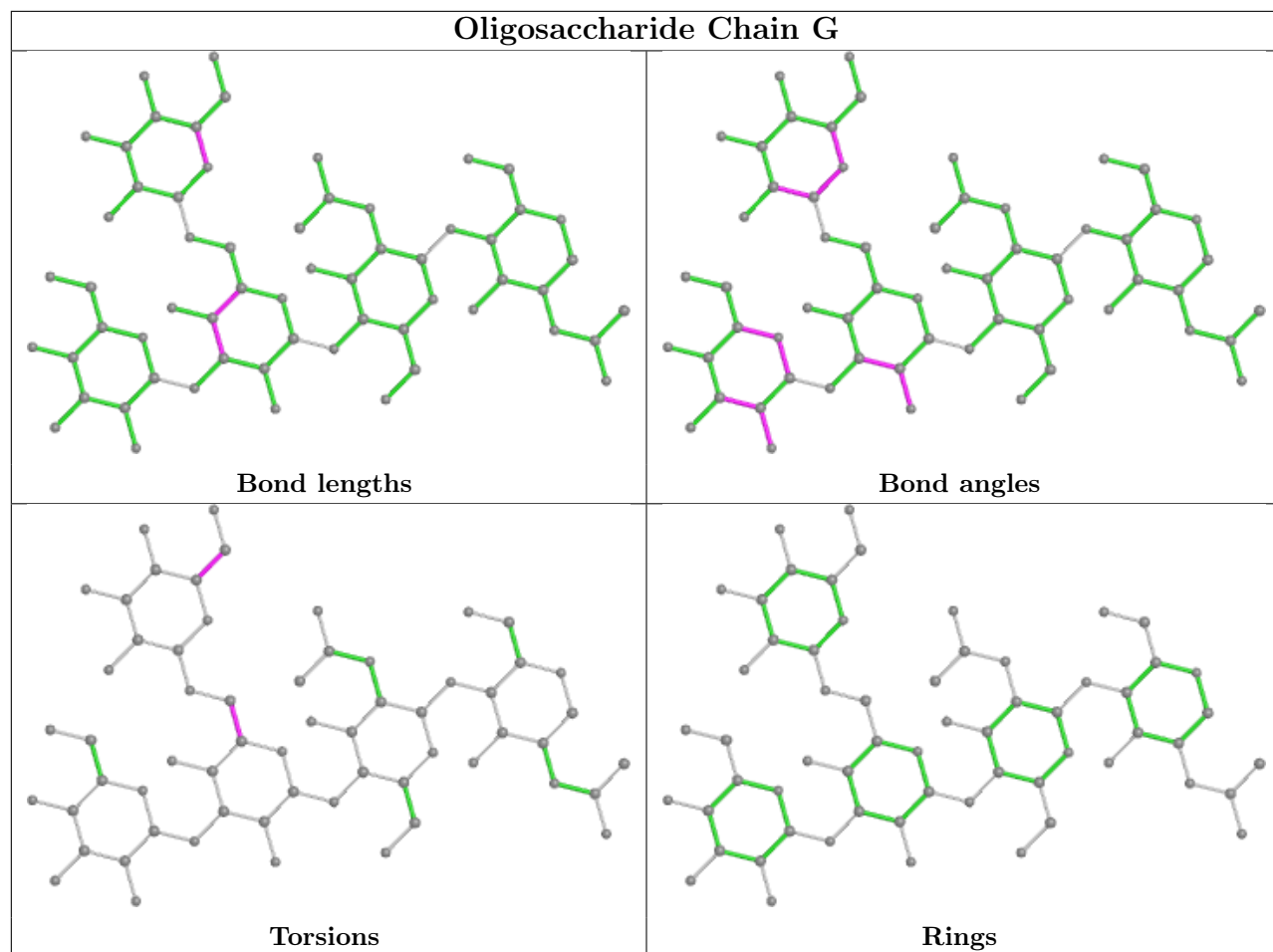
All (16) torsion outliers are listed below:

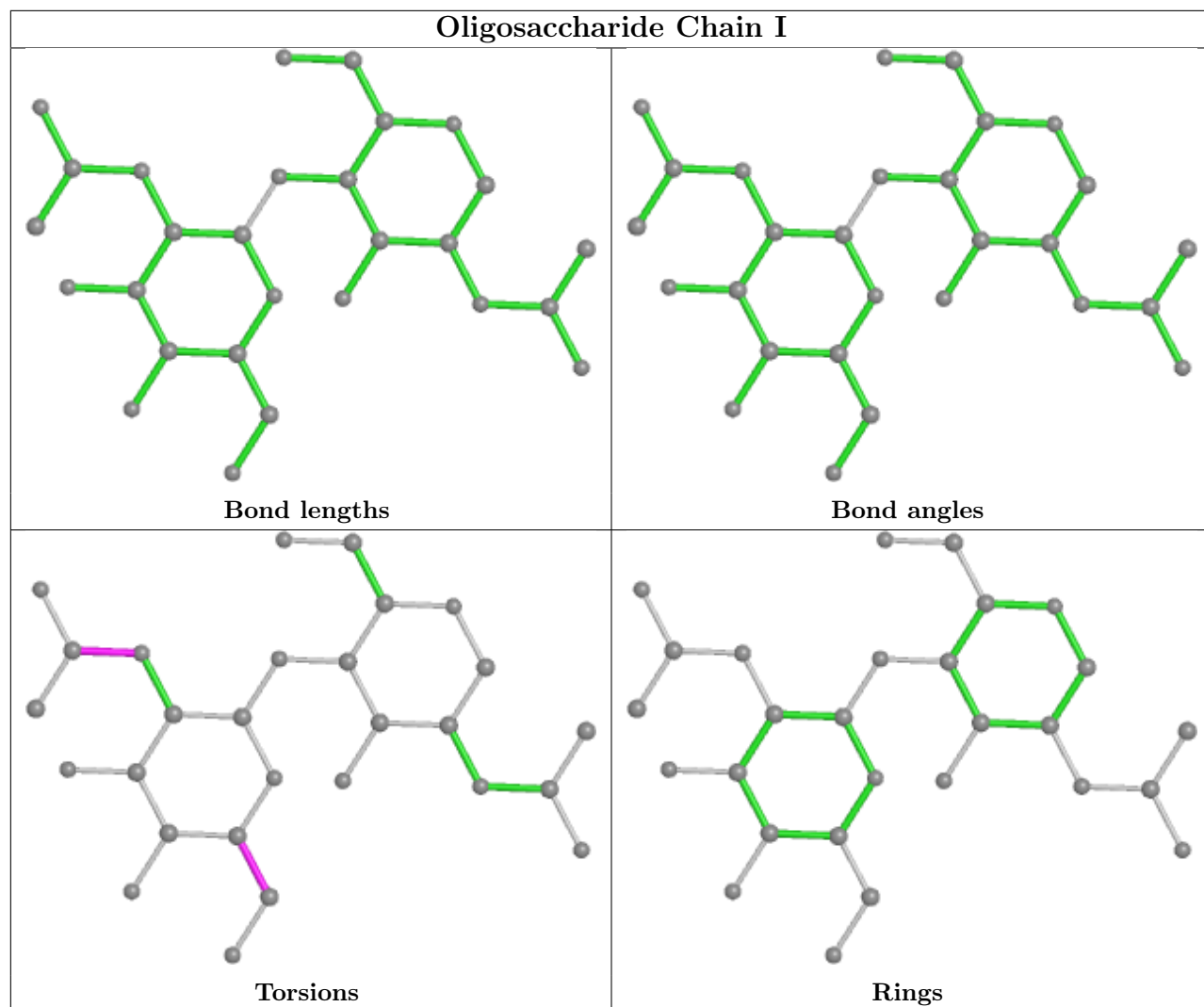
Mol	Chain	Res	Type	Atoms
5	G	5	MAN	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
7	J	2	NAG	C4-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6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

There are no ring outliers.

No monomer is involved in short contacts.

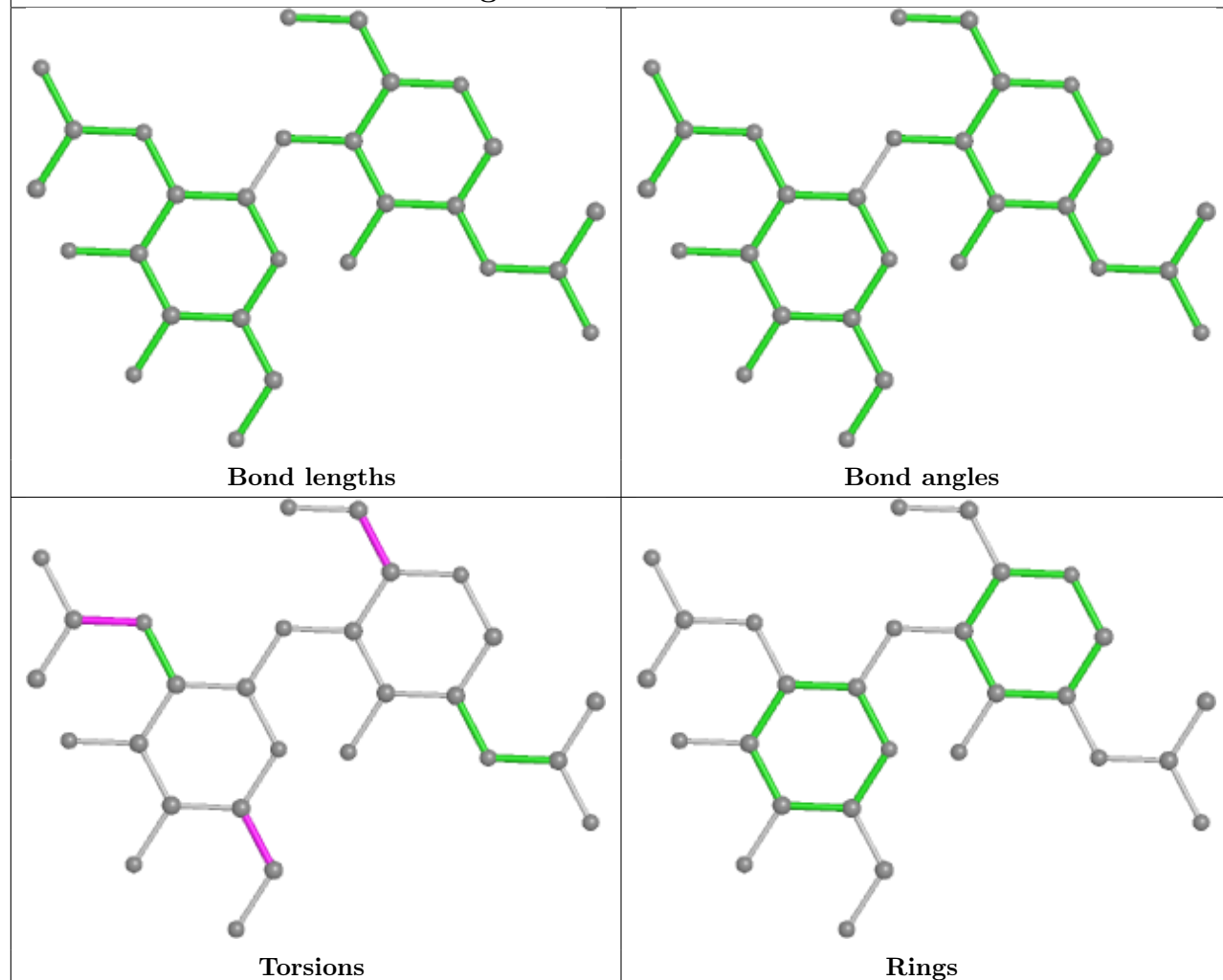
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



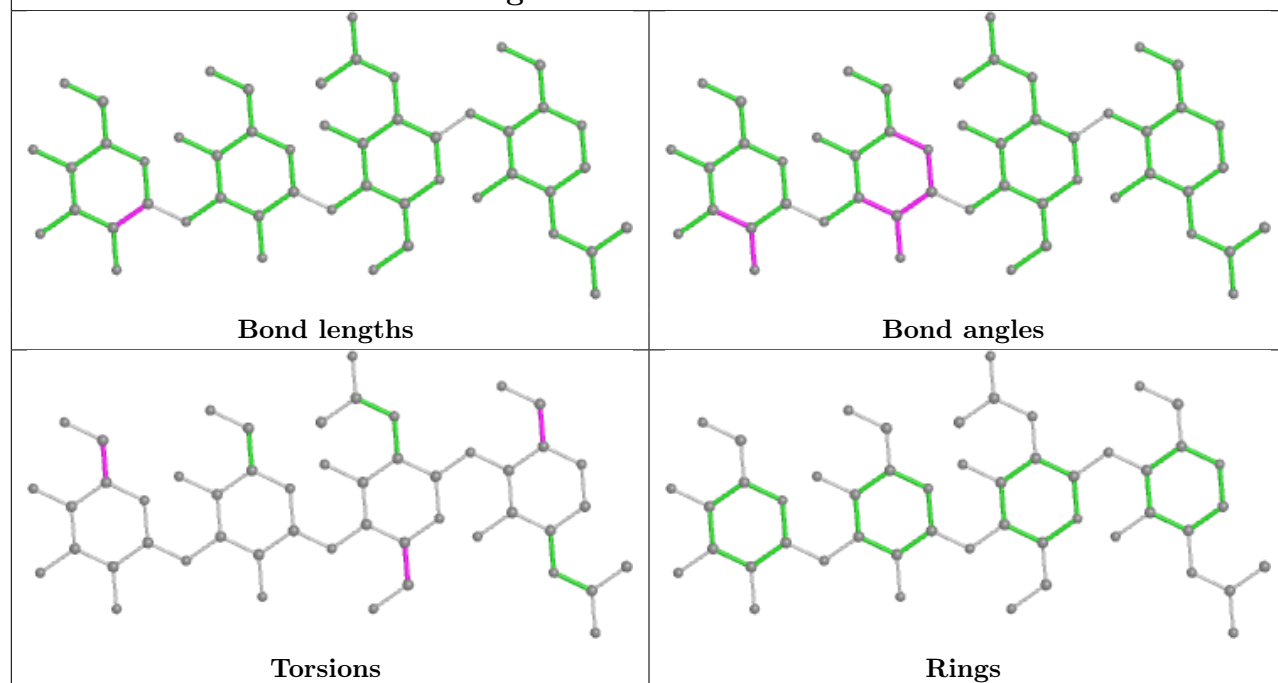




## Oligosaccharide Chain K



## Oligosaccharide Chain J



## 5.6 Ligand geometry

Of 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 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	A	503	-	4,4,4	0.13	0	6,6,6	0.16	0
11	NAG	D	2004	2	14,14,15	0.31	0	17,19,21	0.57	0
12	NB9	B	2005	10	36,36,36	2.59	9 (25%)	44,49,49	1.14	2 (4%)
8	SO4	A	502	-	4,4,4	0.16	0	6,6,6	0.09	0
8	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.10	0
11	NAG	B	2004	2	14,14,15	0.29	0	17,19,21	0.57	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.11	0
8	SO4	C	502	-	4,4,4	0.16	0	6,6,6	0.14	0
8	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.10	0
12	NB9	D	2005	10	36,36,36	2.57	9 (25%)	44,49,49	1.15	2 (4%)
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.11	0
8	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.26	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	NB9	D	2005	10	-	3/29/39/39	0/3/3/3
11	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
11	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
12	NB9	B	2005	10	-	2/29/39/39	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2005	NB9	C12-N03	10.25	1.49	1.34
12	B	2005	NB9	C12-N03	10.21	1.49	1.34
12	B	2005	NB9	C24-N23	7.18	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2005	NB9	C24-N23	7.03	1.49	1.34
12	B	2005	NB9	O13-C12	-4.56	1.14	1.22
12	D	2005	NB9	O13-C12	-4.43	1.14	1.22
12	D	2005	NB9	C32-N34	4.26	1.44	1.33
12	B	2005	NB9	C32-N34	4.16	1.44	1.33
12	B	2005	NB9	C02-N03	2.78	1.52	1.47
12	D	2005	NB9	C02-N03	2.68	1.51	1.47
12	B	2005	NB9	C04-N03	2.67	1.51	1.47
12	D	2005	NB9	C04-N03	2.67	1.51	1.47
12	B	2005	NB9	C15-C16	2.55	1.57	1.51
12	D	2005	NB9	C15-C16	2.52	1.57	1.51
12	B	2005	NB9	C26-C24	2.45	1.55	1.50
12	B	2005	NB9	C14-N23	2.39	1.50	1.45
12	D	2005	NB9	C26-C24	2.34	1.55	1.50
12	D	2005	NB9	C14-N23	2.30	1.50	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2005	NB9	C02-C01-C06	3.54	114.21	110.32
12	D	2005	NB9	C02-C01-C06	3.21	113.85	110.32
12	B	2005	NB9	C01-C02-N03	3.17	115.65	110.82
12	D	2005	NB9	C04-C05-C06	3.06	113.69	110.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	2004	NAG	O5-C5-C6-O6
11	B	2004	NAG	C4-C5-C6-O6
12	D	2005	NB9	O07-C08-C09-O11
12	D	2005	NB9	C09-C08-O07-C06
12	D	2005	NB9	O07-C08-C09-O10
12	B	2005	NB9	O07-C08-C09-O11
12	B	2005	NB9	N23-C14-C15-C16

There are no ring outliers.

2 monomers are involved in 3 short contacts:

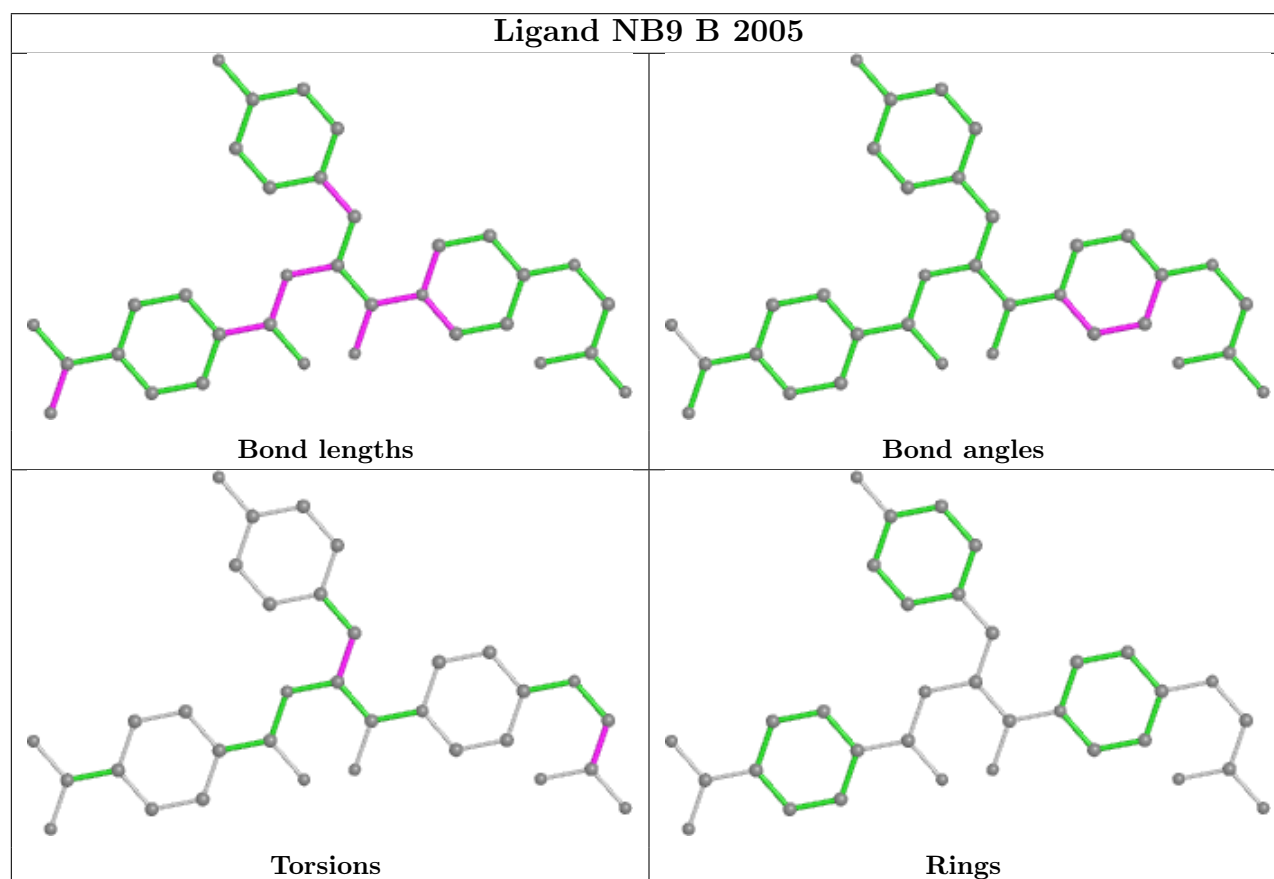
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	2005	NB9	2	0

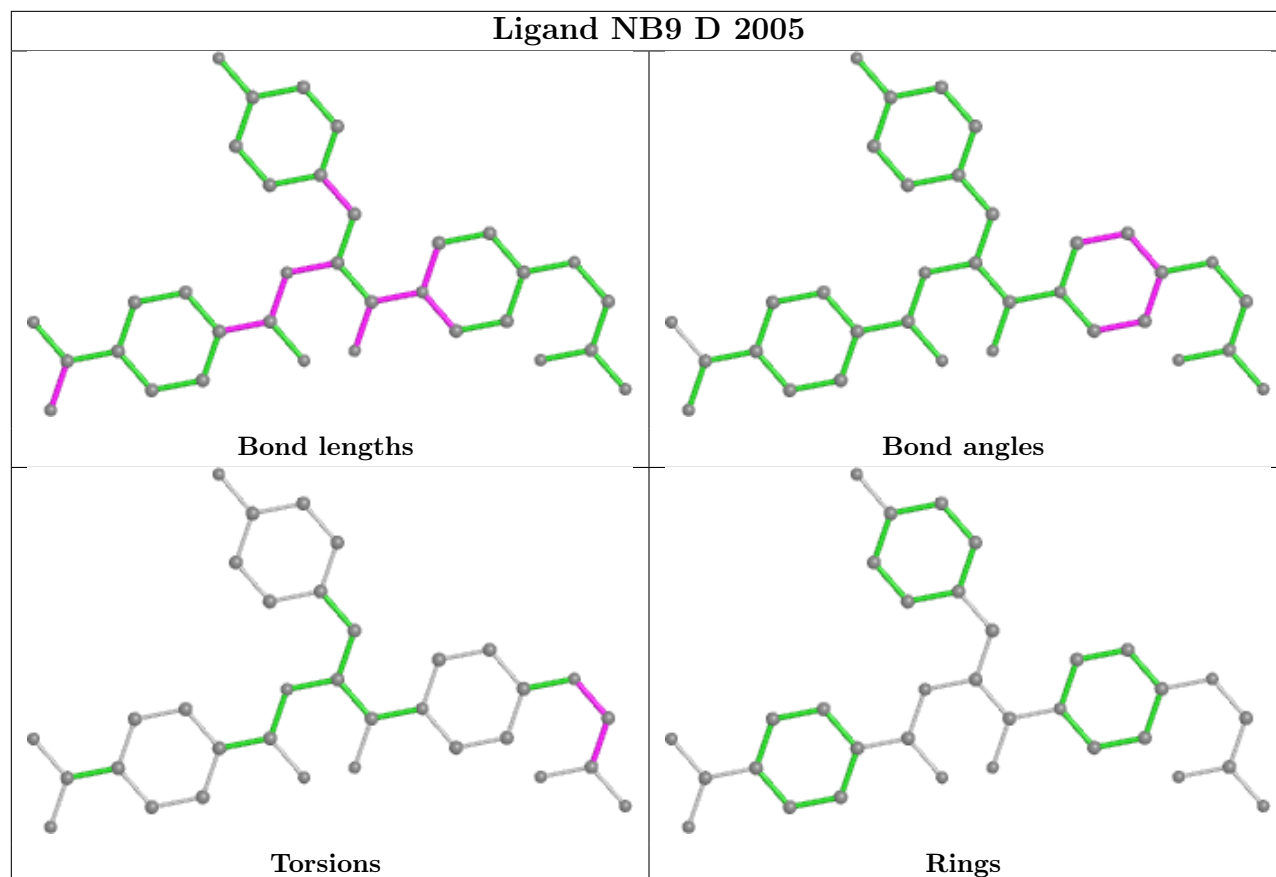
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2005	NB9	1	0

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

### 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%)	0.38	4 (0%) 84 82	46, 58, 78, 96	0
1	C	453/457 (99%)	0.33	4 (0%) 84 82	55, 77, 97, 113	0
2	B	466/472 (98%)	0.58	39 (8%) 11 7	49, 84, 142, 154	1 (0%)
2	D	471/472 (99%)	0.49	34 (7%) 15 11	61, 97, 133, 149	1 (0%)
3	E	214/221 (96%)	1.72	68 (31%) 0 0	97, 133, 187, 197	0
3	H	216/221 (97%)	0.45	14 (6%) 18 14	72, 106, 139, 142	0
4	F	214/214 (100%)	1.48	71 (33%) 0 0	98, 139, 185, 196	0
4	L	214/214 (100%)	0.27	4 (1%) 66 62	76, 100, 113, 137	0
All	All	2702/2728 (99%)	0.62	238 (8%) 10 7	46, 90, 165, 197	2 (0%)

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	216	ILE	10.0
3	E	147	LEU	9.8
3	E	201	CYS	9.1
3	E	133	VAL	9.1
4	F	115	VAL	9.0
3	E	134	CYS	8.1
4	F	214	CYS	7.6
3	E	196	SER	7.5
4	F	130	ALA	7.5
4	F	193	THR	7.5
3	E	199	ILE	7.5
3	E	212	VAL	7.2
3	E	142	VAL	7.0
4	F	148	TRP	7.0
3	E	130	LEU	6.9
3	E	194	TRP	6.7

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Mol	Chain	Res	Type	RSRZ
4	F	179	LEU	6.5
3	E	144	LEU	6.5
2	B	33	LEU	6.4
2	D	375	LEU	6.4
3	E	160	TRP	6.1
3	E	218	PRO	6.0
4	F	209	PHE	6.0
4	F	180	THR	5.9
4	F	134	CYS	5.9
4	F	195	GLU	5.8
2	D	1	GLY	5.8
3	H	216	ILE	5.7
4	L	214	CYS	5.5
3	E	210	THR	5.5
2	D	469	SER	5.4
4	F	181	LEU	5.3
3	E	188	THR	5.2
4	F	207	LYS	5.1
3	E	219	ARG	5.1
3	E	200	THR	5.1
4	F	125	LEU	5.1
3	E	132	PRO	5.1
3	E	131	ALA	5.0
4	F	206	VAL	5.0
3	E	16	ALA	4.9
3	E	145	GLY	4.9
3	E	156	VAL	4.9
3	E	143	THR	4.8
3	E	195	PRO	4.8
4	F	178	THR	4.7
3	E	129	PRO	4.6
4	F	150	ILE	4.6
3	E	198	SER	4.6
4	F	213	GLU	4.5
3	H	165	LEU	4.5
4	F	132	VAL	4.5
4	F	133	VAL	4.4
4	F	208	SER	4.4
3	E	165	LEU	4.3
4	F	146	VAL	4.3
3	E	149	LYS	4.3
3	E	217	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	181	LYS	4.2
4	F	147	LYS	4.2
4	F	135	PHE	4.1
3	E	158	LEU	4.0
2	D	33	LEU	4.0
2	D	2	PRO	4.0
2	D	380	ILE	4.0
2	B	8	ARG	3.9
4	F	182	THR	3.9
3	H	198	SER	3.9
4	F	194	CYS	3.8
2	D	44	LEU	3.8
2	B	34	GLY	3.8
3	E	146	CYS	3.8
2	B	36	PRO	3.7
4	F	159	VAL	3.7
3	H	144	LEU	3.6
4	F	204	PRO	3.6
2	D	36	PRO	3.6
2	B	77	SER	3.6
2	B	2	PRO	3.6
2	D	181	LYS	3.6
4	F	160	LEU	3.6
2	B	54	ILE	3.6
2	D	90	LEU	3.6
3	E	120	ALA	3.5
2	B	376	ASN	3.5
2	B	375	LEU	3.5
3	E	176	LEU	3.5
3	E	205	HIS	3.5
2	B	28	ASP	3.5
2	D	54	ILE	3.5
3	E	148	VAL	3.4
2	B	44	LEU	3.4
3	E	204	ALA	3.4
4	F	154	GLU	3.4
4	F	117	ILE	3.3
3	E	85	SER	3.3
2	B	75	GLY	3.3
4	F	111	ALA	3.3
4	F	149	LYS	3.3
3	E	183	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	157	ASN	3.2
2	D	468	GLY	3.2
4	F	119	PRO	3.2
3	E	215	LYS	3.2
3	E	189	VAL	3.2
4	F	192	TYR	3.2
4	F	203	SER	3.2
2	B	76	ASP	3.1
4	F	129	GLY	3.1
2	B	46	LYS	3.1
4	F	126	THR	3.1
3	H	215	LYS	3.1
2	D	471	CYS	3.1
3	E	84	SER	3.1
3	E	141	SER	3.0
3	H	138	THR	3.0
3	E	214	LYS	3.0
4	F	197	THR	3.0
3	E	127	VAL	3.0
4	F	155	ARG	3.0
4	L	212	ASN	3.0
4	F	122	SER	3.0
3	E	115	VAL	3.0
2	B	466	TRP	3.0
3	E	83	LEU	2.9
3	H	134	CYS	2.9
2	D	35	SER	2.9
4	F	156	GLN	2.9
2	D	378	GLU	2.9
4	F	210	ASN	2.9
4	F	106	ILE	2.9
2	B	378	GLU	2.9
2	D	58	VAL	2.9
4	F	151	ASP	2.8
4	F	200	THR	2.8
3	E	140	SER	2.8
3	E	203	VAL	2.8
2	B	383	LEU	2.8
2	B	10	VAL	2.7
2	D	470	GLN	2.7
4	F	191	SER	2.7
4	F	186	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	159	THR	2.7
2	D	26	CYS	2.7
3	E	128	TYR	2.7
4	F	144	ILE	2.7
4	F	201	SER	2.7
3	E	121	LYS	2.7
3	H	147	LEU	2.6
4	F	120	PRO	2.6
2	D	383	LEU	2.6
4	F	205	ILE	2.6
3	H	133	VAL	2.6
3	H	168	GLY	2.6
4	F	212	ASN	2.6
3	E	20	LEU	2.6
4	F	128	GLY	2.5
4	F	131	SER	2.5
2	B	52	GLU	2.5
2	B	49	CYS	2.5
2	D	34	GLY	2.5
2	B	26	CYS	2.5
4	F	15	LEU	2.5
2	B	51	PRO	2.4
4	F	136	LEU	2.4
2	B	1	GLY	2.4
4	F	202	THR	2.4
1	A	337	PRO	2.4
3	E	177	GLN	2.4
3	H	162	SER	2.4
4	F	127	SER	2.4
2	D	451	GLY	2.4
1	A	338	HIS	2.3
2	D	53	SER	2.3
3	E	119	SER	2.3
4	F	104	LEU	2.3
2	B	29	GLU	2.3
4	F	183	LYS	2.3
2	D	57	PRO	2.3
2	B	27	SER	2.3
2	B	458	GLY	2.3
3	H	189	VAL	2.3
4	F	198	HIS	2.3
2	B	48	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	35	SER	2.3
3	E	4	LEU	2.3
3	E	114	SER	2.3
1	C	130	CYS	2.3
2	B	399	ILE	2.3
3	E	19	LYS	2.3
3	E	163	GLY	2.2
2	D	8	ARG	2.2
2	D	374	CYS	2.2
4	F	83	PHE	2.2
4	F	118	PHE	2.2
3	E	116	THR	2.2
4	L	213	GLU	2.2
2	D	19	VAL	2.2
2	B	62	ARG	2.2
3	E	12	VAL	2.2
1	A	339	ALA	2.2
3	E	66	GLY	2.2
3	E	94	TYR	2.2
2	B	90	LEU	2.2
3	E	86	LEU	2.2
2	D	40	LEU	2.1
4	F	25	ALA	2.1
4	F	109	ALA	2.1
4	L	206	VAL	2.1
4	F	113	PRO	2.1
2	D	52	GLU	2.1
2	B	67	ARG	2.1
2	B	50	ALA	2.1
2	B	432	ASP	2.1
3	H	169	VAL	2.1
4	F	124	GLN	2.1
1	C	141	ALA	2.1
2	D	46	LYS	2.1
2	D	48	ASN	2.1
3	E	168	GLY	2.1
3	H	217	GLU	2.1
2	B	4	ILE	2.1
1	C	109	PRO	2.1
4	F	75	ILE	2.1
3	E	182	THR	2.1
3	E	191	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	36	LEU	2.0
1	A	186	PRO	2.0
4	F	14	SER	2.0
2	D	83	VAL	2.0
2	D	105	ARG	2.0
2	B	9	GLY	2.0
2	D	39	ASP	2.0
1	C	213	LEU	2.0
2	D	31	LEU	2.0
2	B	379	VAL	2.0
3	E	179	ASP	2.0
2	B	79	GLN	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](#)

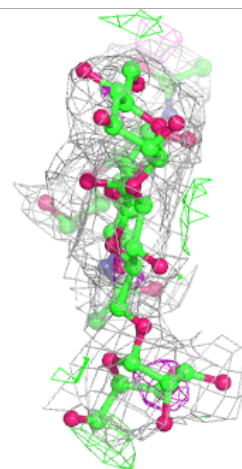
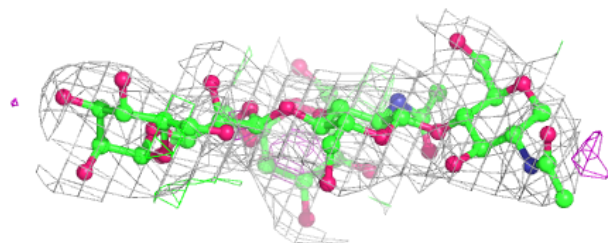
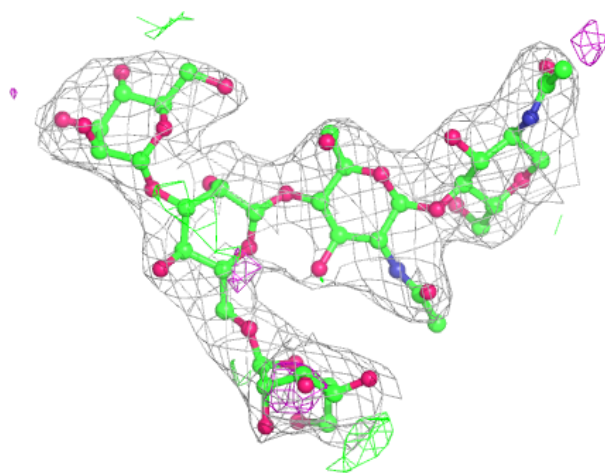
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	BMA	J	3	11/12	0.79	0.29	104,104,104,104	0
5	MAN	G	5	11/12	0.80	0.25	101,101,101,101	0
5	BMA	G	3	11/12	0.87	0.15	93,93,93,93	0
6	NAG	K	1	14/15	0.88	0.22	116,116,116,116	0
7	MAN	J	4	11/12	0.88	0.25	103,103,103,103	0
6	NAG	K	2	14/15	0.89	0.23	118,118,118,118	0
7	NAG	J	2	14/15	0.89	0.27	98,98,98,98	0
6	NAG	I	2	14/15	0.90	0.20	114,114,114,114	0
5	MAN	G	4	11/12	0.91	0.15	91,91,91,91	0
6	NAG	I	1	14/15	0.91	0.20	112,112,112,112	0
5	NAG	G	2	14/15	0.93	0.15	84,84,84,84	0
7	NAG	J	1	14/15	0.94	0.12	88,88,88,88	0
5	NAG	G	1	14/15	0.95	0.16	71,71,71,71	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.

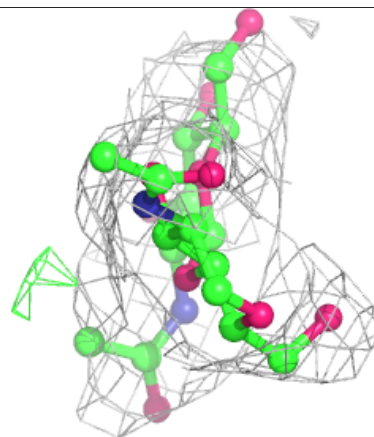
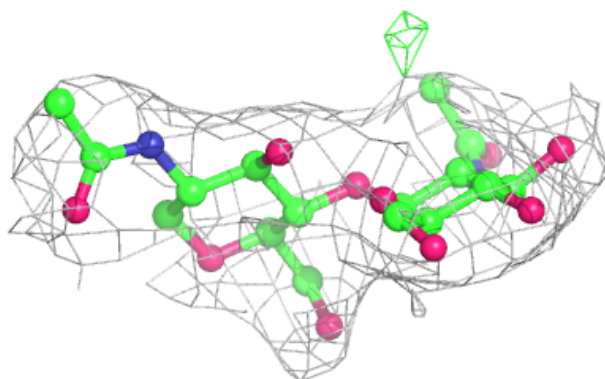
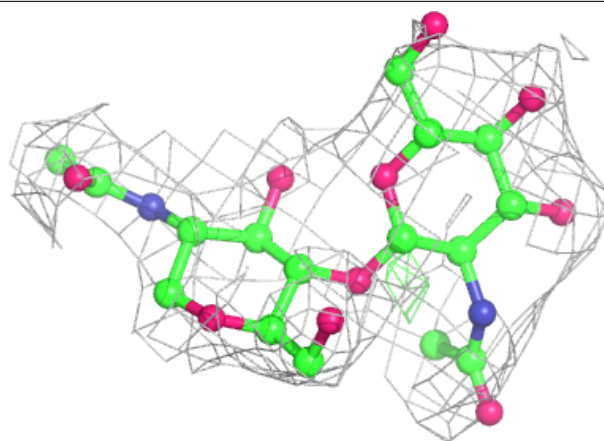
**Electron density around Chain G:**

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



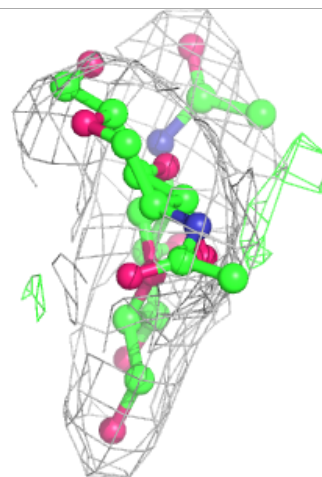
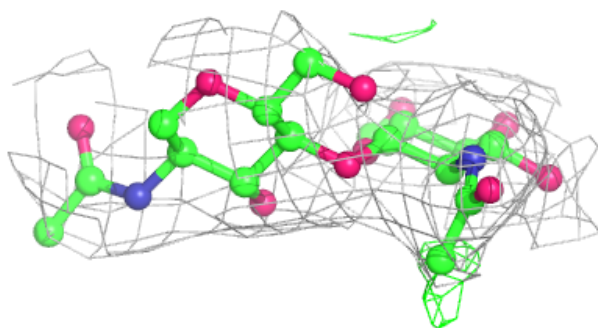
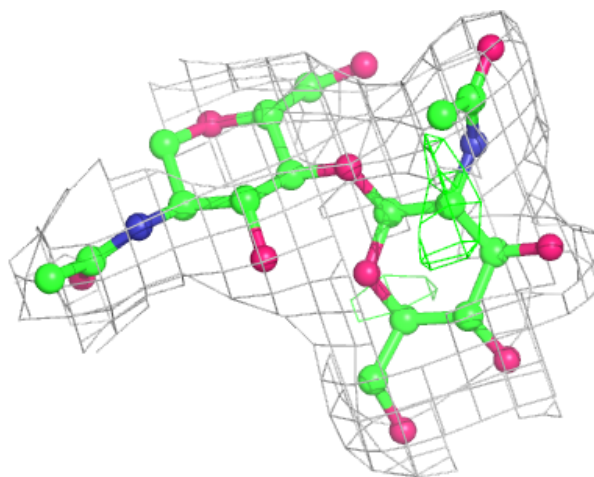
**Electron density around Chain I:**

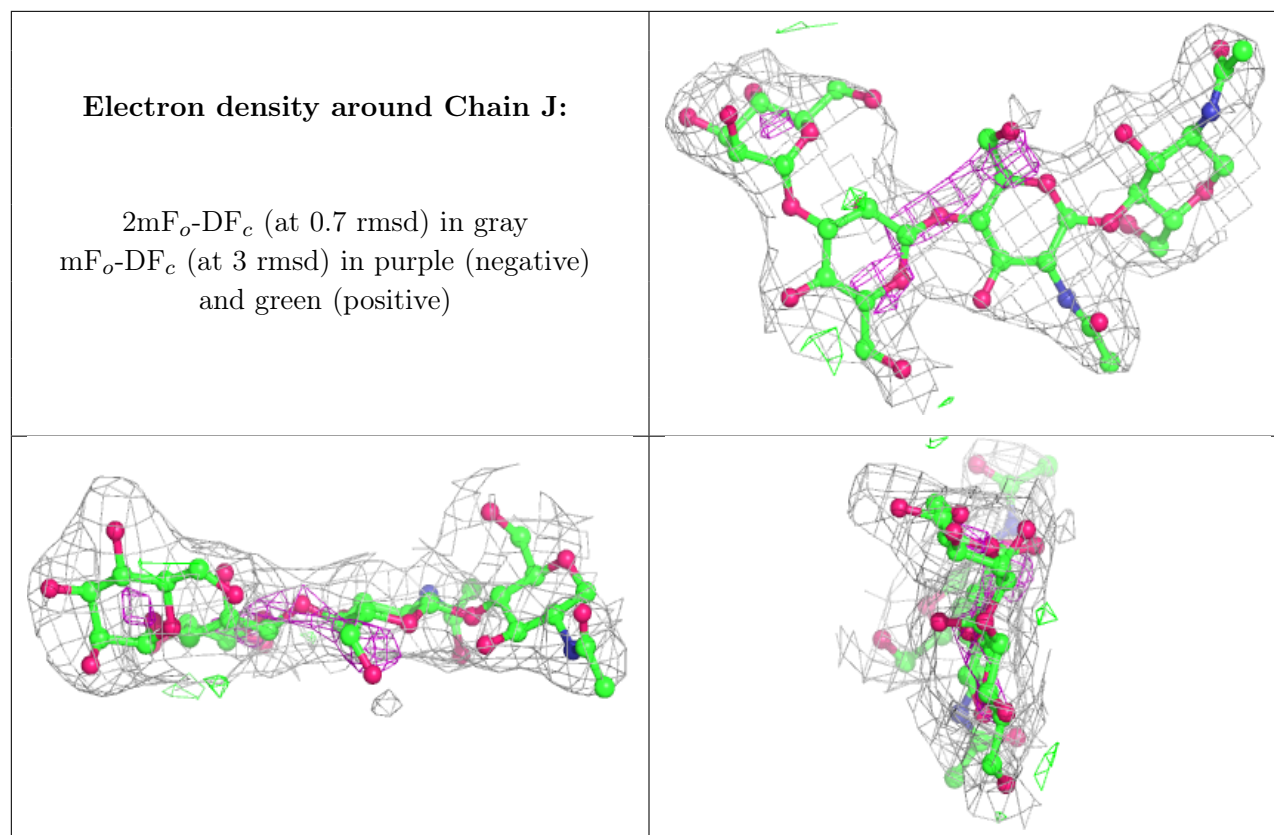
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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
10	MN	B	2002	1/1	0.22	0.21	80,80,80,80	1
9	CA	A	504	1/1	0.77	0.12	68,68,68,68	0
11	NAG	D	2004	14/15	0.86	0.22	113,113,113,113	0
8	SO4	L	301	5/5	0.87	0.14	101,101,101,101	0
8	SO4	C	502	5/5	0.89	0.14	96,96,96,96	0
9	CA	A	505	1/1	0.89	0.16	55,55,55,55	0
9	CA	C	505	1/1	0.91	0.08	95,95,95,95	0
11	NAG	B	2004	14/15	0.91	0.29	110,110,110,110	0
9	CA	C	508	1/1	0.91	0.16	74,74,74,74	0
8	SO4	C	501	5/5	0.92	0.16	91,91,91,91	0
9	CA	C	506	1/1	0.92	0.09	84,84,84,84	0
13	CL	C	504	1/1	0.92	0.22	84,84,84,84	0
12	NB9	B	2005	34/34	0.93	0.23	60,60,60,60	0
12	NB9	D	2005	34/34	0.93	0.22	80,80,80,80	0

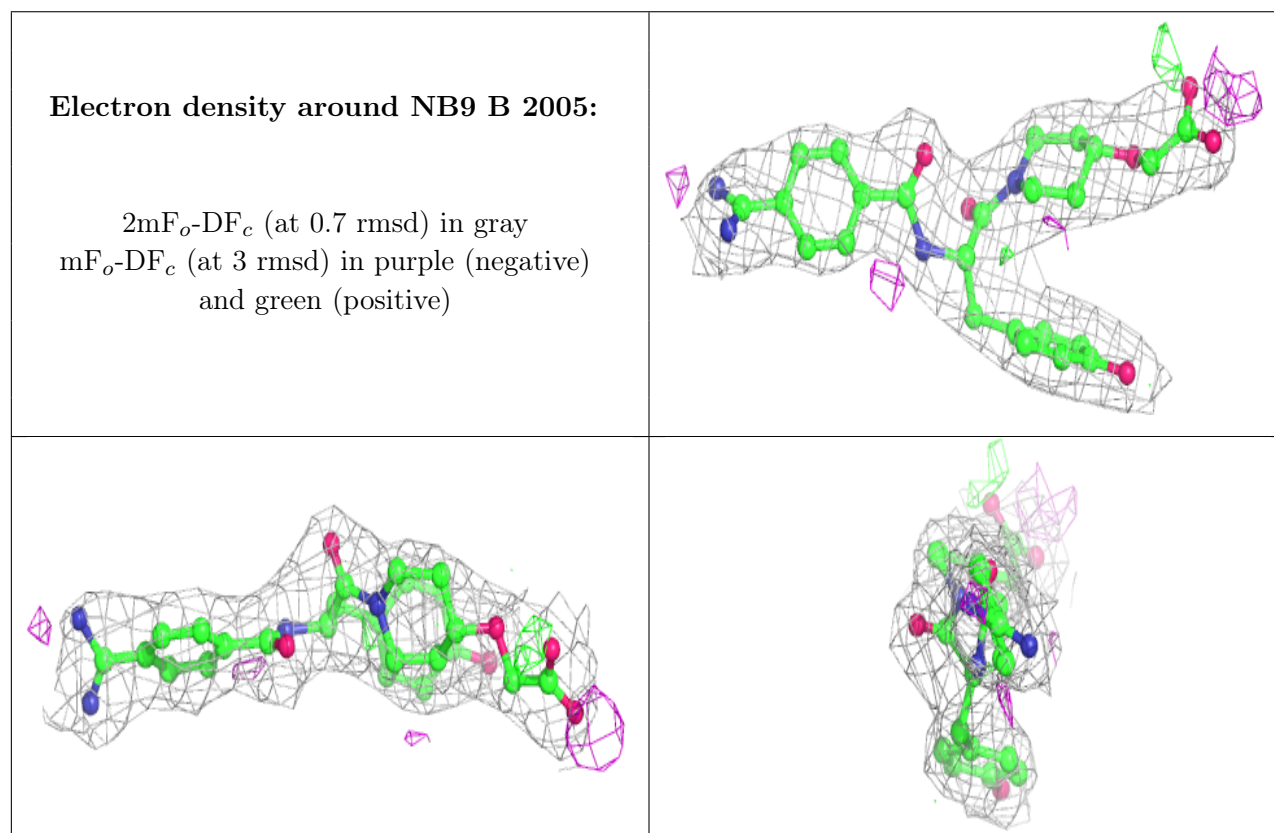
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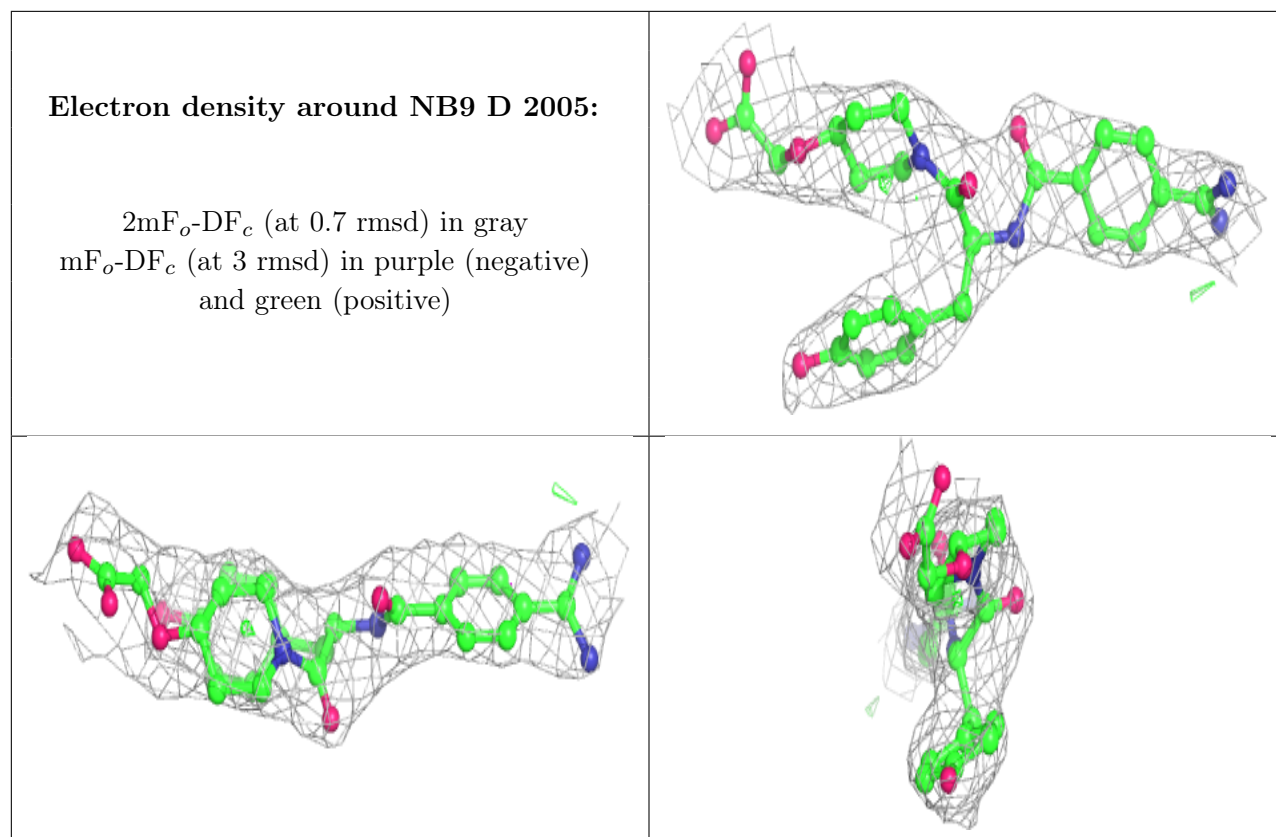


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	A	501	5/5	0.93	0.18	90,90,90,90	0
9	CA	C	507	1/1	0.94	0.16	77,77,77,77	0
8	SO4	A	503	5/5	0.94	0.10	75,75,75,75	0
10	MN	D	2002	1/1	0.95	0.05	98,98,98,98	0
8	SO4	A	508	5/5	0.96	0.09	78,78,78,78	0
8	SO4	C	503	5/5	0.96	0.17	100,100,100,100	0
10	MN	B	2003	1/1	0.96	0.20	53,53,53,53	0
9	CA	A	506	1/1	0.97	0.22	50,50,50,50	0
10	MN	B	2001	1/1	0.97	0.22	55,55,55,55	0
10	MN	D	2003	1/1	0.97	0.18	72,72,72,72	0
8	SO4	A	502	5/5	0.97	0.11	71,71,71,71	0
10	MN	D	2001	1/1	0.98	0.17	75,75,75,75	0
9	CA	A	507	1/1	0.99	0.17	54,54,54,54	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.