



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:21 PM BST

PDB ID : 3GWJ
Title : Crystal structure of Antheraea pernyi arylphorin
Authors : Ryu, K.S.; Lee, J.O.; Kwon, T.H.; Kim, S.
Deposited on : 2009-04-01
Resolution : 2.43 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

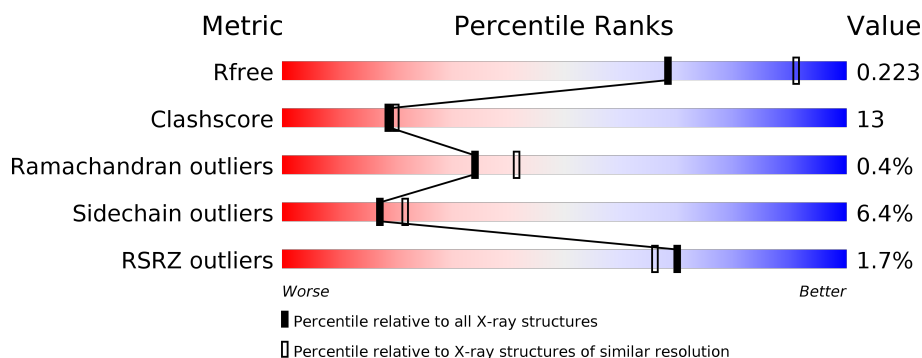
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



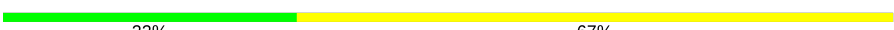




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 ≥ 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	674	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div></div> </div> </div>
1	B	674	<div> <div></div> <div> <div>72%</div> <div>25%</div> <div></div> </div> </div>
1	C	674	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div></div> </div> </div>
1	D	674	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div></div> </div> </div>
1	E	674	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div></div> </div> </div>
1	F	674	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	12	
2	I	12	
2	K	12	
2	M	12	
2	O	12	
2	Q	12	
3	H	2	
3	J	2	
3	L	2	
3	N	2	
3	P	2	
3	R	2	

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
2	MAN	G	12	-	-	-	X
2	MAN	I	12	-	-	-	X
2	MAN	K	10	-	-	-	X
2	MAN	K	12	-	-	-	X
2	MAN	M	12	-	-	-	X
2	MAN	Q	12	-	-	-	X
3	NAG	N	2	-	-	-	X
3	NAG	R	2	-	-	-	X
4	FMT	B	2002	-	-	X	-

2 Entry composition ⓘ

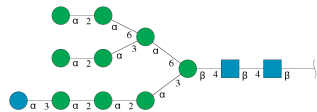
There are 5 unique types of molecules in this entry. The entry contains 36702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Arylphorin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	B	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	C	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	D	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	E	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	F	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			

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



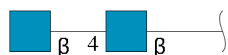
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	12	Total	C	N	O	0	0	0
			138	76	2	60			
2	I	12	Total	C	N	O	0	0	0
			138	76	2	60			
2	K	12	Total	C	N	O	0	0	0
			138	76	2	60			
2	M	12	Total	C	N	O	0	0	0
			138	76	2	60			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	12	Total	C	N	O	0	0	0
			138	76	2	60			
2	Q	12	Total	C	N	O	0	0	0
			138	76	2	60			

- Molecule 3 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
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		

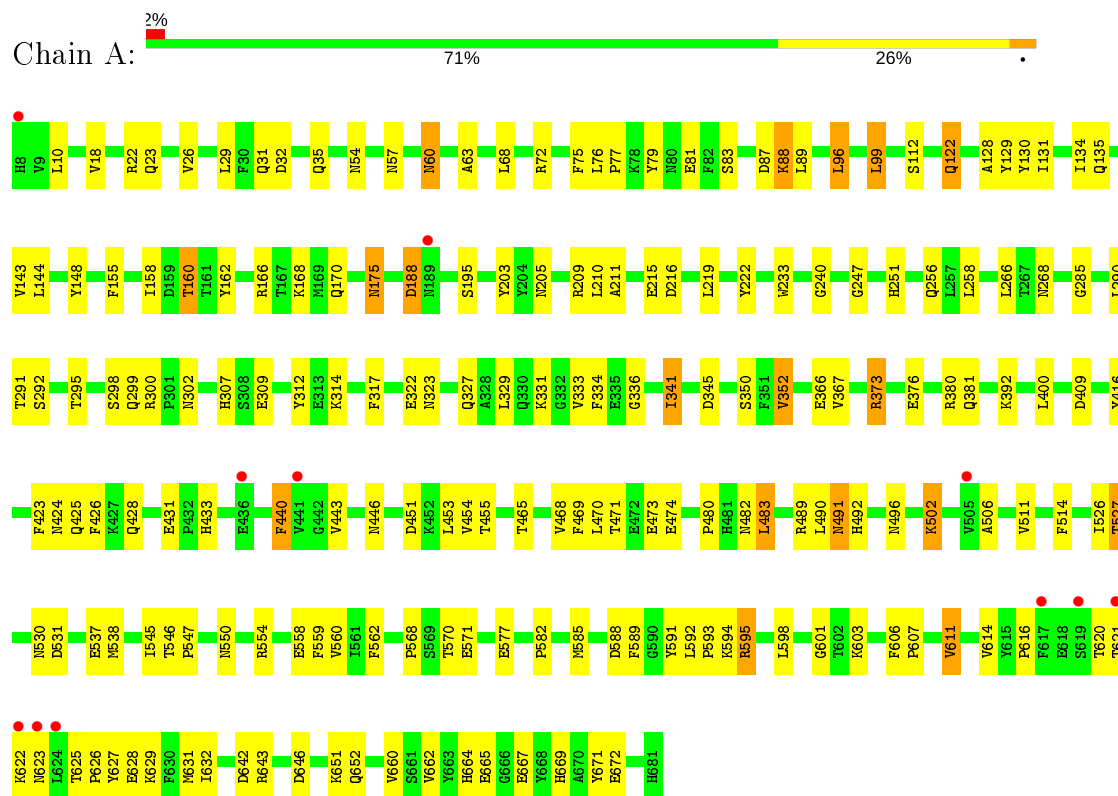
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total	O	0	0
			225	225		
5	B	241	Total	O	0	0
			241	241		
5	C	200	Total	O	0	0
			200	200		
5	D	243	Total	O	0	0
			243	243		
5	E	218	Total	O	0	0
			218	218		
5	F	253	Total	O	0	0
			253	253		

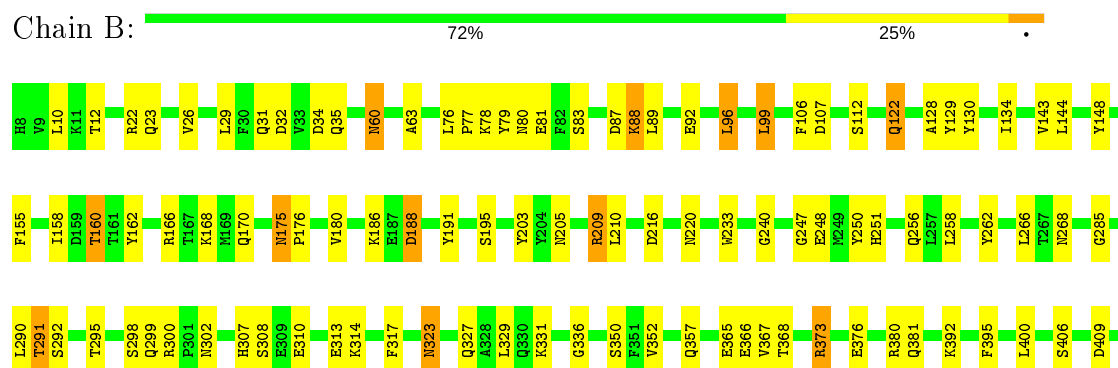
3 Residue-property plots

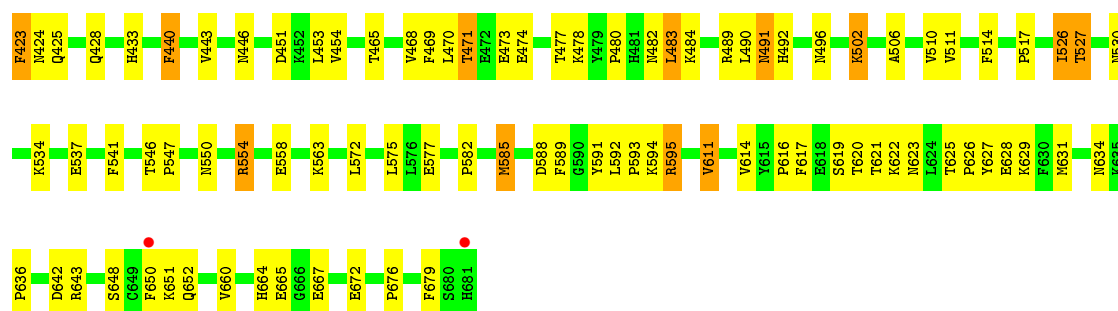
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Arylphorin

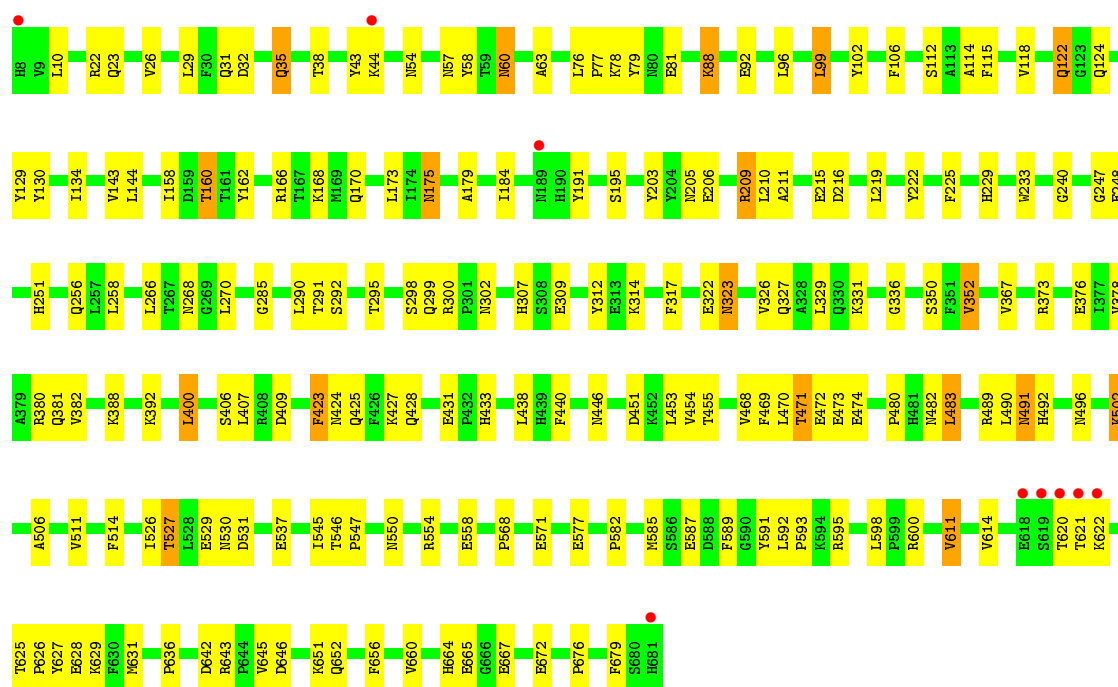


• Molecule 1: Arylphorin

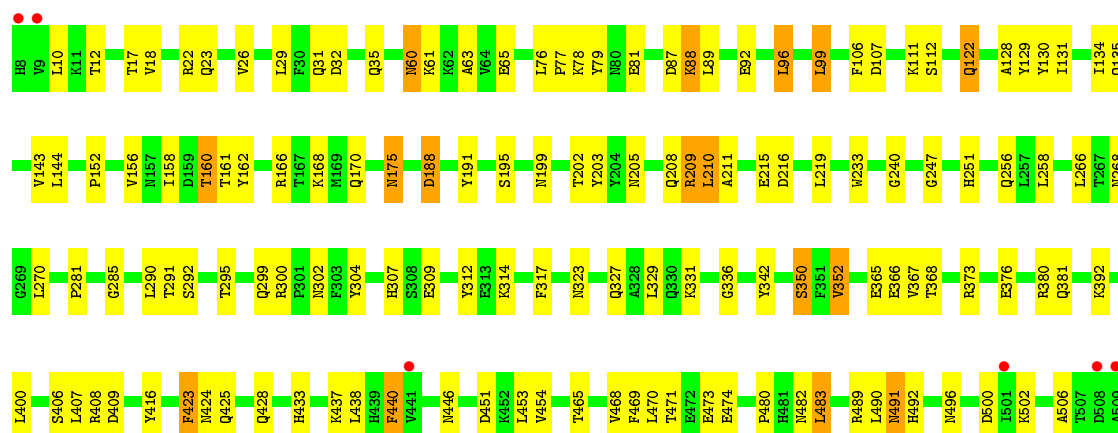


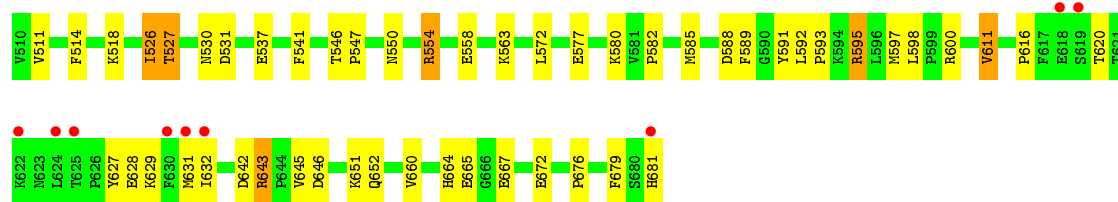


• Molecule 1: Arylphorin

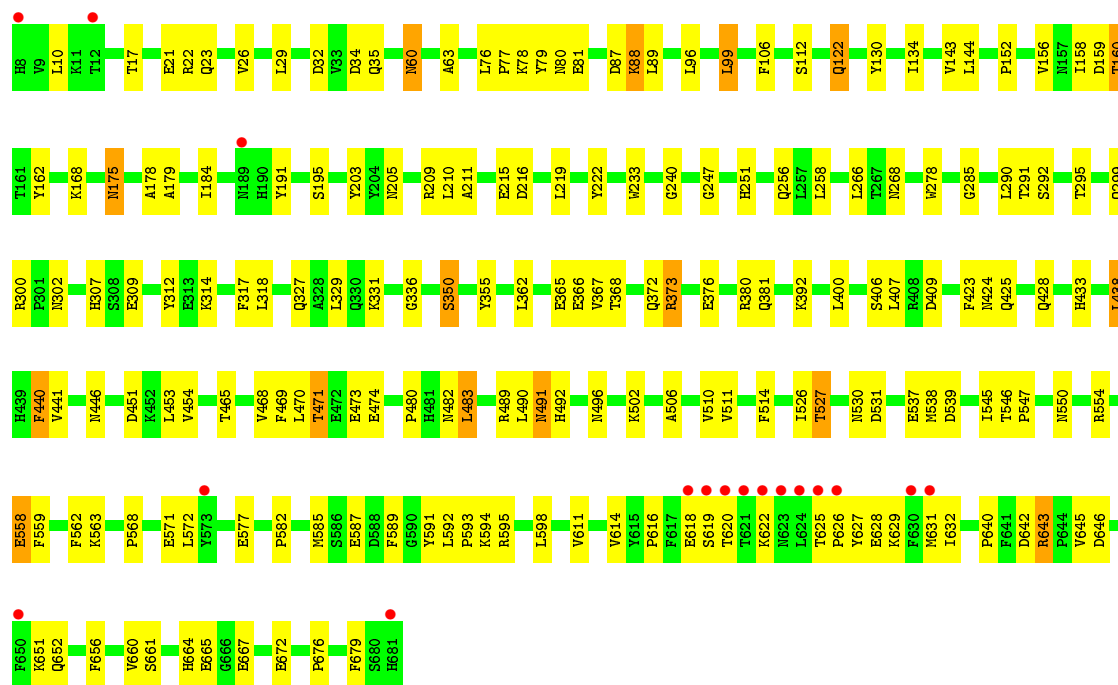
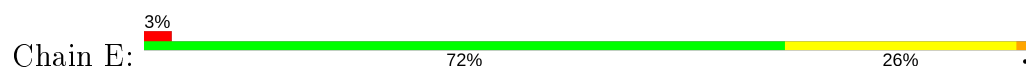


• Molecule 1: Arylphorin

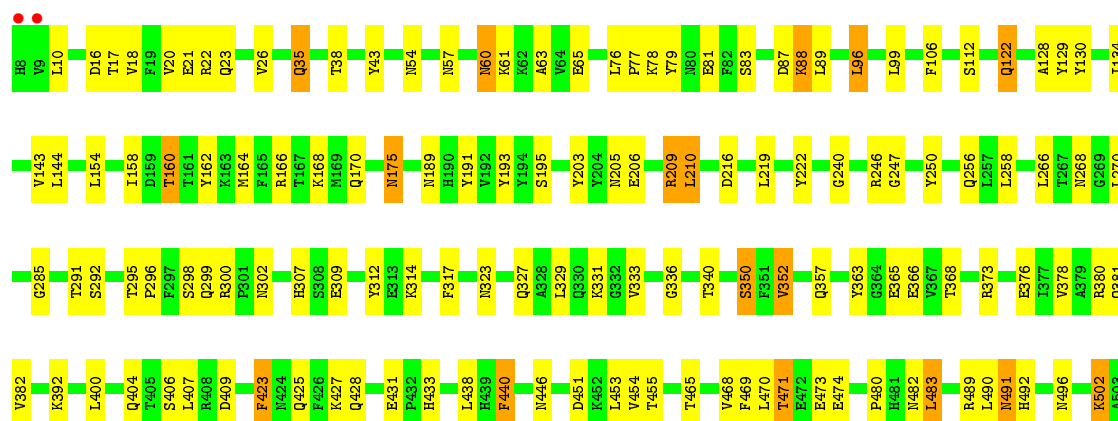


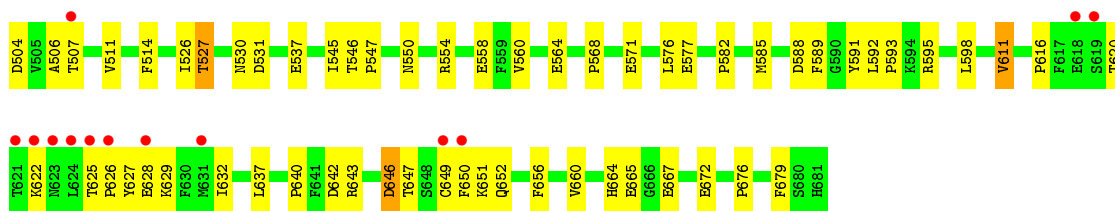


• Molecule 1: Arylphorin



• Molecule 1: Arylphorin





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

Chain G: 



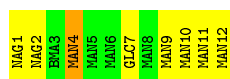
- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-be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

Chain I: 



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

Chain K: 



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

Chain M: 



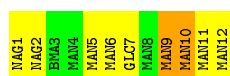
- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-be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

Chain O: 42% 58%



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

Chain Q: 25% 58% 17%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.20Å 119.47Å 319.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.43 48.80 – 2.43	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.80-2.43) 95.8 (48.80-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.182 , 0.229 0.177 , 0.223	Depositor DCC
R_{free} test set	8410 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36702	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, FMT, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/5907	0.58	0/8017
1	B	0.40	0/5907	0.59	0/8017
1	C	0.41	0/5907	0.59	0/8017
1	D	0.40	0/5907	0.58	0/8017
1	E	0.40	0/5907	0.58	0/8017
1	F	0.41	0/5907	0.59	1/8017 (0.0%)
All	All	0.40	0/35442	0.59	1/48102 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	649	CYS	CA-CB-SG	-6.93	101.53	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	342	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	5718	0	5424	151	0
1	B	5718	0	5424	157	0
1	C	5718	0	5424	150	0
1	D	5718	0	5424	159	0
1	E	5718	0	5424	159	0
1	F	5718	0	5424	162	0
2	G	138	0	115	0	0
2	I	138	0	115	1	0
2	K	138	0	115	1	0
2	M	138	0	115	0	0
2	O	138	0	115	0	0
2	Q	138	0	115	2	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	N	28	0	25	0	0
3	P	28	0	25	0	0
3	R	28	0	25	0	0
4	A	3	0	1	1	0
4	B	3	0	1	2	0
4	C	3	0	1	1	0
4	D	3	0	1	1	0
4	E	3	0	1	1	0
4	F	3	0	1	1	0
5	A	225	0	0	7	0
5	B	241	0	0	11	0
5	C	200	0	0	12	0
5	D	243	0	0	11	0
5	E	218	0	0	14	0
5	F	253	0	0	11	0
All	All	36702	0	33390	899	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 13.

All (899) 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:D:134:ILE:HD11	1:D:144:LEU:HD11	1.38	1.06
1:C:134:ILE:HD11	1:C:144:LEU:HD11	1.41	1.02
1:C:23:GLN:HE22	1:C:143:VAL:H	1.06	1.00
1:B:134:ILE:HD11	1:B:144:LEU:HD11	1.48	0.96
1:B:35:GLN:HE22	1:B:470:LEU:H	1.12	0.96
1:E:446:ASN:HD21	1:E:502:LYS:HB2	1.32	0.94
1:A:35:GLN:HE22	1:A:470:LEU:H	1.14	0.94
1:D:425:GLN:O	1:D:428:GLN:HG2	1.67	0.93
1:E:256:GLN:HE22	1:E:537:GLU:H	1.12	0.93
1:E:134:ILE:HD11	1:E:144:LEU:HD11	1.49	0.92
1:C:256:GLN:HE22	1:C:537:GLU:H	1.18	0.92
1:A:23:GLN:HE22	1:A:143:VAL:H	1.18	0.92
1:A:256:GLN:HE22	1:A:537:GLU:H	1.19	0.91
1:E:23:GLN:HE22	1:E:143:VAL:H	1.15	0.90
1:B:209:ARG:HD2	1:B:268:ASN:OD1	1.70	0.90
1:D:23:GLN:HE22	1:D:143:VAL:H	1.19	0.90
1:C:88:LYS:HG2	1:C:392:LYS:HD2	1.54	0.90
1:F:23:GLN:HE22	1:F:143:VAL:H	1.19	0.90
1:B:314:LYS:HE2	1:B:381:GLN:NE2	1.86	0.89
1:D:376:GLU:O	1:D:380:ARG:HG3	1.73	0.88
1:F:491:ASN:HD22	1:F:492:HIS:H	1.17	0.88
1:A:60:ASN:ND2	1:A:63:ALA:H	1.73	0.86
1:D:285:GLY:H	1:D:302:ASN:HD22	1.21	0.86
1:B:285:GLY:H	1:B:302:ASN:HD22	1.23	0.85
1:F:134:ILE:HD11	1:F:144:LEU:HD11	1.58	0.85
1:F:256:GLN:HE22	1:F:537:GLU:H	1.23	0.85
1:C:425:GLN:O	1:C:428:GLN:HG2	1.78	0.84
1:D:256:GLN:HE22	1:D:537:GLU:H	1.24	0.84
1:C:216:ASP:OD1	1:C:489:ARG:HD2	1.78	0.84
1:B:376:GLU:O	1:B:380:ARG:HG3	1.77	0.84
1:D:35:GLN:HE22	1:D:470:LEU:H	1.24	0.84
1:A:88:LYS:HG2	1:A:392:LYS:HD2	1.58	0.84
1:D:514:PHE:HB2	1:D:611:VAL:HG13	1.60	0.83
1:A:285:GLY:H	1:A:302:ASN:HD22	1.23	0.83
1:C:446:ASN:HD21	1:C:502:LYS:HB2	1.43	0.83
1:B:23:GLN:HE22	1:B:143:VAL:H	1.26	0.83
1:E:506:ALA:HB2	1:E:547:PRO:HD3	1.61	0.83
1:F:425:GLN:O	1:F:428:GLN:HG2	1.77	0.83
1:E:35:GLN:HE22	1:E:470:LEU:H	1.23	0.82
1:C:205:ASN:HD22	1:C:302:ASN:HD21	1.27	0.82
1:E:480:PRO:HB2	1:E:482:ASN:HB2	1.61	0.82
1:A:471:THR:HB	1:A:474:GLU:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:THR:H	1:D:550:ASN:HD21	1.24	0.82
1:D:79:TYR:H	1:D:122:GLN:NE2	1.77	0.82
1:A:425:GLN:O	1:A:428:GLN:HG2	1.78	0.81
1:E:546:THR:H	1:E:550:ASN:HD21	1.25	0.81
1:F:209:ARG:HD2	1:F:268:ASN:OD1	1.80	0.81
1:E:425:GLN:O	1:E:428:GLN:HG2	1.80	0.81
1:B:291:THR:HG21	1:F:162:TYR:OH	1.80	0.81
1:B:256:GLN:HE22	1:B:537:GLU:H	1.28	0.81
1:C:546:THR:H	1:C:550:ASN:HD21	1.28	0.81
1:B:546:THR:H	1:B:550:ASN:HD21	1.26	0.81
1:D:209:ARG:HD2	1:D:268:ASN:OD1	1.81	0.80
1:C:317:PHE:CZ	1:C:373:ARG:HG2	2.17	0.80
1:F:446:ASN:HD21	1:F:502:LYS:HB2	1.46	0.80
1:F:79:TYR:H	1:F:122:GLN:NE2	1.79	0.79
1:B:667:GLU:HG2	1:B:672:GLU:CB	2.11	0.79
1:F:35:GLN:HE22	1:F:470:LEU:H	1.29	0.79
1:D:667:GLU:HG2	1:D:672:GLU:CB	2.13	0.78
1:A:446:ASN:HD21	1:A:502:LYS:HB2	1.47	0.78
1:D:437:LYS:HD2	5:D:702:HOH:O	1.84	0.78
1:E:88:LYS:HG2	1:E:392:LYS:HD2	1.63	0.78
1:E:645:VAL:HG12	5:E:707:HOH:O	1.84	0.77
1:E:160:THR:HG21	1:E:195:SER:OG	1.85	0.77
1:B:295:THR:HA	1:F:158:ILE:HD11	1.65	0.77
1:D:134:ILE:HD11	1:D:144:LEU:CD1	2.15	0.77
1:C:480:PRO:HB2	1:C:482:ASN:HB2	1.66	0.76
1:F:667:GLU:HG2	1:F:672:GLU:CB	2.16	0.76
1:E:667:GLU:HG2	1:E:672:GLU:CB	2.16	0.76
1:E:285:GLY:H	1:E:302:ASN:HD22	1.32	0.76
1:B:506:ALA:HB2	1:B:547:PRO:HD3	1.67	0.76
1:F:491:ASN:ND2	1:F:492:HIS:H	1.82	0.76
1:A:491:ASN:HD22	1:A:492:HIS:H	1.34	0.76
1:A:285:GLY:H	1:A:302:ASN:ND2	1.85	0.75
1:C:162:TYR:OH	1:E:291:THR:HG21	1.87	0.75
1:E:79:TYR:H	1:E:122:GLN:NE2	1.83	0.75
1:C:285:GLY:H	1:C:302:ASN:HD22	1.32	0.75
1:A:667:GLU:HG2	1:A:672:GLU:CB	2.17	0.75
1:D:480:PRO:HB2	1:D:482:ASN:HB2	1.69	0.74
1:E:376:GLU:O	1:E:380:ARG:HG3	1.85	0.74
1:E:317:PHE:CZ	1:E:373:ARG:HG2	2.22	0.74
1:F:285:GLY:H	1:F:302:ASN:HD22	1.32	0.74
1:B:122:GLN:NE2	1:B:122:GLN:H	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ASN:HD22	1:E:63:ALA:H	1.35	0.74
1:C:247:GLY:HA3	1:C:350:SER:HA	1.68	0.74
1:F:546:THR:H	1:F:550:ASN:HD21	1.32	0.74
1:F:88:LYS:HG2	1:F:392:LYS:HD2	1.69	0.74
1:A:79:TYR:H	1:A:122:GLN:NE2	1.85	0.74
1:A:60:ASN:HD22	1:A:63:ALA:H	1.31	0.74
1:A:158:ILE:HD11	1:D:295:THR:HA	1.69	0.74
1:D:491:ASN:HD22	1:D:492:HIS:H	1.35	0.74
1:D:645:VAL:HG12	5:D:794:HOH:O	1.87	0.73
1:D:88:LYS:HG2	1:D:392:LYS:HD2	1.68	0.73
1:D:285:GLY:H	1:D:302:ASN:ND2	1.86	0.73
1:A:514:PHE:HB2	1:A:611:VAL:HG13	1.69	0.73
1:D:491:ASN:ND2	1:D:492:HIS:H	1.85	0.73
1:D:99:LEU:HD13	1:D:112:SER:HB3	1.71	0.73
1:A:134:ILE:HD11	1:A:144:LEU:HD11	1.71	0.73
1:A:506:ALA:HB2	1:A:547:PRO:HD3	1.69	0.73
1:C:526:ILE:HD11	5:C:690:HOH:O	1.88	0.73
1:E:471:THR:HG22	1:E:474:GLU:H	1.53	0.73
1:A:489:ARG:HD3	5:A:683:HOH:O	1.89	0.72
1:E:76:LEU:HD12	1:E:77:PRO:HD2	1.69	0.72
1:A:471:THR:HG22	1:A:473:GLU:H	1.54	0.72
1:C:667:GLU:HG2	1:C:672:GLU:CB	2.20	0.72
1:F:60:ASN:ND2	1:F:63:ALA:H	1.87	0.72
1:B:79:TYR:H	1:B:122:GLN:NE2	1.86	0.72
1:D:160:THR:HG21	1:D:195:SER:OG	1.88	0.72
1:F:491:ASN:HD22	1:F:492:HIS:N	1.88	0.72
1:E:667:GLU:HG2	1:E:672:GLU:HB2	1.72	0.72
1:A:209:ARG:HD2	1:A:268:ASN:OD1	1.89	0.72
1:C:79:TYR:H	1:C:122:GLN:NE2	1.88	0.71
1:A:68:LEU:O	1:A:72:ARG:HD2	1.90	0.71
1:C:60:ASN:ND2	1:C:63:ALA:H	1.89	0.71
1:E:23:GLN:HE22	1:E:143:VAL:N	1.88	0.71
1:A:546:THR:H	1:A:550:ASN:HD21	1.35	0.70
1:F:568:PRO:HG2	1:F:571:GLU:HG2	1.73	0.70
1:D:314:LYS:NZ	1:D:381:GLN:HE21	1.88	0.70
1:B:299:GLN:H	1:F:299:GLN:NE2	1.88	0.70
1:A:10:LEU:H	1:A:10:LEU:HD23	1.56	0.70
1:B:160:THR:HG21	1:B:195:SER:OG	1.89	0.70
1:B:514:PHE:HB2	1:B:611:VAL:HG13	1.73	0.70
1:C:60:ASN:HD22	1:C:63:ALA:H	1.36	0.70
1:D:216:ASP:OD1	1:D:489:ARG:HD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LEU:HD23	1:E:10:LEU:H	1.55	0.70
1:C:10:LEU:HD23	1:C:10:LEU:H	1.54	0.70
1:A:376:GLU:O	1:A:380:ARG:HG3	1.91	0.70
1:B:425:GLN:O	1:B:428:GLN:HG2	1.92	0.70
1:E:60:ASN:ND2	1:E:63:ALA:H	1.90	0.69
1:B:446:ASN:HD21	1:B:502:LYS:HB2	1.58	0.69
1:C:134:ILE:HD11	1:C:144:LEU:CD1	2.22	0.69
1:F:582:PRO:HB2	1:F:585:MET:HB2	1.75	0.69
1:B:317:PHE:CZ	1:B:373:ARG:HG2	2.28	0.69
1:E:491:ASN:HD22	1:E:492:HIS:H	1.41	0.69
1:B:205:ASN:HD22	1:B:302:ASN:HD21	1.37	0.69
1:A:454:VAL:CG1	1:A:665:GLU:HG3	2.22	0.69
1:B:490:LEU:O	1:B:595:ARG:HD3	1.93	0.69
1:A:256:GLN:NE2	1:A:537:GLU:H	1.90	0.68
1:B:667:GLU:HG2	1:B:672:GLU:HB2	1.73	0.68
1:B:480:PRO:HB2	1:B:482:ASN:HB2	1.73	0.68
1:B:134:ILE:HD11	1:B:144:LEU:CD1	2.21	0.68
1:F:76:LEU:HD12	1:F:77:PRO:HD2	1.75	0.68
1:D:23:GLN:HE22	1:D:143:VAL:N	1.89	0.68
1:A:480:PRO:HB2	1:A:482:ASN:HB2	1.75	0.68
1:F:216:ASP:OD1	1:F:489:ARG:HD2	1.94	0.68
1:F:314:LYS:NZ	1:F:381:GLN:HE21	1.92	0.68
1:E:446:ASN:ND2	1:E:502:LYS:HB2	2.07	0.68
1:A:433:HIS:HE1	1:A:642:ASP:OD2	1.75	0.68
1:B:88:LYS:HG2	1:B:392:LYS:HD2	1.75	0.68
1:E:134:ILE:HD11	1:E:144:LEU:CD1	2.21	0.68
1:C:295:THR:HA	1:E:158:ILE:HD11	1.77	0.67
1:F:480:PRO:HB2	1:F:482:ASN:HB2	1.75	0.67
1:E:592:LEU:HD22	1:E:593:PRO:HD2	1.76	0.67
1:C:527:THR:HG22	1:C:530:ASN:H	1.58	0.67
1:C:491:ASN:HD22	1:C:492:HIS:H	1.39	0.67
1:E:122:GLN:H	1:E:122:GLN:NE2	1.93	0.67
1:A:256:GLN:HE22	1:A:537:GLU:N	1.91	0.67
1:A:22:ARG:O	1:A:26:VAL:HG13	1.95	0.66
1:C:76:LEU:HD12	1:C:77:PRO:HD2	1.75	0.66
1:B:299:GLN:HE22	1:F:299:GLN:H	1.44	0.66
1:E:209:ARG:HD2	1:E:268:ASN:OD1	1.95	0.66
1:F:490:LEU:O	1:F:595:ARG:HD3	1.94	0.66
1:A:317:PHE:CZ	1:A:373:ARG:HG2	2.30	0.66
1:C:35:GLN:HE22	1:C:470:LEU:H	1.41	0.66
1:D:471:THR:HG22	1:D:473:GLU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:THR:HG21	1:F:195:SER:OG	1.96	0.66
1:F:10:LEU:HD23	1:F:10:LEU:H	1.61	0.66
1:F:65:GLU:HG2	5:F:757:HOH:O	1.96	0.66
1:B:168:LYS:HG2	1:B:468:VAL:HG13	1.75	0.66
1:E:568:PRO:HG2	1:E:571:GLU:HG2	1.78	0.66
1:A:592:LEU:HD22	1:A:593:PRO:HD2	1.76	0.66
1:A:216:ASP:OD1	1:A:489:ARG:HD2	1.96	0.66
1:B:134:ILE:CD1	1:B:144:LEU:HD11	2.23	0.66
1:A:336:GLY:HA3	1:B:331:LYS:HB2	1.77	0.66
1:C:134:ILE:CD1	1:C:144:LEU:HD11	2.22	0.66
1:D:10:LEU:HD23	1:D:10:LEU:H	1.61	0.65
1:D:134:ILE:CD1	1:D:144:LEU:HD11	2.20	0.65
1:F:471:THR:HG22	1:F:473:GLU:H	1.62	0.65
1:D:327:GLN:O	1:D:331:LYS:HG2	1.97	0.65
1:E:175:ASN:HD22	1:E:175:ASN:C	1.98	0.65
1:A:667:GLU:HG2	1:A:672:GLU:HB2	1.79	0.65
1:B:433:HIS:HE1	1:B:642:ASP:OD2	1.80	0.65
1:B:299:GLN:NE2	1:F:299:GLN:H	1.94	0.65
1:D:454:VAL:CG1	1:D:665:GLU:HG3	2.27	0.65
1:D:490:LEU:O	1:D:595:ARG:HD3	1.97	0.65
1:B:307:HIS:HE1	4:B:2002:FMT:O1	1.79	0.65
1:F:514:PHE:HB2	1:F:611:VAL:HG13	1.78	0.65
1:B:158:ILE:HD11	1:F:296:PRO:HD3	1.79	0.65
1:E:514:PHE:HB2	1:E:611:VAL:HG13	1.77	0.65
1:C:205:ASN:HD22	1:C:302:ASN:ND2	1.94	0.65
1:F:168:LYS:HG2	1:F:468:VAL:HG13	1.78	0.65
1:B:162:TYR:OH	1:F:291:THR:HG21	1.97	0.64
1:D:446:ASN:HD21	1:D:502:LYS:HB2	1.61	0.64
1:C:23:GLN:HE22	1:C:143:VAL:N	1.88	0.64
1:C:209:ARG:HD2	1:C:268:ASN:OD1	1.98	0.64
1:F:451:ASP:OD2	1:F:496:ASN:HB2	1.97	0.64
1:B:454:VAL:CG1	1:B:665:GLU:HG3	2.28	0.64
1:D:60:ASN:ND2	1:D:63:ALA:H	1.95	0.64
1:E:642:ASP:OD1	1:E:643:ARG:HG2	1.98	0.64
1:D:331:LYS:HB2	1:F:336:GLY:HA3	1.80	0.64
1:D:205:ASN:HD22	1:D:302:ASN:HD21	1.45	0.64
1:A:162:TYR:OH	1:D:291:THR:HG21	1.98	0.64
1:F:667:GLU:HG2	1:F:672:GLU:HB2	1.80	0.64
1:A:465:THR:HG23	1:A:483:LEU:HD22	1.80	0.64
1:C:667:GLU:HG3	5:C:720:HOH:O	1.98	0.64
1:B:299:GLN:H	1:F:299:GLN:HE22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:ASN:ND2	1:F:502:LYS:HB2	2.13	0.64
1:C:256:GLN:NE2	1:C:537:GLU:H	1.94	0.63
1:E:35:GLN:NE2	1:E:470:LEU:H	1.96	0.63
1:C:645:VAL:HG12	5:C:1005:HOH:O	1.97	0.63
1:D:168:LYS:HG2	1:D:468:VAL:HG13	1.80	0.63
1:B:471:THR:CG2	1:B:473:GLU:H	2.12	0.63
1:D:471:THR:HG22	1:D:473:GLU:N	2.13	0.63
1:E:247:GLY:HA3	1:E:350:SER:HA	1.80	0.63
1:A:446:ASN:ND2	1:A:502:LYS:HB2	2.14	0.63
1:A:582:PRO:HB2	1:A:585:MET:HB2	1.80	0.63
1:F:88:LYS:HA	1:F:88:LYS:HE3	1.80	0.63
1:D:667:GLU:HG2	1:D:672:GLU:HB2	1.78	0.63
1:E:134:ILE:CD1	1:E:144:LEU:HD11	2.23	0.63
1:F:546:THR:N	1:F:550:ASN:HD21	1.97	0.63
1:A:291:THR:HG21	1:D:162:TYR:OH	1.98	0.63
1:A:491:ASN:ND2	1:A:492:HIS:H	1.97	0.62
1:D:317:PHE:CZ	1:D:373:ARG:HG2	2.34	0.62
1:B:300:ARG:HH22	1:B:409:ASP:CG	2.03	0.62
1:E:285:GLY:H	1:E:302:ASN:ND2	1.96	0.62
1:B:88:LYS:HA	1:B:88:LYS:HE3	1.81	0.62
1:E:491:ASN:ND2	1:E:492:HIS:H	1.97	0.62
1:B:285:GLY:H	1:B:302:ASN:ND2	1.97	0.62
1:B:81:GLU:HG2	1:B:292:SER:HB2	1.81	0.62
1:F:205:ASN:HD22	1:F:302:ASN:HD21	1.48	0.62
1:A:160:THR:HG21	1:A:195:SER:OG	2.00	0.62
1:C:160:THR:HG21	1:C:195:SER:OG	2.00	0.62
1:A:454:VAL:HG11	1:A:665:GLU:HG3	1.81	0.62
1:D:307:HIS:HE1	4:D:2001:FMT:O2	1.83	0.62
1:C:168:LYS:HG2	1:C:468:VAL:HG13	1.82	0.61
1:E:216:ASP:OD1	1:E:489:ARG:HD2	2.00	0.61
1:E:527:THR:HG22	1:E:530:ASN:H	1.65	0.61
1:E:23:GLN:NE2	1:E:143:VAL:H	1.93	0.61
1:A:23:GLN:HE22	1:A:143:VAL:N	1.94	0.61
1:A:471:THR:HG22	1:A:473:GLU:N	2.15	0.61
1:F:527:THR:HG22	1:F:530:ASN:H	1.64	0.61
1:D:35:GLN:NE2	1:D:470:LEU:H	1.97	0.61
1:A:168:LYS:HG2	1:A:468:VAL:HG13	1.83	0.61
1:A:526:ILE:HG13	1:A:531:ASP:OD1	1.99	0.61
1:B:158:ILE:HD11	1:F:295:THR:HA	1.82	0.61
1:B:471:THR:HG22	1:B:473:GLU:H	1.65	0.61
1:C:491:ASN:ND2	1:C:492:HIS:H	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:CG	1:C:292:SER:HB2	2.31	0.61
1:D:88:LYS:HA	1:D:88:LYS:HE3	1.83	0.61
1:A:295:THR:HA	1:D:158:ILE:HD11	1.81	0.61
1:E:256:GLN:NE2	1:E:537:GLU:H	1.92	0.61
1:F:506:ALA:HB2	1:F:547:PRO:HD3	1.81	0.61
1:E:465:THR:HG23	1:E:483:LEU:HD22	1.81	0.61
1:F:471:THR:HG22	1:F:473:GLU:N	2.16	0.60
1:B:216:ASP:OD1	1:B:489:ARG:HD2	2.00	0.60
1:B:247:GLY:HA3	1:B:350:SER:HA	1.84	0.60
1:B:471:THR:HG22	1:B:473:GLU:N	2.15	0.60
1:F:206:GLU:HG2	5:F:1237:HOH:O	2.00	0.60
1:D:527:THR:HG22	1:D:530:ASN:H	1.66	0.60
1:C:490:LEU:O	1:C:595:ARG:HD3	2.01	0.60
1:C:134:ILE:HD12	1:C:589:PHE:CZ	2.37	0.60
1:A:527:THR:HG22	1:A:530:ASN:H	1.67	0.60
1:D:471:THR:HB	1:D:474:GLU:HG3	1.84	0.60
1:C:317:PHE:CE2	1:C:373:ARG:HG2	2.37	0.60
1:D:667:GLU:HG3	5:D:694:HOH:O	2.00	0.60
1:B:380:ARG:NH2	1:B:406:SER:OG	2.34	0.59
1:C:514:PHE:HB2	1:C:611:VAL:HG13	1.83	0.59
1:B:621:THR:HG23	1:B:622:LYS:HG3	1.83	0.59
1:D:12:THR:HG23	5:D:695:HOH:O	2.02	0.59
1:B:96:LEU:HD13	1:B:128:ALA:HB3	1.85	0.59
1:D:506:ALA:HB2	1:D:547:PRO:HD3	1.83	0.59
1:C:592:LEU:HD22	1:C:593:PRO:HD2	1.84	0.59
1:A:175:ASN:C	1:A:175:ASN:HD22	2.06	0.59
1:B:99:LEU:HD13	1:B:112:SER:HB3	1.85	0.59
1:D:597:MET:HG3	1:D:598:LEU:HD13	1.84	0.59
1:B:592:LEU:HD22	1:B:593:PRO:HD2	1.83	0.59
1:D:592:LEU:HD22	1:D:593:PRO:HD2	1.85	0.59
1:E:134:ILE:HD12	1:E:589:PHE:CZ	2.38	0.58
1:E:168:LYS:HG2	1:E:468:VAL:HG13	1.83	0.58
1:A:134:ILE:HD12	1:A:589:PHE:CZ	2.38	0.58
1:B:76:LEU:HD12	1:B:77:PRO:HD2	1.84	0.58
1:C:471:THR:HG22	1:C:474:GLU:H	1.68	0.58
1:C:446:ASN:ND2	1:C:502:LYS:HB2	2.17	0.58
1:C:88:LYS:O	1:C:92:GLU:HG3	2.02	0.58
1:E:554:ARG:NH1	1:E:558:GLU:HB3	2.18	0.58
1:B:471:THR:HG22	1:B:474:GLU:H	1.67	0.58
1:B:60:ASN:ND2	1:B:63:ALA:H	2.01	0.58
1:C:506:ALA:HB2	1:C:547:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:H	1:B:10:LEU:HD23	1.68	0.58
1:D:433:HIS:HE1	1:D:642:ASP:OD2	1.85	0.58
1:D:681:HIS:HE1	5:D:1334:HOH:O	1.86	0.58
1:F:454:VAL:CG1	1:F:665:GLU:HG3	2.33	0.58
1:F:471:THR:CG2	1:F:473:GLU:H	2.17	0.58
1:E:314:LYS:NZ	1:E:381:GLN:NE2	2.51	0.58
1:F:564:GLU:HG3	5:F:869:HOH:O	2.03	0.58
1:D:60:ASN:C	1:D:60:ASN:HD22	2.07	0.58
1:E:526:ILE:HD11	5:E:717:HOH:O	2.03	0.58
1:A:568:PRO:HG2	1:A:571:GLU:HG2	1.86	0.58
1:D:491:ASN:HD22	1:D:492:HIS:N	2.01	0.58
1:E:539:ASP:OD1	1:E:559:PHE:HA	2.04	0.58
1:F:99:LEU:CD1	1:F:112:SER:HB3	2.33	0.58
1:A:285:GLY:N	1:A:302:ASN:HD22	2.00	0.58
1:A:627:TYR:CD1	1:A:628:GLU:HG2	2.39	0.58
1:D:514:PHE:HB2	1:D:611:VAL:CG1	2.33	0.58
1:E:219:LEU:HG	1:E:407:LEU:HD23	1.86	0.58
1:F:54:ASN:HB3	1:F:57:ASN:HD22	1.69	0.58
1:D:79:TYR:H	1:D:122:GLN:HE22	1.50	0.57
1:C:23:GLN:NE2	1:C:143:VAL:H	1.89	0.57
1:A:247:GLY:HA3	1:A:350:SER:HA	1.84	0.57
1:B:582:PRO:HB2	1:B:585:MET:HB2	1.86	0.57
1:B:664:HIS:HE1	1:B:667:GLU:O	1.88	0.57
1:F:314:LYS:HZ1	1:F:381:GLN:HE21	1.51	0.57
1:A:99:LEU:HD13	1:A:112:SER:HB3	1.86	0.57
1:E:380:ARG:NH2	1:E:406:SER:OG	2.37	0.57
1:B:175:ASN:HD22	1:B:175:ASN:C	2.06	0.57
1:E:440:PHE:CE1	1:E:616:PRO:HG3	2.40	0.57
1:F:250:TYR:CE1	1:F:357:GLN:HB2	2.40	0.57
1:F:60:ASN:HD22	1:F:63:ALA:H	1.52	0.57
1:C:99:LEU:HD13	1:C:112:SER:HB3	1.87	0.57
1:E:307:HIS:HE1	4:E:2005:FMT:O1	1.87	0.57
1:E:81:GLU:HG2	1:E:292:SER:HB2	1.87	0.57
1:C:327:GLN:O	1:C:331:LYS:HG2	2.05	0.57
1:E:667:GLU:HG3	5:E:745:HOH:O	2.03	0.57
1:F:650:PHE:HB2	5:F:1364:HOH:O	2.04	0.57
1:E:471:THR:HB	1:E:474:GLU:HG3	1.87	0.57
1:A:327:GLN:O	1:A:331:LYS:HG2	2.04	0.57
1:E:546:THR:N	1:E:550:ASN:HD21	2.00	0.57
1:F:642:ASP:OD1	1:F:643:ARG:HG2	2.05	0.57
1:D:122:GLN:H	1:D:122:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:CD1	1:C:112:SER:HB3	2.35	0.56
1:E:620:THR:HG22	1:E:620:THR:O	2.06	0.56
1:B:676:PRO:HA	1:B:679:PHE:CE1	2.40	0.56
1:C:621:THR:HG23	1:C:622:LYS:HG3	1.88	0.56
1:D:76:LEU:HD12	1:D:77:PRO:HD2	1.87	0.56
1:C:433:HIS:HE1	1:C:642:ASP:OD2	1.89	0.56
1:F:191:TYR:HB2	1:F:483:LEU:HD12	1.86	0.56
1:D:256:GLN:NE2	1:D:537:GLU:H	2.00	0.56
1:E:558:GLU:HG2	5:E:1059:HOH:O	2.05	0.56
1:B:81:GLU:CG	1:B:292:SER:HB2	2.35	0.56
1:A:134:ILE:HD11	1:A:144:LEU:CD1	2.35	0.56
1:A:35:GLN:HE22	1:A:470:LEU:N	1.95	0.56
1:B:295:THR:CA	1:F:158:ILE:HD11	2.33	0.56
1:A:490:LEU:O	1:A:595:ARG:HD3	2.05	0.56
1:D:446:ASN:ND2	1:D:502:LYS:HB2	2.19	0.56
1:D:23:GLN:NE2	1:D:143:VAL:H	1.95	0.55
1:D:365:GLU:OE2	1:D:368:THR:HA	2.06	0.55
1:D:526:ILE:HD11	5:D:1109:HOH:O	2.06	0.55
1:F:376:GLU:O	1:F:380:ARG:HG3	2.05	0.55
1:F:314:LYS:NZ	1:F:381:GLN:NE2	2.54	0.55
1:B:23:GLN:HE22	1:B:143:VAL:N	2.01	0.55
1:A:219:LEU:O	1:A:222:TYR:HB3	2.06	0.55
1:C:168:LYS:HG2	1:C:468:VAL:CG1	2.36	0.55
1:F:17:THR:O	1:F:21:GLU:HG2	2.07	0.55
1:F:23:GLN:HE22	1:F:143:VAL:N	1.97	0.55
5:B:791:HOH:O	2:I:10:MAN:H4	2.06	0.55
1:C:22:ARG:HD2	1:C:106:PHE:CD1	2.41	0.55
1:C:627:TYR:CD1	1:C:628:GLU:HG2	2.41	0.55
1:E:300:ARG:HD2	5:E:708:HOH:O	2.07	0.55
1:F:627:TYR:CD1	1:F:628:GLU:HG2	2.41	0.55
1:D:175:ASN:HD22	1:D:175:ASN:C	2.10	0.55
1:D:314:LYS:NZ	1:D:381:GLN:NE2	2.55	0.55
1:E:454:VAL:CG1	1:E:665:GLU:HG3	2.37	0.55
1:E:88:LYS:HE3	1:E:88:LYS:HA	1.89	0.55
1:A:471:THR:HB	1:A:474:GLU:CG	2.35	0.54
1:C:291:THR:HG21	1:E:162:TYR:OH	2.08	0.54
1:E:490:LEU:O	1:E:595:ARG:HD3	2.06	0.54
1:F:504:ASP:O	1:F:547:PRO:HB3	2.07	0.54
1:F:440:PHE:CE1	1:F:616:PRO:HG3	2.42	0.54
1:C:667:GLU:HG2	1:C:672:GLU:HB2	1.87	0.54
1:E:627:TYR:CD1	1:E:628:GLU:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLY:H	1:C:302:ASN:ND2	2.04	0.54
1:F:676:PRO:HA	1:F:679:PHE:CE1	2.42	0.54
1:E:300:ARG:HH22	1:E:409:ASP:CG	2.10	0.54
1:F:134:ILE:CD1	1:F:144:LEU:HD11	2.34	0.54
1:F:545:ILE:HG23	1:F:550:ASN:ND2	2.22	0.54
1:C:568:PRO:HG2	1:C:571:GLU:HG2	1.90	0.54
1:B:314:LYS:HE2	1:B:381:GLN:HE22	1.72	0.54
1:C:471:THR:HB	1:C:474:GLU:HG3	1.90	0.54
1:B:627:TYR:CD1	1:B:628:GLU:HG2	2.43	0.54
5:F:945:HOH:O	2:Q:9:MAN:H2	2.08	0.54
1:B:300:ARG:NH2	1:B:409:ASP:OD2	2.40	0.54
1:C:158:ILE:HD11	1:E:295:THR:HA	1.89	0.54
1:E:205:ASN:HD22	1:E:302:ASN:HD21	1.55	0.54
1:F:256:GLN:HE22	1:F:537:GLU:N	2.01	0.54
1:F:380:ARG:NH2	1:F:406:SER:OG	2.40	0.54
1:F:489:ARG:HD3	5:F:700:HOH:O	2.07	0.54
1:F:134:ILE:HD12	1:F:589:PHE:CZ	2.43	0.54
1:C:591:TYR:OH	1:C:629:LYS:HB2	2.08	0.54
1:C:256:GLN:HE22	1:C:537:GLU:N	1.98	0.53
1:C:471:THR:HG22	1:C:473:GLU:N	2.22	0.53
1:D:468:VAL:CG1	1:D:469:PHE:N	2.71	0.53
1:F:433:HIS:HE1	1:F:642:ASP:OD2	1.91	0.53
1:B:527:THR:HG22	1:B:530:ASN:H	1.71	0.53
1:D:23:GLN:O	1:D:26:VAL:HG22	2.08	0.53
1:F:81:GLU:HG2	1:F:292:SER:HB2	1.89	0.53
1:A:603:LYS:HE2	5:E:1182:HOH:O	2.09	0.53
1:C:380:ARG:NH2	1:C:406:SER:OG	2.42	0.53
1:E:433:HIS:HE1	1:E:642:ASP:OD2	1.92	0.53
1:B:471:THR:HB	1:B:474:GLU:HG3	1.90	0.53
1:D:22:ARG:O	1:D:26:VAL:HG13	2.09	0.53
1:A:81:GLU:HG2	1:A:292:SER:HB2	1.90	0.53
1:B:168:LYS:HG2	1:B:468:VAL:CG1	2.39	0.53
1:B:628:GLU:HB2	1:B:631:MET:SD	2.48	0.53
1:D:152:PRO:O	1:D:156:VAL:HG12	2.09	0.53
1:D:314:LYS:HZ1	1:D:381:GLN:HE21	1.57	0.53
1:E:22:ARG:O	1:E:26:VAL:HG13	2.08	0.53
1:F:317:PHE:CZ	1:F:373:ARG:HG2	2.43	0.53
1:A:32:ASP:OD2	1:A:35:GLN:HB3	2.09	0.53
1:B:642:ASP:OD1	1:B:643:ARG:HG2	2.08	0.53
1:C:502:LYS:HB2	1:C:502:LYS:HZ2	1.73	0.53
1:F:546:THR:H	1:F:550:ASN:ND2	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:HD11	5:A:708:HOH:O	2.09	0.53
1:F:122:GLN:NE2	1:F:122:GLN:H	2.07	0.53
1:A:205:ASN:HD22	1:A:302:ASN:HD21	1.57	0.53
1:D:18:VAL:O	1:D:22:ARG:HG3	2.09	0.53
1:B:191:TYR:HB2	1:B:483:LEU:HD12	1.89	0.53
1:C:88:LYS:HE3	1:C:88:LYS:HA	1.90	0.53
1:B:454:VAL:HG11	1:B:665:GLU:HG3	1.91	0.52
1:B:667:GLU:HG3	5:B:1197:HOH:O	2.09	0.52
1:D:380:ARG:NH2	1:D:406:SER:OG	2.42	0.52
1:D:600:ARG:HG3	1:D:664:HIS:CD2	2.44	0.52
1:A:620:THR:O	1:A:620:THR:HG22	2.09	0.52
1:B:291:THR:HG21	1:F:162:TYR:HH	1.71	0.52
1:F:256:GLN:NE2	1:F:537:GLU:H	2.01	0.52
1:A:502:LYS:HZ2	1:A:502:LYS:HB2	1.74	0.52
1:D:300:ARG:HD2	5:D:5:HOH:O	2.09	0.52
1:D:166:ARG:O	1:D:170:GLN:HG3	2.09	0.52
1:D:591:TYR:OH	1:D:629:LYS:HB2	2.10	0.52
1:D:131:ILE:O	1:D:135:GLN:HG2	2.10	0.52
1:D:285:GLY:N	1:D:302:ASN:HD22	2.00	0.52
1:D:465:THR:HG23	1:D:483:LEU:HD22	1.91	0.52
1:E:538:MET:O	1:E:559:PHE:HB3	2.10	0.52
1:C:664:HIS:HE1	1:C:667:GLU:O	1.92	0.52
1:E:285:GLY:N	1:E:302:ASN:HD22	2.05	0.52
1:E:454:VAL:HG11	1:E:665:GLU:CD	2.30	0.52
1:B:298:SER:HA	1:F:299:GLN:HE22	1.75	0.52
1:F:620:THR:O	1:F:620:THR:HG22	2.09	0.52
1:C:299:GLN:H	1:E:299:GLN:HE22	1.58	0.52
1:D:628:GLU:HB2	1:D:631:MET:SD	2.50	0.52
1:F:365:GLU:OE2	1:F:368:THR:HA	2.10	0.52
1:B:526:ILE:HD11	5:B:753:HOH:O	2.10	0.52
1:E:632:ILE:HG21	5:E:1284:HOH:O	2.10	0.52
1:A:440:PHE:CE1	1:A:616:PRO:HG3	2.45	0.51
1:F:247:GLY:HA3	1:F:350:SER:HA	1.92	0.51
1:B:491:ASN:ND2	1:B:492:HIS:H	2.08	0.51
1:A:233:TRP:O	1:A:367:VAL:HA	2.10	0.51
1:D:247:GLY:HA3	1:D:350:SER:HA	1.93	0.51
1:F:526:ILE:HD11	5:F:694:HOH:O	2.10	0.51
1:F:88:LYS:CA	1:F:88:LYS:HE3	2.41	0.51
1:C:300:ARG:HH22	1:C:409:ASP:CG	2.13	0.51
5:A:814:HOH:O	1:D:471:THR:HG23	2.09	0.51
1:A:468:VAL:CG1	1:A:469:PHE:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LYS:O	1:D:79:TYR:HB2	2.09	0.51
1:C:300:ARG:HD2	5:C:748:HOH:O	2.09	0.51
1:C:471:THR:CG2	1:C:473:GLU:H	2.24	0.51
1:D:620:THR:HG22	1:D:620:THR:O	2.11	0.51
1:E:582:PRO:HB2	1:E:585:MET:HB2	1.91	0.51
1:F:300:ARG:HH22	1:F:409:ASP:CG	2.13	0.51
1:A:300:ARG:HH22	1:A:409:ASP:CG	2.13	0.51
1:E:480:PRO:HD3	5:E:705:HOH:O	2.10	0.51
1:F:591:TYR:OH	1:F:629:LYS:HB2	2.11	0.51
1:A:491:ASN:HD22	1:A:492:HIS:N	2.05	0.51
1:D:336:GLY:HA3	1:E:331:LYS:HB2	1.93	0.51
1:D:588:ASP:HB3	1:D:591:TYR:CD1	2.46	0.51
1:E:81:GLU:CG	1:E:292:SER:HB2	2.41	0.51
1:F:363:TYR:HB2	1:F:365:GLU:HG2	1.91	0.51
1:C:175:ASN:C	1:C:175:ASN:HD22	2.13	0.51
1:C:620:THR:O	1:C:620:THR:HG22	2.11	0.50
1:C:81:GLU:HG2	1:C:292:SER:HB2	1.92	0.50
1:C:299:GLN:H	1:E:299:GLN:NE2	2.10	0.50
1:C:628:GLU:HB2	1:C:631:MET:SD	2.51	0.50
1:C:454:VAL:CG1	1:C:665:GLU:HG3	2.41	0.50
1:F:471:THR:HG22	1:F:474:GLU:H	1.77	0.50
1:B:188:ASP:OD2	1:B:188:ASP:N	2.44	0.50
1:E:473:GLU:HG2	5:E:744:HOH:O	2.10	0.50
1:F:307:HIS:HE1	4:F:2006:FMT:O2	1.95	0.50
1:D:233:TRP:O	1:D:367:VAL:HA	2.11	0.50
1:D:81:GLU:HG2	1:D:292:SER:HB2	1.92	0.50
1:E:152:PRO:O	1:E:156:VAL:HG12	2.11	0.50
1:A:642:ASP:OD1	1:A:643:ARG:HG2	2.11	0.50
1:B:81:GLU:HG2	5:B:1164:HOH:O	2.10	0.50
1:D:26:VAL:HA	1:D:129:TYR:OH	2.12	0.50
1:A:546:THR:N	1:A:550:ASN:HD21	2.08	0.50
1:A:299:GLN:HE22	1:D:299:GLN:H	1.59	0.50
1:C:491:ASN:HD22	1:C:492:HIS:N	2.08	0.50
1:B:491:ASN:HD22	1:B:492:HIS:H	1.59	0.50
1:D:96:LEU:HD13	1:D:128:ALA:HB3	1.94	0.50
1:F:23:GLN:NE2	1:F:143:VAL:H	2.00	0.50
1:F:61:LYS:O	1:F:65:GLU:HG3	2.12	0.50
1:B:563:LYS:HB3	1:B:591:TYR:HB2	1.93	0.50
1:B:648:SER:C	1:B:650:PHE:H	2.15	0.50
1:E:651:LYS:HG2	1:E:652:GLN:O	2.12	0.49
1:A:35:GLN:NE2	1:A:470:LEU:H	1.97	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:THR:HG22	1:B:620:THR:O	2.12	0.49
1:B:623:ASN:ND2	1:B:625:THR:OG1	2.45	0.49
1:B:88:LYS:O	1:B:92:GLU:HG3	2.12	0.49
1:E:365:GLU:OE2	1:E:368:THR:HA	2.12	0.49
1:F:168:LYS:HG2	1:F:468:VAL:CG1	2.40	0.49
1:B:299:GLN:HE22	1:F:298:SER:HA	1.77	0.49
1:C:468:VAL:CG1	1:C:469:PHE:N	2.74	0.49
1:D:300:ARG:HH22	1:D:409:ASP:CG	2.15	0.49
1:F:352:VAL:HG22	1:F:423:PHE:CZ	2.48	0.49
1:F:526:ILE:HG13	1:F:531:ASP:OD1	2.12	0.49
1:E:77:PRO:HB3	2:K:4:MAN:H61	1.94	0.49
1:B:468:VAL:CG1	1:B:469:PHE:N	2.76	0.49
1:E:592:LEU:HD22	1:E:593:PRO:CD	2.42	0.49
1:F:455:THR:OG1	1:F:664:HIS:HD2	1.94	0.49
1:C:81:GLU:HG3	1:C:292:SER:HB2	1.93	0.49
1:E:300:ARG:NH2	1:E:409:ASP:OD2	2.45	0.49
1:D:307:HIS:HD2	5:E:726:HOH:O	1.95	0.49
1:E:211:ALA:O	1:E:215:GLU:HB2	2.13	0.49
1:F:154:LEU:HD13	1:F:404:GLN:CG	2.43	0.49
1:B:291:THR:HG23	1:B:292:SER:O	2.13	0.49
1:C:219:LEU:O	1:C:222:TYR:HB3	2.12	0.49
1:C:314:LYS:NZ	1:C:381:GLN:HE21	2.10	0.49
1:C:526:ILE:HG13	1:C:531:ASP:OD1	2.13	0.49
1:D:251:HIS:HD2	5:D:818:HOH:O	1.96	0.49
1:C:32:ASP:OD2	1:C:35:GLN:HB3	2.13	0.49
1:D:168:LYS:HG2	1:D:468:VAL:CG1	2.42	0.49
1:D:526:ILE:HG13	1:D:531:ASP:OD1	2.11	0.49
1:D:582:PRO:HB2	1:D:585:MET:HB2	1.94	0.49
1:A:18:VAL:O	1:A:22:ARG:HG3	2.13	0.49
1:B:256:GLN:NE2	1:B:537:GLU:H	2.03	0.49
1:E:468:VAL:CG1	1:E:469:PHE:N	2.76	0.49
1:A:168:LYS:HG2	1:A:468:VAL:CG1	2.42	0.49
1:A:621:THR:HG23	1:A:622:LYS:HG3	1.95	0.48
1:C:489:ARG:HD3	5:C:682:HOH:O	2.12	0.48
1:F:134:ILE:HD11	1:F:144:LEU:CD1	2.38	0.48
1:F:611:VAL:HA	1:F:656:PHE:O	2.13	0.48
1:E:327:GLN:O	1:E:331:LYS:HG2	2.13	0.48
1:C:376:GLU:O	1:C:380:ARG:HG3	2.14	0.48
1:D:667:GLU:HG2	1:D:672:GLU:HB3	1.92	0.48
1:A:314:LYS:NZ	1:A:381:GLN:NE2	2.62	0.48
1:D:627:TYR:CD1	1:D:628:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:VAL:HA	1:F:129:TYR:OH	2.14	0.48
1:A:314:LYS:NZ	1:A:381:GLN:HE21	2.12	0.48
1:A:440:PHE:CE2	1:A:443:VAL:HG21	2.49	0.48
1:E:191:TYR:HB2	1:E:483:LEU:HD12	1.95	0.48
1:A:298:SER:HA	1:D:299:GLN:HE22	1.79	0.48
1:A:664:HIS:HE1	1:A:667:GLU:O	1.96	0.48
1:B:484:LYS:HE2	5:B:837:HOH:O	2.12	0.48
1:F:620:THR:HG23	1:F:632:ILE:O	2.14	0.48
1:B:308:SER:OG	1:B:310:GLU:HG2	2.14	0.48
1:B:323:ASN:ND2	5:B:1017:HOH:O	2.46	0.48
1:D:300:ARG:NH2	1:D:409:ASP:OD2	2.47	0.48
1:D:88:LYS:O	1:D:92:GLU:HG3	2.14	0.48
1:A:251:HIS:HE1	1:A:424:ASN:OD1	1.96	0.48
1:B:99:LEU:CD1	1:B:112:SER:HB3	2.44	0.48
1:B:307:HIS:CE1	4:B:2002:FMT:O1	2.65	0.48
1:B:575:LEU:HD23	1:B:582:PRO:HD3	1.95	0.48
1:B:78:LYS:O	1:B:79:TYR:HB2	2.14	0.48
1:C:299:GLN:NE2	1:E:299:GLN:H	2.12	0.48
1:D:219:LEU:HG	1:D:407:LEU:HD23	1.94	0.48
1:C:166:ARG:O	1:C:170:GLN:HG3	2.14	0.48
1:D:188:ASP:N	1:D:188:ASP:OD2	2.47	0.48
1:E:506:ALA:HA	1:E:545:ILE:O	2.14	0.48
1:F:22:ARG:HD2	1:F:106:PHE:CG	2.49	0.48
1:A:299:GLN:H	1:D:299:GLN:NE2	2.12	0.47
1:B:122:GLN:HE21	1:B:122:GLN:H	1.58	0.47
1:F:38:THR:HG22	1:F:43:TYR:CZ	2.49	0.47
1:A:23:GLN:NE2	1:A:143:VAL:H	1.98	0.47
1:B:248:GLU:OE2	1:B:636:PRO:HA	2.14	0.47
1:C:114:ALA:O	1:C:118:VAL:HG23	2.14	0.47
1:D:199:ASN:HB3	1:D:208:GLN:O	2.14	0.47
1:E:168:LYS:HG2	1:E:468:VAL:CG1	2.44	0.47
1:E:222:TYR:CD2	1:E:592:LEU:HD23	2.48	0.47
1:B:256:GLN:HE22	1:B:537:GLU:N	2.06	0.47
1:D:134:ILE:HD12	1:D:589:PHE:CZ	2.50	0.47
1:F:468:VAL:CG1	1:F:469:PHE:N	2.77	0.47
1:D:107:ASP:OD1	1:D:111:LYS:HE3	2.15	0.47
1:D:256:GLN:HE22	1:D:537:GLU:N	2.03	0.47
1:E:219:LEU:O	1:E:222:TYR:HB3	2.14	0.47
1:E:451:ASP:OD2	1:E:496:ASN:HB2	2.14	0.47
1:E:471:THR:CG2	1:E:473:GLU:H	2.27	0.47
1:A:131:ILE:O	1:A:135:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:VAL:HG22	1:C:423:PHE:CZ	2.50	0.47
1:C:78:LYS:O	1:C:79:TYR:HB2	2.13	0.47
1:F:219:LEU:HG	1:F:407:LEU:HD23	1.95	0.47
1:A:222:TYR:CD2	1:A:592:LEU:HD23	2.50	0.47
1:C:471:THR:HG22	1:C:473:GLU:H	1.78	0.47
1:D:446:ASN:HB2	1:D:500:ASP:OD1	2.14	0.47
1:A:307:HIS:HE1	4:A:2003:FMT:O2	1.98	0.47
1:B:629:LYS:HG2	5:B:727:HOH:O	2.14	0.47
1:A:299:GLN:NE2	1:D:299:GLN:H	2.13	0.47
1:B:220:ASN:ND2	5:B:776:HOH:O	2.41	0.47
1:B:313:GLU:OE2	1:B:373:ARG:NH1	2.46	0.47
1:B:440:PHE:CE1	1:B:616:PRO:HG3	2.50	0.47
1:E:546:THR:H	1:E:550:ASN:ND2	2.04	0.47
1:F:35:GLN:NE2	1:F:470:LEU:H	2.05	0.47
1:F:502:LYS:HZ2	1:F:502:LYS:HB2	1.80	0.47
1:B:446:ASN:ND2	1:B:502:LYS:HB2	2.29	0.47
1:D:408:ARG:HD3	5:D:1143:HOH:O	2.15	0.47
1:D:433:HIS:CD2	1:D:643:ARG:HD2	2.49	0.47
1:E:471:THR:HG23	5:E:744:HOH:O	2.14	0.47
1:E:514:PHE:HB2	1:E:611:VAL:CG1	2.44	0.47
1:C:529:GLU:OE2	2:Q:10:MAN:H61	2.15	0.47
1:A:562:PHE:HB2	1:A:594:LYS:HB3	1.96	0.47
1:B:327:GLN:O	1:B:331:LYS:HG2	2.15	0.47
1:B:35:GLN:NE2	1:B:470:LEU:H	1.95	0.47
1:B:502:LYS:HB2	1:B:502:LYS:NZ	2.29	0.47
1:C:10:LEU:CD2	1:C:10:LEU:H	2.27	0.47
1:D:642:ASP:OD1	1:D:643:ARG:HG2	2.14	0.47
1:E:314:LYS:HZ2	1:E:381:GLN:NE2	2.12	0.47
1:B:22:ARG:HD2	1:B:106:PHE:CD1	2.50	0.47
1:C:248:GLU:OE2	1:C:636:PRO:HA	2.15	0.47
1:D:251:HIS:HE1	1:D:424:ASN:OD1	1.98	0.47
1:D:440:PHE:CE1	1:D:616:PRO:HG3	2.50	0.47
1:F:78:LYS:O	1:F:79:TYR:HB2	2.14	0.47
1:A:76:LEU:HD12	1:A:77:PRO:HD2	1.97	0.46
1:C:211:ALA:O	1:C:215:GLU:HB2	2.16	0.46
1:A:83:SER:H	1:A:89:LEU:HD23	1.80	0.46
1:B:60:ASN:HD22	1:B:63:ALA:H	1.62	0.46
1:C:472:GLU:HB2	5:C:706:HOH:O	2.15	0.46
1:D:471:THR:CG2	1:D:473:GLU:H	2.26	0.46
1:E:78:LYS:O	1:E:79:TYR:HB2	2.15	0.46
1:B:619:SER:O	1:B:634:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLN:H	1:C:122:GLN:NE2	2.13	0.46
1:C:642:ASP:OD1	1:C:643:ARG:HG2	2.15	0.46
1:E:10:LEU:CD2	1:E:10:LEU:H	2.26	0.46
1:E:17:THR:O	1:E:21:GLU:HG2	2.16	0.46
1:A:333:VAL:HG23	1:A:341:ILE:O	2.16	0.46
1:C:285:GLY:HA2	1:C:300:ARG:HH11	1.79	0.46
1:C:54:ASN:HD22	1:C:57:ASN:HD22	1.63	0.46
1:D:352:VAL:HG22	1:D:423:PHE:CZ	2.51	0.46
1:D:454:VAL:HG11	1:D:665:GLU:HG3	1.95	0.46
1:B:365:GLU:OE2	1:B:368:THR:HA	2.15	0.46
1:E:233:TRP:O	1:E:367:VAL:HA	2.15	0.46
1:B:651:LYS:HG2	1:B:652:GLN:O	2.16	0.46
1:B:88:LYS:HE3	1:B:88:LYS:CA	2.45	0.46
1:E:664:HIS:HE1	1:E:667:GLU:O	1.98	0.46
1:B:299:GLN:N	1:F:299:GLN:HE22	2.12	0.46
1:F:427:LYS:HD3	1:F:642:ASP:O	2.16	0.46
1:B:148:TYR:HA	1:B:155:PHE:CD1	2.50	0.46
1:C:427:LYS:HD3	1:C:642:ASP:O	2.16	0.46
1:F:378:VAL:O	1:F:382:VAL:HG13	2.15	0.46
1:A:148:TYR:HA	1:A:155:PHE:CD1	2.51	0.46
1:B:26:VAL:HA	1:B:129:TYR:OH	2.16	0.46
1:C:299:GLN:HE22	1:E:299:GLN:H	1.62	0.46
1:E:336:GLY:HA3	1:F:331:LYS:HB2	1.97	0.46
1:B:451:ASP:OD2	1:B:496:ASN:HB2	2.16	0.46
1:B:527:THR:O	1:B:527:THR:HG22	2.14	0.46
1:E:122:GLN:H	1:E:122:GLN:HE21	1.64	0.46
1:F:309:GLU:HA	1:F:312:TYR:CE1	2.51	0.46
1:F:433:HIS:CD2	1:F:643:ARG:HD2	2.51	0.46
1:B:176:PRO:O	1:B:180:VAL:HG23	2.16	0.45
1:B:336:GLY:HA3	1:C:331:LYS:HB2	1.98	0.45
1:E:179:ALA:HB1	1:E:184:ILE:HB	1.98	0.45
1:C:428:GLN:NE2	5:C:794:HOH:O	2.48	0.45
1:C:611:VAL:HA	1:C:656:PHE:O	2.16	0.45
1:D:89:LEU:N	1:D:89:LEU:CD1	2.79	0.45
1:A:309:GLU:HA	1:A:312:TYR:CE1	2.51	0.45
1:A:651:LYS:HG2	1:A:652:GLN:O	2.16	0.45
1:C:124:GLN:NE2	5:C:688:HOH:O	2.49	0.45
1:E:175:ASN:C	1:E:175:ASN:ND2	2.68	0.45
1:F:168:LYS:HD3	1:F:468:VAL:HG11	1.99	0.45
1:F:300:ARG:NH2	1:F:409:ASP:OD2	2.50	0.45
1:C:455:THR:OG1	1:C:664:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:CD1	1:D:112:SER:HB3	2.44	0.45
1:E:563:LYS:HB3	1:E:591:TYR:HB2	1.98	0.45
1:E:625:THR:N	1:E:626:PRO:CD	2.80	0.45
1:A:331:LYS:HB2	1:C:336:GLY:HA3	1.98	0.45
1:A:54:ASN:HB3	1:A:57:ASN:HD22	1.80	0.45
1:B:489:ARG:HD3	5:B:682:HOH:O	2.15	0.45
1:C:300:ARG:NH2	1:C:409:ASP:OD2	2.50	0.45
1:C:483:LEU:HD13	1:C:483:LEU:N	2.32	0.45
1:A:451:ASP:OD2	1:A:496:ASN:HB2	2.16	0.45
1:D:89:LEU:N	1:D:89:LEU:HD12	2.31	0.45
1:A:88:LYS:HE3	1:A:88:LYS:HA	1.97	0.45
1:B:517:PRO:HG2	1:B:526:ILE:HG12	1.99	0.45
1:A:211:ALA:O	1:A:215:GLU:HB2	2.16	0.45
1:D:22:ARG:HD2	1:D:106:PHE:CD1	2.52	0.45
1:A:26:VAL:HA	1:A:129:TYR:OH	2.16	0.45
1:B:299:GLN:HE22	1:F:299:GLN:N	2.13	0.45
1:C:206:GLU:HG2	5:C:721:HOH:O	2.17	0.45
1:C:307:HIS:HE1	4:C:2004:FMT:O2	1.99	0.45
1:C:667:GLU:HG2	1:C:672:GLU:HB3	1.97	0.45
1:E:433:HIS:HB3	1:E:438:LEU:HD13	1.98	0.45
1:E:491:ASN:HD22	1:E:492:HIS:N	2.10	0.45
1:F:667:GLU:HG2	1:F:672:GLU:HB3	1.94	0.45
1:C:179:ALA:HB1	1:C:184:ILE:HB	1.98	0.44
1:C:676:PRO:HA	1:C:679:PHE:CE1	2.52	0.44
1:E:160:THR:HG21	1:E:195:SER:CB	2.47	0.44
1:F:219:LEU:O	1:F:222:TYR:HB3	2.17	0.44
1:A:601:GLY:HA3	1:A:662:VAL:HG12	2.00	0.44
1:B:652:GLN:OE1	1:B:652:GLN:HA	2.16	0.44
1:C:600:ARG:HG3	1:C:664:HIS:CD2	2.52	0.44
1:F:81:GLU:CG	1:F:292:SER:HB2	2.47	0.44
1:A:322:GLU:HB2	5:A:793:HOH:O	2.17	0.44
1:A:433:HIS:CD2	1:A:643:ARG:HD2	2.52	0.44
1:B:186:LYS:HE2	1:B:191:TYR:CZ	2.52	0.44
1:C:219:LEU:HG	1:C:407:LEU:HD23	1.97	0.44
1:C:652:GLN:HA	1:C:652:GLN:OE1	2.17	0.44
1:D:211:ALA:O	1:D:215:GLU:HB2	2.17	0.44
1:F:592:LEU:HD22	1:F:593:PRO:HD2	1.99	0.44
1:C:251:HIS:HE1	1:C:424:ASN:OD1	2.01	0.44
1:D:309:GLU:HA	1:D:312:TYR:CE1	2.52	0.44
1:D:592:LEU:HD13	1:D:593:PRO:O	2.17	0.44
1:F:168:LYS:CD	1:F:468:VAL:HG11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:N	1:A:188:ASP:OD2	2.51	0.44
1:B:34:ASP:OD2	1:B:122:GLN:HG3	2.17	0.44
1:E:99:LEU:HD13	1:E:112:SER:HB3	2.00	0.44
1:E:256:GLN:HE22	1:E:537:GLU:N	1.95	0.44
1:E:483:LEU:HD13	1:E:483:LEU:N	2.32	0.44
1:E:622:LYS:HB3	1:E:622:LYS:HZ3	1.83	0.44
1:E:643:ARG:HH11	1:E:643:ARG:HG2	1.83	0.44
1:F:18:VAL:O	1:F:22:ARG:HG3	2.17	0.44
1:A:341:ILE:HG22	1:A:345:ASP:OD1	2.17	0.44
1:A:591:TYR:OH	1:A:629:LYS:HB2	2.17	0.44
1:B:134:ILE:HD12	1:B:589:PHE:CZ	2.53	0.44
1:C:225:PHE:O	1:C:229:HIS:HB2	2.17	0.44
1:D:160:THR:HG21	1:D:195:SER:CB	2.48	0.44
1:F:154:LEU:HD13	1:F:404:GLN:HG3	1.98	0.44
1:F:210:LEU:HD13	1:F:270:LEU:HD12	1.99	0.44
1:F:246:ARG:HG2	5:F:744:HOH:O	2.17	0.44
1:A:166:ARG:O	1:A:170:GLN:HG3	2.17	0.44
1:A:300:ARG:NH2	1:A:409:ASP:OD2	2.51	0.44
1:C:322:GLU:O	1:C:326:VAL:HG23	2.18	0.44
1:E:22:ARG:HD2	1:E:106:PHE:CG	2.52	0.44
1:E:168:LYS:CD	1:E:468:VAL:HG11	2.48	0.44
1:E:489:ARG:HD3	5:E:683:HOH:O	2.18	0.44
1:D:22:ARG:HD2	1:D:106:PHE:CG	2.53	0.44
1:E:611:VAL:HA	1:E:656:PHE:O	2.17	0.44
1:E:88:LYS:HE3	1:E:88:LYS:CA	2.47	0.44
1:F:175:ASN:C	1:F:175:ASN:HD22	2.21	0.44
1:A:502:LYS:NZ	1:A:502:LYS:HB2	2.32	0.44
1:C:451:ASP:OD2	1:C:496:ASN:HB2	2.18	0.44
1:A:483:LEU:HD13	1:A:483:LEU:N	2.33	0.43
1:A:570:THR:HG23	5:A:1027:HOH:O	2.16	0.43
1:F:96:LEU:HD13	1:F:128:ALA:HB3	1.99	0.43
1:B:251:HIS:HE1	1:B:424:ASN:OD1	2.01	0.43
1:B:667:GLU:HG2	1:B:672:GLU:HB3	1.95	0.43
1:C:625:THR:N	1:C:626:PRO:CD	2.82	0.43
1:D:202:THR:HG23	1:D:202:THR:O	2.19	0.43
1:F:560:VAL:HG11	5:F:736:HOH:O	2.18	0.43
1:A:134:ILE:CD1	1:A:144:LEU:HD11	2.44	0.43
1:C:175:ASN:ND2	5:C:1174:HOH:O	2.51	0.43
1:E:251:HIS:HE1	1:E:424:ASN:OD1	2.01	0.43
1:F:23:GLN:O	1:F:26:VAL:HG22	2.18	0.43
1:B:166:ARG:O	1:B:170:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:PRO:HB2	1:C:585:MET:HB2	1.99	0.43
1:C:88:LYS:HE3	1:C:88:LYS:CA	2.48	0.43
1:B:546:THR:N	1:B:550:ASN:HD21	2.06	0.43
1:D:314:LYS:HZ3	1:D:381:GLN:HE21	1.63	0.43
1:D:468:VAL:HG13	1:D:469:PHE:N	2.33	0.43
1:F:506:ALA:O	1:F:507:THR:HG23	2.17	0.43
1:B:541:PHE:CE1	1:B:554:ARG:HG3	2.54	0.43
1:D:664:HIS:HE1	1:D:667:GLU:O	2.01	0.43
1:E:34:ASP:OD2	1:E:122:GLN:HG3	2.19	0.43
1:E:618:GLU:HG3	1:E:619:SER:H	1.83	0.43
1:A:455:THR:OG1	1:A:664:HIS:HD2	2.01	0.43
1:F:471:THR:HB	1:F:474:GLU:HG3	1.99	0.43
1:A:96:LEU:HD13	1:A:128:ALA:HB3	2.00	0.43
1:A:465:THR:HA	1:A:483:LEU:HD23	2.00	0.43
1:A:560:VAL:HG11	5:A:865:HOH:O	2.18	0.43
1:E:175:ASN:ND2	1:E:178:ALA:H	2.17	0.43
1:F:22:ARG:HD2	1:F:106:PHE:CD1	2.54	0.43
1:F:99:LEU:HD13	1:F:112:SER:HB3	1.98	0.43
1:A:99:LEU:CD1	1:A:112:SER:HB3	2.49	0.43
1:A:606:PHE:CG	1:A:607:PRO:HD2	2.54	0.43
5:C:737:HOH:O	1:E:159:ASP:HB3	2.18	0.43
1:E:510:VAL:O	1:E:614:VAL:HA	2.19	0.43
1:E:620:THR:HG21	5:E:1361:HOH:O	2.18	0.43
1:F:16:ASP:O	1:F:20:VAL:HG23	2.19	0.43
1:A:628:GLU:HB2	1:A:631:MET:SD	2.58	0.43
1:B:233:TRP:O	1:B:367:VAL:HA	2.18	0.43
1:B:83:SER:H	1:B:89:LEU:HD23	1.83	0.43
1:C:233:TRP:O	1:C:367:VAL:HA	2.19	0.43
1:C:31:GLN:O	1:C:32:ASP:C	2.58	0.43
1:F:79:TYR:H	1:F:122:GLN:HE22	1.61	0.43
1:B:465:THR:HG23	1:B:483:LEU:HD22	2.01	0.42
1:B:262:TYR:CE1	1:B:534:LYS:HD3	2.54	0.42
1:B:96:LEU:HD13	1:B:128:ALA:CB	2.48	0.42
1:E:676:PRO:HA	1:E:679:PHE:CE1	2.54	0.42
1:C:400:LEU:HD12	1:C:400:LEU:HA	1.84	0.42
1:D:10:LEU:CD2	1:D:10:LEU:H	2.30	0.42
1:A:295:THR:CA	1:D:158:ILE:HD11	2.49	0.42
1:D:489:ARG:HD3	5:D:711:HOH:O	2.19	0.42
1:E:620:THR:HG23	1:E:632:ILE:O	2.18	0.42
1:A:380:ARG:NH1	1:A:416:TYR:OH	2.52	0.42
1:B:625:THR:N	1:B:626:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:LYS:HE2	5:D:773:HOH:O	2.19	0.42
1:E:441:VAL:HG23	1:E:441:VAL:O	2.20	0.42
1:A:168:LYS:CD	1:A:468:VAL:HG11	2.48	0.42
1:A:623:ASN:ND2	1:A:625:THR:OG1	2.52	0.42
1:B:285:GLY:HA2	1:B:300:ARG:HH11	1.84	0.42
1:B:395:PHE:HA	5:B:1230:HOH:O	2.19	0.42
1:F:327:GLN:O	1:F:331:LYS:HG2	2.19	0.42
1:F:83:SER:H	1:F:89:LEU:HD23	1.84	0.42
1:B:477:THR:OG1	1:B:478:LYS:N	2.52	0.42
1:E:32:ASP:OD2	1:E:35:GLN:HB3	2.20	0.42
1:E:526:ILE:HG13	1:E:531:ASP:OD1	2.19	0.42
1:A:352:VAL:HG11	1:A:426:PHE:CE2	2.54	0.42
1:A:546:THR:H	1:A:550:ASN:ND2	2.11	0.42
1:D:563:LYS:HB3	1:D:591:TYR:HB2	2.00	0.42
1:D:676:PRO:HA	1:D:679:PHE:CE1	2.55	0.42
1:B:440:PHE:CE2	1:B:443:VAL:HG21	2.55	0.42
1:B:433:HIS:CD2	1:B:643:ARG:HD2	2.55	0.42
1:D:31:GLN:O	1:D:32:ASP:C	2.58	0.42
1:F:88:LYS:HA	1:F:88:LYS:CE	2.46	0.42
1:A:175:ASN:C	1:A:175:ASN:ND2	2.72	0.42
1:A:309:GLU:HA	1:A:312:TYR:CD1	2.54	0.42
1:A:620:THR:HG23	1:A:632:ILE:O	2.20	0.42
1:B:60:ASN:HD22	1:B:60:ASN:C	2.22	0.42
1:D:158:ILE:HA	1:D:161:THR:HB	2.02	0.42
1:D:643:ARG:HG2	1:D:643:ARG:HH11	1.83	0.42
1:A:81:GLU:CG	1:A:292:SER:HB2	2.50	0.42
1:B:492:HIS:HE1	1:B:594:LYS:O	2.02	0.42
1:D:12:THR:OG1	1:D:580:LYS:HB3	2.19	0.42
1:D:651:LYS:HG2	1:D:652:GLN:O	2.20	0.42
1:E:667:GLU:HG2	1:E:672:GLU:HB3	1.99	0.42
1:F:637:LEU:HA	5:F:1043:HOH:O	2.20	0.42
1:F:651:LYS:HG3	1:F:652:GLN:O	2.20	0.42
1:F:285:GLY:H	1:F:302:ASN:ND2	2.09	0.42
1:B:250:TYR:CE1	1:B:357:GLN:HB2	2.55	0.41
1:E:632:ILE:CG2	5:E:1284:HOH:O	2.68	0.41
1:F:454:VAL:HG11	1:F:665:GLU:HG3	2.02	0.41
1:C:210:LEU:HD13	1:C:270:LEU:HD12	2.02	0.41
1:C:378:VAL:O	1:C:382:VAL:HG13	2.20	0.41
1:E:309:GLU:HA	1:E:312:TYR:CE1	2.55	0.41
1:F:625:THR:N	1:F:626:PRO:CD	2.83	0.41
1:A:352:VAL:HG11	1:A:426:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LEU:HD21	1:C:184:ILE:HG21	2.01	0.41
1:C:506:ALA:HA	1:C:545:ILE:O	2.20	0.41
1:D:209:ARG:HD2	1:D:268:ASN:CG	2.37	0.41
1:D:210:LEU:HD13	1:D:270:LEU:HD12	2.02	0.41
1:E:314:LYS:HZ1	1:E:381:GLN:NE2	2.17	0.41
1:E:554:ARG:HH11	1:E:558:GLU:HB3	1.85	0.41
1:E:562:PHE:HB2	1:E:594:LYS:HB3	2.03	0.41
1:B:468:VAL:HG13	1:B:469:PHE:N	2.34	0.41
1:C:26:VAL:HA	1:C:129:TYR:OH	2.20	0.41
1:C:298:SER:HA	1:E:299:GLN:HE22	1.86	0.41
1:D:61:LYS:O	1:D:65:GLU:HG3	2.20	0.41
1:A:506:ALA:HA	1:A:545:ILE:O	2.20	0.41
1:A:625:THR:N	1:A:626:PRO:CD	2.83	0.41
1:D:191:TYR:HB2	1:D:483:LEU:HD12	2.03	0.41
1:F:455:THR:OG1	1:F:664:HIS:CD2	2.72	0.41
1:F:502:LYS:HB2	1:F:502:LYS:NZ	2.35	0.41
1:A:10:LEU:CD2	1:A:10:LEU:H	2.26	0.41
1:A:299:GLN:H	1:D:299:GLN:HE22	1.69	0.41
1:A:588:ASP:HB3	1:A:591:TYR:CD1	2.56	0.41
1:B:588:ASP:HB3	1:B:591:TYR:CD1	2.56	0.41
1:D:32:ASP:OD2	1:D:35:GLN:NE2	2.51	0.41
1:D:380:ARG:NH1	1:D:416:TYR:OH	2.53	0.41
1:F:646:ASP:O	1:F:647:THR:C	2.59	0.41
1:A:538:MET:O	1:A:559:PHE:HB3	2.21	0.41
1:B:291:THR:HG21	1:F:162:TYR:CZ	2.55	0.41
1:D:309:GLU:HA	1:D:312:TYR:CD1	2.56	0.41
1:E:89:LEU:N	1:E:89:LEU:HD12	2.36	0.41
1:A:492:HIS:HE1	1:A:594:LYS:O	2.04	0.41
1:E:628:GLU:HB2	1:E:631:MET:SD	2.61	0.41
1:C:112:SER:O	1:C:115:PHE:HB3	2.21	0.41
1:D:285:GLY:HA2	1:D:300:ARG:HH11	1.86	0.41
1:F:164:MET:HG2	1:F:193:TYR:CE2	2.55	0.41
1:F:622:LYS:NZ	1:F:622:LYS:CB	2.83	0.41
1:A:334:PHE:HB2	1:A:341:ILE:HG13	2.03	0.41
1:A:669:HIS:HB3	1:A:671:TYR:CE1	2.56	0.41
1:B:12:THR:HG22	5:B:1093:HOH:O	2.20	0.41
1:D:168:LYS:CD	1:D:468:VAL:HG11	2.51	0.41
1:E:35:GLN:HE22	1:E:470:LEU:N	2.04	0.41
1:F:166:ARG:O	1:F:170:GLN:HG3	2.21	0.41
1:A:468:VAL:HG13	1:A:469:PHE:N	2.36	0.41
1:B:31:GLN:O	1:B:32:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:VAL:HG22	1:B:423:PHE:CZ	2.55	0.41
1:C:22:ARG:HD2	1:C:106:PHE:CG	2.56	0.41
1:C:471:THR:CG2	1:C:472:GLU:N	2.84	0.41
1:E:314:LYS:HZ1	1:E:381:GLN:HE21	1.69	0.41
1:E:591:TYR:OH	1:E:629:LYS:HB2	2.21	0.41
1:F:465:THR:HA	1:F:483:LEU:HD23	2.02	0.41
1:A:31:GLN:O	1:A:32:ASP:C	2.60	0.40
1:C:323:ASN:ND2	5:C:724:HOH:O	2.51	0.40
1:C:58:TYR:HA	1:C:102:TYR:O	2.20	0.40
1:D:541:PHE:CE1	1:D:554:ARG:HG3	2.56	0.40
1:E:440:PHE:CD1	1:E:616:PRO:HG3	2.56	0.40
1:F:23:GLN:HG2	1:F:576:LEU:HD21	2.02	0.40
1:F:588:ASP:HB3	1:F:591:TYR:CD1	2.56	0.40
1:C:309:GLU:HA	1:C:312:TYR:CD1	2.57	0.40
1:C:38:THR:HA	1:C:43:TYR:CG	2.56	0.40
1:C:191:TYR:HB2	1:C:483:LEU:HD12	2.03	0.40
1:C:88:LYS:HG2	1:C:392:LYS:CD	2.39	0.40
1:E:278:TRP:CZ2	1:E:318:LEU:HD13	2.57	0.40
1:E:365:GLU:OE2	1:E:372:GLN:OE1	2.39	0.40
1:A:667:GLU:HG2	1:A:672:GLU:HB3	1.99	0.40
1:B:186:LYS:HE2	1:B:191:TYR:CE2	2.56	0.40
1:B:510:VAL:HG23	1:B:617:PHE:HB2	2.02	0.40
1:C:35:GLN:NE2	1:C:470:LEU:H	2.13	0.40
1:D:281:PRO:HA	1:D:304:TYR:O	2.22	0.40
1:D:451:ASP:OD2	1:D:496:ASN:HB2	2.22	0.40
1:F:189:ASN:HB2	5:F:755:HOH:O	2.22	0.40
1:F:314:LYS:HZ3	1:F:381:GLN:HE21	1.67	0.40
1:F:454:VAL:HG13	1:F:665:GLU:HG3	2.03	0.40
1:A:168:LYS:HE3	1:A:468:VAL:CG1	2.51	0.40
1:B:32:ASP:OD2	1:B:35:GLN:HB3	2.22	0.40
1:C:388:LYS:HB2	1:C:388:LYS:HE3	1.90	0.40
1:E:355:TYR:HA	1:E:362:LEU:HD22	2.03	0.40
1:A:75:PHE:HB3	5:A:772:HOH:O	2.21	0.40
1:C:433:HIS:CD2	1:C:643:ARG:HD2	2.57	0.40
1:C:651:LYS:HG2	1:C:652:GLN:O	2.21	0.40
1:E:22:ARG:HD2	1:E:106:PHE:CD1	2.57	0.40
1:F:333:VAL:HG21	1:F:340:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	672/674 (100%)	649 (97%)	20 (3%)	3 (0%)	34	41
1	B	672/674 (100%)	649 (97%)	21 (3%)	2 (0%)	41	49
1	C	672/674 (100%)	653 (97%)	17 (2%)	2 (0%)	41	49
1	D	672/674 (100%)	655 (98%)	13 (2%)	4 (1%)	25	29
1	E	672/674 (100%)	651 (97%)	18 (3%)	3 (0%)	34	41
1	F	672/674 (100%)	649 (97%)	20 (3%)	3 (0%)	34	41
All	All	4032/4044 (100%)	3906 (97%)	109 (3%)	17 (0%)	34	41

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	ASP
1	C	646	ASP
1	E	240	GLY
1	F	240	GLY
1	F	646	ASP
1	A	87	ASP
1	A	240	GLY
1	C	240	GLY
1	E	646	ASP
1	E	87	ASP
1	F	87	ASP
1	B	240	GLY
1	D	646	ASP
1	A	646	ASP
1	D	87	ASP
1	D	632	ILE
1	D	240	GLY

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	613/613 (100%)	574 (94%)	39 (6%)	17	22
1	B	613/613 (100%)	570 (93%)	43 (7%)	15	18
1	C	613/613 (100%)	574 (94%)	39 (6%)	17	22
1	D	613/613 (100%)	573 (94%)	40 (6%)	17	21
1	E	613/613 (100%)	575 (94%)	38 (6%)	18	23
1	F	613/613 (100%)	576 (94%)	37 (6%)	19	25
All	All	3678/3678 (100%)	3442 (94%)	236 (6%)	17	22

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	60	ASN
1	A	88	LYS
1	A	96	LEU
1	A	99	LEU
1	A	122	GLN
1	A	130	TYR
1	A	160	THR
1	A	175	ASN
1	A	188	ASP
1	A	203	TYR
1	A	210	LEU
1	A	258	LEU
1	A	266	LEU
1	A	290	LEU
1	A	323	ASN
1	A	329	LEU
1	A	341	ILE
1	A	352	VAL
1	A	366	GLU
1	A	373	ARG
1	A	400	LEU

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Mol	Chain	Res	Type
1	A	423	PHE
1	A	431	GLU
1	A	440	PHE
1	A	453	LEU
1	A	483	LEU
1	A	491	ASN
1	A	502	LYS
1	A	511	VAL
1	A	527	THR
1	A	554	ARG
1	A	558	GLU
1	A	577	GLU
1	A	595	ARG
1	A	598	LEU
1	A	611	VAL
1	A	614	VAL
1	A	660	VAL
1	B	29	LEU
1	B	60	ASN
1	B	80	ASN
1	B	88	LYS
1	B	96	LEU
1	B	99	LEU
1	B	107	ASP
1	B	122	GLN
1	B	130	TYR
1	B	160	THR
1	B	175	ASN
1	B	188	ASP
1	B	203	TYR
1	B	209	ARG
1	B	210	LEU
1	B	258	LEU
1	B	266	LEU
1	B	290	LEU
1	B	291	THR
1	B	323	ASN
1	B	329	LEU
1	B	366	GLU
1	B	373	ARG
1	B	400	LEU
1	B	423	PHE

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Mol	Chain	Res	Type
1	B	440	PHE
1	B	453	LEU
1	B	471	THR
1	B	483	LEU
1	B	491	ASN
1	B	502	LYS
1	B	511	VAL
1	B	526	ILE
1	B	527	THR
1	B	554	ARG
1	B	558	GLU
1	B	572	LEU
1	B	577	GLU
1	B	585	MET
1	B	595	ARG
1	B	611	VAL
1	B	614	VAL
1	B	660	VAL
1	C	29	LEU
1	C	35	GLN
1	C	44	LYS
1	C	60	ASN
1	C	88	LYS
1	C	96	LEU
1	C	99	LEU
1	C	122	GLN
1	C	130	TYR
1	C	160	THR
1	C	175	ASN
1	C	203	TYR
1	C	209	ARG
1	C	258	LEU
1	C	266	LEU
1	C	290	LEU
1	C	323	ASN
1	C	329	LEU
1	C	352	VAL
1	C	400	LEU
1	C	423	PHE
1	C	431	GLU
1	C	438	LEU
1	C	440	PHE

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Mol	Chain	Res	Type
1	C	453	LEU
1	C	471	THR
1	C	483	LEU
1	C	491	ASN
1	C	502	LYS
1	C	511	VAL
1	C	527	THR
1	C	554	ARG
1	C	558	GLU
1	C	577	GLU
1	C	587	GLU
1	C	598	LEU
1	C	611	VAL
1	C	614	VAL
1	C	660	VAL
1	D	17	THR
1	D	29	LEU
1	D	60	ASN
1	D	88	LYS
1	D	96	LEU
1	D	99	LEU
1	D	122	GLN
1	D	130	TYR
1	D	160	THR
1	D	175	ASN
1	D	188	ASP
1	D	203	TYR
1	D	209	ARG
1	D	210	LEU
1	D	258	LEU
1	D	266	LEU
1	D	290	LEU
1	D	323	ASN
1	D	329	LEU
1	D	350	SER
1	D	352	VAL
1	D	366	GLU
1	D	400	LEU
1	D	423	PHE
1	D	438	LEU
1	D	440	PHE
1	D	453	LEU

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Mol	Chain	Res	Type
1	D	483	LEU
1	D	491	ASN
1	D	511	VAL
1	D	526	ILE
1	D	527	THR
1	D	554	ARG
1	D	558	GLU
1	D	572	LEU
1	D	577	GLU
1	D	595	ARG
1	D	611	VAL
1	D	643	ARG
1	D	660	VAL
1	E	29	LEU
1	E	60	ASN
1	E	80	ASN
1	E	88	LYS
1	E	96	LEU
1	E	99	LEU
1	E	122	GLN
1	E	130	TYR
1	E	160	THR
1	E	175	ASN
1	E	203	TYR
1	E	210	LEU
1	E	258	LEU
1	E	266	LEU
1	E	290	LEU
1	E	329	LEU
1	E	350	SER
1	E	366	GLU
1	E	373	ARG
1	E	400	LEU
1	E	423	PHE
1	E	438	LEU
1	E	440	PHE
1	E	453	LEU
1	E	471	THR
1	E	483	LEU
1	E	491	ASN
1	E	511	VAL
1	E	527	THR

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Mol	Chain	Res	Type
1	E	558	GLU
1	E	572	LEU
1	E	577	GLU
1	E	587	GLU
1	E	598	LEU
1	E	640	PRO
1	E	643	ARG
1	E	660	VAL
1	E	661	SER
1	F	35	GLN
1	F	60	ASN
1	F	88	LYS
1	F	96	LEU
1	F	122	GLN
1	F	130	TYR
1	F	160	THR
1	F	175	ASN
1	F	203	TYR
1	F	209	ARG
1	F	210	LEU
1	F	258	LEU
1	F	266	LEU
1	F	323	ASN
1	F	329	LEU
1	F	350	SER
1	F	352	VAL
1	F	366	GLU
1	F	400	LEU
1	F	423	PHE
1	F	431	GLU
1	F	438	LEU
1	F	440	PHE
1	F	453	LEU
1	F	471	THR
1	F	483	LEU
1	F	491	ASN
1	F	502	LYS
1	F	511	VAL
1	F	527	THR
1	F	554	ARG
1	F	558	GLU
1	F	577	GLU

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Mol	Chain	Res	Type
1	F	598	LEU
1	F	611	VAL
1	F	640	PRO
1	F	660	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (183) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	GLN
1	A	54	ASN
1	A	60	ASN
1	A	80	ASN
1	A	119	HIS
1	A	122	GLN
1	A	124	GLN
1	A	170	GLN
1	A	175	ASN
1	A	220	ASN
1	A	251	HIS
1	A	256	GLN
1	A	299	GLN
1	A	302	ASN
1	A	307	HIS
1	A	327	GLN
1	A	381	GLN
1	A	433	HIS
1	A	439	HIS
1	A	446	ASN
1	A	487	GLN
1	A	491	ASN
1	A	492	HIS
1	A	493	GLN
1	A	530	ASN
1	A	550	ASN
1	A	623	ASN
1	A	664	HIS
1	A	669	HIS
1	B	23	GLN
1	B	35	GLN
1	B	54	ASN
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	80	ASN
1	B	86	HIS
1	B	119	HIS
1	B	122	GLN
1	B	124	GLN
1	B	170	GLN
1	B	175	ASN
1	B	220	ASN
1	B	251	HIS
1	B	256	GLN
1	B	299	GLN
1	B	302	ASN
1	B	307	HIS
1	B	323	ASN
1	B	327	GLN
1	B	339	GLN
1	B	381	GLN
1	B	428	GLN
1	B	433	HIS
1	B	446	ASN
1	B	487	GLN
1	B	491	ASN
1	B	492	HIS
1	B	493	GLN
1	B	549	GLN
1	B	550	ASN
1	B	623	ASN
1	B	664	HIS
1	C	23	GLN
1	C	35	GLN
1	C	54	ASN
1	C	60	ASN
1	C	80	ASN
1	C	86	HIS
1	C	119	HIS
1	C	122	GLN
1	C	124	GLN
1	C	170	GLN
1	C	175	ASN
1	C	220	ASN
1	C	251	HIS
1	C	256	GLN

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Mol	Chain	Res	Type
1	C	299	GLN
1	C	302	ASN
1	C	307	HIS
1	C	323	ASN
1	C	327	GLN
1	C	339	GLN
1	C	381	GLN
1	C	428	GLN
1	C	439	HIS
1	C	446	ASN
1	C	487	GLN
1	C	491	ASN
1	C	493	GLN
1	C	550	ASN
1	C	664	HIS
1	C	681	HIS
1	D	23	GLN
1	D	35	GLN
1	D	54	ASN
1	D	60	ASN
1	D	80	ASN
1	D	86	HIS
1	D	119	HIS
1	D	122	GLN
1	D	124	GLN
1	D	170	GLN
1	D	175	ASN
1	D	220	ASN
1	D	251	HIS
1	D	256	GLN
1	D	299	GLN
1	D	302	ASN
1	D	307	HIS
1	D	327	GLN
1	D	339	GLN
1	D	381	GLN
1	D	433	HIS
1	D	446	ASN
1	D	487	GLN
1	D	491	ASN
1	D	492	HIS
1	D	493	GLN

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Mol	Chain	Res	Type
1	D	498	ASN
1	D	550	ASN
1	D	664	HIS
1	E	23	GLN
1	E	35	GLN
1	E	54	ASN
1	E	60	ASN
1	E	80	ASN
1	E	86	HIS
1	E	119	HIS
1	E	122	GLN
1	E	124	GLN
1	E	170	GLN
1	E	175	ASN
1	E	220	ASN
1	E	251	HIS
1	E	256	GLN
1	E	286	HIS
1	E	299	GLN
1	E	302	ASN
1	E	307	HIS
1	E	323	ASN
1	E	327	GLN
1	E	339	GLN
1	E	381	GLN
1	E	417	ASN
1	E	433	HIS
1	E	439	HIS
1	E	446	ASN
1	E	487	GLN
1	E	491	ASN
1	E	493	GLN
1	E	550	ASN
1	E	664	HIS
1	E	669	HIS
1	F	23	GLN
1	F	35	GLN
1	F	54	ASN
1	F	57	ASN
1	F	60	ASN
1	F	80	ASN
1	F	119	HIS

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Mol	Chain	Res	Type
1	F	122	GLN
1	F	124	GLN
1	F	175	ASN
1	F	220	ASN
1	F	251	HIS
1	F	256	GLN
1	F	299	GLN
1	F	302	ASN
1	F	307	HIS
1	F	323	ASN
1	F	327	GLN
1	F	339	GLN
1	F	381	GLN
1	F	433	HIS
1	F	439	HIS
1	F	446	ASN
1	F	487	GLN
1	F	491	ASN
1	F	492	HIS
1	F	493	GLN
1	F	543	HIS
1	F	550	ASN
1	F	664	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

84 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	G	1	1,2	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
2	MAN	G	10	2	11,11,12	0.54	0	15,15,17	0.66	1 (6%)
2	MAN	G	11	2	11,11,12	0.61	0	15,15,17	0.64	1 (6%)
2	MAN	G	12	2	11,11,12	0.58	0	15,15,17	0.75	1 (6%)
2	NAG	G	2	2	14,14,15	0.57	0	17,19,21	0.79	0
2	BMA	G	3	2	11,11,12	0.42	0	15,15,17	0.40	0
2	MAN	G	4	2	11,11,12	0.37	0	15,15,17	0.71	1 (6%)
2	MAN	G	5	2	11,11,12	0.52	0	15,15,17	0.61	0
2	MAN	G	6	2	11,11,12	0.59	0	15,15,17	0.68	1 (6%)
2	GLC	G	7	2	11,11,12	0.44	0	15,15,17	1.34	1 (6%)
2	MAN	G	8	2	11,11,12	0.55	0	15,15,17	0.73	1 (6%)
2	MAN	G	9	2	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.45	0	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.55	0	17,19,21	0.66	0
2	NAG	I	1	1,2	14,14,15	0.50	0	17,19,21	0.59	0
2	MAN	I	10	2	11,11,12	0.78	0	15,15,17	1.66	1 (6%)
2	MAN	I	11	2	11,11,12	0.66	0	15,15,17	0.67	1 (6%)
2	MAN	I	12	2	11,11,12	0.56	0	15,15,17	1.01	1 (6%)
2	NAG	I	2	2	14,14,15	0.58	0	17,19,21	0.82	0
2	BMA	I	3	2	11,11,12	0.46	0	15,15,17	0.32	0
2	MAN	I	4	2	11,11,12	0.56	0	15,15,17	0.61	0
2	MAN	I	5	2	11,11,12	0.55	0	15,15,17	0.71	1 (6%)
2	MAN	I	6	2	11,11,12	0.45	0	15,15,17	0.59	1 (6%)
2	GLC	I	7	2	11,11,12	0.49	0	15,15,17	0.66	1 (6%)
2	MAN	I	8	2	11,11,12	0.62	0	15,15,17	0.67	1 (6%)
2	MAN	I	9	2	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.66	0	17,19,21	0.65	0
3	NAG	J	2	3	14,14,15	0.57	0	17,19,21	0.63	0
2	NAG	K	1	1,2	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
2	MAN	K	10	2	11,11,12	0.63	0	15,15,17	0.72	1 (6%)
2	MAN	K	11	2	11,11,12	0.54	0	15,15,17	0.69	1 (6%)
2	MAN	K	12	2	11,11,12	0.57	0	15,15,17	0.74	1 (6%)
2	NAG	K	2	2	14,14,15	0.43	0	17,19,21	0.89	1 (5%)
2	BMA	K	3	2	11,11,12	0.52	0	15,15,17	0.38	0
2	MAN	K	4	2	11,11,12	0.52	0	15,15,17	0.73	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	K	5	2	11,11,12	0.49	0	15,15,17	0.65	0
2	MAN	K	6	2	11,11,12	0.46	0	15,15,17	0.58	0
2	GLC	K	7	2	11,11,12	0.51	0	15,15,17	0.73	1 (6%)
2	MAN	K	8	2	11,11,12	0.56	0	15,15,17	0.65	0
2	MAN	K	9	2	11,11,12	0.71	0	15,15,17	0.91	1 (6%)
3	NAG	L	1	1,3	14,14,15	0.74	0	17,19,21	0.66	0
3	NAG	L	2	3	14,14,15	0.64	0	17,19,21	0.58	0
2	NAG	M	1	1,2	14,14,15	0.50	0	17,19,21	0.74	1 (5%)
2	MAN	M	10	2	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
2	MAN	M	11	2	11,11,12	0.71	0	15,15,17	0.73	1 (6%)
2	MAN	M	12	2	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
2	NAG	M	2	2	14,14,15	0.52	0	17,19,21	0.83	0
2	BMA	M	3	2	11,11,12	0.56	0	15,15,17	0.36	0
2	MAN	M	4	2	11,11,12	0.36	0	15,15,17	0.72	1 (6%)
2	MAN	M	5	2	11,11,12	0.50	0	15,15,17	0.64	0
2	MAN	M	6	2	11,11,12	0.49	0	15,15,17	0.55	0
2	GLC	M	7	2	11,11,12	0.42	0	15,15,17	0.76	1 (6%)
2	MAN	M	8	2	11,11,12	0.55	0	15,15,17	0.67	1 (6%)
2	MAN	M	9	2	11,11,12	0.72	0	15,15,17	1.25	2 (13%)
3	NAG	N	1	1,3	14,14,15	0.67	0	17,19,21	0.63	0
3	NAG	N	2	3	14,14,15	0.68	0	17,19,21	0.56	0
2	NAG	O	1	1,2	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
2	MAN	O	10	2	11,11,12	0.66	0	15,15,17	1.31	1 (6%)
2	MAN	O	11	2	11,11,12	0.56	0	15,15,17	0.59	1 (6%)
2	MAN	O	12	2	11,11,12	0.57	0	15,15,17	0.76	1 (6%)
2	NAG	O	2	2	14,14,15	0.51	0	17,19,21	0.77	0
2	BMA	O	3	2	11,11,12	0.59	0	15,15,17	0.38	0
2	MAN	O	4	2	11,11,12	0.46	0	15,15,17	0.72	0
2	MAN	O	5	2	11,11,12	0.55	0	15,15,17	0.56	0
2	MAN	O	6	2	11,11,12	0.66	0	15,15,17	0.65	0
2	GLC	O	7	2	11,11,12	0.52	0	15,15,17	1.23	1 (6%)
2	MAN	O	8	2	11,11,12	0.54	0	15,15,17	0.75	1 (6%)
2	MAN	O	9	2	11,11,12	0.79	0	15,15,17	1.26	1 (6%)
3	NAG	P	1	1,3	14,14,15	0.64	0	17,19,21	0.61	0
3	NAG	P	2	3	14,14,15	0.52	0	17,19,21	0.69	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.48	0	17,19,21	0.67	1 (5%)
2	MAN	Q	10	2	11,11,12	0.53	0	15,15,17	0.71	1 (6%)
2	MAN	Q	11	2	11,11,12	0.50	0	15,15,17	0.58	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	Q	12	2	11,11,12	0.60	0	15,15,17	0.72	1 (6%)
2	NAG	Q	2	2	14,14,15	0.51	0	17,19,21	0.93	1 (5%)
2	BMA	Q	3	2	11,11,12	0.41	0	15,15,17	0.32	0
2	MAN	Q	4	2	11,11,12	0.56	0	15,15,17	0.62	0
2	MAN	Q	5	2	11,11,12	0.51	0	15,15,17	0.80	1 (6%)
2	MAN	Q	6	2	11,11,12	0.46	0	15,15,17	0.65	1 (6%)
2	GLC	Q	7	2	11,11,12	0.43	0	15,15,17	0.61	1 (6%)
2	MAN	Q	8	2	11,11,12	0.51	0	15,15,17	0.59	0
2	MAN	Q	9	2	11,11,12	0.74	0	15,15,17	0.95	1 (6%)
3	NAG	R	1	1,3	14,14,15	0.49	0	17,19,21	0.71	1 (5%)
3	NAG	R	2	3	14,14,15	0.59	0	17,19,21	0.64	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
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	G	10	2	-	0/2/19/22	1/1/1/1
2	MAN	G	11	2	-	0/2/19/22	0/1/1/1
2	MAN	G	12	2	-	2/2/19/22	1/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1
2	GLC	G	7	2	-	2/2/19/22	0/1/1/1
2	MAN	G	8	2	-	0/2/19/22	0/1/1/1
2	MAN	G	9	2	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	I	10	2	-	2/2/19/22	0/1/1/1
2	MAN	I	11	2	-	0/2/19/22	0/1/1/1
2	MAN	I	12	2	-	1/2/19/22	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	I	6	2	-	1/2/19/22	0/1/1/1
2	GLC	I	7	2	-	0/2/19/22	0/1/1/1
2	MAN	I	8	2	-	0/2/19/22	0/1/1/1
2	MAN	I	9	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	K	10	2	-	0/2/19/22	1/1/1/1
2	MAN	K	11	2	-	1/2/19/22	0/1/1/1
2	MAN	K	12	2	-	2/2/19/22	1/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	0/2/19/22	0/1/1/1
2	MAN	K	6	2	-	1/2/19/22	0/1/1/1
2	GLC	K	7	2	-	0/2/19/22	0/1/1/1
2	MAN	K	8	2	-	0/2/19/22	0/1/1/1
2	MAN	K	9	2	-	1/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	M	10	2	-	2/2/19/22	0/1/1/1
2	MAN	M	11	2	-	2/2/19/22	0/1/1/1
2	MAN	M	12	2	-	1/2/19/22	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
2	MAN	M	5	2	-	0/2/19/22	0/1/1/1
2	MAN	M	6	2	-	0/2/19/22	0/1/1/1
2	GLC	M	7	2	-	0/2/19/22	0/1/1/1
2	MAN	M	8	2	-	0/2/19/22	0/1/1/1
2	MAN	M	9	2	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	O	10	2	-	2/2/19/22	0/1/1/1
2	MAN	O	11	2	-	0/2/19/22	0/1/1/1
2	MAN	O	12	2	-	2/2/19/22	1/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	BMA	O	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
2	MAN	O	5	2	-	0/2/19/22	0/1/1/1
2	MAN	O	6	2	-	0/2/19/22	0/1/1/1
2	GLC	O	7	2	-	0/2/19/22	0/1/1/1
2	MAN	O	8	2	-	0/2/19/22	0/1/1/1
2	MAN	O	9	2	-	0/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	Q	10	2	-	0/2/19/22	1/1/1/1
2	MAN	Q	11	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	12	2	-	0/2/19/22	1/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	5	2	-	1/2/19/22	0/1/1/1
2	MAN	Q	6	2	-	0/2/19/22	0/1/1/1
2	GLC	Q	7	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	8	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	9	2	-	0/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	10	MAN	C1-C2-C3	-5.92	102.39	109.67
2	G	7	GLC	C1-O5-C5	4.57	118.38	112.19
2	M	10	MAN	C1-O5-C5	4.39	118.14	112.19
2	O	10	MAN	C1-O5-C5	4.32	118.04	112.19
2	O	7	GLC	C1-O5-C5	4.14	117.80	112.19
2	O	9	MAN	C1-C2-C3	3.76	114.29	109.67
2	M	9	MAN	C1-C2-C3	3.63	114.13	109.67
2	M	12	MAN	C1-O5-C5	3.23	116.57	112.19
2	I	12	MAN	C1-O5-C5	3.07	116.35	112.19
2	K	1	NAG	C2-N2-C7	-2.70	119.06	122.90
2	Q	5	MAN	C1-O5-C5	2.53	115.62	112.19
2	M	7	GLC	C1-O5-C5	2.51	115.60	112.19
2	Q	10	MAN	C1-O5-C5	2.50	115.58	112.19
2	I	9	MAN	C2-C3-C4	-2.46	106.63	110.89
2	G	12	MAN	C1-O5-C5	2.43	115.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	12	MAN	C1-O5-C5	2.42	115.48	112.19
2	M	11	MAN	C1-O5-C5	2.42	115.47	112.19
2	Q	9	MAN	C1-C2-C3	2.41	112.63	109.67
2	K	10	MAN	C1-O5-C5	2.41	115.45	112.19
2	O	12	MAN	C1-O5-C5	2.36	115.39	112.19
2	O	8	MAN	C1-O5-C5	2.35	115.37	112.19
2	K	9	MAN	C1-C2-C3	2.33	112.53	109.67
2	O	1	NAG	C2-N2-C7	-2.33	119.58	122.90
2	K	7	GLC	C1-O5-C5	2.32	115.34	112.19
2	K	11	MAN	C1-O5-C5	2.31	115.32	112.19
2	M	1	NAG	C2-N2-C7	-2.30	119.63	122.90
2	I	7	GLC	C1-O5-C5	2.30	115.31	112.19
2	K	4	MAN	C1-O5-C5	2.27	115.26	112.19
2	G	10	MAN	C1-O5-C5	2.26	115.26	112.19
2	G	11	MAN	C1-O5-C5	2.25	115.24	112.19
2	Q	12	MAN	C1-O5-C5	2.25	115.24	112.19
2	G	4	MAN	C1-O5-C5	2.25	115.23	112.19
2	I	8	MAN	C1-O5-C5	2.24	115.23	112.19
2	Q	2	NAG	C2-N2-C7	-2.22	119.75	122.90
2	G	9	MAN	C1-C2-C3	2.22	112.39	109.67
2	Q	1	NAG	C2-N2-C7	-2.20	119.77	122.90
2	Q	7	GLC	C1-O5-C5	2.19	115.15	112.19
2	I	5	MAN	C1-O5-C5	2.17	115.13	112.19
2	I	11	MAN	C1-O5-C5	2.16	115.12	112.19
2	G	6	MAN	C1-O5-C5	2.13	115.08	112.19
2	M	4	MAN	C1-O5-C5	2.11	115.05	112.19
2	G	8	MAN	C1-O5-C5	2.11	115.05	112.19
2	I	9	MAN	C1-O5-C5	2.09	115.03	112.19
2	M	8	MAN	C1-O5-C5	2.08	115.01	112.19
3	R	1	NAG	C2-N2-C7	-2.08	119.95	122.90
3	P	2	NAG	C2-N2-C7	-2.07	119.96	122.90
2	G	1	NAG	C2-N2-C7	-2.06	119.97	122.90
2	O	11	MAN	C1-O5-C5	2.03	114.95	112.19
2	Q	11	MAN	C1-O5-C5	2.03	114.94	112.19
2	Q	6	MAN	C1-O5-C5	2.02	114.93	112.19
2	M	9	MAN	C2-C3-C4	2.02	114.39	110.89
2	I	6	MAN	C1-O5-C5	2.01	114.92	112.19
2	K	2	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	O	10	MAN	O5-C5-C6-O6
2	M	10	MAN	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
2	I	10	MAN	C4-C5-C6-O6
2	O	10	MAN	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
2	M	10	MAN	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	I	10	MAN	O5-C5-C6-O6
2	G	7	GLC	C4-C5-C6-O6
2	K	12	MAN	C4-C5-C6-O6
2	O	12	MAN	C4-C5-C6-O6
2	G	12	MAN	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
2	M	11	MAN	C4-C5-C6-O6
2	K	12	MAN	O5-C5-C6-O6
2	O	12	MAN	O5-C5-C6-O6
2	G	12	MAN	O5-C5-C6-O6
2	Q	5	MAN	C4-C5-C6-O6
2	I	12	MAN	C4-C5-C6-O6
3	N	1	NAG	C1-C2-N2-C7
2	K	6	MAN	C4-C5-C6-O6
2	M	11	MAN	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	K	11	MAN	C4-C5-C6-O6
2	I	6	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	M	12	MAN	C4-C5-C6-O6
2	K	9	MAN	C4-C5-C6-O6
2	G	7	GLC	O5-C5-C6-O6

All (7) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	12	MAN	C1-C2-C3-C4-C5-O5
2	K	10	MAN	C1-C2-C3-C4-C5-O5

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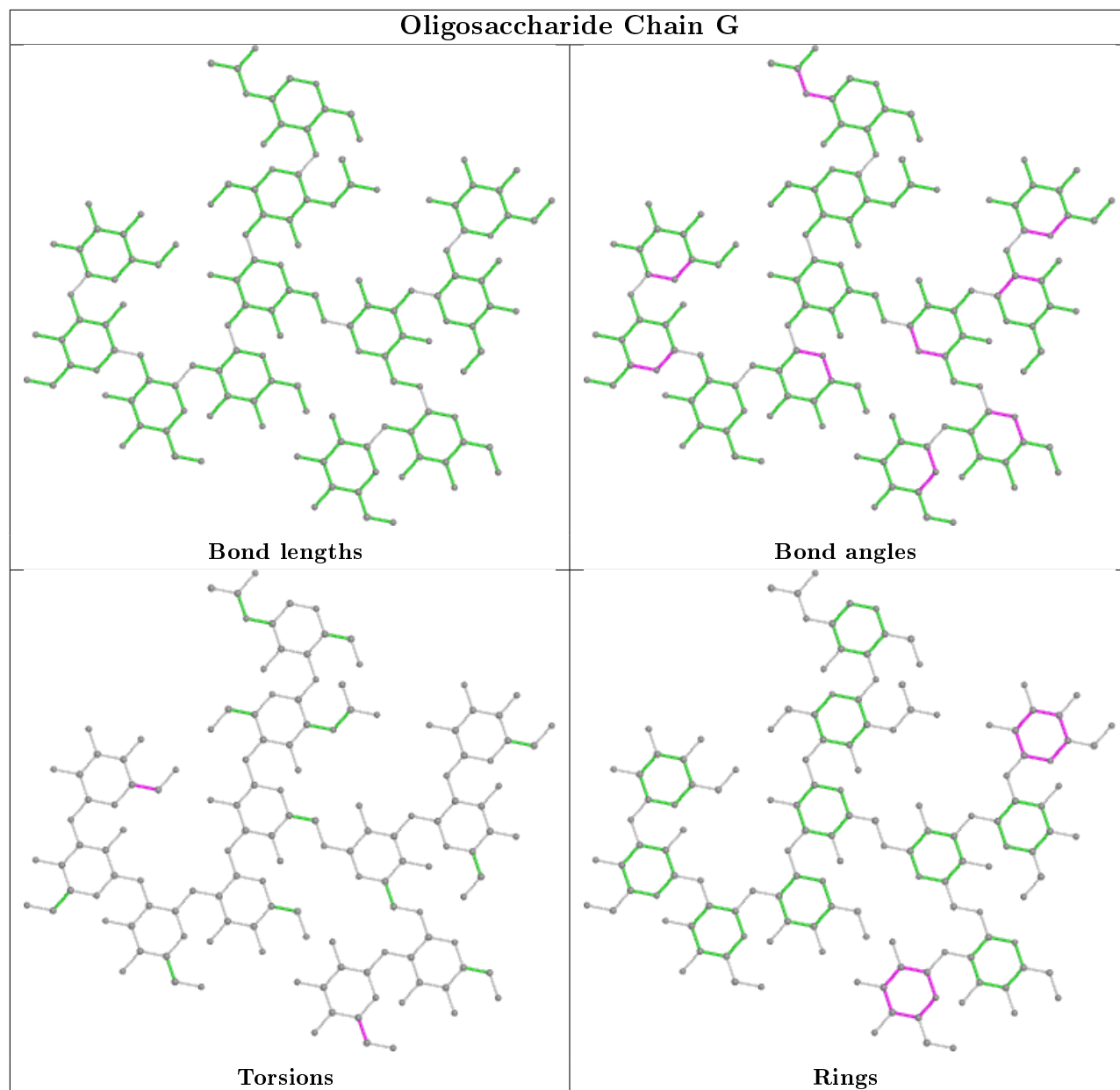
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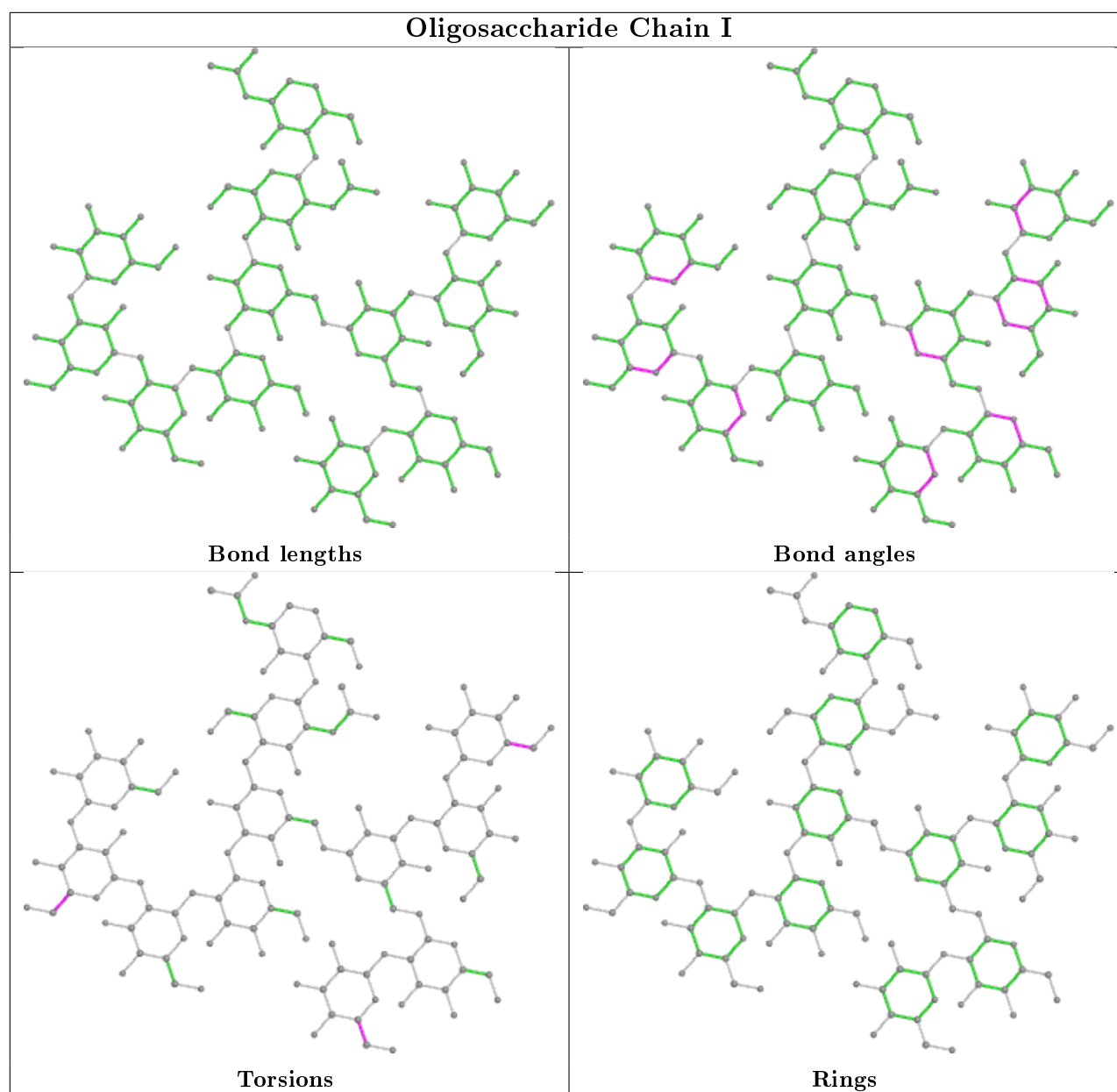
Mol	Chain	Res	Type	Atoms
2	G	12	MAN	C1-C2-C3-C4-C5-O5
2	Q	10	MAN	C1-C2-C3-C4-C5-O5
2	K	12	MAN	C1-C2-C3-C4-C5-O5
2	O	12	MAN	C1-C2-C3-C4-C5-O5
2	G	10	MAN	C1-C2-C3-C4-C5-O5

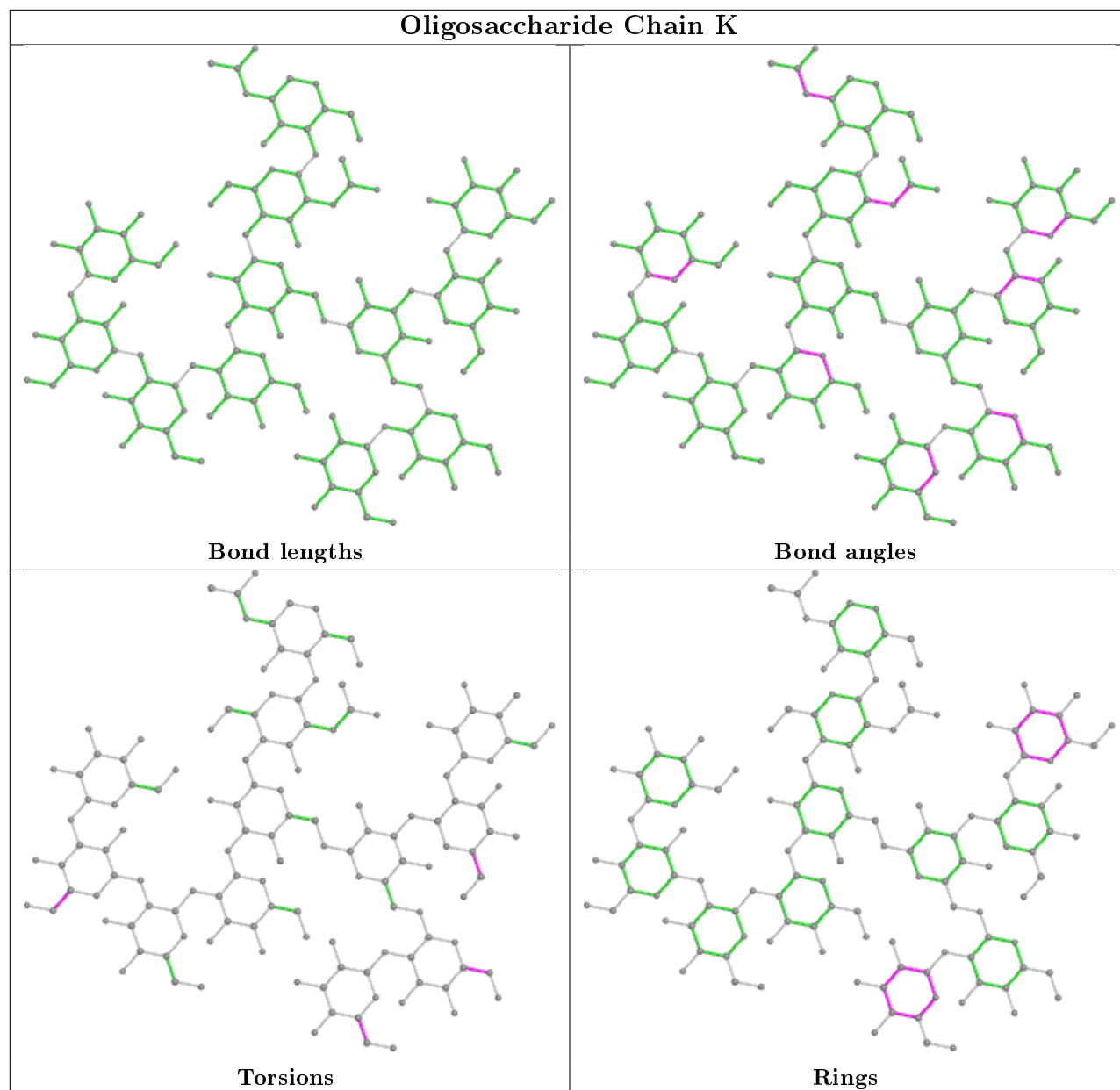
4 monomers are involved in 4 short contacts:

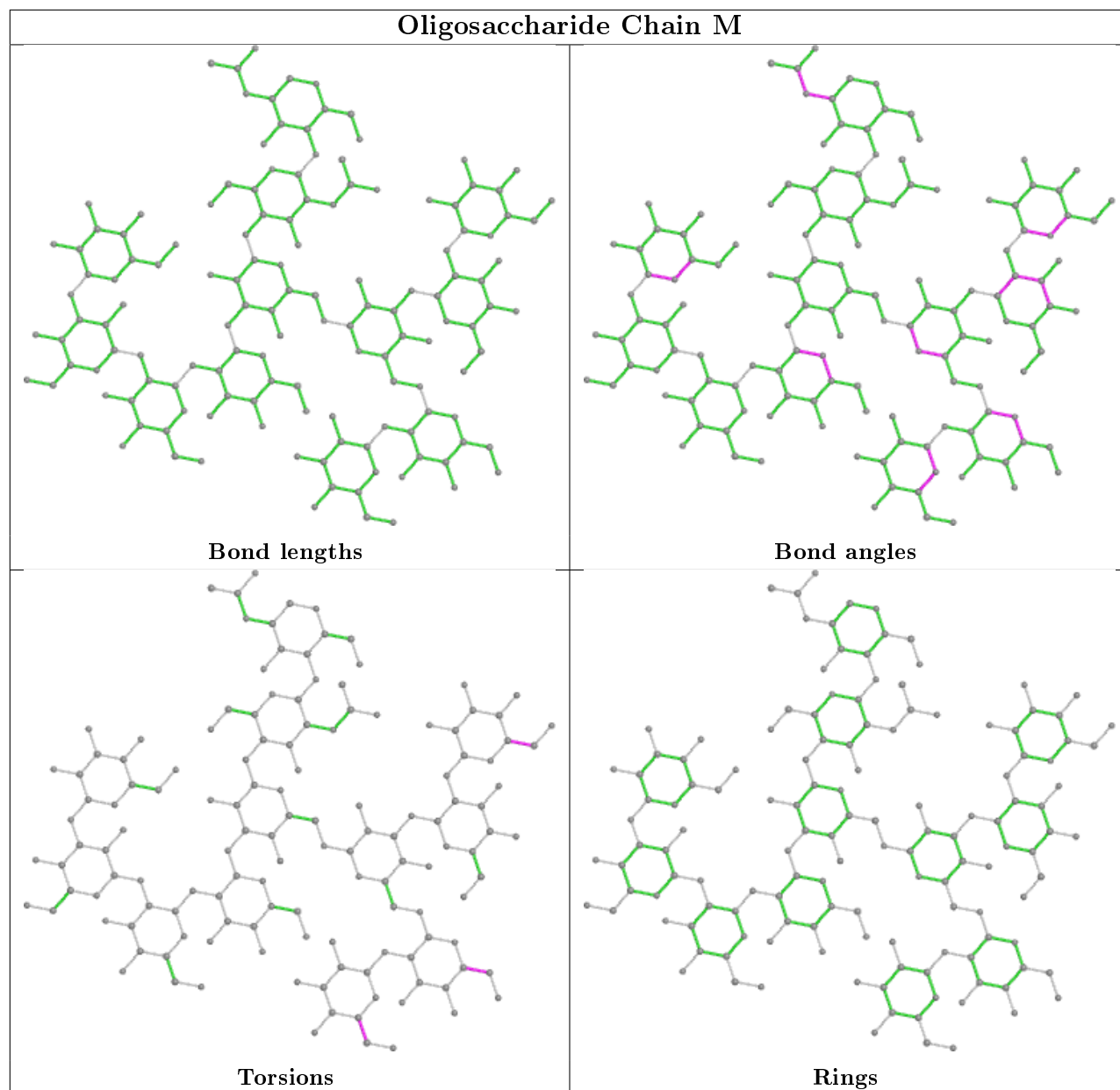
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	9	MAN	1	0
2	I	10	MAN	1	0
2	K	4	MAN	1	0
2	Q	10	MAN	1	0

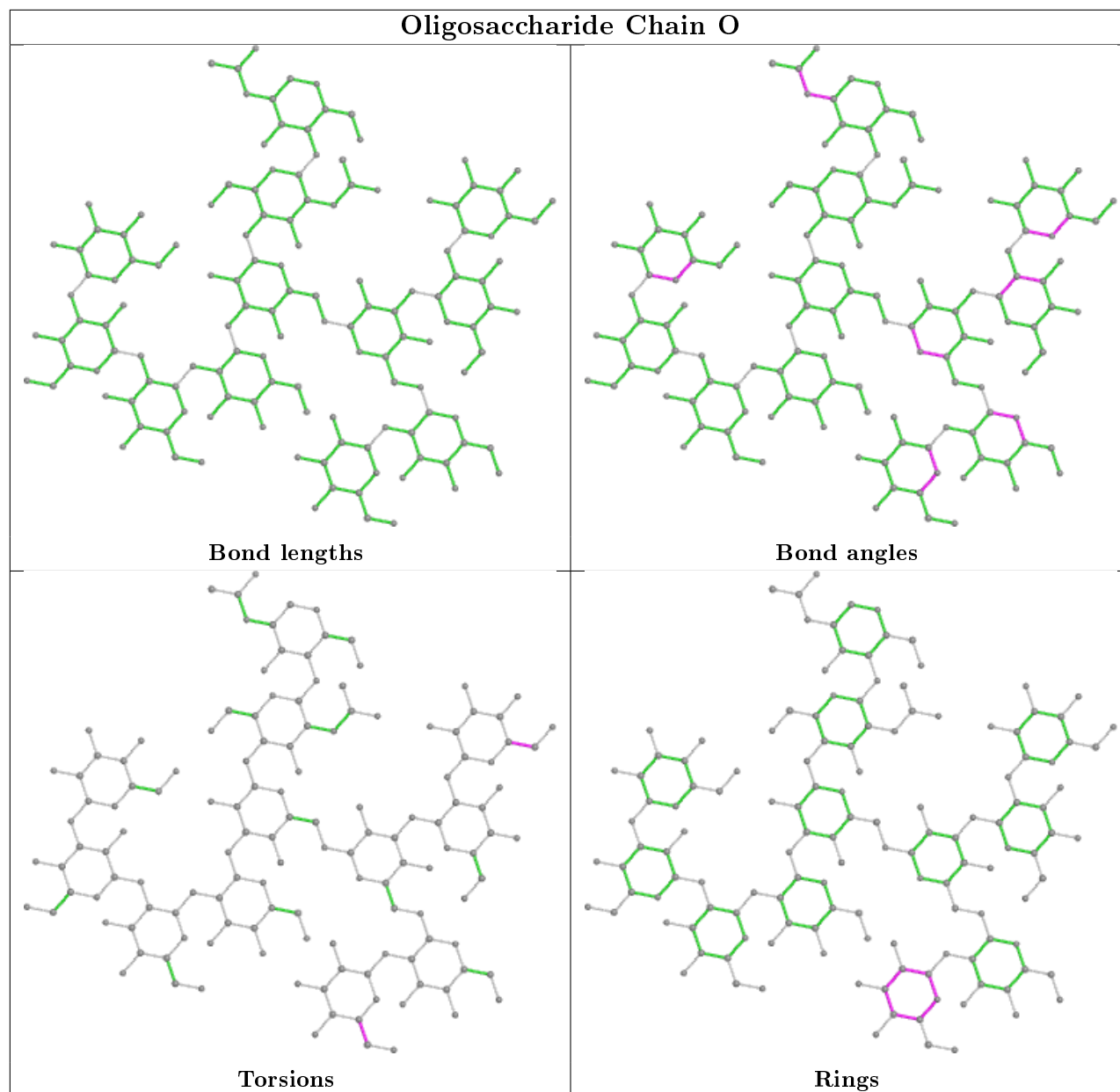
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

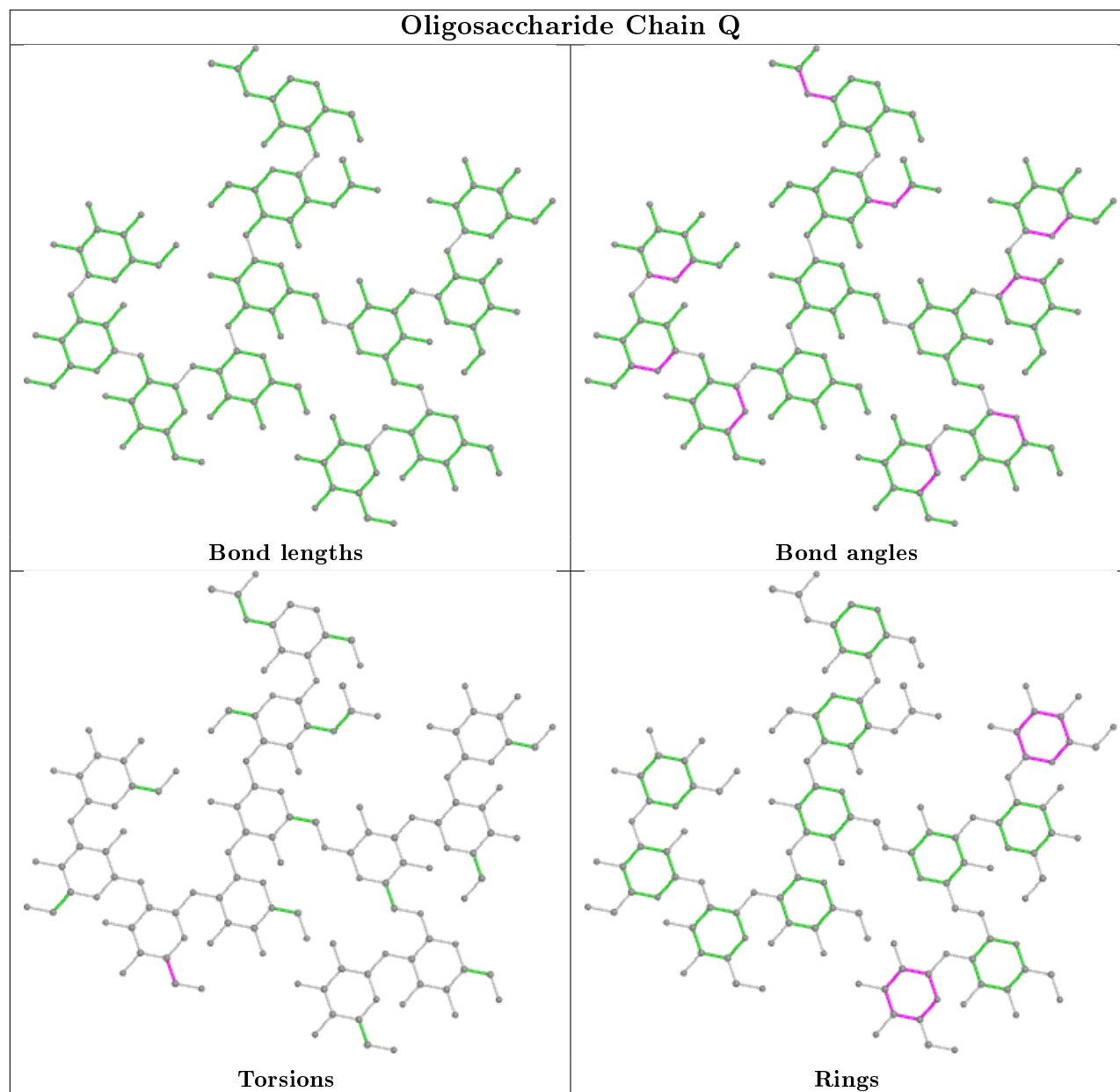


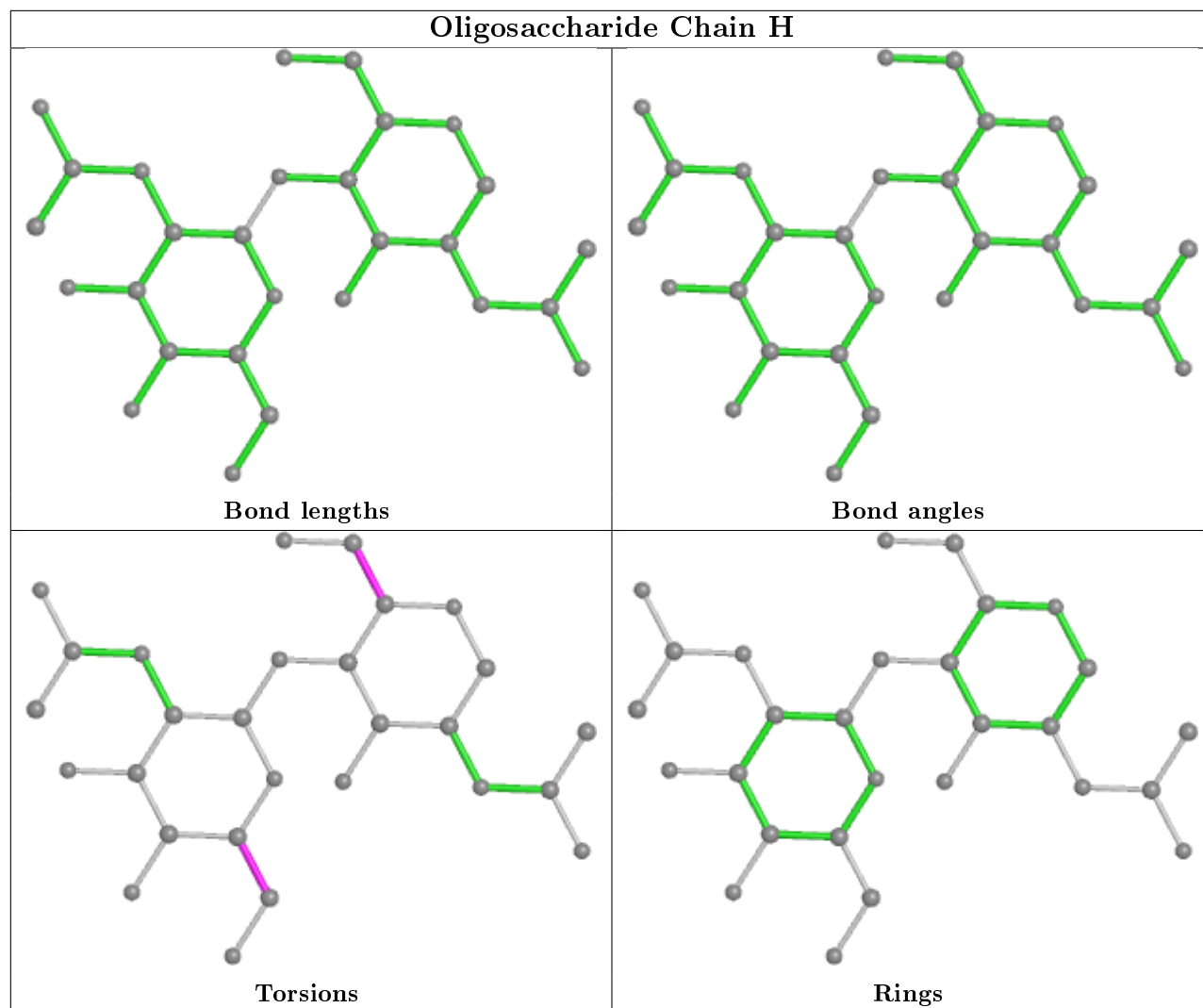


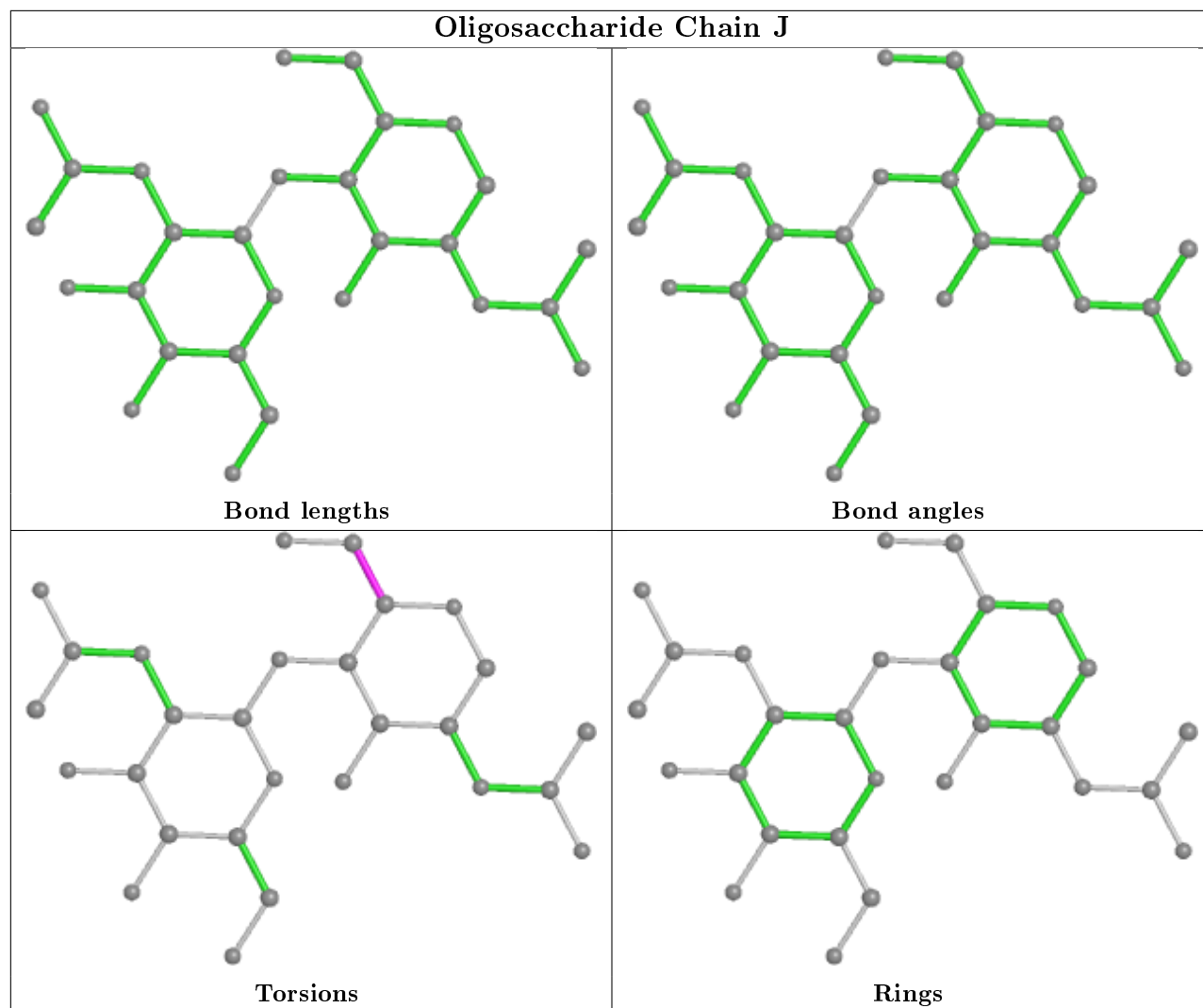


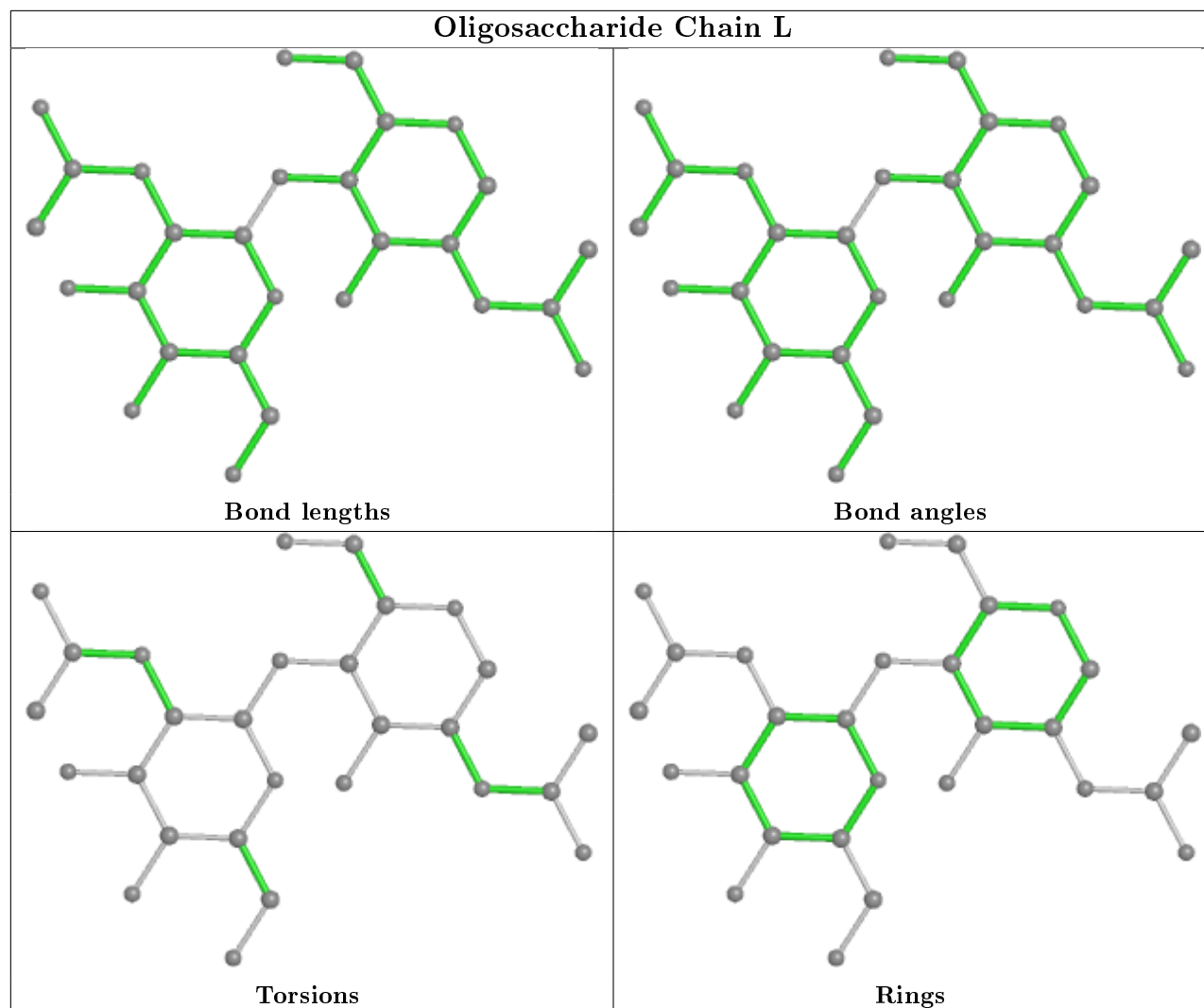


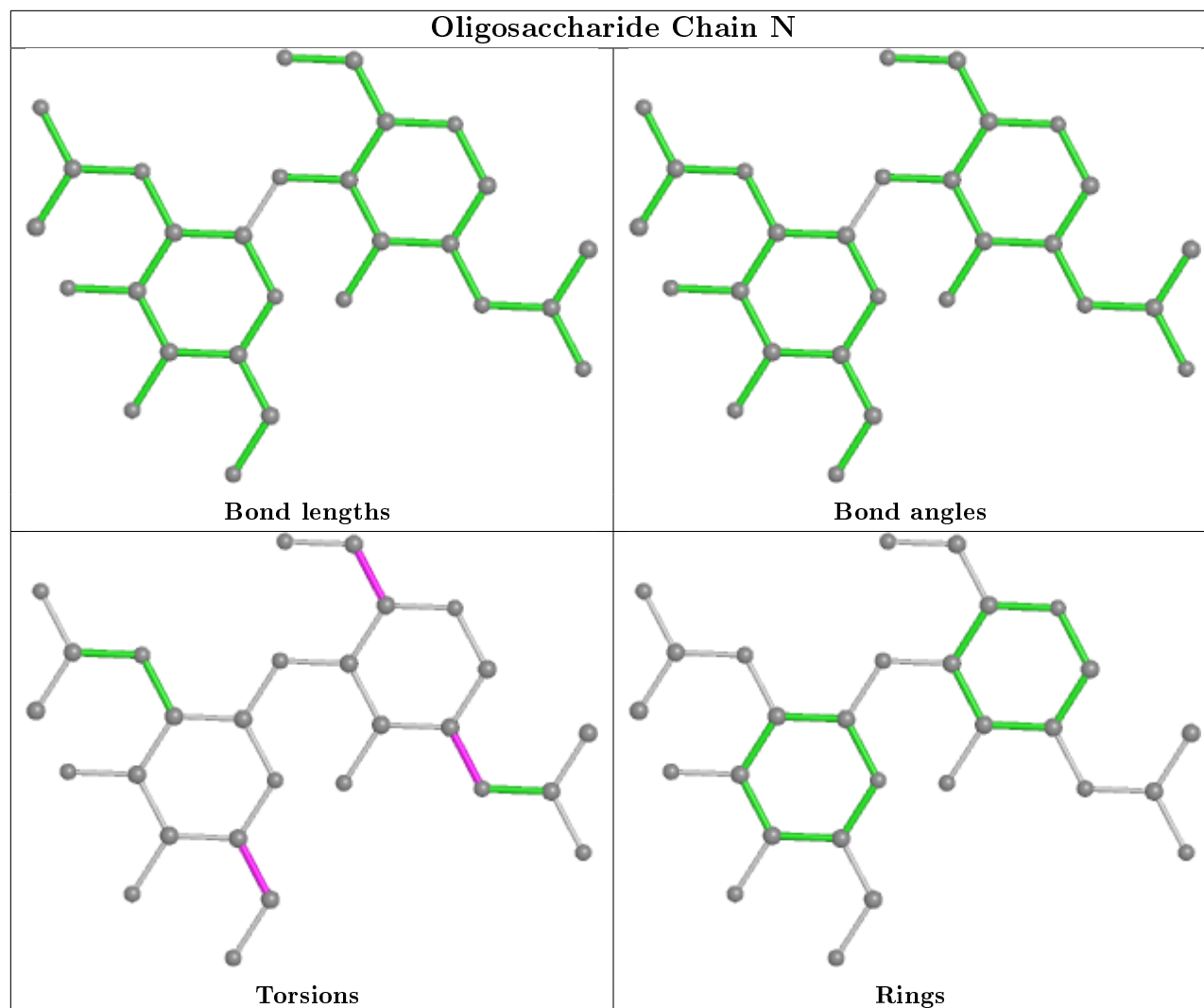


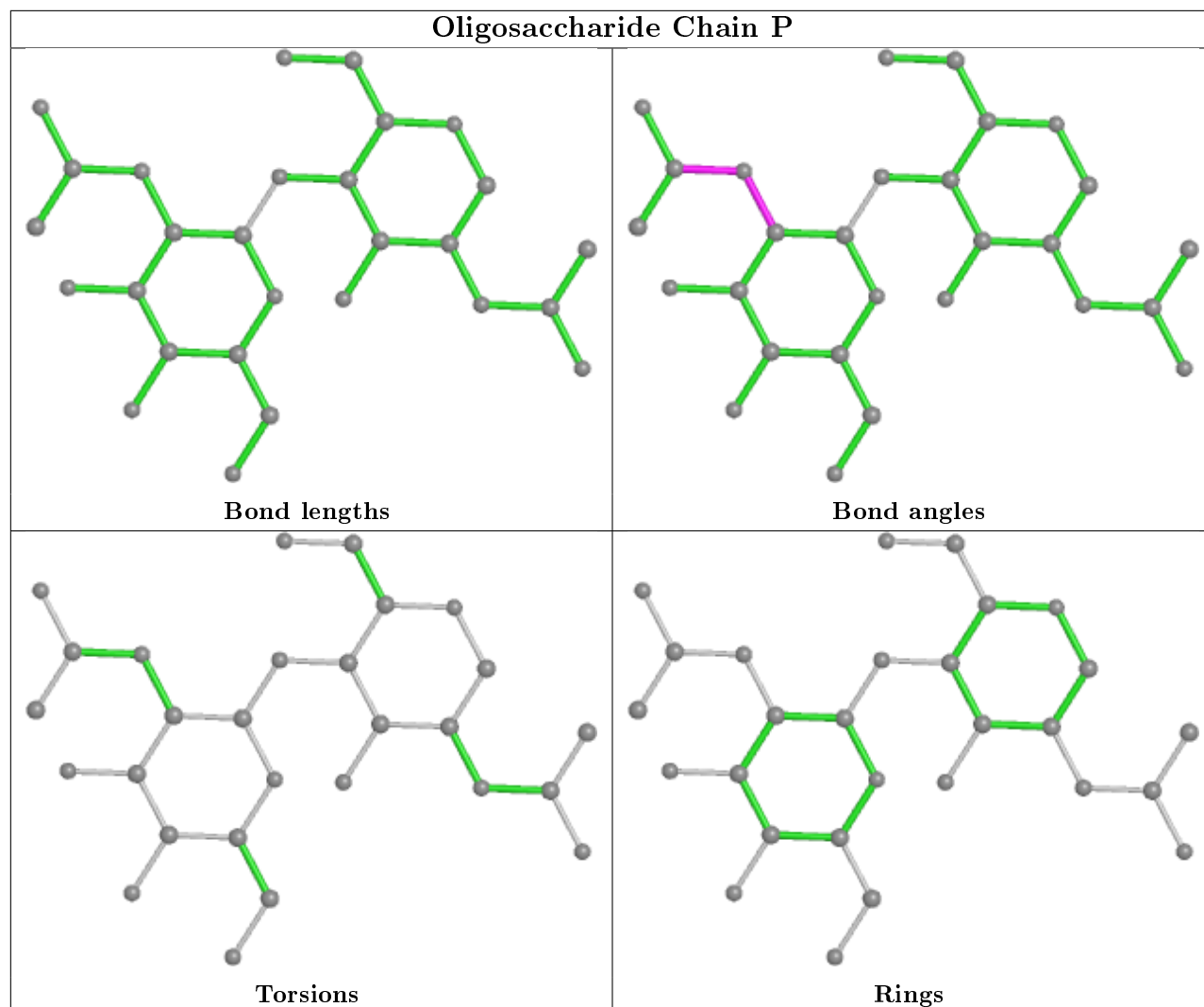


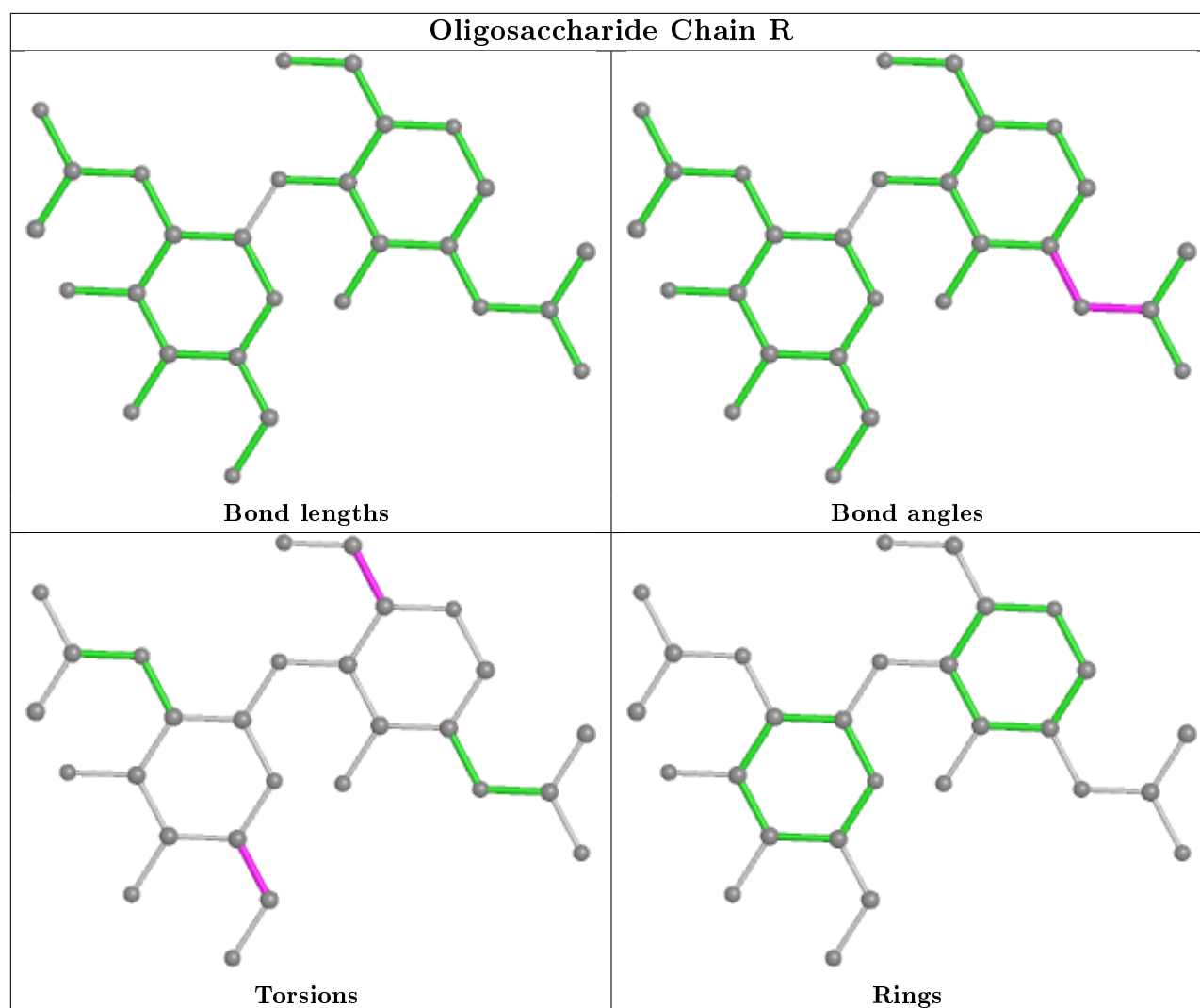












5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
4	FMT	B	2002	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	F	2006	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	2003	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	2005	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	C	2004	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	2001	-	0,2,2	0.00	-	0,1,1	0.00	-

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.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2002	FMT	2	0
4	F	2006	FMT	1	0
4	A	2003	FMT	1	0
4	E	2005	FMT	1	0
4	C	2004	FMT	1	0
4	D	2001	FMT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	674/674 (100%)	-0.52	11 (1%) 72 69	18, 33, 64, 96	0
1	B	674/674 (100%)	-0.54	2 (0%) 94 94	16, 32, 63, 94	0
1	C	674/674 (100%)	-0.46	9 (1%) 77 75	17, 34, 65, 97	0
1	D	674/674 (100%)	-0.42	15 (2%) 62 58	17, 33, 63, 96	0
1	E	674/674 (100%)	-0.38	17 (2%) 57 53	17, 34, 65, 97	0
1	F	674/674 (100%)	-0.46	15 (2%) 62 58	17, 33, 66, 96	0
All	All	4044/4044 (100%)	-0.46	69 (1%) 70 66	16, 33, 65, 97	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	621	THR	6.5
1	F	631	MET	5.5
1	A	8	HIS	5.5
1	F	624	LEU	5.4
1	B	650	PHE	5.4
1	E	681	HIS	4.7
1	D	681	HIS	4.5
1	F	8	HIS	4.4
1	A	622	LYS	4.4
1	F	625	THR	4.2
1	E	624	LEU	4.2
1	E	621	THR	4.1
1	E	618	GLU	4.1
1	F	626	PRO	4.1
1	C	621	THR	3.9
1	C	8	HIS	3.8
1	C	622	LYS	3.7
1	F	649	CYS	3.7
1	D	624	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	619	SER	3.6
1	D	501	ILE	3.5
1	E	8	HIS	3.4
1	F	650	PHE	3.4
1	E	622	LYS	3.3
1	F	622	LYS	3.3
1	E	650	PHE	3.2
1	F	618	GLU	3.2
1	A	624	LEU	3.2
1	F	623	ASN	3.2
1	E	573	TYR	3.0
1	C	681	HIS	3.0
1	D	441	VAL	3.0
1	F	628	GLU	3.0
1	B	681	HIS	3.0
1	E	626	PRO	2.9
1	D	622	LYS	2.9
1	C	618	GLU	2.9
1	D	618	GLU	2.8
1	D	619	SER	2.8
1	D	630	PHE	2.8
1	C	619	SER	2.8
1	E	189	ASN	2.7
1	E	630	PHE	2.7
1	E	620	THR	2.7
1	E	625	THR	2.6
1	D	631	MET	2.6
1	E	623	ASN	2.5
1	C	620	THR	2.5
1	E	12	THR	2.5
1	D	632	ILE	2.4
1	A	441	VAL	2.4
1	A	617	PHE	2.3
1	D	508	ASP	2.3
1	D	8	HIS	2.3
1	F	619	SER	2.2
1	D	509	ALA	2.2
1	A	619	SER	2.2
1	F	9	VAL	2.1
1	D	625	THR	2.1
1	A	505	VAL	2.1
1	D	9	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	189	ASN	2.1
1	C	189	ASN	2.1
1	E	631	MET	2.1
1	C	44	LYS	2.1
1	A	621	THR	2.0
1	F	507	THR	2.0
1	A	623	ASN	2.0
1	A	436	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	K	10	11/12	0.53	0.47	86,91,92,92	0
2	MAN	M	12	11/12	0.55	0.71	97,100,101,102	0
2	MAN	O	10	11/12	0.56	0.36	87,89,91,92	0
2	MAN	I	12	11/12	0.60	0.54	95,99,101,103	0
3	NAG	N	2	14/15	0.61	0.44	98,102,104,105	0
2	MAN	Q	12	11/12	0.69	0.48	97,99,100,100	0
3	NAG	R	2	14/15	0.71	0.41	86,89,92,92	0
2	MAN	K	12	11/12	0.72	0.58	97,99,101,101	0
2	MAN	M	10	11/12	0.72	0.37	87,91,93,93	0
2	MAN	G	10	11/12	0.72	0.35	86,90,92,93	0
2	MAN	I	10	11/12	0.73	0.28	88,89,91,91	0
3	NAG	J	2	14/15	0.74	0.25	88,90,91,91	0
3	NAG	N	1	14/15	0.74	0.26	79,86,90,95	0
2	MAN	G	12	11/12	0.74	0.41	96,98,100,100	0
2	MAN	M	11	11/12	0.76	0.36	88,90,91,96	0
2	MAN	Q	10	11/12	0.76	0.25	85,90,91,91	0
2	MAN	G	11	11/12	0.76	0.38	84,88,90,94	0
2	MAN	I	11	11/12	0.77	0.30	83,87,90,94	0
3	NAG	L	2	14/15	0.77	0.31	79,82,84,85	0
2	MAN	G	8	11/12	0.83	0.22	66,70,77,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	O	12	11/12	0.83	0.37	96,99,100,101	0
3	NAG	J	1	14/15	0.83	0.20	67,72,77,81	0
2	MAN	Q	11	11/12	0.84	0.30	86,87,90,94	0
3	NAG	H	2	14/15	0.84	0.18	63,68,70,71	0
2	MAN	K	9	11/12	0.86	0.28	79,80,83,86	0
2	GLC	K	7	11/12	0.87	0.21	53,55,58,58	0
3	NAG	R	1	14/15	0.88	0.18	67,74,79,81	0
2	MAN	O	11	11/12	0.89	0.19	86,88,90,95	0
2	MAN	O	8	11/12	0.89	0.11	61,65,75,84	0
2	MAN	K	11	11/12	0.89	0.24	85,87,89,94	0
2	GLC	G	7	11/12	0.89	0.18	53,57,59,60	0
2	MAN	G	9	11/12	0.89	0.20	79,82,83,86	0
3	NAG	P	2	14/15	0.89	0.21	72,74,76,76	0
2	MAN	M	9	11/12	0.89	0.25	81,83,85,87	0
2	MAN	M	8	11/12	0.90	0.10	63,70,76,83	0
2	MAN	K	8	11/12	0.91	0.16	62,66,75,83	0
2	MAN	Q	9	11/12	0.91	0.20	79,80,82,84	0
2	MAN	O	9	11/12	0.91	0.17	78,81,82,85	0
2	MAN	I	9	11/12	0.91	0.14	78,79,81,86	0
3	NAG	L	1	14/15	0.92	0.24	63,68,72,76	0
2	MAN	Q	8	11/12	0.92	0.13	63,67,76,84	0
2	GLC	I	7	11/12	0.92	0.20	56,57,59,61	0
2	MAN	O	6	11/12	0.92	0.13	44,45,50,54	0
3	NAG	P	1	14/15	0.92	0.17	60,65,68,70	0
2	MAN	I	8	11/12	0.92	0.14	63,69,77,84	0
2	GLC	O	7	11/12	0.93	0.14	57,60,62,62	0
2	GLC	M	7	11/12	0.94	0.15	51,55,59,60	0
2	BMA	G	3	11/12	0.94	0.10	36,39,48,59	0
2	MAN	M	6	11/12	0.94	0.11	39,43,45,49	0
2	BMA	M	3	11/12	0.95	0.09	35,38,47,56	0
2	BMA	O	3	11/12	0.95	0.09	31,39,44,55	0
2	MAN	G	6	11/12	0.95	0.10	40,42,45,49	0
2	GLC	Q	7	11/12	0.95	0.16	50,53,55,58	0
2	BMA	Q	3	11/12	0.96	0.08	33,35,42,53	0
2	MAN	I	6	11/12	0.96	0.10	40,42,46,50	0
2	MAN	Q	6	11/12	0.96	0.10	40,40,43,46	0
2	MAN	G	5	11/12	0.96	0.11	33,35,39,42	0
2	MAN	G	4	11/12	0.96	0.09	36,37,39,40	0
2	MAN	K	6	11/12	0.96	0.09	40,41,43,50	0
2	NAG	M	2	14/15	0.96	0.11	24,32,39,40	0
3	NAG	H	1	14/15	0.96	0.11	39,49,52,56	0
2	MAN	O	5	11/12	0.96	0.10	29,34,38,44	0

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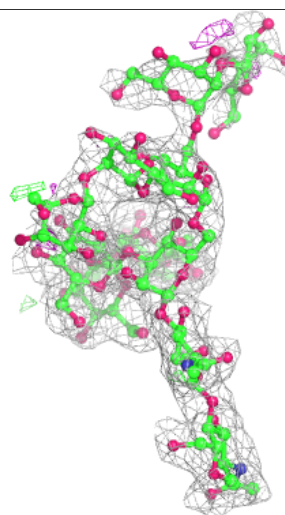
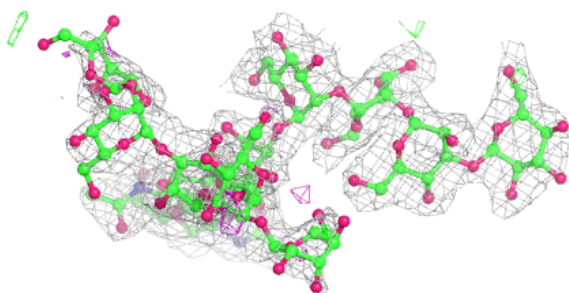
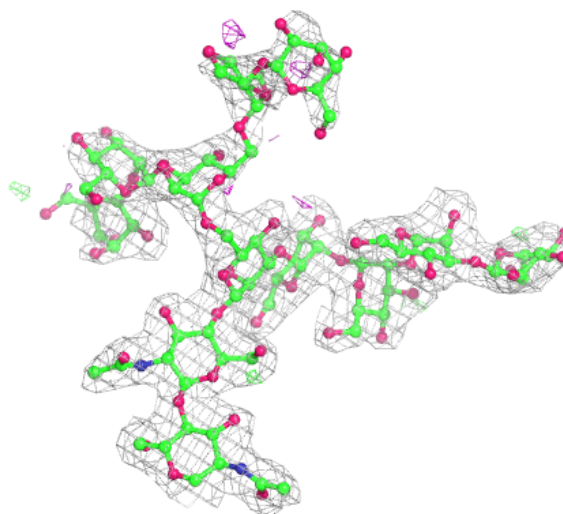
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	O	4	11/12	0.96	0.12	34,36,39,41	0
2	NAG	G	1	14/15	0.97	0.09	20,26,31,31	0
2	MAN	Q	4	11/12	0.97	0.07	34,35,37,38	0
2	NAG	I	1	14/15	0.97	0.10	22,24,29,32	0
2	MAN	I	5	11/12	0.97	0.10	32,35,38,41	0
2	NAG	G	2	14/15	0.97	0.09	29,33,37,43	0
2	NAG	O	2	14/15	0.97	0.11	29,32,34,37	0
2	MAN	K	4	11/12	0.97	0.10	32,32,34,35	0
2	NAG	M	1	14/15	0.97	0.08	22,24,29,30	0
2	BMA	I	3	11/12	0.97	0.09	36,39,48,57	0
2	NAG	I	2	14/15	0.97	0.10	28,32,37,38	0
2	MAN	I	4	11/12	0.97	0.08	34,36,37,38	0
2	NAG	Q	2	14/15	0.97	0.10	29,31,33,39	0
2	MAN	M	5	11/12	0.97	0.09	33,35,36,40	0
2	NAG	O	1	14/15	0.98	0.10	24,27,29,29	0
2	MAN	K	5	11/12	0.98	0.09	32,33,36,38	0
2	MAN	M	4	11/12	0.98	0.08	34,36,39,40	0
2	NAG	K	1	14/15	0.98	0.09	20,25,28,30	0
2	NAG	K	2	14/15	0.98	0.09	25,31,37,40	0
2	NAG	Q	1	14/15	0.98	0.09	21,24,26,27	0
2	BMA	K	3	11/12	0.98	0.08	32,37,46,55	0
2	MAN	Q	5	11/12	0.98	0.10	28,32,36,37	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

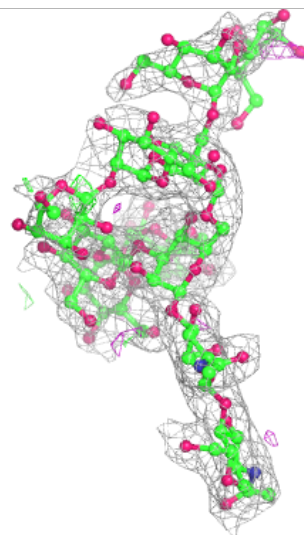
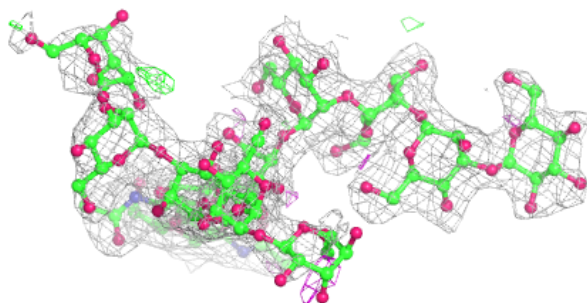
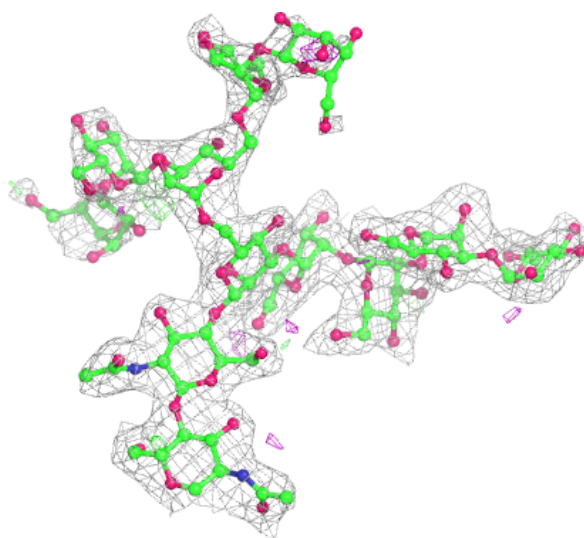
Electron density around Chain G:

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



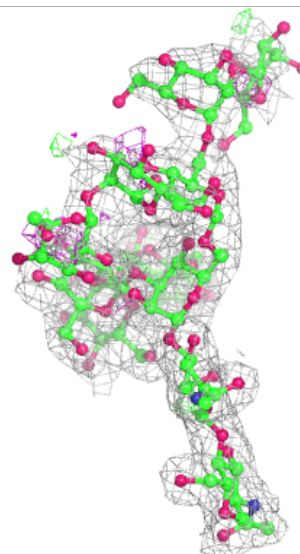
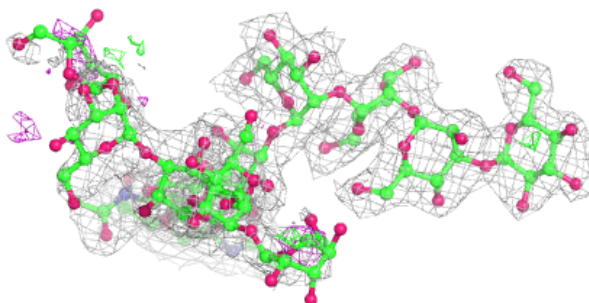
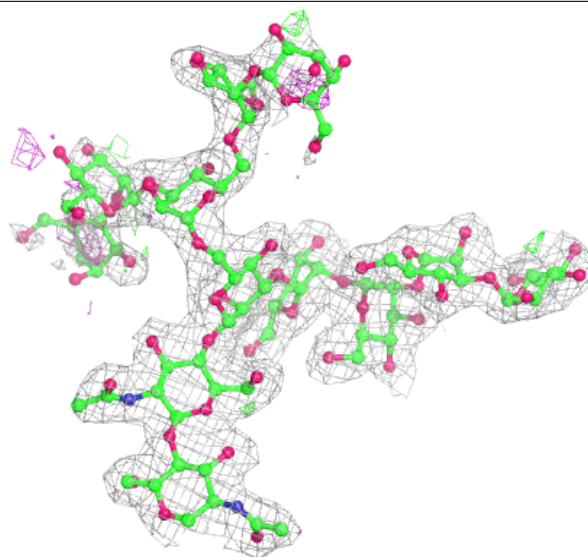
Electron density around Chain I:

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



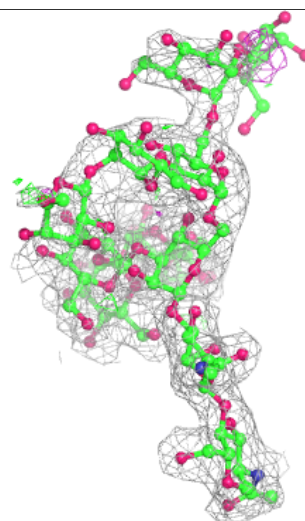
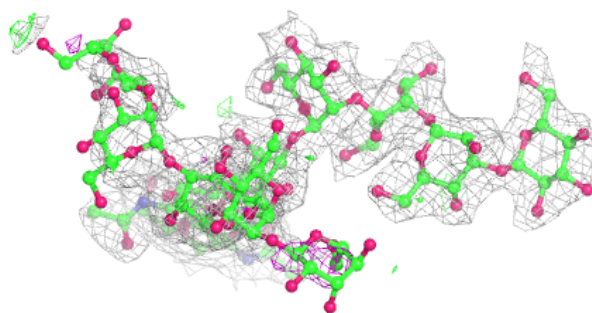
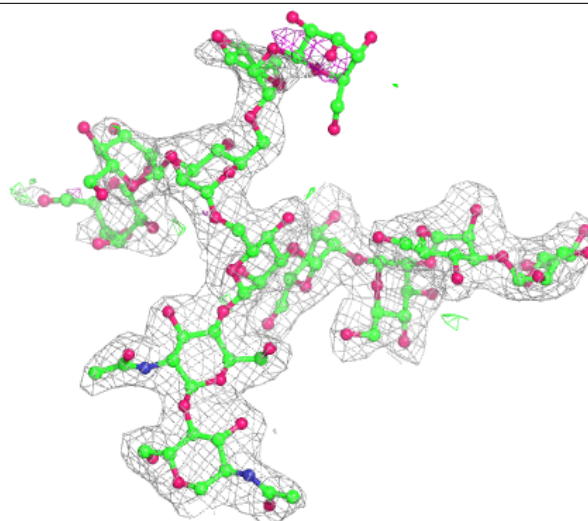
Electron density around Chain K:

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



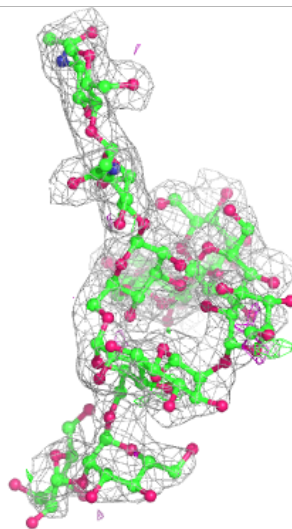
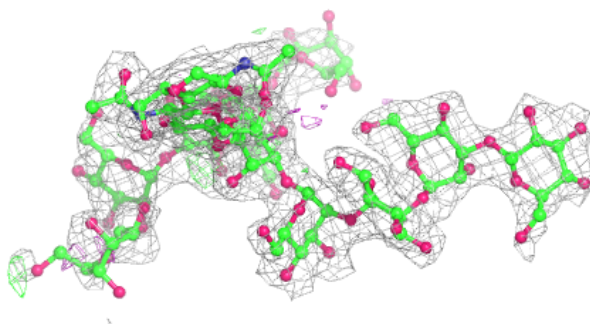
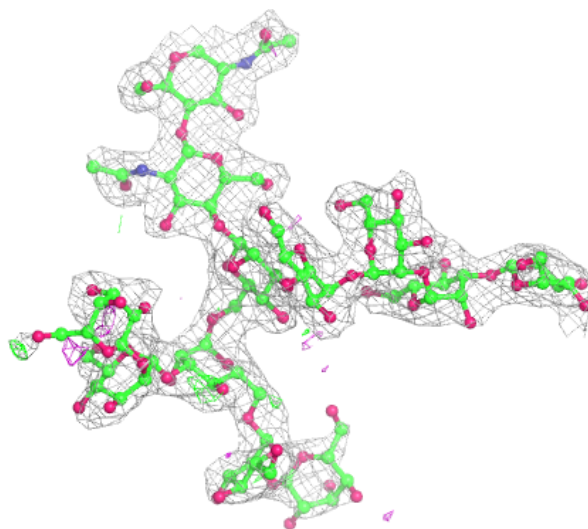
Electron density around Chain M:

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



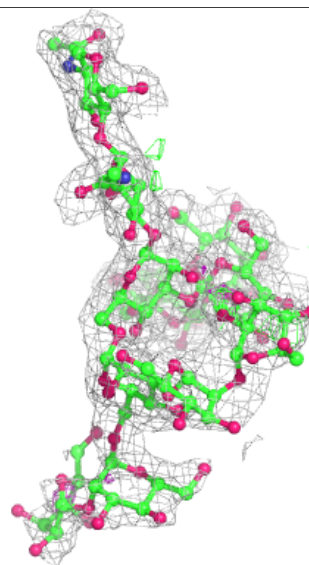
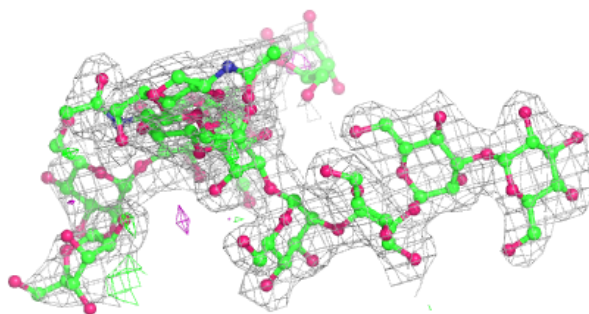
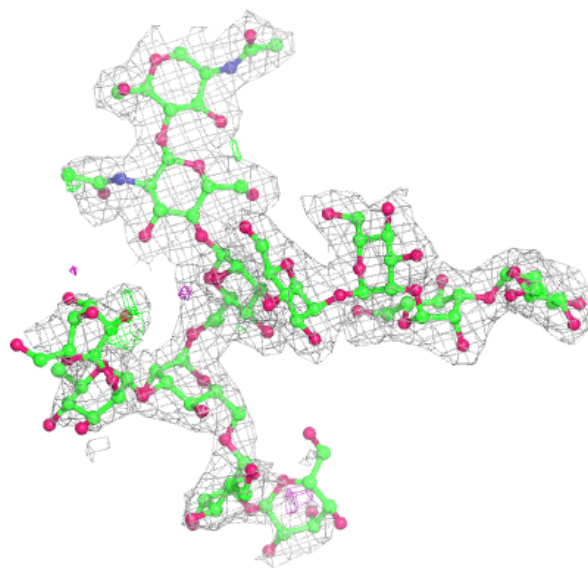
Electron density around Chain O:

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



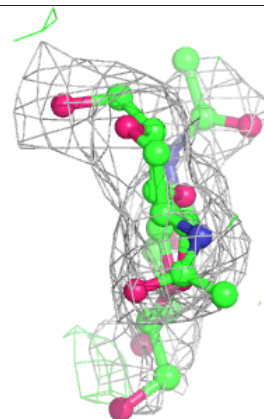
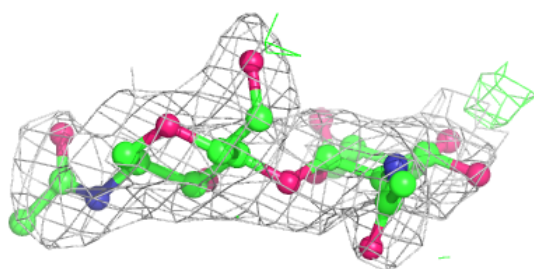
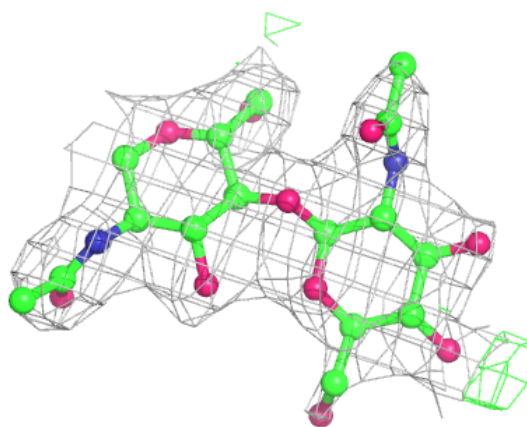
Electron density around Chain Q:

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

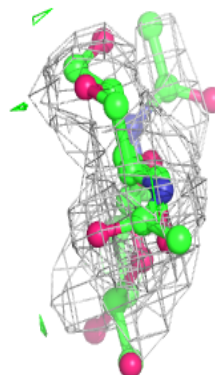
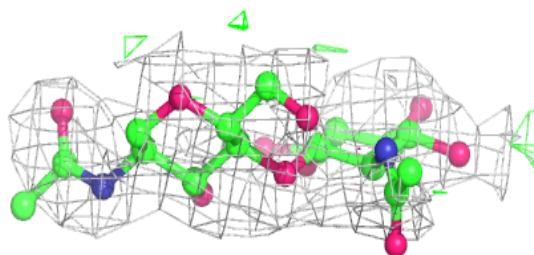
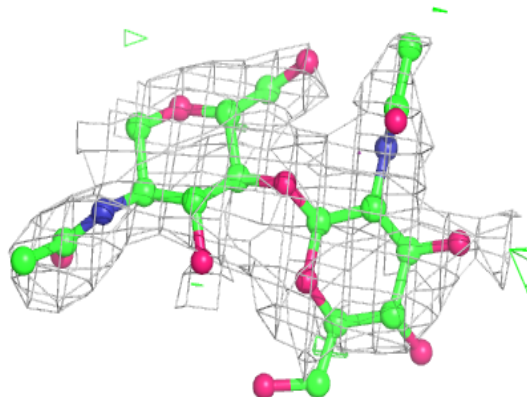


Electron density around Chain H:

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

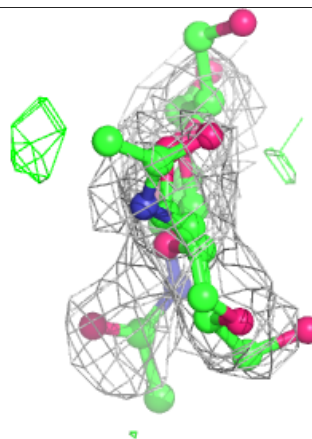
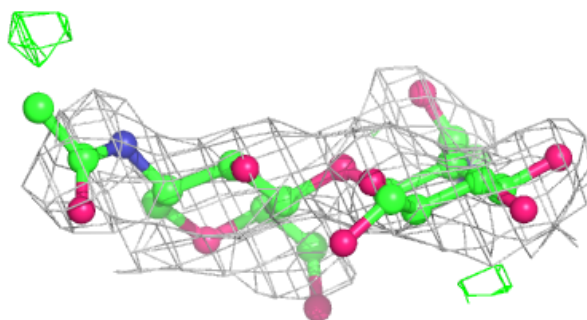
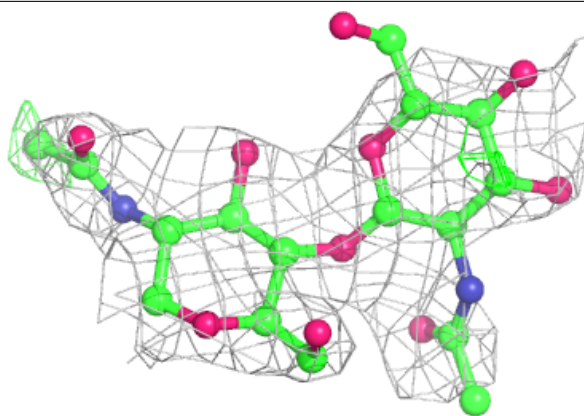
**Electron density around Chain J:**

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



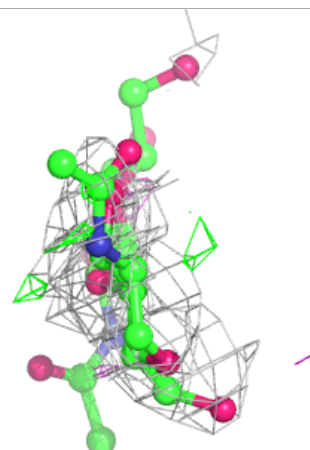
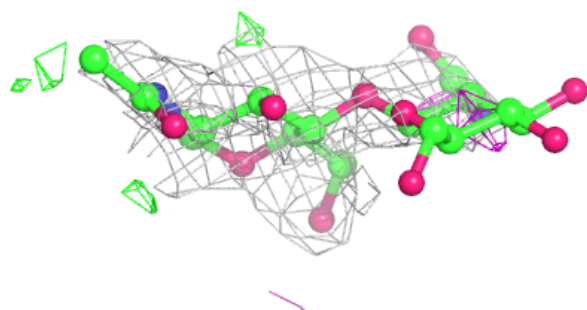
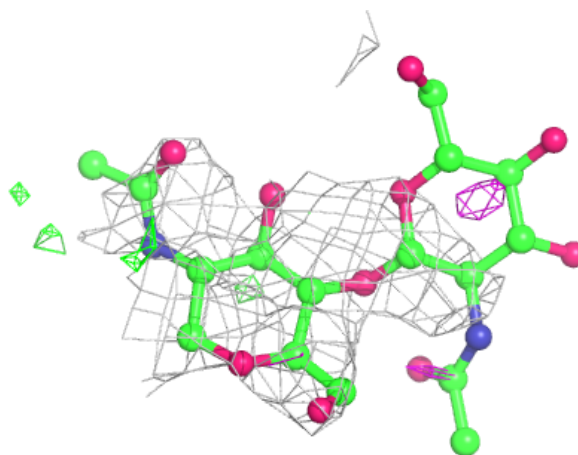
Electron density around Chain L:

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

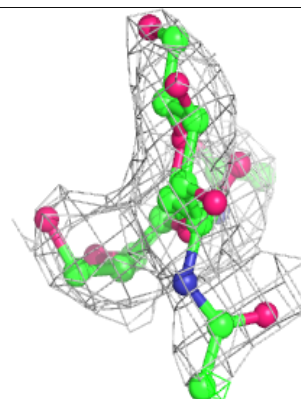
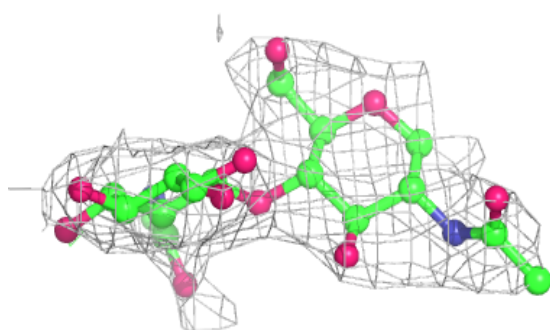
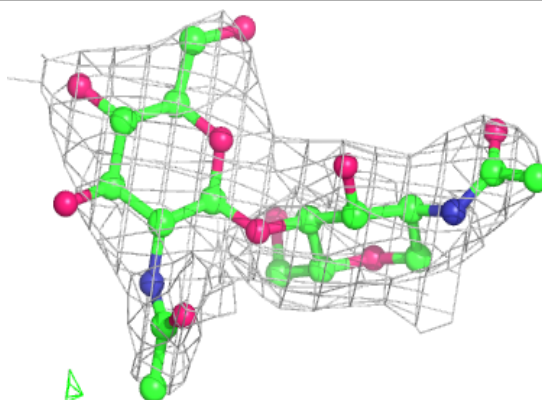


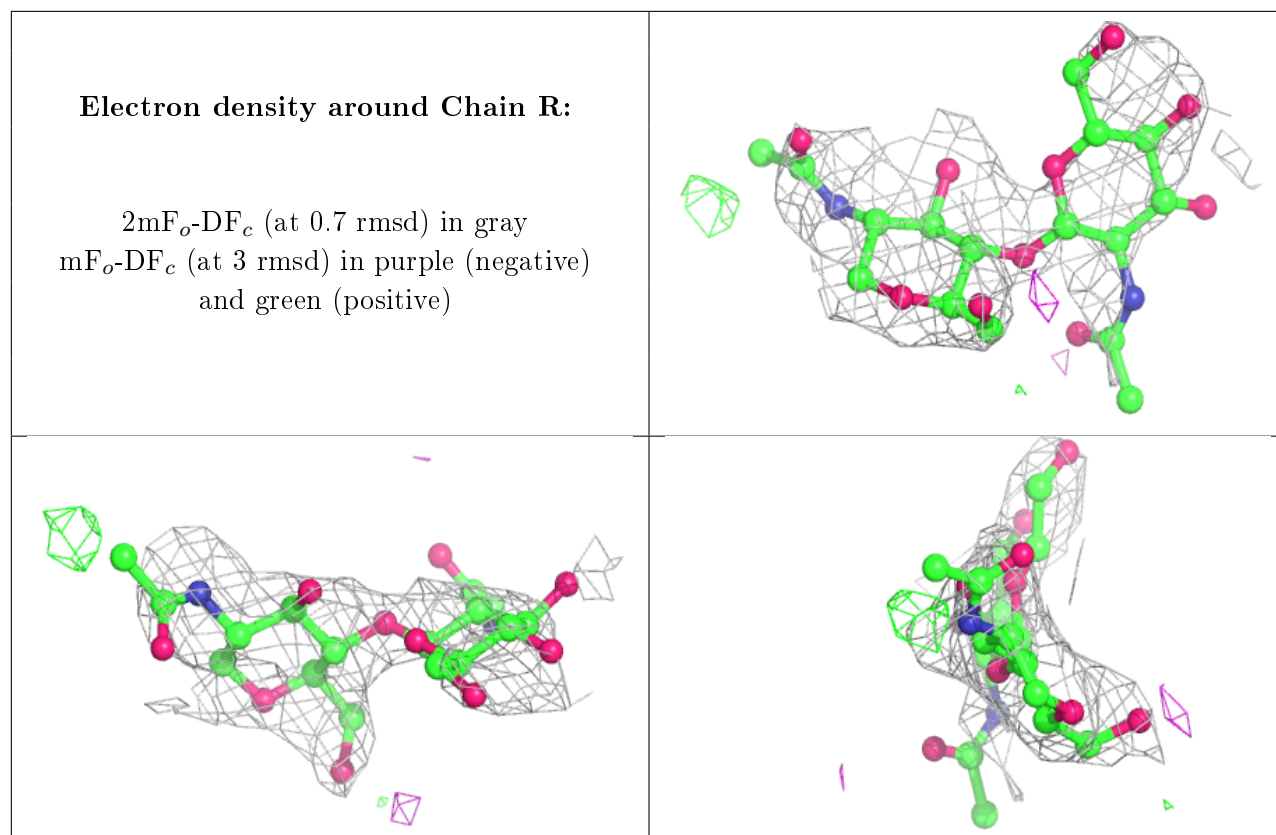
Electron density around Chain N:

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

**Electron density around Chain P:**

$2mF_o-DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FMT	B	2002	3/3	0.98	0.11	21,21,22,23	0
4	FMT	E	2005	3/3	0.98	0.09	12,12,16,18	0
4	FMT	C	2004	3/3	0.98	0.07	23,23,25,28	0
4	FMT	F	2006	3/3	0.99	0.09	23,23,26,26	0
4	FMT	A	2003	3/3	0.99	0.07	22,22,29,31	0
4	FMT	D	2001	3/3	0.99	0.07	30,30,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.