



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:27 AM BST

PDB ID : 1IVG  
Title : STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS  
NEURAMINIDASE  
Authors : Jedrzejas, M.J.; Luo, M.  
Deposited on : 1994-12-12  
Resolution : 1.90 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

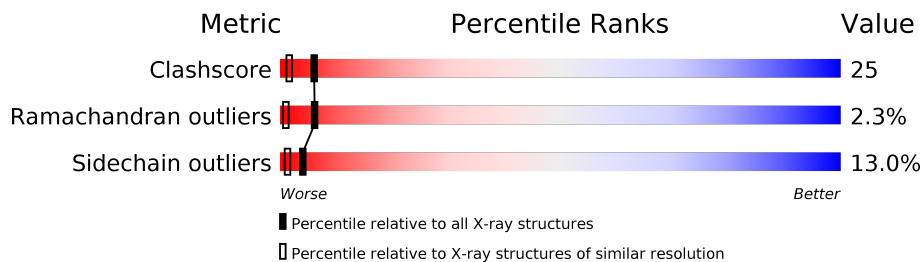
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.



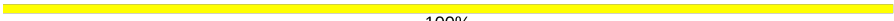
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	388	61% 31% 7% .
1	B	388	63% 29% 7% .
2	C	2	100%
2	E	2	50% 50%
2	G	2	100%
2	J	2	50% 50%
3	D	4	75% 25%
4	F	6	100%
4	I	6	100%

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Mol	Chain	Length	Quality of chain
5	H	4	 100%

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
4	NAG	F	1	-	-	X	-
4	MAN	F	4	-	-	X	-
4	MAN	F	6	-	-	X	-
4	MAN	I	4	-	-	X	-
4	MAN	I	5	-	-	X	-
5	FUC	H	4	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8557 atoms, of which 2032 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 INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	388	3745	1866	723	545	588	23	0	0	0
1	B	388	3745	1866	723	545	588	23	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

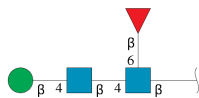
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820
B	339	ASP	ASN	conflict	UNP P06820

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



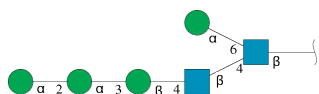
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	55	16	27	2	10	0	0	0
2	E	2	55	16	27	2	10	0	0	0
2	G	2	55	16	27	2	10	0	0	0
2	J	2	55	16	27	2	10	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



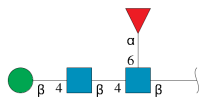
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
3	D	4	96	28	47	2	19	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
4	F	6	139	40	67	2	30	0	0	0
4	I	6	139	40	67	2	30	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
5	H	4	96	28	47	2	19	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		


- Molecule 7 is water.

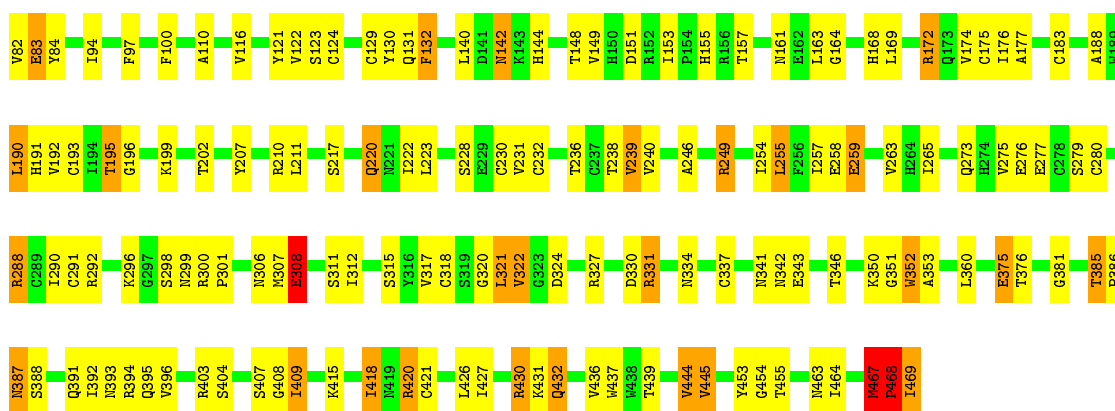
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
7	A	120	Total	H	O	0	0
			360	240	120		
7	B	5	Total	H	O	0	0
			15	10	5		

### 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. 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. 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.

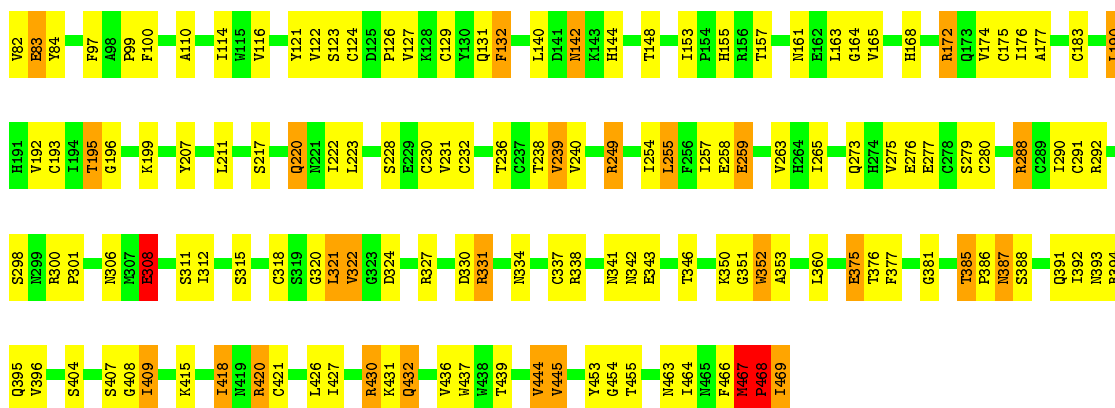
- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain A: 



- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain B: 




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

Chain C: 



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

Chain E:  50% 50%


MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain J:  50% 50%

MAG1  
MAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  75% 25%

MAG1  
MAG2  
BMA3  
FUL4

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



Chain H:

100%

IMG1  
IMG2  
BGLA3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.97Å 141.14Å 142.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90 9.65 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-1.90) 34.1 (9.65-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.80Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.205 , (Not available) 0.256 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtrriage
Anisotropy	0.461	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 78.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, CA, FUC, FUL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.55	0/3092	0.84	3/4194 (0.1%)
1	B	0.55	0/3092	0.84	3/4194 (0.1%)
All	All	0.55	0/6184	0.84	6/8388 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	MET	N-CA-C	6.16	127.63	111.00
1	B	467	MET	N-CA-C	6.16	127.63	111.00
1	A	468	PRO	CA-N-CD	-5.38	103.96	111.50
1	B	468	PRO	CA-N-CD	-5.38	103.96	111.50
1	A	190	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	190	LEU	CA-CB-CG	5.15	127.15	115.30

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	3022	723	2851	136	75
1	B	3022	723	2850	167	4
2	C	28	27	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	27	25	1	0
2	G	28	27	25	2	0
2	J	28	27	25	1	0
3	D	49	47	43	1	0
4	F	72	67	49	49	0
4	I	72	67	59	2	74
5	H	49	47	43	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	120	240	0	18	3
7	B	5	10	0	2	0
All	All	6525	2032	5995	306	78

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 25.

All (306) 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:B:453:TYR:HD1	4:F:1:NAG:C8	1.33	1.41
1:B:453:TYR:CD1	4:F:1:NAG:C8	2.04	1.38
1:B:453:TYR:CD1	4:F:1:NAG:H81	1.64	1.27
1:B:377:PHE:HB3	4:F:4:MAN:H3	1.25	1.14
1:B:394:ARG:HD3	4:F:3:BMA:H3	1.14	1.14
1:B:453:TYR:CD1	4:F:1:NAG:H82	1.81	1.11
1:A:467:MET:HB3	1:A:468:PRO:HD2	1.15	1.10
1:B:467:MET:HB3	1:B:468:PRO:HD2	1.15	1.10
1:A:172:ARG:HG2	1:B:165:VAL:HG12	1.10	1.09
1:B:352:TRP:CD1	1:B:409:ILE:HB	1.92	1.04
1:A:352:TRP:CD1	1:A:409:ILE:HB	1.92	1.03
1:B:453:TYR:HD1	4:F:1:NAG:H81	1.00	1.02
1:B:455:THR:OG1	4:F:6:MAN:H2	1.62	1.00
1:B:454:GLY:O	4:F:1:NAG:C8	2.09	1.00
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.44	0.99
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.44	0.97
1:A:172:ARG:CG	1:B:165:VAL:HG12	1.94	0.96
1:B:455:THR:HB	4:F:6:MAN:H3	1.48	0.95
1:B:454:GLY:O	4:F:1:NAG:C7	2.14	0.95
1:A:437:TRP:H	1:A:469:ILE:HG21	1.31	0.94
1:B:455:THR:CB	4:F:6:MAN:H3	1.96	0.94
1:B:437:TRP:H	1:B:469:ILE:HG21	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ARG:HD3	4:F:3:BMA:C3	1.98	0.93
1:A:467:MET:HB3	1:A:468:PRO:CD	1.99	0.92
1:B:454:GLY:CA	4:F:1:NAG:H83	1.99	0.92
1:B:454:GLY:N	4:F:1:NAG:H83	1.84	0.91
1:B:467:MET:HB3	1:B:468:PRO:CD	1.99	0.91
1:B:279:SER:HB3	1:B:352:TRP:CE2	2.06	0.91
1:A:279:SER:HB3	1:A:352:TRP:CE2	2.06	0.90
1:B:352:TRP:NE1	1:B:409:ILE:HB	1.86	0.90
1:A:352:TRP:NE1	1:A:409:ILE:HB	1.86	0.89
1:B:454:GLY:O	4:F:1:NAG:H83	1.72	0.89
1:B:453:TYR:CE1	4:F:1:NAG:H81	2.08	0.89
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.38	0.87
1:A:288:ARG:HH11	1:A:288:ARG:HG3	1.38	0.87
1:B:455:THR:CB	4:F:6:MAN:C3	2.47	0.86
1:B:391:GLN:C	4:F:4:MAN:O6	2.13	0.86
1:B:352:TRP:CE3	1:B:408:GLY:HA2	2.11	0.85
1:A:352:TRP:CE3	1:A:408:GLY:HA2	2.11	0.85
1:B:436:VAL:HA	1:B:469:ILE:HG22	1.60	0.84
1:A:436:VAL:HA	1:A:469:ILE:HG22	1.60	0.84
1:B:455:THR:OG1	4:F:6:MAN:C2	2.25	0.84
1:A:169:LEU:HD13	1:B:114:ILE:HD11	1.59	0.83
1:B:455:THR:HB	4:F:6:MAN:C3	2.08	0.83
1:A:418:ILE:HD11	1:A:420:ARG:NH2	1.94	0.83
1:B:394:ARG:CD	4:F:3:BMA:H3	2.05	0.82
1:B:418:ILE:HD11	1:B:420:ARG:NH2	1.94	0.82
1:A:172:ARG:HG2	1:B:165:VAL:CG1	2.04	0.82
1:B:394:ARG:HD2	4:F:4:MAN:O4	1.79	0.82
1:B:392:ILE:N	4:F:4:MAN:O6	2.12	0.81
1:B:377:PHE:HB3	4:F:4:MAN:C3	2.11	0.78
1:B:352:TRP:CZ3	1:B:408:GLY:HA2	2.19	0.78
1:A:352:TRP:CZ3	1:A:408:GLY:HA2	2.19	0.78
1:B:394:ARG:O	4:F:5:MAN:H3	1.82	0.77
1:B:394:ARG:O	4:F:5:MAN:C3	2.31	0.76
1:B:454:GLY:C	4:F:1:NAG:H83	2.06	0.76
1:B:453:TYR:CE1	4:F:1:NAG:C8	2.66	0.76
1:B:279:SER:HA	1:B:352:TRP:CZ2	2.22	0.75
1:A:279:SER:HA	1:A:352:TRP:CZ2	2.22	0.75
1:A:296:LYS:HD2	7:A:589:HOH:O	1.86	0.74
1:B:376:THR:O	4:F:5:MAN:O6	2.03	0.74
1:B:377:PHE:CB	4:F:4:MAN:H3	2.12	0.73
1:B:255:LEU:HD13	1:B:265:ILE:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG13	7:A:527:HOH:O	1.89	0.71
1:B:376:THR:OG1	4:F:5:MAN:O6	2.04	0.71
1:A:255:LEU:HD13	1:A:265:ILE:HG12	1.72	0.71
1:A:467:MET:CB	1:A:468:PRO:HD2	2.07	0.71
1:B:467:MET:CB	1:B:468:PRO:HD2	2.07	0.70
1:A:375:GLU:HG3	1:A:394:ARG:NH1	2.07	0.69
1:B:375:GLU:HG3	1:B:394:ARG:NH1	2.07	0.69
1:A:148:THR:HG22	1:A:439:THR:HB	1.75	0.69
1:B:279:SER:HB3	1:B:352:TRP:CD2	2.27	0.69
1:A:279:SER:HB3	1:A:352:TRP:CD2	2.27	0.69
1:A:144:HIS:HE2	1:B:463:ASN:H	1.38	0.68
1:B:148:THR:HG22	1:B:439:THR:HB	1.75	0.68
1:A:409:ILE:HG12	1:A:421:CYS:O	1.96	0.66
1:B:409:ILE:HG12	1:B:421:CYS:O	1.96	0.66
1:A:321:LEU:O	1:A:322:VAL:HB	1.97	0.65
1:B:321:LEU:O	1:B:322:VAL:HB	1.97	0.64
1:B:418:ILE:HD11	1:B:420:ARG:CZ	2.29	0.63
1:B:258:GLU:HG3	1:B:263:VAL:HG11	1.80	0.63
1:A:249:ARG:HH22	1:A:273:GLN:NE2	1.97	0.62
1:A:418:ILE:HD11	1:A:420:ARG:CZ	2.29	0.62
1:A:258:GLU:HG3	1:A:263:VAL:HG11	1.80	0.62
1:A:207:TYR:CE2	1:A:259:GLU:HG3	2.35	0.62
1:B:127:VAL:O	7:B:513:HOH:O	2.16	0.62
1:B:454:GLY:HA2	4:F:1:NAG:HN2	1.64	0.61
1:B:249:ARG:HH22	1:B:273:GLN:NE2	1.97	0.61
1:B:207:TYR:CE2	1:B:259:GLU:HG3	2.35	0.61
1:B:455:THR:OG1	4:F:6:MAN:H3	1.99	0.61
1:A:279:SER:HB2	1:A:290:ILE:O	2.02	0.60
1:B:455:THR:CG2	4:F:6:MAN:O3	2.50	0.60
1:B:394:ARG:CD	4:F:4:MAN:H2	1.78	0.60
1:A:97:PHE:H	1:A:395:GLN:HE22	1.49	0.59
1:B:97:PHE:H	1:B:395:GLN:HE22	1.49	0.59
1:B:279:SER:HB2	1:B:290:ILE:O	2.02	0.59
1:B:392:ILE:N	4:F:4:MAN:HO6	2.01	0.58
1:B:426:LEU:HD11	1:B:444:VAL:HG22	1.85	0.58
1:B:352:TRP:NE1	1:B:409:ILE:CB	2.64	0.58
1:A:436:VAL:HA	1:A:469:ILE:CG2	2.32	0.58
1:B:288:ARG:NH1	1:B:288:ARG:HG3	2.15	0.58
6:A:470:CA:CA	7:A:592:HOH:O	1.79	0.57
1:B:436:VAL:HA	1:B:469:ILE:CG2	2.32	0.57
1:A:426:LEU:HD11	1:A:444:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:CD	1:A:84:TYR:H	2.08	0.57
1:B:83:GLU:CD	1:B:84:TYR:H	2.08	0.57
1:B:300:ARG:CZ	1:B:351:GLY:HA3	2.35	0.56
1:B:350:LYS:HE3	1:B:352:TRP:CZ3	2.40	0.56
1:A:130:TYR:HB2	7:A:506:HOH:O	2.04	0.56
1:A:317:VAL:HG23	7:A:543:HOH:O	2.04	0.56
1:B:157:THR:HG22	1:B:176:ILE:HA	1.87	0.56
1:A:249:ARG:HH22	1:A:273:GLN:CD	2.09	0.56
1:A:351:GLY:O	1:A:352:TRP:CE3	2.59	0.56
1:B:436:VAL:CA	1:B:469:ILE:HG22	2.36	0.56
1:A:300:ARG:CZ	1:A:351:GLY:HA3	2.35	0.56
1:B:454:GLY:HA2	4:F:1:NAG:N2	2.21	0.56
1:A:157:THR:HG22	1:A:176:ILE:HA	1.87	0.55
1:A:239:VAL:HG12	1:A:255:LEU:HB2	1.88	0.55
1:A:436:VAL:CA	1:A:469:ILE:HG22	2.36	0.55
1:B:351:GLY:O	1:B:352:TRP:CE3	2.59	0.55
1:A:306:ASN:HD21	1:A:308:GLU:CD	2.09	0.55
1:A:350:LYS:HE3	1:A:352:TRP:CZ3	2.40	0.55
1:B:249:ARG:HH22	1:B:273:GLN:CD	2.09	0.55
1:B:324:ASP:O	1:B:327:ARG:HD3	2.06	0.55
1:B:306:ASN:HD21	1:B:308:GLU:CD	2.09	0.55
1:A:324:ASP:O	1:A:327:ARG:HD3	2.06	0.55
1:A:352:TRP:NE1	1:A:409:ILE:CB	2.64	0.55
1:B:239:VAL:HG12	1:B:255:LEU:HB2	1.88	0.54
1:B:279:SER:CB	1:B:352:TRP:CE2	2.87	0.54
1:B:148:THR:HG21	1:B:439:THR:O	2.07	0.54
1:A:334:ASN:HB3	1:A:387:ASN:HD21	1.73	0.54
1:A:148:THR:HG21	1:A:439:THR:O	2.07	0.54
1:B:157:THR:HB	1:B:175:CYS:O	2.08	0.54
1:A:437:TRP:H	1:A:469:ILE:CG2	2.14	0.53
1:A:157:THR:HB	1:A:175:CYS:O	2.08	0.53
1:A:437:TRP:N	1:A:469:ILE:HG21	2.13	0.53
1:A:191:HIS:CE1	7:A:507:HOH:O	2.62	0.53
1:B:276:GLU:O	1:B:291:CYS:HB3	2.09	0.53
1:B:279:SER:CA	1:B:352:TRP:CZ2	2.92	0.53
1:B:404:SER:O	1:B:427:ILE:HG22	2.09	0.53
1:B:430:ARG:HD3	1:B:436:VAL:O	2.08	0.53
1:A:404:SER:O	1:A:427:ILE:HG22	2.09	0.53
1:B:334:ASN:HB3	1:B:387:ASN:HD21	1.73	0.53
1:A:430:ARG:HD3	1:A:436:VAL:O	2.08	0.52
1:B:453:TYR:C	4:F:1:NAG:C8	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:O	1:A:291:CYS:HB3	2.09	0.52
1:A:279:SER:CA	1:A:352:TRP:CZ2	2.92	0.52
1:A:246:ALA:HB3	7:A:599:HOH:O	2.09	0.52
1:A:110:ALA:HA	1:A:468:PRO:HG2	1.92	0.52
1:B:453:TYR:O	7:B:512:HOH:O	2.18	0.52
1:A:352:TRP:HE1	1:A:409:ILE:CG2	2.22	0.52
1:B:352:TRP:CD2	1:B:408:GLY:HA2	2.43	0.52
1:B:352:TRP:HE1	1:B:409:ILE:CG2	2.22	0.51
1:A:279:SER:CB	1:A:352:TRP:CE2	2.87	0.51
4:I:2:NAG:H5	4:I:3:BMA:O5	2.10	0.51
1:B:110:ALA:HA	1:B:468:PRO:HG2	1.92	0.51
1:A:352:TRP:CD2	1:A:408:GLY:HA2	2.43	0.51
4:F:1:NAG:O3	4:F:2:NAG:N2	2.41	0.51
1:B:454:GLY:CA	4:F:1:NAG:C8	2.83	0.50
1:A:210:ARG:NH2	1:B:126:PRO:O	2.45	0.50
4:F:2:NAG:H5	4:F:3:BMA:O5	2.10	0.50
4:I:1:NAG:O3	4:I:2:NAG:N2	2.41	0.50
1:B:437:TRP:H	1:B:469:ILE:CG2	2.14	0.50
1:A:321:LEU:O	1:A:322:VAL:CB	2.59	0.50
1:A:352:TRP:HZ2	7:A:525:HOH:O	1.94	0.50
1:B:121:TYR:CG	1:B:228:SER:HA	2.47	0.50
1:B:321:LEU:O	1:B:322:VAL:CB	2.59	0.50
1:B:350:LYS:NZ	1:B:352:TRP:CH2	2.78	0.49
2:G:1:NAG:H61	2:G:2:NAG:O7	2.12	0.49
1:A:288:ARG:NH1	1:A:288:ARG:HG3	2.15	0.49
1:B:377:PHE:CB	4:F:4:MAN:C3	2.82	0.49
2:C:1:NAG:H61	2:C:2:NAG:O7	2.12	0.49
1:A:121:TYR:CG	1:A:228:SER:HA	2.47	0.49
1:A:320:GLY:N	1:A:388:SER:O	2.46	0.49
1:A:259:GLU:HA	7:A:520:HOH:O	2.12	0.49
1:A:258:GLU:HG3	1:A:263:VAL:CG1	2.43	0.48
1:A:353:ALA:HB1	1:A:360:LEU:HD11	1.95	0.48
1:B:350:LYS:HE3	1:B:352:TRP:HZ3	1.78	0.48
1:B:453:TYR:C	4:F:1:NAG:H83	2.31	0.48
1:B:430:ARG:NH2	1:B:437:TRP:CZ3	2.82	0.48
1:B:394:ARG:HD3	4:F:4:MAN:H2	1.85	0.48
1:A:273:GLN:HE21	1:A:273:GLN:HA	1.79	0.48
1:A:199:LYS:HA	1:A:220:GLN:O	2.14	0.48
1:A:430:ARG:NH2	1:A:437:TRP:CZ3	2.82	0.48
1:B:142:ASN:HD22	1:B:144:HIS:H	1.62	0.48
1:B:353:ALA:HB1	1:B:360:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:HG2	7:A:604:HOH:O	2.14	0.48
1:A:426:LEU:HD11	1:A:444:VAL:CG2	2.44	0.48
1:B:273:GLN:HA	1:B:273:GLN:HE21	1.79	0.48
1:B:426:LEU:HD11	1:B:444:VAL:CG2	2.44	0.48
1:B:258:GLU:HG3	1:B:263:VAL:CG1	2.43	0.48
1:B:320:GLY:N	1:B:388:SER:O	2.46	0.48
1:B:437:TRP:N	1:B:469:ILE:HG21	2.13	0.48
1:B:392:ILE:C	4:F:4:MAN:O3	2.52	0.48
1:A:142:ASN:HD22	1:A:144:HIS:H	1.62	0.47
1:B:199:LYS:HA	1:B:220:GLN:O	2.14	0.47
1:A:176:ILE:HD12	1:B:99:PRO:HB3	1.94	0.47
2:C:1:NAG:C6	2:C:2:NAG:O7	2.62	0.47
1:B:273:GLN:HA	1:B:273:GLN:NE2	2.29	0.47
1:A:273:GLN:HA	1:A:273:GLN:NE2	2.29	0.47
1:A:82:VAL:HG12	1:A:83:GLU:N	2.29	0.47
1:B:254:ILE:HD12	1:B:254:ILE:N	2.29	0.47
1:A:142:ASN:HD21	1:B:110:ALA:HB3	1.78	0.47
1:B:466:PHE:HZ	3:D:4:FUL:HO3	1.62	0.47
1:A:254:ILE:N	1:A:254:ILE:HD12	2.29	0.47
1:A:350:LYS:NZ	1:A:352:TRP:CH2	2.78	0.47
1:B:279:SER:HA	1:B:352:TRP:CH2	2.49	0.47
2:G:1:NAG:C6	2:G:2:NAG:O7	2.62	0.47
1:A:279:SER:HA	1:A:352:TRP:CH2	2.49	0.47
1:B:82:VAL:HG12	1:B:83:GLU:N	2.29	0.47
1:B:217:SER:HA	1:B:223:LEU:HD22	1.96	0.47
1:A:217:SER:HA	1:A:223:LEU:HD22	1.96	0.47
1:A:307:MET:N	7:A:529:HOH:O	2.48	0.47
1:B:392:ILE:C	4:F:4:MAN:HO3	2.18	0.47
1:A:467:MET:CB	1:A:468:PRO:CD	2.81	0.46
1:A:321:LEU:HD11	1:A:391:GLN:HB3	1.98	0.46
1:B:131:GLN:NE2	1:B:164:GLY:H	2.13	0.46
1:B:334:ASN:CB	1:B:387:ASN:HD21	2.28	0.46
1:B:392:ILE:HG12	1:B:393:ASN:H	1.80	0.46
1:A:195:THR:HG22	1:A:196:GLY:H	1.80	0.46
1:A:311:SER:O	1:A:312:ILE:HD13	2.16	0.46
1:A:301:PRO:HA	1:A:315:SER:O	2.16	0.46
1:B:311:SER:O	1:B:312:ILE:HD13	2.16	0.46
1:B:195:THR:HG22	1:B:196:GLY:H	1.80	0.46
1:A:131:GLN:NE2	1:A:164:GLY:H	2.13	0.46
1:A:300:ARG:NH2	1:A:351:GLY:HA3	2.30	0.46
1:B:124:CYS:HA	1:B:129:CYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HG23	7:A:553:HOH:O	2.16	0.46
1:B:275:VAL:O	1:B:276:GLU:HG2	2.16	0.46
1:B:334:ASN:HA	1:B:387:ASN:HD21	1.81	0.46
1:A:334:ASN:CB	1:A:387:ASN:HD21	2.28	0.46
1:B:321:LEU:HD11	1:B:391:GLN:HB3	1.98	0.46
1:A:392:ILE:HG12	1:A:393:ASN:H	1.80	0.45
1:B:301:PRO:HA	1:B:315:SER:O	2.16	0.45
1:A:124:CYS:HA	1:A:129:CYS:HA	1.97	0.45
1:B:300:ARG:NH2	1:B:351:GLY:HA3	2.30	0.45
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.81	0.45
1:B:455:THR:OG1	4:F:6:MAN:C3	2.59	0.45
1:A:275:VAL:O	1:A:276:GLU:HG2	2.16	0.45
1:B:131:GLN:HG2	1:B:163:LEU:HA	1.98	0.45
1:A:350:LYS:HE3	1:A:352:TRP:HZ3	1.78	0.44
1:B:337:CYS:SG	1:B:386:PRO:HB3	2.57	0.44
1:A:131:GLN:HG2	1:A:163:LEU:HA	1.98	0.44
1:A:337:CYS:SG	1:A:386:PRO:HB3	2.57	0.44
1:B:140:LEU:CD2	1:B:468:PRO:HB3	2.48	0.44
1:A:409:ILE:HD12	7:A:523:HOH:O	2.18	0.44
1:A:352:TRP:HE1	1:A:409:ILE:HG22	1.82	0.44
1:A:183:CYS:HB3	1:A:230:CYS:O	2.18	0.43
1:A:392:ILE:HG12	1:A:393:ASN:N	2.34	0.43
1:B:352:TRP:HE1	1:B:409:ILE:HG22	1.82	0.43
1:A:140:LEU:CD2	1:A:468:PRO:HB3	2.48	0.43
1:A:232:CYS:HA	1:A:236:THR:O	2.18	0.43
1:A:299:ASN:N	1:A:299:ASN:OD1	2.51	0.43
1:B:132:PHE:CD1	1:B:132:PHE:N	2.86	0.43
1:B:331:ARG:HD2	1:B:331:ARG:N	2.34	0.43
1:A:432:GLN:HE21	1:A:432:GLN:C	2.22	0.43
1:B:392:ILE:HG12	1:B:393:ASN:N	2.34	0.43
1:B:183:CYS:HB3	1:B:230:CYS:O	2.18	0.43
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.84	0.43
1:A:331:ARG:HD2	1:A:331:ARG:N	2.34	0.43
1:B:116:VAL:HG13	1:B:439:THR:O	2.19	0.43
2:E:2:NAG:H3	2:E:2:NAG:O7	2.19	0.42
1:B:232:CYS:HA	1:B:236:THR:O	2.18	0.42
1:A:116:VAL:HG13	1:A:439:THR:O	2.19	0.42
1:A:132:PHE:N	1:A:132:PHE:CD1	2.86	0.42
1:B:153:ILE:HG13	1:B:155:HIS:H	1.84	0.42
1:B:280:CYS:HA	1:B:288:ARG:O	2.20	0.42
1:A:151:ASP:N	7:A:586:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:O	1:A:394:ARG:HA	2.20	0.42
1:A:352:TRP:CZ3	1:A:407:SER:O	2.73	0.42
1:B:381:GLY:O	1:B:385:THR:HG23	2.19	0.42
1:B:376:THR:O	1:B:394:ARG:HA	2.20	0.42
1:A:188:ALA:HB1	7:A:510:HOH:O	2.20	0.42
1:B:82:VAL:HG12	1:B:83:GLU:O	2.20	0.42
2:J:2:NAG:O7	2:J:2:NAG:H3	2.19	0.42
1:A:341:ASN:O	1:A:343:GLU:HG3	2.20	0.42
1:B:279:SER:OG	1:B:351:GLY:O	2.38	0.42
1:B:432:GLN:C	1:B:432:GLN:HE21	2.22	0.42
1:A:350:LYS:CE	1:A:352:TRP:HZ3	2.33	0.42
1:B:318:CYS:HB3	1:B:385:THR:O	2.20	0.42
1:B:437:TRP:HB2	1:B:469:ILE:HD13	2.02	0.42
1:A:153:ILE:HG13	1:A:155:HIS:H	1.84	0.41
1:A:318:CYS:HB3	1:A:385:THR:O	2.20	0.41
1:B:350:LYS:CE	1:B:352:TRP:HZ3	2.33	0.41
1:A:381:GLY:O	1:A:385:THR:HG23	2.19	0.41
1:A:437:TRP:HB2	1:A:469:ILE:HD13	2.02	0.41
1:B:350:LYS:CE	1:B:352:TRP:CZ3	3.03	0.41
1:B:453:TYR:C	4:F:1:NAG:H82	2.40	0.41
1:A:279:SER:OG	1:A:351:GLY:O	2.38	0.41
1:A:280:CYS:HA	1:A:288:ARG:O	2.20	0.41
1:B:350:LYS:NZ	1:B:352:TRP:HH2	2.17	0.41
1:B:352:TRP:CZ3	1:B:407:SER:O	2.73	0.41
1:B:308:GLU:HG3	1:B:308:GLU:H	1.67	0.41
1:A:149:VAL:HB	7:A:572:HOH:O	2.21	0.41
1:A:409:ILE:HG21	7:A:523:HOH:O	2.20	0.41
1:A:202:THR:O	1:A:202:THR:HG23	2.21	0.41
1:A:352:TRP:NE1	1:A:409:ILE:CG2	2.84	0.41
1:A:350:LYS:CE	1:A:352:TRP:CZ3	3.03	0.40
1:B:467:MET:CB	1:B:468:PRO:CD	2.81	0.40
1:A:100:PHE:HB3	1:A:445:VAL:HG22	2.02	0.40
1:A:168:HIS:CD2	1:A:168:HIS:H	2.40	0.40
1:A:82:VAL:HG12	1:A:83:GLU:O	2.20	0.40
1:B:168:HIS:CD2	1:B:168:HIS:H	2.40	0.40
1:A:132:PHE:HE2	7:A:507:HOH:O	2.01	0.40
1:B:341:ASN:O	1:B:343:GLU:HG3	2.20	0.40
1:B:100:PHE:HB3	1:B:445:VAL:HG22	2.02	0.40

All (78) 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)
1:A:394:ARG:CB	4:I:4:MAN:C2[4_555]	0.65	1.55
1:A:394:ARG:N	4:I:5:MAN:C1[4_555]	0.82	1.38
1:A:394:ARG:CA	4:I:4:MAN:O2[4_555]	0.91	1.29
1:A:394:ARG:CA	4:I:5:MAN:C1[4_555]	1.10	1.10
1:A:391:GLN:OE1	4:I:4:MAN:C4[4_555]	1.11	1.09
1:A:393:ASN:C	4:I:5:MAN:C2[4_555]	1.20	1.00
1:B:338:ARG:HH11	7:A:489:HOH:H2[7_544]	0.70	0.90
1:A:393:ASN:C	4:I:5:MAN:O2[4_555]	1.34	0.86
1:A:395:GLN:N	4:I:5:MAN:C5[4_555]	1.37	0.83
1:A:391:GLN:OE1	4:I:4:MAN:C5[4_555]	1.37	0.83
1:A:394:ARG:CB	4:I:4:MAN:O2[4_555]	1.38	0.82
1:A:393:ASN:C	4:I:5:MAN:C1[4_555]	1.41	0.79
1:A:393:ASN:O	4:I:5:MAN:O2[4_555]	1.41	0.79
1:A:395:GLN:CB	4:I:5:MAN:C6[4_555]	1.41	0.79
1:A:395:GLN:CG	4:I:5:MAN:O4[4_555]	1.41	0.79
1:A:394:ARG:C	4:I:5:MAN:H5[4_555]	0.83	0.77
1:A:394:ARG:N	4:I:4:MAN:O2[4_555]	1.43	0.77
1:A:394:ARG:C	4:I:5:MAN:C5[4_555]	1.47	0.73
1:A:455:THR:CG2	4:I:6:MAN:O2[4_555]	1.48	0.72
1:A:394:ARG:CB	4:I:4:MAN:H2[4_555]	0.90	0.70
1:A:391:GLN:CG	4:I:4:MAN:H61[4_555]	0.91	0.69
1:A:394:ARG:N	4:I:5:MAN:C2[4_555]	1.54	0.66
1:A:393:ASN:CA	4:I:5:MAN:O2[4_555]	1.56	0.64
1:A:391:GLN:CG	4:I:4:MAN:C6[4_555]	1.57	0.63
1:A:395:GLN:CA	4:I:5:MAN:H62[4_555]	0.98	0.62
1:A:395:GLN:N	4:I:5:MAN:H5[4_555]	1.02	0.58
1:A:394:ARG:CG	4:I:4:MAN:H2[4_555]	1.03	0.57
1:A:394:ARG:CA	4:I:5:MAN:O5[4_555]	1.65	0.55
1:A:391:GLN:OE1	4:I:4:MAN:H4[4_555]	1.06	0.54
1:A:376:THR:HG1	4:I:5:MAN:HO6[4_555]	1.08	0.52
1:A:394:ARG:C	4:I:4:MAN:O2[4_555]	1.69	0.51
1:A:395:GLN:CB	4:I:5:MAN:H62[4_555]	1.10	0.50
1:A:391:GLN:CD	4:I:4:MAN:H61[4_555]	1.10	0.50
1:A:391:GLN:OE1	4:I:4:MAN:C6[4_555]	1.70	0.50
1:A:391:GLN:CD	4:I:4:MAN:C6[4_555]	1.71	0.49
1:A:395:GLN:N	4:I:5:MAN:C6[4_555]	1.72	0.48
1:A:395:GLN:CG	4:I:5:MAN:C4[4_555]	1.74	0.46
1:A:394:ARG:CB	4:I:4:MAN:C3[4_555]	1.75	0.45
1:A:395:GLN:CA	4:I:5:MAN:C6[4_555]	1.75	0.45
1:A:394:ARG:C	4:I:5:MAN:O5[4_555]	1.75	0.45
1:A:393:ASN:CB	4:I:5:MAN:O2[4_555]	1.78	0.42
1:A:394:ARG:N	4:I:5:MAN:H1[4_555]	1.22	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HH12	7:A:505:HOH:H2[4_555]	1.24	0.36
1:A:393:ASN:O	4:I:5:MAN:C1[4_555]	1.87	0.33
1:A:394:ARG:CA	4:I:4:MAN:C2[4_555]	1.88	0.32
1:A:376:THR:OG1	4:I:5:MAN:HO6[4_555]	1.29	0.31
1:A:391:GLN:CB	4:I:4:MAN:O6[4_555]	1.90	0.30
1:A:395:GLN:CB	4:I:5:MAN:H61[4_555]	1.31	0.29
1:A:463:ASN:H	1:B:144:HIS:HE2[4_555]	1.31	0.29
1:A:391:GLN:CG	4:I:4:MAN:O6[4_555]	1.91	0.29
1:A:394:ARG:O	4:I:5:MAN:H5[4_555]	1.32	0.28
1:A:393:ASN:O	4:I:5:MAN:C2[4_555]	1.92	0.28
1:A:393:ASN:CA	4:I:5:MAN:C2[4_555]	1.92	0.28
1:A:455:THR:OG1	4:I:6:MAN:H2[4_555]	1.37	0.23
1:A:391:GLN:OE1	4:I:4:MAN:O4[4_555]	1.97	0.23
1:A:394:ARG:C	4:I:5:MAN:C1[4_555]	1.97	0.23
1:A:393:ASN:O	4:I:5:MAN:O5[4_555]	1.98	0.22
1:A:391:GLN:C	4:I:4:MAN:HO6[4_555]	1.39	0.21
1:A:393:ASN:C	4:I:5:MAN:H1[4_555]	1.40	0.20
1:A:391:GLN:CB	4:I:4:MAN:HO6[4_555]	1.40	0.20
1:A:394:ARG:CG	4:I:4:MAN:C2[4_555]	2.00	0.20
1:A:395:GLN:N	4:I:5:MAN:O5[4_555]	2.02	0.18
1:A:395:GLN:CG	4:I:5:MAN:C6[4_555]	2.03	0.17
1:A:376:THR:O	4:I:5:MAN:O6[4_555]	2.03	0.17
1:A:453:TYR:CD1	4:I:1:NAG:C8[4_555]	2.04	0.16
1:A:376:THR:OG1	4:I:5:MAN:O6[4_555]	2.04	0.16
1:A:394:ARG:O	4:I:5:MAN:C5[4_555]	2.06	0.14
1:A:395:GLN:CG	4:I:5:MAN:H61[4_555]	1.47	0.13
1:A:454:GLY:O	4:I:1:NAG:C8[4_555]	2.09	0.11
1:A:395:GLN:CA	4:I:5:MAN:C5[4_555]	2.10	0.10
1:A:392:ILE:N	4:I:4:MAN:O6[4_555]	2.12	0.08
1:A:391:GLN:CA	4:I:4:MAN:HO6[4_555]	1.53	0.07
1:A:394:ARG:O	4:I:4:MAN:O2[4_555]	2.13	0.07
1:A:391:GLN:C	4:I:4:MAN:O6[4_555]	2.13	0.07
1:A:454:GLY:O	4:I:1:NAG:C7[4_555]	2.14	0.06
1:B:338:ARG:NH1	7:A:489:HOH:H2[7_544]	1.58	0.02
1:A:391:GLN:CD	4:I:4:MAN:C5[4_555]	2.19	0.01
1:A:394:ARG:CA	4:I:5:MAN:H1[4_555]	1.60	0.00

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	386/388 (100%)	344 (89%)	33 (8%)	9 (2%)	6 1
1	B	386/388 (100%)	344 (89%)	33 (8%)	9 (2%)	6 1
All	All	772/776 (100%)	688 (89%)	66 (8%)	18 (2%)	6 1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	A	467	MET
1	A	468	PRO
1	B	322	VAL
1	B	467	MET
1	B	468	PRO
1	A	321	LEU
1	A	330	ASP
1	B	321	LEU
1	B	330	ASP
1	A	430	ARG
1	B	430	ARG
1	A	222	ILE
1	A	277	GLU
1	A	308	GLU
1	B	222	ILE
1	B	277	GLU
1	B	308	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/338 (100%)	294 (87%)	44 (13%)	4	1
1	B	338/338 (100%)	294 (87%)	44 (13%)	4	1
All	All	676/676 (100%)	588 (87%)	88 (13%)	4	1

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	122	VAL
1	A	123	SER
1	A	132	PHE
1	A	142	ASN
1	A	161	ASN
1	A	172	ARG
1	A	174	VAL
1	A	190	LEU
1	A	192	VAL
1	A	195	THR
1	A	211	LEU
1	A	220	GLN
1	A	231	VAL
1	A	238	THR
1	A	239	VAL
1	A	240	VAL
1	A	249	ARG
1	A	255	LEU
1	A	257	ILE
1	A	259	GLU
1	A	288	ARG
1	A	292	ARG
1	A	298	SER
1	A	308	GLU
1	A	331	ARG
1	A	342	ASN
1	A	346	THR
1	A	352	TRP
1	A	375	GLU
1	A	385	THR
1	A	387	ASN
1	A	396	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	409	ILE
1	A	415	LYS
1	A	418	ILE
1	A	420	ARG
1	A	431	LYS
1	A	432	GLN
1	A	444	VAL
1	A	445	VAL
1	A	464	ILE
1	A	467	MET
1	A	469	ILE
1	B	83	GLU
1	B	122	VAL
1	B	123	SER
1	B	132	PHE
1	B	142	ASN
1	B	161	ASN
1	B	172	ARG
1	B	174	VAL
1	B	190	LEU
1	B	192	VAL
1	B	195	THR
1	B	211	LEU
1	B	220	GLN
1	B	231	VAL
1	B	238	THR
1	B	239	VAL
1	B	240	VAL
1	B	249	ARG
1	B	255	LEU
1	B	257	ILE
1	B	259	GLU
1	B	288	ARG
1	B	292	ARG
1	B	298	SER
1	B	308	GLU
1	B	331	ARG
1	B	342	ASN
1	B	346	THR
1	B	352	TRP
1	B	375	GLU
1	B	385	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	387	ASN
1	B	396	VAL
1	B	409	ILE
1	B	415	LYS
1	B	418	ILE
1	B	420	ARG
1	B	431	LYS
1	B	432	GLN
1	B	444	VAL
1	B	445	VAL
1	B	464	ILE
1	B	467	MET
1	B	469	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	104	ASN
1	A	131	GLN
1	A	142	ASN
1	A	173	GLN
1	A	273	GLN
1	A	387	ASN
1	A	393	ASN
1	A	395	GLN
1	A	402	ASN
1	A	419	ASN
1	A	432	GLN
1	A	465	ASN
1	B	104	ASN
1	B	131	GLN
1	B	142	ASN
1	B	273	GLN
1	B	387	ASN
1	B	393	ASN
1	B	395	GLN
1	B	402	ASN
1	B	419	ASN
1	B	432	GLN
1	B	465	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

28 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
2	NAG	C	1	1,2	14,14,15	1.37	3 (21%)	17,19,21	2.47	7 (41%)
2	NAG	C	2	2	14,14,15	1.61	3 (21%)	17,19,21	2.82	7 (41%)
3	NAG	D	1	1,3	14,14,15	1.27	1 (7%)	17,19,21	3.41	5 (29%)
3	NAG	D	2	3	14,14,15	1.49	3 (21%)	17,19,21	2.81	6 (35%)
3	BMA	D	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.82	6 (40%)
3	FUL	D	4	3	10,10,11	1.27	2 (20%)	14,14,16	1.18	1 (7%)
2	NAG	E	1	1,2	14,14,15	1.39	1 (7%)	17,19,21	2.00	4 (23%)
2	NAG	E	2	2	14,14,15	1.10	2 (14%)	17,19,21	2.01	4 (23%)
4	NAG	F	1	1,4	14,14,15	1.62	3 (21%)	17,19,21	3.66	6 (35%)
4	NAG	F	2	4	14,14,15	2.34	7 (50%)	17,19,21	3.69	9 (52%)
4	BMA	F	3	4	11,11,12	3.74	8 (72%)	15,15,17	2.08	5 (33%)
4	MAN	F	4	4	11,11,12	2.19	5 (45%)	15,15,17	2.69	5 (33%)
4	MAN	F	5	4	11,11,12	1.44	1 (9%)	15,15,17	1.28	2 (13%)
4	MAN	F	6	4	11,11,12	1.79	2 (18%)	15,15,17	3.28	8 (53%)
2	NAG	G	1	1,2	14,14,15	1.37	3 (21%)	17,19,21	2.47	7 (41%)
2	NAG	G	2	2	14,14,15	1.61	3 (21%)	17,19,21	2.82	7 (41%)
5	NAG	H	1	1,5	14,14,15	1.27	1 (7%)	17,19,21	3.41	5 (29%)
5	NAG	H	2	5	14,14,15	1.49	3 (21%)	17,19,21	2.81	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	H	3	5	11,11,12	1.28	2 (18%)	15,15,17	1.82	6 (40%)
5	FUC	H	4	5	10,10,11	1.27	2 (20%)	14,14,16	1.18	1 (7%)
4	NAG	I	1	1,4	14,14,15	1.62	3 (21%)	17,19,21	3.66	6 (35%)
4	NAG	I	2	4	14,14,15	2.34	7 (50%)	17,19,21	3.69	9 (52%)
4	BMA	I	3	4	11,11,12	3.74	8 (72%)	15,15,17	2.08	5 (33%)
4	MAN	I	4	4	11,11,12	2.19	5 (45%)	15,15,17	2.69	5 (33%)
4	MAN	I	5	4	11,11,12	1.44	1 (9%)	15,15,17	1.28	2 (13%)
4	MAN	I	6	4	11,11,12	1.79	2 (18%)	15,15,17	3.28	8 (53%)
2	NAG	J	1	1,2	14,14,15	1.39	1 (7%)	17,19,21	2.00	4 (23%)
2	NAG	J	2	2	14,14,15	1.10	2 (14%)	17,19,21	2.01	4 (23%)

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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	FUL	D	4	3	-	-	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	1/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	2/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	FUC	H	4	5	1/1/5/5	-	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	I	3	4	-	1/2/19/22	1/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	0/1/1/1
4	MAN	I	6	4	-	2/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C2-C3	6.52	1.62	1.52
4	I	3	BMA	C2-C3	6.52	1.62	1.52
4	F	3	BMA	C4-C5	6.30	1.66	1.53
4	I	3	BMA	C4-C5	6.30	1.66	1.53
4	F	2	NAG	C4-C3	4.90	1.64	1.52
4	I	2	NAG	C4-C3	4.90	1.64	1.52
4	F	6	MAN	C1-C2	4.66	1.62	1.52
4	I	6	MAN	C1-C2	4.66	1.62	1.52
4	F	3	BMA	C1-C2	4.51	1.62	1.52
4	I	3	BMA	C1-C2	4.51	1.62	1.52
4	F	3	BMA	O3-C3	4.31	1.53	1.43
4	I	3	BMA	O3-C3	4.31	1.53	1.43
4	F	4	MAN	O5-C5	4.05	1.51	1.43
4	I	4	MAN	O5-C5	4.05	1.51	1.43
4	I	5	MAN	C2-C3	3.94	1.58	1.52
4	F	5	MAN	C2-C3	3.94	1.58	1.52
4	F	1	NAG	O3-C3	-3.70	1.34	1.43
4	I	1	NAG	O3-C3	-3.70	1.34	1.43
4	F	2	NAG	C6-C5	3.56	1.63	1.51
4	I	2	NAG	C6-C5	3.56	1.63	1.51
3	D	1	NAG	O5-C5	3.50	1.50	1.43
5	H	1	NAG	O5-C5	3.50	1.50	1.43
4	F	4	MAN	O2-C2	3.49	1.50	1.43
4	I	4	MAN	O2-C2	3.49	1.50	1.43
2	C	2	NAG	C4-C3	3.47	1.61	1.52
2	G	2	NAG	C4-C3	3.47	1.61	1.52
2	G	1	NAG	C1-C2	-3.45	1.47	1.52
2	C	1	NAG	C1-C2	-3.45	1.47	1.52
4	F	2	NAG	C1-C2	3.40	1.57	1.52
4	I	2	NAG	C1-C2	3.40	1.57	1.52
4	F	3	BMA	C4-C3	3.39	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	BMA	C4-C3	3.39	1.61	1.52
3	D	3	BMA	C2-C3	2.92	1.56	1.52
5	H	3	BMA	C2-C3	2.92	1.56	1.52
4	F	2	NAG	C4-C5	2.92	1.59	1.53
4	I	2	NAG	C4-C5	2.92	1.59	1.53
4	F	4	MAN	C1-C2	2.88	1.58	1.52
4	I	4	MAN	C1-C2	2.88	1.58	1.52
2	C	2	NAG	C3-C2	2.79	1.58	1.52
2	G	2	NAG	C3-C2	2.79	1.58	1.52
4	F	6	MAN	C4-C5	2.78	1.58	1.53
4	I	6	MAN	C4-C5	2.78	1.58	1.53
4	F	3	BMA	O5-C1	2.74	1.48	1.43
4	I	3	BMA	O5-C1	2.74	1.48	1.43
4	F	4	MAN	O5-C1	2.69	1.48	1.43
4	I	4	MAN	O5-C1	2.69	1.48	1.43
4	F	1	NAG	O5-C1	-2.68	1.39	1.43
4	I	1	NAG	O5-C1	-2.68	1.39	1.43
3	D	2	NAG	C4-C5	2.67	1.58	1.53
5	H	2	NAG	C4-C5	2.67	1.58	1.53
2	J	1	NAG	O4-C4	2.65	1.49	1.43
2	E	1	NAG	O4-C4	2.65	1.49	1.43
3	D	2	NAG	O5-C5	2.56	1.48	1.43
5	H	2	NAG	O5-C5	2.56	1.48	1.43
4	F	3	BMA	C6-C5	2.51	1.60	1.51
4	I	3	BMA	C6-C5	2.51	1.60	1.51
4	F	1	NAG	C3-C2	-2.49	1.47	1.52
4	I	1	NAG	C3-C2	-2.49	1.47	1.52
3	D	4	FUL	O5-C1	2.37	1.47	1.43
5	H	4	FUC	O5-C1	2.37	1.47	1.43
2	G	1	NAG	O4-C4	2.30	1.48	1.43
2	C	1	NAG	O4-C4	2.30	1.48	1.43
4	F	2	NAG	C3-C2	2.20	1.57	1.52
4	I	2	NAG	C3-C2	2.20	1.57	1.52
2	J	2	NAG	C4-C5	-2.18	1.48	1.53
2	E	2	NAG	C4-C5	-2.18	1.48	1.53
4	F	2	NAG	O4-C4	2.18	1.48	1.43
4	I	2	NAG	O4-C4	2.18	1.48	1.43
4	F	3	BMA	O5-C5	2.11	1.47	1.43
4	I	3	BMA	O5-C5	2.11	1.47	1.43
2	C	2	NAG	C1-C2	2.09	1.55	1.52
2	G	2	NAG	C1-C2	2.09	1.55	1.52
2	J	2	NAG	C3-C2	2.08	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C3-C2	2.08	1.56	1.52
2	G	1	NAG	C4-C5	2.07	1.57	1.53
2	C	1	NAG	C4-C5	2.07	1.57	1.53
3	D	3	BMA	C4-C3	2.03	1.57	1.52
5	H	3	BMA	C4-C3	2.03	1.57	1.52
3	D	4	FUL	C4-C3	2.02	1.57	1.52
5	H	4	FUC	C4-C3	2.02	1.57	1.52
3	D	2	NAG	O5-C1	2.02	1.46	1.43
5	H	2	NAG	O5-C1	2.02	1.46	1.43
4	F	4	MAN	C2-C3	2.01	1.55	1.52
4	I	4	MAN	C2-C3	2.01	1.55	1.52
4	F	2	NAG	C2-N2	2.01	1.49	1.46
4	I	2	NAG	C2-N2	2.01	1.49	1.46

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C6-C5-C4	10.61	137.86	113.00
4	I	1	NAG	C6-C5-C4	10.61	137.86	113.00
3	D	1	NAG	C1-C2-N2	10.02	127.61	110.49
5	H	1	NAG	C1-C2-N2	10.02	127.61	110.49
3	D	1	NAG	C1-O5-C5	8.24	123.36	112.19
5	H	1	NAG	C1-O5-C5	8.24	123.36	112.19
4	F	2	NAG	C1-C2-N2	7.90	123.98	110.49
4	I	2	NAG	C1-C2-N2	7.90	123.98	110.49
4	F	2	NAG	C2-N2-C7	7.78	133.98	122.90
4	I	2	NAG	C2-N2-C7	7.78	133.98	122.90
4	F	6	MAN	O2-C2-C1	7.31	124.10	109.15
4	I	6	MAN	O2-C2-C1	7.31	124.10	109.15
3	D	2	NAG	C1-C2-N2	6.70	121.93	110.49
5	H	2	NAG	C1-C2-N2	6.70	121.93	110.49
4	F	2	NAG	C1-O5-C5	6.61	121.15	112.19
4	I	2	NAG	C1-O5-C5	6.61	121.15	112.19
2	G	1	NAG	C6-C5-C4	6.40	127.98	113.00
2	C	1	NAG	C6-C5-C4	6.40	127.98	113.00
4	F	1	NAG	C2-N2-C7	6.39	132.00	122.90
4	I	1	NAG	C2-N2-C7	6.39	132.00	122.90
2	C	2	NAG	C1-O5-C5	6.31	120.74	112.19
2	G	2	NAG	C1-O5-C5	6.31	120.74	112.19
2	J	2	NAG	C1-C2-N2	-5.91	100.39	110.49
2	E	2	NAG	C1-C2-N2	-5.91	100.39	110.49
3	D	2	NAG	C4-C3-C2	-5.91	102.36	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	C4-C3-C2	-5.91	102.36	111.02
4	F	6	MAN	O5-C1-C2	-5.74	101.91	110.77
4	I	6	MAN	O5-C1-C2	-5.74	101.91	110.77
4	F	4	MAN	C1-O5-C5	5.69	119.90	112.19
4	I	4	MAN	C1-O5-C5	5.69	119.90	112.19
4	F	4	MAN	C1-C2-C3	-5.41	103.01	109.67
4	I	4	MAN	C1-C2-C3	-5.41	103.01	109.67
4	F	3	BMA	C2-C3-C4	-5.15	101.98	110.89
4	I	3	BMA	C2-C3-C4	-5.15	101.98	110.89
2	J	1	NAG	C1-C2-N2	-5.01	101.94	110.49
2	E	1	NAG	C1-C2-N2	-5.01	101.94	110.49
2	C	2	NAG	O7-C7-C8	-4.90	112.96	122.06
2	G	2	NAG	O7-C7-C8	-4.90	112.96	122.06
4	F	4	MAN	O5-C1-C2	4.89	118.32	110.77
4	I	4	MAN	O5-C1-C2	4.89	118.32	110.77
2	C	2	NAG	C8-C7-N2	4.86	124.33	116.10
2	G	2	NAG	C8-C7-N2	4.86	124.33	116.10
4	F	6	MAN	O4-C4-C3	-4.68	99.54	110.35
4	I	6	MAN	O4-C4-C3	-4.68	99.54	110.35
3	D	2	NAG	O5-C1-C2	-4.63	103.98	111.29
5	H	2	NAG	O5-C1-C2	-4.63	103.98	111.29
4	F	1	NAG	O5-C5-C6	-4.59	100.00	107.20
4	I	1	NAG	O5-C5-C6	-4.59	100.00	107.20
4	F	3	BMA	C1-O5-C5	4.41	118.16	112.19
4	I	3	BMA	C1-O5-C5	4.41	118.16	112.19
2	G	1	NAG	C3-C4-C5	-4.21	102.73	110.24
2	C	1	NAG	C3-C4-C5	-4.21	102.73	110.24
2	C	2	NAG	C1-C2-N2	4.19	117.65	110.49
2	G	2	NAG	C1-C2-N2	4.19	117.65	110.49
4	F	1	NAG	C3-C4-C5	-4.07	102.98	110.24
4	I	1	NAG	C3-C4-C5	-4.07	102.98	110.24
4	F	6	MAN	O2-C2-C3	-3.81	102.51	110.14
4	I	6	MAN	O2-C2-C3	-3.81	102.51	110.14
4	F	2	NAG	C6-C5-C4	3.74	121.77	113.00
4	I	2	NAG	C6-C5-C4	3.74	121.77	113.00
4	F	2	NAG	O5-C1-C2	-3.59	105.62	111.29
4	I	2	NAG	O5-C1-C2	-3.59	105.62	111.29
4	F	1	NAG	C1-O5-C5	3.58	117.05	112.19
4	I	1	NAG	C1-O5-C5	3.58	117.05	112.19
4	F	2	NAG	O7-C7-C8	-3.56	115.45	122.06
4	I	2	NAG	O7-C7-C8	-3.56	115.45	122.06
3	D	3	BMA	C1-O5-C5	3.49	116.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	BMA	C1-O5-C5	3.49	116.92	112.19
4	F	6	MAN	C1-O5-C5	3.48	116.90	112.19
4	I	6	MAN	C1-O5-C5	3.48	116.90	112.19
2	J	1	NAG	C6-C5-C4	3.28	120.69	113.00
2	E	1	NAG	C6-C5-C4	3.28	120.69	113.00
4	F	2	NAG	C8-C7-N2	3.14	121.42	116.10
4	I	2	NAG	C8-C7-N2	3.14	121.42	116.10
2	G	1	NAG	O4-C4-C5	2.93	116.57	109.30
2	C	1	NAG	O4-C4-C5	2.93	116.57	109.30
2	G	1	NAG	O5-C1-C2	-2.91	106.69	111.29
2	C	1	NAG	O5-C1-C2	-2.91	106.69	111.29
4	F	1	NAG	O4-C4-C5	2.90	116.49	109.30
4	I	1	NAG	O4-C4-C5	2.90	116.49	109.30
4	I	5	MAN	C1-C2-C3	2.86	113.18	109.67
4	F	5	MAN	C1-C2-C3	2.86	113.18	109.67
2	J	1	NAG	O5-C1-C2	-2.82	106.83	111.29
2	E	1	NAG	O5-C1-C2	-2.82	106.83	111.29
3	D	1	NAG	C6-C5-C4	-2.80	106.44	113.00
5	H	1	NAG	C6-C5-C4	-2.80	106.44	113.00
3	D	2	NAG	O3-C3-C4	2.78	116.77	110.35
5	H	2	NAG	O3-C3-C4	2.78	116.77	110.35
3	D	1	NAG	O5-C5-C6	-2.76	102.87	107.20
5	H	1	NAG	O5-C5-C6	-2.76	102.87	107.20
4	F	6	MAN	O3-C3-C4	-2.75	103.98	110.35
4	I	6	MAN	O3-C3-C4	-2.75	103.98	110.35
4	F	4	MAN	C6-C5-C4	-2.74	106.59	113.00
4	I	4	MAN	C6-C5-C4	-2.74	106.59	113.00
2	J	2	NAG	C6-C5-C4	2.71	119.36	113.00
2	E	2	NAG	C6-C5-C4	2.71	119.36	113.00
3	D	2	NAG	O4-C4-C3	2.71	116.61	110.35
5	H	2	NAG	O4-C4-C3	2.71	116.61	110.35
2	C	2	NAG	C2-N2-C7	2.67	126.71	122.90
2	G	2	NAG	C2-N2-C7	2.67	126.71	122.90
3	D	1	NAG	O5-C5-C4	2.66	117.31	110.83
5	H	1	NAG	O5-C5-C4	2.66	117.31	110.83
4	F	3	BMA	O5-C5-C6	-2.62	103.09	107.20
4	I	3	BMA	O5-C5-C6	-2.62	103.09	107.20
2	C	2	NAG	C4-C3-C2	2.62	114.86	111.02
2	G	2	NAG	C4-C3-C2	2.62	114.86	111.02
3	D	3	BMA	C3-C4-C5	-2.60	105.59	110.24
5	H	3	BMA	C3-C4-C5	-2.60	105.59	110.24
4	I	5	MAN	C1-O5-C5	2.58	115.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5	MAN	C1-O5-C5	2.58	115.69	112.19
2	J	2	NAG	O5-C5-C4	-2.58	104.56	110.83
2	E	2	NAG	O5-C5-C4	-2.58	104.56	110.83
4	F	4	MAN	O2-C2-C3	2.57	115.29	110.14
4	I	4	MAN	O2-C2-C3	2.57	115.29	110.14
3	D	3	BMA	C1-C2-C3	2.50	112.74	109.67
5	H	3	BMA	C1-C2-C3	2.50	112.74	109.67
3	D	3	BMA	O5-C5-C4	-2.44	104.89	110.83
5	H	3	BMA	O5-C5-C4	-2.44	104.89	110.83
3	D	3	BMA	O5-C1-C2	2.41	114.49	110.77
5	H	3	BMA	O5-C1-C2	2.41	114.49	110.77
3	D	2	NAG	C1-O5-C5	2.41	115.45	112.19
5	H	2	NAG	C1-O5-C5	2.41	115.45	112.19
4	F	2	NAG	O5-C5-C4	-2.38	105.04	110.83
4	I	2	NAG	O5-C5-C4	-2.38	105.04	110.83
4	F	6	MAN	C2-C3-C4	2.37	114.99	110.89
4	I	6	MAN	C2-C3-C4	2.37	114.99	110.89
3	D	3	BMA	O5-C5-C6	2.34	110.88	107.20
5	H	3	BMA	O5-C5-C6	2.34	110.88	107.20
4	F	6	MAN	C6-C5-C4	2.34	118.49	113.00
4	I	6	MAN	C6-C5-C4	2.34	118.49	113.00
2	G	1	NAG	O7-C7-C8	-2.34	117.71	122.06
2	C	1	NAG	O7-C7-C8	-2.34	117.71	122.06
2	J	1	NAG	C1-O5-C5	2.33	115.35	112.19
2	E	1	NAG	C1-O5-C5	2.33	115.35	112.19
2	C	2	NAG	O5-C5-C6	2.29	110.80	107.20
2	G	2	NAG	O5-C5-C6	2.29	110.80	107.20
4	F	2	NAG	O6-C6-C5	2.24	118.99	111.29
4	I	2	NAG	O6-C6-C5	2.24	118.99	111.29
3	D	4	FUL	C3-C4-C5	2.23	113.25	109.77
5	H	4	FUC	C3-C4-C5	2.23	113.25	109.77
4	F	3	BMA	O3-C3-C4	2.19	115.42	110.35
4	I	3	BMA	O3-C3-C4	2.19	115.42	110.35
2	G	1	NAG	C1-O5-C5	2.13	115.08	112.19
2	C	1	NAG	C1-O5-C5	2.13	115.08	112.19
4	F	3	BMA	C3-C4-C5	2.11	114.00	110.24
4	I	3	BMA	C3-C4-C5	2.11	114.00	110.24
2	G	1	NAG	C2-N2-C7	-2.10	119.92	122.90
2	C	1	NAG	C2-N2-C7	-2.10	119.92	122.90
2	J	2	NAG	O5-C5-C6	2.04	110.41	107.20
2	E	2	NAG	O5-C5-C6	2.04	110.41	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	4	FUC	C1

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
4	F	5	MAN	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	F	6	MAN	C4-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
5	H	1	NAG	C1-C2-N2-C7
2	J	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
4	I	6	MAN	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7

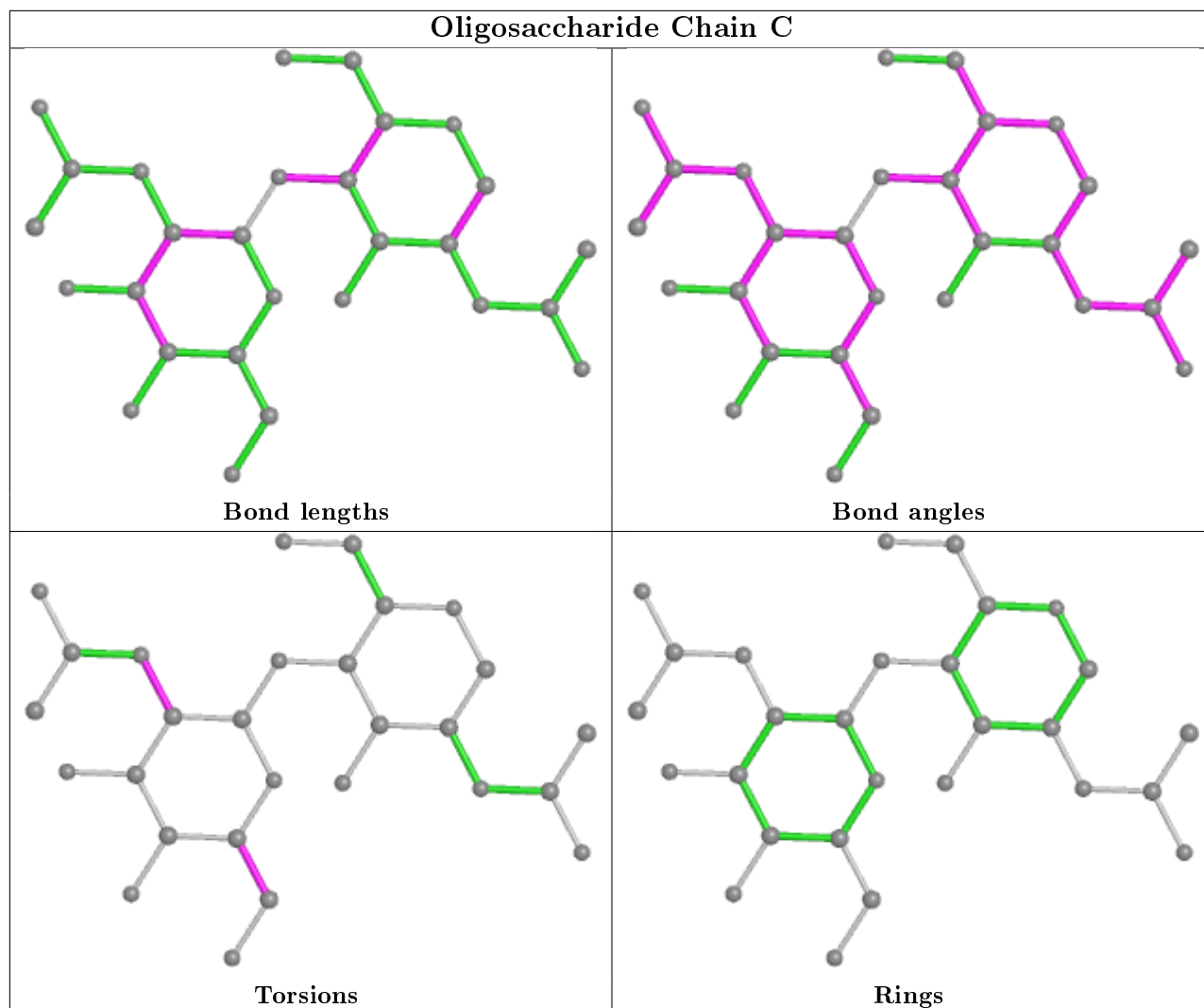
All (2) ring outliers are listed below:

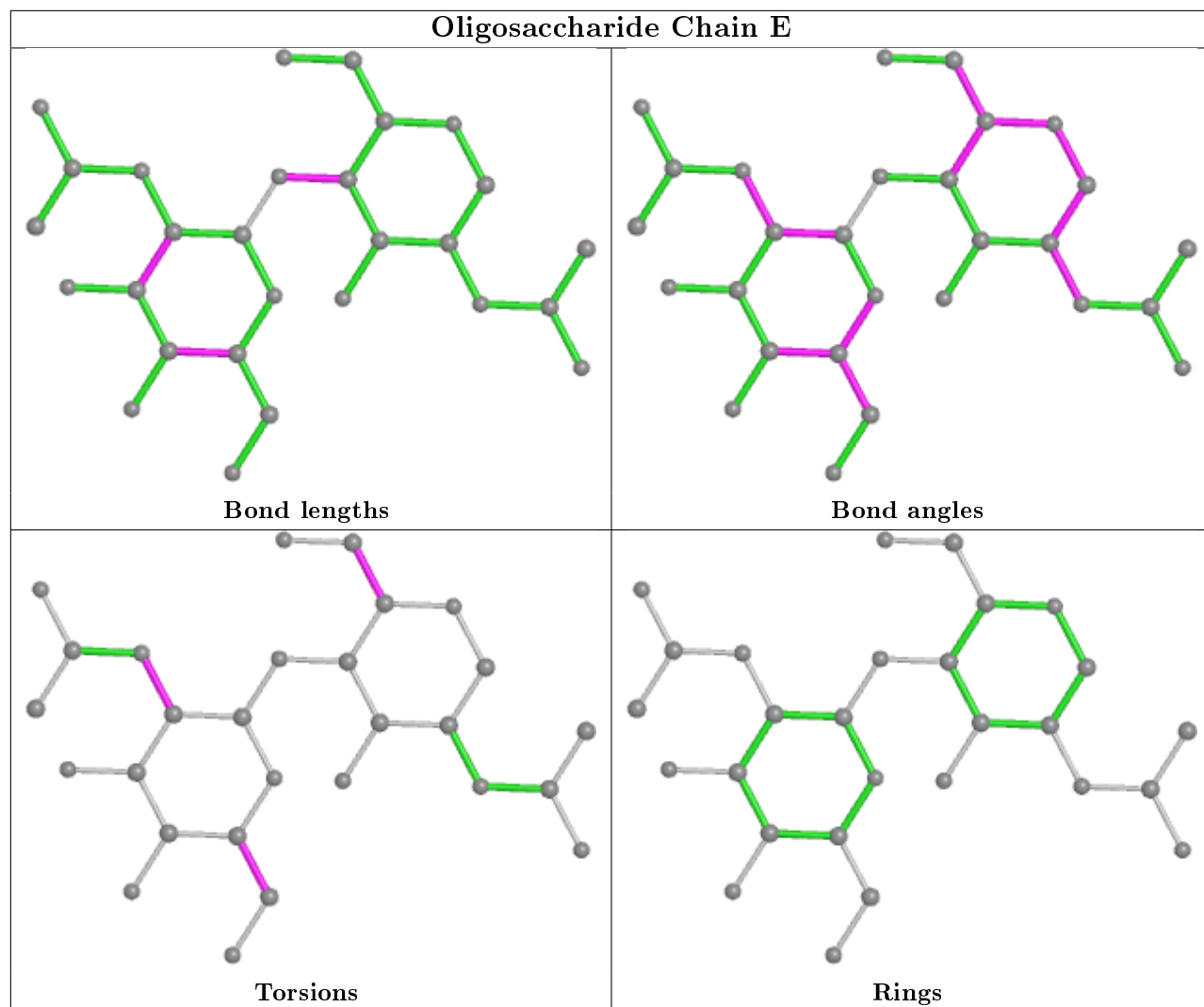
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C1-C2-C3-C4-C5-O5
4	I	3	BMA	C1-C2-C3-C4-C5-O5

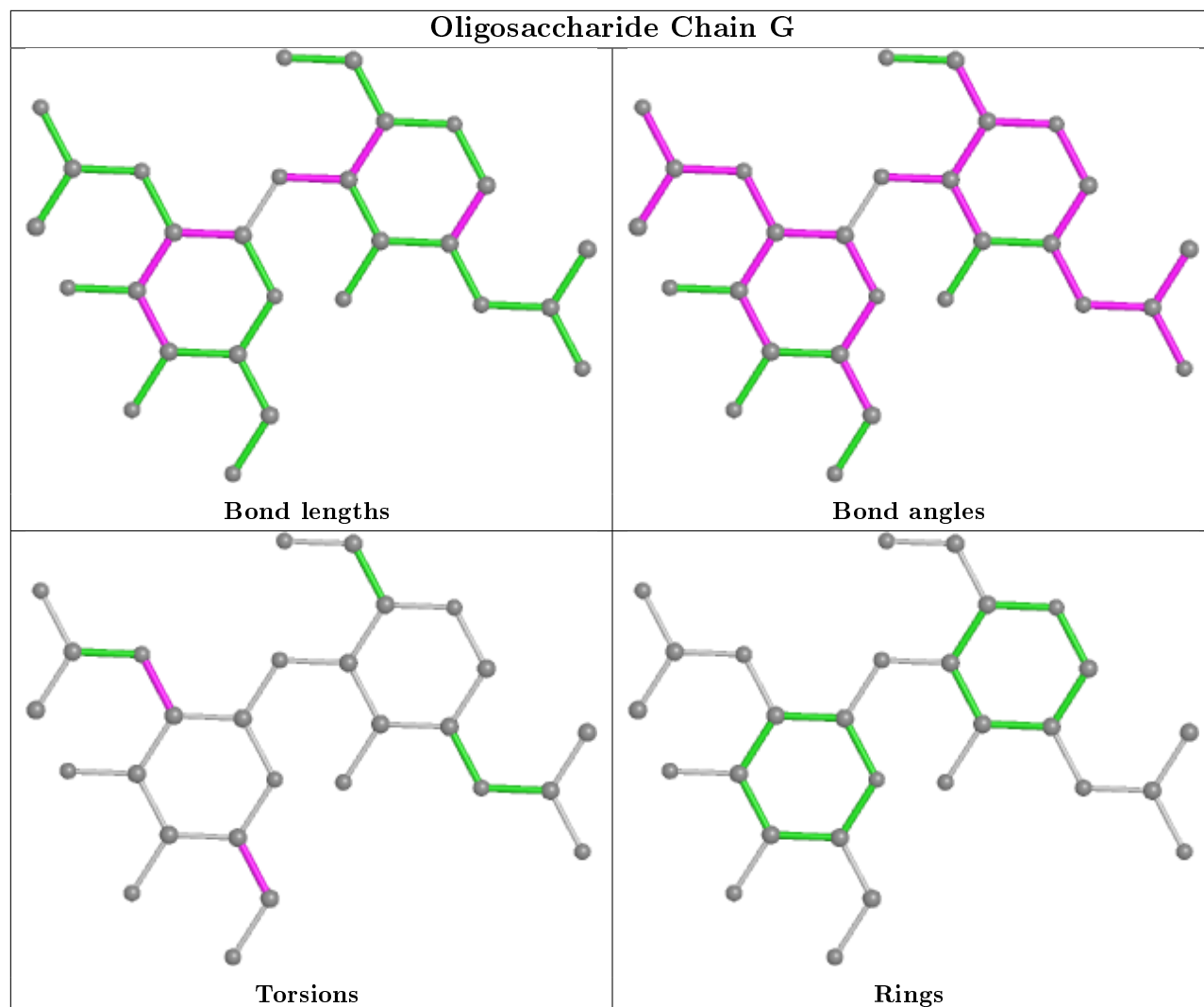
19 monomers are involved in 132 short contacts:

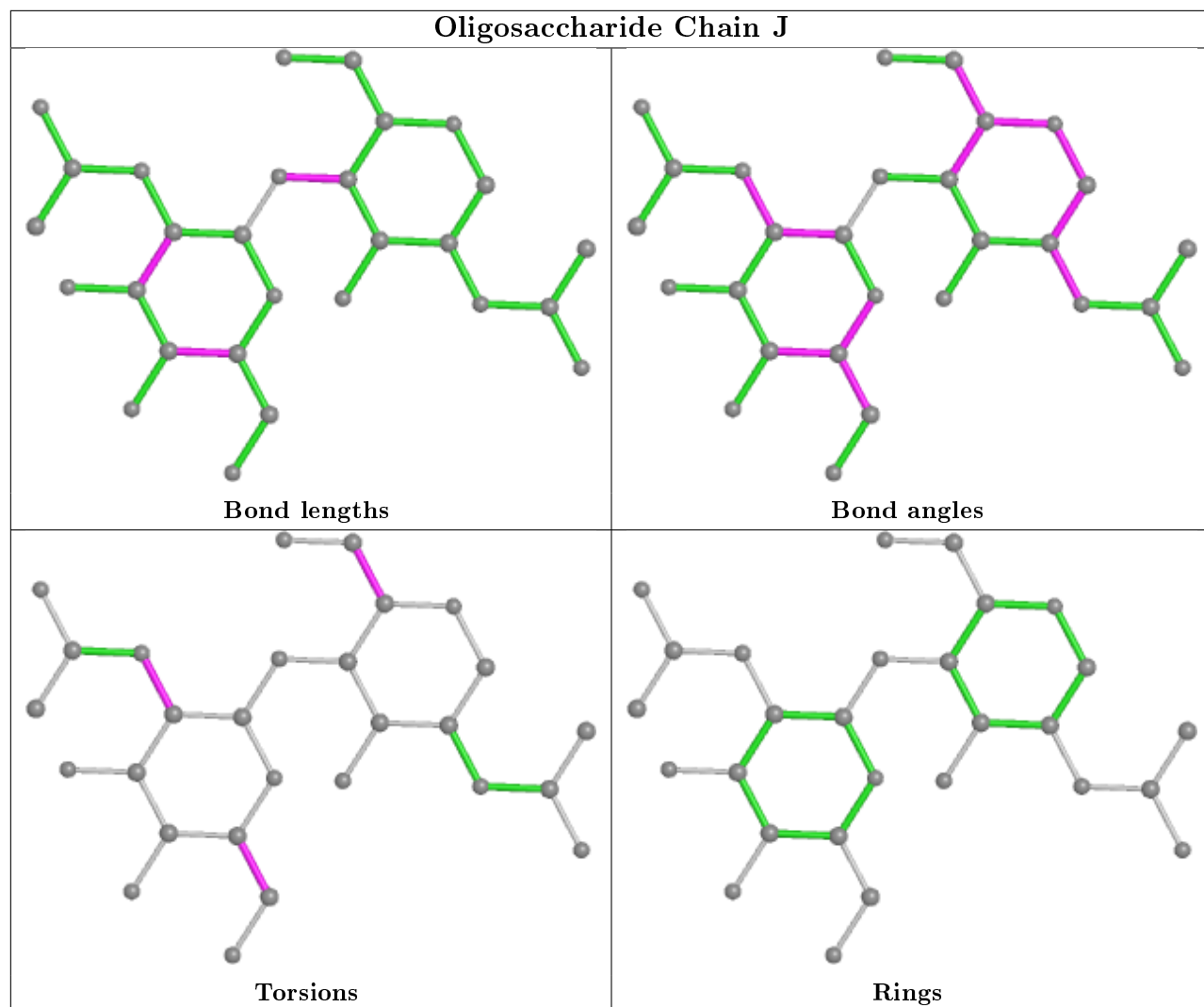
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
4	F	3	BMA	4	0
4	F	2	NAG	2	0
4	I	5	MAN	0	41
4	F	5	MAN	4	0
4	F	6	MAN	9	0
4	F	4	MAN	12	0
4	I	2	NAG	2	0
2	G	2	NAG	2	0
4	I	4	MAN	0	28
3	D	4	FUL	1	0
2	J	2	NAG	1	0
2	G	1	NAG	2	0
4	I	6	MAN	0	2
4	I	3	BMA	1	0
2	E	2	NAG	1	0
4	F	1	NAG	20	0
4	I	1	NAG	1	3
2	C	1	NAG	2	0

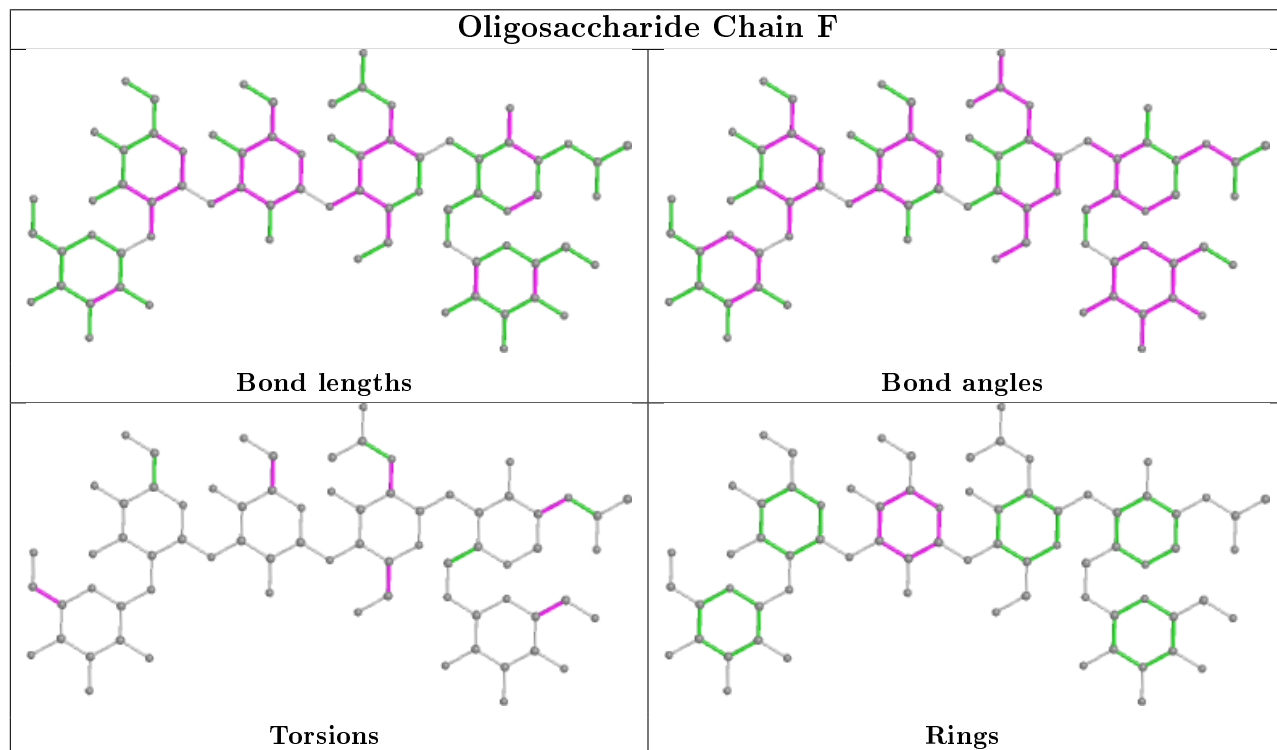
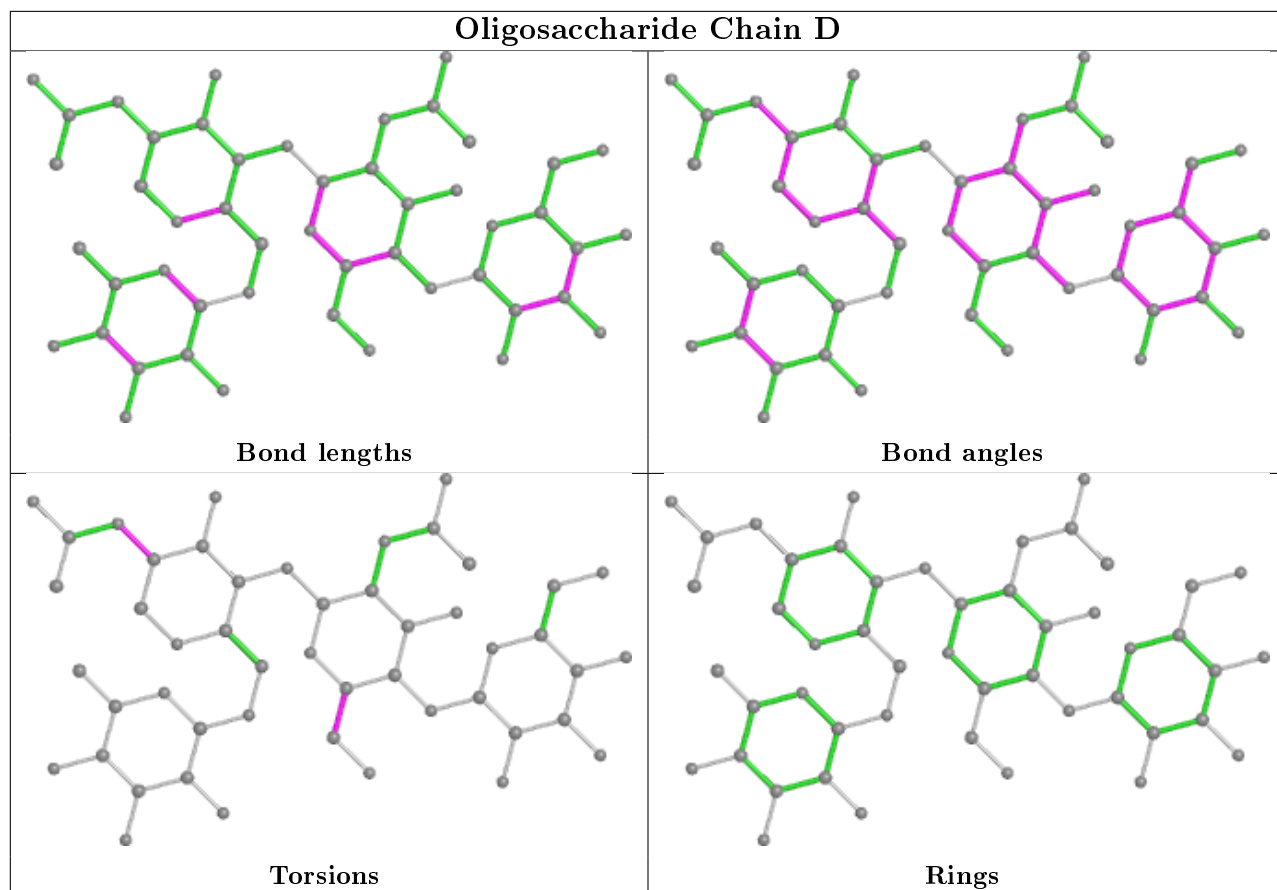
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



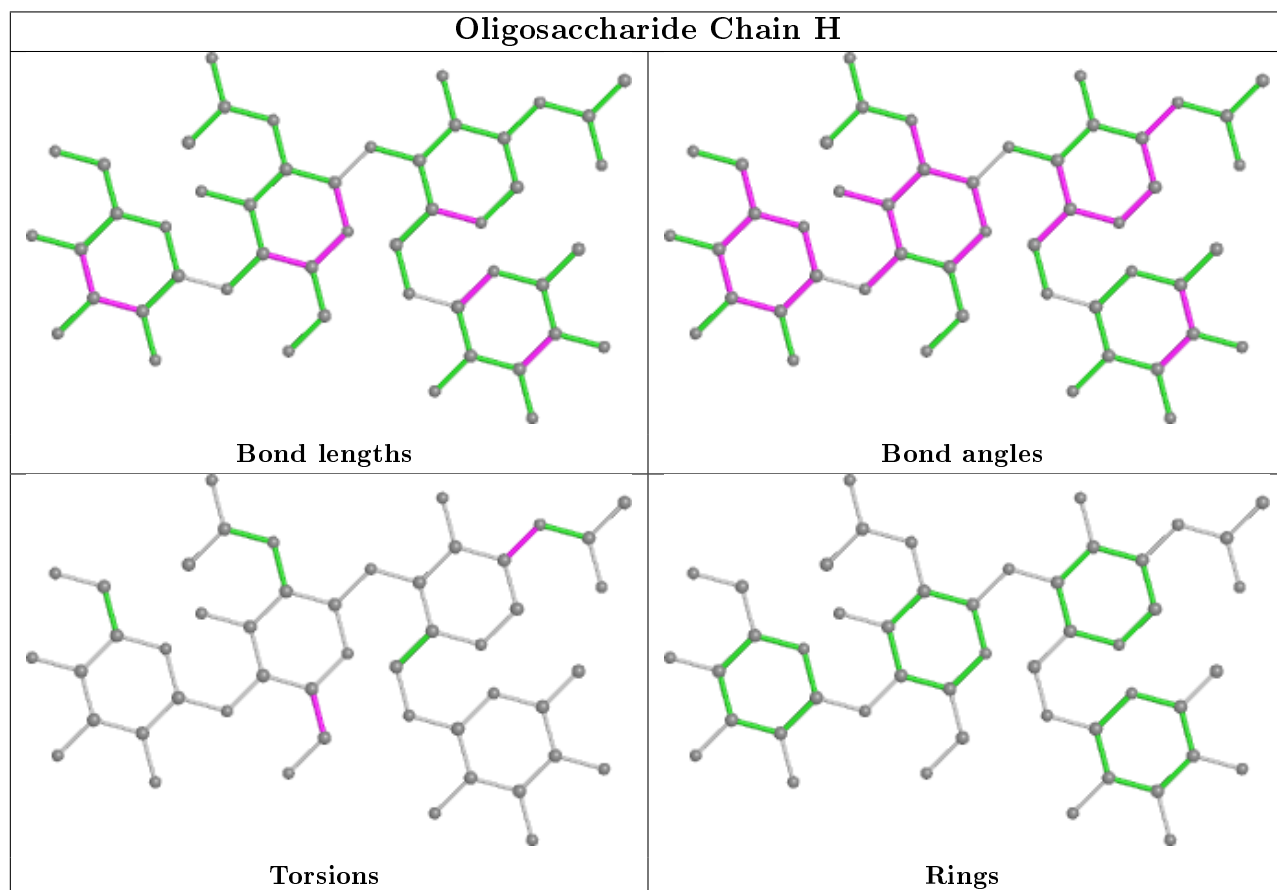
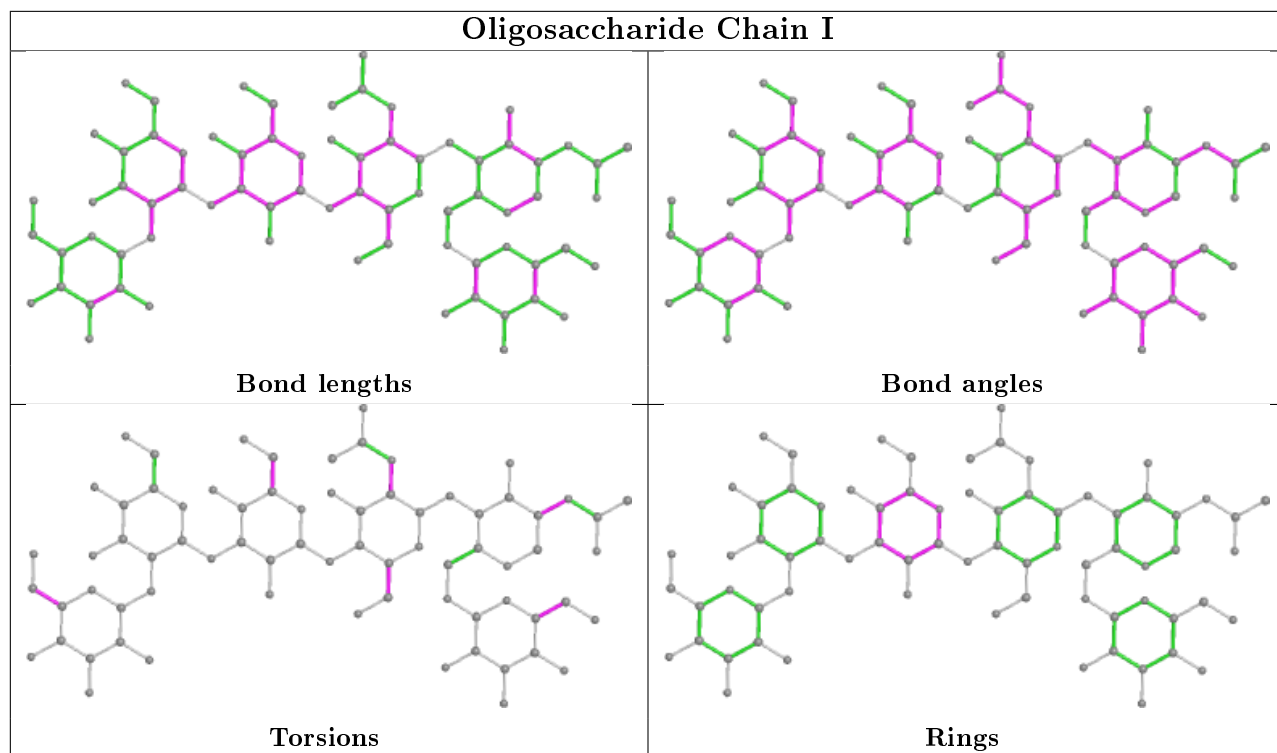












## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

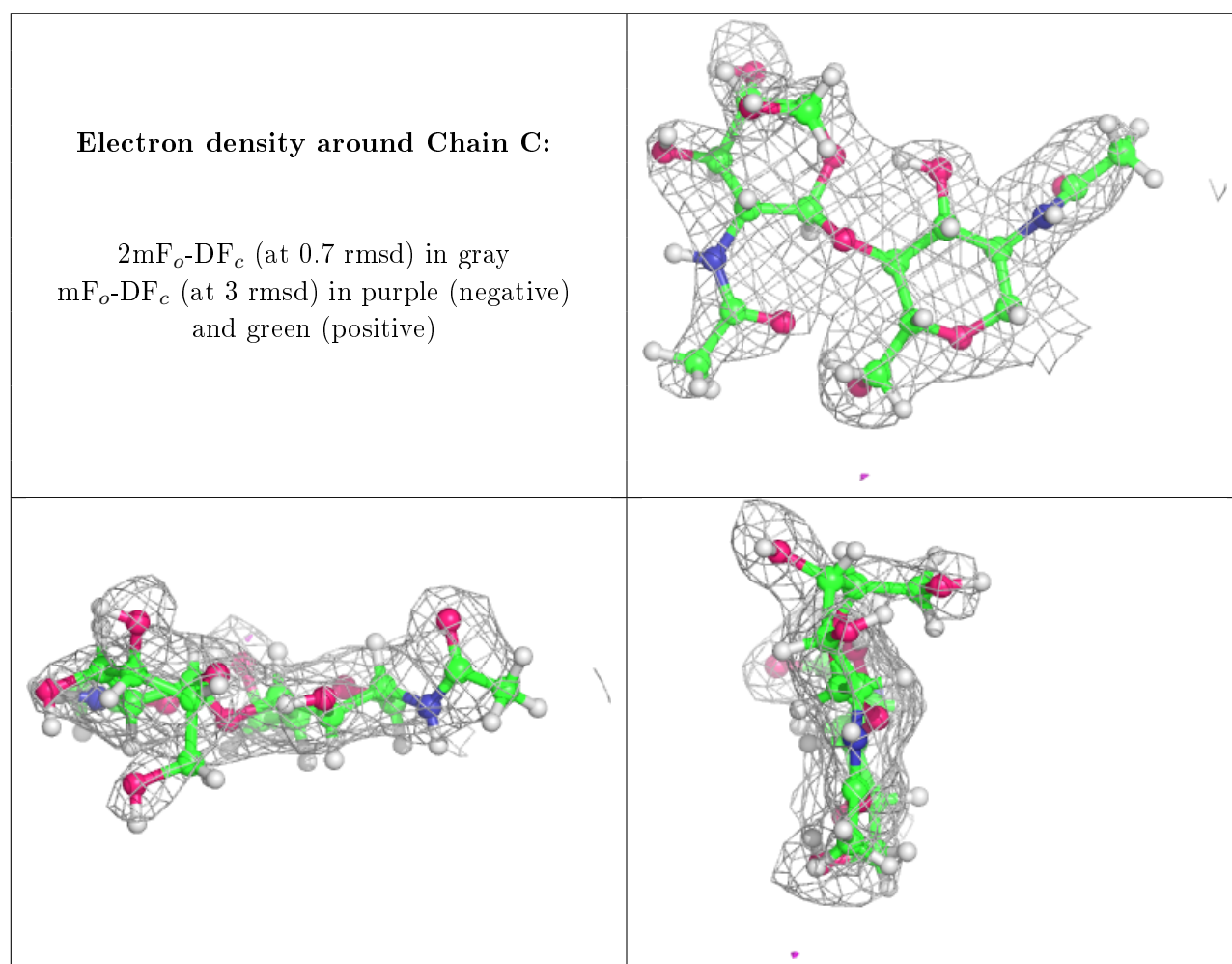
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

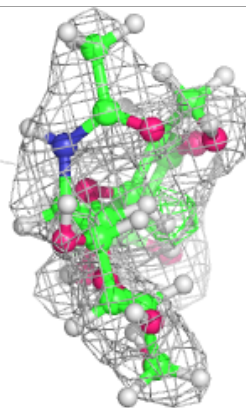
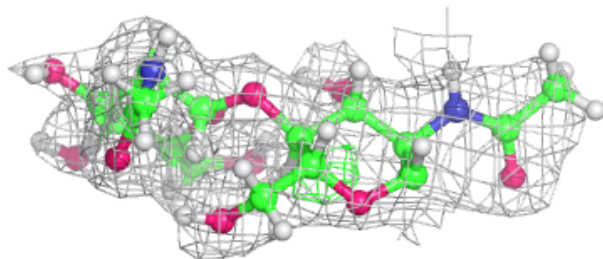
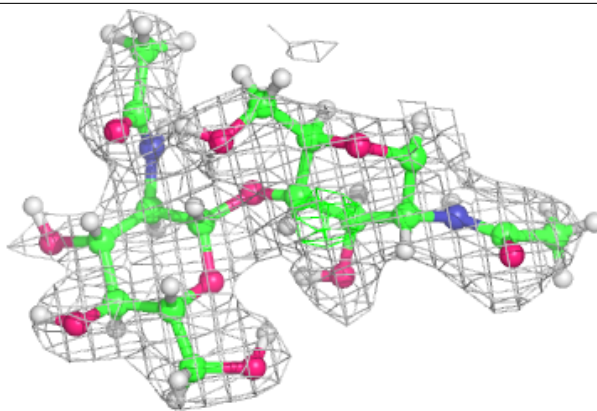
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

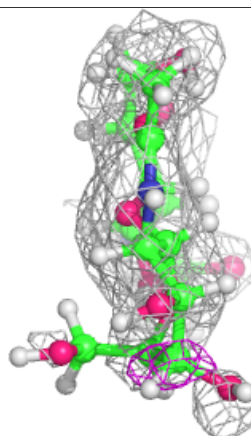
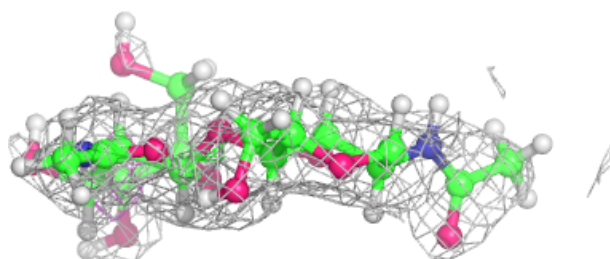
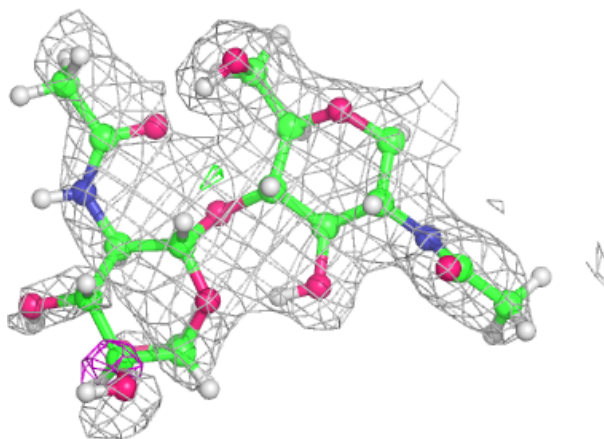


**Electron density around Chain E:**

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

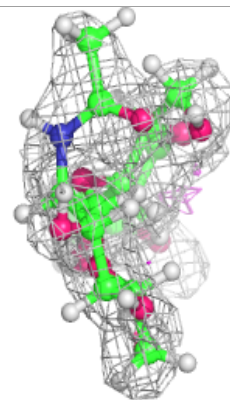
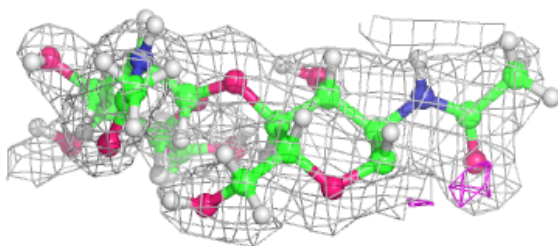
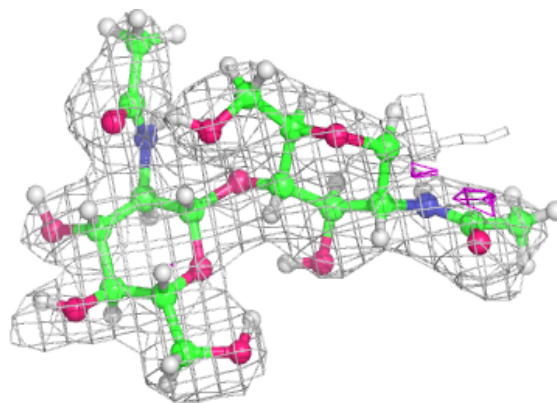
**Electron density around Chain G:**

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

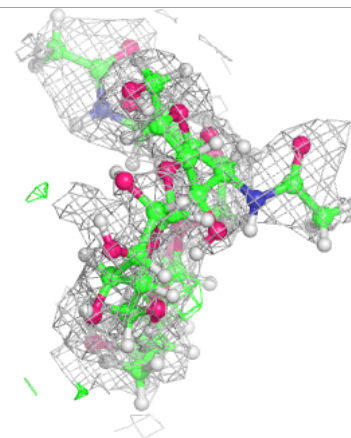
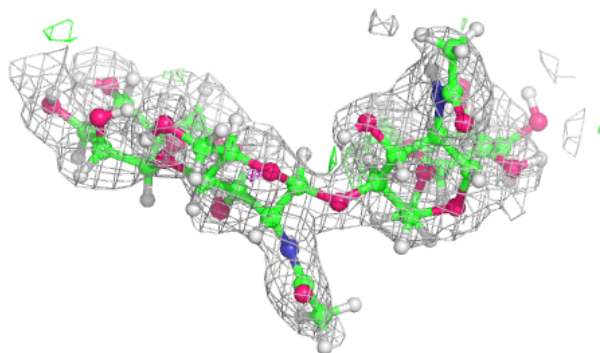
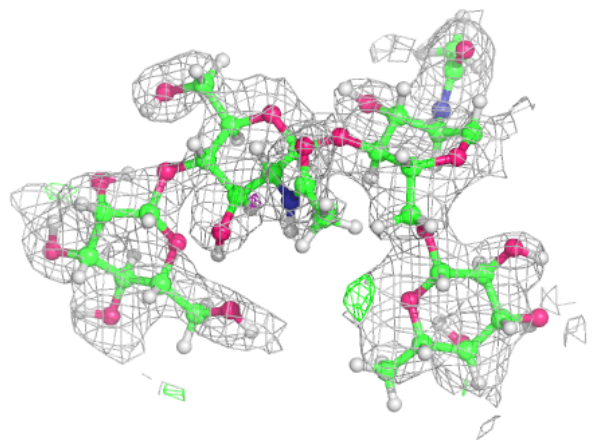


**Electron density around Chain J:**

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

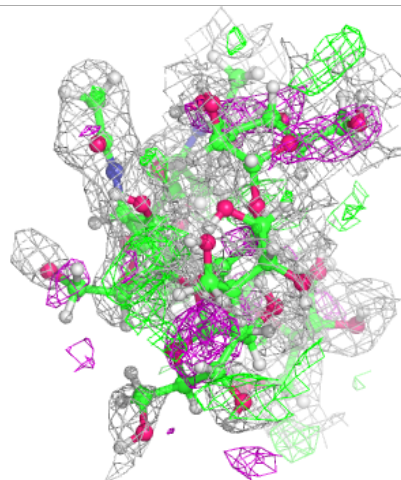
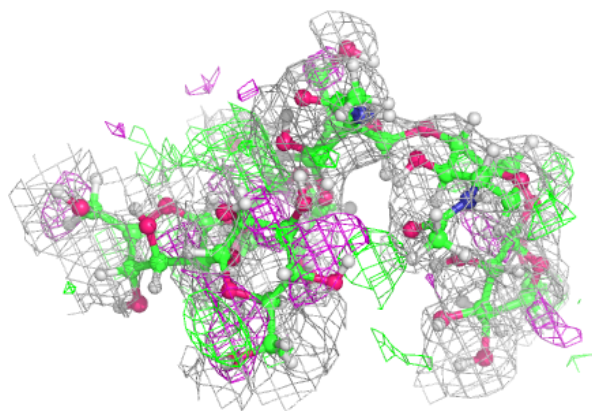
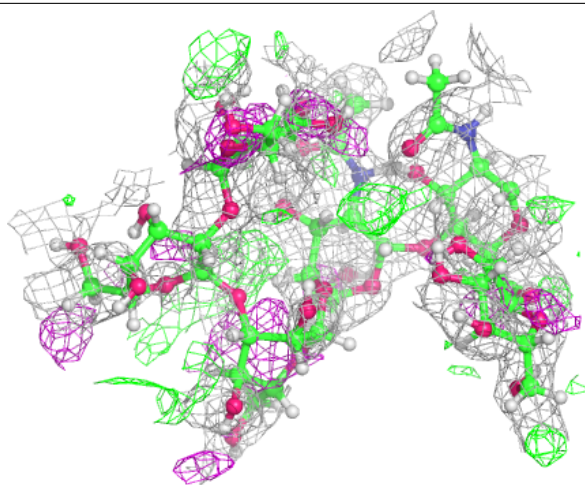
**Electron density around Chain D:**

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



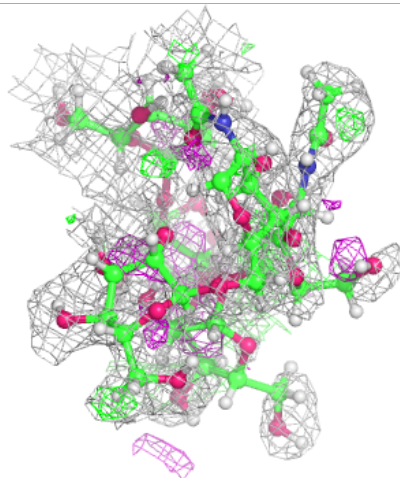
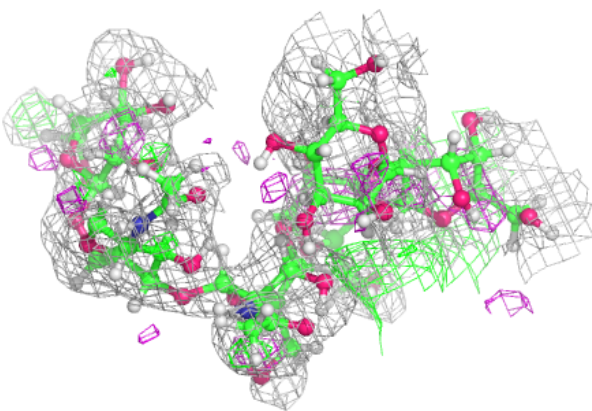
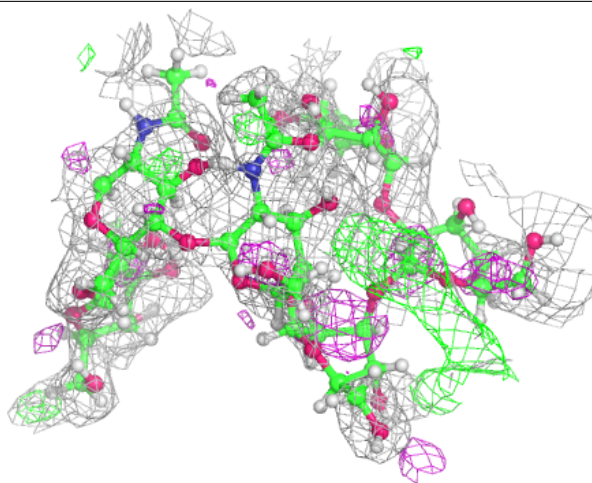
**Electron density around Chain F:**

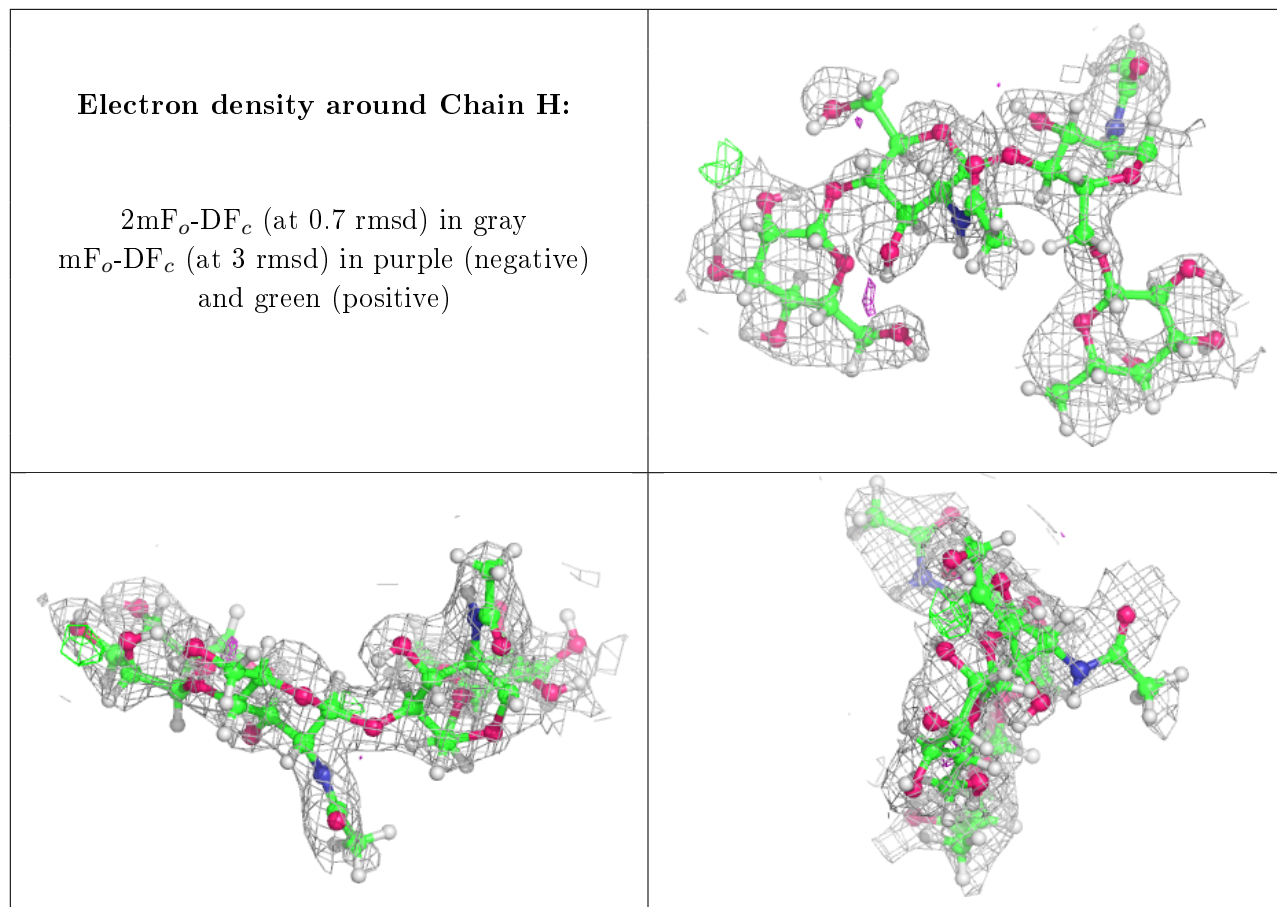
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.