



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 07:53 AM EST

PDB ID : 1TKR  
Title : Human Dipeptidyl Peptidase IV/CD26 inhibited with Diisopropyl FluoroPhosphate  
Authors : Bjelke, J.R.; Christensen, J.; Branner, S.; Wagtmann, N.; Olsen, C.; Kanstrup, A.B.; Rasmussen, H.B.  
Deposited on : 2004-06-09  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

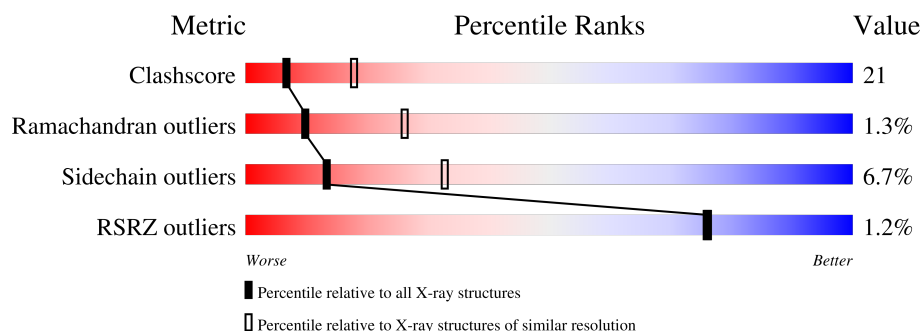
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.







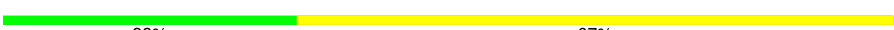


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div></div> <div> <div></div> <div>63%</div> <div>32%</div> <div>.</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>5%</div> </div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>
3	D	3	<div> <div>33%</div> <div>67%</div> </div>
4	E	2	<div> <div>50%</div> <div>50%</div> </div>
4	G	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	2	 50% 50%
4	J	2	 50% 50%
5	F	3	 33% 67%
6	I	2	 50% 50%
7	K	3	 33% 67%
7	L	3	 67% 33%
8	M	2	 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
3	NAG	D	1	X	-	-	-
4	NAG	J	1	X	-	-	-
8	NAG	M	1	X	-	X	-
8	NDG	M	2	-	-	X	-

## 2 Entry composition [i](#)

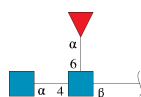
There are 11 unique types of molecules in this entry. The entry contains 12996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase IV.

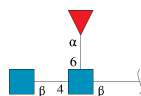
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



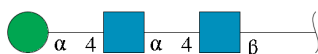
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 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
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



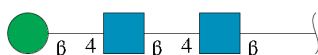
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 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.



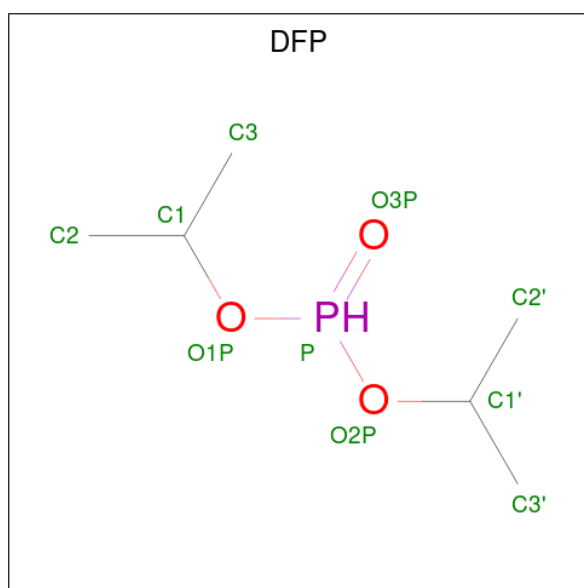
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 9 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	P	0	0
			10	6	3	1		
9	B	1	Total	C	O	P	0	0
			10	6	3	1		

- Molecule 10 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>).



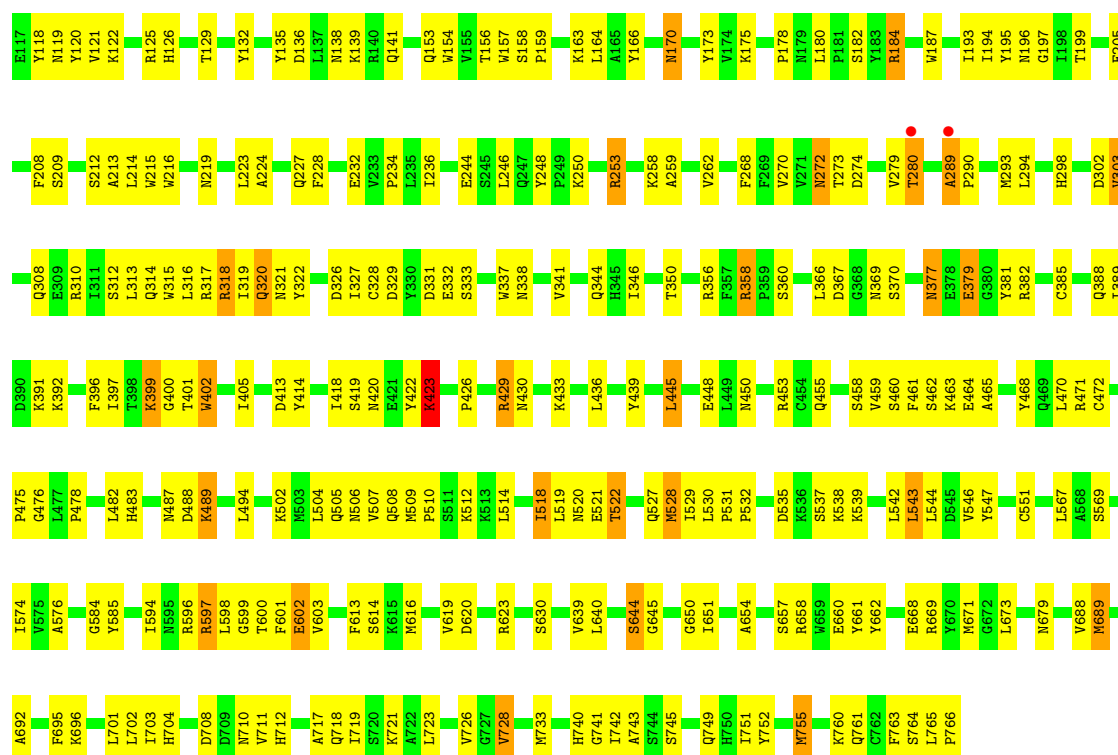
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	378	Total	O	0	0
			378	378		
11	B	315	Total	O	0	0
			315	315		







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

Chain C: 33% 67%



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

Chain D: 33% 67%



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

Chain E: 50% 50%



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

Chain G: 100%



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

Chain H:  50% 50%



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

Chain J:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%

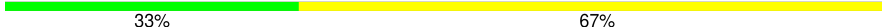


- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



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

Chain K:  33% 67%



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

Chain L:  67% 33%



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

Chain M:  100%

HA31  
ADG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.22Å 123.46Å 131.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.60 – 2.70 30.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (30.60-2.70) 92.6 (30.60-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.23 (at 2.68Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.203 , 0.268 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: FUC, NAG, MAN, BMA, DFP, NDG

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	0.36	0/6119	0.62	0/8321
1	B	0.37	0/6136	0.61	0/8344
All	All	0.37	0/12255	0.61	0/16665

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5948	0	5659	227	0
1	B	5964	0	5676	267	0
2	C	38	0	33	1	0
3	D	38	0	34	6	0
4	E	28	0	25	1	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	J	28	0	25	2	0
5	F	39	0	33	4	0
6	I	24	0	22	2	0
7	K	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	39	0	34	0	0
8	M	28	0	24	9	0
9	A	10	0	14	2	0
9	B	10	0	14	2	0
10	B	14	0	13	0	0
11	A	378	0	0	21	0
11	B	315	0	0	21	0
All	All	12996	0	11690	505	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 21.

All (505) 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)
9:A:1:DFP:H21	11:A:1159:HOH:O	1.30	1.28
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.34	1.08
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.38	1.03
1:B:458:SER:HB3	1:B:471:ARG:HB2	1.44	0.99
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.22	0.98
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.61	0.96
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.62	0.96
1:B:72:GLN:HE21	1:B:77:LEU:HD21	1.26	0.96
1:A:172:ILE:H	1:A:186:THR:HG22	1.35	0.90
1:B:657:SER:HB2	1:B:689:MET:HE1	1.57	0.87
1:B:77:LEU:HD23	1:B:77:LEU:H	1.37	0.87
1:B:620:ASP:OD2	1:B:623:ARG:HD3	1.75	0.87
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.58	0.85
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.06	0.85
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.58	0.85
1:A:184:ARG:NH1	1:A:187:TRP:HA	1.93	0.84
1:A:194:ILE:HG12	5:F:1:NAG:H82	1.60	0.82
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.09	0.81
1:A:253:ARG:HH22	1:B:253:ARG:HH22	0.83	0.80
1:B:308:GLN:HB3	4:J:1:NAG:H62	1.62	0.80
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.79	0.80
1:B:121:VAL:HB	1:B:129:THR:HG23	1.64	0.79
1:B:40:ARG:NH1	1:B:508:GLN:HG2	1.97	0.79
1:B:332:GLU:HB2	11:B:1011:HOH:O	1.83	0.78
1:A:438:ASP:OD1	1:A:440:THR:HG22	1.82	0.78
1:B:657:SER:HB2	1:B:689:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.86	0.75
3:D:1:NAG:H4	3:D:2:NAG:N2	2.00	0.75
1:A:75:ASN:HD22	1:A:88:VAL:HG13	1.51	0.74
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.67	0.74
1:B:651:ILE:HD13	1:B:755:MET:HG3	1.67	0.74
1:B:377:ASN:C	1:B:377:ASN:HD22	1.91	0.74
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.88	0.73
1:B:170:ASN:N	1:B:170:ASN:HD22	1.86	0.73
1:B:272:ASN:ND2	1:B:274:ASP:H	1.87	0.73
1:A:310:ARG:HG3	1:A:329:ASP:OD2	1.88	0.72
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.70	0.72
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.24	0.71
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.25	0.71
1:A:597:ARG:HG3	1:A:600:THR:HG21	1.71	0.70
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.27	0.70
1:A:600:THR:O	1:A:603:VAL:HG13	1.92	0.70
1:B:433:LYS:HB2	1:B:445:LEU:HD21	1.74	0.69
1:B:538:LYS:HD3	1:B:539:LYS:N	2.07	0.69
1:A:64:SER:HA	1:A:463:LYS:HG3	1.74	0.69
1:B:272:ASN:C	1:B:272:ASN:HD22	1.96	0.69
1:A:317:ARG:HD2	1:A:322:TYR:HB3	1.74	0.69
1:B:74:ASN:HD22	1:B:92:ASN:HD22	1.39	0.69
1:B:651:ILE:HD13	1:B:755:MET:CG	2.23	0.69
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.92	0.69
1:B:344:GLN:HE21	1:B:346:ILE:HD11	1.58	0.69
1:B:232:GLU:HB3	1:B:262:VAL:HG11	1.75	0.68
1:B:93:SER:HA	1:B:96:ASP:CG	2.14	0.68
1:B:377:ASN:ND2	1:B:381:TYR:H	1.92	0.68
1:B:594:ILE:HG21	1:B:602:GLU:HG2	1.76	0.68
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.29	0.67
1:A:489:LYS:HE2	11:A:1092:HOH:O	1.93	0.67
1:A:91:GLU:C	1:A:93:SER:H	1.99	0.66
1:A:293:MET:CE	1:A:317:ARG:HG3	2.26	0.66
1:A:463:LYS:HA	1:A:463:LYS:HE2	1.78	0.66
1:A:756:SER:O	1:A:760:LYS:HG2	1.96	0.66
1:A:172:ILE:H	1:A:186:THR:CG2	2.07	0.66
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.11	0.66
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.76	0.66
1:B:164:LEU:HB2	1:B:175:LYS:HB2	1.78	0.66
1:A:193:ILE:HG22	1:A:194:ILE:HD12	1.78	0.65
1:A:141:GLN:HG3	11:A:892:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:OD1	1:B:82:GLU:HB3	1.96	0.65
1:B:596:ARG:O	1:B:597:ARG:HD2	1.97	0.65
1:B:721:LYS:HG2	11:B:1061:HOH:O	1.95	0.64
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.78	0.64
1:B:657:SER:CB	1:B:689:MET:HE1	2.27	0.64
8:M:1:NAG:H62	8:M:2:NDG:H8C1	1.78	0.64
8:M:1:NAG:H62	8:M:2:NDG:HA	1.62	0.64
1:A:648:LYS:HD3	1:A:762:CYS:SG	2.38	0.63
1:B:308:GLN:HB3	4:J:1:NAG:C6	2.28	0.63
1:A:341:VAL:C	1:A:343:ARG:H	2.00	0.63
1:B:528:MET:HG3	1:B:576:ALA:HB2	1.80	0.63
1:A:197:GLY:C	1:A:213:ALA:HB3	2.19	0.63
1:A:272:ASN:ND2	1:A:274:ASP:H	1.96	0.63
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.34	0.63
1:A:535:ASP:OD1	1:A:537:SER:HB3	1.98	0.62
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.80	0.62
1:A:410:LEU:HD13	1:A:415:LEU:HD22	1.79	0.62
1:A:413:ASP:HB3	1:A:414:TYR:CD1	2.34	0.62
1:A:352:GLY:HA2	1:A:595:ASN:ND2	2.15	0.62
1:B:77:LEU:H	1:B:77:LEU:CD2	2.12	0.62
1:B:414:TYR:HA	1:B:436:LEU:HD13	1.81	0.62
1:A:410:LEU:HD13	1:A:415:LEU:CD2	2.30	0.62
1:B:399:LYS:HB2	1:B:402:TRP:CZ2	2.35	0.61
1:B:370:SER:HB3	1:B:388:GLN:NE2	2.15	0.61
1:A:203:TYR:HA	1:A:207:VAL:CG1	2.31	0.61
1:B:74:ASN:HD22	1:B:92:ASN:ND2	1.99	0.60
1:A:93:SER:HB2	1:A:96:ASP:OD2	1.99	0.60
5:F:2:NDG:H6C2	5:F:3:MAN:H2	1.83	0.60
1:A:536:LYS:NZ	1:A:536:LYS:HB3	2.17	0.60
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.32	0.60
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.83	0.60
1:A:379:GLU:O	1:A:379:GLU:HG2	2.01	0.60
1:B:614:SER:HA	1:B:619:VAL:HB	1.82	0.60
1:B:279:VAL:O	1:B:280:THR:HB	2.01	0.60
1:A:341:VAL:HG22	1:A:342:ALA:H	1.67	0.59
1:A:458:SER:HB3	1:A:471:ARG:HB2	1.83	0.59
1:B:689:MET:HE1	1:B:719:ILE:HG12	1.84	0.59
1:B:69:LEU:HD11	1:B:107:ILE:HD12	1.84	0.59
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.85	0.59
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.38	0.59
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.84	0.59
1:B:289:ALA:CB	1:B:290:PRO:HA	2.24	0.59
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.18	0.59
1:A:289:ALA:HB3	11:A:1097:HOH:O	2.03	0.59
8:M:1:NAG:H4	8:M:2:NDG:HA	1.68	0.59
1:A:293:MET:HE2	1:A:317:ARG:HG3	1.84	0.58
1:A:319:ILE:HG22	1:A:321:ASN:HB2	1.84	0.58
1:A:486:VAL:HG13	1:A:487:ASN:N	2.19	0.58
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.83	0.58
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.37	0.58
1:A:512:LYS:HE3	1:A:527:GLN:OE1	2.03	0.58
1:B:279:VAL:O	1:B:280:THR:CB	2.51	0.58
1:A:80:ASN:OD1	1:A:82:GLU:HB3	2.04	0.58
1:A:90:LEU:HA	11:A:886:HOH:O	2.03	0.58
1:A:734:TRP:HE1	1:A:736:THR:HG22	1.69	0.58
1:B:139:LYS:HG3	1:B:141:GLN:HB2	1.85	0.58
1:B:341:VAL:HG12	11:B:962:HOH:O	2.03	0.58
1:B:358:ARG:HH11	1:B:358:ARG:CB	2.06	0.58
1:A:75:ASN:HB3	1:A:91:GLU:HA	1.85	0.57
1:A:681:ASP:HB2	11:A:1134:HOH:O	2.04	0.57
1:A:370:SER:HB2	1:A:387:PHE:O	2.05	0.57
1:A:327:ILE:HD13	1:A:389:ILE:HG22	1.86	0.57
1:B:72:GLN:HE21	1:B:77:LEU:CD2	2.10	0.57
1:A:214:LEU:O	1:A:214:LEU:HD12	2.04	0.57
11:A:1001:HOH:O	5:F:3:MAN:H61	2.04	0.57
1:B:418:ILE:HA	1:B:430:ASN:O	2.05	0.57
1:B:518:ILE:HD13	1:B:518:ILE:C	2.25	0.57
1:B:538:LYS:HD3	1:B:539:LYS:H	1.69	0.57
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.70	0.57
1:A:289:ALA:CB	1:A:290:PRO:HA	2.24	0.57
1:B:93:SER:HA	1:B:96:ASP:OD2	2.04	0.57
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.70	0.57
1:A:414:TYR:HA	1:A:436:LEU:HD13	1.87	0.56
1:B:450:ASN:HB2	11:B:814:HOH:O	2.04	0.56
1:B:316:LEU:HD12	1:B:322:TYR:O	2.05	0.56
1:B:529:ILE:N	1:B:529:ILE:HD12	2.20	0.56
1:B:385:CYS:HB3	1:B:396:PHE:CD1	2.40	0.56
1:A:76:ILE:HB	1:A:90:LEU:HD11	1.87	0.56
1:B:219:ASN:CB	1:B:308:GLN:OE1	2.53	0.56
1:A:334:SER:OG	1:A:336:ARG:HG3	2.05	0.56
1:A:409:ALA:HA	11:A:1005:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:O	1:B:47:ASP:HB2	2.06	0.56
1:B:93:SER:HA	1:B:96:ASP:OD1	2.05	0.56
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.88	0.56
1:B:544:LEU:HD12	1:B:576:ALA:O	2.06	0.56
1:B:272:ASN:HD22	1:B:273:THR:N	2.04	0.56
1:B:662:TYR:CE2	9:B:1:DFP:H3'3	2.41	0.56
1:A:289:ALA:CB	1:A:290:PRO:CA	2.82	0.55
1:B:429:ARG:HD3	11:B:901:HOH:O	2.06	0.55
1:B:197:GLY:C	1:B:213:ALA:HB3	2.26	0.55
1:A:218:PRO:HB2	1:A:308:GLN:HE22	1.71	0.55
1:A:651:ILE:HG23	1:A:701:LEU:HD13	1.87	0.55
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.88	0.55
1:B:422:TYR:CZ	1:B:423:LYS:HD3	2.41	0.55
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.88	0.55
1:B:193:ILE:O	1:B:194:ILE:HD13	2.07	0.55
1:B:293:MET:HG2	1:B:315:TRP:HB3	1.88	0.55
1:A:597:ARG:HD3	1:A:682:HIS:CE1	2.42	0.55
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.89	0.55
1:B:289:ALA:CB	1:B:290:PRO:CA	2.83	0.55
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.42	0.55
1:A:276:LEU:H	1:A:276:LEU:HD23	1.72	0.55
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.88	0.55
1:A:221:THR:HB	11:A:1133:HOH:O	2.07	0.54
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.43	0.54
1:B:308:GLN:HB2	11:B:977:HOH:O	2.07	0.54
1:B:219:ASN:HB3	1:B:308:GLN:OE1	2.07	0.54
1:A:341:VAL:HG22	1:A:342:ALA:N	2.22	0.54
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.08	0.54
1:B:689:MET:CE	1:B:719:ILE:HG12	2.37	0.54
1:B:703:ILE:HA	1:B:733:MET:O	2.08	0.54
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.06	0.54
1:A:47:ASP:HA	1:A:52:THR:HG23	1.90	0.54
1:A:325:MET:HE1	1:A:327:ILE:HD11	1.89	0.54
1:A:736:THR:HG21	1:B:717:ALA:O	2.08	0.54
1:B:703:ILE:HG12	1:B:733:MET:HB3	1.89	0.54
5:F:2:NDG:O7	5:F:2:NDG:H3	2.08	0.54
1:A:341:VAL:O	1:A:342:ALA:HB3	2.07	0.53
1:B:453:ARG:HG3	1:B:476:GLY:HA3	1.88	0.53
1:B:118:TYR:CD2	1:B:119:ASN:ND2	2.76	0.53
1:B:471:ARG:NE	11:B:805:HOH:O	2.41	0.53
1:B:745:SER:O	1:B:749:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:NAG:H4	2:C:2:NDG:H3	1.89	0.53
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.91	0.53
1:A:40:ARG:HB3	1:A:506:ASN:O	2.08	0.53
1:B:44:THR:HB	11:B:843:HOH:O	2.07	0.53
1:B:258:LYS:NZ	1:B:712:HIS:HD2	2.07	0.53
1:A:290:PRO:HD3	1:A:315:TRP:CD1	2.43	0.53
1:A:319:ILE:O	1:A:321:ASN:N	2.36	0.53
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.44	0.53
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.44	0.53
1:A:285:ILE:HG12	1:A:335:GLY:O	2.09	0.52
1:A:356:ARG:HD3	1:A:551:CYS:SG	2.49	0.52
1:B:77:LEU:HA	1:B:89:PHE:H	1.75	0.52
1:B:542:LEU:HD12	1:B:574:ILE:O	2.09	0.52
8:M:1:NAG:C6	8:M:2:NDG:HA	2.22	0.52
1:A:693:GLU:OE1	1:A:696:LYS:HE2	2.09	0.52
1:B:219:ASN:HB2	1:B:308:GLN:CD	2.29	0.52
1:B:433:LYS:CB	1:B:445:LEU:HD21	2.39	0.52
1:B:765:LEU:HA	1:B:766:PRO:OXT	2.09	0.52
1:B:599:GLY:H	1:B:602:GLU:CD	2.13	0.52
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.44	0.52
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.44	0.52
1:A:736:THR:HG23	11:B:848:HOH:O	2.08	0.52
1:A:579:ASP:HB3	1:A:583:SER:OG	2.10	0.52
1:A:658:ARG:HD2	1:A:661:TYR:CE1	2.44	0.52
1:B:318:ARG:HD3	1:B:668:GLU:OE1	2.10	0.52
1:A:65:ASP:HB3	1:A:66:HIS:CE1	2.45	0.52
1:A:734:TRP:NE1	1:A:736:THR:HG22	2.25	0.52
1:A:147:ARG:HD2	3:D:1:NAG:H83	1.92	0.51
1:B:272:ASN:HD22	1:B:274:ASP:H	1.58	0.51
1:A:405:ILE:HG13	1:A:429:ARG:CD	2.40	0.51
1:A:322:TYR:OH	1:A:346:ILE:HD13	2.10	0.51
1:A:195:TYR:HB3	1:A:198:ILE:HG13	1.93	0.51
1:A:595:ASN:OD1	1:A:596:ARG:HG3	2.10	0.51
3:D:2:NAG:O7	3:D:2:NAG:H3	2.09	0.51
1:B:377:ASN:HD21	1:B:381:TYR:H	1.58	0.51
1:B:115:LEU:HD11	1:B:132:TYR:HB3	1.93	0.51
1:B:289:ALA:HA	1:B:294:LEU:HG	1.93	0.51
1:B:358:ARG:HB3	1:B:358:ARG:NH1	2.06	0.51
8:M:1:NAG:H4	8:M:2:NDG:H3	1.93	0.51
11:A:1076:HOH:O	4:E:1:NAG:H82	2.10	0.51
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:HB3	11:A:1137:HOH:O	2.11	0.50
1:A:542:LEU:HD23	1:A:542:LEU:C	2.32	0.50
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.76	0.50
1:A:272:ASN:HD22	1:A:273:THR:N	2.09	0.50
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.94	0.50
1:A:546:VAL:HG22	1:A:547:TYR:N	2.26	0.50
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.12	0.50
1:B:46:THR:HG23	11:B:999:HOH:O	2.10	0.50
1:B:535:ASP:OD1	1:B:537:SER:HB2	2.11	0.50
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.47	0.50
1:B:86:SER:O	1:B:87:SER:HB3	2.11	0.50
1:B:760:LYS:HE3	1:B:766:PRO:HD3	1.93	0.50
1:B:72:GLN:NE2	1:B:77:LEU:HD21	2.10	0.50
1:B:118:TYR:CE2	1:B:119:ASN:ND2	2.80	0.49
1:B:504:LEU:HD22	1:B:509:MET:CE	2.42	0.49
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.94	0.49
1:B:250:LYS:HB2	1:B:250:LYS:NZ	2.26	0.49
1:B:312:SER:O	1:B:313:LEU:HD12	2.12	0.49
1:B:392:LYS:HG2	11:B:861:HOH:O	2.12	0.49
1:A:452:GLU:HB2	11:A:859:HOH:O	2.11	0.49
1:A:91:GLU:C	1:A:93:SER:N	2.66	0.49
1:A:602:GLU:HG2	1:A:603:VAL:N	2.28	0.49
1:B:76:ILE:HG23	1:B:76:ILE:O	2.12	0.49
1:A:242:SER:OG	1:A:243:ASP:N	2.44	0.49
1:B:184:ARG:NH1	1:B:187:TRP:HA	2.27	0.49
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.12	0.49
1:B:520:ASN:O	1:B:522:THR:HG22	2.13	0.49
1:A:244:GLU:CD	1:B:689:MET:HG3	2.32	0.48
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.34	0.48
1:A:193:ILE:HG22	1:A:194:ILE:CD1	2.42	0.48
1:B:489:LYS:O	1:B:489:LYS:HG3	2.14	0.48
1:A:262:VAL:HG23	11:A:939:HOH:O	2.12	0.48
1:A:693:GLU:CA	1:A:726:VAL:HG11	2.39	0.48
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.48	0.48
1:B:184:ARG:HD2	1:B:187:TRP:NE1	2.28	0.48
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.49	0.48
11:B:913:HOH:O	6:I:1:NAG:H83	2.13	0.48
1:A:669:ARG:NH2	11:A:839:HOH:O	2.43	0.48
1:B:195:TYR:O	1:B:227:GLN:HA	2.13	0.48
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.49	0.48
1:B:487:ASN:O	1:B:488:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.95	0.48
1:A:186:THR:HG21	1:A:196:ASN:CB	2.43	0.48
1:B:405:ILE:HG12	1:B:419:SER:HA	1.96	0.48
1:B:546:VAL:HG22	1:B:547:TYR:N	2.28	0.48
1:B:290:PRO:HG3	1:B:326:ASP:OD2	2.13	0.48
1:A:40:ARG:N	11:A:1152:HOH:O	2.46	0.47
1:B:272:ASN:ND2	1:B:272:ASN:C	2.65	0.47
1:B:279:VAL:O	1:B:280:THR:HG22	2.14	0.47
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.29	0.47
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.57	0.47
1:B:377:ASN:C	1:B:377:ASN:ND2	2.63	0.47
1:B:600:THR:OG1	1:B:601:PHE:N	2.43	0.47
1:B:696:LYS:HA	11:B:958:HOH:O	2.14	0.47
1:A:405:ILE:N	1:A:418:ILE:O	2.46	0.47
1:B:208:PHE:O	1:B:209:SER:C	2.52	0.47
1:A:65:ASP:HB2	1:A:464:GLU:HG2	1.96	0.47
1:A:170:ASN:N	1:A:170:ASN:HD22	2.12	0.47
1:B:450:ASN:N	11:B:838:HOH:O	2.35	0.47
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.49	0.47
1:A:109:PRO:HG2	1:A:161:GLY:O	2.14	0.47
1:A:184:ARG:HH12	1:A:187:TRP:HA	1.76	0.47
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.96	0.47
1:A:325:MET:HE3	1:A:364:PHE:HZ	1.80	0.47
1:B:184:ARG:HB3	1:B:187:TRP:CZ2	2.50	0.47
1:A:279:VAL:HG12	1:A:279:VAL:O	2.15	0.47
1:B:688:VAL:HB	1:B:689:MET:CE	2.45	0.47
1:A:633:GLY:HA3	1:A:655:PRO:HB3	1.96	0.47
1:B:170:ASN:ND2	1:B:170:ASN:N	2.57	0.47
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.50	0.47
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.48	0.47
1:A:596:ARG:HA	1:A:670:TYR:O	2.15	0.47
1:A:39:SER:O	1:A:508:GLN:NE2	2.48	0.46
1:A:377:ASN:HB2	1:A:381:TYR:H	1.80	0.46
1:B:521:GLU:OE1	1:B:521:GLU:HA	2.16	0.46
8:M:1:NAG:H4	8:M:2:NDG:N2	2.25	0.46
1:A:91:GLU:HB3	1:A:93:SER:OG	2.15	0.46
1:B:328:CYS:HA	1:B:338:ASN:O	2.15	0.46
1:A:341:VAL:C	1:A:343:ARG:N	2.68	0.46
1:A:704:HIS:HD2	1:A:716:SER:OG	1.98	0.46
1:B:740:HIS:CD2	9:B:1:DFP:H21	2.51	0.46
1:B:77:LEU:CB	1:B:88:VAL:HA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HG23	1:A:415:LEU:HD11	1.97	0.46
1:B:512:LYS:HE3	1:B:527:GLN:CD	2.36	0.46
1:B:742:ILE:O	1:B:742:ILE:HG22	2.16	0.46
1:A:88:VAL:HG11	1:A:91:GLU:OE2	2.16	0.46
1:A:272:ASN:HD22	1:A:272:ASN:C	2.17	0.46
1:A:597:ARG:HG3	1:A:600:THR:CG2	2.44	0.46
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.50	0.46
1:B:54:ARG:HG3	11:B:1071:HOH:O	2.16	0.46
1:B:259:ALA:HB3	1:B:660:GLU:HA	1.98	0.46
1:B:532:PRO:HD3	1:B:569:SER:HA	1.97	0.46
1:B:598:LEU:HA	1:B:602:GLU:OE2	2.15	0.46
1:B:385:CYS:HB3	1:B:396:PHE:HA	1.97	0.46
1:A:388:GLN:O	1:A:390:ASP:N	2.49	0.46
1:A:718:GLN:NE2	1:A:718:GLN:HA	2.30	0.46
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.46	0.46
1:B:293:MET:HG3	1:B:298:HIS:CB	2.46	0.46
3:D:1:NAG:C4	3:D:2:NAG:N2	2.76	0.46
1:B:319:ILE:O	1:B:321:ASN:N	2.40	0.46
3:D:1:NAG:H2	3:D:2:NAG:H83	1.98	0.46
1:A:316:LEU:HD21	1:A:320:GLN:HG2	1.98	0.45
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.98	0.45
1:B:87:SER:HB3	6:I:1:NAG:H81	1.99	0.45
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.46	0.45
1:A:422:TYR:C	1:A:424:GLY:H	2.19	0.45
1:B:331:ASP:OD1	1:B:333:SER:HB3	2.16	0.45
1:B:154:TRP:O	1:B:166:TYR:HA	2.17	0.45
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.80	0.45
1:B:382:ARG:NH2	11:B:975:HOH:O	2.49	0.45
1:B:584:GLY:O	1:B:585:TYR:HB2	2.17	0.45
1:A:293:MET:HE1	1:A:317:ARG:HG3	1.96	0.45
1:B:77:LEU:HD23	1:B:77:LEU:N	2.18	0.45
1:B:74:ASN:HB3	1:B:92:ASN:HD22	1.82	0.45
1:B:112:GLN:HB3	1:B:138:ASN:HD21	1.82	0.45
1:B:399:LYS:HA	11:B:965:HOH:O	2.15	0.45
1:B:459:VAL:HG22	1:B:460:SER:N	2.31	0.45
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.83	0.45
1:A:542:LEU:HD23	1:A:543:LEU:N	2.31	0.45
1:B:630:SER:HA	1:B:654:ALA:O	2.16	0.45
1:B:751:ILE:HG23	1:B:752:TYR:N	2.31	0.45
1:A:630:SER:HA	1:A:654:ALA:O	2.17	0.45
1:B:399:LYS:HB3	1:B:400:GLY:H	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:CG1	1:A:487:ASN:N	2.79	0.45
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.98	0.45
1:B:658:ARG:HD3	1:B:660:GLU:HB2	1.98	0.45
1:A:554:LYS:HG3	11:A:916:HOH:O	2.16	0.45
1:B:518:ILE:O	1:B:519:LEU:HD23	2.16	0.45
1:A:276:LEU:H	1:A:276:LEU:CD2	2.29	0.44
1:A:386:TYR:O	1:A:394:CYS:HB2	2.17	0.44
1:A:536:LYS:HB3	1:A:536:LYS:HZ3	1.81	0.44
1:B:268:PHE:CD2	1:B:313:LEU:HD21	2.51	0.44
1:B:356:ARG:HG2	1:B:551:CYS:SG	2.57	0.44
1:B:413:ASP:O	1:B:436:LEU:HD13	2.17	0.44
1:B:763:PHE:O	1:B:764:SER:HB2	2.17	0.44
1:A:266:VAL:HG22	1:A:267:LYS:N	2.32	0.44
1:A:701:LEU:HD22	1:A:703:ILE:HG13	2.00	0.44
1:B:215:TRP:CE2	1:B:303:VAL:HG13	2.53	0.44
1:A:270:VAL:HG11	1:A:337:TRP:CZ2	2.52	0.44
1:A:301:CYS:SG	1:A:359:PRO:HG2	2.56	0.44
1:B:272:ASN:ND2	1:B:274:ASP:N	2.63	0.44
1:B:369:ASN:HA	1:B:389:ILE:HD13	1.99	0.44
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.53	0.44
1:A:41:LYS:HG2	1:A:42:THR:N	2.32	0.44
1:B:718:GLN:HA	1:B:718:GLN:NE2	2.31	0.44
1:A:314:GLN:NE2	1:A:359:PRO:HB2	2.32	0.44
1:A:689:MET:HB3	1:A:722:ALA:HB2	2.00	0.44
1:A:734:TRP:CD1	1:A:736:THR:HG22	2.53	0.44
1:B:317:ARG:HD2	1:B:322:TYR:HB3	1.99	0.44
1:B:399:LYS:HB2	1:B:402:TRP:HZ2	1.83	0.44
1:B:669:ARG:NH2	11:B:785:HOH:O	2.32	0.44
1:B:741:GLY:C	1:B:743:ALA:N	2.68	0.44
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.44
1:A:313:LEU:O	1:A:325:MET:HA	2.18	0.44
1:A:361:GLU:HG3	11:A:987:HOH:O	2.18	0.44
1:A:536:LYS:NZ	1:A:536:LYS:CB	2.80	0.44
1:B:346:ILE:HD12	1:B:346:ILE:N	2.33	0.44
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.99	0.43
1:A:321:ASN:OD1	1:A:349:SER:O	2.35	0.43
1:A:340:LEU:O	1:A:343:ARG:HB3	2.18	0.43
1:A:520:ASN:O	1:A:521:GLU:HB2	2.19	0.43
1:A:689:MET:HG3	1:B:244:GLU:CD	2.38	0.43
1:B:49:LEU:HD22	1:B:749:GLN:HA	2.00	0.43
1:B:61:ARG:HG3	11:B:827:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:HD3	1:B:216:TRP:HB2	2.00	0.43
1:B:219:ASN:HB2	1:B:308:GLN:OE1	2.18	0.43
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.16	0.43
1:A:91:GLU:O	1:A:93:SER:N	2.47	0.43
1:A:551:CYS:HA	1:A:584:GLY:HA3	2.00	0.43
1:B:156:THR:OG1	1:B:214:LEU:HD11	2.18	0.43
1:B:472:CYS:O	1:B:478:PRO:HA	2.18	0.43
1:A:666:TYR:O	1:A:669:ARG:HB3	2.18	0.43
1:B:74:ASN:ND2	1:B:92:ASN:HD22	2.10	0.43
1:B:77:LEU:HB2	1:B:88:VAL:HA	1.99	0.43
1:B:418:ILE:CG2	1:B:429:ARG:HG2	2.48	0.43
1:B:613:PHE:O	1:B:616:MET:HB2	2.18	0.43
1:A:662:TYR:CE2	9:A:1:DFP:H3'3	2.54	0.43
1:B:651:ILE:HD13	1:B:755:MET:HG2	1.99	0.43
1:A:149:PRO:HG3	11:A:919:HOH:O	2.18	0.43
1:B:708:ASP:OD2	1:B:740:HIS:HA	2.18	0.43
1:B:455:GLN:HB2	1:B:475:PRO:HD3	2.00	0.43
1:B:546:VAL:CG2	1:B:547:TYR:N	2.81	0.43
1:A:135:TYR:CE2	1:A:137:LEU:HD23	2.53	0.43
1:A:290:PRO:HG3	1:A:326:ASP:OD2	2.19	0.43
1:A:325:MET:HE2	1:A:327:ILE:CG1	2.49	0.43
1:A:472:CYS:O	1:A:478:PRO:HA	2.18	0.43
1:B:528:MET:HG3	1:B:576:ALA:CB	2.46	0.43
1:A:689:MET:HB3	1:A:722:ALA:CB	2.49	0.43
1:B:129:THR:HG22	11:B:964:HOH:O	2.18	0.43
1:B:350:THR:HA	8:M:1:NAG:O7	2.18	0.43
1:A:95:PHE:HB3	1:A:98:PHE:HB2	2.00	0.43
1:B:40:ARG:CZ	1:B:508:GLN:HG2	2.49	0.43
3:D:1:NAG:O3	3:D:2:NAG:C7	2.66	0.43
1:A:208:PHE:O	1:A:209:SER:C	2.57	0.43
1:A:504:LEU:O	1:A:507:VAL:HG13	2.17	0.43
1:B:318:ARG:NH1	1:B:668:GLU:OE2	2.51	0.43
1:B:377:ASN:ND2	1:B:379:GLU:H	2.17	0.43
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.18	0.42
1:A:374:ILE:CD1	1:A:406:GLY:HA2	2.48	0.42
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.49	0.42
1:A:248:TYR:CE2	1:B:234:PRO:HB2	2.54	0.42
1:B:175:LYS:HG2	1:B:182:SER:HB3	2.01	0.42
1:A:106:SER:HB3	1:A:115:LEU:HB3	2.02	0.42
1:A:405:ILE:HG13	1:A:429:ARG:HD2	2.01	0.42
1:A:658:ARG:HG3	1:A:658:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TRP:HB3	11:A:793:HOH:O	2.18	0.42
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.84	0.42
1:B:377:ASN:ND2	1:B:379:GLU:N	2.67	0.42
1:A:546:VAL:CG2	1:A:547:TYR:N	2.82	0.42
1:B:175:LYS:HE2	1:B:180:LEU:O	2.20	0.42
1:B:270:VAL:HG11	1:B:337:TRP:CE2	2.53	0.42
1:B:62:TRP:CD2	1:B:462:SER:HA	2.55	0.42
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.88	0.42
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.02	0.42
1:B:367:ASP:OD1	1:B:369:ASN:N	2.50	0.42
1:A:310:ARG:NH1	1:A:329:ASP:OD2	2.53	0.42
1:A:446:SER:HB2	1:A:457:TYR:CD1	2.55	0.42
1:B:420:ASN:HB2	1:B:426:PRO:HA	2.01	0.42
1:B:509:MET:HG3	1:B:510:PRO:HD2	2.01	0.42
1:B:733:MET:CE	11:B:897:HOH:O	2.67	0.42
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.50	0.42
1:A:254:VAL:HA	1:A:255:PRO:HD3	1.93	0.42
1:B:464:GLU:O	1:B:465:ALA:HB3	2.19	0.42
1:B:40:ARG:HA	1:B:506:ASN:O	2.20	0.41
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.19	0.41
1:B:93:SER:O	1:B:95:PHE:N	2.53	0.41
1:B:113:PHE:CE2	1:B:178:PRO:HG2	2.55	0.41
1:B:120:TYR:OH	1:B:122:LYS:HB2	2.19	0.41
1:B:463:LYS:HE3	1:B:463:LYS:HB3	1.85	0.41
1:B:482:LEU:HB2	1:B:494:LEU:HD11	2.01	0.41
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.01	0.41
1:A:513:LYS:HE3	1:A:513:LYS:HB2	1.94	0.41
1:B:66:HIS:ND1	1:B:66:HIS:N	2.68	0.41
1:B:125:ARG:HH21	1:B:205:GLU:CD	2.22	0.41
1:A:597:ARG:HD3	1:A:682:HIS:ND1	2.34	0.41
1:A:127:SER:O	1:A:128:TYR:HB3	2.20	0.41
1:A:379:GLU:O	1:A:379:GLU:CG	2.69	0.41
1:B:102:ILE:HD12	1:B:116:LEU:HB3	2.03	0.41
1:B:279:VAL:O	1:B:280:THR:CG2	2.68	0.41
1:B:400:GLY:O	1:B:402:TRP:N	2.53	0.41
8:M:1:NAG:C4	8:M:2:NDG:N2	2.83	0.41
1:B:156:THR:HG22	1:B:157:TRP:O	2.20	0.41
1:B:704:HIS:NE2	1:B:711:VAL:O	2.50	0.41
1:A:77:LEU:CD2	1:A:88:VAL:HA	2.51	0.41
1:A:161:GLY:HA3	11:A:998:HOH:O	2.19	0.41
1:A:293:MET:HE2	1:A:317:ARG:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:C	1:A:390:ASP:H	2.24	0.41
1:A:655:PRO:O	1:A:711:VAL:HG11	2.21	0.41
1:A:735:TYR:OH	1:A:751:ILE:HA	2.21	0.41
1:B:104:ASP:OD1	1:B:105:TYR:O	2.39	0.41
1:B:136:ASP:OD1	1:B:138:ASN:N	2.54	0.41
1:B:199:THR:HA	1:B:228:PHE:CE2	2.56	0.41
1:B:293:MET:HG2	1:B:315:TRP:CB	2.51	0.41
1:A:156:THR:HG21	1:A:214:LEU:CD1	2.51	0.41
1:A:276:LEU:CD2	1:A:276:LEU:N	2.84	0.41
1:A:378:GLU:HB3	11:A:1141:HOH:O	2.21	0.41
1:A:459:VAL:HG22	1:A:460:SER:N	2.36	0.41
1:A:598:LEU:O	1:A:682:HIS:NE2	2.45	0.41
1:B:94:THR:HG22	1:B:94:THR:O	2.21	0.41
1:B:139:LYS:HE2	1:B:139:LYS:HB3	1.87	0.41
1:A:66:HIS:ND1	1:A:66:HIS:N	2.69	0.40
1:B:121:VAL:HB	1:B:129:THR:CG2	2.43	0.40
1:B:502:LYS:O	1:B:505:GLN:HG2	2.20	0.40
1:B:644:SER:OG	1:B:645:GLY:N	2.55	0.40
1:A:603:VAL:HG22	1:A:604:GLU:N	2.36	0.40
1:A:640:LEU:HD11	1:A:650:GLY:HA3	2.02	0.40
1:B:598:LEU:HD22	1:B:671:MET:HG2	2.04	0.40
1:B:692:ALA:O	1:B:695:PHE:HB2	2.21	0.40
8:M:1:NAG:C4	8:M:2:NDG:HA	2.30	0.40
1:A:246:LEU:HD22	1:A:248:TYR:O	2.21	0.40
1:B:154:TRP:HE1	1:B:156:THR:HG1	1.66	0.40
1:B:320:GLN:NE2	1:B:669:ARG:HB2	2.37	0.40
1:B:413:ASP:HB3	1:B:414:TYR:HD1	1.83	0.40
1:A:170:ASN:O	1:A:196:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 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	724/728 (100%)	656 (91%)	60 (8%)	8 (1%)	12	30
1	B	726/728 (100%)	641 (88%)	74 (10%)	11 (2%)	8	22
All	All	1450/1456 (100%)	1297 (89%)	134 (9%)	19 (1%)	10	26

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	289	ALA
1	B	320	GLN
1	B	399	LYS
1	B	401	THR
1	A	289	ALA
1	A	389	ILE
1	A	520	ASN
1	B	86	SER
1	B	280	THR
1	B	360	SER
1	B	402	TRP
1	B	423	LYS
1	A	72	GLN
1	A	73	GLU
1	A	332	GLU
1	B	94	THR
1	A	491	LEU
1	B	73	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/653 (100%)	606 (93%)	45 (7%)	13	31
1	B	653/653 (100%)	610 (93%)	43 (7%)	14	33
All	All	1304/1306 (100%)	1216 (93%)	88 (7%)	13	33

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

Mol	Chain	Res	Type
1	A	41	LYS
1	A	51	ASN
1	A	66	HIS
1	A	90	LEU
1	A	91	GLU
1	A	104	ASP
1	A	110	ASP
1	A	125	ARG
1	A	141	GLN
1	A	184	ARG
1	A	207	VAL
1	A	230	ASP
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	272	ASN
1	A	275	SER
1	A	276	LEU
1	A	288	THR
1	A	293	MET
1	A	303	VAL
1	A	332	GLU
1	A	373	LYS
1	A	382	ARG
1	A	385	CYS
1	A	415	LEU
1	A	423	LYS
1	A	448	GLU
1	A	458	SER
1	A	507	VAL
1	A	514	LEU
1	A	536	LYS
1	A	537	SER
1	A	543	LEU
1	A	561	LEU
1	A	566	TYR
1	A	581	ARG
1	A	602	GLU
1	A	603	VAL
1	A	658	ARG
1	A	689	MET
1	A	701	LEU

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	736	THR
1	A	761	GLN
1	B	46	THR
1	B	61	ARG
1	B	66	HIS
1	B	73	GLU
1	B	74	ASN
1	B	75	ASN
1	B	92	ASN
1	B	170	ASN
1	B	184	ARG
1	B	223	LEU
1	B	246	LEU
1	B	253	ARG
1	B	272	ASN
1	B	303	VAL
1	B	318	ARG
1	B	329	ASP
1	B	358	ARG
1	B	366	LEU
1	B	377	ASN
1	B	379	GLU
1	B	423	LYS
1	B	429	ARG
1	B	445	LEU
1	B	448	GLU
1	B	489	LYS
1	B	507	VAL
1	B	514	LEU
1	B	518	ILE
1	B	522	THR
1	B	528	MET
1	B	543	LEU
1	B	597	ARG
1	B	602	GLU
1	B	644	SER
1	B	673	LEU
1	B	679	ASN
1	B	689	MET
1	B	701	LEU
1	B	702	LEU

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Mol	Chain	Res	Type
1	B	710	ASN
1	B	728	VAL
1	B	755	MET
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	119	ASN
1	A	151	ASN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	369	ASN
1	A	435	GLN
1	A	483	HIS
1	A	505	GLN
1	A	533	HIS
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	B	51	ASN
1	B	72	GLN
1	B	74	ASN
1	B	75	ASN
1	B	112	GLN
1	B	119	ASN
1	B	126	HIS
1	B	138	ASN
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	263	ASN
1	B	272	ASN
1	B	314	GLN
1	B	344	GLN
1	B	345	HIS

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Mol	Chain	Res	Type
1	B	369	ASN
1	B	377	ASN
1	B	388	GLN
1	B	435	GLN
1	B	487	ASN
1	B	505	GLN
1	B	520	ASN
1	B	572	ASN
1	B	595	ASN
1	B	679	ASN
1	B	697	GLN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	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 ⓘ

27 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	2,1	14,14,15	0.69	0	17,19,21	1.29	2 (11%)
2	NDG	C	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FUC	C	3	2	10,10,11	0.49	0	14,14,16	0.43	0
3	NAG	D	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	0.99	1 (5%)
3	NAG	D	2	3	14,14,15	0.72	1 (7%)	17,19,21	0.70	0
3	FUC	D	3	3	10,10,11	0.51	0	14,14,16	0.34	0
4	NAG	E	1	4,1	14,14,15	0.53	0	17,19,21	0.92	1 (5%)
4	NAG	E	2	4	14,14,15	0.48	0	17,19,21	0.70	0
5	NAG	F	1	5,1	14,14,15	0.60	0	17,19,21	1.06	2 (11%)
5	NDG	F	2	5	14,14,15	1.01	1 (7%)	17,19,21	0.90	0
5	MAN	F	3	5	11,11,12	0.66	0	15,15,17	0.49	0
4	NAG	G	1	4,1	14,14,15	0.48	0	17,19,21	0.63	0
4	NAG	G	2	4	14,14,15	0.53	0	17,19,21	0.62	0
4	NAG	H	1	4,1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
4	NAG	H	2	4	14,14,15	0.73	0	17,19,21	0.58	0
6	NAG	I	1	6,1	14,14,15	0.55	0	17,19,21	0.66	0
6	FUC	I	2	6	10,10,11	0.52	0	14,14,16	0.39	0
4	NAG	J	1	4,1	14,14,15	0.70	0	17,19,21	0.84	1 (5%)
4	NAG	J	2	4	14,14,15	0.51	0	17,19,21	0.77	0
7	NAG	K	1	7,1	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
7	NAG	K	2	7	14,14,15	0.47	0	17,19,21	0.84	1 (5%)
7	BMA	K	3	7	11,11,12	0.58	0	15,15,17	0.17	0
7	NAG	L	1	7,1	14,14,15	0.52	0	17,19,21	0.63	0
7	NAG	L	2	7	14,14,15	0.65	0	17,19,21	1.13	2 (11%)
7	BMA	L	3	7	11,11,12	0.43	0	15,15,17	0.33	0
8	NAG	M	1	8,1	14,14,15	0.61	0	17,19,21	0.97	1 (5%)
8	NDG	M	2	8	14,14,15	0.78	1 (7%)	17,19,21	0.80	1 (5%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NDG	C	2	2	-	1/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	1/6/23/26	0/1/1/1
5	NDG	F	2	5	-	1/6/23/26	0/1/1/1
5	MAN	F	3	5	-	2/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
6	NAG	I	1	6,1	-	2/6/23/26	0/1/1/1
6	FUC	I	2	6	-	-	0/1/1/1
4	NAG	J	1	4,1	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	NAG	L	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1
8	NAG	M	1	8,1	1/1/5/7	1/6/23/26	0/1/1/1
8	NDG	M	2	8	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NDG	C1-C2	3.12	1.56	1.52
8	M	2	NDG	C1-C2	2.30	1.55	1.52
3	D	2	NAG	C1-C2	2.07	1.55	1.52
3	D	1	NAG	C1-C2	2.04	1.55	1.52
2	C	2	NDG	C1-C2	2.04	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	3.36	115.95	111.02
5	F	1	NAG	C2-N2-C7	-3.03	118.84	122.90
7	K	1	NAG	C2-N2-C7	-2.58	119.44	122.90
8	M	1	NAG	C4-C3-C2	2.57	114.79	111.02
7	L	2	NAG	C2-N2-C7	-2.53	119.52	122.90
7	L	2	NAG	C4-C3-C2	-2.49	107.36	111.02
4	J	1	NAG	C2-N2-C7	-2.44	119.63	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NDG	C2-N2-C7	-2.29	119.83	122.90
8	M	2	NDG	C2-N2-C7	-2.20	119.96	122.90
4	H	1	NAG	C2-N2-C7	-2.19	119.97	122.90
4	E	1	NAG	C4-C3-C2	2.15	114.17	111.02
3	D	1	NAG	C2-N2-C7	-2.08	120.12	122.90
2	C	1	NAG	C3-C4-C5	2.07	113.98	110.23
7	K	2	NAG	C4-C3-C2	2.04	114.00	111.02
5	F	1	NAG	C4-C3-C2	-2.02	108.06	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	NAG	C1
4	J	1	NAG	C1
8	M	1	NAG	C1

All (25) torsion outliers are listed below:

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

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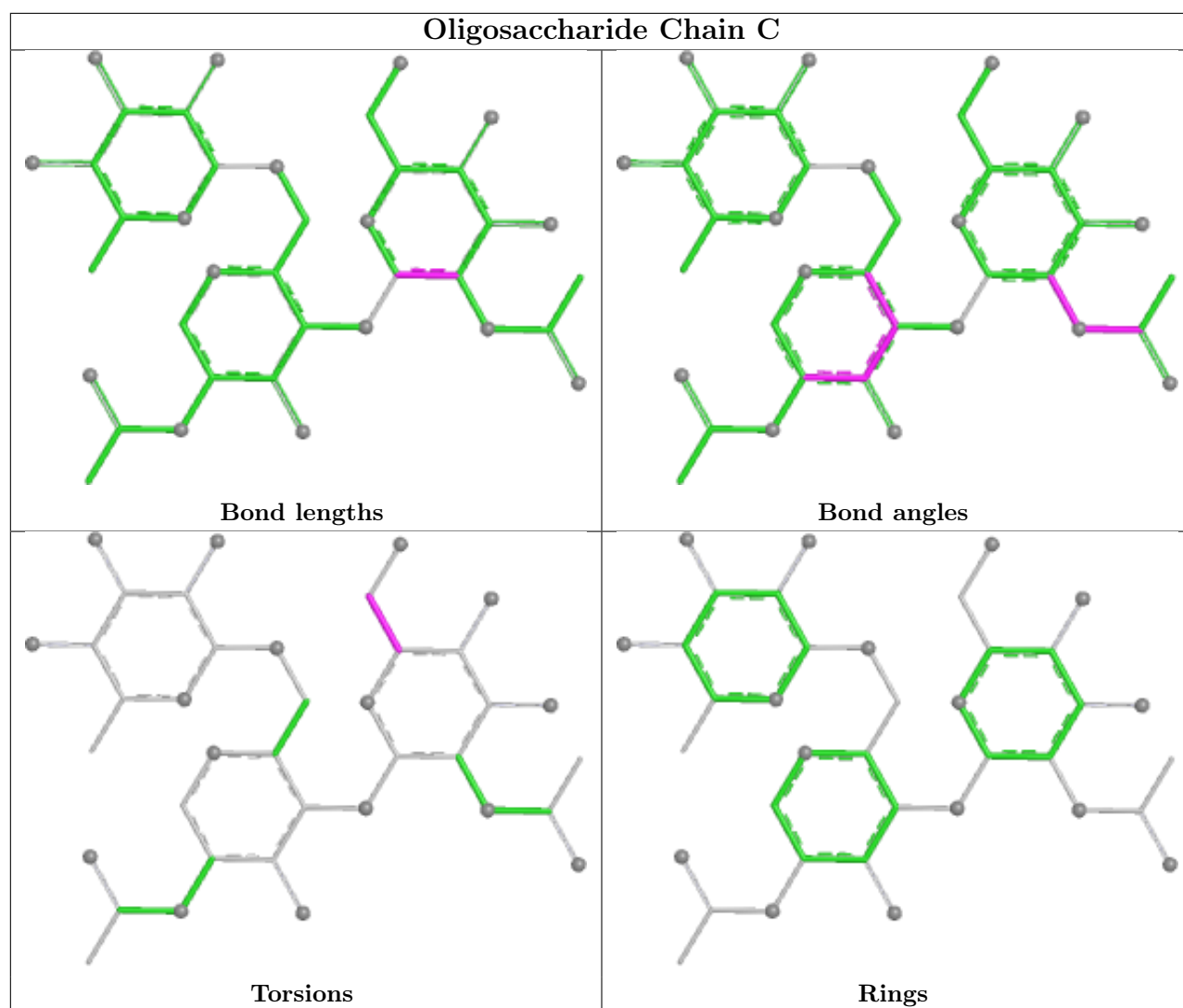
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6

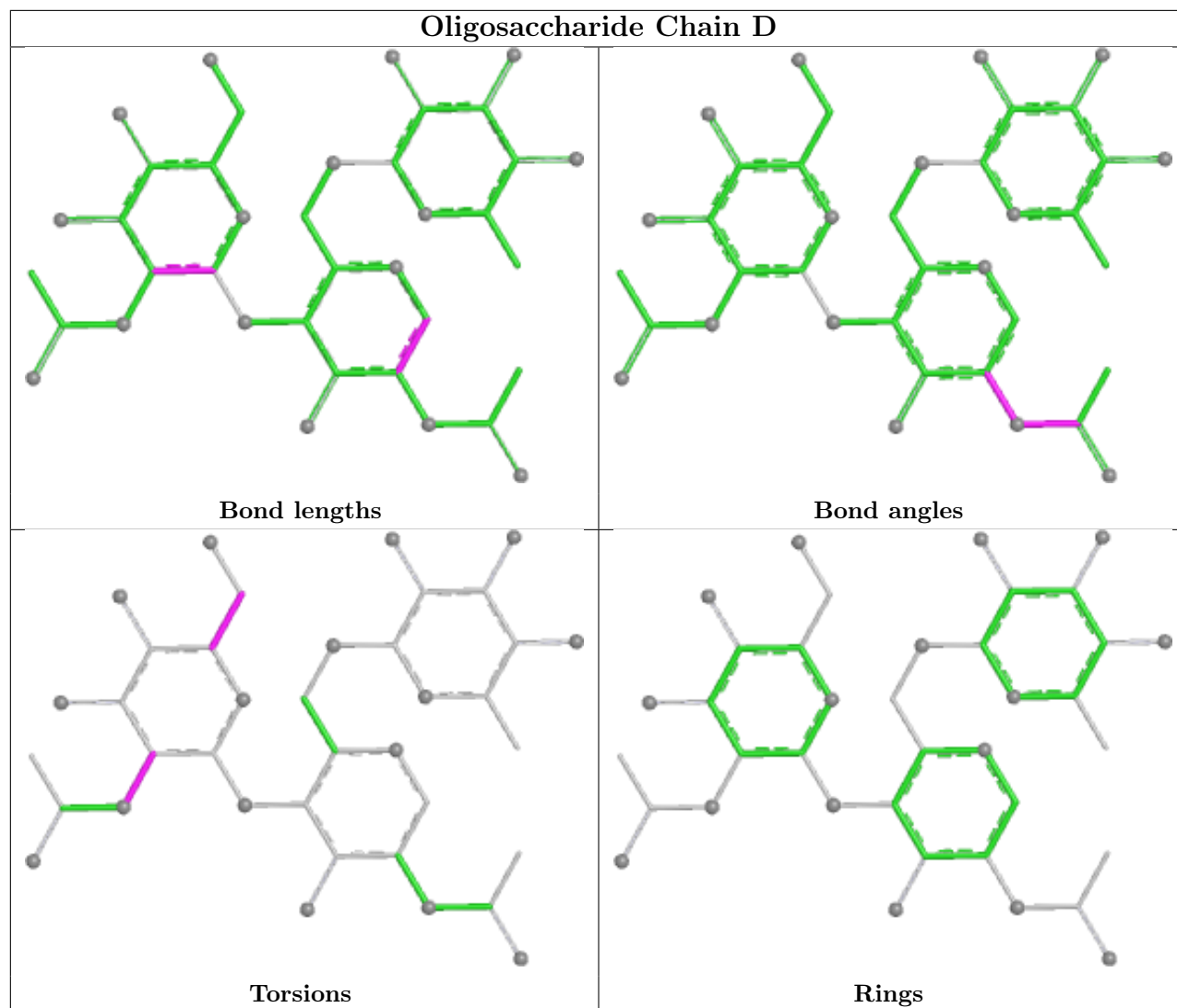
There are no ring outliers.

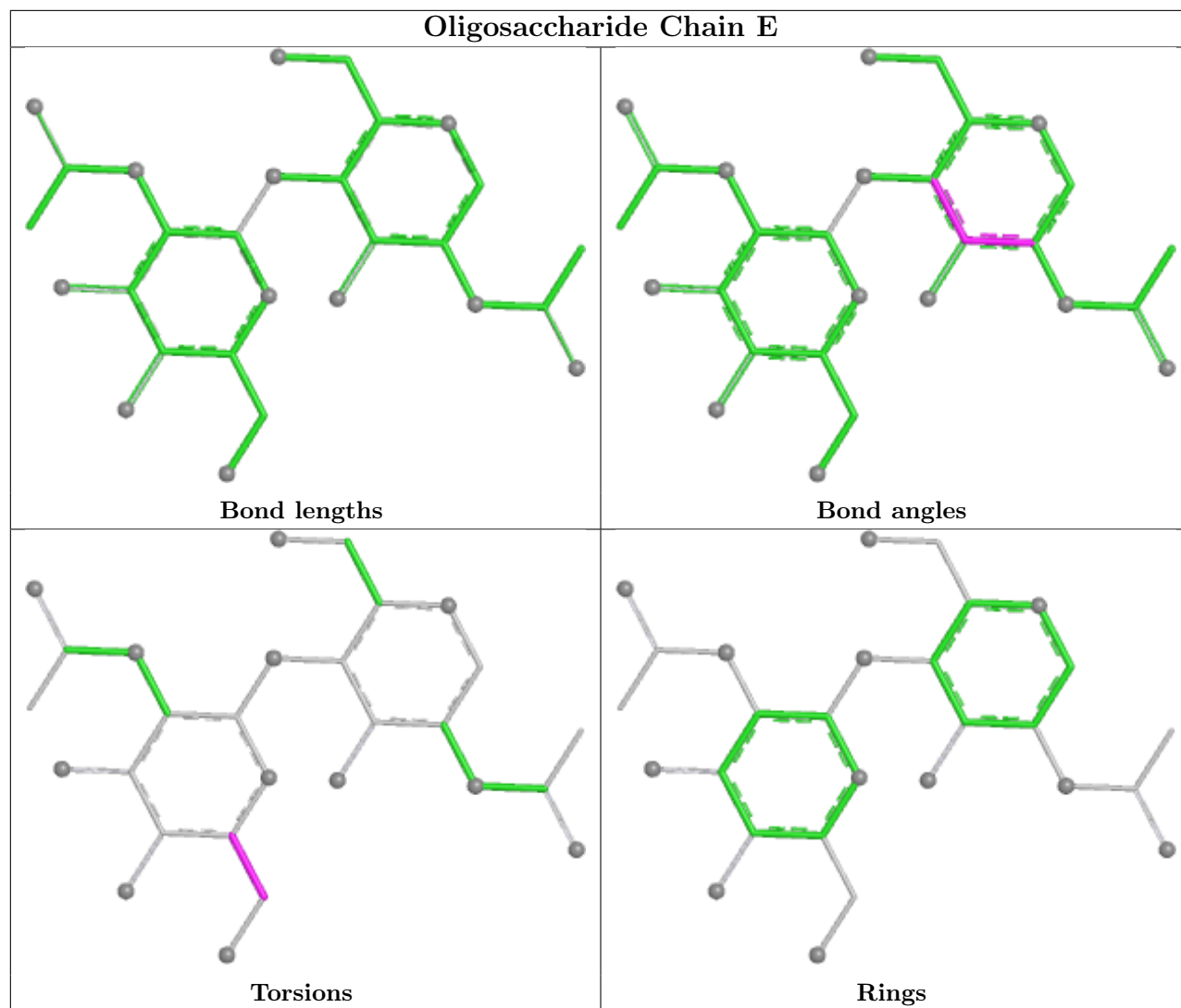
12 monomers are involved in 25 short contacts:

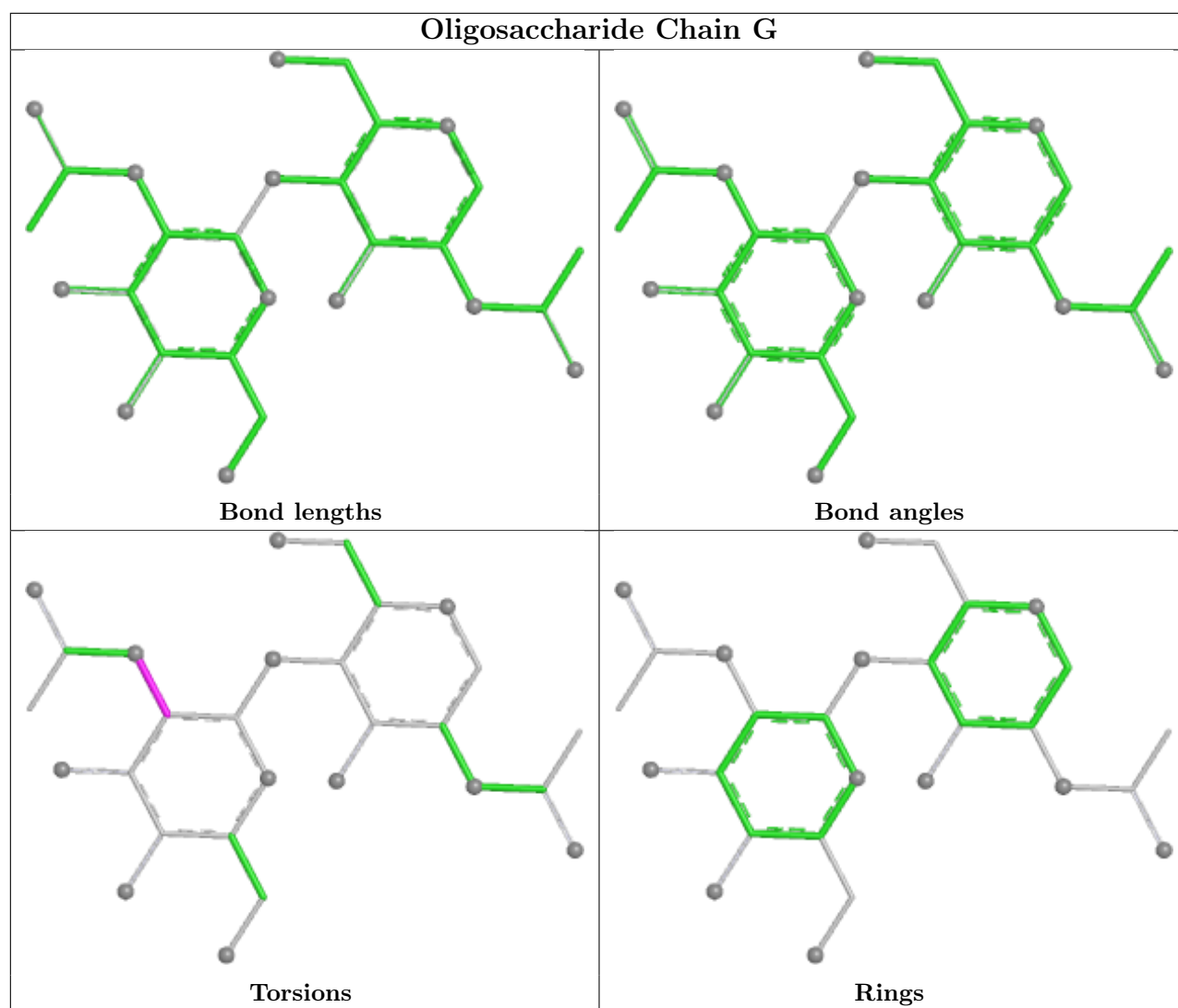
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NDG	1	0
2	C	1	NAG	1	0
4	J	1	NAG	2	0
3	D	2	NAG	5	0
5	F	3	MAN	2	0
4	E	1	NAG	1	0
3	D	1	NAG	5	0
8	M	2	NDG	8	0
6	I	1	NAG	2	0
5	F	1	NAG	1	0
8	M	1	NAG	9	0
5	F	2	NDG	2	0

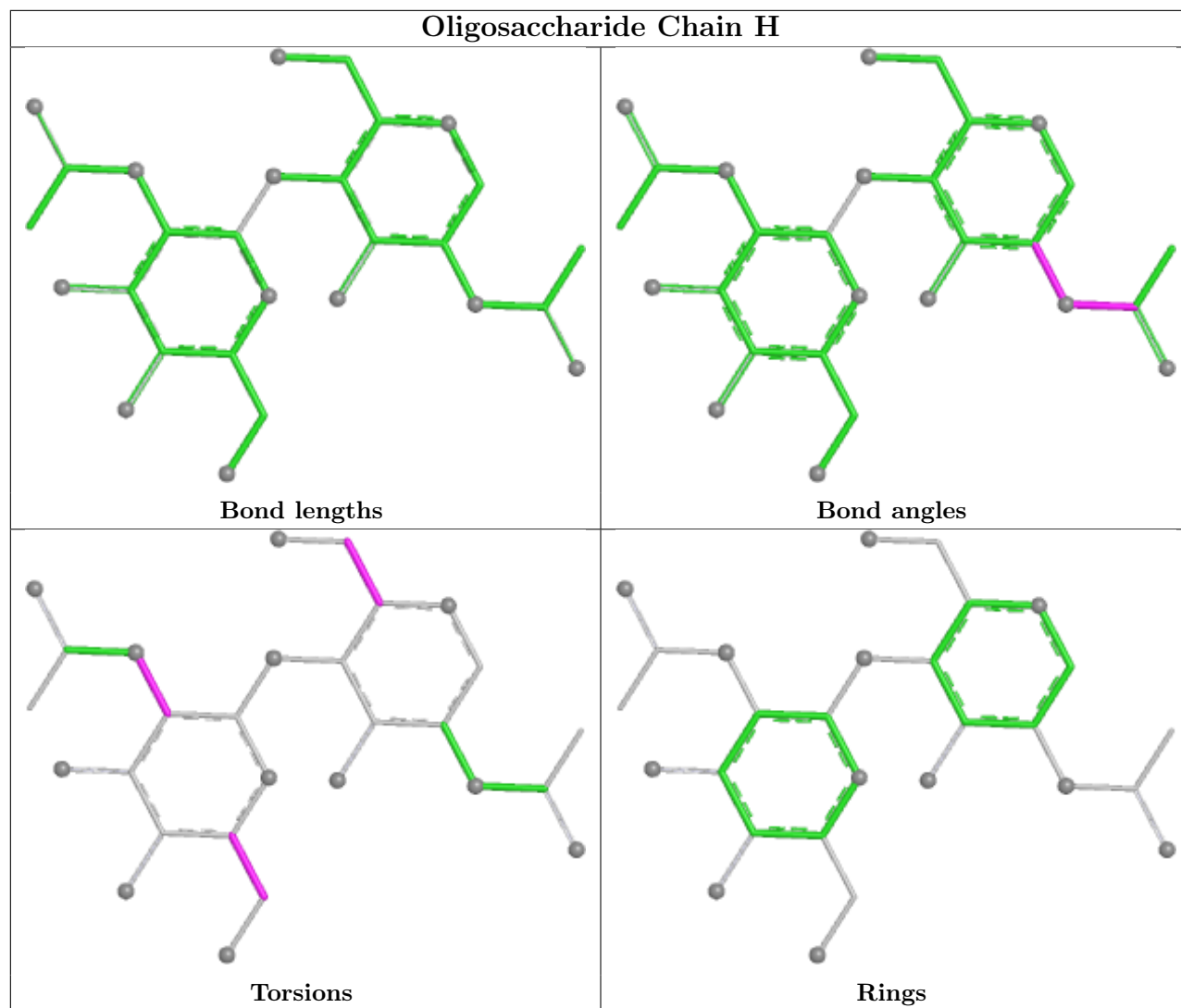
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



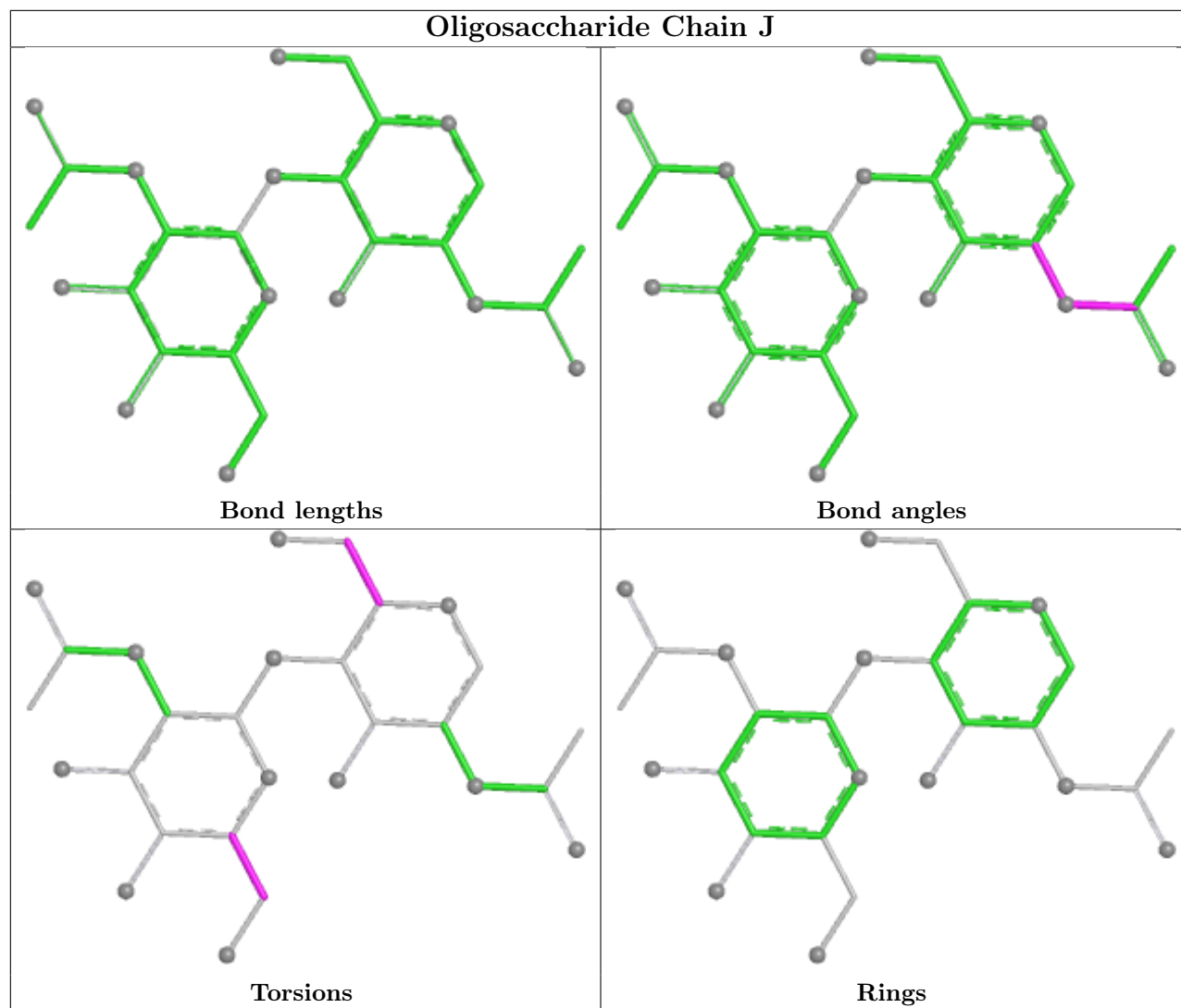


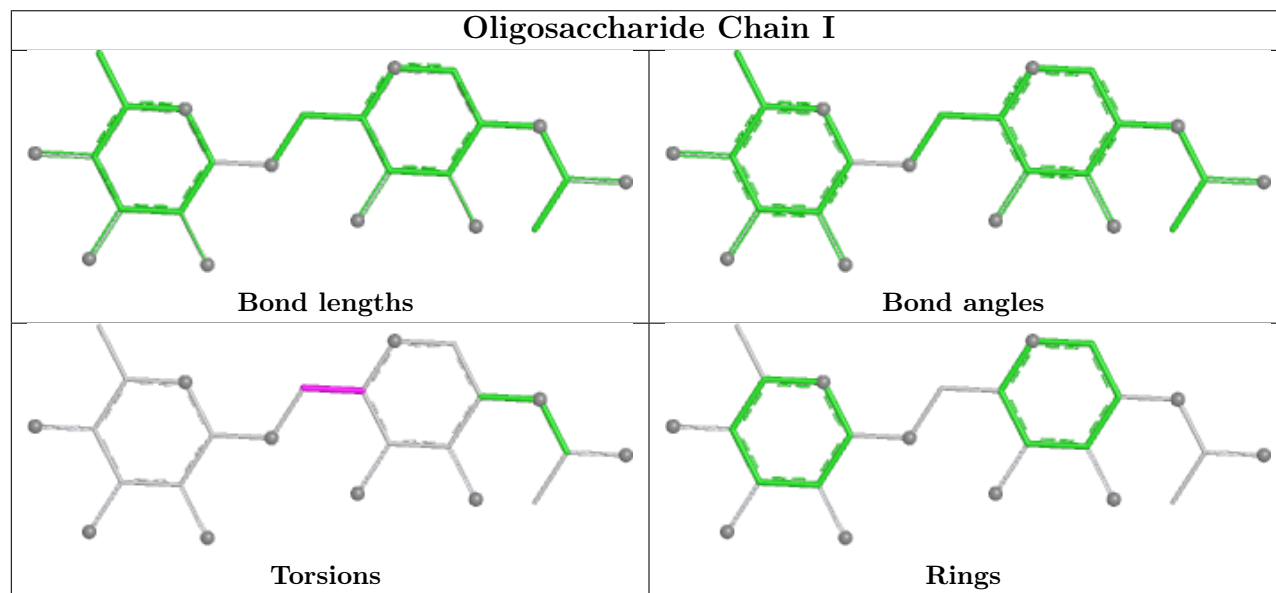
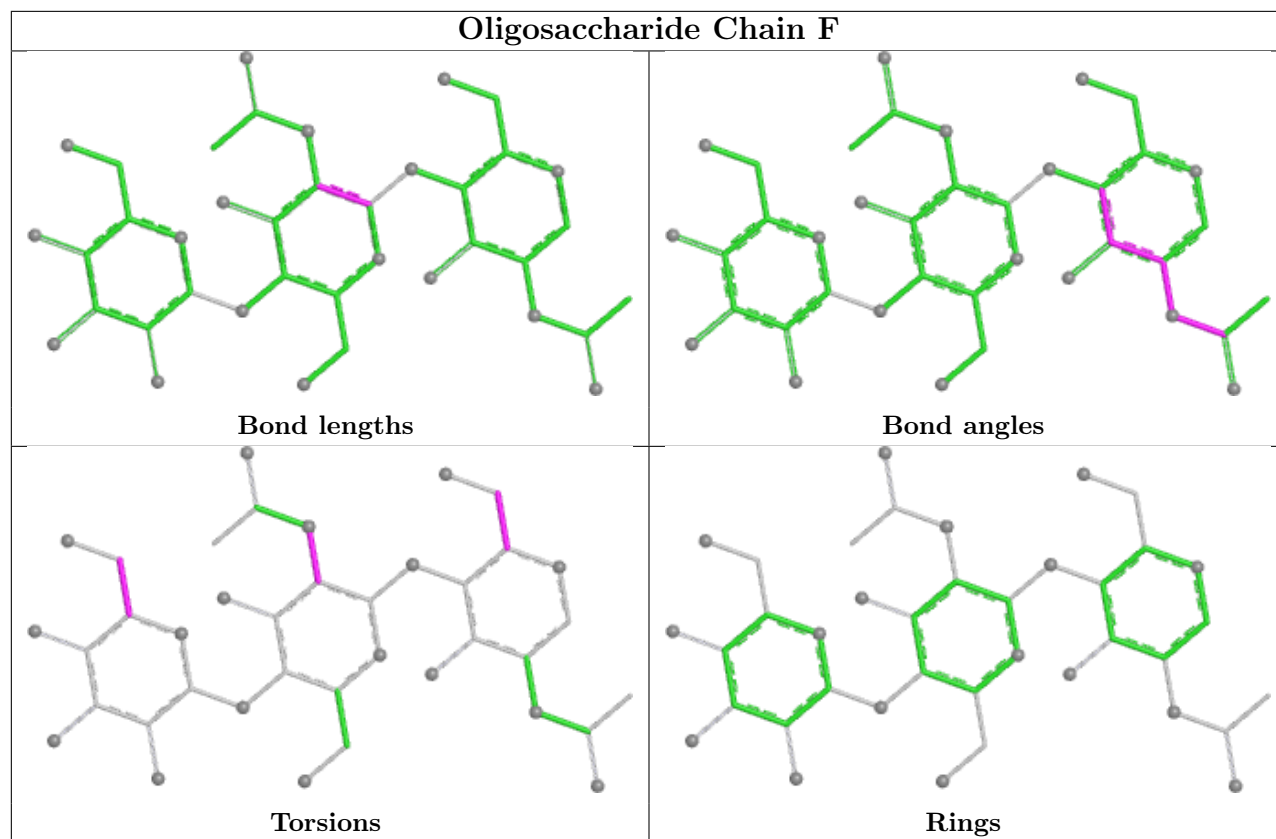


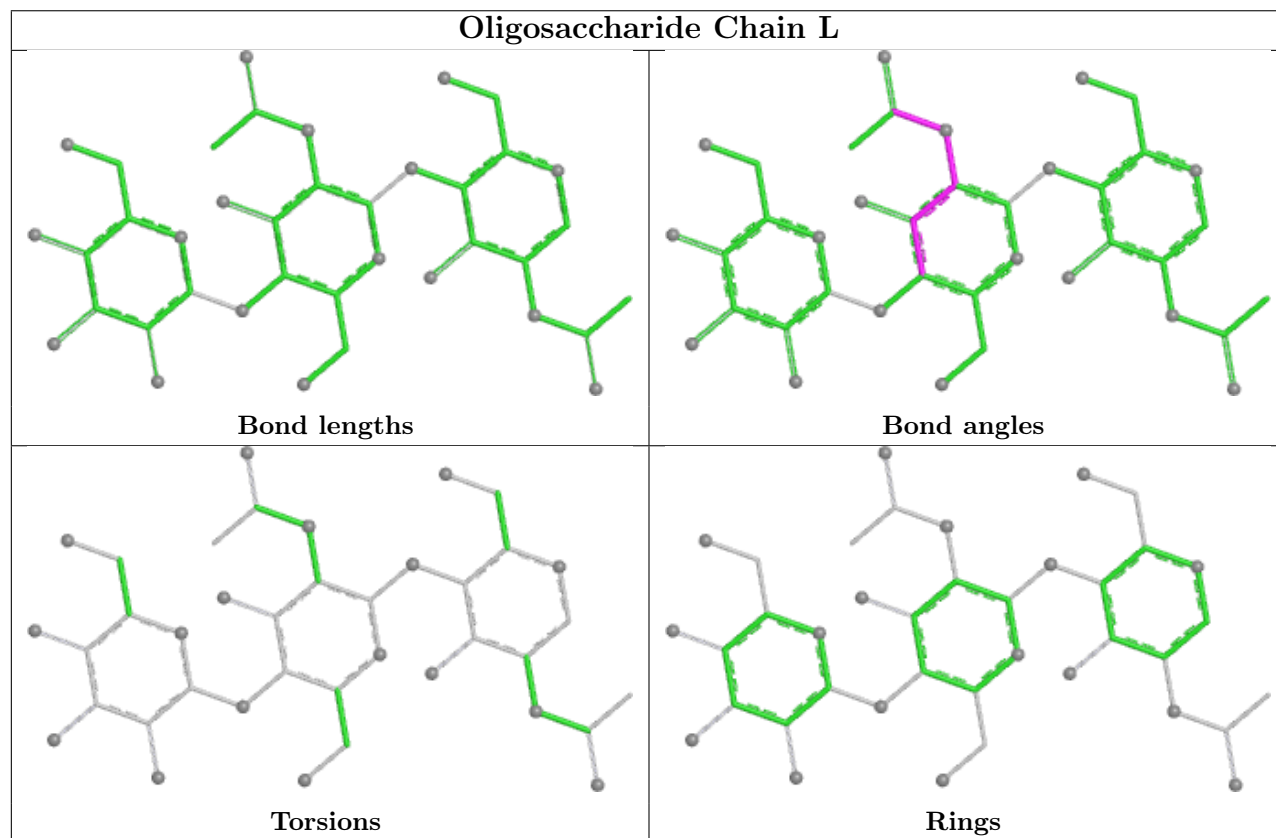
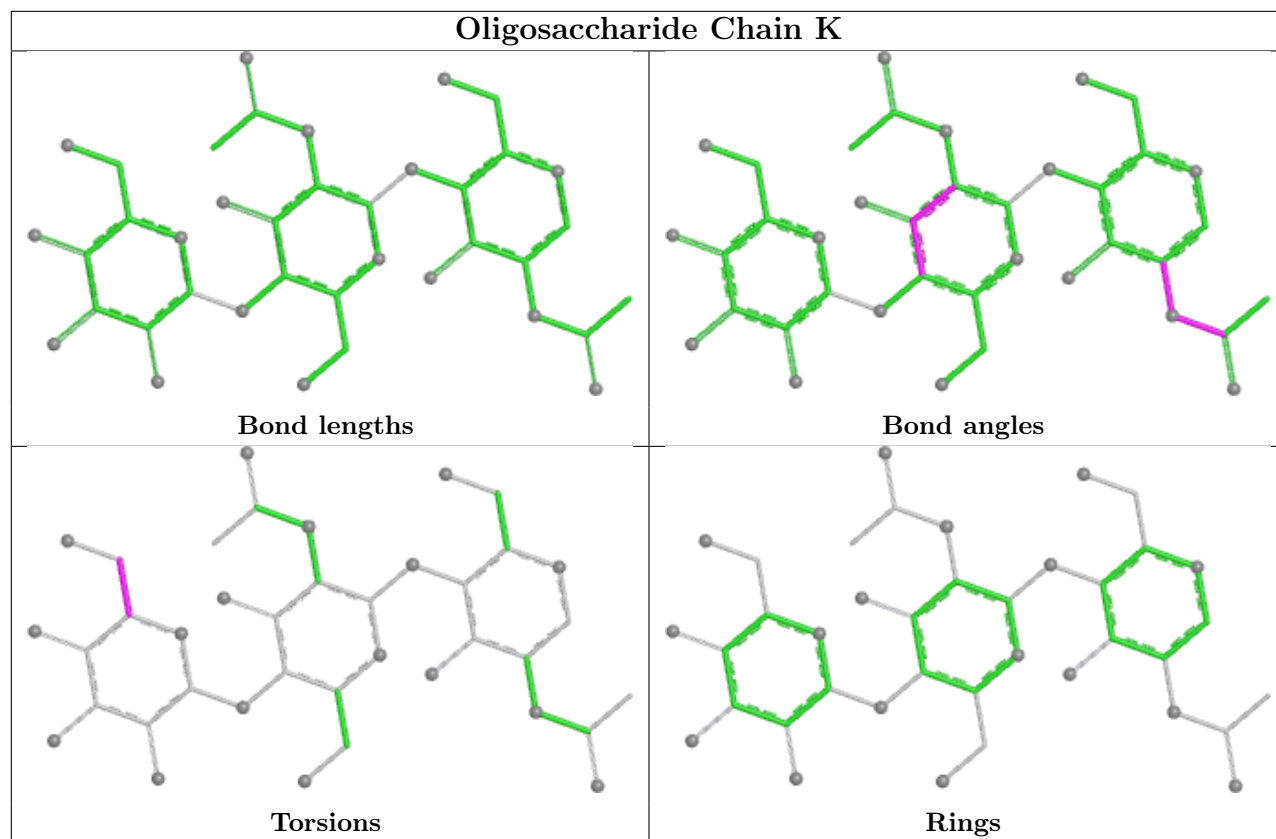


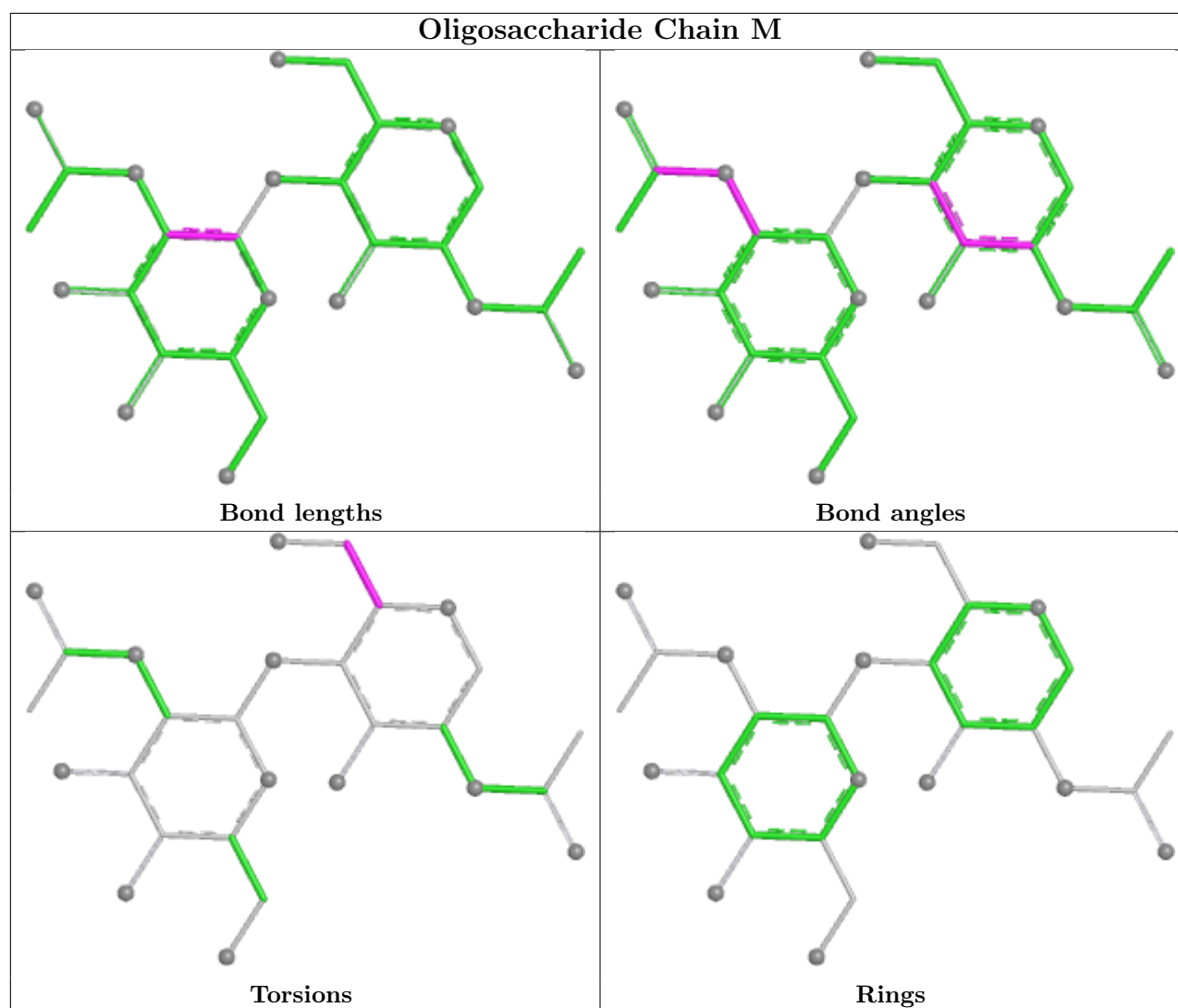












## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
10	NAG	B	769	1	14,14,15	0.54	0	17,19,21	0.70	0
9	DFP	A	1	1	6,9,9	1.20	0	6,11,11	0.42	0
9	DFP	B	1	1	6,9,9	1.20	0	6,11,11	0.43	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
10	NAG	B	769	1	-	1/6/23/26	0/1/1/1
9	DFP	A	1	1	-	2/4/8/8	-
9	DFP	B	1	1	-	2/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1	DFP	C3'-C1'-O2P-P
9	A	1	DFP	C3'-C1'-O2P-P
9	B	1	DFP	C2'-C1'-O2P-P
9	A	1	DFP	C2'-C1'-O2P-P
10	B	769	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1	DFP	2	0
9	B	1	DFP	2	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	726/728 (99%)	-0.38	5 (0%) 84 83	9, 22, 44, 67	0
1	B	728/728 (100%)	-0.27	13 (1%) 67 67	6, 24, 54, 94	0
All	All	1454/1456 (99%)	-0.33	18 (1%) 76 76	6, 23, 48, 94	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	3.5
1	B	39	SER	3.4
1	B	105	TYR	3.3
1	A	289	ALA	3.1
1	B	89	PHE	2.7
1	A	73	GLU	2.5
1	B	280	THR	2.5
1	B	289	ALA	2.5
1	A	74	ASN	2.5
1	B	99	GLY	2.4
1	A	39	SER	2.4
1	B	91	GLU	2.3
1	B	98	PHE	2.3
1	B	97	GLU	2.3
1	B	94	THR	2.1
1	B	100	HIS	2.1
1	B	76	ILE	2.1
1	A	393	ASP	2.1

### 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

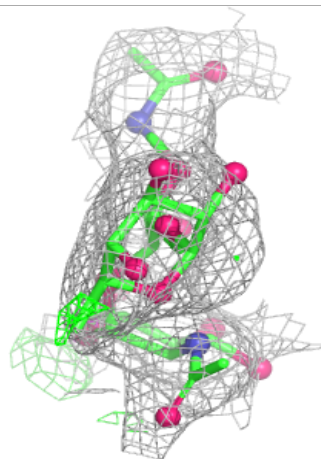
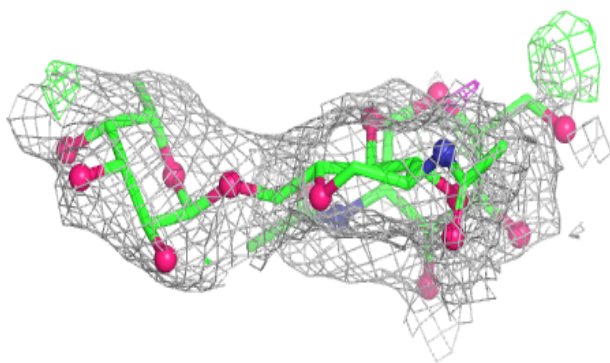
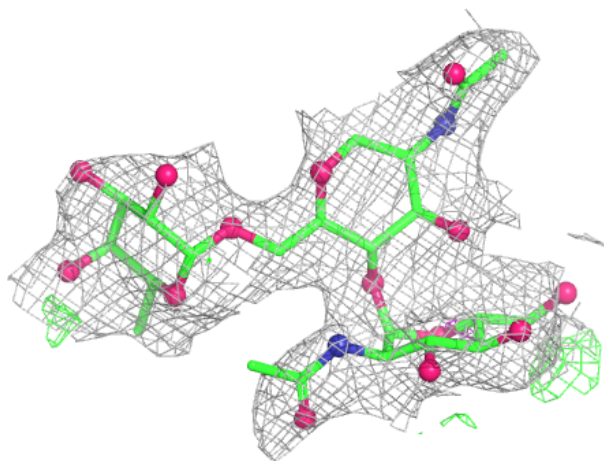
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
5	MAN	F	3	11/12	0.39	0.20	86,88,88,89	0
3	FUC	D	3	10/11	0.42	0.18	83,86,87,88	0
4	NAG	H	2	14/15	0.52	0.19	72,75,76,77	0
3	NAG	D	2	14/15	0.54	0.19	77,79,84,84	0
8	NDG	M	2	14/15	0.54	0.17	79,81,84,85	0
7	BMA	K	3	11/12	0.55	0.16	64,66,67,68	0
2	NDG	C	2	14/15	0.58	0.16	72,74,76,77	0
5	NDG	F	2	14/15	0.59	0.21	67,74,76,82	0
3	NAG	D	1	14/15	0.61	0.17	65,69,77,80	0
7	BMA	L	3	11/12	0.62	0.16	53,56,58,59	0
6	FUC	I	2	10/11	0.65	0.16	74,75,75,75	0
4	NAG	G	2	14/15	0.73	0.16	65,69,71,72	0
4	NAG	E	2	14/15	0.77	0.13	54,56,59,59	0
8	NAG	M	1	14/15	0.77	0.15	63,67,72,76	0
4	NAG	J	2	14/15	0.77	0.14	65,67,68,69	0
6	NAG	I	1	14/15	0.78	0.14	63,66,71,72	0
2	FUC	C	3	10/11	0.79	0.14	63,64,65,65	0
7	NAG	K	2	14/15	0.83	0.13	50,54,59,62	0
4	NAG	H	1	14/15	0.84	0.13	57,61,65,70	0
4	NAG	J	1	14/15	0.84	0.14	55,58,62,64	0
4	NAG	E	1	14/15	0.85	0.10	39,41,45,50	0
2	NAG	C	1	14/15	0.86	0.10	54,58,62,67	0
7	NAG	L	2	14/15	0.89	0.13	32,38,44,47	0
5	NAG	F	1	14/15	0.89	0.11	39,42,48,58	0
4	NAG	G	1	14/15	0.90	0.09	49,52,55,60	0
7	NAG	K	1	14/15	0.93	0.09	28,30,35,43	0
7	NAG	L	1	14/15	0.94	0.09	20,27,32,33	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 C:**

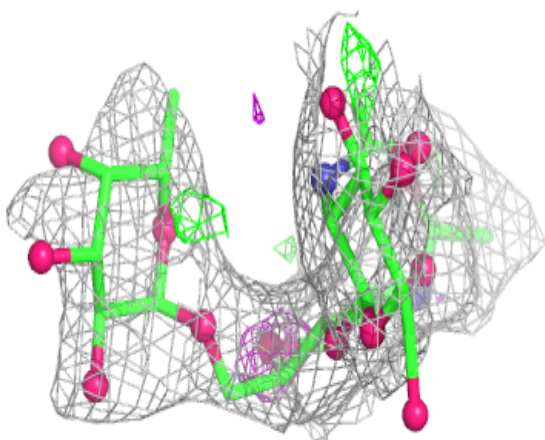
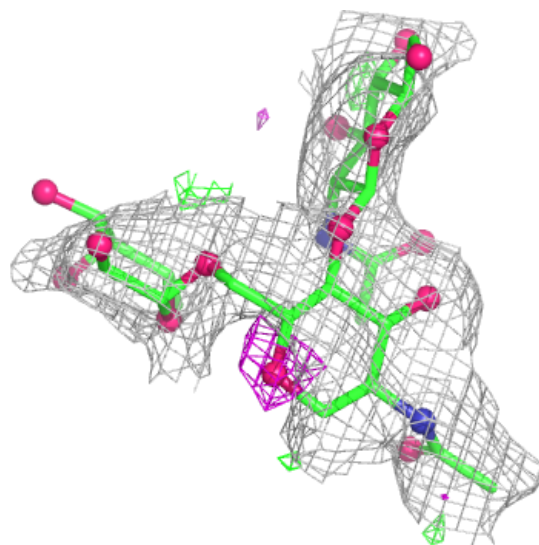
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





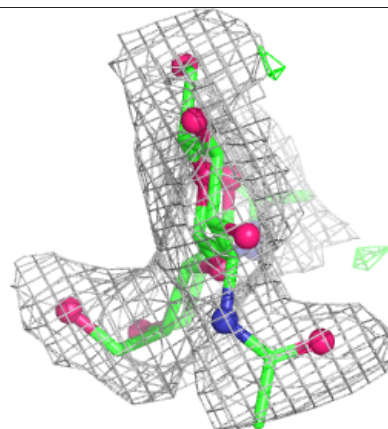
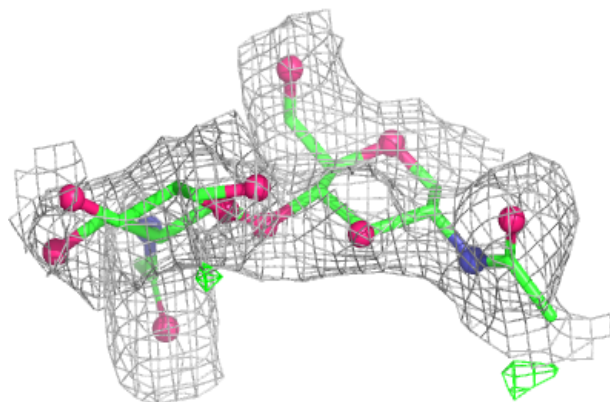
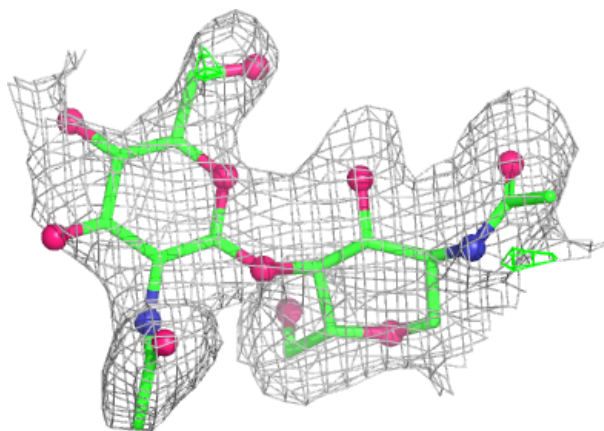
**Electron density around Chain D:**

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

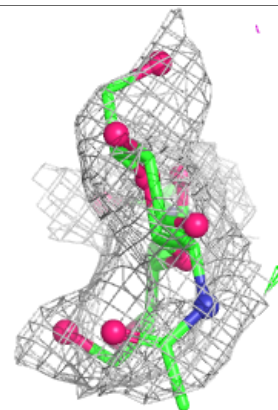
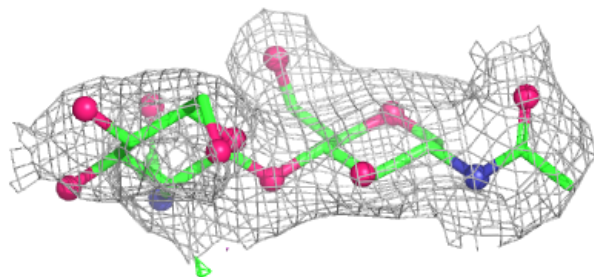
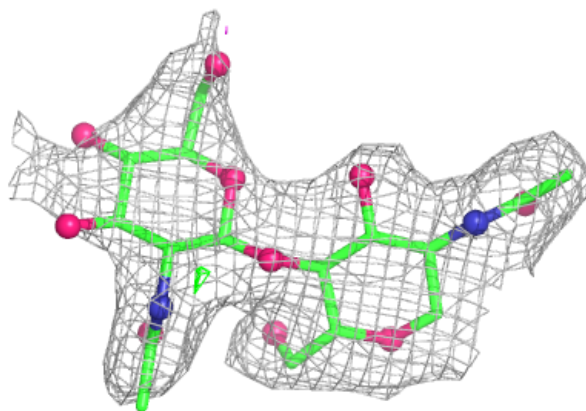


**Electron density around Chain E:**

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

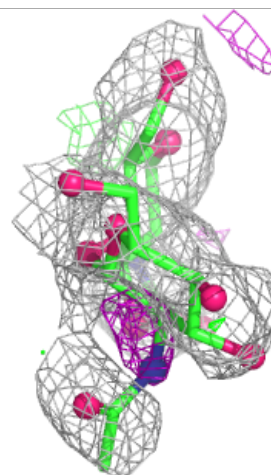
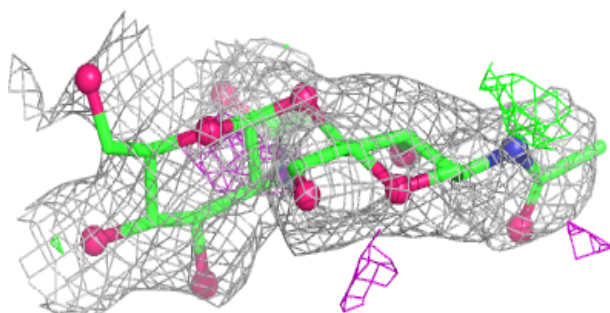
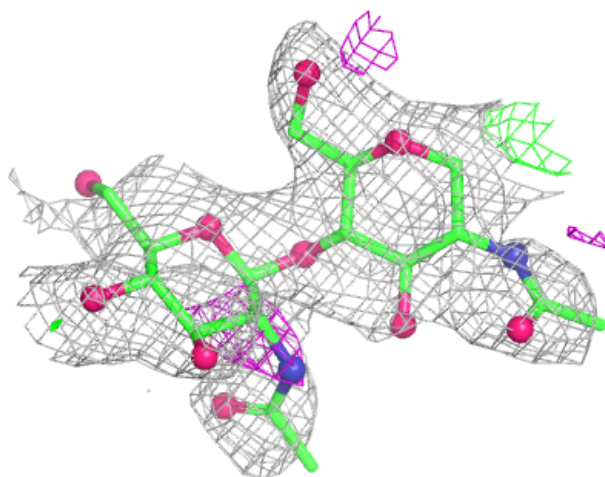
**Electron density around Chain G:**

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



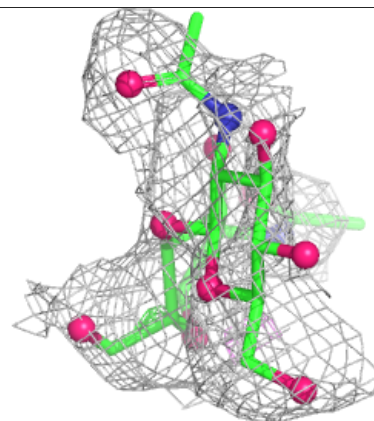
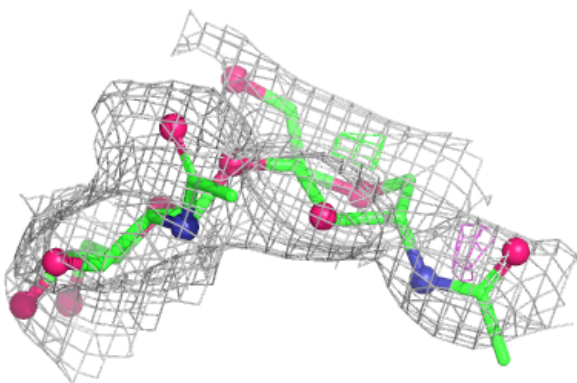
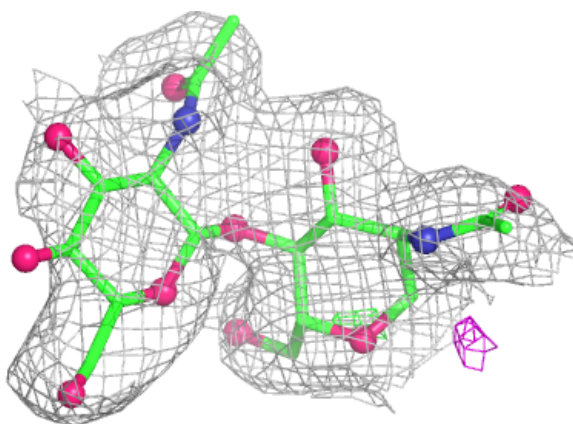
**Electron density around Chain H:**

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

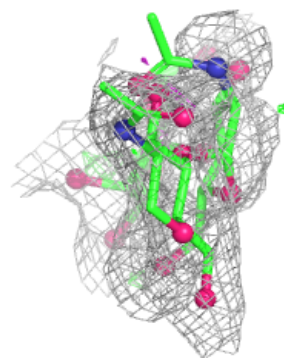
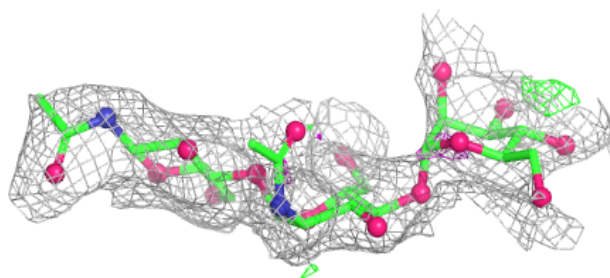
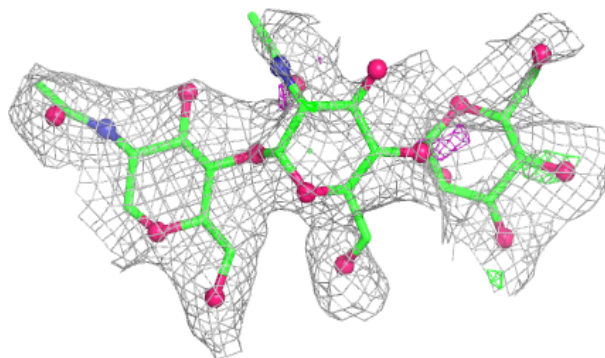


**Electron density around Chain J:**

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

**Electron density around Chain F:**

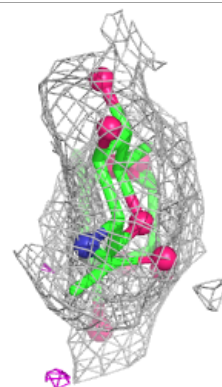
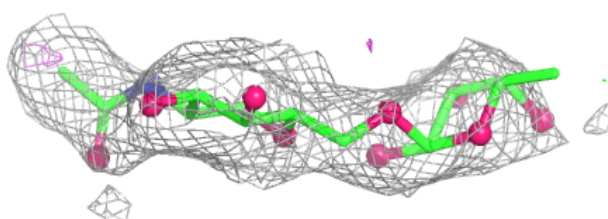
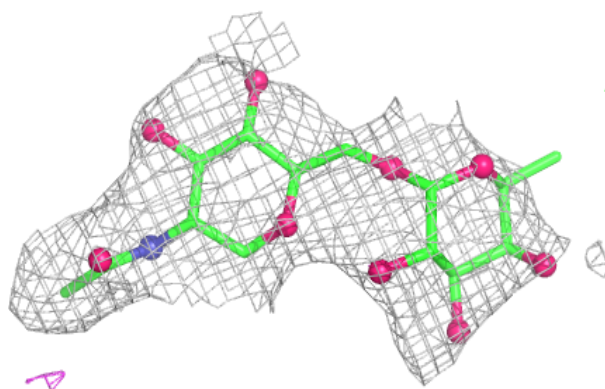
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



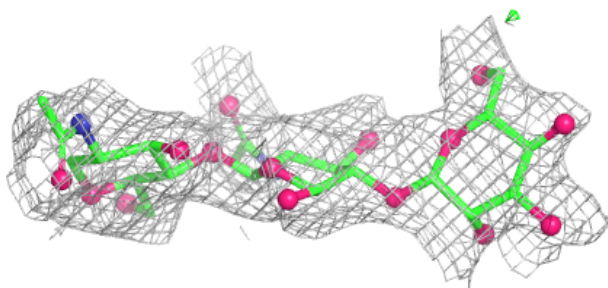
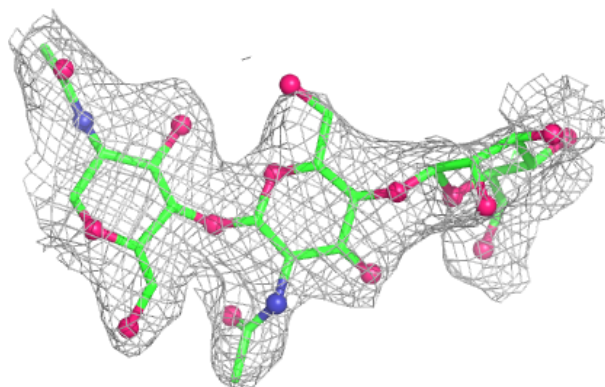


**Electron density around Chain I:**

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

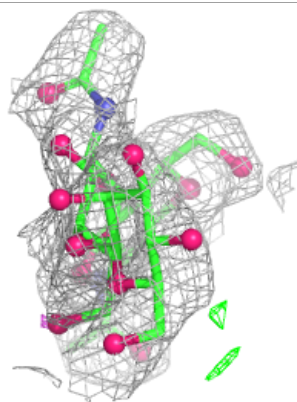
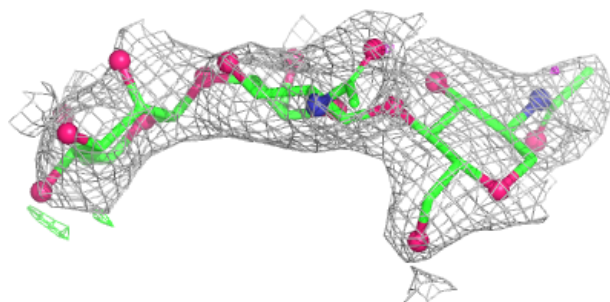
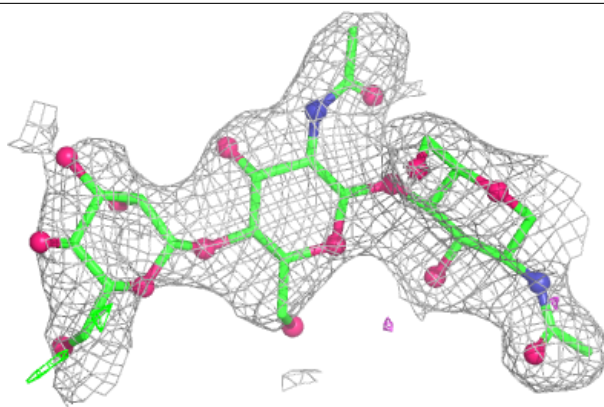
**Electron density around Chain K:**

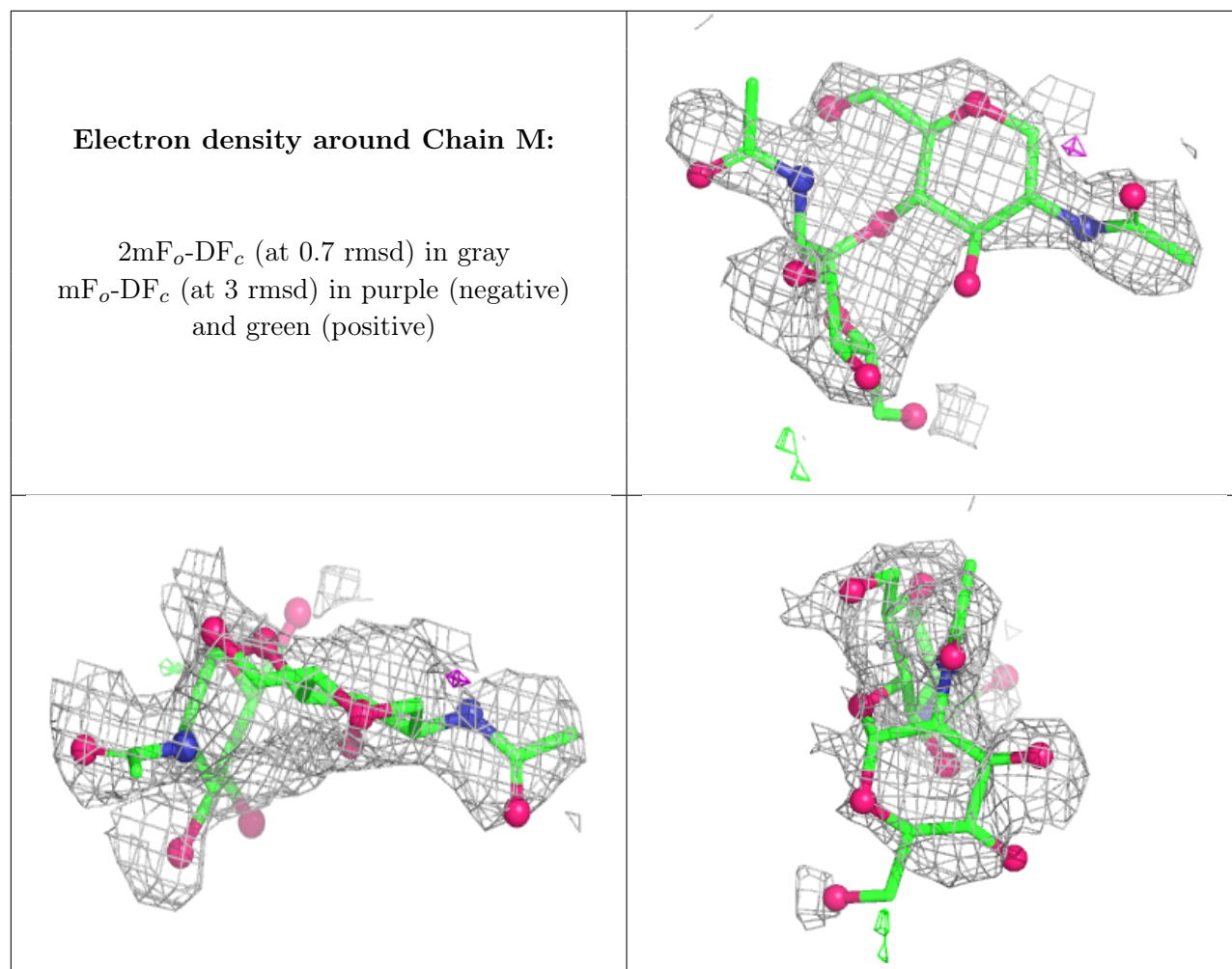
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

$2mF_o - DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
10	NAG	B	769	14/15	0.61	0.15	68,73,74,75	0
9	DFP	A	1	10/10	0.95	0.12	16,23,27,29	0
9	DFP	B	1	10/10	0.96	0.10	25,29,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.