



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:44 AM BST

PDB ID : 6CE0  
Title : Crystal structure of a HIV-1 clade B tier-3 isolate H078.14 UFO-BG Env trimer in complex with broadly neutralizing Fabs PGT124 and 35O22 at 4.6 Angstrom  
Authors : Kumar, S.; Sarkar, A.; Wilson, I.A.  
Deposited on : 2018-02-09  
Resolution : 4.60 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.

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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 : 2.13.1  
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) : 2.13.1

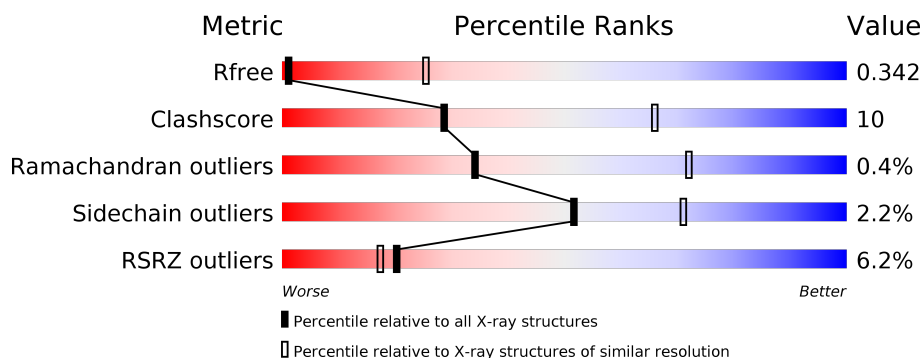
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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.







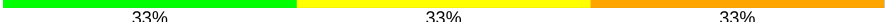
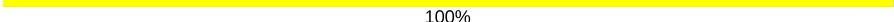



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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 on 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	B	140	<div> <div>81%</div> <div>16%</div> <div>••</div> </div>
2	G	487	<div> <div>4%</div> <div>66%</div> <div>24%</div> <div>•</div> <div>8%</div> </div>
3	D	243	<div> <div>10%</div> <div>82%</div> <div>16%</div> <div>••</div> </div>
4	E	216	<div> <div>4%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>
5	H	236	<div> <div>8%</div> <div>72%</div> <div>22%</div> <div>••</div> </div>
6	L	214	<div> <div>10%</div> <div>80%</div> <div>17%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
7	A	2	 100%
7	C	2	 50% 50%
7	J	2	 50% 50%
8	F	3	 67% 33%
8	K	3	 33% 33% 33%
9	I	5	 100%
9	N	5	 80% 20%
10	M	4	 50% 25% 25%
11	O	7	 29% 71%

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
10	MAN	M	4	-	-	-	X
12	NAG	G	607	-	-	-	X
12	NAG	G	614	-	-	-	X
12	NAG	G	627	-	-	-	X
12	NAG	G	630	-	-	-	X
12	NAG	G	631	-	-	-	X
7	NAG	J	2	-	-	-	X
9	MAN	N	4	-	-	-	X
9	MAN	N	5	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11946 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	137	Total	C	N	O	S	0	0	0
			1086	688	185	206	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	548	ASN	-	linker	UNP Q2N0T3
B	549	PRO	-	linker	UNP Q2N0T3
B	563	ASP	-	linker	UNP Q2N0T3
B	564	TRP	-	linker	UNP Q2N0T3
B	565	LEU	-	linker	UNP Q2N0T3
B	566	PRO	-	linker	UNP Q2N0T3
B	567	ASP	-	linker	UNP Q2N0T3
B	568	MET	-	linker	UNP Q2N0T3
B	569	THR	-	linker	UNP Q2N0T3
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	446	Total	C	N	O	S	0	0	0
			3512	2212	616	659	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	engineered mutation	UNP A4ZPX1
G	507	GLY	-	expression tag	UNP A4ZPX1
G	508	GLY	-	expression tag	UNP A4ZPX1
G	509	GLY	-	expression tag	UNP A4ZPX1
G	510	GLY	-	expression tag	UNP A4ZPX1
G	511	GLY	-	expression tag	UNP A4ZPX1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	512	SER	-	expression tag	UNP A4ZPX1
G	513	GLY	-	expression tag	UNP A4ZPX1
G	514	GLY	-	expression tag	UNP A4ZPX1
G	515	GLY	-	expression tag	UNP A4ZPX1
G	516	GLY	-	expression tag	UNP A4ZPX1
G	517	SER	-	expression tag	UNP A4ZPX1

- Molecule 3 is a protein called 35O22 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 4 is a protein called 35O22 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 5 is a protein called PGT124 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			

- Molecule 6 is a protein called PGT124 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 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
7	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

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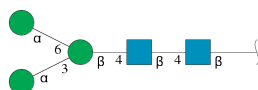
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



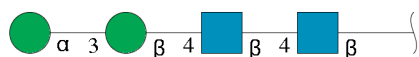
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 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.



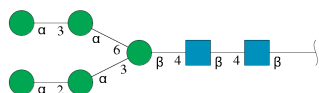
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 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.



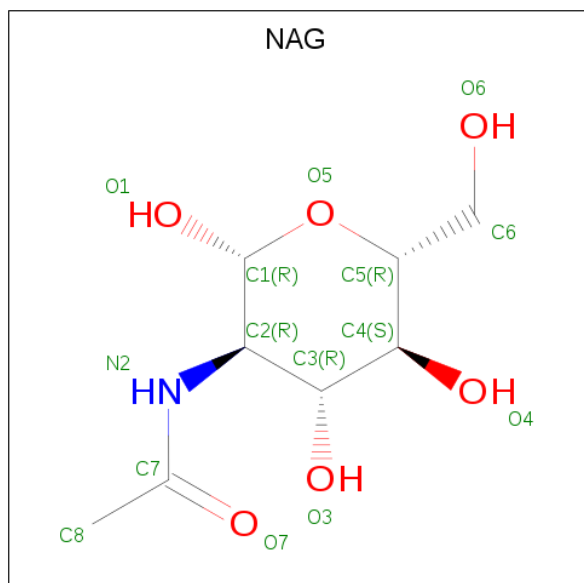
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
11	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		



### 3 Residue-property plots

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.

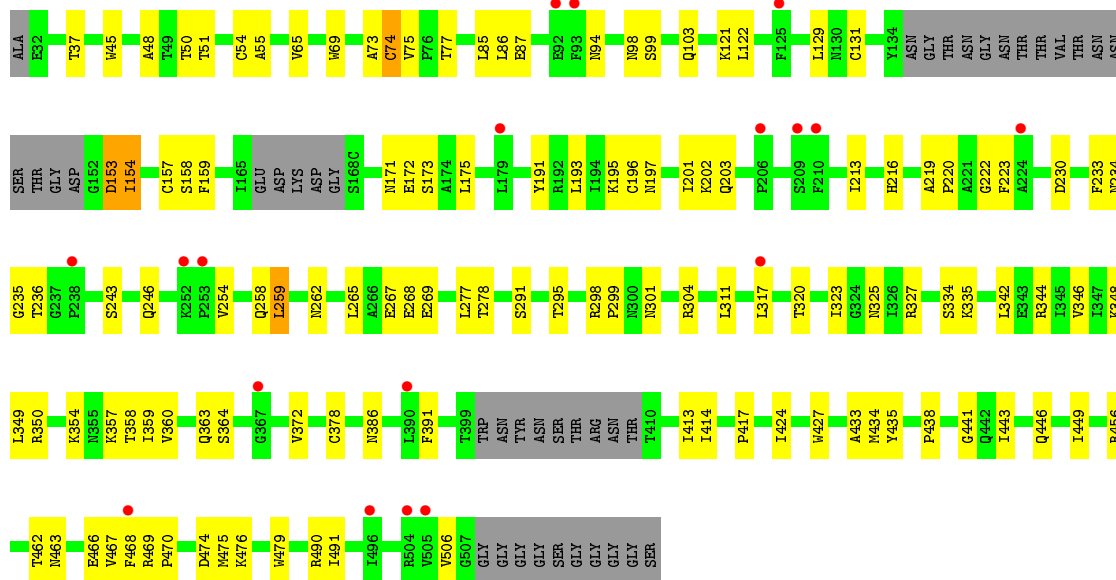
- Molecule 1: Envelope glycoprotein gp160

Chain B: 




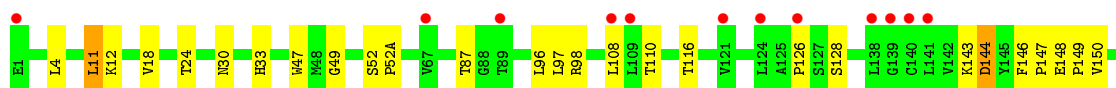
- Molecule 2: Envelope glycoprotein gp160

Chain G: 



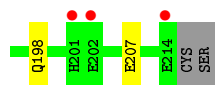
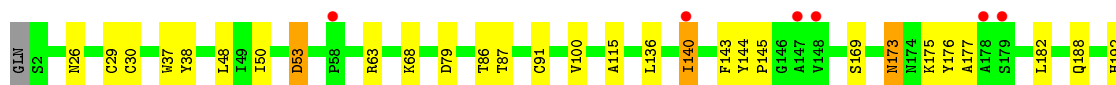
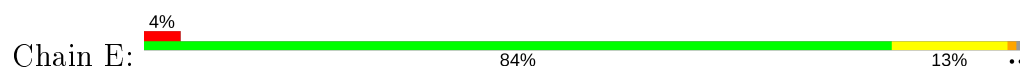
- Molecule 3: 35O22 Heavy chain

Chain D: 

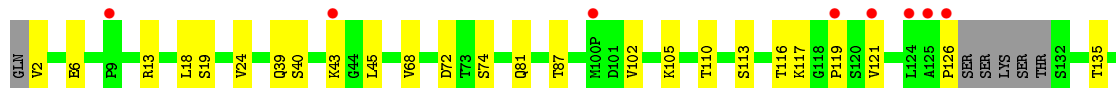
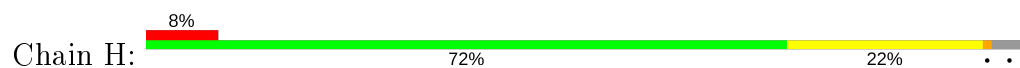




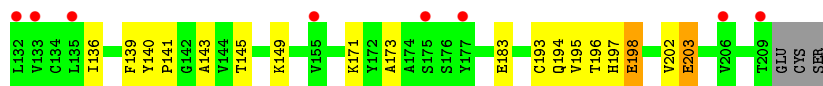
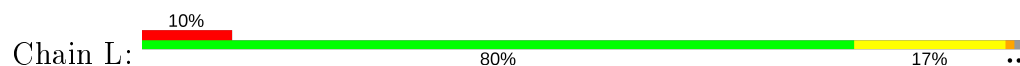
- Molecule 4: 35O22 Light chain



- Molecule 5: PGT124 Heavy chain



- Molecule 6: PGT124 Light chain



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



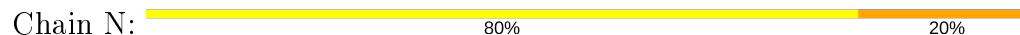
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 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 9: 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 10: 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



- Molecule 11:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -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 O:  29% 71%

MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.35Å 127.35Å 316.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 4.60 48.87 – 4.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.87-4.60) 96.9 (48.87-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 4.64Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.313 , 0.341 0.313 , 0.342	Depositor DCC
$R_{free}$ test set	749 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	181.7	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 210.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.159 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	274.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	0.23	0/1109	0.42	0/1509
2	G	0.24	0/3579	0.44	0/4854
3	D	0.25	0/1860	0.46	0/2533
4	E	0.25	0/1659	0.45	0/2269
5	H	0.25	0/1763	0.48	0/2407
6	L	0.27	0/1644	0.45	0/2246
All	All	0.25	0/11614	0.45	0/15818

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	B	1086	0	1055	21	0
2	G	3512	0	3485	83	0
3	D	1813	0	1784	26	0
4	E	1615	0	1544	21	0
5	H	1720	0	1684	40	0
6	L	1601	0	1545	44	0
7	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	28	0	25	1	0
7	J	28	0	25	1	0
8	F	39	0	34	2	0
8	K	39	0	34	1	0
9	I	61	0	52	1	0
9	N	61	0	50	6	0
10	M	50	0	43	1	0
11	O	83	0	69	0	0
12	G	182	0	165	7	0
All	All	11946	0	11619	228	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 10.

All (228) 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)
6:L:195:VAL:HG23	6:L:202:VAL:CG2	1.45	1.45
6:L:195:VAL:CG2	6:L:202:VAL:HG23	1.48	1.41
6:L:195:VAL:CG2	6:L:202:VAL:CG2	2.02	1.35
6:L:145:THR:HB	6:L:196:THR:HB	1.19	1.19
6:L:195:VAL:HG23	6:L:202:VAL:HG21	1.28	1.10
6:L:194:GLN:CA	6:L:203:GLU:HG2	1.83	1.09
6:L:195:VAL:HG22	6:L:202:VAL:HG23	1.11	1.07
6:L:194:GLN:HB2	6:L:203:GLU:HG3	1.40	1.03
6:L:194:GLN:HA	6:L:203:GLU:HG2	1.03	1.03
6:L:194:GLN:HA	6:L:203:GLU:CG	1.89	1.02
6:L:194:GLN:HB2	6:L:203:GLU:CG	1.96	0.96
6:L:198:GLU:OE1	6:L:198:GLU:N	2.08	0.87
6:L:193:CYS:C	6:L:203:GLU:OE2	2.13	0.87
6:L:143:ALA:HB3	6:L:198:GLU:OE1	1.75	0.85
6:L:194:GLN:CA	6:L:203:GLU:CG	2.51	0.85
6:L:195:VAL:CG2	6:L:202:VAL:HG21	1.86	0.83
3:D:98:ARG:HH11	9:N:1:NAG:H2	1.44	0.83
2:G:158:SER:HB3	12:G:601:NAG:H82	1.63	0.81
4:E:30:CYS:HB2	4:E:68:LYS:HD2	1.63	0.81
6:L:194:GLN:CB	6:L:203:GLU:CG	2.60	0.80
6:L:110:LYS:HD2	6:L:141:PRO:HG3	1.64	0.79
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.65	0.78
5:H:151:THR:HB	5:H:199:ASN:HB2	1.66	0.76
3:D:30:ASN:O	9:N:1:NAG:O6	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:LYS:HB3	2:G:51:THR:HB	1.69	0.75
1:B:572:GLY:HA2	1:B:575:GLN:HB3	1.68	0.74
6:L:145:THR:CB	6:L:196:THR:HB	2.12	0.73
6:L:194:GLN:CB	6:L:203:GLU:HG3	2.16	0.72
2:G:363:GLN:O	2:G:469:ARG:NH1	2.22	0.71
6:L:143:ALA:HB3	6:L:198:GLU:CD	2.09	0.71
6:L:33:VAL:N	6:L:51:ASN:OD1	2.19	0.71
2:G:269:GLU:HB3	2:G:348:LYS:HE2	1.73	0.70
4:E:143:PHE:HB2	4:E:176:TYR:HB2	1.73	0.70
4:E:115:ALA:H	4:E:144:TYR:HB3	1.57	0.69
5:H:119:PRO:HB3	5:H:145:TYR:HB3	1.75	0.69
3:D:11:LEU:HD11	3:D:202:PRO:HB3	1.74	0.68
4:E:136:LEU:HD12	4:E:182:LEU:HD23	1.75	0.68
2:G:301:ASN:ND2	7:J:1:NAG:O7	2.27	0.68
2:G:219:ALA:O	2:G:246:GLN:NE2	2.28	0.67
2:G:277:LEU:O	2:G:456:ARG:NH1	2.28	0.67
5:H:2:VAL:HG22	5:H:102:VAL:HG11	1.77	0.67
3:D:200:HIS:HD2	3:D:203:SER:H	1.42	0.66
6:L:141:PRO:HB2	6:L:198:GLU:OE2	1.95	0.66
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.77	0.66
5:H:121:VAL:HG11	5:H:198:VAL:HG21	1.78	0.66
4:E:140:ILE:HB	4:E:143:PHE:HZ	1.60	0.65
5:H:147:PRO:HD2	5:H:200:HIS:HE2	1.62	0.65
2:G:258:GLN:NE2	2:G:372:VAL:O	2.29	0.64
5:H:155:ASN:HD21	5:H:194:TYR:HA	1.62	0.64
4:E:37:TRP:HB2	4:E:50:ILE:HB	1.80	0.64
6:L:111:ALA:H	6:L:141:PRO:HD3	1.64	0.63
2:G:195:LYS:HZ3	2:G:433:ALA:HB1	1.64	0.62
6:L:111:ALA:HB3	6:L:140:TYR:H	1.64	0.62
4:E:91:CYS:SG	4:E:100:VAL:N	2.72	0.62
2:G:85:LEU:HD23	2:G:243:SER:HB3	1.79	0.62
3:D:108:LEU:HD22	3:D:149:PRO:HD3	1.81	0.62
5:H:147:PRO:HD2	5:H:200:HIS:NE2	2.14	0.62
5:H:105:LYS:HA	6:L:43:ALA:HB2	1.83	0.61
1:B:605:CYS:HA	2:G:37:THR:HG22	1.81	0.61
4:E:144:TYR:CG	4:E:145:PRO:HD3	2.35	0.61
1:B:607:ASN:ND2	1:B:654:GLU:OE1	2.34	0.60
3:D:128:SER:HB2	3:D:220:LEU:HB2	1.84	0.60
10:M:1:NAG:H83	10:M:1:NAG:H3	1.83	0.60
3:D:33:HIS:NE2	9:N:2:NAG:O3	2.23	0.60
2:G:121:LYS:HE3	2:G:202:LYS:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:325:ASN:OD1	6:L:93:SER:OG	2.21	0.59
6:L:140:TYR:CE2	6:L:171:LYS:HG2	2.37	0.59
5:H:13:ARG:NE	5:H:113:SER:O	2.35	0.59
5:H:147:PRO:HG2	5:H:202:PRO:HB2	1.86	0.58
4:E:29:CYS:SG	4:E:30:CYS:N	2.77	0.58
6:L:194:GLN:HB2	6:L:203:GLU:CD	2.24	0.58
2:G:122:LEU:HB2	2:G:201:ILE:HG23	1.85	0.58
2:G:195:LYS:NZ	2:G:433:ALA:HB1	2.19	0.58
5:H:145:TYR:HB2	5:H:200:HIS:CE1	2.39	0.58
2:G:295:THR:HG22	2:G:446:GLN:HG2	1.86	0.58
4:E:26:ASN:HA	4:E:29:CYS:HB2	1.86	0.57
2:G:94:ASN:HA	2:G:236:THR:HG22	1.87	0.57
2:G:298:ARG:NH2	2:G:441:GLY:O	2.36	0.57
5:H:121:VAL:HG12	5:H:142:VAL:HA	1.86	0.57
4:E:140:ILE:HB	4:E:143:PHE:CZ	2.39	0.57
6:L:195:VAL:HG22	6:L:202:VAL:CG2	1.95	0.57
4:E:144:TYR:CD2	4:E:145:PRO:HD3	2.39	0.56
2:G:311:LEU:HG	2:G:317:LEU:HG	1.87	0.56
2:G:265:LEU:HD21	2:G:291:SER:HB3	1.87	0.56
2:G:462:THR:OG1	2:G:463:ASN:N	2.39	0.55
1:B:572:GLY:HA2	1:B:575:GLN:HE21	1.72	0.55
2:G:476:LYS:HA	2:G:479:TRP:CD1	2.41	0.55
2:G:335:LYS:HB2	2:G:414:ILE:HG13	1.89	0.54
4:E:173:ASN:O	4:E:175:LYS:NZ	2.36	0.54
1:B:596:TRP:CD2	1:B:646:LEU:HD23	2.43	0.54
1:B:650:GLN:HG3	1:B:651:ASN:H	1.73	0.54
3:D:126:PRO:HB2	3:D:215:SER:HB2	1.90	0.54
5:H:147:PRO:HD2	5:H:200:HIS:CE1	2.43	0.54
2:G:51:THR:HA	2:G:103:GLN:HE22	1.73	0.53
5:H:116:THR:HA	5:H:146:PHE:HD1	1.72	0.53
2:G:74:CYS:SG	2:G:75:VAL:HG22	2.48	0.53
2:G:201:ILE:HD11	2:G:435:TYR:HB2	1.91	0.53
2:G:153:ASP:N	2:G:153:ASP:OD1	2.40	0.53
2:G:48:ALA:HB3	2:G:490:ARG:HG3	1.91	0.53
6:L:193:CYS:N	6:L:203:GLU:OE2	2.41	0.53
6:L:113:PRO:HB3	6:L:139:PHE:HB3	1.91	0.53
1:B:565:LEU:N	1:B:566:PRO:HD3	2.23	0.53
1:B:650:GLN:O	1:B:654:GLU:N	2.25	0.52
4:E:198:GLN:HG2	4:E:207:GLU:HG3	1.90	0.52
2:G:55:ALA:HA	2:G:75:VAL:HG21	1.92	0.52
2:G:364:SER:HB3	2:G:372:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:469:ARG:NH2	12:G:621:NAG:H2	2.24	0.52
4:E:115:ALA:N	4:E:144:TYR:HB3	2.24	0.52
2:G:299:PRO:HB2	2:G:327:ARG:HB2	1.91	0.52
2:G:154:ILE:HG23	2:G:175:LEU:HD21	1.91	0.52
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.50	0.51
3:D:143:LYS:HG3	3:D:144:ASP:H	1.76	0.51
3:D:98:ARG:O	9:N:2:NAG:H5	2.10	0.51
6:L:193:CYS:O	6:L:203:GLU:OE2	2.28	0.51
2:G:344:ARG:HD3	12:G:615:NAG:H5	1.94	0.50
5:H:39:GLN:HB2	5:H:45:LEU:HD23	1.94	0.50
3:D:189:LEU:HD22	3:D:213:PRO:HB2	1.94	0.50
6:L:136:ILE:HG12	6:L:195:VAL:HG11	1.94	0.50
6:L:145:THR:O	6:L:196:THR:N	2.31	0.50
2:G:122:LEU:HD21	2:G:203:GLN:HB2	1.93	0.49
2:G:474:ASP:OD1	2:G:475:MET:N	2.46	0.49
6:L:35:TRP:HB2	6:L:48:ILE:HB	1.93	0.49
2:G:230:ASP:HB3	2:G:233:PHE:HB2	1.93	0.49
5:H:148:GLU:CB	5:H:149:PRO:HD3	2.42	0.49
8:K:1:NAG:O3	8:K:2:NAG:O5	2.17	0.49
1:B:578:ALA:HB1	2:G:220:PRO:HG3	1.94	0.48
2:G:55:ALA:HA	2:G:75:VAL:CG2	2.43	0.48
5:H:119:PRO:HD3	5:H:200:HIS:ND1	2.28	0.48
2:G:172:GLU:HA	8:F:1:NAG:H82	1.94	0.48
5:H:196:CYS:SG	5:H:209:LYS:HB2	2.54	0.48
6:L:197:HIS:CD2	6:L:198:GLU:OE2	2.66	0.48
2:G:121:LYS:HA	2:G:202:LYS:HA	1.94	0.48
2:G:254:VAL:HG21	2:G:262:ASN:HB2	1.96	0.48
5:H:135:THR:HB	5:H:183:THR:HG22	1.94	0.48
3:D:52(A):PRO:HD2	9:N:2:NAG:H81	1.95	0.48
3:D:116:THR:HG23	3:D:147:PRO:HG2	1.95	0.48
3:D:4:LEU:HG	3:D:24:THR:HG22	1.95	0.48
2:G:346:VAL:HG23	2:G:359:ILE:HD13	1.95	0.48
1:B:571:TRP:O	1:B:575:GLN:N	2.44	0.47
2:G:171:ASN:HB2	12:G:601:NAG:H81	1.96	0.47
3:D:87:THR:HG23	3:D:110:THR:HA	1.96	0.47
1:B:544:LEU:HD12	2:G:222:GLY:HA2	1.95	0.47
5:H:87:THR:HG23	5:H:110:THR:HA	1.96	0.47
4:E:188:GLN:O	4:E:192:HIS:ND1	2.46	0.47
2:G:298:ARG:HB3	2:G:443:ILE:HB	1.95	0.47
3:D:96:LEU:HG	3:D:97:LEU:HG	1.97	0.46
2:G:69:TRP:HB3	2:G:213:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:50:THR:O	2:G:103:GLN:NE2	2.47	0.46
5:H:166:PHE:CE2	6:L:173:ALA:HB1	2.50	0.46
3:D:207:VAL:HG12	3:D:209:LYS:HG2	1.97	0.46
5:H:170:LEU:HD13	5:H:176:TYR:CZ	2.50	0.46
5:H:159:LEU:HD13	5:H:182:VAL:HG11	1.97	0.46
5:H:121:VAL:HG23	5:H:209:LYS:HE3	1.96	0.46
2:G:223:PHE:CE2	2:G:490:ARG:HG2	2.50	0.46
2:G:129:LEU:O	2:G:191:TYR:N	2.49	0.46
2:G:220:PRO:HG2	2:G:223:PHE:CD1	2.50	0.46
3:D:148:GLU:N	3:D:149:PRO:HD2	2.31	0.46
2:G:467:VAL:HG21	12:G:621:NAG:H83	1.56	0.46
2:G:386:ASN:HB3	2:G:417:PRO:HD2	1.99	0.45
5:H:119:PRO:HD2	5:H:205:THR:HG21	1.98	0.45
2:G:304:ARG:NH2	2:G:438:PRO:O	2.42	0.45
2:G:195:LYS:HZ2	2:G:424:ILE:N	2.13	0.45
2:G:349:LEU:HD13	2:G:468:PHE:CE2	2.52	0.45
3:D:12:LYS:HG3	3:D:18:VAL:HB	1.99	0.45
2:G:360:VAL:N	2:G:466:GLU:O	2.50	0.45
2:G:259:LEU:H	2:G:259:LEU:HD23	1.82	0.45
2:G:45:TRP:HB3	2:G:491:ILE:HD13	1.99	0.44
5:H:148:GLU:HB2	5:H:149:PRO:HD3	1.99	0.44
2:G:301:ASN:HB3	2:G:323:ILE:O	2.18	0.44
1:B:516:GLY:N	1:B:535:MET:SD	2.90	0.44
3:D:146:PHE:HB3	3:D:147:PRO:HD3	1.99	0.44
5:H:117:LYS:H	5:H:146:PHE:HB3	1.83	0.44
5:H:200:HIS:ND1	5:H:203:SER:OG	2.44	0.44
1:B:574:LYS:O	2:G:51:THR:OG1	2.28	0.43
5:H:126:PRO:HD3	5:H:138:LEU:HD12	2.00	0.43
6:L:54:ARG:HG2	6:L:58:ILE:HB	2.00	0.43
5:H:169:VAL:HG12	5:H:177:SER:O	2.19	0.43
1:B:568:MET:O	1:B:568:MET:HG3	2.18	0.43
2:G:234:ASN:OD1	2:G:235:GLY:N	2.51	0.43
1:B:523:LEU:O	2:G:86:LEU:HD22	2.18	0.43
5:H:68:VAL:HG13	5:H:81:GLN:HB2	2.00	0.43
6:L:28:LEU:HB2	6:L:94:ARG:HB2	2.01	0.42
1:B:583:VAL:HA	1:B:586:TYR:HB3	2.00	0.42
5:H:116:THR:HA	5:H:146:PHE:CD1	2.52	0.42
9:I:1:NAG:H62	9:I:2:NAG:C7	2.49	0.42
6:L:198:GLU:CD	6:L:198:GLU:N	2.73	0.42
3:D:200:HIS:CD2	3:D:203:SER:H	2.30	0.42
5:H:6:GLU:N	5:H:6:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:31:ARG:HG3	6:L:51:ASN:HD21	1.84	0.42
1:B:659:ASP:O	1:B:663:LEU:HB2	2.19	0.42
2:G:131:CYS:HA	2:G:157:CYS:HA	2.02	0.42
2:G:427:TRP:CD1	2:G:475:MET:HG2	2.53	0.42
5:H:138:LEU:HD11	5:H:211:VAL:HB	2.00	0.42
7:C:1:NAG:H61	7:C:2:NAG:C1	2.49	0.42
2:G:278:THR:O	2:G:456:ARG:NH2	2.51	0.42
2:G:334:SER:HA	2:G:413:ILE:HG23	2.01	0.42
3:D:52:SER:OG	9:N:2:NAG:O7	2.33	0.42
2:G:346:VAL:HG22	2:G:350:ARG:HD2	2.01	0.42
3:D:210:ARG:NH1	3:D:211:VAL:O	2.53	0.42
4:E:86:THR:OG1	4:E:87:THR:N	2.53	0.42
2:G:202:LYS:O	2:G:434:MET:HA	2.20	0.42
12:G:607:NAG:O7	12:G:607:NAG:O3	2.32	0.41
2:G:159:PHE:O	12:G:601:NAG:H83	2.21	0.41
5:H:18:LEU:HD23	5:H:19:SER:N	2.35	0.41
2:G:354:LYS:HD2	2:G:354:LYS:HA	1.69	0.41
1:B:661:LEU:HG	2:G:506:VAL:O	2.21	0.41
2:G:98:ASN:OD1	2:G:99:SER:N	2.54	0.41
2:G:173:SER:N	8:F:1:NAG:H81	2.35	0.41
2:G:391:PHE:CD2	2:G:470:PRO:HG3	2.56	0.41
5:H:72:ASP:OD1	5:H:74:SER:OG	2.32	0.41
5:H:40:SER:HB2	5:H:43:LYS:HD2	2.02	0.41
4:E:169:SER:O	4:E:177:ALA:N	2.53	0.41
5:H:144:ASP:HB3	5:H:175:LEU:HD23	2.03	0.41
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.55	0.41
2:G:267:GLU:HG3	2:G:268:GLU:HG2	2.03	0.41
2:G:363:GLN:HG2	2:G:364:SER:H	1.86	0.41
1:B:565:LEU:HB3	2:G:73:ALA:HB1	2.02	0.41
4:E:63:ARG:HD2	4:E:79:ASP:HB3	2.03	0.41
4:E:38:TYR:CZ	4:E:48:LEU:HD13	2.56	0.40
5:H:163:VAL:HG22	5:H:182:VAL:HG22	2.03	0.40
1:B:574:LYS:HB3	2:G:51:THR:CB	2.46	0.40
3:D:170:LEU:HD13	3:D:176:TYR:CZ	2.56	0.40
4:E:50:ILE:HG23	4:E:53:ASP:O	2.20	0.40
3:D:150:VAL:HG22	3:D:200:HIS:HD1	1.87	0.40
2:G:74:CYS:O	2:G:75:VAL:HG13	2.22	0.40
6:L:87:TYR:CG	6:L:101:ALA:HB2	2.57	0.40
2:G:357:LYS:HB2	2:G:357:LYS:HE3	1.84	0.40
5:H:200:HIS:CE1	5:H:203:SER:HG	2.38	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	B	135/140 (96%)	125 (93%)	9 (7%)	1 (1%)	22	62
2	G	438/487 (90%)	404 (92%)	34 (8%)	0	100	100
3	D	238/243 (98%)	229 (96%)	8 (3%)	1 (0%)	34	72
4	E	211/216 (98%)	202 (96%)	9 (4%)	0	100	100
5	H	222/236 (94%)	207 (93%)	13 (6%)	2 (1%)	17	56
6	L	209/214 (98%)	196 (94%)	11 (5%)	2 (1%)	15	54
All	All	1453/1536 (95%)	1363 (94%)	84 (6%)	6 (0%)	34	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	566	PRO
5	H	148	GLU
6	L	198	GLU
3	D	144	ASP
6	L	6	VAL
5	H	147	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	B	117/118 (99%)	117 (100%)	0	100	100
2	G	400/428 (94%)	386 (96%)	14 (4%)	36	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	203/206 (98%)	201 (99%)	2 (1%)	76	86
4	E	186/189 (98%)	183 (98%)	3 (2%)	62	79
5	H	194/204 (95%)	191 (98%)	3 (2%)	65	80
6	L	177/180 (98%)	171 (97%)	6 (3%)	37	60
All	All	1277/1325 (96%)	1249 (98%)	28 (2%)	52	71

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

Mol	Chain	Res	Type
2	G	54	CYS
2	G	65	VAL
2	G	74	CYS
2	G	77	THR
2	G	87	GLU
2	G	153	ASP
2	G	154	ILE
2	G	197	ASN
2	G	259	LEU
2	G	320	THR
2	G	342	LEU
2	G	358	THR
2	G	378	CYS
2	G	449	ILE
3	D	11	LEU
3	D	164	HIS
4	E	53	ASP
4	E	140	ILE
4	E	173	ASN
5	H	24	VAL
5	H	192	GLN
5	H	205	THR
6	L	51	ASN
6	L	65	THR
6	L	89	HIS
6	L	149	LYS
6	L	183	GLU
6	L	203	GLU

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

Mol	Chain	Res	Type
1	B	575	GLN
2	G	103	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

33 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$
7	NAG	A	1	1,7	14,14,15	0.39	0	17,19,21	0.45	0
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	0.52	0
7	NAG	C	1	2,7	14,14,15	0.78	1 (7%)	17,19,21	1.29	3 (17%)
7	NAG	C	2	7	14,14,15	0.33	0	17,19,21	0.38	0
8	NAG	F	1	8,2	14,14,15	0.22	0	17,19,21	0.71	1 (5%)
8	NAG	F	2	8	14,14,15	0.19	0	17,19,21	0.45	0
8	BMA	F	3	8	11,11,12	0.78	0	15,15,17	0.74	0
9	NAG	I	1	9,2	14,14,15	0.47	0	17,19,21	0.52	0
9	NAG	I	2	9	14,14,15	0.64	0	17,19,21	0.80	0
9	BMA	I	3	9	11,11,12	0.86	0	15,15,17	1.06	1 (6%)
9	MAN	I	4	9	11,11,12	0.78	0	15,15,17	0.85	1 (6%)
9	MAN	I	5	9	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
7	NAG	J	1	2,7	14,14,15	0.54	0	17,19,21	1.46	2 (11%)
7	NAG	J	2	7	14,14,15	0.37	0	17,19,21	0.58	0
8	NAG	K	1	8,2	14,14,15	0.40	0	17,19,21	0.59	0
8	NAG	K	2	8	14,14,15	0.22	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	K	3	8	11,11,12	0.60	0	15,15,17	0.72	0
10	NAG	M	1	10,2	14,14,15	0.51	0	17,19,21	1.28	1 (5%)
10	NAG	M	2	10	14,14,15	0.30	0	17,19,21	0.59	0
10	BMA	M	3	10	11,11,12	0.59	0	15,15,17	0.72	0
10	MAN	M	4	10	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
9	NAG	N	1	9,3,2	14,14,15	0.52	0	17,19,21	1.93	2 (11%)
9	NAG	N	2	9	14,14,15	0.20	0	17,19,21	0.39	0
9	BMA	N	3	9	11,11,12	0.89	1 (9%)	15,15,17	1.03	0
9	MAN	N	4	9	11,11,12	0.71	0	15,15,17	0.85	1 (6%)
9	MAN	N	5	9,3	11,11,12	1.13	1 (9%)	15,15,17	0.81	1 (6%)
11	NAG	O	1	11,2	14,14,15	0.32	0	17,19,21	0.47	0
11	NAG	O	2	11	14,14,15	0.29	0	17,19,21	0.52	0
11	BMA	O	3	11	11,11,12	1.47	1 (9%)	15,15,17	1.46	2 (13%)
11	MAN	O	4	11	11,11,12	1.60	3 (27%)	15,15,17	2.33	3 (20%)
11	MAN	O	5	11,5	11,11,12	0.95	1 (9%)	15,15,17	1.08	2 (13%)
11	MAN	O	6	11	11,11,12	1.38	1 (9%)	15,15,17	1.90	3 (20%)
11	MAN	O	7	11	11,11,12	0.76	1 (9%)	15,15,17	1.29	2 (13%)

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
7	NAG	A	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	NAG	C	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1
8	NAG	F	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	1/2/19/22	0/1/1/1
9	NAG	I	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	4/6/23/26	0/1/1/1
9	BMA	I	3	9	-	1/2/19/22	0/1/1/1
9	MAN	I	4	9	-	0/2/19/22	0/1/1/1
9	MAN	I	5	9	-	1/2/19/22	0/1/1/1
7	NAG	J	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
8	NAG	K	1	8,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
10	NAG	M	1	10,2	-	5/6/23/26	0/1/1/1
10	NAG	M	2	10	-	3/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	MAN	M	4	10	-	0/2/19/22	0/1/1/1
9	NAG	N	1	9,3,2	-	3/6/23/26	0/1/1/1
9	NAG	N	2	9	-	0/6/23/26	0/1/1/1
9	BMA	N	3	9	-	2/2/19/22	0/1/1/1
9	MAN	N	4	9	-	1/2/19/22	0/1/1/1
9	MAN	N	5	9,3	-	2/2/19/22	0/1/1/1
11	NAG	O	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	O	2	11	-	0/6/23/26	0/1/1/1
11	BMA	O	3	11	-	2/2/19/22	0/1/1/1
11	MAN	O	4	11	-	0/2/19/22	0/1/1/1
11	MAN	O	5	11,5	-	0/2/19/22	0/1/1/1
11	MAN	O	6	11	-	0/2/19/22	0/1/1/1
11	MAN	O	7	11	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	3	BMA	O3-C3	3.84	1.52	1.43
9	N	5	MAN	O5-C1	-3.35	1.38	1.43
11	O	4	MAN	C1-C2	3.33	1.59	1.52
11	O	6	MAN	C1-C2	3.27	1.59	1.52
11	O	4	MAN	O5-C5	2.84	1.49	1.43
7	C	1	NAG	O5-C1	-2.70	1.39	1.43
11	O	4	MAN	O5-C1	2.60	1.47	1.43
11	O	5	MAN	C1-C2	2.46	1.57	1.52
11	O	7	MAN	C1-C2	2.28	1.57	1.52
9	N	3	BMA	C4-C3	2.06	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	4	MAN	C1-O5-C5	7.66	122.58	112.19
9	N	1	NAG	C1-O5-C5	6.18	120.57	112.19
11	O	6	MAN	C1-O5-C5	5.62	119.81	112.19
7	J	1	NAG	C2-N2-C7	4.39	129.15	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	3	BMA	O3-C3-C2	4.21	118.06	109.99
10	M	1	NAG	C2-N2-C7	4.17	128.84	122.90
11	O	7	MAN	C1-O5-C5	3.81	117.36	112.19
7	C	1	NAG	C1-O5-C5	3.41	116.82	112.19
11	O	6	MAN	C1-C2-C3	3.24	113.65	109.67
7	J	1	NAG	C1-C2-N2	3.22	115.98	110.49
11	O	4	MAN	O5-C1-C2	3.00	115.40	110.77
10	M	4	MAN	C1-O5-C5	2.80	115.98	112.19
9	N	1	NAG	C3-C4-C5	2.55	114.79	110.24
9	I	5	MAN	C1-O5-C5	2.50	115.57	112.19
7	C	1	NAG	O4-C4-C3	-2.44	104.72	110.35
11	O	6	MAN	O2-C2-C3	-2.41	105.31	110.14
9	N	5	MAN	O2-C2-C3	-2.25	105.64	110.14
11	O	3	BMA	C1-O5-C5	2.24	115.23	112.19
10	M	4	MAN	O2-C2-C3	-2.22	105.69	110.14
9	I	5	MAN	O2-C2-C3	-2.22	105.70	110.14
9	I	4	MAN	O2-C2-C3	-2.21	105.71	110.14
9	N	4	MAN	O2-C2-C3	-2.19	105.75	110.14
8	F	1	NAG	C1-O5-C5	2.18	115.15	112.19
11	O	5	MAN	C1-O5-C5	2.18	115.15	112.19
11	O	5	MAN	O2-C2-C3	-2.18	105.77	110.14
11	O	7	MAN	O2-C2-C3	-2.17	105.80	110.14
8	K	2	NAG	C1-O5-C5	2.11	115.06	112.19
11	O	4	MAN	O2-C2-C3	-2.06	106.02	110.14
9	I	3	BMA	C1-O5-C5	2.05	114.97	112.19
7	C	1	NAG	O5-C5-C6	-2.04	104.01	107.20

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	1	NAG	C1-C2-N2-C7
9	N	3	BMA	O5-C5-C6-O6
9	N	5	MAN	O5-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
11	O	1	NAG	O5-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
11	O	3	BMA	C4-C5-C6-O6
9	N	5	MAN	C4-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
9	N	3	BMA	C4-C5-C6-O6
11	O	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	M	1	NAG	C4-C5-C6-O6
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
9	I	2	NAG	C8-C7-N2-C2
9	I	2	NAG	O7-C7-N2-C2
8	K	1	NAG	O5-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
8	F	3	BMA	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
11	O	3	BMA	O5-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
9	I	2	NAG	C4-C5-C6-O6
9	I	5	MAN	O5-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
7	C	2	NAG	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
9	I	1	NAG	C1-C2-N2-C7
9	I	3	BMA	O5-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
9	N	4	MAN	O5-C5-C6-O6
9	N	1	NAG	C3-C2-N2-C7
10	M	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C3-C2-N2-C7
7	A	2	NAG	O5-C5-C6-O6
7	C	2	NAG	C1-C2-N2-C7
10	M	1	NAG	C3-C2-N2-C7
9	I	1	NAG	C3-C2-N2-C7
10	M	2	NAG	C1-C2-N2-C7

There are no ring outliers.

11 monomers are involved in 13 short contacts:

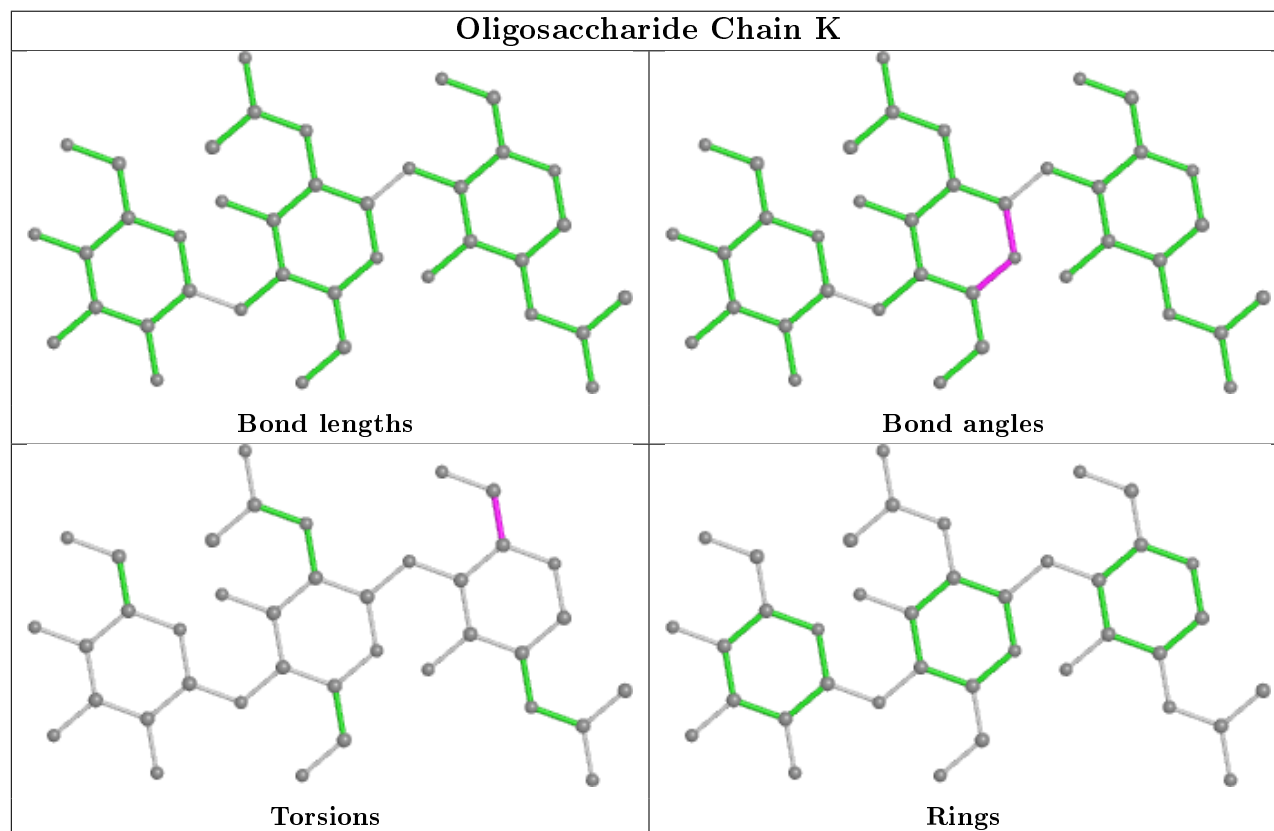
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	2	NAG	4	0
8	F	1	NAG	2	0
7	J	1	NAG	1	0
7	C	2	NAG	1	0
7	C	1	NAG	1	0
10	M	1	NAG	1	0
8	K	1	NAG	1	0

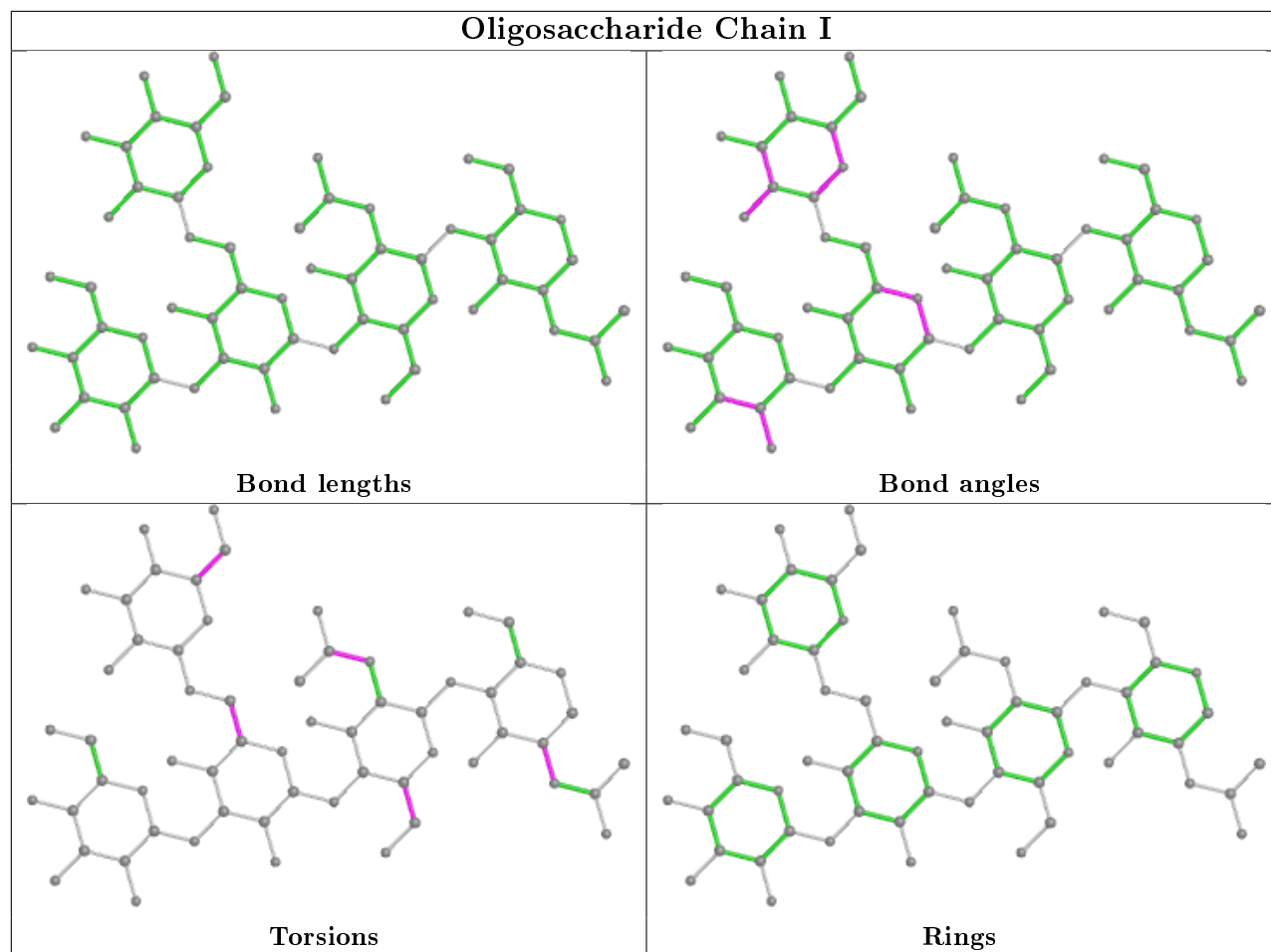
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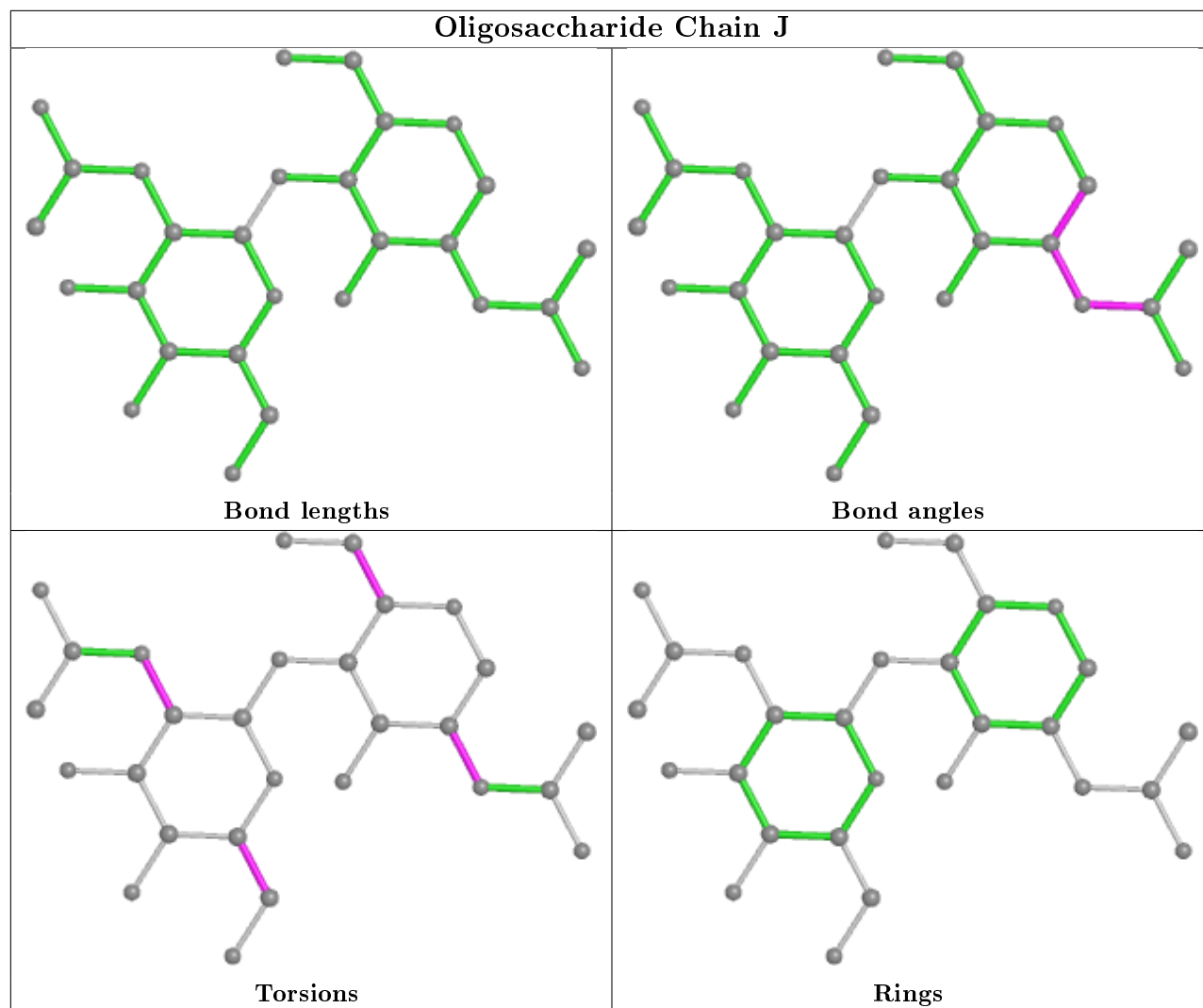
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	1	NAG	2	0
9	I	2	NAG	1	0
8	K	2	NAG	1	0
9	I	1	NAG	1	0

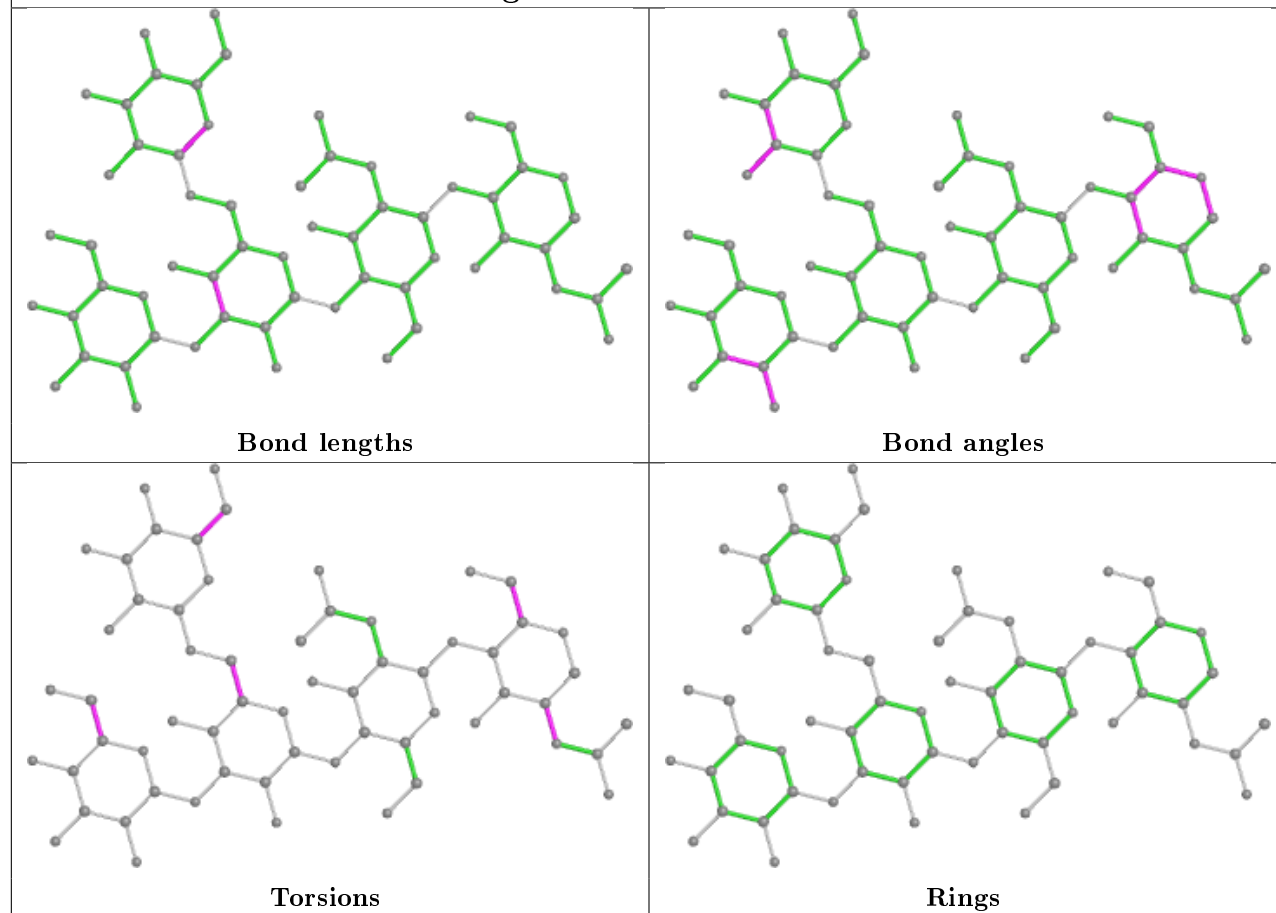
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



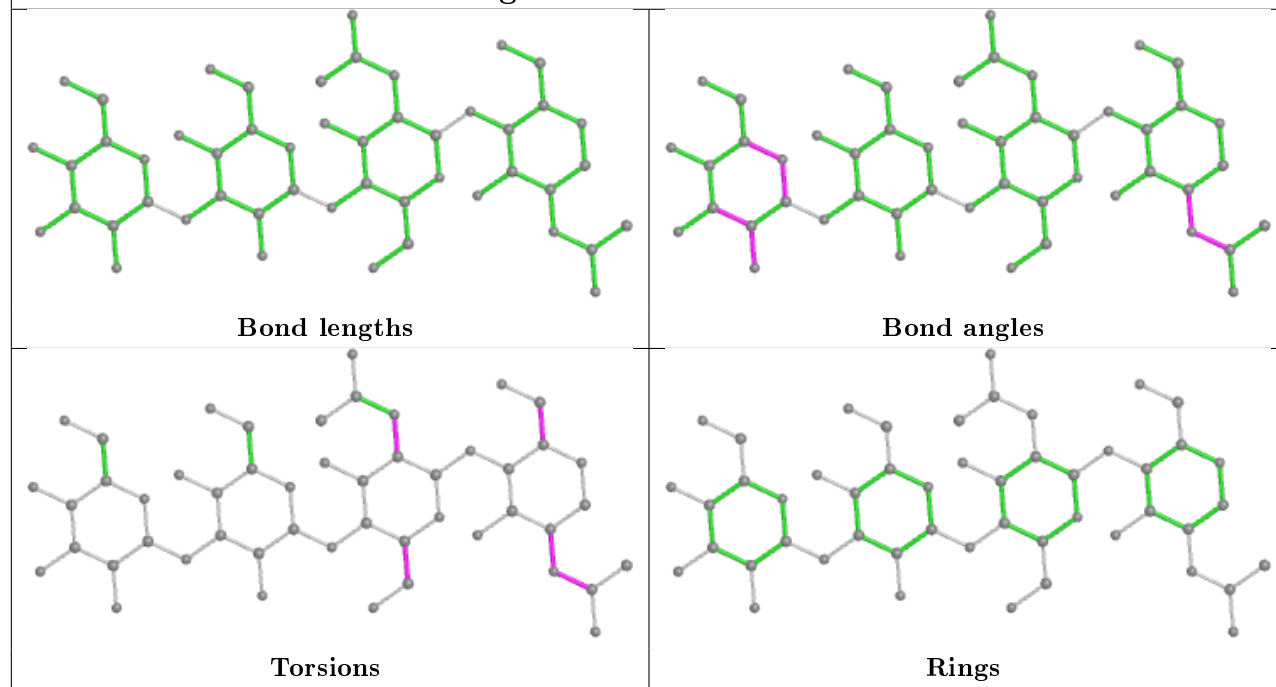


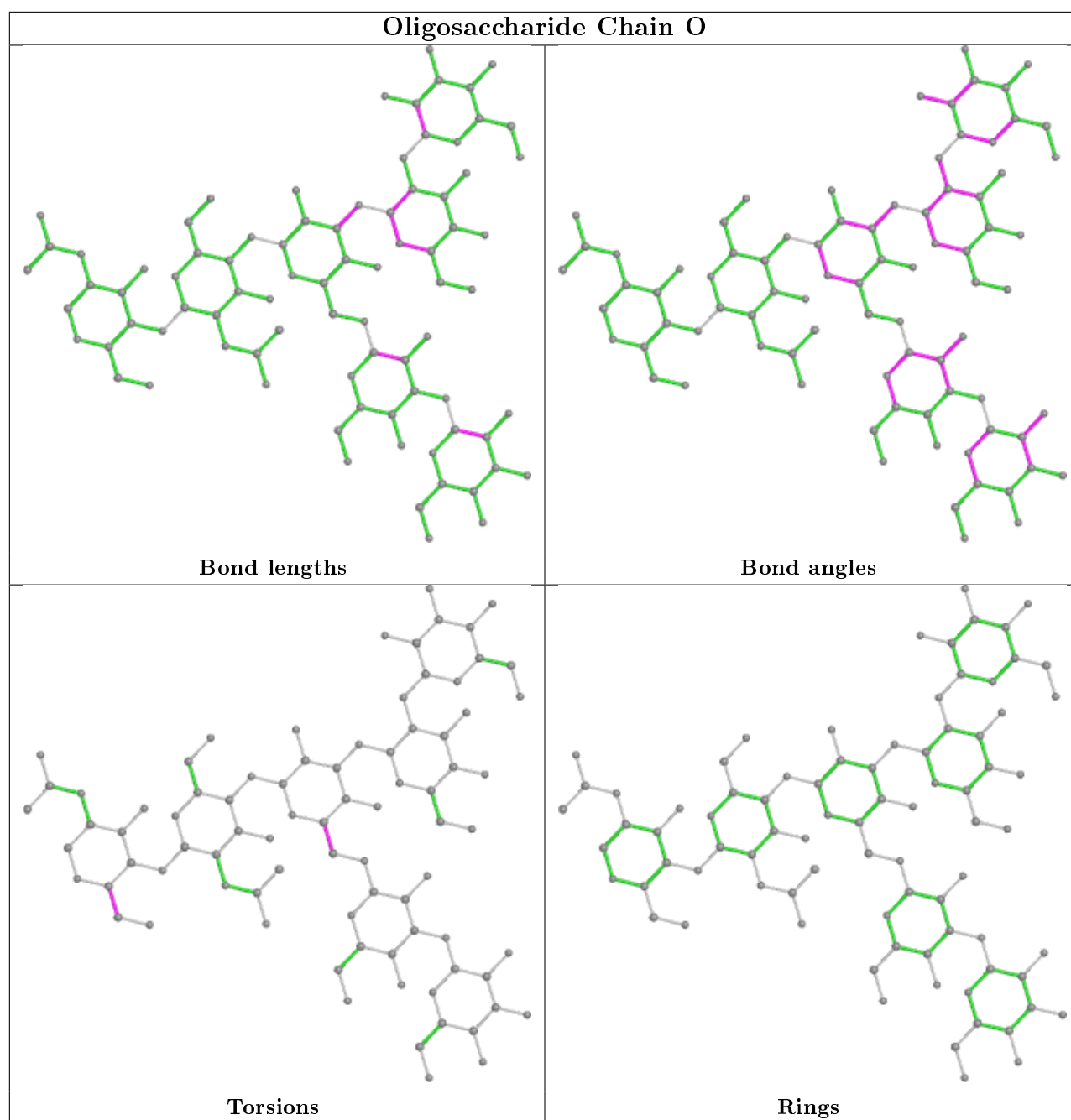


## Oligosaccharide Chain N



## Oligosaccharide Chain M





## 5.6 Ligand geometry [i](#)

13 ligands 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
12	NAG	G	621	2	14,14,15	0.26	0	17,19,21	0.68	1 (5%)
12	NAG	G	615	2	14,14,15	0.26	0	17,19,21	0.60	0
12	NAG	G	607	2	14,14,15	0.33	0	17,19,21	0.42	0
12	NAG	G	628	2	14,14,15	0.28	0	17,19,21	0.41	0
12	NAG	G	626	2	14,14,15	0.27	0	17,19,21	0.52	0
12	NAG	G	629	2	14,14,15	0.32	0	17,19,21	0.37	0
12	NAG	G	632	2	14,14,15	0.36	0	17,19,21	0.44	0
12	NAG	G	631	2	14,14,15	0.24	0	17,19,21	0.37	0
12	NAG	G	608	2	14,14,15	0.44	0	17,19,21	0.76	1 (5%)
12	NAG	G	627	2	14,14,15	0.26	0	17,19,21	0.52	0
12	NAG	G	601	2	14,14,15	0.37	0	17,19,21	0.44	0
12	NAG	G	614	2	14,14,15	0.29	0	17,19,21	0.36	0
12	NAG	G	630	2	14,14,15	0.17	0	17,19,21	0.46	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	NAG	G	621	2	-	0/6/23/26	0/1/1/1
12	NAG	G	615	2	-	1/6/23/26	0/1/1/1
12	NAG	G	607	2	-	4/6/23/26	0/1/1/1
12	NAG	G	628	2	-	0/6/23/26	0/1/1/1
12	NAG	G	626	2	-	0/6/23/26	0/1/1/1
12	NAG	G	629	2	-	4/6/23/26	0/1/1/1
12	NAG	G	632	2	-	1/6/23/26	0/1/1/1
12	NAG	G	631	2	-	2/6/23/26	0/1/1/1
12	NAG	G	608	2	-	2/6/23/26	0/1/1/1
12	NAG	G	627	2	-	2/6/23/26	0/1/1/1
12	NAG	G	601	2	-	3/6/23/26	0/1/1/1
12	NAG	G	614	2	-	0/6/23/26	0/1/1/1
12	NAG	G	630	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	608	NAG	C1-O5-C5	2.67	115.81	112.19
12	G	621	NAG	C1-O5-C5	2.26	115.25	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	NAG	C4-C5-C6-O6
12	G	607	NAG	O5-C5-C6-O6
12	G	608	NAG	O5-C5-C6-O6
12	G	629	NAG	C4-C5-C6-O6
12	G	607	NAG	C1-C2-N2-C7
12	G	629	NAG	C8-C7-N2-C2
12	G	629	NAG	O7-C7-N2-C2
12	G	629	NAG	O5-C5-C6-O6
12	G	608	NAG	C4-C5-C6-O6
12	G	601	NAG	O5-C5-C6-O6
12	G	607	NAG	C4-C5-C6-O6
12	G	627	NAG	O5-C5-C6-O6
12	G	631	NAG	C4-C5-C6-O6
12	G	631	NAG	O5-C5-C6-O6
12	G	627	NAG	C4-C5-C6-O6
12	G	632	NAG	C1-C2-N2-C7
12	G	607	NAG	C3-C2-N2-C7
12	G	601	NAG	C3-C2-N2-C7
12	G	615	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	621	NAG	2	0
12	G	615	NAG	1	0
12	G	607	NAG	1	0
12	G	601	NAG	3	0

## 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	B	137/140 (97%)	-0.12	0 100 100	181, 225, 304, 320	0
2	G	446/487 (91%)	0.01	18 (4%) 38 31	142, 236, 306, 372	0
3	D	240/243 (98%)	0.26	25 (10%) 6 6	158, 270, 425, 444	0
4	E	213/216 (98%)	-0.01	9 (4%) 36 30	183, 292, 389, 429	0
5	H	226/236 (95%)	0.17	18 (7%) 12 11	204, 284, 405, 456	0
6	L	211/214 (98%)	0.13	22 (10%) 6 6	209, 296, 363, 411	0
All	All	1473/1536 (95%)	0.08	92 (6%) 20 17	142, 264, 389, 456	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	126	PRO	14.4
5	H	213	PRO	9.3
5	H	125	ALA	7.9
3	D	138	LEU	7.2
5	H	212	GLU	6.7
4	E	214	GLU	6.3
3	D	214	LYS	6.2
3	D	180	SER	5.7
3	D	139	GLY	5.7
3	D	140	CYS	5.2
3	D	182	VAL	5.1
5	H	121	VAL	5.1
4	E	202	GLU	5.0
5	H	124	LEU	4.9
6	L	133	VAL	4.9
3	D	166	PHE	4.7
3	D	213	PRO	4.7
4	E	148	VAL	4.6
6	L	131	THR	4.6

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Mol	Chain	Res	Type	RSRZ
3	D	181	VAL	4.5
6	L	132	LEU	4.5
4	E	178	ALA	4.4
2	G	253	PRO	4.2
6	L	118	PHE	4.1
3	D	108	LEU	4.0
3	D	109	LEU	4.0
5	H	141	LEU	3.9
6	L	116	THR	3.9
3	D	124	LEU	3.8
3	D	165	THR	3.8
6	L	206	VAL	3.8
5	H	100(P)	MET	3.7
6	L	130	ALA	3.7
6	L	75	ILE	3.7
5	H	210	LYS	3.6
3	D	121	VAL	3.6
3	D	207	VAL	3.5
4	E	179	SER	3.5
3	D	1	GLU	3.4
2	G	367	GLY	3.4
2	G	210	PHE	3.4
5	H	157	GLY	3.4
6	L	120	PRO	3.2
6	L	119	PRO	3.2
5	H	138	LEU	3.2
5	H	119	PRO	3.2
4	E	201	HIS	3.2
3	D	183	THR	3.1
5	H	211	VAL	3.1
4	E	140	ILE	3.1
5	H	142	VAL	3.1
6	L	175	SER	3.0
3	D	89	THR	3.0
2	G	505	VAL	2.9
3	D	126	PRO	2.9
2	G	252	LYS	2.8
6	L	177	TYR	2.8
6	L	135	LEU	2.7
5	H	143	LYS	2.7
3	D	212	GLU	2.6
6	L	47	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	167	PRO	2.6
2	G	206	PRO	2.6
3	D	179	SER	2.5
5	H	139	GLY	2.5
2	G	209	SER	2.5
2	G	468	PHE	2.5
2	G	125	PHE	2.4
6	L	209	THR	2.4
6	L	19	ALA	2.4
5	H	43	LYS	2.4
6	L	82	ASP	2.4
3	D	141	LEU	2.3
6	L	62	PHE	2.3
4	E	58	PRO	2.3
2	G	93	PHE	2.3
4	E	147	ALA	2.3
2	G	179	LEU	2.3
6	L	117	LEU	2.3
3	D	67	VAL	2.3
2	G	238	PRO	2.2
6	L	66(B)	ILE	2.2
2	G	496	ILE	2.2
5	H	9	PRO	2.1
2	G	224	ALA	2.1
2	G	504	ARG	2.1
6	L	155	VAL	2.1
2	G	317	LEU	2.1
3	D	211	VAL	2.0
2	G	92	GLU	2.0
2	G	390	LEU	2.0
6	L	86	TYR	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](#)

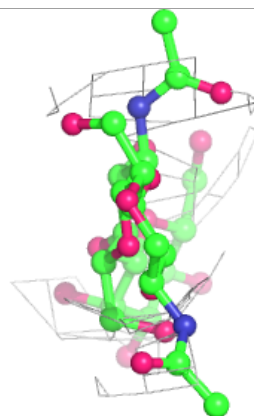
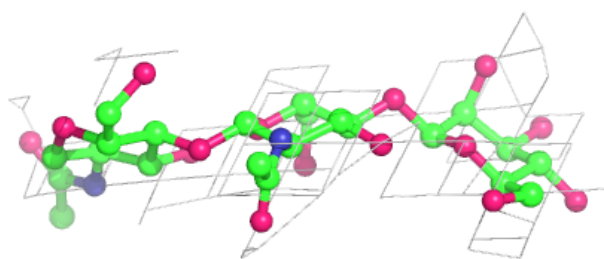
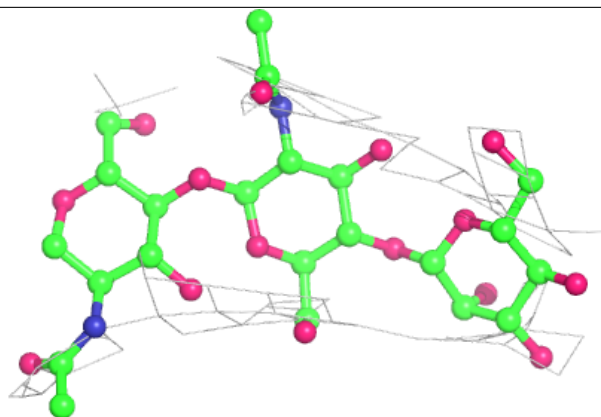
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	N	5	11/12	-0.14	0.44	320,320,320,320	0
10	MAN	M	4	11/12	0.37	0.54	407,407,407,407	0
10	BMA	M	3	11/12	0.43	0.37	404,404,404,404	0
8	BMA	K	3	11/12	0.50	0.34	375,375,375,375	0
10	NAG	M	2	14/15	0.52	0.31	392,392,392,392	0
9	NAG	N	2	14/15	0.54	0.20	295,295,295,295	0
9	BMA	N	3	11/12	0.59	0.27	300,300,300,300	0
7	NAG	J	2	14/15	0.63	0.46	337,337,337,337	0
9	MAN	N	4	11/12	0.69	0.43	317,317,317,317	0
9	NAG	N	1	14/15	0.74	0.21	286,286,286,286	0
7	NAG	A	1	14/15	0.74	0.33	124,124,124,124	0
8	NAG	F	2	14/15	0.75	0.29	396,396,396,396	0
9	NAG	I	1	14/15	0.76	0.27	342,342,342,342	0
9	MAN	I	5	11/12	0.77	0.27	355,355,355,355	0
8	NAG	K	1	14/15	0.79	0.26	343,343,343,343	0
11	NAG	O	1	14/15	0.79	0.20	285,285,285,285	0
8	BMA	F	3	11/12	0.80	0.28	399,399,399,399	0
10	NAG	M	1	14/15	0.82	0.45	357,357,357,357	0
11	BMA	O	3	11/12	0.82	0.15	326,326,326,326	0
7	NAG	C	2	14/15	0.82	0.34	387,387,387,387	0
11	MAN	O	7	11/12	0.83	0.30	124,124,124,124	0
8	NAG	F	1	14/15	0.84	0.21	367,367,367,367	0
7	NAG	J	1	14/15	0.84	0.26	313,313,313,313	0
11	MAN	O	6	11/12	0.84	0.18	327,327,327,327	0
7	NAG	C	1	14/15	0.86	0.24	352,352,352,352	0
9	BMA	I	3	11/12	0.87	0.19	343,343,343,343	0
11	NAG	O	2	14/15	0.88	0.28	313,313,313,313	0
9	MAN	I	4	11/12	0.90	0.26	345,345,345,345	0
11	MAN	O	4	11/12	0.90	0.34	342,342,342,342	0
8	NAG	K	2	14/15	0.92	0.18	365,365,365,365	0
7	NAG	A	2	14/15	0.93	0.37	124,124,124,124	0
11	MAN	O	5	11/12	0.93	0.14	124,124,124,124	0
9	NAG	I	2	14/15	0.95	0.36	326,326,326,326	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.

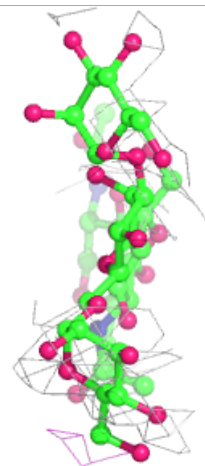
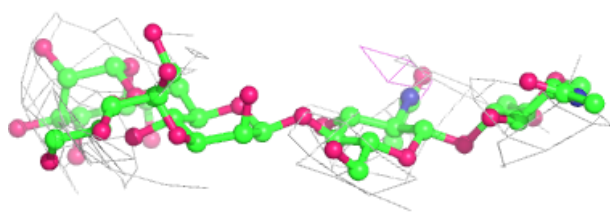
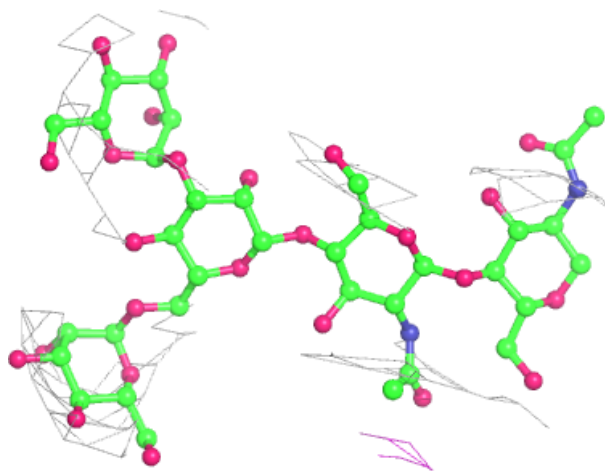
**Electron density around Chain K:**

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



**Electron density around Chain I:**

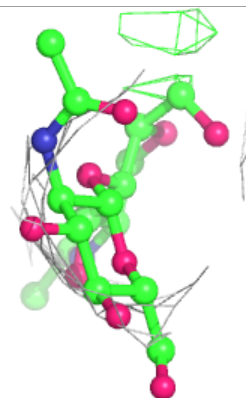
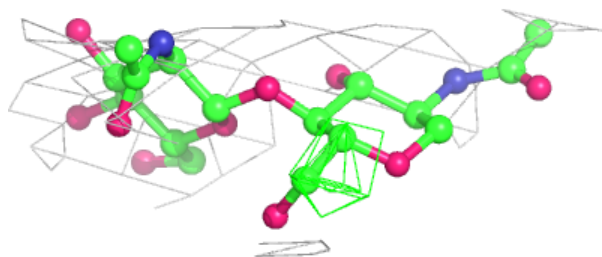
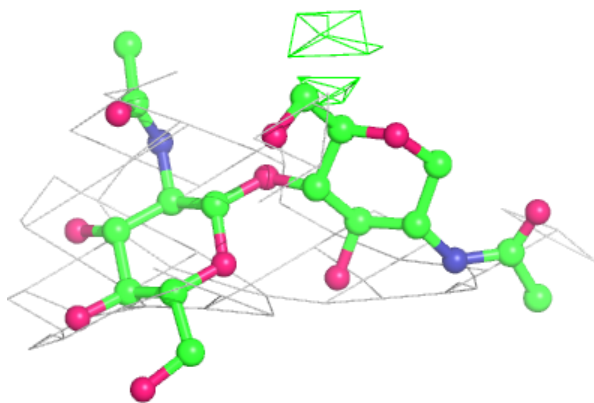
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





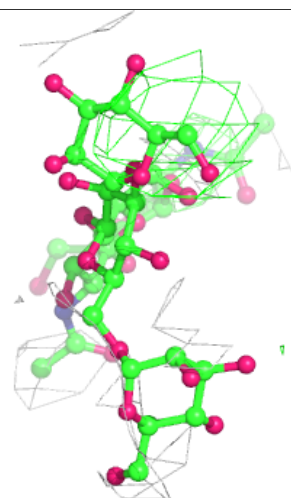
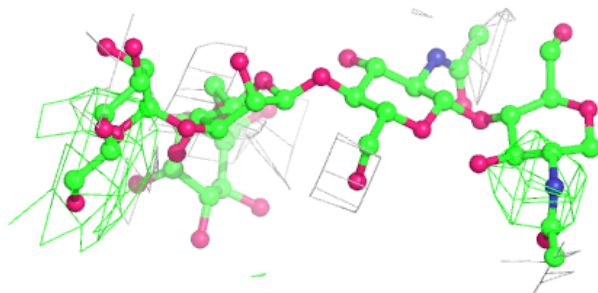
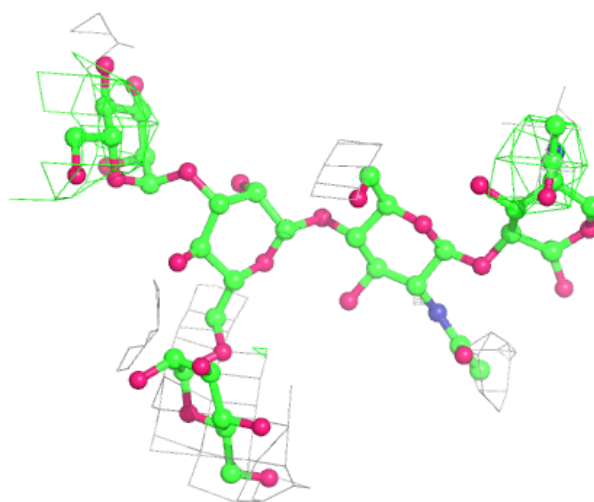
**Electron density around Chain J:**

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



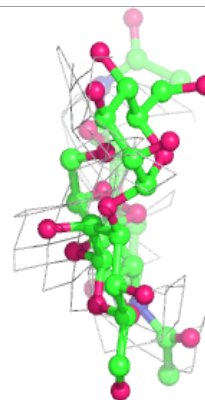
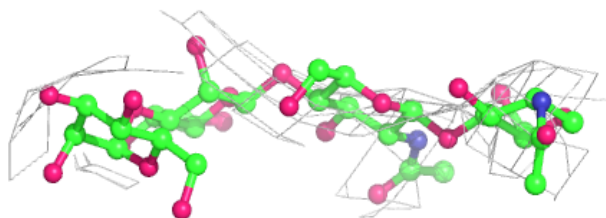
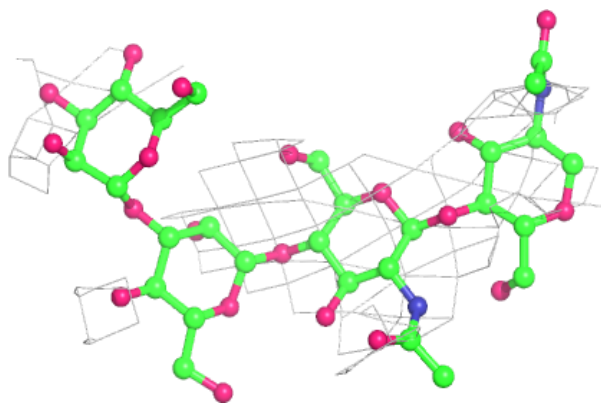
**Electron density around Chain N:**

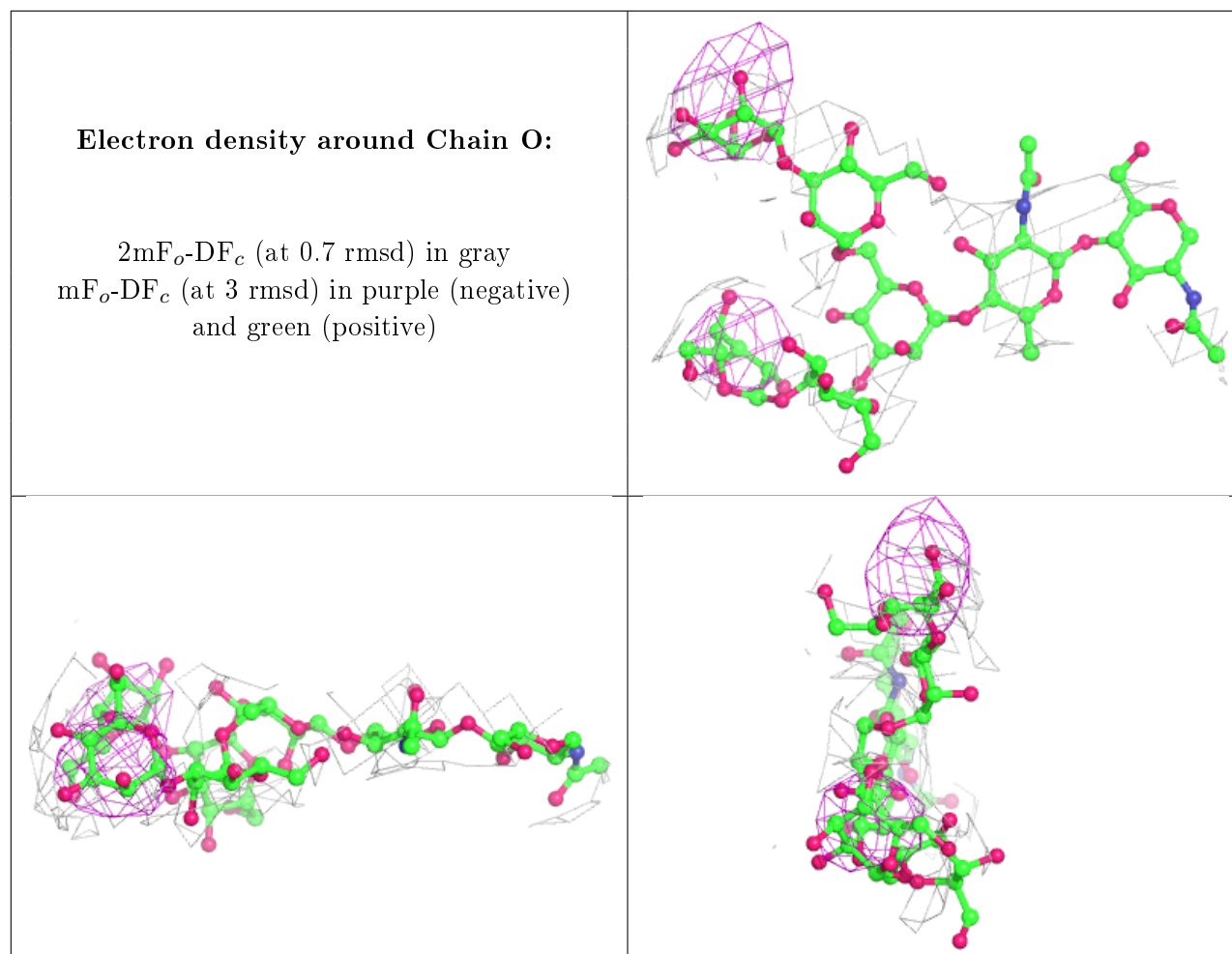
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain M:**

$2mF_o - DF_c$  (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
12	NAG	G	627	14/15	0.35	0.56	352,352,352,352	0
12	NAG	G	607	14/15	0.37	0.89	331,331,331,331	0
12	NAG	G	621	14/15	0.51	0.36	355,355,355,355	0
12	NAG	G	629	14/15	0.52	0.34	345,345,345,345	0
12	NAG	G	631	14/15	0.56	0.63	364,364,364,364	0
12	NAG	G	608	14/15	0.75	0.34	294,294,294,294	0
12	NAG	G	614	14/15	0.75	0.48	379,379,379,379	0
12	NAG	G	630	14/15	0.76	1.31	377,377,377,377	0
12	NAG	G	632	14/15	0.81	0.31	124,124,124,124	0
12	NAG	G	628	14/15	0.85	0.35	371,371,371,371	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	NAG	G	615	14/15	0.85	0.20	327,327,327,327	0
12	NAG	G	601	14/15	0.88	0.25	360,360,360,360	0
12	NAG	G	626	14/15	0.89	0.22	323,323,323,323	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.