



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:41 PM EDT

PDB ID : 7UH8
Title : Integrin α IIb β 3 complex with roxifiban (Mn/Ca)
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-25
Resolution : 2.75 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

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>.

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

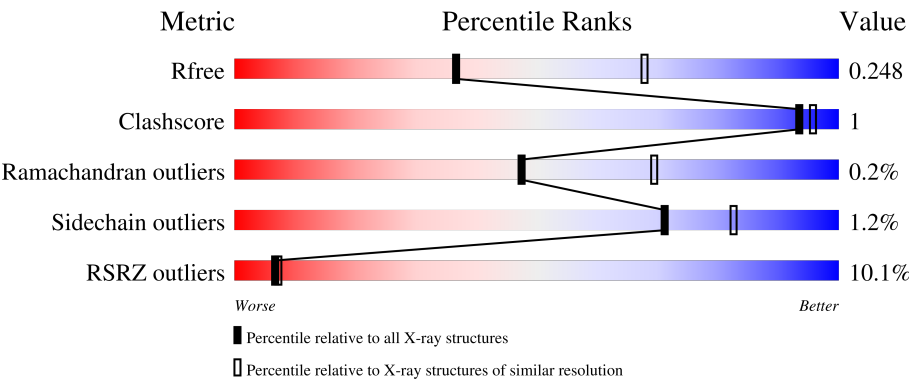
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 ≥ 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></div><div></div><div></div></div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>• •</div></div>
1	C	457	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>5%</div><div>•</div></div>
2	B	472	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>92%</div><div><div></div><div></div><div></div><div></div></div><div>6%</div><div>•</div></div>
2	D	472	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>6%</div><div>•</div></div>
3	E	221	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>91%</div><div><div></div><div></div><div></div><div></div></div><div>5%</div><div>•</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

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21664 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	2	0
			3604	2245	615	710	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: O₄S).



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).

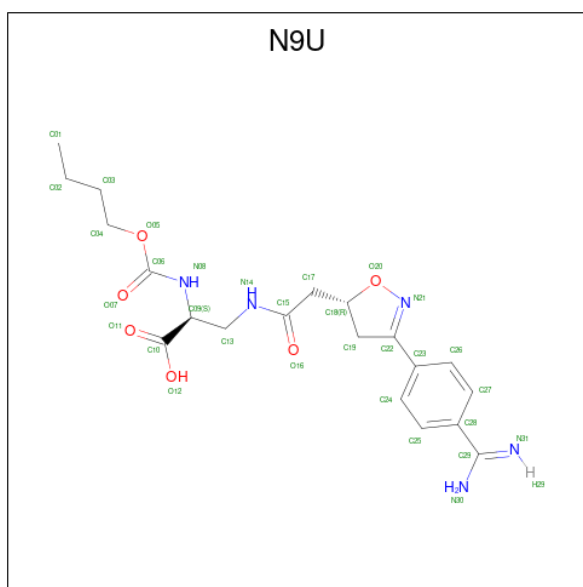
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- 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 Roxifiban (three-letter code: N9U) (formula: $C_{20}H_{27}N_5O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			31	20	5	6		
12	D	1	Total	C	N	O	0	0
			31	20	5	6		

- 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		
13	D	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	260	Total	O	0	0
			260	260		
14	B	105	Total	O	0	0
			105	105		
14	C	100	Total	O	0	0
			100	100		
14	D	61	Total	O	0	0
			61	61		
14	E	6	Total	O	0	0
			6	6		

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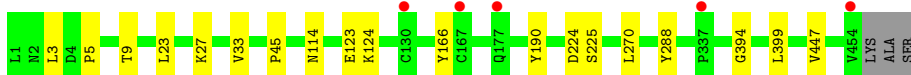
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	F	3	Total 3	O 3	0	0
14	H	16	Total 16	O 16	0	0
14	L	19	Total 19	O 19	0	0

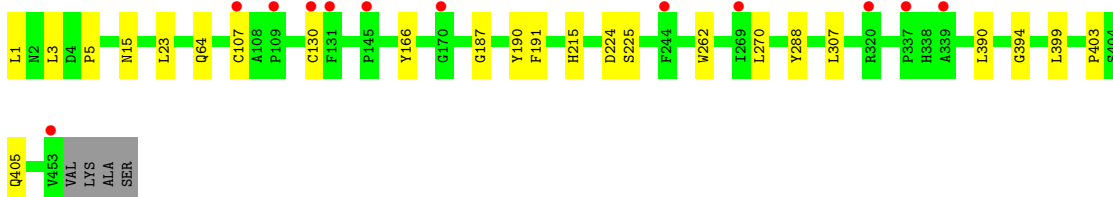
3 Residue-property plots [i](#)

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.

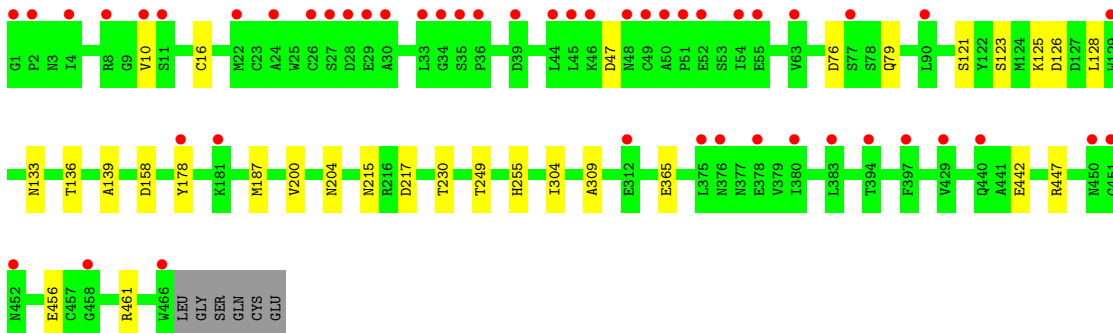
- Molecule 1: Integrin alpha-IIb heavy chain



- Molecule 1: Integrin alpha-IIb heavy chain

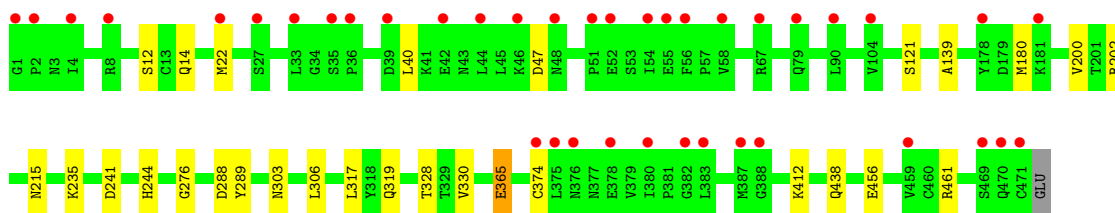


- Molecule 2: Isoform Beta-3C of Integrin beta-3

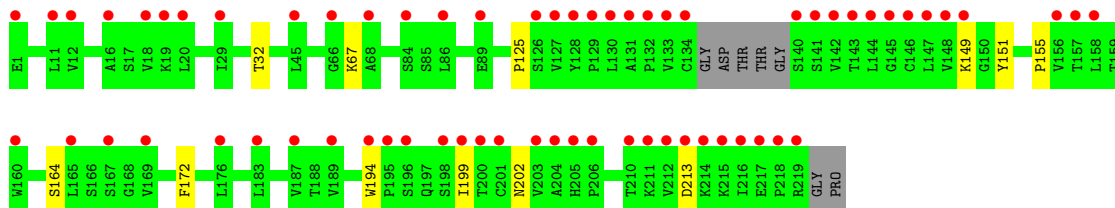
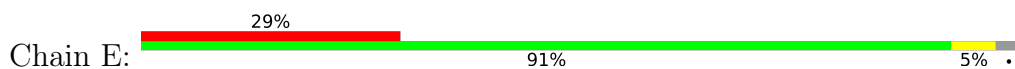


- Molecule 2: Isoform Beta-3C of Integrin beta-3

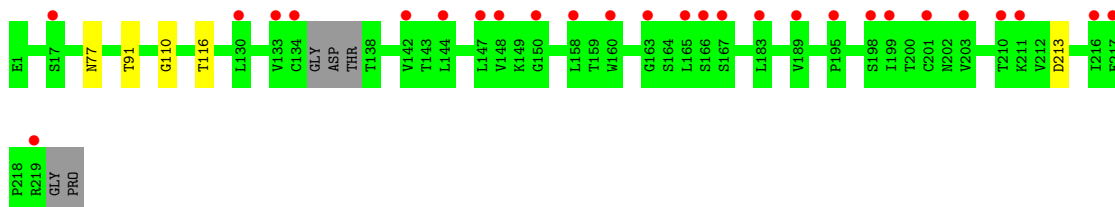




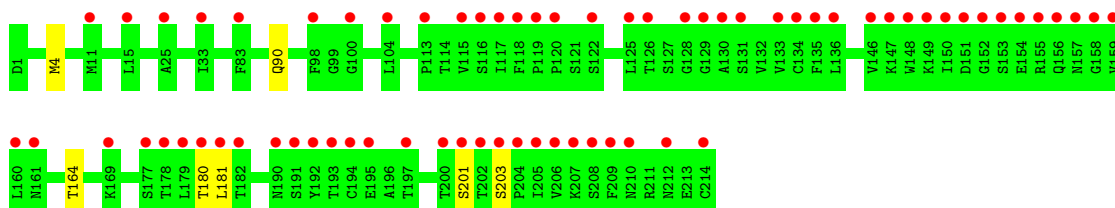
• Molecule 3: 10E5 Fab heavy chain



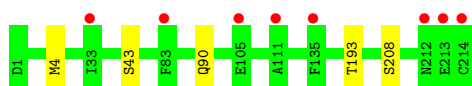
• Molecule 3: 10E5 Fab heavy chain



• 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

Chain G:  60% 40%

WAG1
WAG2
BGA3
MAN4
MAN5

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

Chain I:  100%

WAG1
WAG2

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

Chain K:  100%

WAG1
WAG2

- 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%

WAG1
WAG2
BGA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	258.69Å 144.04Å 104.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.75 49.25 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.25-2.75) 99.5 (49.25-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.229 , 0.248 0.229 , 0.248	Depositor DCC
R_{free} test set	1995 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21664	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, CL, BMA, CA, MAN, N9U, MN, NAG

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	0/3608	0.47	0/4918
1	C	0.26	0/3605	0.46	0/4912
2	B	0.26	0/3674	0.46	0/4981
2	D	0.25	0/3690	0.45	0/5003
3	E	0.27	0/1673	0.46	0/2290
3	H	0.25	0/1684	0.47	0/2305
4	F	0.26	0/1673	0.45	0/2269
4	L	0.25	0/1673	0.46	0/2269
All	All	0.26	0/21280	0.46	0/28947

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	7	0
1	C	3502	0	3334	11	0
2	B	3604	0	3525	14	0
2	D	3623	0	3540	13	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	3	0
4	F	1637	0	1553	4	0
4	L	1637	0	1553	3	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	31	0	0	2	0
12	D	31	0	0	2	0
13	C	2	0	0	0	0
13	D	1	0	0	0	0
14	A	260	0	0	0	1
14	B	105	0	0	0	0
14	C	100	0	0	1	1
14	D	61	0	0	0	0
14	E	6	0	0	0	0
14	F	3	0	0	0	0
14	H	16	0	0	0	0
14	L	19	0	0	0	0
All	All	21664	0	20211	57	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 (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LEU:O	1:C:405:GLN:NE2	2.26	0.69
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.83	0.61
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.85	0.58
2:B:136:THR:OG1	2:B:204:ASN:OD1	2.16	0.58
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ASP:OD1	2:B:126:ASP:N	2.36	0.57
2:D:121:SER:HB2	12:D:2006:N9U:O12	2.06	0.54
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.89	0.53
2:B:133:ASN:OD1	2:B:133:ASN:N	2.41	0.53
2:D:456:GLU:OE2	2:D:461:ARG:NH1	2.41	0.53
1:C:224:ASP:OD1	1:C:225:SER:N	2.38	0.51
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.26	0.51
2:B:230:THR:HG23	2:B:304:ILE:HG13	1.92	0.49
3:H:110:GLY:O	4:L:43:SER:OG	2.24	0.49
1:A:27:LYS:HG2	1:A:33:VAL:HG22	1.94	0.49
1:A:3:LEU:O	1:A:5:PRO:HD3	2.13	0.49
1:A:225:SER:O	12:B:2005:N9U:N30	2.47	0.48
1:C:64:GLN:NE2	14:C:609:HOH:O	2.46	0.48
1:A:9:THR:HB	1:A:447:VAL:HB	1.95	0.47
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.96	0.47
1:C:225:SER:O	12:D:2006:N9U:N30	2.48	0.47
4:L:193:THR:HG23	4:L:208:SER:HB3	1.96	0.47
1:C:107:CYS:HA	1:C:130:CYS:HA	1.96	0.47
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.95	0.47
2:D:319:GLN:HA	2:D:330:VAL:HG21	1.97	0.47
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.50	0.47
1:A:224:ASP:OD1	1:A:225:SER:N	2.40	0.46
2:D:14:GLN:HB2	2:D:438:GLN:HE22	1.81	0.46
2:D:244:HIS:ND1	2:D:303:ASN:O	2.48	0.46
2:D:288:ASP:OD1	2:D:289:TYR:N	2.48	0.45
1:C:390:LEU:HD23	1:C:403:PRO:HG3	1.98	0.45
2:B:158:ASP:HB3	2:B:187[A]:MET:HE3	1.99	0.44
2:B:217:ASP:OD2	2:B:255:HIS:NE2	2.47	0.44
2:D:235:LYS:HE3	2:D:276:GLY:O	2.19	0.43
3:H:213:ASP:OD1	3:H:213:ASP:N	2.52	0.43
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.54	0.42
2:B:442:GLU:OE1	2:B:447:ARG:NH1	2.52	0.42
4:F:4:MET:HE2	4:F:90:GLN:HB3	2.02	0.42
2:B:121:SER:HB2	12:B:2005:N9U:O12	2.20	0.42
2:B:249:THR:HG22	2:B:309:ALA:HB3	2.00	0.42
3:E:67:LYS:HE3	3:E:67:LYS:HB2	1.85	0.42
2:D:22:MET:HG2	2:D:40:LEU:HD22	2.02	0.42
1:C:3:LEU:O	1:C:5:PRO:HD3	2.20	0.42
1:C:394:GLY:HA2	1:C:399:LEU:HD23	2.02	0.41
3:H:91:THR:HG23	3:H:116:THR:HA	2.02	0.41
2:B:365:GLU:H	2:B:365:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.53	0.41
3:E:202:ASN:HA	3:E:213:ASP:HB3	2.03	0.41
1:C:187:GLY:HA2	1:C:191:PHE:HA	2.03	0.41
2:D:139:ALA:HB2	2:D:200:VAL:HG11	2.03	0.41
4:F:201:SER:OG	4:F:203:SER:O	2.20	0.41
1:A:114:ASN:HB2	1:A:124:LYS:HA	2.03	0.41
3:E:194:TRP:CD1	3:E:199:ILE:HD12	2.56	0.40
2:B:204:ASN:N	2:B:204:ASN:HD22	2.19	0.40
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.54	0.40
3:E:125:PRO:HB3	3:E:151:TYR:HB3	2.04	0.40
2:B:10:VAL:HG11	2:B:16:CYS:HA	2.03	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:782:HOH:O	14:C:681:HOH:O[1_554]	2.18	0.02

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%)	15 (3%)	2 (0%)	34	53
1	C	455/457 (100%)	435 (96%)	20 (4%)	0	100	100
2	B	466/472 (99%)	449 (96%)	16 (3%)	1 (0%)	47	69
2	D	469/472 (99%)	447 (95%)	21 (4%)	1 (0%)	47	69
3	E	210/221 (95%)	196 (93%)	12 (6%)	2 (1%)	15	27
3	H	212/221 (96%)	202 (95%)	10 (5%)	0	100	100
4	F	212/214 (99%)	200 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
All	All	2692/2728 (99%)	2570 (96%)	116 (4%)	6 (0%)	47	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	164	SER
2	B	76	ASP
2	D	374	CYS
1	A	123	GLU
1	A	45	PRO
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%)	361 (99%)	5 (1%)	67	79
1	C	365/364 (100%)	357 (98%)	8 (2%)	52	70
2	B	414/417 (99%)	407 (98%)	7 (2%)	60	76
2	D	416/417 (100%)	410 (99%)	6 (1%)	67	79
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	88	92
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	92
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2310/2318 (100%)	2282 (99%)	28 (1%)	71	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR

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Mol	Chain	Res	Type
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	47	ASP
2	B	79	GLN
2	B	123	SER
2	B	125	LYS
2	B	128	LEU
2	B	178	TYR
2	B	215	ASN
1	C	1	LEU
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	270	LEU
1	C	288	TYR
1	C	307	LEU
2	D	47	ASP
2	D	180	MET
2	D	202	ARG
2	D	215	ASN
2	D	241	ASP
2	D	365	GLU
4	F	181	LEU
3	H	77	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	333	GLN
2	D	280	HIS

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	2,5	14,14,15	0.38	0	17,19,21	0.50	0
5	NAG	G	2	5	14,14,15	0.16	0	17,19,21	0.40	0
5	BMA	G	3	5	11,11,12	0.80	0	15,15,17	0.79	0
5	MAN	G	4	5	11,11,12	0.73	0	15,15,17	0.98	2 (13%)
5	MAN	G	5	5	11,11,12	1.01	1 (9%)	15,15,17	1.22	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.42	0	17,19,21	0.39	0
6	NAG	I	2	6	14,14,15	0.31	0	17,19,21	0.38	0
7	NAG	J	1	7,2	14,14,15	0.56	0	17,19,21	0.40	0
7	NAG	J	2	7	14,14,15	0.34	0	17,19,21	0.45	0
7	BMA	J	3	7	11,11,12	0.67	0	15,15,17	0.78	0
7	MAN	J	4	7	11,11,12	0.85	0	15,15,17	1.05	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	K	2	6	14,14,15	0.32	0	17,19,21	0.49	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	2,5	-	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	-	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	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
7	MAN	J	4	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	C1-C2	2.76	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-O5-C5	3.44	116.85	112.19
7	J	4	MAN	O2-C2-C3	-2.32	105.49	110.14
5	G	4	MAN	O2-C2-C3	-2.22	105.69	110.14
5	G	4	MAN	C1-O5-C5	2.22	115.19	112.19
5	G	5	MAN	O2-C2-C3	-2.19	105.74	110.14
7	J	4	MAN	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

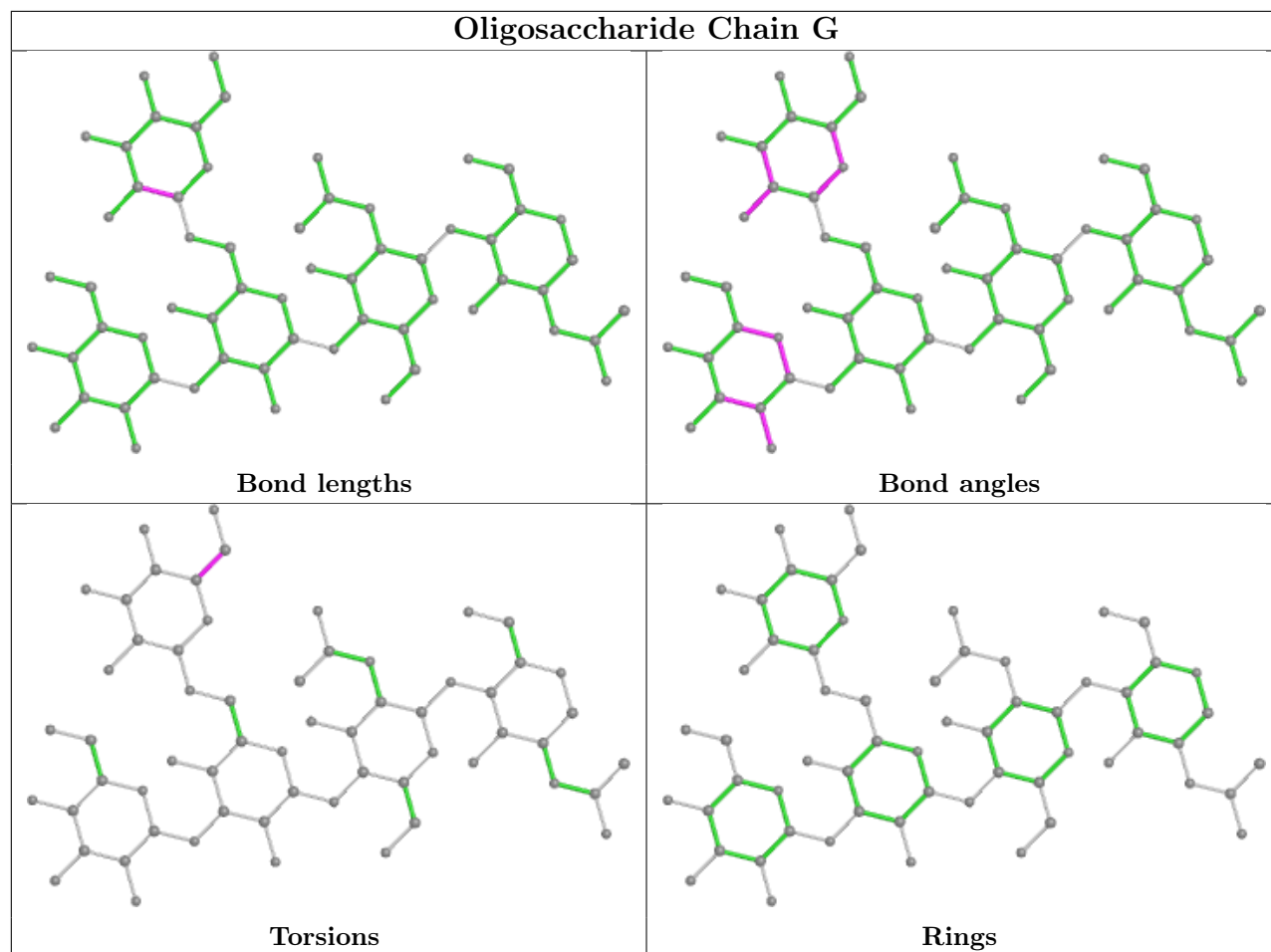
All (13) torsion outliers are listed below:

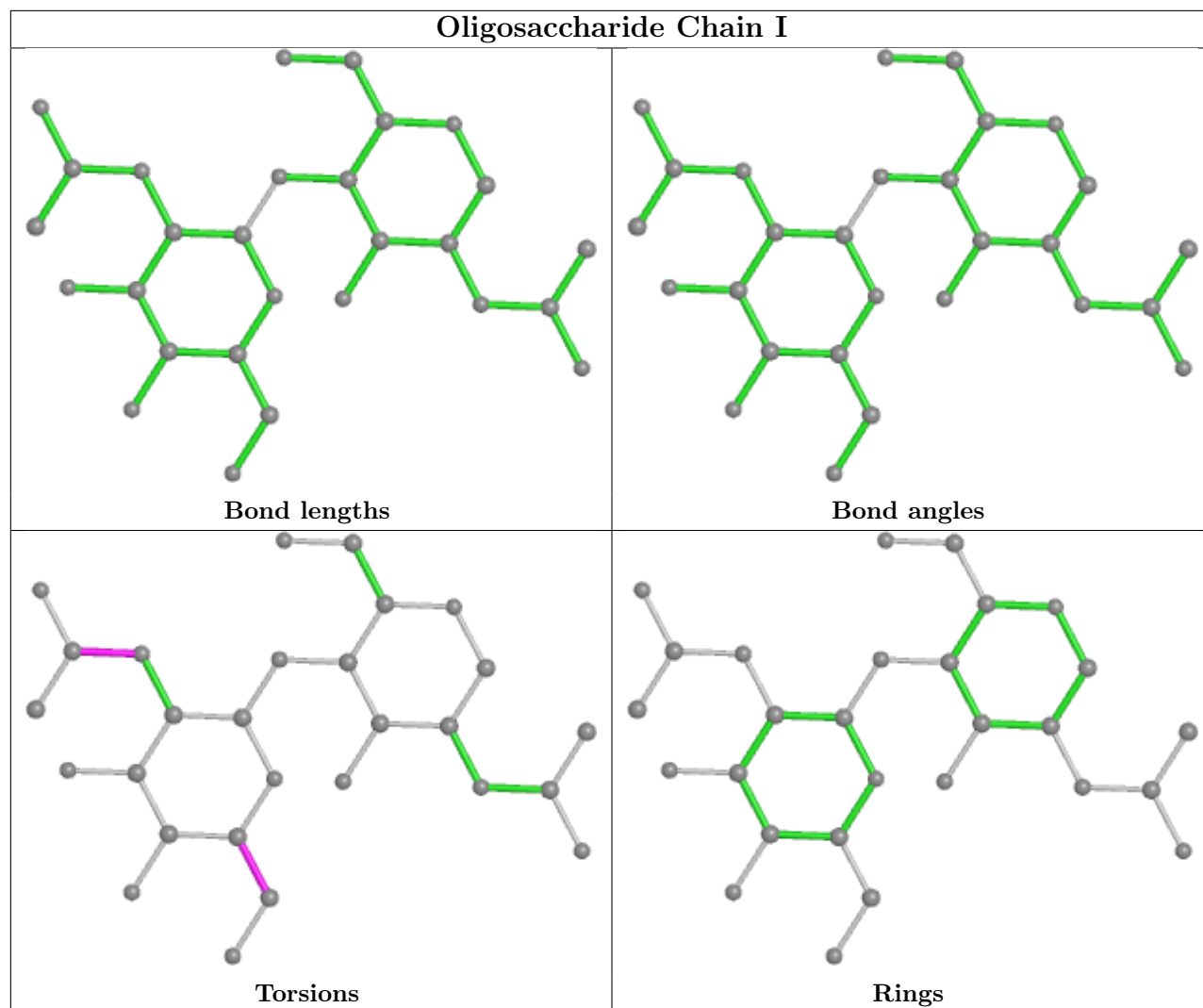
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6

There are no ring outliers.

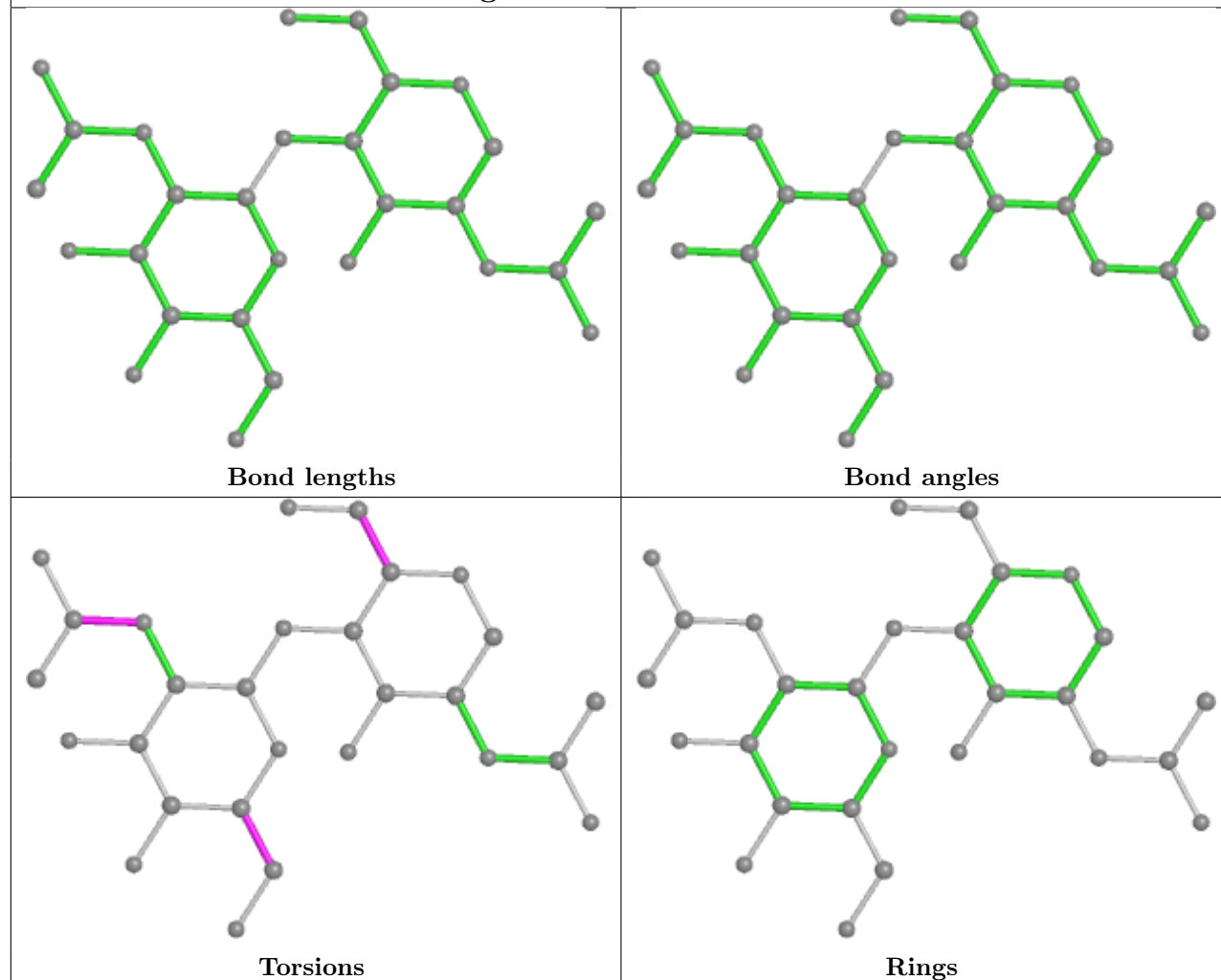
No monomer is involved in short contacts.

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

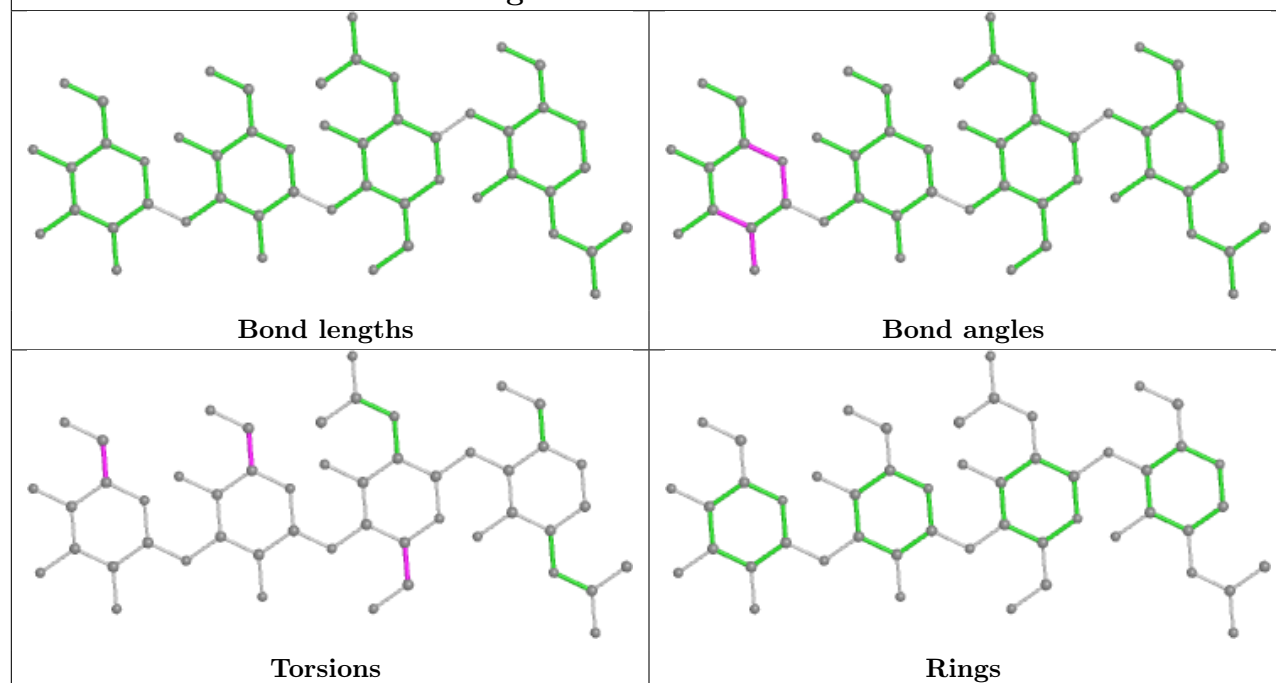




Oligosaccharide Chain K



Oligosaccharide Chain J



5.6 Ligand geometry

Of 30 ligands modelled in this entry, 17 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
11	NAG	B	2004	2	14,14,15	0.75	1 (7%)	17,19,21	0.82	0
11	NAG	D	2004	2	14,14,15	0.31	0	17,19,21	0.58	0
8	SO4	A	501	-	4,4,4	0.17	0	6,6,6	0.17	0
8	SO4	A	502	-	4,4,4	0.13	0	6,6,6	0.14	0
8	SO4	L	301	-	4,4,4	0.15	0	6,6,6	0.12	0
12	N9U	D	2006	10	31,32,32	3.57	12 (38%)	34,42,42	1.83	10 (29%)
12	N9U	B	2005	10	31,32,32	3.55	12 (38%)	34,42,42	1.84	10 (29%)
8	SO4	C	503	-	4,4,4	0.18	0	6,6,6	0.14	0
8	SO4	A	507	-	4,4,4	0.17	0	6,6,6	0.13	0
8	SO4	C	510	-	4,4,4	0.14	0	6,6,6	0.12	0
8	SO4	C	501	-	4,4,4	0.13	0	6,6,6	0.14	0
8	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.14	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
12	N9U	B	2005	10	-	7/30/39/39	0/2/2/2
12	N9U	D	2006	10	-	9/30/39/39	0/2/2/2
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	N9U	C19-C22	-12.88	1.31	1.50
12	D	2006	N9U	C19-C22	-12.86	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	N9U	C22-N21	6.40	1.44	1.28
12	D	2006	N9U	C22-N21	6.33	1.44	1.28
12	D	2006	N9U	C15-N14	5.90	1.46	1.33
12	B	2005	N9U	C15-N14	5.72	1.46	1.33
12	D	2006	N9U	C23-C22	5.59	1.59	1.47
12	B	2005	N9U	C23-C22	5.58	1.58	1.47
12	D	2006	N9U	O20-C18	5.48	1.54	1.46
12	B	2005	N9U	O20-C18	5.32	1.53	1.46
12	D	2006	N9U	C29-N30	4.40	1.45	1.33
12	B	2005	N9U	C29-N30	4.33	1.44	1.33
12	B	2005	N9U	C17-C18	-4.17	1.43	1.51
12	D	2006	N9U	O05-C06	4.15	1.43	1.35
12	B	2005	N9U	O05-C06	3.98	1.42	1.35
12	D	2006	N9U	C17-C18	-3.96	1.43	1.51
12	D	2006	N9U	C28-C29	3.17	1.53	1.47
12	B	2005	N9U	C28-C29	2.77	1.52	1.47
12	D	2006	N9U	O11-C10	2.71	1.30	1.22
12	B	2005	N9U	O11-C10	2.59	1.30	1.22
12	B	2005	N9U	C06-N08	2.55	1.41	1.34
12	B	2005	N9U	C19-C18	-2.55	1.48	1.52
12	D	2006	N9U	C06-N08	2.42	1.40	1.34
11	B	2004	NAG	C1-C2	2.40	1.55	1.52
12	D	2006	N9U	C19-C18	-2.34	1.49	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2006	N9U	O05-C06-N08	5.31	121.29	110.50
12	B	2005	N9U	O05-C06-N08	4.81	120.27	110.50
12	B	2005	N9U	C18-O20-N21	-4.63	103.72	108.86
12	D	2006	N9U	C18-O20-N21	-3.64	104.83	108.86
12	B	2005	N9U	O20-N21-C22	-3.31	104.23	109.17
12	D	2006	N9U	C17-C15-N14	3.26	120.49	115.97
12	D	2006	N9U	O07-C06-N08	-3.14	119.70	124.85
12	D	2006	N9U	O20-N21-C22	-3.01	104.68	109.17
12	B	2005	N9U	O07-C06-N08	-2.83	120.22	124.85
12	B	2005	N9U	C17-C15-N14	2.77	119.80	115.97
12	D	2006	N9U	O05-C06-O07	-2.73	119.01	124.25
12	B	2005	N9U	C18-C19-C22	2.70	103.32	100.85
12	D	2006	N9U	C18-C19-C22	2.66	103.28	100.85
12	B	2005	N9U	C19-C22-C23	-2.65	121.14	124.84
12	B	2005	N9U	O05-C06-O07	-2.47	119.51	124.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2005	N9U	O12-C10-C09	2.19	120.68	113.40
12	D	2006	N9U	O12-C10-C09	2.18	120.64	113.40
12	D	2006	N9U	O12-C10-O11	-2.06	119.40	124.09
12	D	2006	N9U	O16-C15-N14	-2.06	119.13	123.01
12	B	2005	N9U	O12-C10-O11	-2.01	119.54	124.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	N9U	N08-C06-O05-C04
12	B	2005	N9U	O07-C06-O05-C04
12	D	2006	N9U	N08-C09-C13-N14
12	D	2006	N9U	O07-C06-N08-C09
12	D	2006	N9U	N08-C06-O05-C04
12	D	2006	N9U	O07-C06-O05-C04
12	D	2006	N9U	O05-C06-N08-C09
12	B	2005	N9U	O07-C06-N08-C09
11	D	2004	NAG	O5-C5-C6-O6
12	B	2005	N9U	O05-C06-N08-C09
12	D	2006	N9U	C03-C04-O05-C06
12	D	2006	N9U	C02-C03-C04-O05
12	B	2005	N9U	C03-C04-O05-C06
12	B	2005	N9U	C10-C09-C13-N14
12	D	2006	N9U	C10-C09-C13-N14
11	D	2004	NAG	C4-C5-C6-O6
12	D	2006	N9U	C13-C09-N08-C06
12	B	2005	N9U	C02-C03-C04-O05

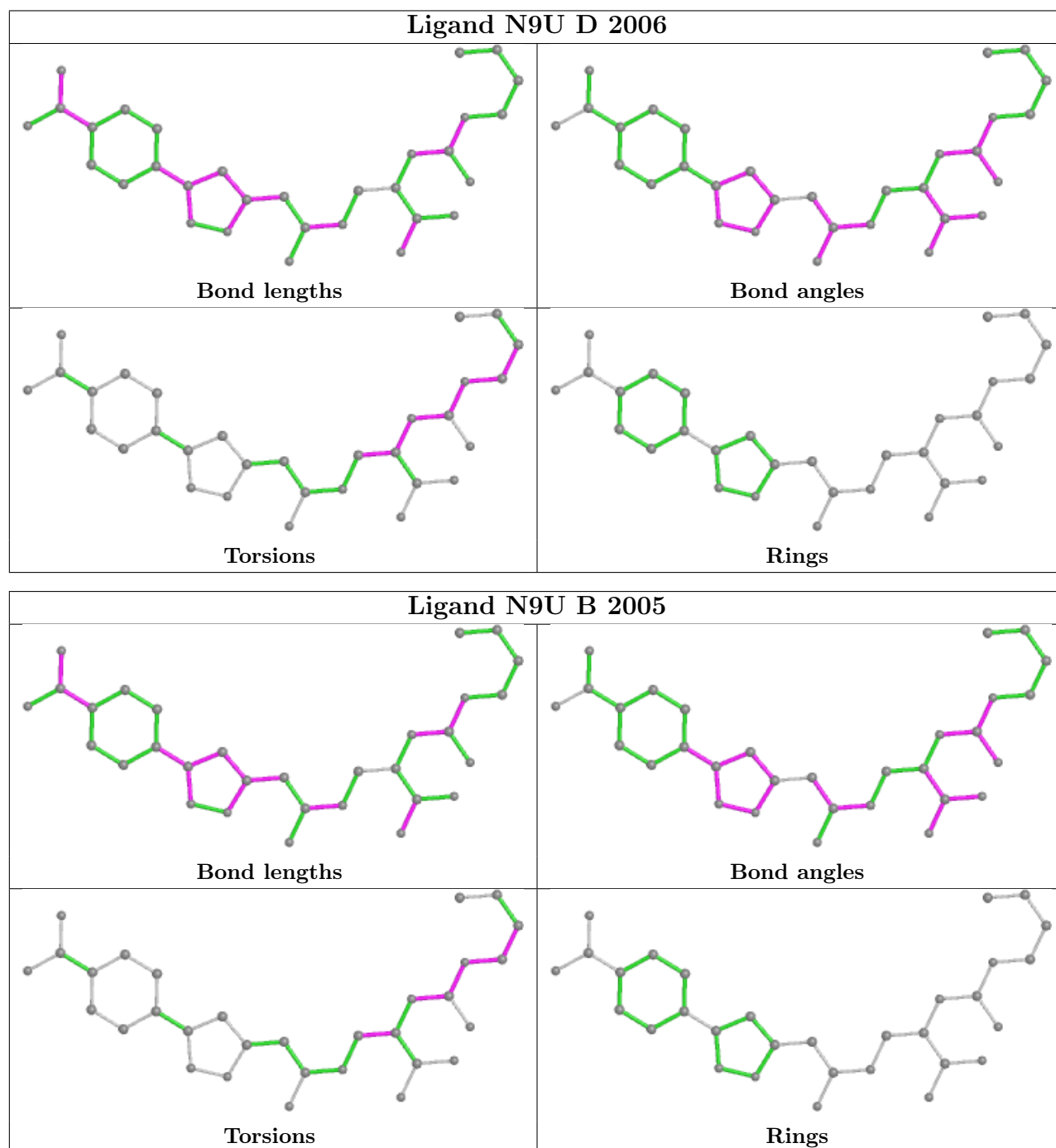
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2006	N9U	2	0
12	B	2005	N9U	2	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, 95th 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 ²)	Q<0.9
1	A	454/457 (99%)	0.52	5 (1%) 80 86	41, 55, 75, 96	0
1	C	453/457 (99%)	0.50	12 (2%) 56 65	50, 74, 99, 121	0
2	B	466/472 (98%)	0.78	49 (10%) 6 7	43, 84, 148, 168	1 (0%)
2	D	471/472 (99%)	0.69	39 (8%) 11 13	58, 100, 135, 151	1 (0%)
3	E	214/221 (96%)	1.68	65 (30%) 0 0	93, 132, 186, 190	0
3	H	216/221 (97%)	0.76	27 (12%) 3 4	67, 106, 141, 146	0
4	F	214/214 (100%)	1.54	69 (32%) 0 0	96, 141, 182, 191	0
4	L	214/214 (100%)	0.43	8 (3%) 41 49	70, 102, 119, 142	0
All	All	2702/2728 (99%)	0.77	274 (10%) 7 7	41, 90, 165, 191	2 (0%)

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	10.4
2	D	375	LEU	8.5
2	D	469	SER	8.1
3	E	142	VAL	8.0
2	B	33	LEU	7.9
3	E	133	VAL	7.8
3	E	147	LEU	7.6
3	E	201	CYS	7.4
3	E	196	SER	7.3
4	F	115	VAL	7.1
4	F	148	TRP	7.1
4	F	214	CYS	6.9
4	F	159	VAL	6.9
3	E	216	ILE	6.9
2	D	1	GLY	6.8
3	E	194	TRP	6.7

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Mol	Chain	Res	Type	RSRZ
3	E	134	CYS	6.5
3	E	144	LEU	6.5
3	E	203	VAL	6.4
2	B	466	TRP	6.4
3	E	160	TRP	6.4
4	F	117	ILE	6.2
4	F	193	THR	6.1
3	E	127	VAL	6.1
3	E	132	PRO	6.0
4	F	130	ALA	6.0
4	F	160	LEU	5.9
4	F	125	LEU	5.6
2	D	181	LYS	5.5
3	E	219	ARG	5.5
4	F	146	VAL	5.5
2	B	77	SER	5.4
2	B	181	LYS	5.4
3	E	143	THR	5.3
3	E	213	ASP	5.3
4	F	154	GLU	5.2
4	F	135	PHE	5.1
4	F	180	THR	5.1
3	E	165	LEU	5.1
4	L	214	CYS	5.1
2	B	34	GLY	5.0
4	F	179	LEU	5.0
3	H	195	PRO	5.0
3	H	165	LEU	4.9
3	H	216	ILE	4.8
2	B	458	GLY	4.8
2	B	375	LEU	4.8
4	F	181	LEU	4.7
4	F	194	CYS	4.7
2	B	10	VAL	4.7
4	F	178	THR	4.7
4	F	156	GLN	4.7
2	B	44	LEU	4.6
1	A	454	VAL	4.6
4	F	191	SER	4.6
4	F	195	GLU	4.6
2	B	49	CYS	4.5
3	E	145	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	33	LEU	4.5
4	F	208	SER	4.5
3	E	204	ALA	4.4
2	B	8	ARG	4.4
3	E	131	ALA	4.4
3	E	158	LEU	4.4
3	E	195	PRO	4.3
3	E	129	PRO	4.2
3	H	130	LEU	4.2
3	E	215	LYS	4.2
4	F	204	PRO	4.2
2	D	36	PRO	4.1
4	F	120	PRO	4.1
3	E	140	SER	4.1
3	E	130	LEU	4.1
2	D	35	SER	4.1
3	H	217	GLU	4.1
2	D	54	ILE	4.1
2	D	8	ARG	4.0
4	F	147	LYS	4.0
3	E	210	THR	4.0
4	F	116	SER	4.0
3	E	156	VAL	4.0
3	E	199	ILE	4.0
3	E	18	VAL	3.9
4	F	150	ILE	3.9
3	H	189	VAL	3.8
2	B	2	PRO	3.8
4	F	209	PHE	3.8
2	D	471	CYS	3.7
3	H	133	VAL	3.7
4	F	133	VAL	3.7
4	F	207	LYS	3.7
4	L	212	ASN	3.7
3	E	146	CYS	3.7
4	F	149	LYS	3.7
4	F	201	SER	3.7
3	E	20	LEU	3.7
2	B	36	PRO	3.7
4	F	134	CYS	3.6
2	B	48	ASN	3.5
2	D	2	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	129	GLY	3.5
3	E	183	LEU	3.5
3	E	128	TYR	3.5
2	B	29	GLU	3.5
4	F	177	SER	3.5
1	C	339	ALA	3.4
4	F	118	PHE	3.4
4	F	152	GLY	3.4
4	F	119	PRO	3.3
2	B	54	ILE	3.3
2	D	380	ILE	3.3
2	B	380	ILE	3.3
2	D	44	LEU	3.3
4	F	104	LEU	3.3
2	B	46	LYS	3.3
3	H	211	LYS	3.3
2	B	63	VAL	3.2
2	D	388	GLY	3.2
4	F	131	SER	3.2
3	E	205	HIS	3.2
3	H	144	LEU	3.2
3	E	198	SER	3.2
4	F	155	ARG	3.2
3	E	200	THR	3.2
4	F	200	THR	3.2
4	L	135	PHE	3.2
2	D	22	MET	3.1
3	E	148	VAL	3.1
4	F	206	VAL	3.1
4	F	15	LEU	3.1
1	C	453	VAL	3.1
3	E	189	VAL	3.1
3	E	16	ALA	3.1
4	F	11	MET	3.0
3	E	176	LEU	3.0
2	D	79	GLN	3.0
3	E	29	ILE	3.0
3	H	167	SER	3.0
2	D	378	GLU	3.0
2	D	387	MET	3.0
3	H	142	VAL	3.0
2	B	452	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	470	GLN	3.0
4	F	126	THR	3.0
3	E	187	VAL	3.0
2	D	376	ASN	3.0
2	B	55	GLU	3.0
3	H	158	LEU	3.0
1	C	320	ARG	3.0
3	H	134	CYS	3.0
3	H	198	SER	2.9
2	D	58	VAL	2.9
2	D	39	ASP	2.9
2	D	48	ASN	2.9
4	F	122	SER	2.9
3	E	214	LYS	2.9
4	F	197	THR	2.9
2	D	52	GLU	2.9
2	B	90	LEU	2.9
2	B	11	SER	2.9
4	F	83	PHE	2.9
2	B	450	ASN	2.8
3	H	199	ILE	2.8
2	B	26	CYS	2.8
3	H	203	VAL	2.8
2	B	1	GLY	2.8
3	E	12	VAL	2.8
4	L	213	GLU	2.7
2	B	30	ALA	2.7
3	E	211	LYS	2.7
4	F	153	SER	2.7
2	D	55	GLU	2.7
3	E	89	GLU	2.7
4	F	113	PRO	2.7
2	D	104	VAL	2.7
1	C	130	CYS	2.7
3	E	19	LYS	2.7
4	L	111	ALA	2.7
3	E	217	GLU	2.7
4	F	100	GLY	2.7
4	F	157	ASN	2.7
2	B	4	ILE	2.7
1	C	107	CYS	2.6
2	D	178	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	42	GLU	2.6
2	D	46	LYS	2.6
2	B	129	TRP	2.6
1	C	244	PHE	2.6
3	E	167	SER	2.6
4	L	105	GLU	2.6
3	H	201	CYS	2.6
4	F	33	ILE	2.6
2	B	378	GLU	2.6
2	B	28	ASP	2.5
4	F	161	ASN	2.5
3	H	150	GLY	2.5
3	H	166	SER	2.5
3	E	86	LEU	2.5
3	H	219	ARG	2.5
2	D	67	ARG	2.5
3	E	157	THR	2.5
4	F	158	GLY	2.5
2	B	52	GLU	2.5
3	E	11	LEU	2.5
4	F	98	PHE	2.5
2	D	383	LEU	2.5
3	H	147	LEU	2.5
2	D	56	PHE	2.4
2	D	4	ILE	2.4
3	H	183	LEU	2.4
2	D	51	PRO	2.4
2	B	39	ASP	2.4
2	B	440	GLN	2.4
4	F	128	GLY	2.4
4	F	169	LYS	2.4
2	D	90	LEU	2.4
3	H	163	GLY	2.4
1	C	337	PRO	2.4
2	B	27	SER	2.4
2	B	35	SER	2.3
2	B	376	ASN	2.3
3	H	160	TRP	2.3
2	B	50	ALA	2.3
3	E	126	SER	2.3
4	F	202	THR	2.3
2	B	45	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	178	TYR	2.3
4	F	182	THR	2.3
4	L	83	PHE	2.3
4	F	205	ILE	2.3
1	A	130	CYS	2.3
4	F	203	SER	2.2
2	D	459	VAL	2.2
3	E	141	SER	2.2
4	F	190	ASN	2.2
2	B	24	ALA	2.2
1	A	167	CYS	2.2
1	C	269	ILE	2.2
3	E	84	SER	2.2
3	E	68	ALA	2.2
3	E	66	GLY	2.2
3	E	206	PRO	2.2
1	C	131	PHE	2.2
3	E	149	LYS	2.2
4	F	210	ASN	2.2
2	D	27	SER	2.2
3	E	1	GLU	2.2
2	B	451	GLY	2.2
1	C	109	PRO	2.1
2	D	374	CYS	2.1
3	E	218	PRO	2.1
4	F	25	ALA	2.1
4	F	192	TYR	2.1
3	E	45	LEU	2.1
4	L	33	ILE	2.1
4	F	151	ASP	2.1
4	F	212	ASN	2.1
2	B	22	MET	2.1
1	C	170	GLY	2.1
2	D	382	GLY	2.1
3	H	148	VAL	2.1
3	H	210	THR	2.1
2	B	397	PHE	2.1
2	B	383	LEU	2.1
2	B	429	VAL	2.1
2	B	51	PRO	2.1
3	H	17	SER	2.1
1	A	177	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	136	LEU	2.0
2	B	312	GLU	2.0
2	B	394	THR	2.0
1	A	337	PRO	2.0
1	C	145	PRO	2.0
3	E	169	VAL	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](#)

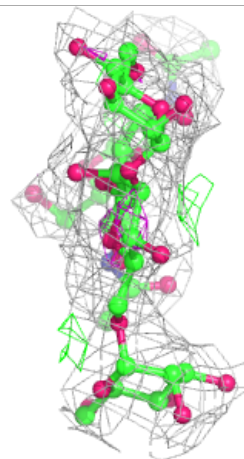
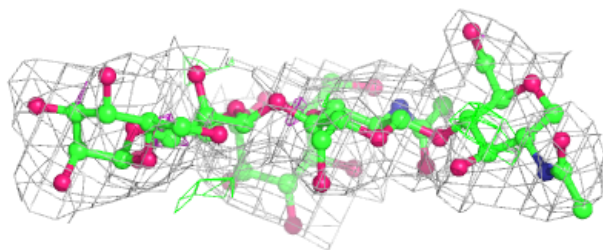
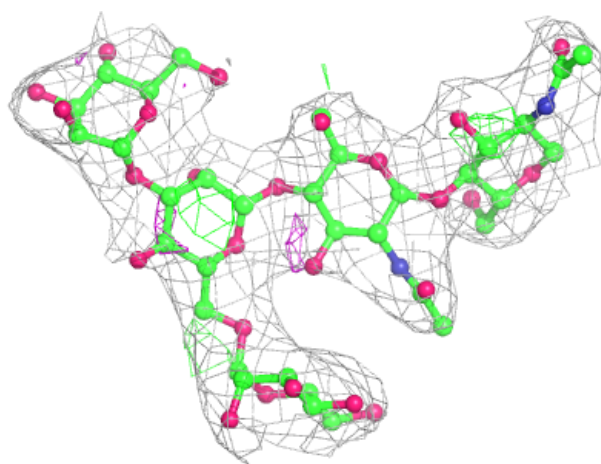
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	G	3	11/12	0.83	0.14	88,88,88,88	0
7	NAG	J	2	14/15	0.85	0.24	100,100,100,100	0
6	NAG	K	2	14/15	0.86	0.20	122,122,122,122	0
7	BMA	J	3	11/12	0.86	0.29	108,108,108,108	0
7	MAN	J	4	11/12	0.86	0.37	107,107,107,107	0
6	NAG	I	2	14/15	0.87	0.21	115,115,115,115	0
6	NAG	K	1	14/15	0.88	0.22	120,120,120,120	0
5	MAN	G	5	11/12	0.90	0.15	95,95,95,95	0
7	NAG	J	1	14/15	0.91	0.21	90,90,90,90	0
5	MAN	G	4	11/12	0.91	0.17	87,87,87,87	0
5	NAG	G	2	14/15	0.92	0.14	76,76,76,76	0
6	NAG	I	1	14/15	0.94	0.15	110,110,110,110	0
5	NAG	G	1	14/15	0.94	0.19	64,64,64,64	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.

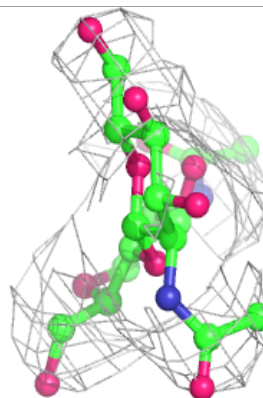
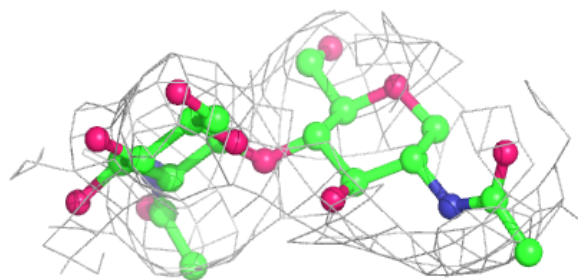
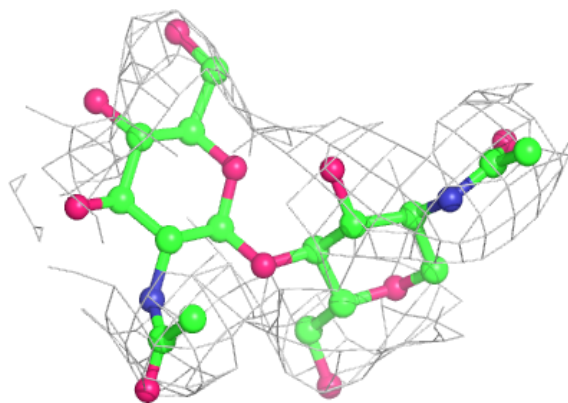
Electron density around Chain G:

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

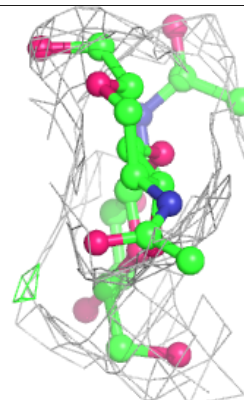
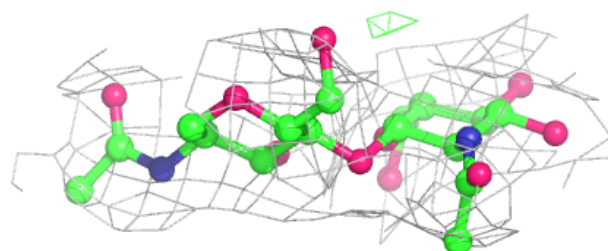
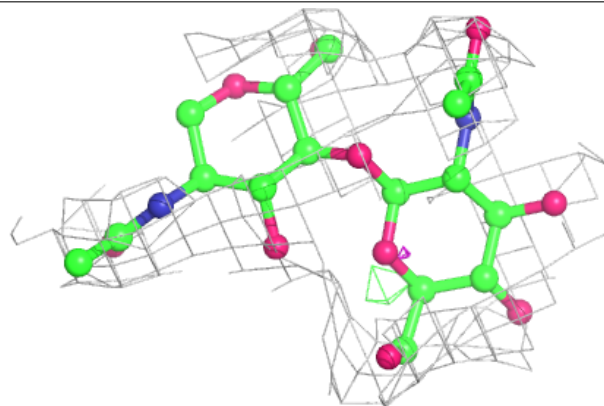


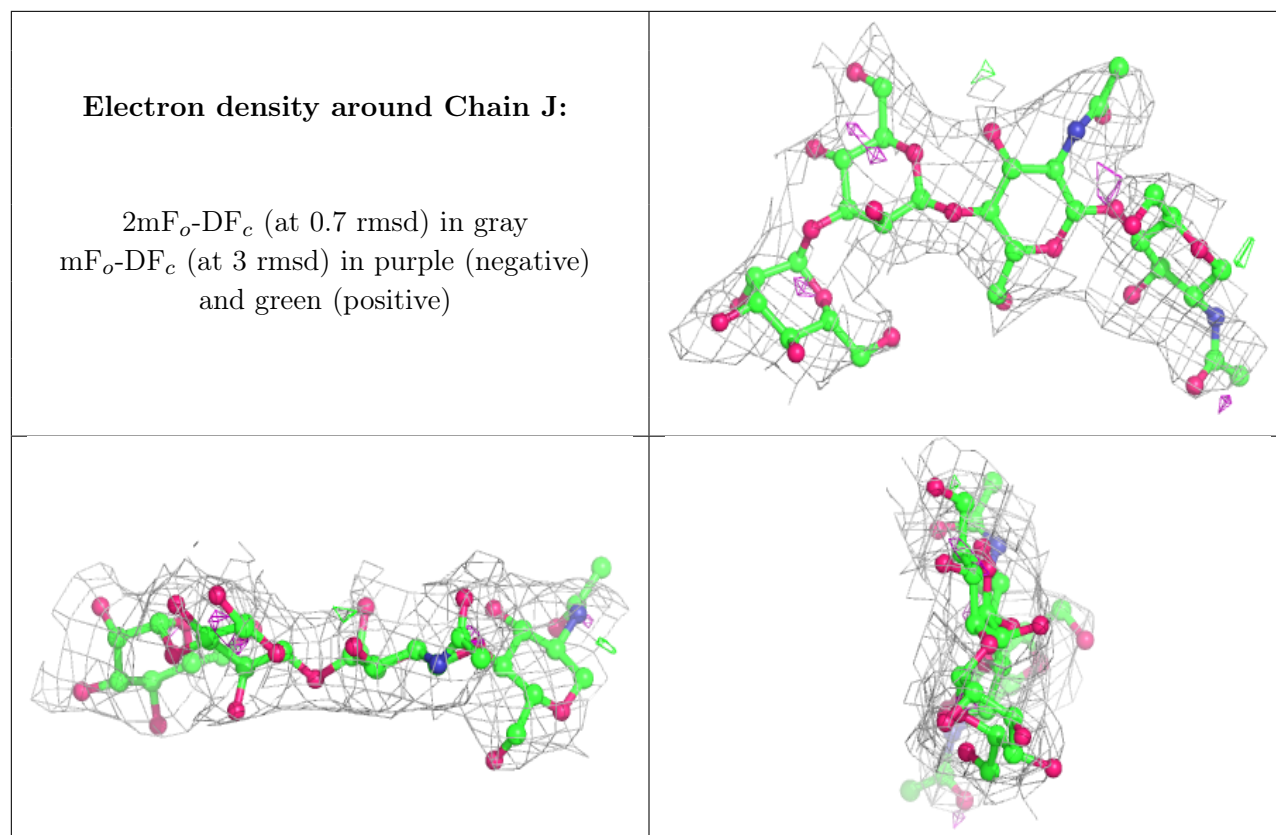
Electron density around Chain I:

$2mF_o-DF_c$ (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, 95th 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.

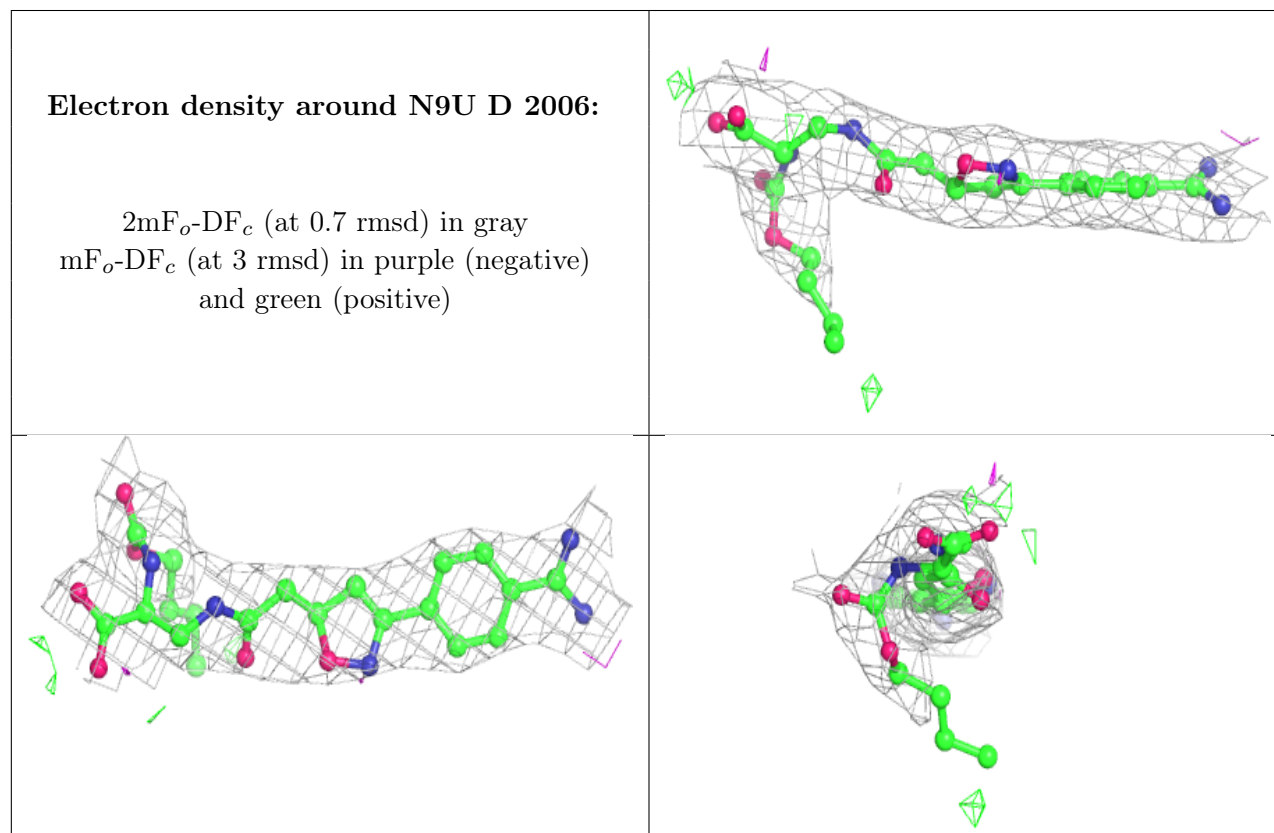
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	CL	C	505	1/1	0.74	0.56	93,93,93,93	0
9	CA	C	508	1/1	0.80	0.14	73,73,73,73	0
11	NAG	D	2004	14/15	0.82	0.24	113,113,113,113	0
10	MN	D	2002	1/1	0.84	0.12	98,98,98,98	0
13	CL	D	2005	1/1	0.84	0.17	99,99,99,99	0
8	SO4	C	503	5/5	0.85	0.22	108,108,108,108	0
9	CA	C	507	1/1	0.85	0.10	87,87,87,87	0
11	NAG	B	2004	14/15	0.85	0.30	115,115,115,115	0
8	SO4	C	502	5/5	0.87	0.16	96,96,96,96	0
9	CA	C	509	1/1	0.89	0.13	67,67,67,67	0
8	SO4	C	510	5/5	0.89	0.19	106,106,106,106	0
8	SO4	A	508	5/5	0.91	0.18	85,85,85,85	0
8	SO4	A	507	5/5	0.91	0.27	84,84,84,84	0
10	MN	B	2002	1/1	0.92	0.09	79,79,79,79	0

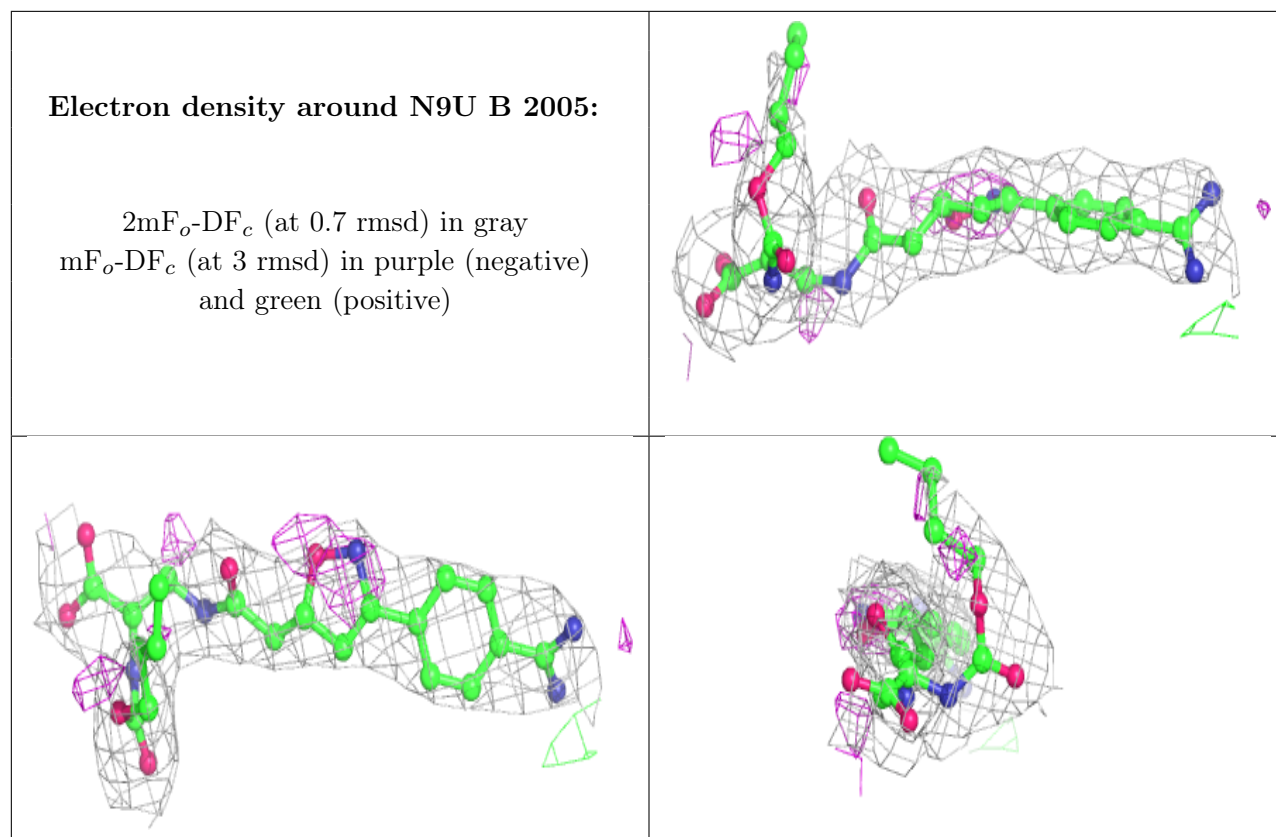
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	N9U	D	2006	31/31	0.92	0.20	79,79,79,79	0
9	CA	A	505	1/1	0.92	0.17	48,48,48,48	0
9	CA	A	503	1/1	0.92	0.11	62,62,62,62	0
8	SO4	C	501	5/5	0.93	0.20	90,90,90,90	0
8	SO4	A	501	5/5	0.93	0.19	66,66,66,66	0
12	N9U	B	2005	31/31	0.94	0.23	58,58,58,58	0
13	CL	C	504	1/1	0.94	0.30	76,76,76,76	0
9	CA	A	504	1/1	0.95	0.16	52,52,52,52	0
10	MN	D	2003	1/1	0.96	0.18	73,73,73,73	0
9	CA	C	506	1/1	0.96	0.07	102,102,102,102	0
8	SO4	A	502	5/5	0.97	0.10	66,66,66,66	0
8	SO4	L	301	5/5	0.97	0.14	90,90,90,90	0
10	MN	D	2001	1/1	0.97	0.20	75,75,75,75	0
10	MN	B	2001	1/1	0.98	0.20	51,51,51,51	0
9	CA	A	506	1/1	0.98	0.15	51,51,51,51	0
10	MN	B	2003	1/1	0.99	0.16	51,51,51,51	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.