



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:56 AM EDT

PDB ID : 7UH8  
Title : Integrin alpha IIB beta3 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](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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

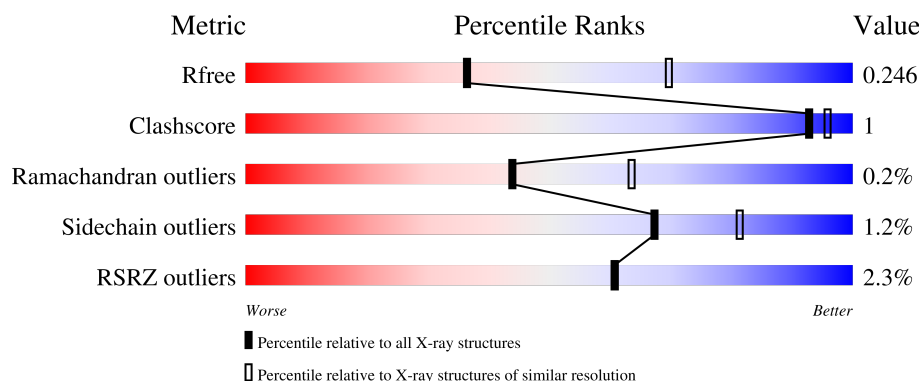
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (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  $\geq 3$ , 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>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	C	457	<div> <div>94%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	B	472	<div> <div>92%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	D	472	<div> <div>94%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
3	E	221	<div> <div>91%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	H	221	<div><div></div><div>2%</div><div>95%</div><div></div></div>
4	F	214	<div><div></div><div>4%</div><div>97%</div><div></div></div>
4	L	214	<div><div></div><div>%</div><div>98%</div><div></div></div>
5	G	5	<div><div></div><div>60%</div><div>40%</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>75%</div><div>25%</div><div></div></div>

## 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: 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	C	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

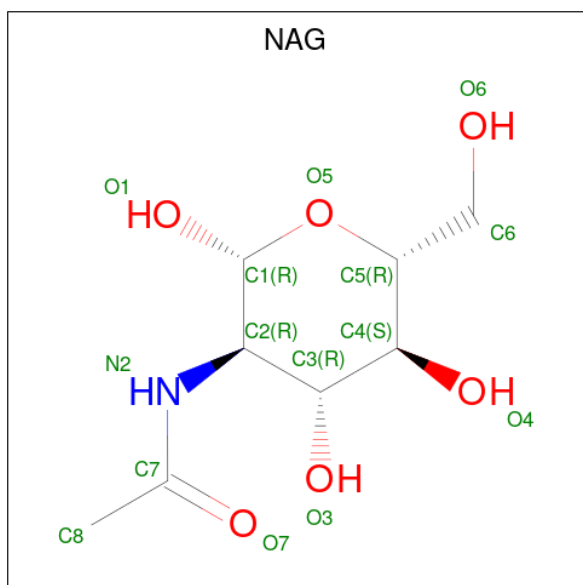
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

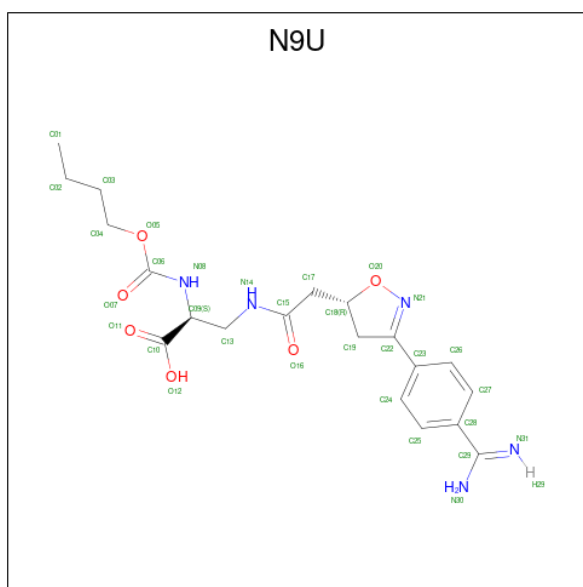
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- 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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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

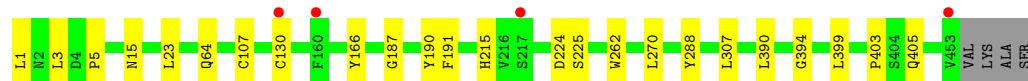
### 3 Residue-property plots [i](#)

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.

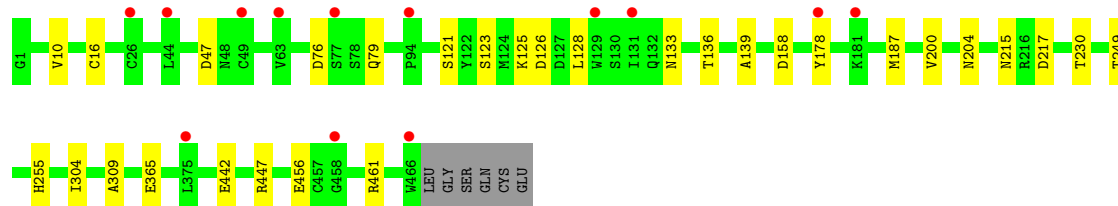
- Molecule 1: Integrin alpha-IIb heavy chain



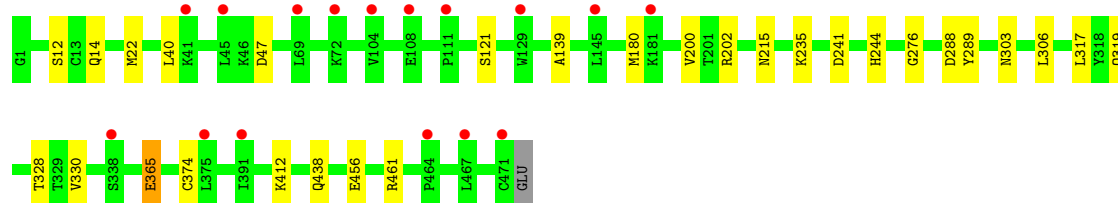
- Molecule 1: Integrin alpha-IIb heavy chain



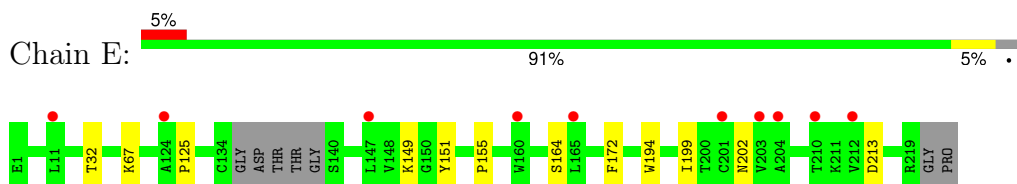
- Molecule 2: Isoform Beta-3C of Integrin beta-3



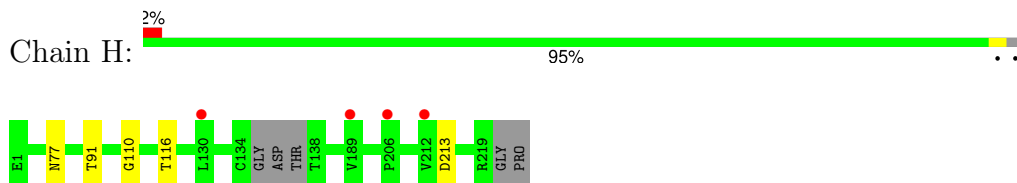
- Molecule 2: Isoform Beta-3C of Integrin beta-3



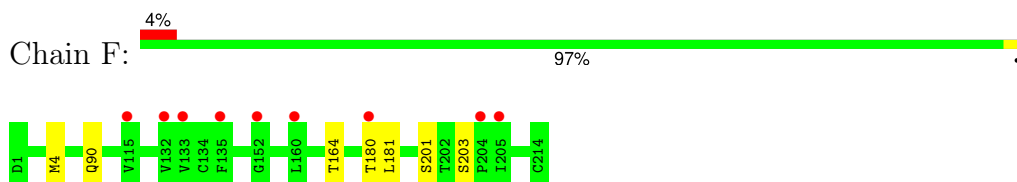
- Molecule 3: 10E5 Fab heavy chain



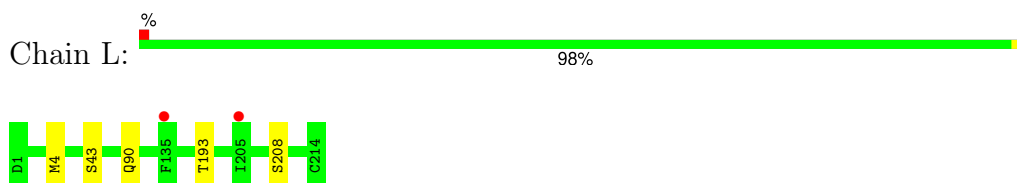
- Molecule 3: 10E5 Fab heavy chain



- Molecule 4: 10E5 Fab light chain



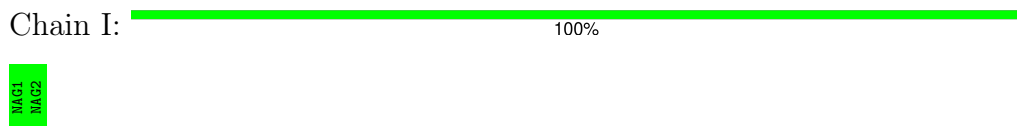
- Molecule 4: 10E5 Fab light chain



- 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



- 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



NAG1  
NAG2

- 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:



NAG1  
NAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.229 , 0.248 0.230 , 0.246	Depositor DCC
$R_{free}$ test set	101158 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.3	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: N9U, CA, BMA, CL, MAN, NAG, SO4, MN

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%)	30	47
1	C	455/457 (100%)	435 (96%)	20 (4%)	0	100	100
2	B	466/472 (99%)	449 (96%)	16 (3%)	1 (0%)	44	63
2	D	469/472 (99%)	447 (95%)	21 (4%)	1 (0%)	44	63
3	E	210/221 (95%)	196 (93%)	12 (6%)	2 (1%)	13	23
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%)	44	63

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%)	62	78
1	C	365/364 (100%)	357 (98%)	8 (2%)	47	68
2	B	414/417 (99%)	407 (98%)	7 (2%)	56	74
2	D	416/417 (100%)	410 (99%)	6 (1%)	62	78
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	86	92
4	F	188/188 (100%)	187 (100%)	1 (0%)	86	92
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2310/2318 (100%)	2282 (99%)	28 (1%)	67	81

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	0.40	0	17,19,21	0.51	0
5	NAG	G	2	5	14,14,15	0.16	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.79	0	15,15,17	0.75	0
5	MAN	G	4	5	11,11,12	0.70	0	15,15,17	0.95	2 (13%)
5	MAN	G	5	5	11,11,12	0.98	1 (9%)	15,15,17	1.18	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.43	0	17,19,21	0.40	0
6	NAG	I	2	6	14,14,15	0.33	0	17,19,21	0.39	0
7	NAG	J	1	2,7	14,14,15	0.54	0	17,19,21	0.41	0
7	NAG	J	2	7	14,14,15	0.32	0	17,19,21	0.46	0
7	BMA	J	3	7	11,11,12	0.66	0	15,15,17	0.74	0
7	MAN	J	4	7	11,11,12	0.83	0	15,15,17	1.02	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.42	0	17,19,21	0.45	0
6	NAG	K	2	6	14,14,15	0.31	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	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	2,7	-	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	2.63	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	3.48	116.85	112.19
7	J	4	MAN	O2-C2-C3	-2.25	105.49	110.15
5	G	4	MAN	C1-O5-C5	2.24	115.19	112.19
5	G	4	MAN	O2-C2-C3	-2.15	105.69	110.15
7	J	4	MAN	C1-O5-C5	2.13	115.04	112.19
5	G	5	MAN	O2-C2-C3	-2.13	105.74	110.15

There are no chirality outliers.

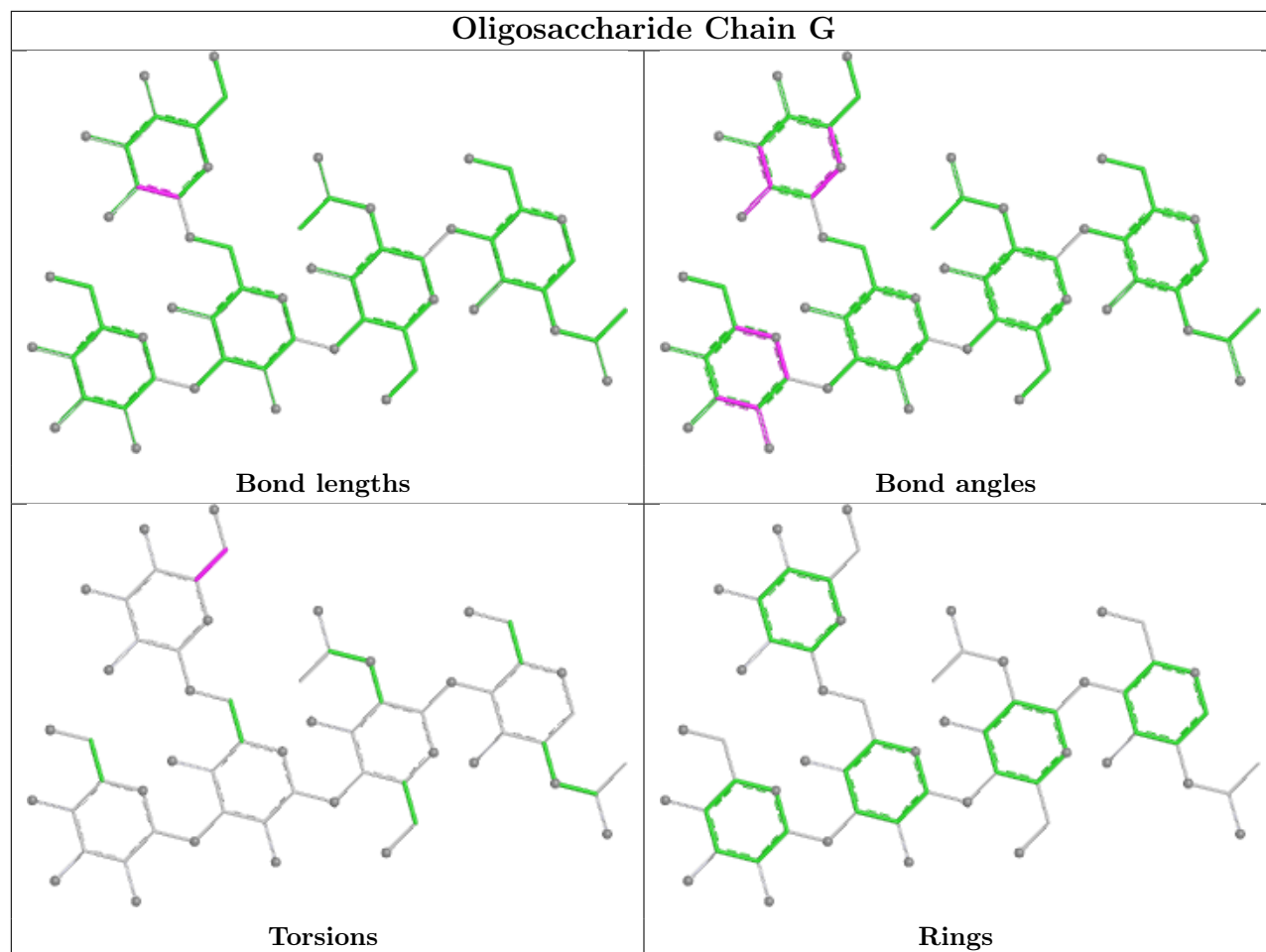
All (13) torsion outliers are listed below:

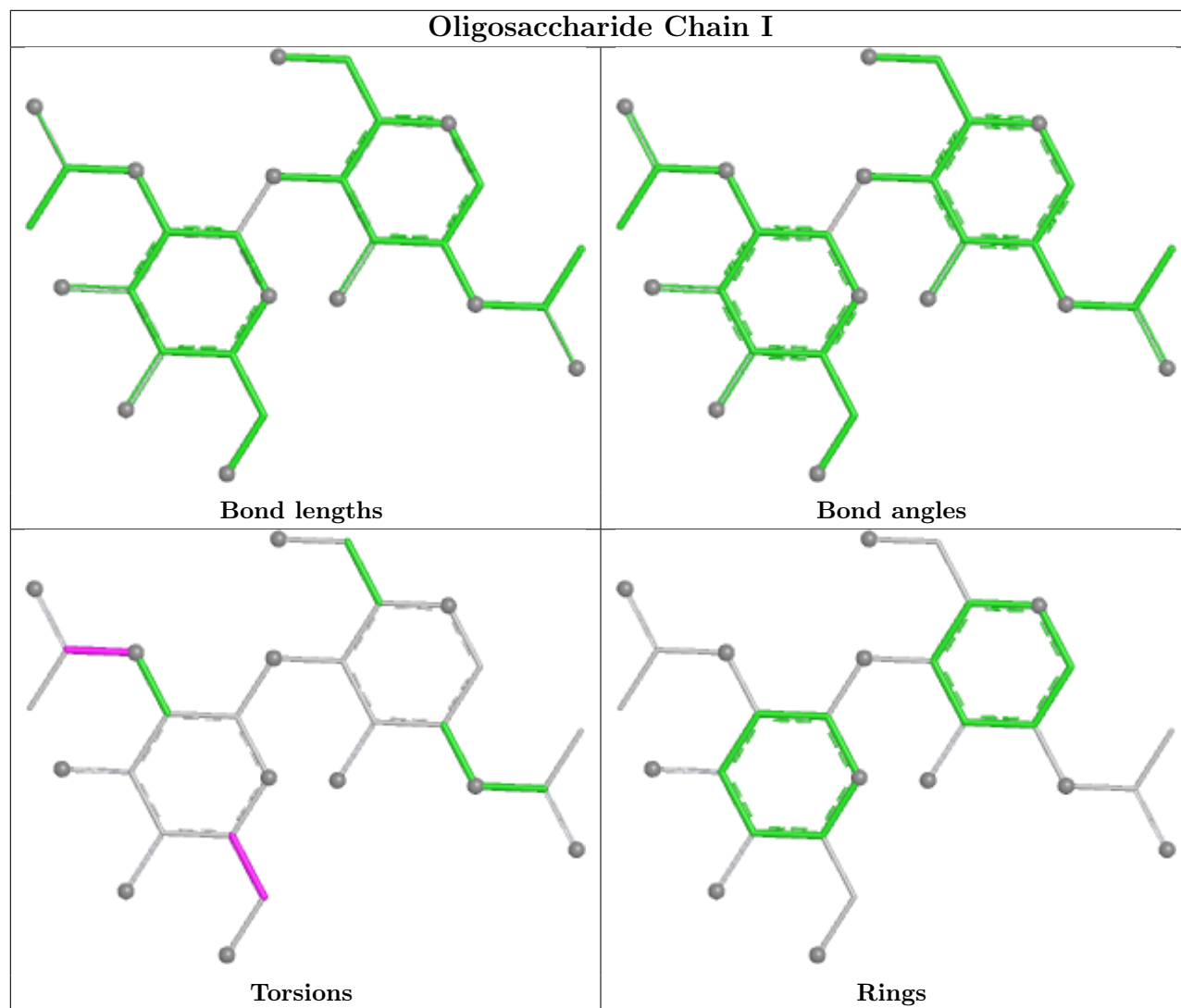
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6

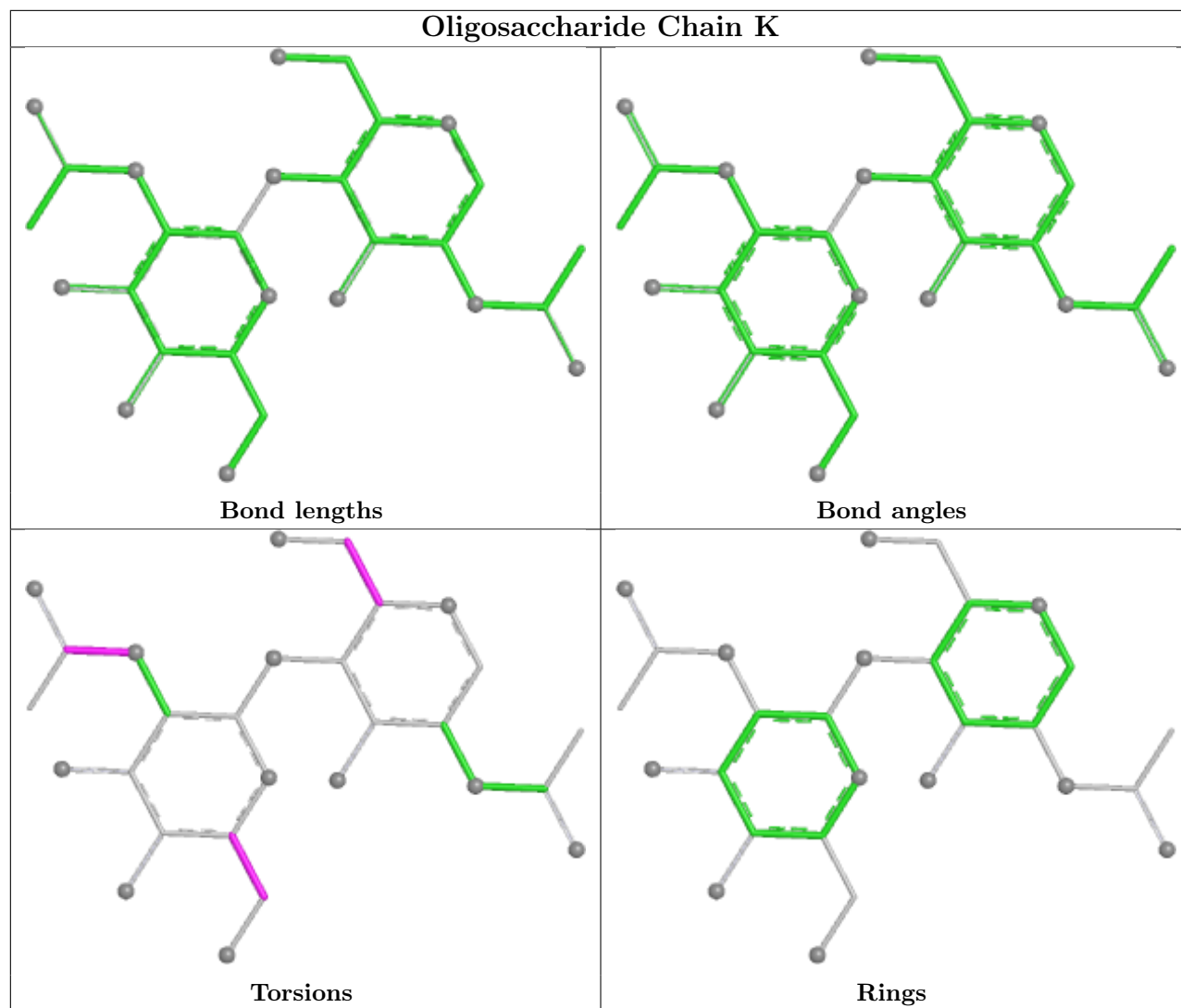
There are no ring outliers.

No monomer is involved in short contacts.

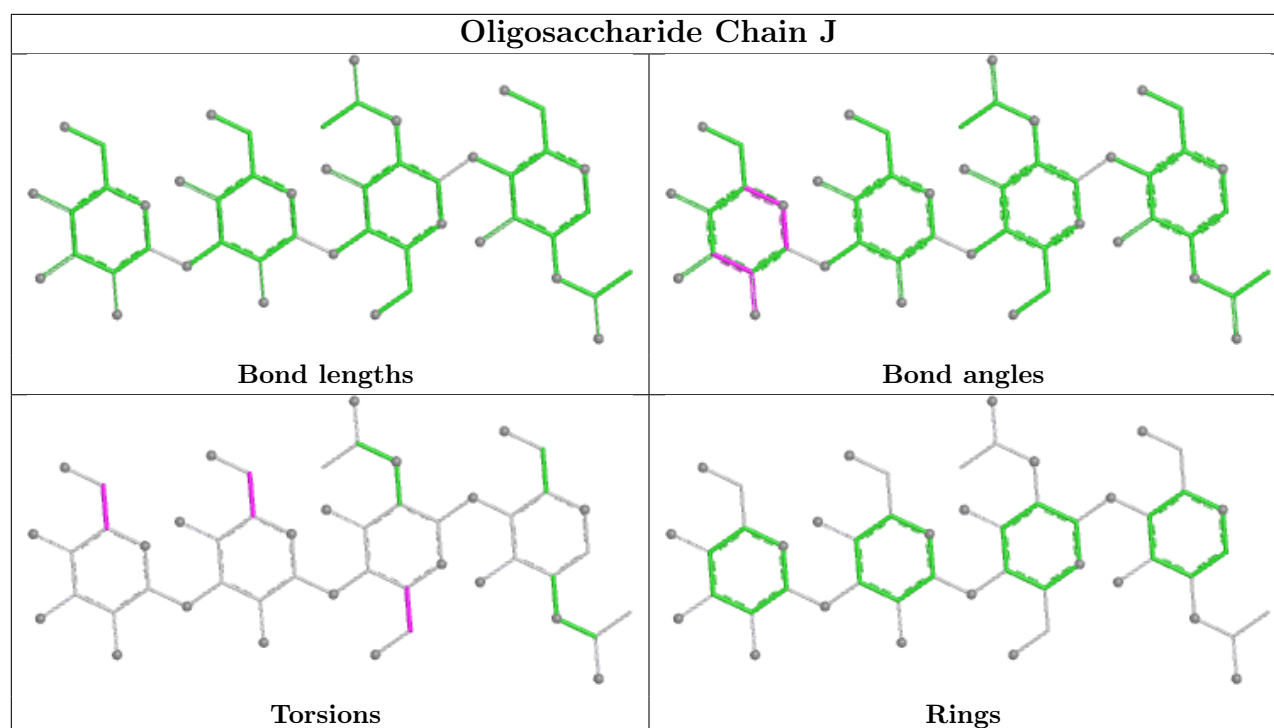
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
8	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.15	0
8	SO4	C	503	-	4,4,4	0.29	0	6,6,6	0.18	0
11	NAG	D	2004	2	14,14,15	0.33	0	17,19,21	0.60	0
8	SO4	A	508	-	4,4,4	0.25	0	6,6,6	0.15	0
8	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.17	0
8	SO4	C	510	-	4,4,4	0.25	0	6,6,6	0.14	0
8	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.12	0
8	SO4	C	502	-	4,4,4	0.26	0	6,6,6	0.10	0
11	NAG	B	2004	2	14,14,15	0.80	1 (7%)	17,19,21	0.84	0
8	SO4	A	507	-	4,4,4	0.27	0	6,6,6	0.12	0
12	N9U	D	2006	10	32,32,32	3.49	12 (37%)	34,42,42	1.81	9 (26%)
8	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	N9U	B	2005	10	32,32,32	3.48	12 (37%)	34,42,42	1.85	10 (29%)

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	D	2006	10	-	10/30/39/39	0/2/2/2
12	N9U	B	2005	10	-	7/30/39/39	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	-12.55	1.31	1.50
12	D	2006	N9U	C19-C22	-12.54	1.31	1.50
12	B	2005	N9U	C22-N21	6.75	1.44	1.28
12	D	2006	N9U	C22-N21	6.67	1.44	1.28
12	D	2006	N9U	C23-C22	5.84	1.59	1.47
12	B	2005	N9U	C23-C22	5.83	1.58	1.47
12	D	2006	N9U	C15-N14	5.66	1.46	1.33
12	B	2005	N9U	C15-N14	5.48	1.46	1.33
12	D	2006	N9U	O20-C18	5.18	1.54	1.46
12	B	2005	N9U	O20-C18	5.03	1.53	1.46
12	B	2005	N9U	C17-C18	-4.37	1.43	1.51
12	D	2006	N9U	C29-N30	4.32	1.45	1.33
12	B	2005	N9U	C29-N30	4.25	1.44	1.33
12	D	2006	N9U	C17-C18	-4.15	1.43	1.51
12	D	2006	N9U	O05-C06	3.98	1.43	1.35
12	B	2005	N9U	O05-C06	3.82	1.42	1.35
12	D	2006	N9U	C28-C29	3.08	1.53	1.47
12	D	2006	N9U	O11-C10	2.80	1.30	1.22
12	B	2005	N9U	C28-C29	2.70	1.52	1.47
12	B	2005	N9U	O11-C10	2.68	1.30	1.22
11	B	2004	NAG	C1-C2	2.63	1.55	1.52
12	B	2005	N9U	C19-C18	-2.58	1.48	1.52
12	B	2005	N9U	C06-N08	2.52	1.41	1.34
12	D	2006	N9U	C06-N08	2.39	1.40	1.34
12	D	2006	N9U	C19-C18	-2.38	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2006	N9U	O05-C06-N08	5.07	121.29	110.45
12	B	2005	N9U	C18-O20-N21	-4.82	103.72	108.86
12	B	2005	N9U	O05-C06-N08	4.59	120.27	110.45
12	D	2006	N9U	C18-O20-N21	-3.78	104.83	108.86
12	B	2005	N9U	O20-N21-C22	-3.49	104.23	109.20
12	D	2006	N9U	O20-N21-C22	-3.18	104.68	109.20
12	D	2006	N9U	O07-C06-N08	-3.15	119.70	124.86
12	D	2006	N9U	C17-C15-N14	2.92	120.49	115.97
12	B	2005	N9U	O07-C06-N08	-2.83	120.22	124.86
12	B	2005	N9U	C18-C19-C22	2.80	103.32	100.82
12	D	2006	N9U	C18-C19-C22	2.75	103.28	100.82
12	D	2006	N9U	O05-C06-O07	-2.74	119.01	124.26
12	B	2005	N9U	C19-C22-C23	-2.73	121.14	124.83
12	B	2005	N9U	O05-C06-O07	-2.48	119.51	124.26
12	B	2005	N9U	C17-C15-N14	2.48	119.80	115.97
12	B	2005	N9U	O12-C10-C09	2.12	120.68	113.51
12	D	2006	N9U	O12-C10-C09	2.11	120.64	113.51
12	D	2006	N9U	O12-C10-O11	-2.06	119.40	124.08
12	B	2005	N9U	O12-C10-O11	-2.00	119.54	124.08

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	2005	N9U	N08-C06-O05-C04
12	D	2006	N9U	O05-C06-N08-C09
12	B	2005	N9U	O07-C06-O05-C04
12	D	2006	N9U	N08-C09-C13-N14
11	D	2004	NAG	O5-C5-C6-O6
12	B	2005	N9U	O07-C06-N08-C09
12	B	2005	N9U	O05-C06-N08-C09
12	D	2006	N9U	C03-C04-O05-C06
12	B	2005	N9U	C03-C04-O05-C06
12	D	2006	N9U	C02-C03-C04-O05
12	D	2006	N9U	C10-C09-C13-N14
12	D	2006	N9U	C13-C09-C10-O12
11	D	2004	NAG	C4-C5-C6-O6
12	D	2006	N9U	C13-C09-N08-C06

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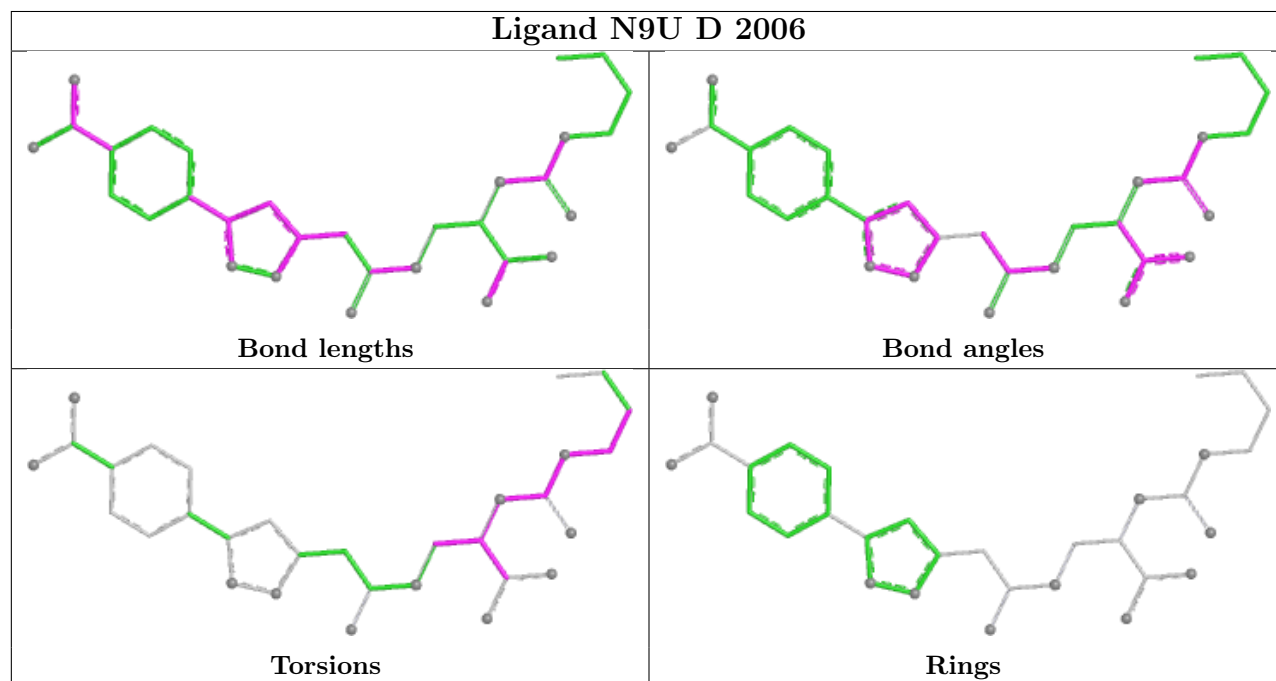
Mol	Chain	Res	Type	Atoms
12	B	2005	N9U	C10-C09-C13-N14
12	B	2005	N9U	C02-C03-C04-O05

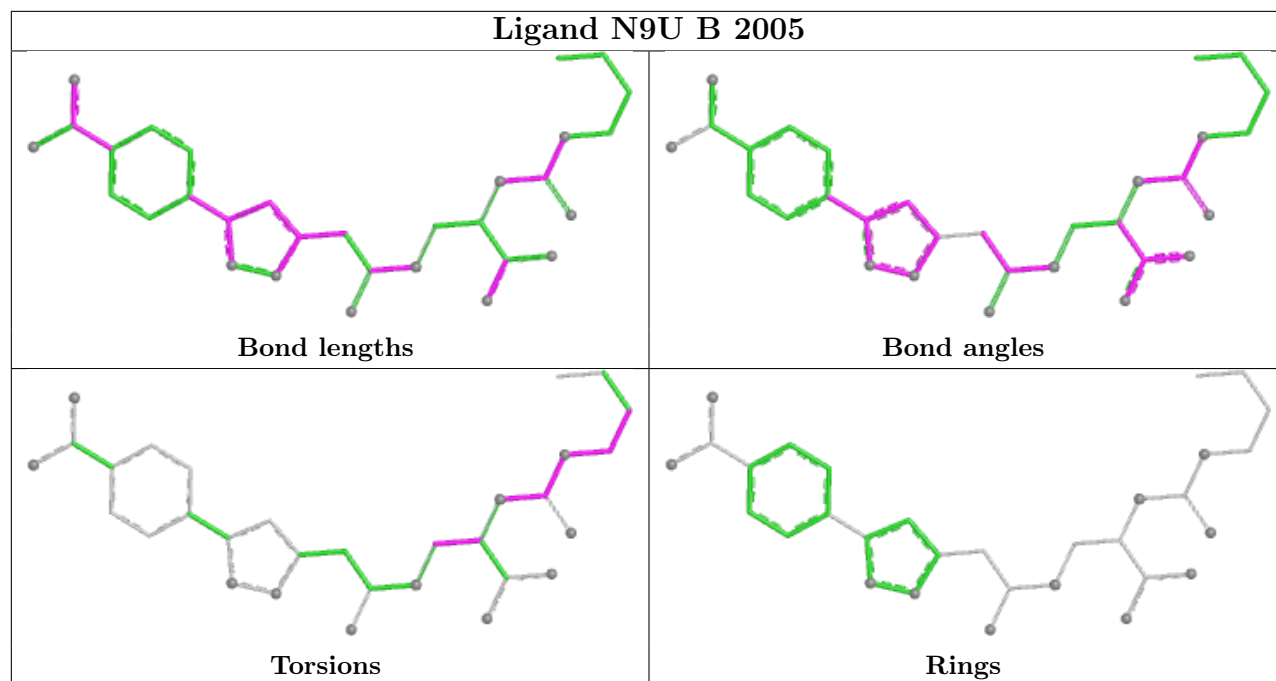
There are no ring outliers.

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, 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%)	-0.07	4 (0%) 81 83	30, 55, 75, 96	4 (0%)
1	C	453/457 (99%)	0.31	4 (0%) 81 83	30, 74, 99, 121	4 (0%)
2	B	466/472 (98%)	0.37	13 (2%) 55 56	26, 84, 148, 168	3 (0%)
2	D	471/472 (99%)	0.62	16 (3%) 48 50	58, 99, 135, 151	1 (0%)
3	E	214/221 (96%)	0.92	10 (4%) 37 39	93, 132, 186, 190	0
3	H	216/221 (97%)	0.54	4 (1%) 66 67	67, 106, 141, 146	0
4	F	214/214 (100%)	0.74	9 (4%) 41 42	96, 141, 182, 191	0
4	L	214/214 (100%)	0.44	2 (0%) 81 83	70, 102, 119, 142	0
All	All	2702/2728 (99%)	0.42	62 (2%) 61 61	26, 89, 165, 191	12 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	VAL	4.7
3	E	212	VAL	4.4
2	D	375	LEU	4.3
1	A	217	SER	3.5
3	E	147	LEU	3.5
2	B	77	SER	3.4
4	F	135	PHE	3.4
3	E	203	VAL	3.3
2	D	391	ILE	3.3
1	C	453	VAL	3.3
1	C	217	SER	3.2
2	B	131	ILE	3.1
2	B	129	TRP	3.0
3	E	165	LEU	3.0
1	A	130	CYS	3.0
2	B	466	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	458	GLY	2.8
1	C	130	CYS	2.8
3	H	206	PRO	2.8
2	D	145	LEU	2.7
4	F	160	LEU	2.7
2	D	338	SER	2.6
4	F	152	GLY	2.6
3	E	204	ALA	2.6
2	B	49	CYS	2.5
4	F	205	ILE	2.5
2	D	104	VAL	2.5
4	L	135	PHE	2.5
2	D	72	LYS	2.5
4	F	115	VAL	2.4
4	F	133	VAL	2.4
1	A	61	GLU	2.4
2	D	181	LYS	2.4
4	F	204	PRO	2.4
2	D	467	LEU	2.3
2	D	108	GLU	2.3
2	B	181	LYS	2.3
3	E	201	CYS	2.3
3	E	210	THR	2.2
3	E	124	ALA	2.2
2	B	44	LEU	2.2
2	B	178	TYR	2.2
2	D	69	LEU	2.2
3	E	160	TRP	2.2
2	D	111	PRO	2.2
3	H	130	LEU	2.2
2	B	94	PRO	2.1
1	C	160	PHE	2.1
3	H	189	VAL	2.1
3	E	11	LEU	2.1
2	B	375	LEU	2.1
2	D	129	TRP	2.1
2	D	41	LYS	2.1
4	L	205	ILE	2.1
4	F	132	VAL	2.1
2	D	45	LEU	2.1
2	B	26	CYS	2.0
2	D	471	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	H	212	VAL	2.0
2	D	464	PRO	2.0
4	F	180	THR	2.0
2	B	63	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](#)

SUGAR-RSR INFOmissingINFO

## 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( $\text{\AA}^2$ )	Q<0.9
11	NAG	B	2004	14/15	0.55	0.13	115,115,115,115	0
11	NAG	D	2004	14/15	0.63	0.12	113,113,113,113	0
8	SO4	C	502	5/5	0.67	0.19	96,96,96,96	0
8	SO4	C	510	5/5	0.74	0.14	106,106,106,106	0
8	SO4	C	503	5/5	0.76	0.15	108,108,108,108	0
8	SO4	A	507	5/5	0.76	0.24	84,84,84,84	0
13	CL	D	2005	1/1	0.82	0.15	99,99,99,99	0
8	SO4	A	508	5/5	0.83	0.17	85,85,85,85	0
8	SO4	C	501	5/5	0.83	0.23	90,90,90,90	0
8	SO4	L	301	5/5	0.85	0.18	90,90,90,90	0
13	CL	C	505	1/1	0.86	0.19	93,93,93,93	0
8	SO4	A	501	5/5	0.88	0.26	66,66,66,66	0
10	MN	D	2002	1/1	0.88	0.12	98,98,98,98	0
12	N9U	D	2006	31/31	0.89	0.13	79,79,79,79	0
12	N9U	B	2005	31/31	0.90	0.12	58,58,58,58	0
13	CL	C	504	1/1	0.93	0.08	76,76,76,76	0
8	SO4	A	502	5/5	0.94	0.09	66,66,66,66	0
10	MN	B	2002	1/1	0.95	0.10	79,79,79,79	0
9	CA	C	506	1/1	0.96	0.06	102,102,102,102	0

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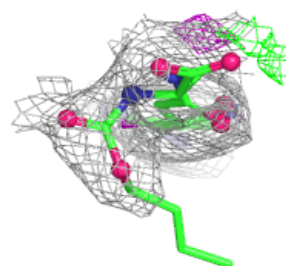
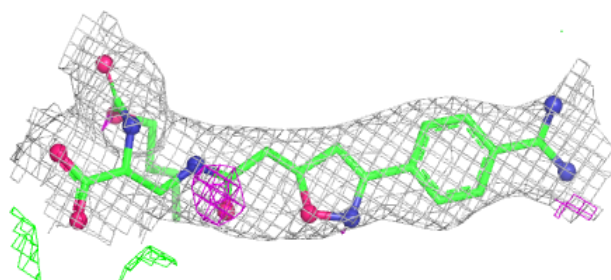
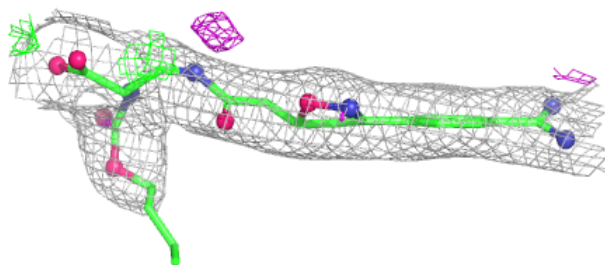
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CA	A	505	1/1	0.96	0.06	48,48,48,48	0
9	CA	C	508	1/1	0.97	0.04	73,73,73,73	0
9	CA	C	507	1/1	0.97	0.04	87,87,87,87	0
9	CA	A	504	1/1	0.98	0.03	52,52,52,52	0
9	CA	C	509	1/1	0.98	0.04	67,67,67,67	0
9	CA	A	503	1/1	0.98	0.04	62,62,62,62	0
10	MN	D	2001	1/1	0.98	0.05	75,75,75,75	0
10	MN	B	2003	1/1	0.99	0.04	51,51,51,51	0
10	MN	D	2003	1/1	0.99	0.03	73,73,73,73	0
9	CA	A	506	1/1	0.99	0.03	51,51,51,51	0
10	MN	B	2001	1/1	1.00	0.02	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.

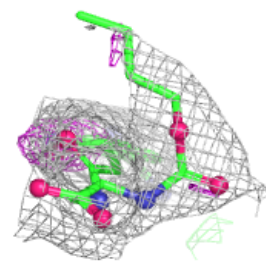
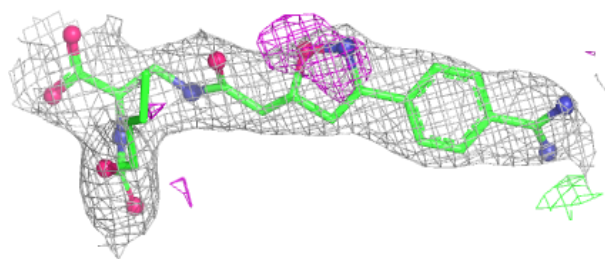
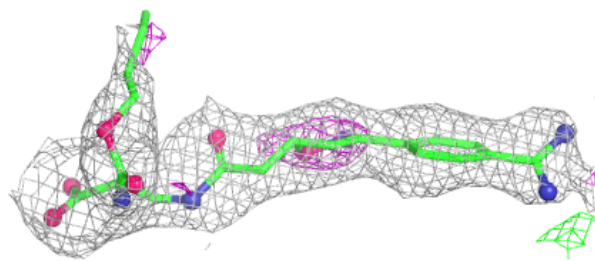
**Electron density around N9U D 2006:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around N9U B 2005:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.