



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2022 – 06:14 PM JST

PDB ID : 7DRB
Title : Crystal structure of plant receptor like protein RXEG1 with xyloglucanase XEG1
Authors : Sun, Y.; Wang, Y.; Zhang, X.X.; Chen, Z.D.; Xia, Y.Q.; Sun, Y.J.; Zhang, M.M.; Xiao, Y.; Han, Z.F.; Wang, Y.C.; Chai, J.J.
Deposited on : 2020-12-27
Resolution : 3.30 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 : 2.28.1
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) : 2.28.1

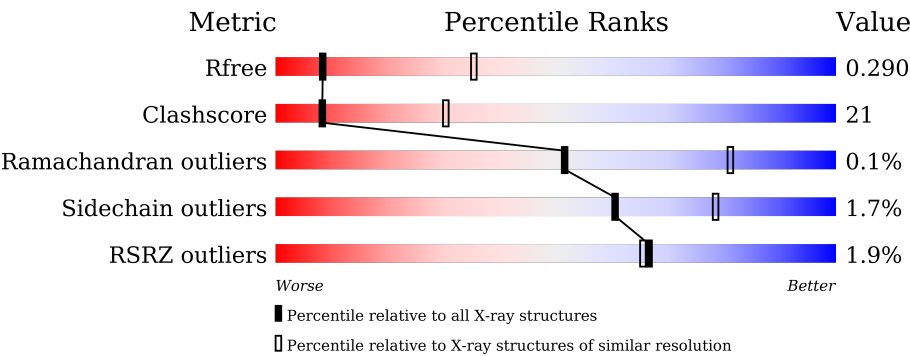
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	241	<div><div></div><div>58%34%8%</div></div>
1	B	241	<div><div>3%</div><div>60%32%8%</div></div>
2	C	934	<div><div>%</div><div>49%30%19%</div></div>
2	D	934	<div><div>2%</div><div>46%33%19%</div></div>
3	E	10	<div><div>10%90%</div></div>
3	L	10	<div><div>40%50%10%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	G	2	 50% 50%
4	J	2	 50% 50%
4	K	2	 50% 50%
4	M	2	 100%
4	Q	2	 100%
5	H	3	 33% 67%
5	N	3	 33% 67%
5	O	3	 33% 67%
5	R	3	 67% 33%
6	I	7	 43% 57%
6	P	7	 43% 57%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	M	2	-	-	-	X
7	NAG	D	1001	-	-	-	X
7	NAG	D	1003	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16004 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.

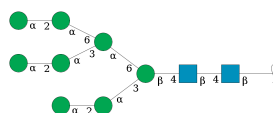
- Molecule 1 is a protein called Cell 12A endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1675	1068	269	333	5			
1	B	222	Total	C	N	O	S	0	0	0
			1675	1068	269	333	5			

- Molecule 2 is a protein called Membrane-localized LRR receptor-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	752	Total	C	N	O	S	0	0	0
			5924	3792	984	1122	26			
2	D	752	Total	C	N	O	S	0	0	0
			5924	3792	984	1122	26			

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



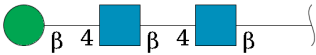
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			116	64	2	50			
3	L	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



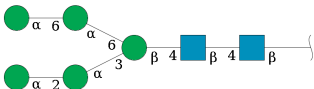
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



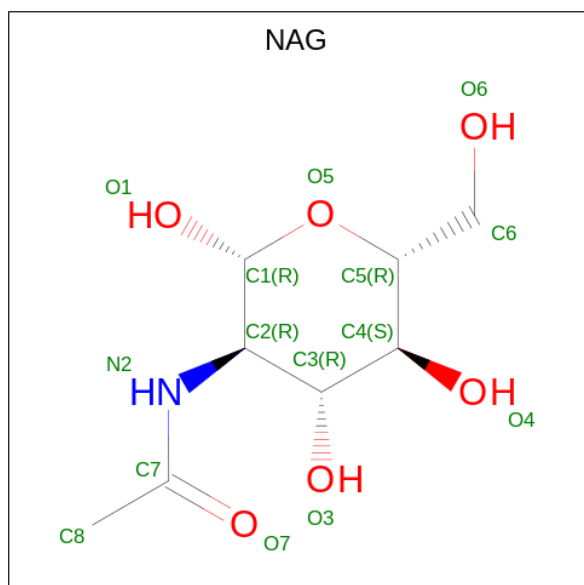
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.

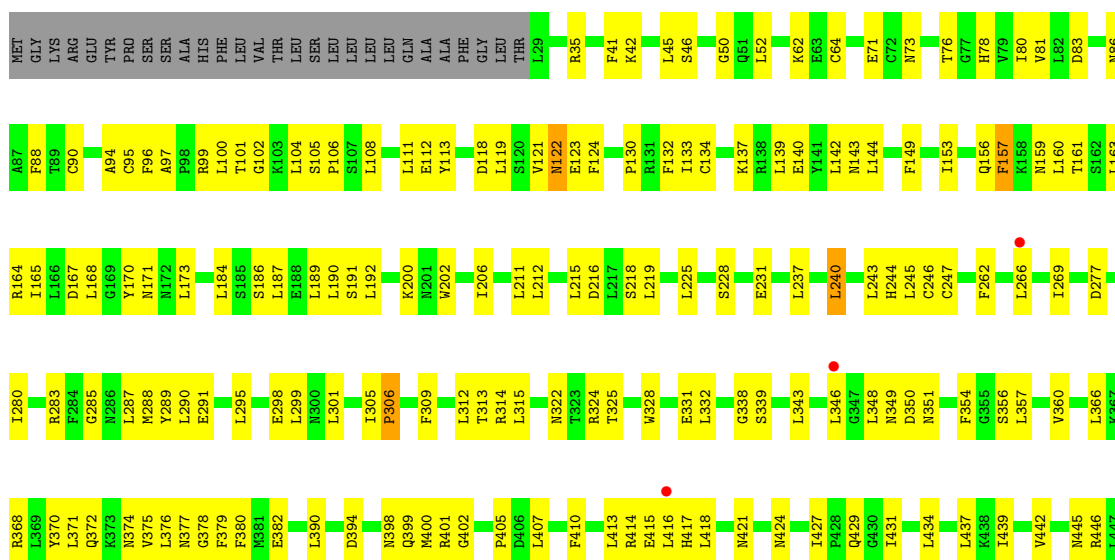


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	P	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		



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

Chain G:  50% 50%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain M:  100%



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

Chain Q:  100%



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

Chain H:  33% 67%



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

Chain N:  33% 67%



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

Chain O:  33% 67%



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

Chain R:  67% 33%



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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:  43% 57%



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 P:  43% 57%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.89Å 92.84Å 154.53Å 90.00° 107.91° 90.00°	Depositor
Resolution (Å)	49.01 – 3.30 49.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.01-3.30) 97.2 (49.01-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.284 0.241 , 0.290	Depositor DCC
R_{free} test set	2064 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	0/1716	0.84	0/2333
1	B	0.53	0/1716	0.78	0/2333
2	C	0.57	0/6051	0.86	1/8202 (0.0%)
2	D	0.52	0/6051	0.82	1/8202 (0.0%)
All	All	0.55	0/15534	0.83	2/21070 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	723	LEU	CA-CB-CG	6.01	129.13	115.30
2	D	637	PHE	CB-CA-C	-5.12	100.17	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1675	0	1624	70	0
1	B	1675	0	1624	69	0
2	C	5924	0	5889	242	1
2	D	5924	0	5887	289	0
3	E	116	0	97	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	116	0	97	2	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	Q	28	0	25	0	0
5	H	39	0	34	3	0
5	N	39	0	34	0	0
5	O	39	0	34	0	0
5	R	39	0	34	6	0
6	I	83	0	70	0	0
6	P	83	0	70	0	0
7	C	42	0	39	1	0
7	D	42	0	39	1	0
All	All	16004	0	15722	666	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (666) 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)
2:D:614:PHE:HA	2:D:637:PHE:HA	1.24	1.09
2:D:90:CYS:HA	2:D:95:CYS:HA	1.37	1.03
2:D:628:THR:HA	2:D:651:LEU:HA	1.49	0.94
2:C:479:LEU:HA	2:C:482:LEU:HD21	1.49	0.94
2:C:470:LEU:HB2	2:C:493:ASN:HD22	1.36	0.90
1:B:38:ASN:HB2	1:B:53:THR:HG21	1.53	0.90
2:C:498:LYS:HE2	2:C:520:GLY:HA2	1.55	0.87
2:C:313:THR:O	2:C:339:SER:HB3	1.76	0.86
1:B:84:ASN:ND2	1:B:218:GLU:OE1	2.09	0.86
2:D:349:ASN:HD22	2:D:372:GLN:NE2	1.75	0.84
1:B:119:VAL:HG22	1:B:221:THR:HG22	1.57	0.84
2:D:596:LEU:HD11	2:D:619:SER:HB2	1.60	0.84
1:A:159:THR:HG22	1:A:168:LYS:HD3	1.57	0.83
2:C:280:ILE:HD11	2:C:305:ILE:HA	1.60	0.83
1:B:159:THR:HG22	1:B:168:LYS:HD3	1.60	0.82
2:C:171:ASN:HB2	2:C:173:LEU:HD22	1.60	0.81
1:B:49:GLY:HA3	1:B:71:TRP:CE3	2.15	0.81
2:D:41:PHE:HB2	2:D:108:LEU:HD21	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ASP:HB2	2:D:118:ASP:HB3	1.63	0.79
2:D:554:LEU:HD21	2:D:577:GLU:HB2	1.64	0.79
2:C:202:TRP:HD1	2:C:206:ILE:HD12	1.48	0.79
1:A:209:PRO:HG2	1:A:212:GLN:HG2	1.65	0.79
2:D:349:ASN:HD22	2:D:372:GLN:HE22	1.30	0.79
2:C:535:VAL:HG23	2:C:560:ILE:HB	1.65	0.79
2:C:617:ILE:HD11	2:C:641:LEU:HD22	1.65	0.79
2:D:165:ILE:HG23	2:D:189:LEU:HD22	1.65	0.79
1:B:149:PRO:HG2	1:B:170:TYR:CD2	2.18	0.78
2:D:468:ASN:HB2	2:D:470:LEU:HD23	1.64	0.78
1:A:108:TYR:HE2	1:A:115:PHE:HZ	1.30	0.78
2:D:280:ILE:HD11	2:D:305:ILE:HA	1.65	0.78
2:D:228:SER:HB3	2:D:231:GLU:HG3	1.65	0.77
1:A:149:PRO:HG2	1:A:170:TYR:HD2	1.49	0.77
2:D:476:GLU:OE1	2:D:500:SER:N	2.17	0.77
2:C:86:ASN:O	2:C:121:VAL:HB	1.85	0.77
2:D:630:LEU:HD23	2:D:651:LEU:HD11	1.66	0.76
2:D:655:ASN:HA	2:D:679:TYR:HB2	1.67	0.76
1:B:149:PRO:HG2	1:B:170:TYR:HD2	1.49	0.76
2:C:510:GLN:HA	2:C:533:TYR:HA	1.67	0.75
2:D:71:GLU:HB2	2:D:81:VAL:HB	1.68	0.75
2:C:165:ILE:HG23	2:C:189:LEU:HD22	1.69	0.75
2:D:45:LEU:HD23	2:D:100:LEU:HD23	1.67	0.75
2:C:90:CYS:HA	2:C:95:CYS:HA	1.68	0.75
2:D:458:SER:H	2:D:482:LEU:HD23	1.51	0.75
1:B:97:ILE:HD13	1:B:100:ILE:HD11	1.69	0.75
2:C:306:PRO:O	2:C:335:ARG:HD3	1.88	0.73
2:D:171:ASN:HB2	2:D:173:LEU:HD22	1.71	0.73
1:A:57:LYS:HB3	1:A:64:ALA:HB3	1.70	0.73
1:A:59:SER:OG	1:A:62:THR:HG23	1.89	0.73
1:A:108:TYR:CE2	1:A:115:PHE:HZ	2.06	0.73
2:C:134:CYS:SG	2:C:156:GLN:HB3	2.29	0.72
1:A:123:LEU:HD22	1:A:217:LEU:HG	1.70	0.72
2:C:202:TRP:CD1	2:C:206:ILE:HD12	2.25	0.72
2:D:299:LEU:O	2:D:324:ARG:NH1	2.22	0.72
2:C:470:LEU:HB2	2:C:493:ASN:ND2	2.03	0.72
2:D:491:SER:HA	2:D:515:PRO:HD2	1.73	0.71
2:D:86:ASN:HD22	2:D:122:ASN:HD21	1.37	0.71
1:A:97:ILE:HG21	1:A:100:ILE:HG13	1.72	0.71
1:B:93:GLN:HG2	1:B:213:TYR:CD1	2.26	0.71
2:D:237:LEU:HD11	7:D:1001:NAG:H81	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:PHE:HD1	2:D:402:GLY:HA3	1.57	0.70
2:C:519:LEU:HD12	2:C:538:ILE:HG23	1.74	0.70
1:B:53:THR:HA	1:B:67:THR:HA	1.74	0.70
3:L:9:MAN:H2	3:L:10:MAN:H5	1.74	0.69
2:C:248:ASN:O	2:C:274:ASN:ND2	2.20	0.69
2:C:738:SER:HB3	2:C:740:ILE:HG12	1.75	0.69
1:B:93:GLN:HG2	1:B:213:TYR:CE1	2.27	0.69
2:D:665:LEU:HB2	2:D:690:PRO:HD3	1.75	0.69
2:C:672:LEU:HD23	2:C:675:LEU:HD13	1.75	0.69
1:B:195:LEU:HA	1:B:198:PHE:HD2	1.57	0.69
2:C:515:PRO:HG3	2:C:537:ASP:OD1	1.93	0.69
2:D:86:ASN:HD22	2:D:122:ASN:ND2	1.91	0.68
2:D:512:ILE:HG23	2:D:536:LEU:HA	1.75	0.68
2:C:244:HIS:HA	2:C:270:ASP:HB3	1.75	0.68
1:B:169:LEU:HD13	1:B:182:PHE:CE1	2.29	0.68
2:D:500:SER:HB3	2:D:503:TRP:HB2	1.74	0.68
2:D:501:ILE:HD12	2:D:501:ILE:H	1.58	0.67
2:D:510:GLN:HA	2:D:533:TYR:HA	1.76	0.67
2:D:644:CYS:HB3	5:R:1:NAG:H82	1.77	0.67
2:C:638:SER:HA	2:C:660:ASN:O	1.95	0.67
1:A:124:PHE:HE2	2:C:792:TYR:HE1	1.43	0.67
1:A:171:LYS:HE2	1:A:180:PHE:CE1	2.28	0.67
2:D:351:ASN:O	2:D:374:ASN:HA	1.95	0.67
2:C:675:LEU:HD21	2:C:678:LEU:HD13	1.77	0.67
2:D:663:GLY:O	2:D:685:PHE:HD1	1.78	0.67
2:D:643:ASP:OD1	2:D:666:PRO:HB3	1.95	0.66
2:C:201:ASN:HB2	2:C:204:GLN:OE1	1.96	0.66
2:D:88:PHE:HB3	2:D:97:ALA:HB2	1.77	0.66
1:B:47:ALA:HB1	1:B:72:THR:O	1.96	0.65
2:D:288:MET:HG3	2:D:289:TYR:HD1	1.59	0.65
5:H:1:NAG:H61	5:H:2:NAG:H82	1.76	0.65
2:D:577:GLU:HG3	2:D:578:ASN:H	1.62	0.65
1:A:156:ALA:HB2	1:A:170:TYR:HE1	1.61	0.65
2:C:188:GLU:HA	2:C:211:LEU:O	1.96	0.65
2:D:191:SER:HA	2:D:216:ASP:HB3	1.79	0.64
2:C:460:LEU:HD21	2:C:463:PHE:HB2	1.79	0.64
2:C:605:ILE:HG22	2:C:629:SER:HB3	1.79	0.64
2:D:589:SER:H	2:D:610:LYS:HB2	1.63	0.64
2:C:681:ARG:HG2	2:C:704:GLY:H	1.63	0.64
1:B:182:PHE:CD2	1:B:198:PHE:HD1	2.16	0.64
2:D:246:CYS:SG	2:D:247:CYS:N	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:ILE:HD11	2:C:306:PRO:HD3	1.79	0.64
1:A:159:THR:HG23	2:C:219:LEU:HD21	1.80	0.64
2:C:709:THR:HA	2:C:732:LYS:O	1.97	0.63
2:C:79:VAL:HB	2:C:111:LEU:HD12	1.79	0.63
2:C:144:LEU:HB3	2:C:149:PHE:CE2	2.33	0.63
2:D:86:ASN:ND2	2:D:122:ASN:HD21	1.97	0.63
2:C:458:SER:HA	2:C:482:LEU:HA	1.81	0.63
2:C:295:LEU:O	2:C:298:GLU:HG2	1.99	0.63
2:C:85:HIS:HB2	2:C:120:SER:OG	1.99	0.63
1:B:169:LEU:HD13	1:B:182:PHE:HE1	1.64	0.63
1:A:215:ILE:HG22	1:A:216:THR:HG23	1.81	0.63
2:D:83:ASP:CB	2:D:118:ASP:HB3	2.29	0.62
2:D:654:LEU:HD23	2:D:678:LEU:CD1	2.29	0.62
2:C:55:TRP:CZ2	2:C:70:ILE:HD11	2.34	0.62
2:C:503:TRP:CH2	2:C:505:PRO:HB3	2.35	0.62
1:B:165:ASN:OD1	1:B:186:LYS:HD2	1.98	0.62
2:D:515:PRO:HG3	2:D:537:ASP:OD1	1.99	0.62
1:B:67:THR:HG21	1:B:83:SER:OG	1.99	0.62
2:D:202:TRP:HE3	2:D:206:ILE:HD12	1.64	0.62
2:C:88:PHE:HB3	2:C:97:ALA:HB2	1.82	0.61
2:C:120:SER:HB2	3:E:1:NAG:H62	1.82	0.61
2:C:698:LEU:HD21	2:C:720:LEU:HD21	1.82	0.61
2:D:519:LEU:HD23	2:D:541:ALA:HB2	1.80	0.61
1:A:38:ASN:HB2	1:A:53:THR:HG21	1.82	0.61
2:C:467:TYR:CE1	2:C:492:PHE:HD2	2.19	0.61
2:C:197:PHE:HB3	2:C:220:CYS:O	2.00	0.61
2:C:178:LEU:HG	2:C:181:LEU:HD13	1.82	0.61
1:A:150:ILE:HD12	2:C:92:ALA:O	2.02	0.60
2:D:41:PHE:CB	2:D:108:LEU:HD21	2.31	0.60
2:C:680:MET:HB2	2:C:703:LEU:HD13	1.83	0.60
2:D:216:ASP:HA	2:D:244:HIS:HB2	1.83	0.60
5:H:2:NAG:H3	5:H:2:NAG:H83	1.82	0.60
1:B:50:SER:O	1:B:69:TYR:HA	2.01	0.60
2:C:351:ASN:O	2:C:374:ASN:HA	2.01	0.60
1:B:158:ALA:HA	2:D:219:LEU:HD21	1.83	0.60
2:D:376:LEU:HB2	2:D:398:ASN:HB3	1.84	0.60
1:A:169:LEU:HD13	1:A:182:PHE:CE1	2.36	0.60
1:B:126:SER:HB3	1:B:215:ILE:HD11	1.83	0.60
2:C:304:GLY:HA3	2:C:327:GLN:OE1	2.01	0.59
1:B:70:THR:HG23	1:B:227:THR:HA	1.83	0.59
2:D:164:ARG:HA	2:D:187:LEU:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:LEU:HB2	2:C:690:PRO:HD3	1.84	0.59
2:C:722:ASN:O	2:C:723:LEU:HB2	2.01	0.59
2:C:327:GLN:HE21	2:C:331:GLU:HG3	1.68	0.59
2:D:508:GLN:NE2	2:D:529:SER:O	2.25	0.59
2:D:652:ALA:HA	2:D:675:LEU:HA	1.83	0.59
2:C:314:ARG:HA	2:C:342:THR:HG21	1.84	0.59
2:D:533:TYR:CE1	2:D:555:PRO:HG2	2.38	0.59
1:A:124:PHE:HE2	2:C:792:TYR:CE1	2.21	0.59
1:A:182:PHE:CD2	1:A:198:PHE:HD2	2.20	0.59
2:C:88:PHE:HB2	2:C:96:PHE:O	2.02	0.59
2:C:581:ASP:OD1	2:C:602:ASN:ND2	2.34	0.59
1:A:128:THR:HG23	1:A:131:GLY:CA	2.32	0.59
2:D:139:LEU:HD13	2:D:142:LEU:HD12	1.85	0.59
2:C:577:GLU:HG2	2:C:580:TYR:CZ	2.37	0.59
1:A:108:TYR:HE2	1:A:115:PHE:CZ	2.18	0.59
1:A:149:PRO:HG2	1:A:170:TYR:CD2	2.35	0.59
1:A:182:PHE:CE2	1:A:198:PHE:HD2	2.21	0.59
2:C:668:SER:O	2:C:671:SER:HB3	2.03	0.59
2:C:655:ASN:HA	2:C:679:TYR:HB2	1.84	0.58
2:D:666:PRO:HD2	2:D:669:LEU:HD12	1.85	0.58
2:C:498:LYS:NZ	2:C:521:PRO:HD3	2.18	0.58
2:D:99:ARG:HA	2:D:122:ASN:HD22	1.67	0.58
2:C:33:LYS:HB3	2:D:328:TRP:CD2	2.38	0.58
2:C:479:LEU:HD12	2:C:503:TRP:CH2	2.39	0.58
2:C:596:LEU:HD23	2:C:617:ILE:HG22	1.85	0.58
1:B:69:TYR:CZ	1:B:223:PRO:HB3	2.38	0.58
2:D:622:LYS:HD3	5:R:1:NAG:H2	1.85	0.58
2:D:86:ASN:O	2:D:121:VAL:HB	2.04	0.58
1:B:186:LYS:O	1:B:188:ILE:HG13	2.03	0.58
2:D:665:LEU:HD11	2:D:708:LEU:HD11	1.84	0.58
2:C:349:ASN:HD22	2:C:372:GLN:HE22	1.51	0.57
2:D:487:ASP:HA	2:D:511:VAL:HG13	1.86	0.57
1:A:156:ALA:HA	1:A:170:TYR:CD1	2.39	0.57
2:C:112:GLU:HG2	2:C:113:TYR:CE1	2.39	0.57
2:D:134:CYS:HG	2:D:157:PHE:HD1	1.52	0.57
2:C:59:GLU:O	2:C:62:LYS:HB3	2.05	0.57
2:D:645:TRP:HE1	2:D:666:PRO:HG2	1.70	0.57
2:D:664:LYS:HA	2:D:686:SER:O	2.04	0.57
2:D:41:PHE:CG	2:D:108:LEU:HD21	2.40	0.57
2:C:512:ILE:HG23	2:C:536:LEU:HA	1.86	0.57
2:C:103:LYS:HD2	2:C:125:GLU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:658:TYR:HD1	2:D:682:GLN:HB2	1.70	0.57
1:A:128:THR:HG23	1:A:131:GLY:HA3	1.87	0.56
2:C:101:THR:N	2:C:123:GLU:O	2.37	0.56
2:C:131:ARG:HD2	2:C:156:GLN:NE2	2.20	0.56
2:C:479:LEU:HD12	2:C:503:TRP:HH2	1.70	0.56
2:C:652:ALA:HA	2:C:675:LEU:HA	1.86	0.56
2:D:348:LEU:HB2	2:D:371:LEU:HD23	1.86	0.56
2:D:509:LEU:HD23	2:D:530:GLN:HG2	1.85	0.56
1:B:108:TYR:CE1	1:B:231:MET:HB2	2.39	0.56
2:C:329:LEU:HD21	2:C:333:PHE:CE2	2.40	0.56
2:C:41:PHE:CD2	2:C:108:LEU:HD21	2.41	0.56
2:D:243:LEU:HB3	2:D:245:LEU:HD23	1.86	0.56
2:D:161:THR:O	2:D:186:SER:OG	2.17	0.56
2:D:600:PRO:HB2	2:D:603:VAL:HB	1.88	0.56
2:C:130:PRO:HD2	2:C:133:ILE:HD11	1.88	0.56
2:D:200:LYS:HA	2:D:225:LEU:HD22	1.88	0.56
2:D:644:CYS:HA	2:D:646:MET:SD	2.46	0.56
1:A:57:LYS:HE2	1:A:64:ALA:HB2	1.87	0.55
2:C:664:LYS:HD3	2:C:687:GLY:HA3	1.87	0.55
2:C:163:LEU:HD13	2:C:166:LEU:HG	1.87	0.55
2:D:295:LEU:O	2:D:298:GLU:HG2	2.06	0.55
2:D:521:PRO:HA	2:D:542:ASN:O	2.05	0.55
2:C:164:ARG:HG2	2:C:165:ILE:HG13	1.88	0.55
2:C:336:LEU:HD23	2:C:343:LEU:HD11	1.89	0.55
2:D:277:ASP:HB2	2:D:299:LEU:HD23	1.87	0.55
2:D:313:THR:O	2:D:339:SER:OG	2.15	0.55
1:A:47:ALA:HB2	1:A:80:LYS:HE2	1.89	0.55
2:C:508:GLN:HA	2:C:530:GLN:OE1	2.07	0.55
2:D:418:LEU:HB2	2:D:442:VAL:HG12	1.89	0.55
2:C:166:LEU:HD22	2:C:168:LEU:HD11	1.89	0.55
2:C:681:ARG:NE	2:C:702:ASP:OD2	2.31	0.55
2:D:475:THR:O	2:D:478:HIS:HB3	2.05	0.55
2:D:689:LEU:HD21	2:D:713:PRO:HD3	1.89	0.55
1:B:77:THR:HG23	1:B:78:GLU:HG3	1.88	0.55
2:D:558:ILE:HD11	2:D:582:TYR:OH	2.07	0.55
2:C:491:SER:HA	2:C:515:PRO:HD2	1.88	0.55
2:D:100:LEU:HD13	2:D:122:ASN:OD1	2.07	0.55
2:C:109:LEU:HD21	2:C:135:SER:HB2	1.90	0.54
2:C:192:LEU:O	2:C:220:CYS:SG	2.65	0.54
2:D:184:LEU:HB3	2:D:187:LEU:HG	1.88	0.54
2:D:301:LEU:HB2	2:D:325:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:654:LEU:HD23	2:D:678:LEU:HD11	1.89	0.54
1:B:38:ASN:HB2	1:B:53:THR:CG2	2.31	0.54
2:D:410:PHE:O	2:D:434:LEU:HD21	2.06	0.54
1:A:105:LYS:HE3	1:A:190:ASN:ND2	2.22	0.54
2:C:47:ASP:O	2:C:49:PHE:N	2.38	0.54
2:C:103:LYS:HD3	2:C:125:GLU:OE2	2.08	0.54
1:A:109:SER:O	1:A:229:ALA:HA	2.08	0.54
2:D:101:THR:N	2:D:123:GLU:O	2.40	0.54
2:D:507:PHE:CE1	2:D:509:LEU:HD22	2.43	0.54
2:D:794:ARG:HD3	2:D:796:TYR:CZ	2.43	0.54
1:A:79:VAL:HG22	1:A:224:PHE:CE1	2.42	0.53
1:A:95:LYS:HG2	1:A:210:SER:HB3	1.89	0.53
2:C:479:LEU:N	2:C:479:LEU:HD23	2.23	0.53
2:D:457:LEU:HB2	2:D:482:LEU:HD21	1.89	0.53
2:D:170:TYR:HE1	2:D:219:LEU:HD12	1.74	0.53
2:D:511:VAL:HG23	2:D:535:VAL:CG1	2.38	0.53
1:B:195:LEU:HA	1:B:198:PHE:CD2	2.40	0.53
2:D:445:ASN:O	2:D:468:ASN:HA	2.08	0.53
2:D:622:LYS:HD3	5:R:1:NAG:C2	2.37	0.53
2:C:266:LEU:HD13	2:C:269:ILE:HD11	1.90	0.53
2:D:168:LEU:O	2:D:171:ASN:ND2	2.41	0.53
2:D:429:GLN:OE1	2:D:451:PRO:HB2	2.09	0.53
2:D:266:LEU:HD13	2:D:269:ILE:HD11	1.90	0.53
2:D:547:LEU:HD22	2:D:575:LEU:HD13	1.90	0.53
2:D:664:LYS:HE3	2:D:687:GLY:HA3	1.88	0.53
2:D:535:VAL:HG23	2:D:560:ILE:HB	1.90	0.53
1:A:126:SER:HB3	1:A:215:ILE:HD11	1.89	0.53
2:D:343:LEU:HD21	2:D:346:LEU:HB2	1.90	0.53
2:D:450:LEU:HB3	2:D:478:HIS:HE1	1.74	0.53
2:C:571:ARG:NH1	2:C:595:PRO:HD3	2.24	0.53
2:D:46:SER:OG	2:D:101:THR:HG23	2.09	0.53
2:D:642:PRO:HB2	2:D:644:CYS:SG	2.49	0.53
1:B:91:LYS:NZ	1:B:129:ALA:O	2.26	0.53
1:B:182:PHE:CE2	1:B:198:PHE:HD1	2.26	0.53
2:C:658:TYR:N	2:C:658:TYR:HD1	2.07	0.52
2:C:47:ASP:HB2	2:C:50:GLY:O	2.09	0.52
2:D:140:GLU:HA	2:D:163:LEU:HA	1.89	0.52
2:C:246:CYS:SG	2:C:247:CYS:SG	3.02	0.52
2:C:685:PHE:O	2:C:706:ASN:O	2.28	0.52
1:A:28:TRP:HE1	2:C:674:ASN:ND2	2.07	0.52
2:C:298:GLU:HB2	2:C:323:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:596:LEU:HD22	2:C:620:ILE:HD11	1.90	0.52
2:C:33:LYS:HB3	2:D:328:TRP:CE3	2.44	0.52
2:C:800:GLY:O	2:C:802:LEU:HD12	2.10	0.52
1:A:69:TYR:CZ	1:A:223:PRO:HB3	2.44	0.52
2:C:681:ARG:HG2	2:C:704:GLY:N	2.24	0.52
2:C:710:GLY:HA2	2:C:734:TYR:CZ	2.45	0.52
1:B:72:THR:HA	1:B:225:VAL:HG13	1.90	0.52
2:D:508:GLN:OE1	2:D:530:GLN:HA	2.11	0.52
2:C:658:TYR:N	2:C:658:TYR:CD1	2.78	0.51
2:C:703:LEU:HD23	2:C:728:LEU:CD2	2.39	0.51
2:D:289:TYR:HB3	2:D:314:ARG:HH11	1.74	0.51
2:D:35:ARG:NH1	2:D:62:LYS:HB2	2.25	0.51
2:D:99:ARG:HA	2:D:122:ASN:ND2	2.25	0.51
2:D:458:SER:HA	2:D:482:LEU:HA	1.93	0.51
2:C:559:LYS:NZ	2:C:788:PHE:O	2.44	0.51
2:D:503:TRP:CH2	2:D:505:PRO:HA	2.45	0.51
2:D:354:PHE:HA	2:D:375:VAL:O	2.11	0.51
1:A:28:TRP:CH2	2:C:650:ASN:HB3	2.45	0.51
2:D:240:LEU:HD23	2:D:262:PHE:CZ	2.46	0.51
2:D:291:GLU:HA	2:D:315:LEU:HA	1.91	0.51
1:A:87:LEU:HD11	1:A:238:ALA:HB3	1.91	0.51
2:C:305:ILE:HD11	2:C:332:LEU:HG	1.92	0.51
2:D:613:PHE:O	2:D:636:GLN:HB2	2.11	0.51
2:C:501:ILE:HG13	2:C:502:ASP:N	2.25	0.51
1:A:94:ILE:HG12	1:A:199:LEU:HD23	1.92	0.51
1:B:40:LEU:CD2	1:B:51:GLN:HB3	2.41	0.51
1:B:182:PHE:HD2	1:B:198:PHE:CD1	2.27	0.51
2:D:658:TYR:HE1	2:D:682:GLN:HG3	1.76	0.51
1:A:128:THR:HG23	1:A:131:GLY:N	2.27	0.50
2:D:139:LEU:HB3	2:D:163:LEU:HD21	1.93	0.50
2:C:142:LEU:HD22	2:C:166:LEU:HD21	1.94	0.50
2:D:289:TYR:HB2	2:D:314:ARG:HD2	1.93	0.50
2:D:356:SER:OG	2:D:378:GLY:HA3	2.11	0.50
2:C:702:ASP:C	2:C:703:LEU:HD22	2.32	0.50
2:D:164:ARG:HG3	2:D:165:ILE:HG13	1.92	0.50
2:D:659:ASN:O	2:D:683:ASN:HA	2.11	0.50
1:A:53:THR:HA	1:A:67:THR:HA	1.94	0.50
1:A:97:ILE:HG21	1:A:100:ILE:CG1	2.39	0.50
2:C:434:LEU:HD12	2:C:437:LEU:HD22	1.94	0.50
2:D:618:SER:HA	2:D:642:PRO:HG3	1.93	0.50
1:B:111:SER:HB2	1:B:227:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:TRP:O	2:D:331:GLU:HG2	2.11	0.50
1:A:125:THR:OG1	1:A:135:TYR:HB2	2.11	0.50
2:C:680:MET:O	2:C:706:ASN:ND2	2.44	0.50
2:C:114:LEU:O	2:C:114:LEU:HD12	2.12	0.50
2:D:572:VAL:HG21	2:D:587:LEU:HD13	1.93	0.50
1:A:53:THR:OG1	1:A:67:THR:HG22	2.12	0.50
1:A:167:PHE:HE1	1:A:184:ALA:HB2	1.77	0.50
1:B:45:ALA:CB	1:B:80:LYS:HE3	2.42	0.50
2:D:476:GLU:HB3	2:D:499:THR:HA	1.94	0.50
2:D:794:ARG:HD3	2:D:796:TYR:CE2	2.47	0.50
2:C:160:LEU:HD13	2:C:163:LEU:HD11	1.94	0.49
1:B:125:THR:HG22	1:B:214:LEU:HA	1.94	0.49
2:D:646:MET:SD	5:R:1:NAG:H81	2.53	0.49
2:D:133:ILE:O	2:D:160:LEU:HD11	2.12	0.49
1:A:157:ILE:HD11	1:A:169:LEU:HG	1.94	0.49
2:C:59:GLU:O	2:C:62:LYS:HD2	2.13	0.49
2:D:641:LEU:HB3	2:D:645:TRP:HZ2	1.77	0.49
2:D:641:LEU:HG	2:D:685:PHE:HE1	1.77	0.49
2:D:747:LEU:HD21	2:D:750:LEU:HD13	1.93	0.49
2:C:445:ASN:O	2:C:468:ASN:HA	2.13	0.49
2:D:173:LEU:HD23	2:D:173:LEU:H	1.78	0.49
2:C:99:ARG:HB3	2:C:123:GLU:H	1.77	0.49
2:C:379:PHE:HD1	2:C:402:GLY:HA3	1.78	0.49
2:C:689:LEU:H	2:C:689:LEU:HD23	1.78	0.49
2:D:505:PRO:HG3	2:D:529:SER:OG	2.12	0.49
1:B:45:ALA:O	1:B:46:ALA:HB3	2.13	0.49
1:B:92:LYS:NZ	1:B:241:ASN:O	2.33	0.49
1:B:108:TYR:CD1	1:B:231:MET:HB2	2.48	0.49
2:D:100:LEU:HD13	2:D:122:ASN:CG	2.33	0.49
2:C:525:LYS:HE2	2:C:528:GLN:NE2	2.28	0.49
2:C:664:LYS:CD	2:C:687:GLY:HA3	2.43	0.49
2:D:462:SER:HA	2:D:487:ASP:HB3	1.95	0.49
2:D:599:VAL:HG11	2:D:625:THR:HB	1.95	0.49
2:C:306:PRO:HD2	2:C:309:PHE:CD1	2.47	0.48
2:D:219:LEU:HG	2:D:247:CYS:CB	2.43	0.48
2:C:651:LEU:O	2:C:674:ASN:O	2.32	0.48
2:C:698:LEU:CD1	2:C:723:LEU:HD13	2.43	0.48
1:B:94:ILE:HG12	1:B:199:LEU:HD23	1.93	0.48
2:D:144:LEU:HB3	2:D:149:PHE:HE2	1.78	0.48
2:D:559:LYS:HG2	2:D:560:ILE:HG13	1.94	0.48
1:A:75:ALA:O	1:A:80:LYS:NZ	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:ARG:HG2	2:C:64:CYS:HB3	1.94	0.48
1:A:119:VAL:HG22	1:A:221:THR:HG22	1.96	0.48
1:B:97:ILE:HG21	1:B:100:ILE:HG13	1.95	0.48
1:B:182:PHE:CD2	1:B:198:PHE:CD1	2.98	0.48
2:D:90:CYS:HB3	2:D:94:ALA:O	2.14	0.48
2:D:562:ASN:HA	2:D:586:ASP:OD1	2.13	0.48
2:D:630:LEU:HD11	2:D:654:LEU:HD12	1.95	0.48
2:D:156:GLN:O	2:D:159:ASN:HB2	2.13	0.48
2:D:612:GLN:HA	2:D:636:GLN:HG3	1.96	0.48
2:D:645:TRP:HD1	2:D:668:SER:HB2	1.78	0.48
2:C:323:THR:OG1	2:C:325:THR:HG23	2.12	0.48
2:D:104:LEU:HD11	2:D:130:PRO:HG2	1.96	0.48
2:D:487:ASP:HA	2:D:511:VAL:CG1	2.44	0.48
2:D:617:ILE:HD11	2:D:641:LEU:HD22	1.94	0.48
1:A:83:SER:O	1:A:220:GLY:HA3	2.13	0.48
1:A:169:LEU:HD13	1:A:182:PHE:CD1	2.48	0.48
2:D:306:PRO:HD2	2:D:309:PHE:CE1	2.48	0.48
2:D:313:THR:HA	2:D:338:GLY:O	2.14	0.48
1:B:160:VAL:HG12	1:B:162:ILE:HG13	1.96	0.48
2:C:470:LEU:HD13	2:C:493:ASN:HD21	1.77	0.48
2:C:572:VAL:HG23	2:C:597:PRO:HG3	1.94	0.48
2:C:228:SER:HB3	2:C:231:GLU:HG3	1.94	0.48
2:D:585:ILE:HD11	2:D:600:PRO:HG2	1.95	0.48
2:C:39:LEU:HD11	2:C:56:GLY:HA2	1.95	0.47
2:D:450:LEU:HB3	2:D:478:HIS:CE1	2.49	0.47
2:C:558:ILE:HD11	2:C:582:TYR:CE1	2.50	0.47
2:D:215:LEU:HB2	2:D:240:LEU:HD11	1.96	0.47
2:D:592:PHE:O	2:D:612:GLN:HB2	2.14	0.47
2:D:693:SER:HB3	2:D:719:ASP:OD2	2.15	0.47
2:C:202:TRP:CH2	2:C:227:PRO:HD3	2.48	0.47
2:C:451:PRO:O	2:C:454:MET:HG2	2.14	0.47
2:D:470:LEU:HB3	2:D:495:LEU:HD13	1.97	0.47
2:D:558:ILE:HG13	2:D:582:TYR:CE1	2.49	0.47
1:A:156:ALA:HA	1:A:170:TYR:HD1	1.79	0.47
2:C:210:PRO:HB2	2:C:211:LEU:HD22	1.96	0.47
2:C:237:LEU:HD21	7:C:1001:NAG:H81	1.95	0.47
1:A:97:ILE:HD13	1:A:100:ILE:HD11	1.95	0.47
1:B:169:LEU:HD12	1:B:170:TYR:N	2.30	0.47
2:D:106:PRO:HB3	2:D:132:PHE:CD2	2.50	0.47
2:D:143:ASN:OD1	2:D:167:ASP:HB3	2.15	0.47
2:D:218:SER:HB2	2:D:246:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:511:VAL:HG23	2:D:535:VAL:HG11	1.96	0.47
2:D:80:ILE:HG13	2:D:81:VAL:HG23	1.96	0.47
2:D:144:LEU:HB3	2:D:149:PHE:CE2	2.50	0.47
2:C:698:LEU:HD21	2:C:720:LEU:CD2	2.45	0.47
2:D:471:LYS:HD2	2:D:471:LYS:C	2.35	0.47
1:A:108:TYR:CE1	1:A:231:MET:HB2	2.50	0.47
1:A:142:ALA:HB1	1:A:144:TYR:CE1	2.50	0.47
1:A:214:LEU:HD21	1:A:217:LEU:HD11	1.97	0.47
2:C:301:LEU:HB2	2:C:325:THR:HG22	1.97	0.47
1:B:99:SER:OG	1:B:101:PRO:HD3	2.15	0.47
2:D:492:PHE:HA	2:D:516:SER:HB3	1.96	0.47
2:C:572:VAL:HA	2:C:575:LEU:HB2	1.97	0.47
2:C:698:LEU:HD11	2:C:720:LEU:HG	1.96	0.47
2:C:782:GLU:HB2	2:C:796:TYR:O	2.14	0.47
1:B:62:THR:HG22	1:B:237:SER:HB2	1.97	0.47
2:D:305:ILE:HD11	2:D:332:LEU:HG	1.97	0.47
2:C:373:LYS:HE3	2:C:373:LYS:HB3	1.82	0.46
1:B:85:ALA:HB3	1:B:236:PHE:CE2	2.51	0.46
2:D:313:THR:HG22	2:D:314:ARG:H	1.80	0.46
2:C:336:LEU:HD23	2:C:343:LEU:CD1	2.45	0.46
2:C:469:VAL:HG12	2:C:469:VAL:O	2.16	0.46
2:D:133:ILE:CG2	2:D:142:LEU:HD11	2.46	0.46
2:D:219:LEU:HG	2:D:247:CYS:HB2	1.97	0.46
2:D:280:ILE:HD11	2:D:306:PRO:HD3	1.98	0.46
1:A:93:GLN:HG2	1:A:213:TYR:CE1	2.51	0.46
2:D:366:LEU:HD23	2:D:390:LEU:HD11	1.97	0.46
1:A:171:LYS:HE2	1:A:180:PHE:CZ	2.50	0.46
1:B:37:TYR:HB2	1:B:84:ASN:OD1	2.16	0.46
2:D:572:VAL:HG13	2:D:576:ILE:HG23	1.97	0.46
2:C:251:SER:HA	2:C:276:LEU:HA	1.96	0.46
1:B:216:THR:HG22	1:B:218:GLU:HG3	1.98	0.46
2:C:299:LEU:O	2:C:324:ARG:NH1	2.49	0.46
2:C:514:LEU:N	2:C:515:PRO:HD3	2.30	0.46
1:B:167:PHE:HE1	1:B:184:ALA:HB2	1.79	0.46
2:D:586:ASP:HB2	2:D:607:TYR:HB2	1.97	0.46
1:A:45:ALA:HB3	1:A:80:LYS:HE3	1.98	0.46
1:A:62:THR:OG1	1:A:235:SER:OG	2.16	0.46
2:C:212:LEU:O	2:C:240:LEU:HD12	2.15	0.46
2:D:42:LYS:HE3	2:D:52:LEU:O	2.15	0.46
2:D:102:GLY:O	2:D:124:PHE:HB3	2.16	0.46
2:D:599:VAL:CG1	2:D:625:THR:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:ARG:HH22	2:C:62:LYS:HA	1.81	0.46
2:C:479:LEU:CA	2:C:482:LEU:HD21	2.33	0.46
2:C:509:LEU:HD21	2:C:512:ILE:HD12	1.97	0.46
2:D:153:ILE:HD11	2:D:168:LEU:HD22	1.97	0.46
2:D:400:MET:N	2:D:421:ASN:OD1	2.33	0.46
2:C:131:ARG:HG2	2:C:154:PRO:HB3	1.98	0.46
2:D:313:THR:HG22	2:D:314:ARG:N	2.31	0.46
2:C:139:LEU:HD13	2:C:142:LEU:HD12	1.98	0.45
2:D:35:ARG:HE	2:D:35:ARG:HB3	1.38	0.45
2:D:187:LEU:O	2:D:211:LEU:HB2	2.16	0.45
2:D:799:LEU:HD12	2:D:799:LEU:HA	1.80	0.45
1:A:99:SER:OG	1:A:101:PRO:HD3	2.16	0.45
2:D:122:ASN:HD22	2:D:122:ASN:HA	1.46	0.45
2:D:285:GLY:HA2	2:D:312:LEU:HD21	1.97	0.45
2:C:50:GLY:O	2:C:52:LEU:N	2.42	0.45
2:C:509:LEU:O	2:C:533:TYR:HB3	2.16	0.45
2:C:693:SER:HB3	2:C:719:ASP:OD2	2.17	0.45
2:D:486:VAL:HG13	2:D:510:GLN:HB2	1.98	0.45
2:D:528:GLN:HG2	2:D:550:TRP:CD2	2.52	0.45
2:D:669:LEU:O	2:D:672:LEU:HB2	2.17	0.45
3:L:9:MAN:H2	3:L:10:MAN:C5	2.43	0.45
1:A:57:LYS:O	1:A:58:ILE:HD13	2.16	0.45
2:C:349:ASN:HD22	2:C:372:GLN:NE2	2.12	0.45
2:C:384:PHE:HD2	2:C:386:GLN:HB2	1.81	0.45
2:D:288:MET:HG3	2:D:289:TYR:CD1	2.47	0.45
2:D:322:ASN:HA	2:D:350:ASP:O	2.16	0.45
2:D:586:ASP:CB	2:D:607:TYR:HB2	2.47	0.45
2:C:541:ALA:O	2:C:566:ASN:OD1	2.34	0.45
2:C:617:ILE:HD11	2:C:641:LEU:CD2	2.42	0.45
2:C:688:MET:HA	2:C:709:THR:O	2.17	0.45
2:D:118:ASP:O	2:D:119:LEU:HD23	2.17	0.45
2:D:583:MET:HG3	2:D:584:VAL:HG23	1.98	0.45
2:C:503:TRP:CZ3	2:C:505:PRO:HB3	2.52	0.45
1:B:40:LEU:HD22	1:B:51:GLN:HB3	1.98	0.45
1:B:156:ALA:HB2	1:B:170:TYR:HE1	1.81	0.45
2:D:88:PHE:HB3	2:D:97:ALA:CB	2.46	0.45
2:D:695:CYS:O	2:D:698:LEU:HD23	2.17	0.45
2:C:180:TRP:CZ3	2:C:181:LEU:HD12	2.52	0.45
2:C:306:PRO:C	2:C:335:ARG:HD3	2.37	0.45
2:C:558:ILE:HG13	2:C:558:ILE:O	2.16	0.45
1:B:49:GLY:HA2	1:B:70:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:505:PRO:HG3	2:D:530:GLN:OE1	2.16	0.45
2:D:622:LYS:HD3	5:R:1:NAG:N2	2.32	0.45
1:A:49:GLY:HA3	1:A:70:THR:O	2.16	0.45
2:C:166:LEU:HD13	2:C:168:LEU:HD11	1.98	0.45
2:D:41:PHE:HB2	2:D:108:LEU:CD2	2.39	0.45
2:D:645:TRP:CD1	2:D:668:SER:HB2	2.52	0.45
1:B:171:LYS:HG2	1:B:172:GLY:N	2.32	0.45
2:D:78:HIS:CG	2:D:113:TYR:HD2	2.34	0.45
2:D:470:LEU:HB2	2:D:493:ASN:ND2	2.31	0.45
1:A:153:THR:HG22	1:A:155:LYS:HG3	1.99	0.44
2:C:313:THR:HA	2:C:338:GLY:O	2.17	0.44
2:D:309:PHE:CD2	2:D:312:LEU:HD11	2.53	0.44
2:D:427:ILE:HD12	2:D:450:LEU:HD22	1.98	0.44
2:C:80:ILE:HA	2:C:114:LEU:HA	1.99	0.44
2:D:509:LEU:CD2	2:D:530:GLN:HG2	2.47	0.44
2:D:622:LYS:NZ	2:D:644:CYS:HB3	2.32	0.44
2:D:514:LEU:N	2:D:515:PRO:HD3	2.33	0.44
2:D:645:TRP:HB2	2:D:668:SER:C	2.38	0.44
2:D:658:TYR:CE1	2:D:682:GLN:HG3	2.53	0.44
1:A:79:VAL:HG22	1:A:224:PHE:HE1	1.82	0.44
2:C:114:LEU:HD11	2:C:136:PHE:CE1	2.52	0.44
2:C:317:TYR:HD2	2:C:345:VAL:HB	1.82	0.44
2:D:105:SER:O	2:D:108:LEU:HD23	2.17	0.44
2:D:683:ASN:HD22	2:D:685:PHE:HE2	1.65	0.44
2:D:702:ASP:CB	2:D:727:SER:HB3	2.48	0.44
2:C:498:LYS:HE2	2:C:521:PRO:HD3	1.99	0.44
2:D:654:LEU:HD23	2:D:678:LEU:HD12	1.98	0.44
2:C:291:GLU:HA	2:C:315:LEU:HA	1.99	0.44
2:C:324:ARG:CZ	2:C:324:ARG:HB2	2.45	0.44
2:D:287:LEU:HB2	2:D:290:LEU:HD22	1.98	0.44
2:D:357:LEU:HG	2:D:360:VAL:HG22	1.98	0.44
2:D:641:LEU:HB2	2:D:666:PRO:CG	2.48	0.44
1:A:186:LYS:O	1:A:188:ILE:HG13	2.16	0.44
2:C:64:CYS:HA	2:C:67:TRP:CE2	2.53	0.44
2:C:243:LEU:HB3	2:C:245:LEU:CD2	2.47	0.44
1:B:221:THR:HG23	1:B:231:MET:HE2	2.00	0.44
2:D:738:SER:HB3	2:D:740:ILE:HG12	2.00	0.44
2:C:680:MET:HB2	2:C:703:LEU:CD1	2.47	0.44
2:C:614:PHE:HA	2:C:637:PHE:HA	1.99	0.43
2:C:677:ALA:HB1	2:C:679:TYR:CE1	2.53	0.43
1:B:53:THR:OG1	1:B:67:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ASN:HB3	2:D:76:THR:O	2.18	0.43
1:A:28:TRP:HE1	2:C:674:ASN:HD21	1.63	0.43
2:C:128:GLU:OE1	2:C:151:GLY:HA3	2.17	0.43
2:C:202:TRP:O	2:C:203:PHE:C	2.57	0.43
2:C:659:ASN:O	2:C:683:ASN:OD1	2.35	0.43
2:D:533:TYR:CZ	2:D:555:PRO:HG2	2.54	0.43
2:D:645:TRP:CD1	2:D:669:LEU:HG	2.53	0.43
2:C:724:ARG:HH12	2:C:780:PRO:HG2	1.84	0.43
2:D:379:PHE:HA	2:D:401:ARG:O	2.18	0.43
2:D:467:TYR:CE1	2:D:492:PHE:HD2	2.36	0.43
2:D:468:ASN:CB	2:D:470:LEU:HD23	2.42	0.43
2:D:715:TRP:CZ3	2:D:716:ILE:HG12	2.54	0.43
2:C:41:PHE:CG	2:C:108:LEU:HD21	2.53	0.43
2:C:199:VAL:O	2:C:225:LEU:HD13	2.19	0.43
2:D:170:TYR:CE1	2:D:219:LEU:HD12	2.50	0.43
2:C:181:LEU:O	2:C:182:SER:C	2.56	0.43
2:C:508:GLN:NE2	2:C:529:SER:O	2.52	0.43
2:D:202:TRP:CE3	2:D:206:ILE:HD12	2.47	0.43
2:D:215:LEU:HB3	2:D:243:LEU:HD23	2.00	0.43
2:C:244:HIS:C	2:C:245:LEU:HD22	2.39	0.43
2:C:710:GLY:HA2	2:C:734:TYR:CE2	2.54	0.43
2:D:596:LEU:HD21	2:D:619:SER:HB2	2.00	0.43
2:C:39:LEU:HD21	2:C:67:TRP:HH2	1.83	0.43
2:C:86:ASN:O	2:C:121:VAL:CB	2.62	0.43
2:C:394:ASP:HA	2:C:417:HIS:HB2	2.01	0.43
2:D:380:PHE:O	2:D:405:PRO:HD3	2.19	0.43
2:C:339:SER:HB2	2:C:342:THR:OG1	2.19	0.43
2:C:498:LYS:HZ1	2:C:521:PRO:HD3	1.82	0.43
2:D:190:LEU:HD21	2:D:192:LEU:CD1	2.49	0.43
2:D:689:LEU:H	2:D:689:LEU:HG	1.43	0.43
2:C:724:ARG:HA	2:C:747:LEU:HA	2.01	0.43
2:D:111:LEU:O	2:D:112:GLU:HB2	2.18	0.43
2:D:399:GLN:N	2:D:421:ASN:OD1	2.52	0.43
2:D:613:PHE:HB3	2:D:637:PHE:CE2	2.54	0.43
2:C:698:LEU:HD11	2:C:720:LEU:HD23	2.00	0.42
2:D:617:ILE:HD11	2:D:641:LEU:CD2	2.49	0.42
1:B:69:TYR:HB2	1:B:71:TRP:NE1	2.33	0.42
2:D:646:MET:HG2	2:D:647:ASN:N	2.33	0.42
2:C:361:THR:HB	2:C:382:GLU:OE2	2.19	0.42
1:B:40:LEU:HD21	1:B:51:GLN:HG2	2.01	0.42
2:D:111:LEU:H	2:D:111:LEU:HG	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:GLU:CD	2:D:439:ILE:HD12	2.40	0.42
2:D:665:LEU:HA	2:D:666:PRO:HD3	1.72	0.42
2:C:130:PRO:HD2	2:C:133:ILE:CD1	2.50	0.42
2:D:99:ARG:HB3	2:D:123:GLU:H	1.84	0.42
2:C:71:GLU:HB2	2:C:81:VAL:HB	2.00	0.42
2:C:498:LYS:CE	2:C:521:PRO:HD3	2.50	0.42
2:D:414:ARG:HA	2:D:437:LEU:HA	2.01	0.42
2:D:434:LEU:HA	2:D:434:LEU:HD23	1.79	0.42
2:D:517:CYS:O	2:D:519:LEU:HD22	2.19	0.42
2:D:621:CYS:HB2	2:D:644:CYS:HB2	1.64	0.42
2:D:622:LYS:HD3	5:R:1:NAG:HN2	1.85	0.42
2:C:303:GLY:O	2:C:325:THR:HB	2.20	0.42
1:B:103:LYS:HE2	1:B:103:LYS:HB3	1.76	0.42
2:D:100:LEU:HD13	2:D:122:ASN:ND2	2.34	0.42
1:B:169:LEU:HD13	1:B:182:PHE:CD1	2.54	0.42
2:C:114:LEU:HD21	2:C:136:PHE:CE1	2.55	0.42
2:D:622:LYS:HE2	2:D:622:LYS:HB2	1.85	0.42
5:H:2:NAG:H3	5:H:2:NAG:C8	2.50	0.42
2:C:187:LEU:HD23	2:C:187:LEU:HA	1.75	0.42
2:C:281:ASP:CG	2:C:283:ARG:HE	2.24	0.42
2:C:312:LEU:HD23	2:C:312:LEU:HA	1.92	0.42
1:B:69:TYR:HB2	1:B:71:TRP:CD1	2.55	0.42
2:D:448:GLU:O	2:D:471:LYS:HG3	2.20	0.42
2:D:498:LYS:HE2	2:D:520:GLY:HA2	2.02	0.42
2:D:606:PHE:O	2:D:630:LEU:HA	2.19	0.42
2:D:663:GLY:O	2:D:685:PHE:CD1	2.65	0.42
2:C:134:CYS:HA	2:C:160:LEU:HG	2.01	0.42
2:C:289:TYR:O	2:C:290:LEU:C	2.58	0.42
2:C:375:VAL:HG23	2:C:375:VAL:O	2.20	0.42
1:B:156:ALA:HA	1:B:170:TYR:CD1	2.55	0.42
2:D:289:TYR:CB	2:D:314:ARG:HD2	2.48	0.42
2:D:379:PHE:CD1	2:D:402:GLY:HA3	2.47	0.42
2:D:802:LEU:HD12	2:D:802:LEU:HA	1.82	0.42
2:C:547:LEU:N	2:C:569:SER:O	2.45	0.41
1:B:58:ILE:HD13	1:B:63:ILE:HG13	2.02	0.41
2:D:543:ILE:HG22	2:D:568:ILE:HG12	2.01	0.41
2:C:125:GLU:O	2:C:127:SER:N	2.54	0.41
2:C:560:ILE:HG12	2:C:584:VAL:HB	2.02	0.41
2:D:88:PHE:HB2	2:D:96:PHE:O	2.20	0.41
2:D:104:LEU:HD23	2:D:104:LEU:H	1.85	0.41
2:D:212:LEU:HD12	2:D:212:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:519:LEU:CD2	2:D:538:ILE:HG23	2.51	0.41
2:D:728:LEU:HB2	2:D:752:LEU:HD23	2.01	0.41
2:C:88:PHE:HB2	2:C:96:PHE:C	2.41	0.41
2:C:222:LEU:HA	2:C:222:LEU:HD12	1.80	0.41
2:C:224:LYS:HD2	2:C:224:LYS:HA	1.83	0.41
2:C:250:PHE:O	2:C:251:SER:HB2	2.20	0.41
2:C:280:ILE:CG1	2:C:306:PRO:HD3	2.50	0.41
2:D:52:LEU:HD13	2:D:52:LEU:HA	1.88	0.41
2:D:240:LEU:HD23	2:D:262:PHE:CE2	2.54	0.41
2:D:560:ILE:HG12	2:D:584:VAL:HB	2.02	0.41
2:D:702:ASP:HB3	2:D:727:SER:HB3	2.01	0.41
2:C:282:ASP:OD2	2:C:282:ASP:N	2.53	0.41
2:C:467:TYR:CE1	2:C:492:PHE:CD2	3.05	0.41
2:C:715:TRP:HA	2:C:718:THR:HB	2.01	0.41
2:D:35:ARG:CG	2:D:64:CYS:HB3	2.50	0.41
2:D:407:LEU:HD12	2:D:431:ILE:HD12	2.02	0.41
2:D:413:LEU:HD13	2:D:416:LEU:HD13	2.01	0.41
2:D:424:ASN:HA	2:D:446:ARG:O	2.21	0.41
2:D:609:HIS:HB2	2:D:633:SER:OG	2.21	0.41
2:C:76:THR:HG23	4:J:1:NAG:O6	2.20	0.41
2:C:617:ILE:O	2:C:642:PRO:HG3	2.21	0.41
1:B:81:SER:O	1:B:223:PRO:HD2	2.19	0.41
2:D:713:PRO:HG2	2:D:716:ILE:HG13	2.02	0.41
4:F:1:NAG:H61	4:F:2:NAG:H82	2.02	0.41
1:A:123:LEU:HA	1:A:216:THR:O	2.21	0.41
2:C:137:LYS:HB3	2:C:137:LYS:HE2	1.92	0.41
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.93	0.41
2:D:621:CYS:SG	2:D:622:LYS:N	2.94	0.41
2:D:681:ARG:HG2	2:D:704:GLY:H	1.85	0.41
1:A:81:SER:O	1:A:223:PRO:HD2	2.20	0.41
2:C:288:MET:HG3	2:C:314:ARG:HH12	1.86	0.41
2:C:645:TRP:HD1	2:C:668:SER:HB2	1.85	0.41
1:A:133:ASN:H	1:A:133:ASN:ND2	2.18	0.41
2:C:689:LEU:HD11	2:C:713:PRO:CD	2.51	0.41
2:C:698:LEU:HD11	2:C:720:LEU:CD2	2.51	0.41
1:B:45:ALA:O	1:B:74:GLY:HA3	2.20	0.41
1:B:68:SER:HA	1:B:229:ALA:O	2.21	0.41
2:D:394:ASP:OD1	2:D:417:HIS:HB2	2.20	0.41
2:C:142:LEU:CD2	2:C:144:LEU:HG	2.51	0.41
2:C:166:LEU:HD22	2:C:168:LEU:CD1	2.50	0.41
2:C:280:ILE:HG22	2:C:301:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HE3	1:B:43:LYS:HB2	1.76	0.41
1:B:100:ILE:HG22	1:B:100:ILE:O	2.21	0.41
2:D:382:GLU:OE1	2:D:382:GLU:HA	2.21	0.41
2:D:609:HIS:HD2	2:D:610:LYS:HG2	1.85	0.41
2:D:616:SER:HG	2:D:618:SER:HG	1.65	0.41
2:D:645:TRP:O	2:D:672:LEU:HD11	2.21	0.41
1:A:165:ASN:OD1	1:A:186:LYS:HD2	2.21	0.41
2:C:361:THR:HG21	2:C:386:GLN:C	2.41	0.41
2:C:368:ARG:HG2	2:C:392:TYR:HB2	2.02	0.41
2:C:698:LEU:HD11	2:C:720:LEU:CG	2.51	0.41
2:D:50:GLY:O	2:D:52:LEU:N	2.49	0.41
2:D:190:LEU:HD21	2:D:192:LEU:HD12	2.02	0.41
2:D:507:PHE:CD1	2:D:509:LEU:HD22	2.55	0.41
2:C:191:SER:HA	2:C:216:ASP:HB3	2.03	0.40
2:C:217:LEU:HD13	2:C:222:LEU:HD11	2.02	0.40
2:C:501:ILE:HG13	2:C:502:ASP:H	1.86	0.40
1:A:32:THR:OG1	1:A:33:ASN:N	2.54	0.40
2:C:535:VAL:O	2:C:535:VAL:HG13	2.22	0.40
2:D:596:LEU:HD21	2:D:619:SER:CB	2.51	0.40
2:C:478:HIS:HB2	2:C:479:LEU:HD23	2.04	0.40
2:C:631:ASP:HA	2:C:655:ASN:HB3	2.03	0.40
2:D:137:LYS:H	2:D:160:LEU:HD23	1.87	0.40
2:D:219:LEU:HD23	2:D:219:LEU:HA	1.91	0.40
2:D:596:LEU:HD21	2:D:619:SER:H	1.85	0.40
2:C:357:LEU:HA	2:C:357:LEU:HD12	1.88	0.40
2:C:434:LEU:CD1	2:C:437:LEU:HD22	2.51	0.40
2:C:571:ARG:O	2:C:571:ARG:HG3	2.21	0.40
2:C:582:TYR:CG	2:C:585:ILE:HD11	2.57	0.40
2:D:218:SER:HA	2:D:246:CYS:O	2.21	0.40
1:A:171:LYS:HG2	1:A:172:GLY:N	2.36	0.40
2:D:368:ARG:HD3	2:D:370:TYR:HE2	1.86	0.40
2:D:578:ASN:OD1	2:D:598:LEU:HB2	2.21	0.40
2:D:630:LEU:HD11	2:D:654:LEU:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:ASN:OD1	2:C:711:ARG:NH1[1_455]	2.14	0.06

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	220/241 (91%)	202 (92%)	18 (8%)	0	100	100
1	B	220/241 (91%)	204 (93%)	16 (7%)	0	100	100
2	C	748/934 (80%)	681 (91%)	67 (9%)	0	100	100
2	D	748/934 (80%)	676 (90%)	71 (10%)	1 (0%)	51	81
All	All	1936/2350 (82%)	1763 (91%)	172 (9%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	306	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/191 (95%)	180 (99%)	1 (1%)	86	91
1	B	181/191 (95%)	181 (100%)	0	100	100
2	C	680/839 (81%)	666 (98%)	14 (2%)	53	75
2	D	680/839 (81%)	665 (98%)	15 (2%)	52	74
All	All	1722/2060 (84%)	1692 (98%)	30 (2%)	60	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
2	C	114	LEU
2	C	166	LEU
2	C	167	ASP
2	C	179	THR
2	C	181	LEU
2	C	211	LEU
2	C	219	LEU
2	C	282	ASP
2	C	283	ARG
2	C	340	ARG
2	C	479	LEU
2	C	482	LEU
2	C	660	ASN
2	C	698	LEU
2	D	122	ASN
2	D	157	PHE
2	D	240	LEU
2	D	283	ARG
2	D	377	ASN
2	D	471	LYS
2	D	572	VAL
2	D	622	LYS
2	D	624	THR
2	D	628	THR
2	D	643	ASP
2	D	644	CYS
2	D	646	MET
2	D	689	LEU
2	D	799	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	349	ASN
2	C	493	ASN
2	C	531	ASN
2	D	122	ASN
2	D	372	GLN
2	D	478	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 ⓘ

58 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
3	NAG	E	1	2,3	14,14,15	0.48	0	17,19,21	0.75	0
3	MAN	E	10	3	11,11,12	1.94	4 (36%)	15,15,17	2.36	5 (33%)
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.62	0
3	BMA	E	3	3	11,11,12	1.81	3 (27%)	15,15,17	1.59	4 (26%)
3	MAN	E	4	3	11,11,12	1.59	2 (18%)	15,15,17	2.21	3 (20%)
3	MAN	E	5	3	11,11,12	1.50	2 (18%)	15,15,17	1.81	3 (20%)
3	MAN	E	6	3	11,11,12	1.31	1 (9%)	15,15,17	1.43	2 (13%)
3	MAN	E	7	3	11,11,12	1.24	1 (9%)	15,15,17	2.63	4 (26%)
3	MAN	E	8	3	11,11,12	2.41	5 (45%)	15,15,17	2.10	5 (33%)
3	MAN	E	9	3	11,11,12	1.65	3 (27%)	15,15,17	1.79	5 (33%)
4	NAG	F	1	2,4	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
4	NAG	F	2	4	14,14,15	0.68	1 (7%)	17,19,21	0.56	0
4	NAG	G	1	2,4	14,14,15	0.79	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	G	2	4	14,14,15	0.58	0	17,19,21	0.70	0
5	NAG	H	1	2,5	14,14,15	0.68	0	17,19,21	1.08	1 (5%)
5	NAG	H	2	5	14,14,15	0.52	0	17,19,21	1.63	2 (11%)
5	BMA	H	3	5	11,11,12	0.87	1 (9%)	15,15,17	0.94	0
6	NAG	I	1	2,6	14,14,15	0.67	0	17,19,21	1.03	1 (5%)
6	NAG	I	2	6	14,14,15	0.56	0	17,19,21	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	I	3	6	11,11,12	0.48	0	15,15,17	0.87	0
6	MAN	I	4	6	11,11,12	0.49	0	15,15,17	0.72	0
6	MAN	I	5	6	11,11,12	0.40	0	15,15,17	0.82	0
6	MAN	I	6	6	11,11,12	0.30	0	15,15,17	0.99	1 (6%)
6	MAN	I	7	6	11,11,12	0.42	0	15,15,17	1.03	1 (6%)
4	NAG	J	1	2,4	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	0.79	1 (5%)
4	NAG	K	1	2,4	14,14,15	0.66	0	17,19,21	0.62	0
4	NAG	K	2	4	14,14,15	0.58	0	17,19,21	0.82	1 (5%)
3	NAG	L	1	2,3	14,14,15	0.45	0	17,19,21	0.55	0
3	MAN	L	10	3	11,11,12	0.25	0	15,15,17	0.77	0
3	NAG	L	2	3	14,14,15	0.32	0	17,19,21	0.84	0
3	BMA	L	3	3	11,11,12	1.72	2 (18%)	15,15,17	1.49	3 (20%)
3	MAN	L	4	3	11,11,12	0.78	0	15,15,17	1.40	3 (20%)
3	MAN	L	5	3	11,11,12	0.64	0	15,15,17	1.67	3 (20%)
3	MAN	L	6	3	11,11,12	0.51	0	15,15,17	0.87	0
3	MAN	L	7	3	11,11,12	0.56	0	15,15,17	1.08	1 (6%)
3	MAN	L	8	3	11,11,12	0.32	0	15,15,17	0.87	0
3	MAN	L	9	3	11,11,12	1.66	3 (27%)	15,15,17	1.36	2 (13%)
4	NAG	M	1	2,4	14,14,15	0.30	0	17,19,21	0.74	0
4	NAG	M	2	4	14,14,15	0.40	0	17,19,21	0.79	0
5	NAG	N	1	2,5	14,14,15	0.42	0	17,19,21	0.92	1 (5%)
5	NAG	N	2	5	14,14,15	0.45	0	17,19,21	0.96	1 (5%)
5	BMA	N	3	5	11,11,12	0.39	0	15,15,17	0.61	0
5	NAG	O	1	2,5	14,14,15	0.78	1 (7%)	17,19,21	1.34	2 (11%)
5	NAG	O	2	5	14,14,15	0.41	0	17,19,21	0.67	0
5	BMA	O	3	5	11,11,12	1.51	3 (27%)	15,15,17	1.07	0
6	NAG	P	1	2,6	14,14,15	0.52	0	17,19,21	0.94	1 (5%)
6	NAG	P	2	6	14,14,15	0.64	0	17,19,21	1.01	1 (5%)
6	BMA	P	3	6	11,11,12	0.51	0	15,15,17	1.26	1 (6%)
6	MAN	P	4	6	11,11,12	0.50	0	15,15,17	0.78	0
6	MAN	P	5	6	11,11,12	0.35	0	15,15,17	0.95	0
6	MAN	P	6	6	11,11,12	0.35	0	15,15,17	0.84	0
6	MAN	P	7	6	11,11,12	0.23	0	15,15,17	1.15	1 (6%)
4	NAG	Q	1	2,4	14,14,15	0.58	0	17,19,21	0.78	0
4	NAG	Q	2	4	14,14,15	0.36	0	17,19,21	1.05	0
5	NAG	R	1	2,5	14,14,15	0.52	0	17,19,21	0.81	1 (5%)
5	NAG	R	2	5	14,14,15	0.40	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	R	3	5	11,11,12	0.30	0	15,15,17	0.87	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
3	NAG	E	1	2,3	-	4/6/23/26	0/1/1/1
3	MAN	E	10	3	-	0/2/19/22	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
3	MAN	E	8	3	-	2/2/19/22	0/1/1/1
3	MAN	E	9	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	5/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	1/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
6	MAN	I	6	6	-	2/2/19/22	0/1/1/1
6	MAN	I	7	6	-	0/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
3	NAG	L	1	2,3	-	2/6/23/26	0/1/1/1
3	MAN	L	10	3	-	0/2/19/22	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8	MAN	C1-C2	5.42	1.64	1.52
3	E	3	BMA	C4-C5	4.23	1.61	1.53
3	L	3	BMA	O5-C1	-4.10	1.37	1.43
3	E	4	MAN	C4-C3	3.68	1.61	1.52
3	E	10	MAN	O5-C1	3.56	1.49	1.43
3	L	9	MAN	O5-C5	3.54	1.50	1.43
3	E	8	MAN	O5-C1	3.39	1.49	1.43
3	E	9	MAN	O5-C5	3.27	1.50	1.43
3	E	8	MAN	C4-C5	3.16	1.59	1.53
3	L	3	BMA	C4-C5	3.10	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	10	MAN	O5-C5	3.09	1.49	1.43
5	O	3	BMA	C1-C2	3.06	1.59	1.52
3	E	3	BMA	C2-C3	-2.80	1.48	1.52
3	E	9	MAN	C4-C3	2.79	1.59	1.52
3	E	10	MAN	C1-C2	2.68	1.58	1.52
3	E	9	MAN	O2-C2	2.57	1.48	1.43
3	E	10	MAN	C4-C3	2.48	1.58	1.52
3	L	9	MAN	C4-C5	2.44	1.58	1.53
3	E	5	MAN	O5-C1	-2.35	1.40	1.43
3	E	6	MAN	C1-C2	2.31	1.57	1.52
3	E	8	MAN	O5-C5	2.28	1.48	1.43
5	O	1	NAG	O5-C1	2.23	1.47	1.43
3	E	5	MAN	C2-C3	2.21	1.55	1.52
3	L	9	MAN	O5-C1	-2.17	1.40	1.43
3	E	8	MAN	C2-C3	2.14	1.55	1.52
5	O	3	BMA	O5-C1	2.12	1.47	1.43
4	F	2	NAG	O5-C1	2.12	1.47	1.43
4	G	1	NAG	O5-C1	2.10	1.47	1.43
3	E	4	MAN	C4-C5	2.10	1.57	1.53
3	E	7	MAN	C6-C5	2.06	1.58	1.51
5	H	3	BMA	C1-C2	2.04	1.56	1.52
3	E	3	BMA	O5-C1	-2.03	1.40	1.43
5	O	3	BMA	C2-C3	2.02	1.55	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	MAN	C1-O5-C5	8.31	123.45	112.19
3	E	10	MAN	C1-O5-C5	6.73	121.31	112.19
3	E	4	MAN	C1-O5-C5	6.13	120.50	112.19
5	H	2	NAG	C2-N2-C7	5.19	130.29	122.90
3	E	8	MAN	C1-O5-C5	4.86	118.78	112.19
3	E	5	MAN	O2-C2-C3	-4.82	100.48	110.14
3	E	4	MAN	C3-C4-C5	4.37	118.03	110.24
3	E	9	MAN	C1-C2-C3	-4.08	104.65	109.67
5	O	1	NAG	O4-C4-C5	3.86	118.89	109.30
6	I	2	NAG	C2-N2-C7	-3.76	117.55	122.90
3	E	6	MAN	O2-C2-C3	-3.60	102.93	110.14
3	E	8	MAN	C1-C2-C3	3.38	113.81	109.67
3	L	5	MAN	C2-C3-C4	-3.35	105.10	110.89
6	P	3	BMA	O3-C3-C2	-3.32	103.63	109.99
3	L	3	BMA	O5-C5-C6	-3.32	102.00	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C1-O5-C5	3.32	116.69	112.19
3	E	3	BMA	O2-C2-C3	-3.30	103.52	110.14
3	L	5	MAN	O2-C2-C3	-3.25	103.62	110.14
3	E	7	MAN	O5-C1-C2	3.16	115.65	110.77
3	E	10	MAN	O5-C1-C2	3.09	115.54	110.77
6	P	7	MAN	C1-O5-C5	3.06	116.34	112.19
3	E	7	MAN	O5-C5-C4	2.97	118.05	110.83
3	E	3	BMA	O5-C5-C6	-2.90	102.65	107.20
3	E	5	MAN	O3-C3-C2	2.86	115.46	109.99
3	L	4	MAN	O3-C3-C2	-2.84	104.55	109.99
3	E	8	MAN	O5-C1-C2	2.80	115.09	110.77
3	L	5	MAN	O5-C1-C2	-2.78	106.47	110.77
3	E	3	BMA	C6-C5-C4	2.72	119.38	113.00
3	L	9	MAN	O2-C2-C3	-2.70	104.73	110.14
3	E	9	MAN	C1-O5-C5	2.69	115.83	112.19
3	E	8	MAN	O2-C2-C1	2.67	114.62	109.15
3	E	6	MAN	O2-C2-C1	2.64	114.56	109.15
4	J	2	NAG	C1-O5-C5	2.63	115.76	112.19
3	L	9	MAN	C1-C2-C3	-2.59	106.48	109.67
4	K	2	NAG	C1-O5-C5	2.53	115.63	112.19
3	L	3	BMA	O5-C1-C2	-2.52	106.88	110.77
3	L	3	BMA	C6-C5-C4	2.50	118.85	113.00
4	F	1	NAG	C1-O5-C5	2.43	115.49	112.19
6	I	1	NAG	C1-C2-N2	-2.40	106.38	110.49
5	N	2	NAG	O4-C4-C3	-2.40	104.80	110.35
5	H	2	NAG	C1-C2-N2	2.35	114.49	110.49
3	L	4	MAN	C1-O5-C5	2.34	115.36	112.19
3	E	4	MAN	O5-C1-C2	-2.33	107.18	110.77
3	E	9	MAN	O5-C1-C2	-2.32	107.19	110.77
3	E	8	MAN	O3-C3-C2	2.29	114.38	109.99
3	E	10	MAN	O3-C3-C4	2.29	115.64	110.35
3	E	10	MAN	O4-C4-C3	2.25	115.56	110.35
3	E	9	MAN	O3-C3-C2	2.24	114.28	109.99
3	E	9	MAN	O2-C2-C3	-2.23	105.66	110.14
3	E	5	MAN	C1-C2-C3	-2.23	106.93	109.67
6	P	1	NAG	C4-C3-C2	-2.23	107.76	111.02
3	L	7	MAN	O2-C2-C3	-2.22	105.68	110.14
3	E	3	BMA	O5-C1-C2	-2.20	107.37	110.77
3	E	7	MAN	C1-C2-C3	2.14	112.29	109.67
6	I	7	MAN	C2-C3-C4	-2.13	107.20	110.89
3	L	4	MAN	O3-C3-C4	-2.13	105.43	110.35
5	H	1	NAG	C1-O5-C5	2.07	115.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	2.07	115.00	112.19
5	N	1	NAG	O4-C4-C3	-2.07	105.57	110.35
3	E	10	MAN	C3-C4-C5	-2.06	106.56	110.24
6	P	2	NAG	O4-C4-C3	-2.03	105.66	110.35
5	R	1	NAG	C4-C3-C2	-2.02	108.05	111.02
6	I	6	MAN	O5-C5-C6	2.02	110.38	107.20
4	G	1	NAG	C1-O5-C5	2.01	114.91	112.19
6	I	2	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C1-C2-N2-C7
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
3	E	8	MAN	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	F	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
6	I	6	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	8	MAN	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
4	K	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C1-C2-N2-C7
5	H	2	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
6	I	6	MAN	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
6	P	7	MAN	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C3-C2-N2-C7
5	R	2	NAG	C3-C2-N2-C7
3	E	5	MAN	C4-C5-C6-O6
5	N	1	NAG	C3-C2-N2-C7
3	E	4	MAN	O5-C5-C6-O6
6	I	1	NAG	C1-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 14 short contacts:

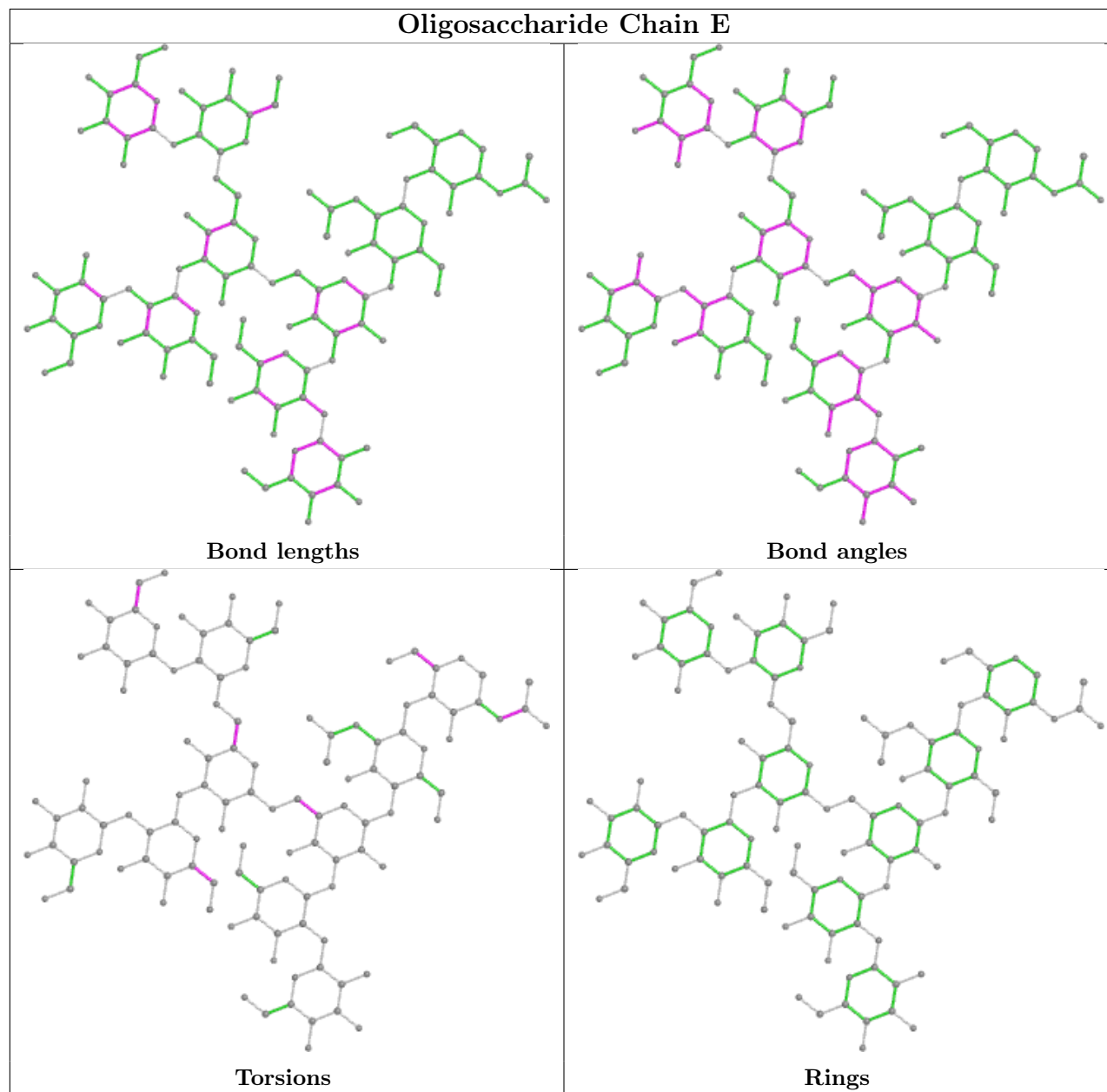
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	3	0
4	F	2	NAG	1	0
5	R	1	NAG	6	0
3	L	10	MAN	2	0
3	L	9	MAN	2	0
3	E	1	NAG	1	0
5	H	1	NAG	1	0
4	F	1	NAG	1	0

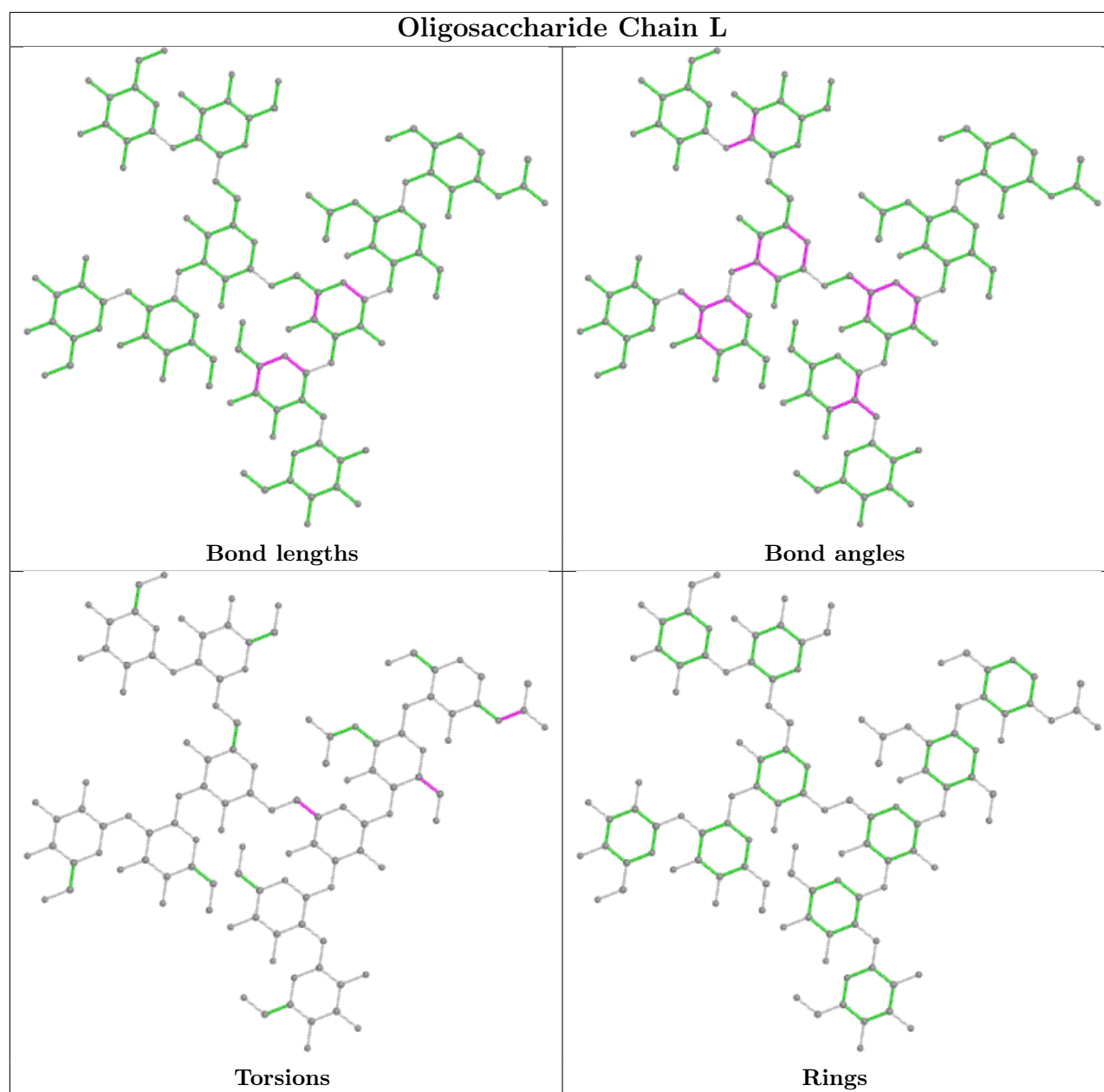
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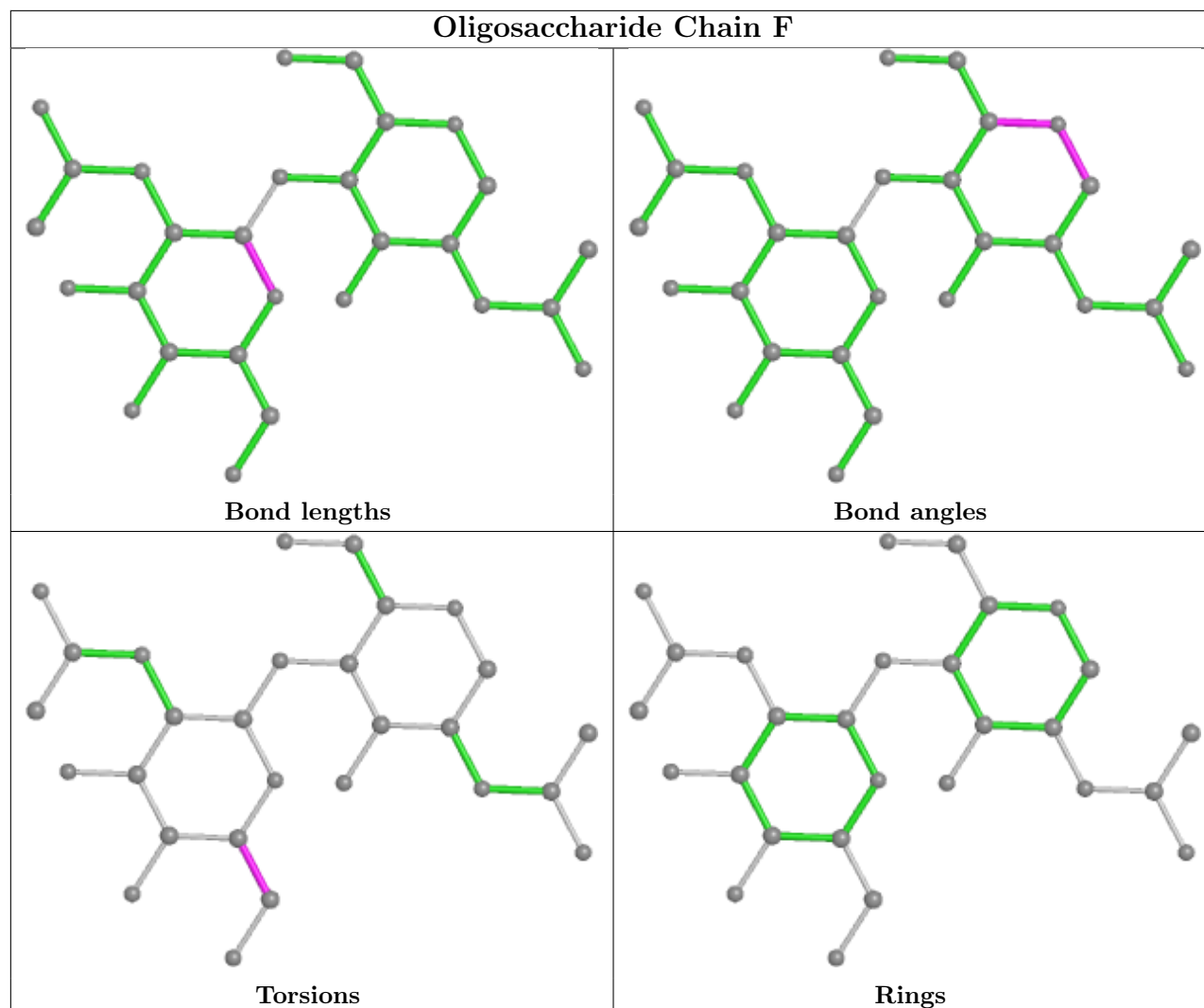
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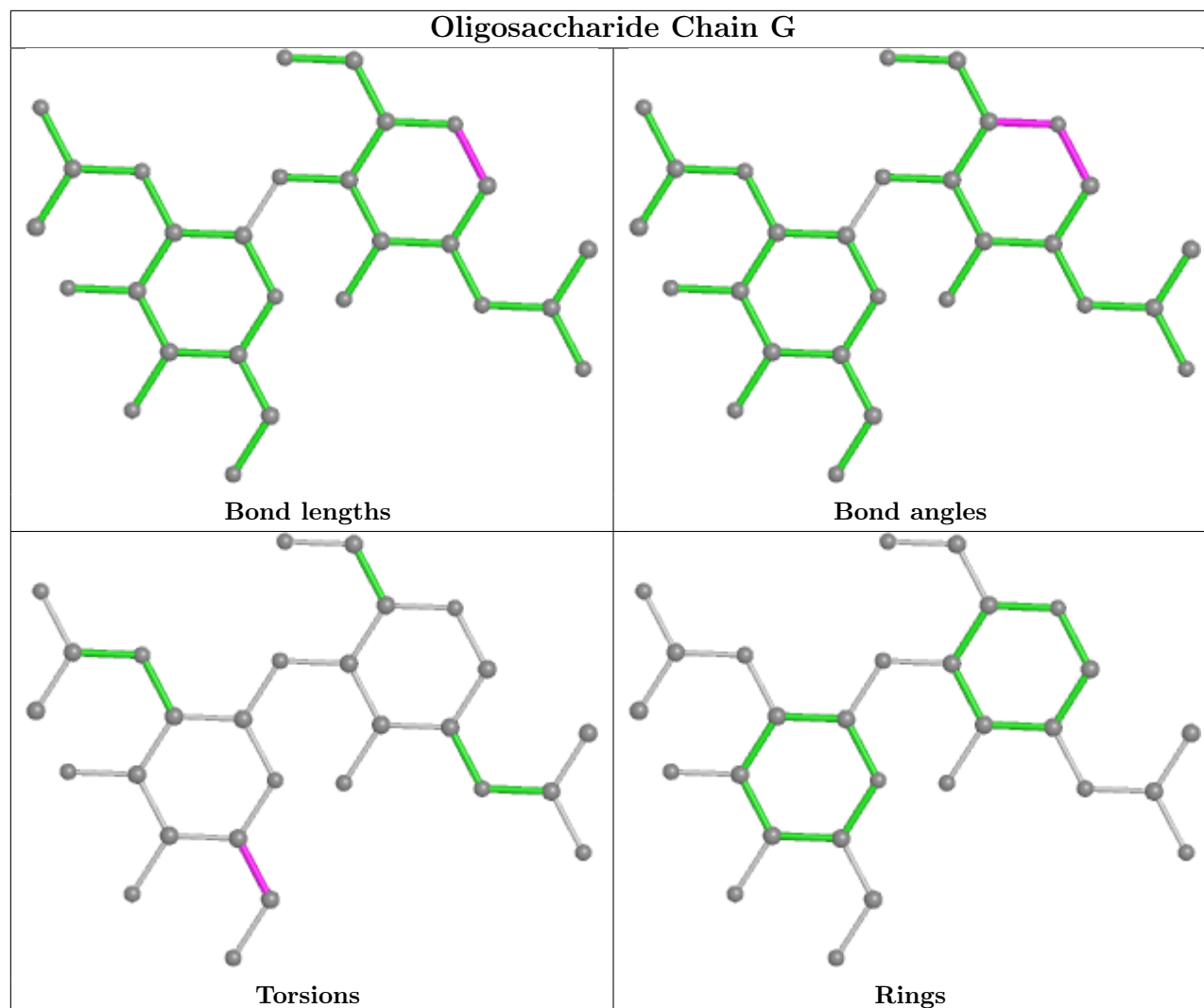
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	1	0

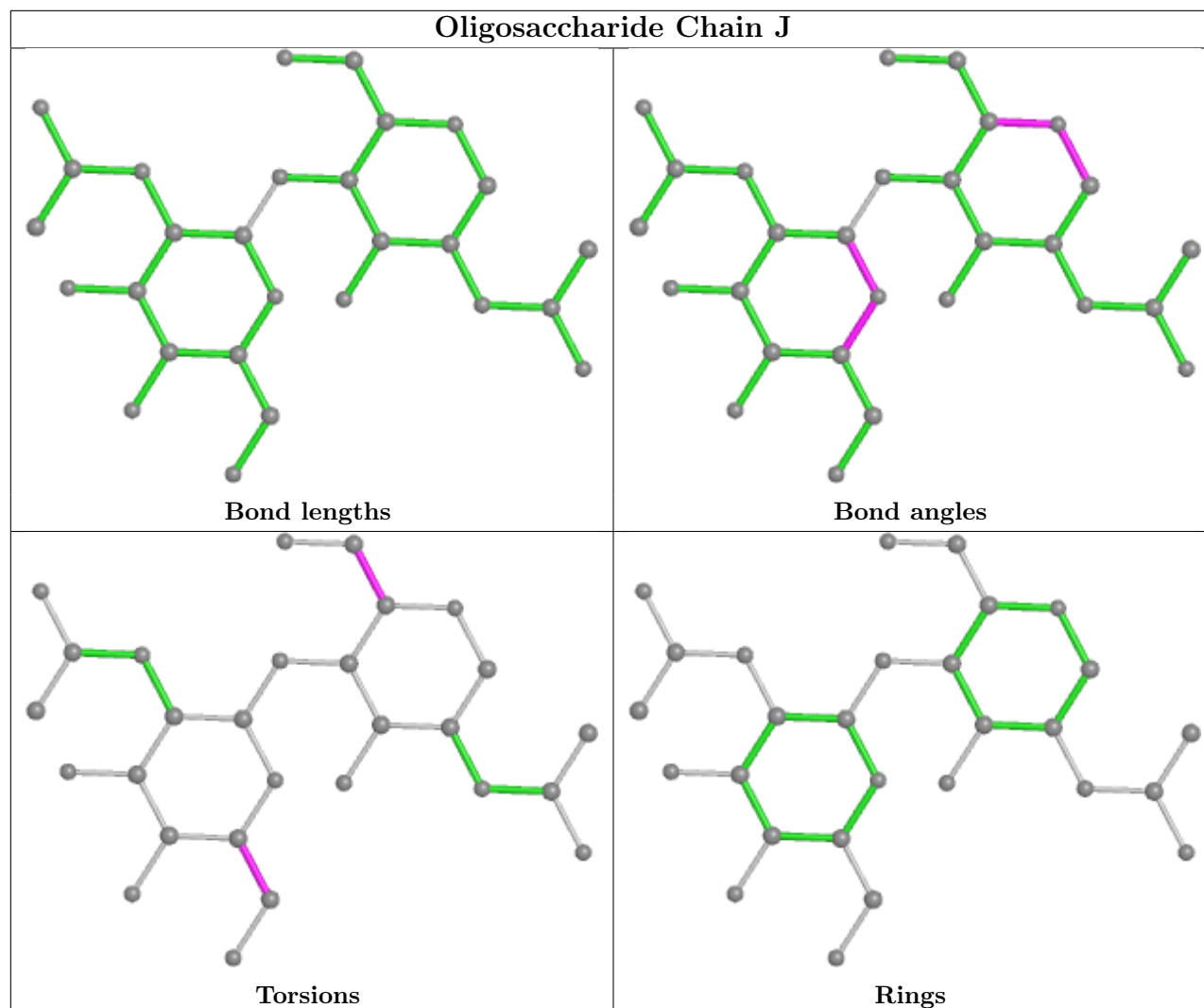
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

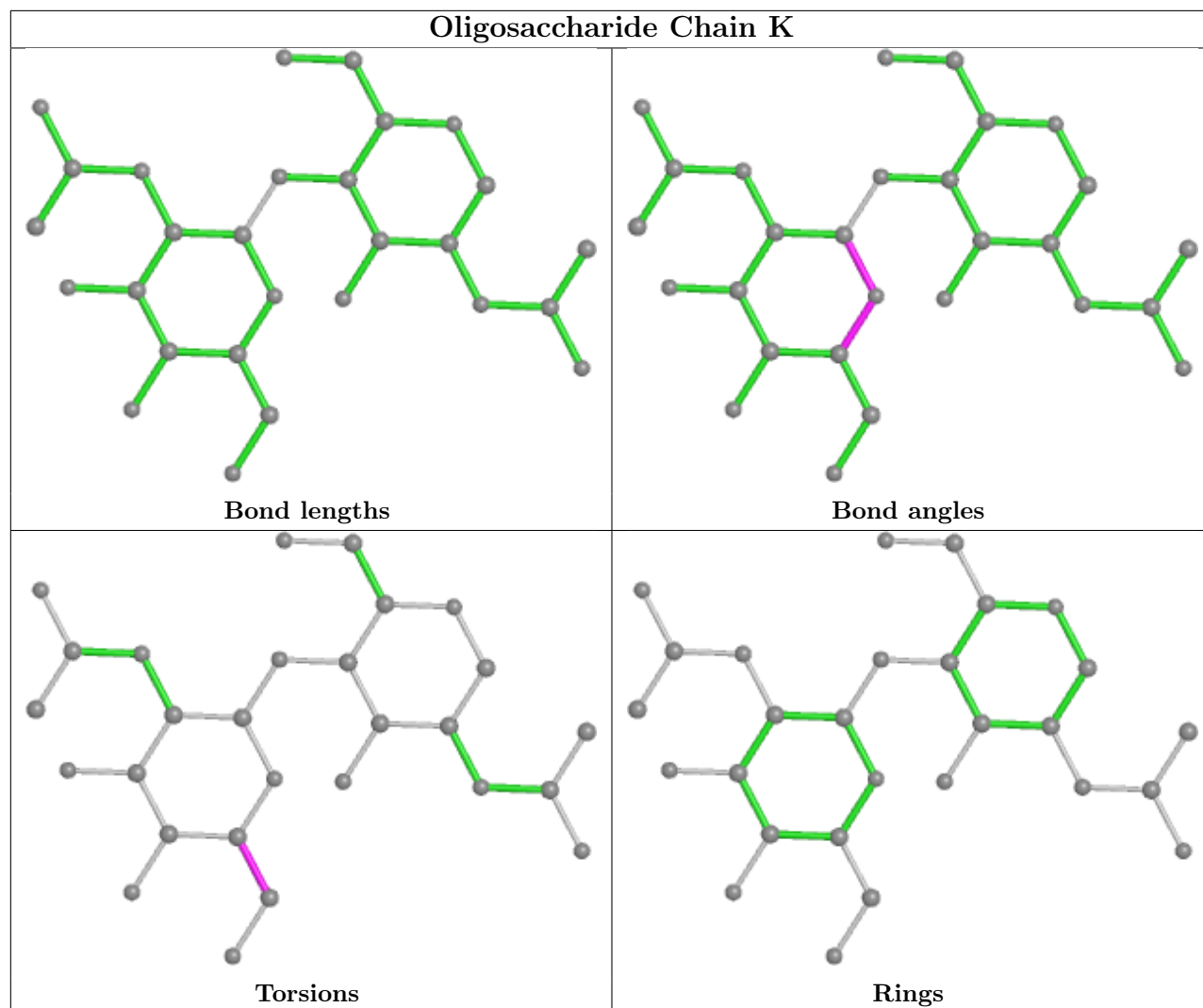


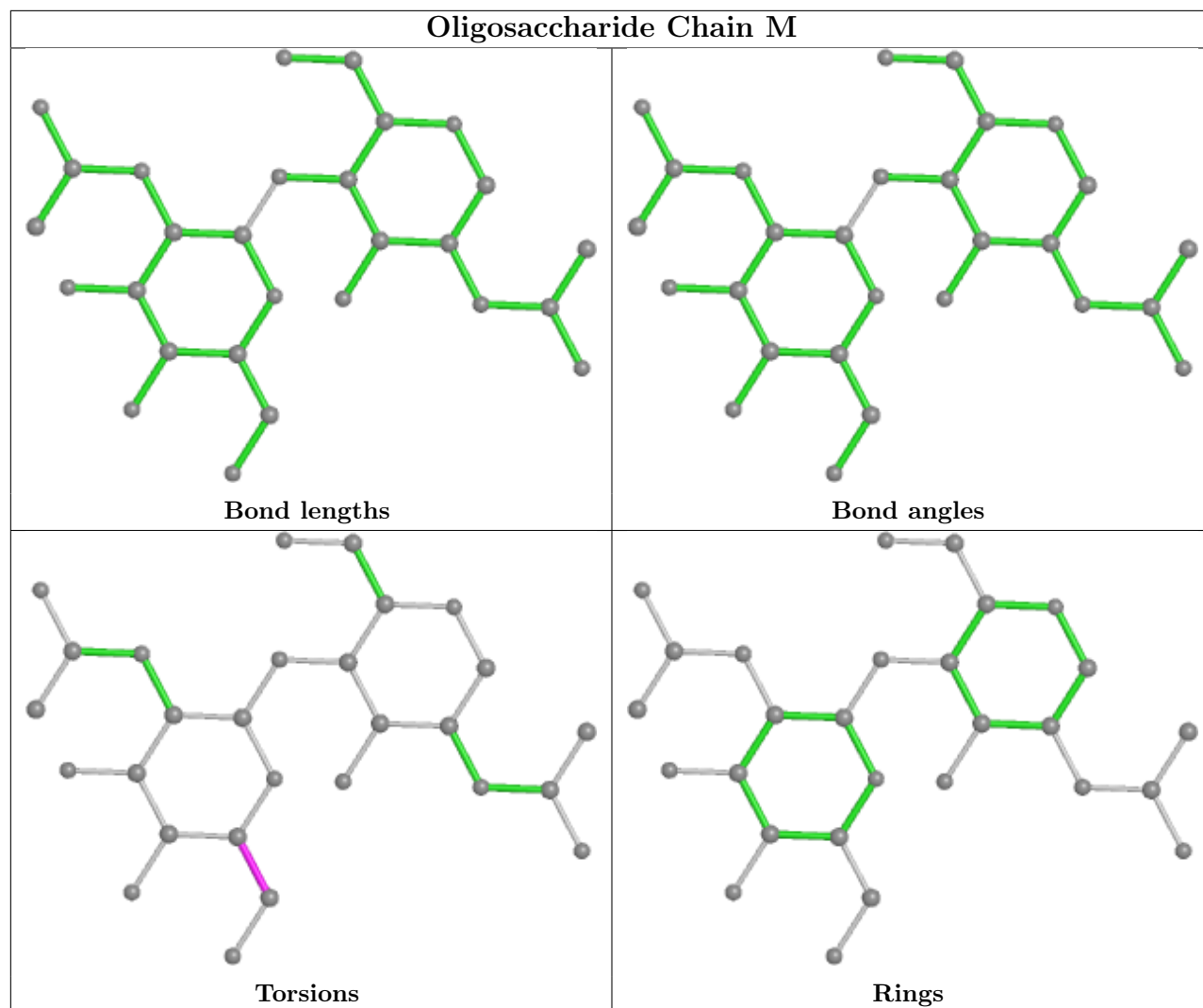


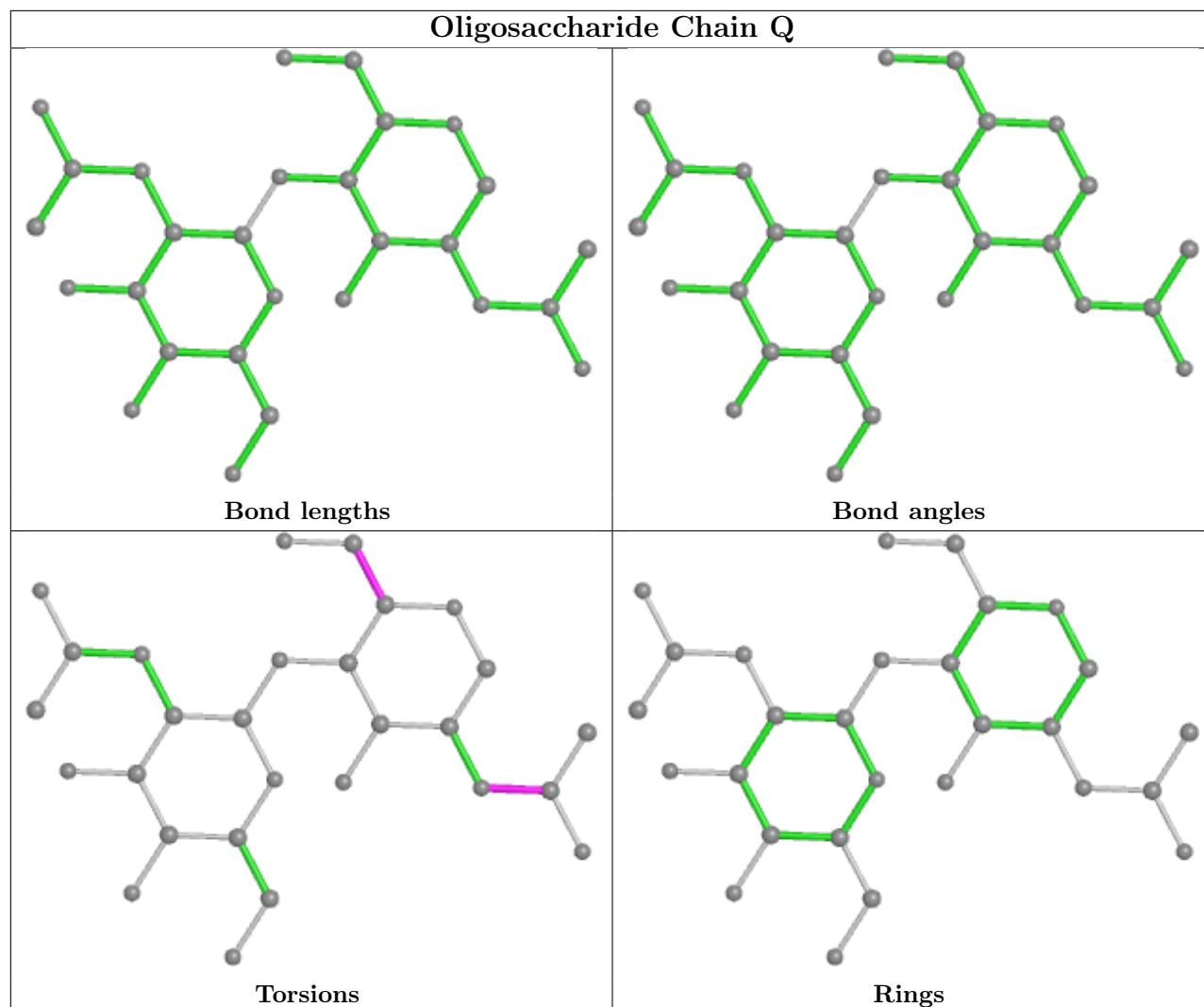


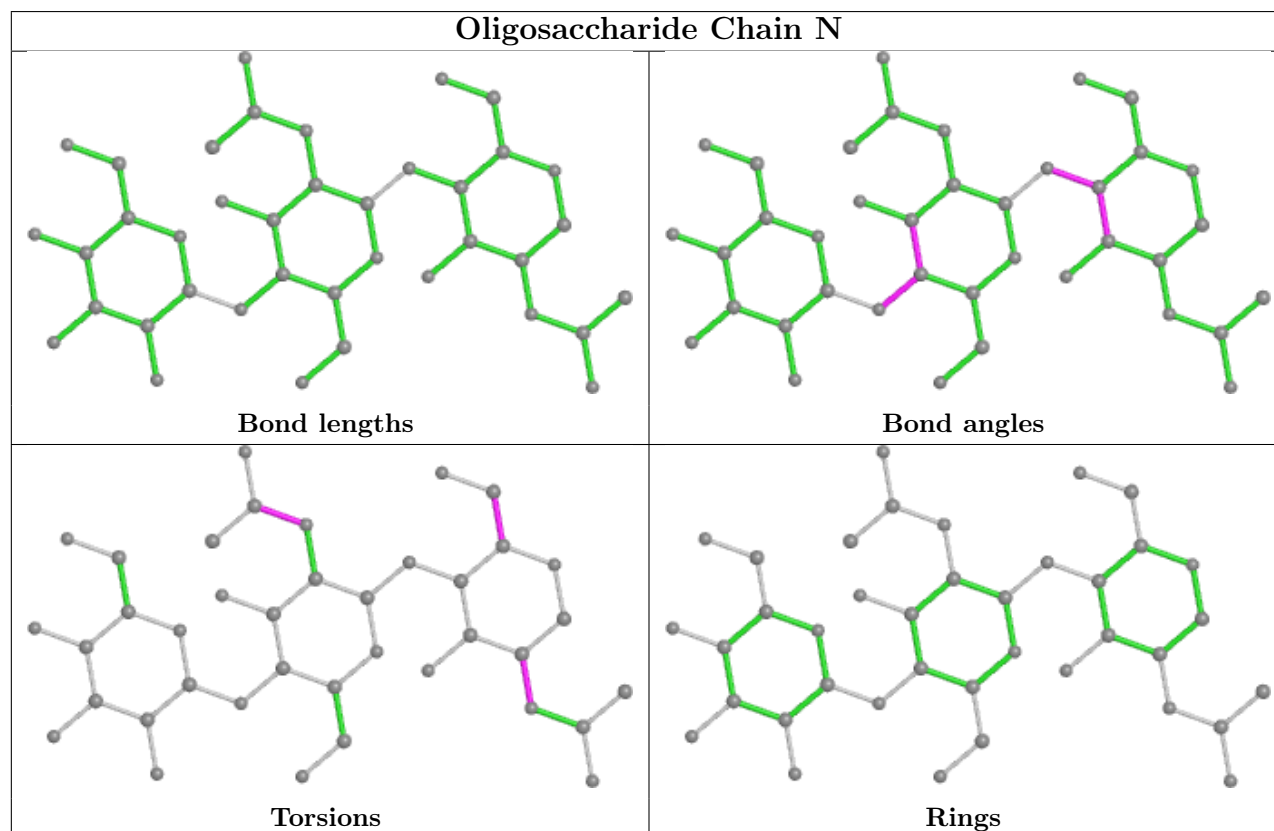
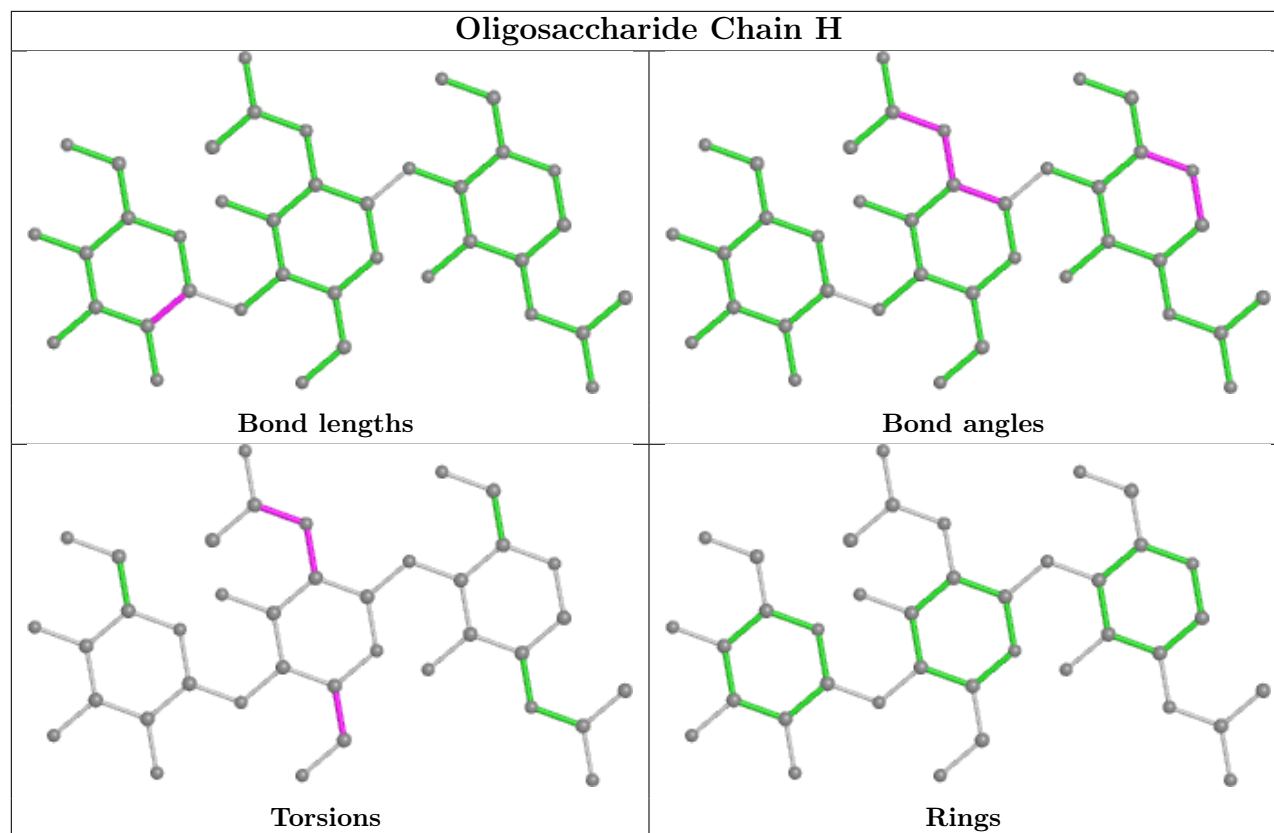


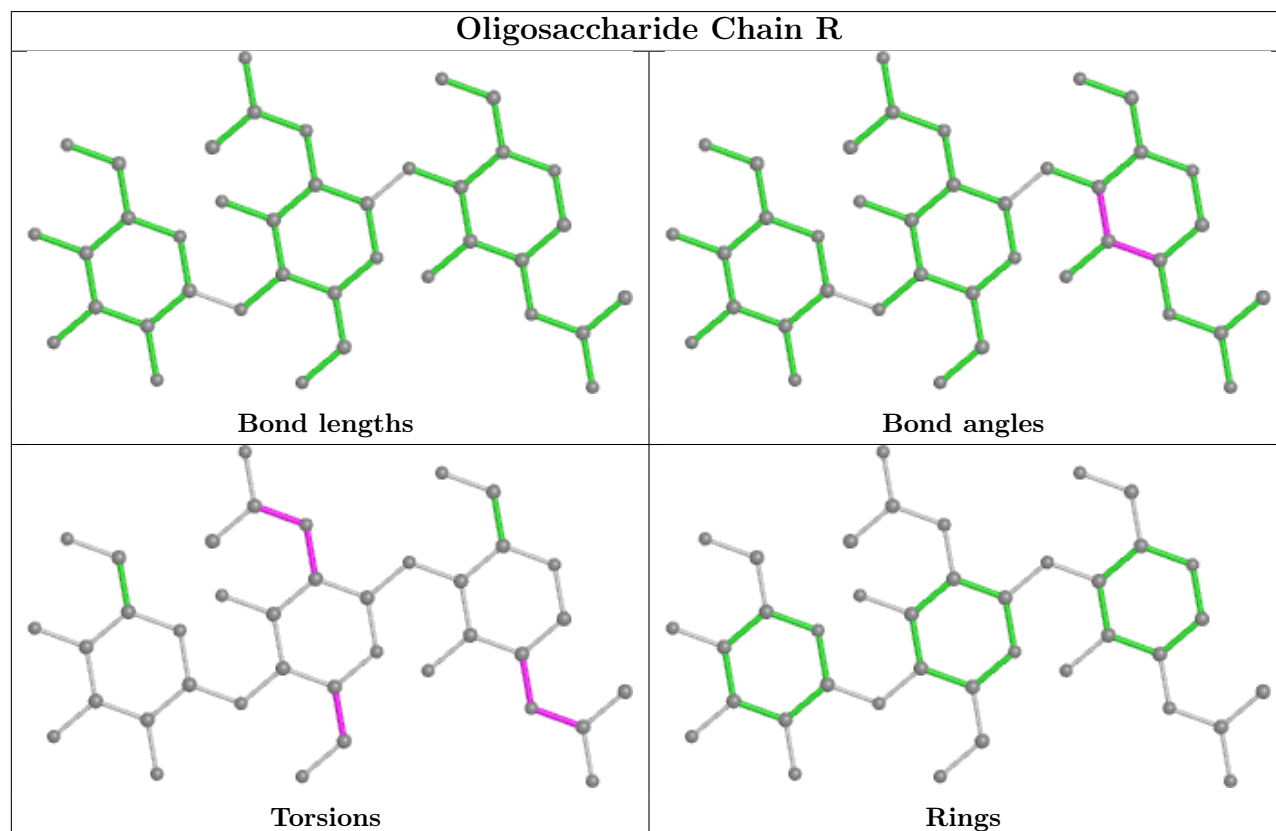
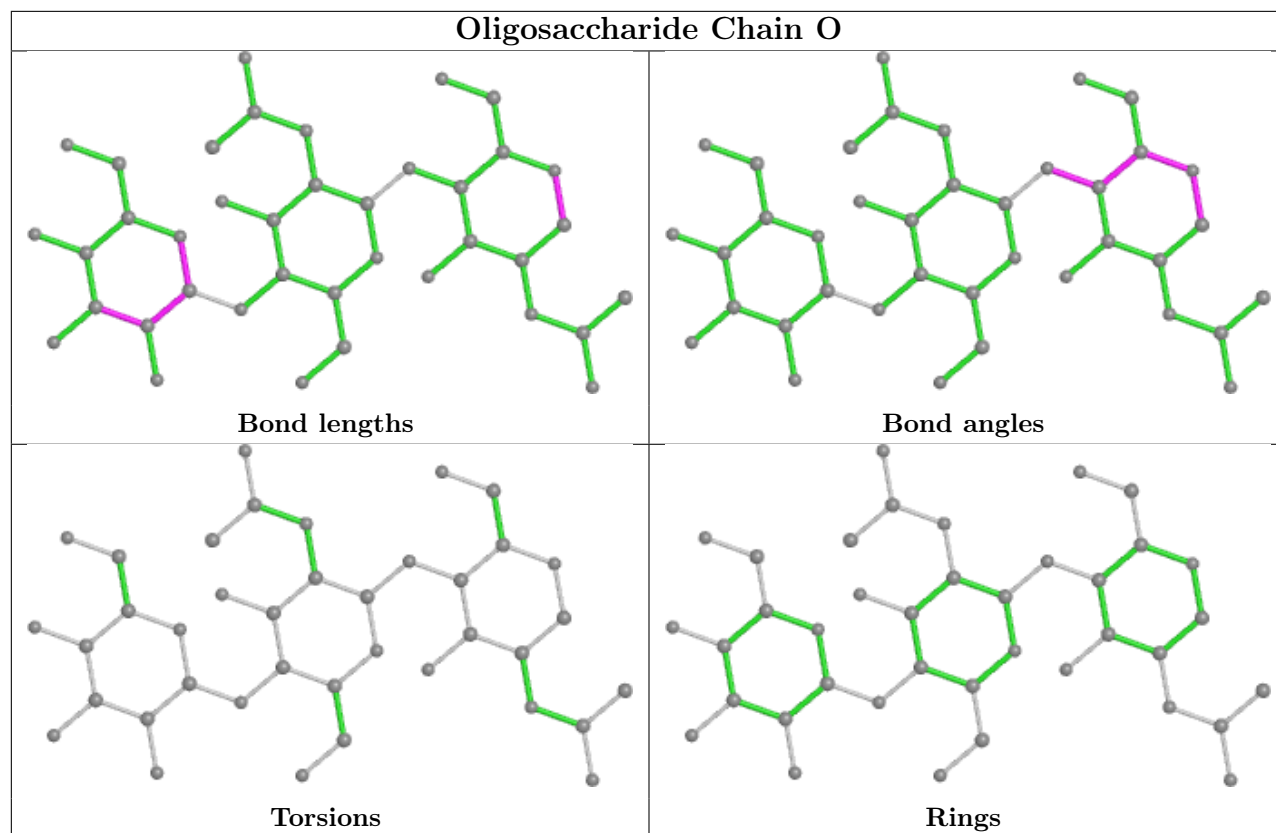


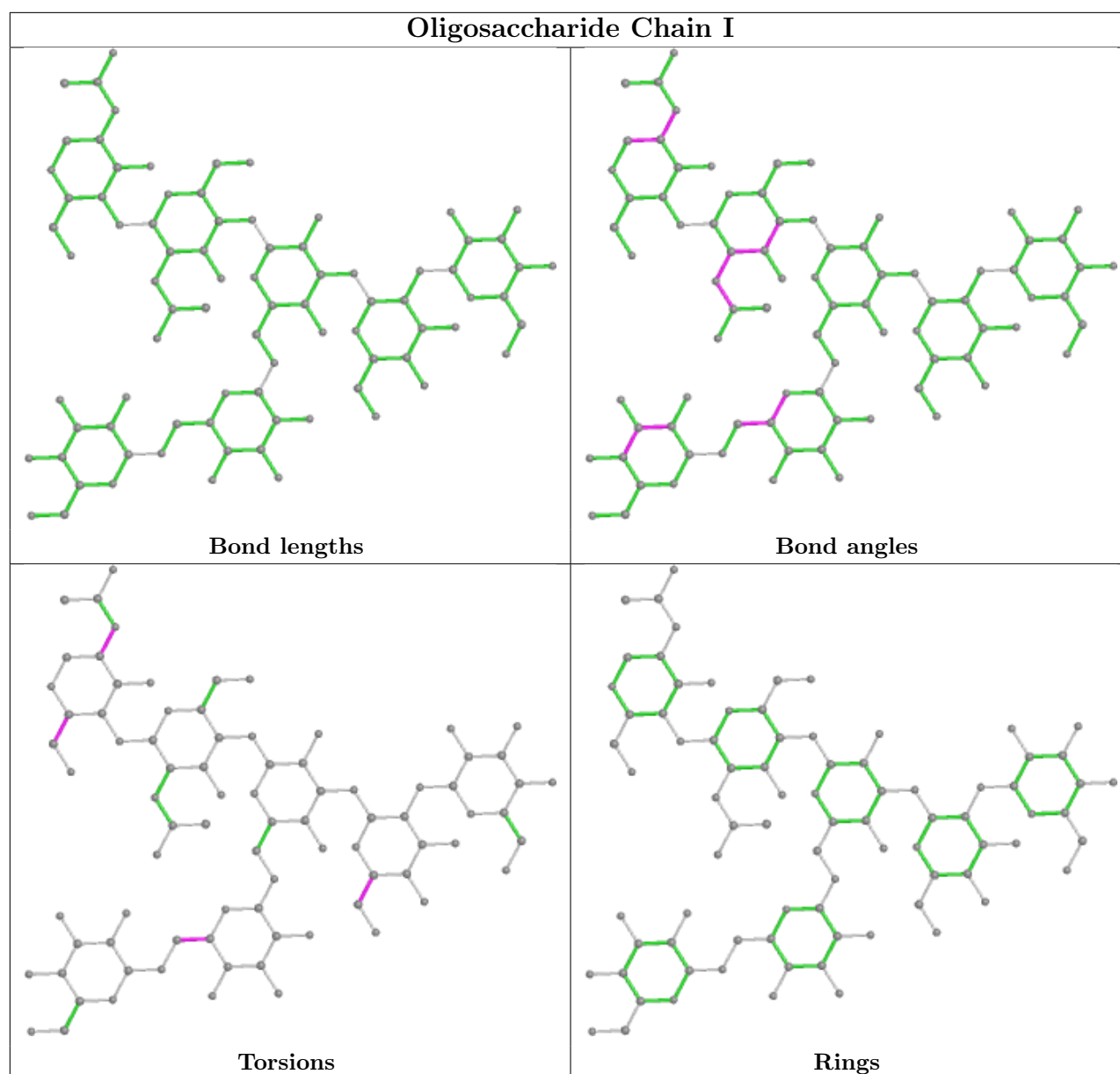


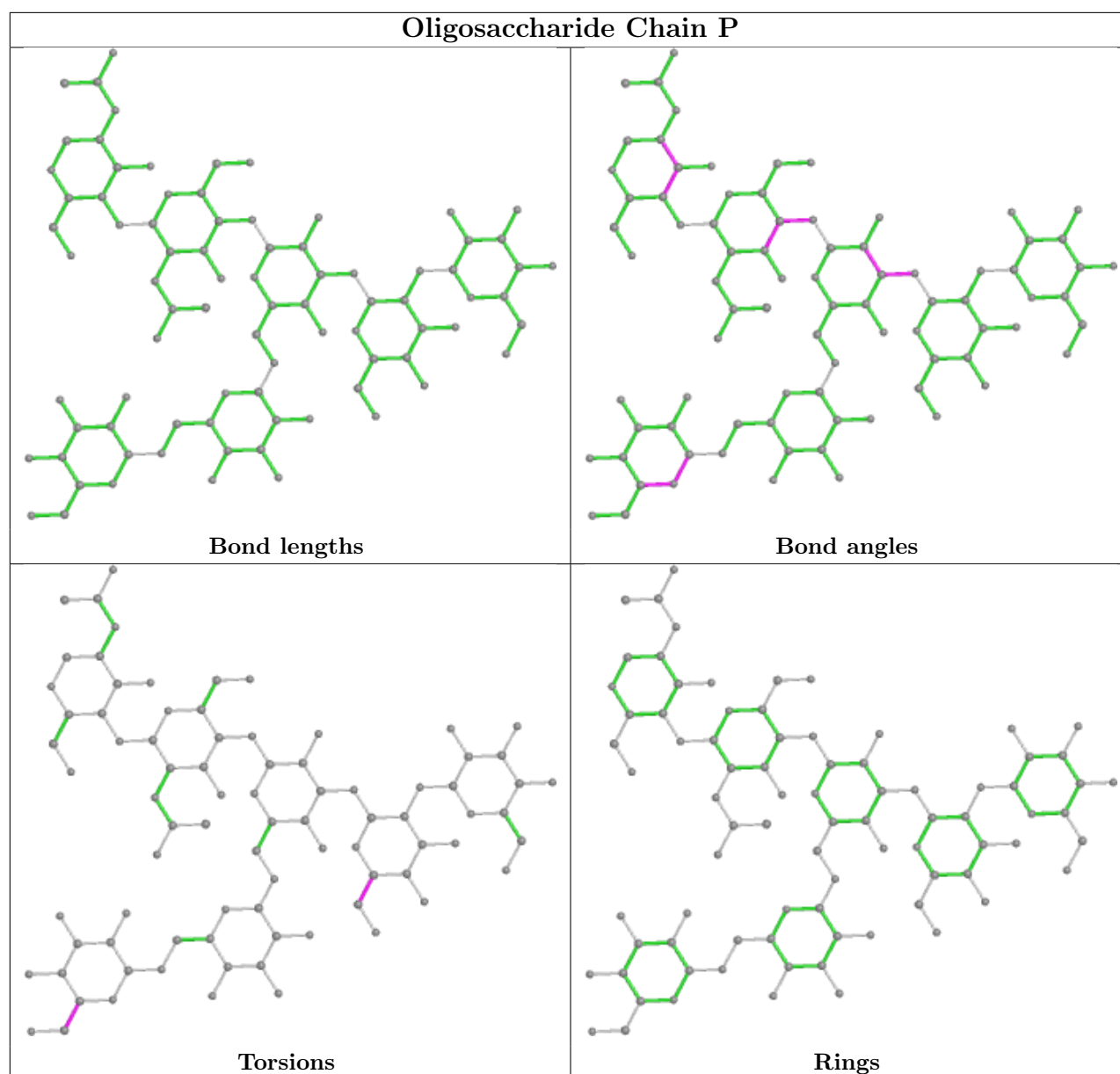












5.6 Ligand geometry [i](#)

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
7	NAG	C	1002	2	14,14,15	0.67	1 (7%)	17,19,21	0.83	1 (5%)
7	NAG	C	1001	2	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
7	NAG	D	1001	2	14,14,15	0.44	0	17,19,21	0.73	0
7	NAG	D	1002	2	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
7	NAG	D	1003	2	14,14,15	0.39	0	17,19,21	0.57	0
7	NAG	C	1003	2	14,14,15	0.77	1 (7%)	17,19,21	0.76	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
7	NAG	C	1002	2	-	0/6/23/26	0/1/1/1
7	NAG	C	1001	2	-	2/6/23/26	0/1/1/1
7	NAG	D	1001	2	-	2/6/23/26	0/1/1/1
7	NAG	D	1002	2	-	0/6/23/26	0/1/1/1
7	NAG	D	1003	2	-	2/6/23/26	0/1/1/1
7	NAG	C	1003	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1003	NAG	C1-C2	2.34	1.55	1.52
7	C	1002	NAG	O5-C1	2.10	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1002	NAG	C1-O5-C5	2.23	115.21	112.19
7	C	1001	NAG	C1-O5-C5	2.21	115.19	112.19
7	D	1002	NAG	C2-N2-C7	-2.08	119.94	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1003	NAG	C8-C7-N2-C2
7	D	1003	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	C	1001	NAG	O5-C5-C6-O6
7	C	1001	NAG	C4-C5-C6-O6
7	C	1003	NAG	C8-C7-N2-C2
7	C	1003	NAG	O7-C7-N2-C2
7	D	1001	NAG	C8-C7-N2-C2
7	D	1001	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1001	NAG	1	0
7	D	1001	NAG	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	222/241 (92%)	-0.07	1 (0%) 91 91	56, 89, 116, 128	0
1	B	222/241 (92%)	0.10	7 (3%) 47 46	68, 105, 132, 147	0
2	C	752/934 (80%)	-0.12	8 (1%) 80 81	59, 84, 119, 157	0
2	D	752/934 (80%)	0.10	21 (2%) 53 51	76, 109, 144, 160	0
All	All	1948/2350 (82%)	-0.00	37 (1%) 66 65	56, 97, 138, 160	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	802	LEU	4.8
2	D	497	LEU	4.6
2	D	592	PHE	4.4
2	D	752	LEU	4.2
2	D	519	LEU	3.6
2	D	578	ASN	3.4
1	B	76	ALA	3.1
2	D	524	PRO	3.0
1	B	77	THR	2.8
2	D	606	PHE	2.8
2	D	536	LEU	2.8
2	C	83	ASP	2.7
2	C	737	ILE	2.7
2	D	533	TYR	2.6
2	C	726	LEU	2.6
2	D	736	SER	2.6
2	C	800	GLY	2.6
2	D	580	TYR	2.5
2	D	590	ASN	2.5
1	B	72	THR	2.5
2	C	738	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	266	LEU	2.4
2	C	750	LEU	2.4
2	C	741	ILE	2.4
2	C	56	GLY	2.4
2	D	712	ILE	2.4
2	D	757	LEU	2.4
2	D	703	LEU	2.4
1	B	217	LEU	2.3
2	D	517	CYS	2.2
1	B	231	MET	2.2
2	D	416	LEU	2.2
1	B	147	ALA	2.2
1	A	226	GLY	2.1
2	D	346	LEU	2.1
1	B	71	TRP	2.1
2	D	456	GLN	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(Å ²)	Q<0.9
4	NAG	M	1	14/15	0.42	0.22	135,148,163,165	0
5	NAG	R	1	14/15	0.69	0.17	128,149,157,159	0
5	NAG	N	2	14/15	0.70	0.24	119,138,147,148	0
4	NAG	F	2	14/15	0.70	0.21	130,142,151,151	0
5	NAG	O	2	14/15	0.72	0.23	148,166,173,175	0
6	BMA	I	3	11/12	0.72	0.21	99,101,104,110	0
5	NAG	O	1	14/15	0.73	0.16	126,144,155,156	0
5	BMA	N	3	11/12	0.76	0.21	128,143,150,152	0
6	MAN	I	6	11/12	0.76	0.27	30,30,30,30	0
3	MAN	E	8	11/12	0.77	0.25	113,117,127,133	0
5	BMA	R	3	11/12	0.78	0.19	150,155,161,164	0
6	MAN	P	5	11/12	0.78	0.25	127,134,143,145	0

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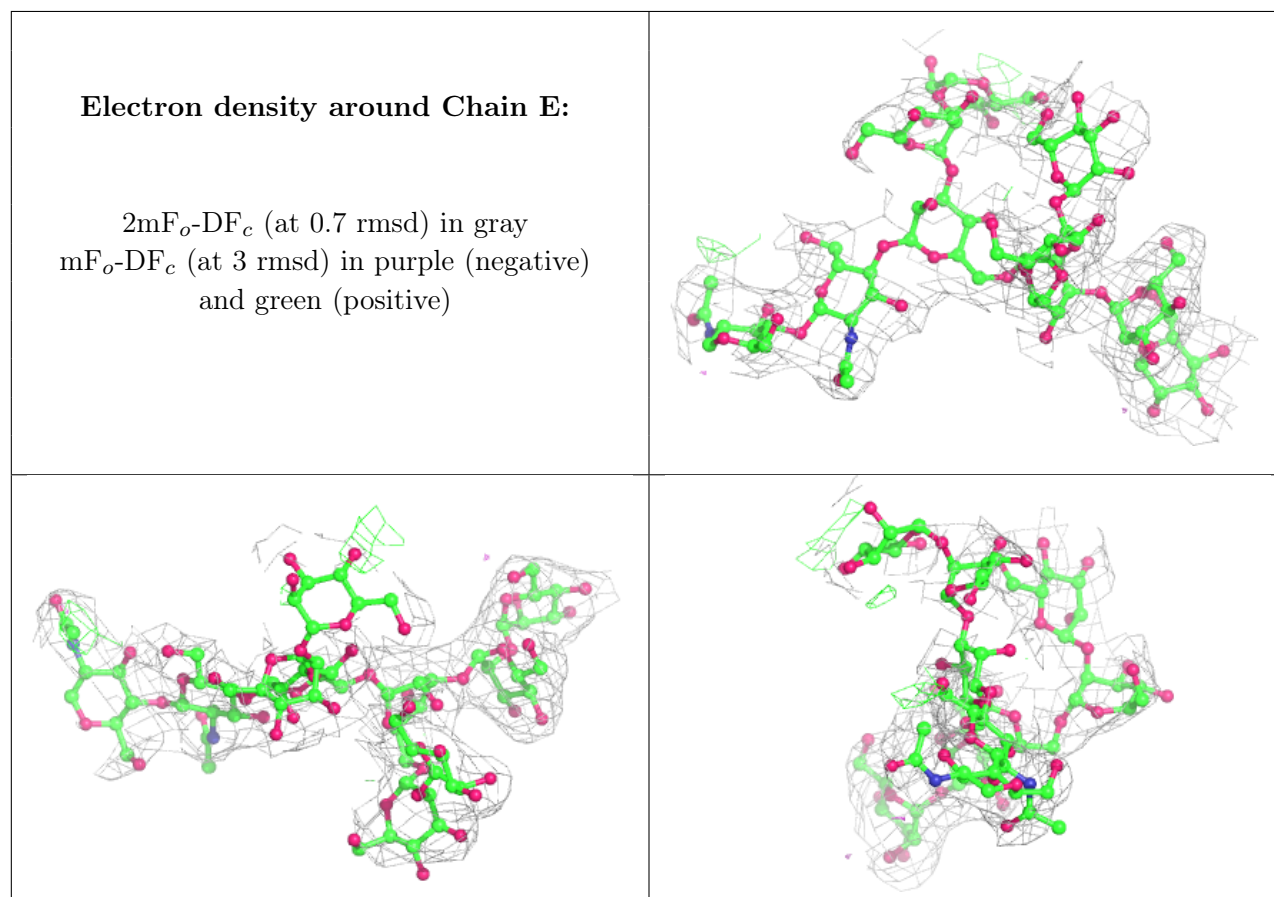
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	M	2	14/15	0.79	0.44	159,170,174,177	0
3	MAN	L	10	11/12	0.79	0.22	116,131,143,145	0
5	NAG	N	1	14/15	0.80	0.19	113,131,140,142	0
6	MAN	P	7	11/12	0.81	0.38	30,30,30,30	0
5	BMA	H	3	11/12	0.82	0.23	137,150,153,157	0
3	MAN	L	8	11/12	0.83	0.20	124,131,139,141	0
5	BMA	O	3	11/12	0.84	0.21	163,174,176,178	0
6	BMA	P	3	11/12	0.84	0.16	118,123,125,125	0
5	NAG	H	2	14/15	0.85	0.25	116,136,143,151	0
4	NAG	K	2	14/15	0.85	0.18	129,141,143,147	0
4	NAG	Q	1	14/15	0.85	0.17	101,124,132,142	0
4	NAG	G	2	14/15	0.86	0.21	92,111,122,127	0
5	NAG	R	2	14/15	0.86	0.15	148,161,165,165	0
4	NAG	G	1	14/15	0.87	0.23	79,86,100,102	0
4	NAG	F	1	14/15	0.87	0.20	118,133,142,144	0
3	MAN	E	7	11/12	0.87	0.22	114,119,126,127	0
4	NAG	Q	2	14/15	0.87	0.26	129,146,150,151	0
6	NAG	P	1	14/15	0.88	0.19	98,113,120,121	0
3	BMA	L	3	11/12	0.88	0.26	104,108,113,123	0
5	NAG	H	1	14/15	0.88	0.12	79,102,112,122	0
3	MAN	L	4	11/12	0.88	0.26	95,101,112,116	0
4	NAG	J	2	14/15	0.89	0.23	135,140,145,146	0
4	NAG	K	1	14/15	0.89	0.16	117,126,129,131	0
4	NAG	J	1	14/15	0.89	0.26	116,125,136,137	0
6	MAN	I	7	11/12	0.89	0.33	30,30,30,30	0
6	MAN	P	4	11/12	0.90	0.31	115,124,134,137	0
6	NAG	P	2	14/15	0.90	0.17	111,116,126,129	0
6	MAN	P	6	11/12	0.90	0.26	30,30,30,30	0
6	MAN	I	5	11/12	0.90	0.19	107,114,118,120	0
3	MAN	L	7	11/12	0.91	0.17	118,126,130,132	0
6	MAN	I	4	11/12	0.91	0.17	83,97,106,108	0
3	MAN	E	10	11/12	0.91	0.21	91,110,115,120	0
3	MAN	L	6	11/12	0.91	0.24	72,84,92,96	0
3	NAG	L	1	14/15	0.92	0.20	80,89,92,98	0
3	MAN	E	4	11/12	0.92	0.17	77,85,95,100	0
3	NAG	E	2	14/15	0.92	0.18	76,80,92,95	0
3	MAN	L	5	11/12	0.92	0.25	79,87,90,91	0
3	MAN	L	9	11/12	0.93	0.15	111,123,126,126	0
3	MAN	E	9	11/12	0.93	0.14	105,108,116,118	0
6	NAG	I	2	14/15	0.93	0.14	72,88,100,100	0
6	NAG	I	1	14/15	0.94	0.20	54,61,74,74	0
3	NAG	E	1	14/15	0.94	0.22	60,70,76,85	0

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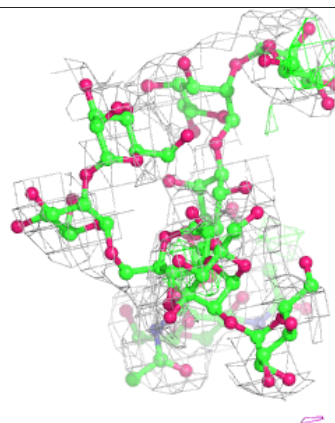
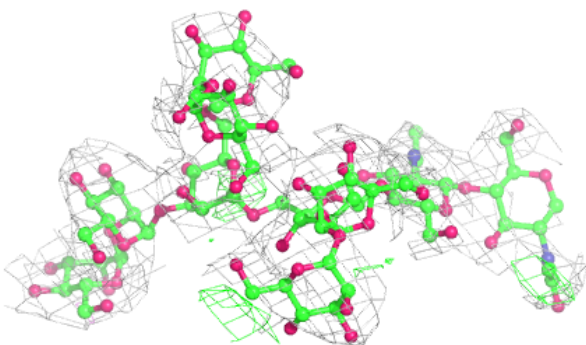
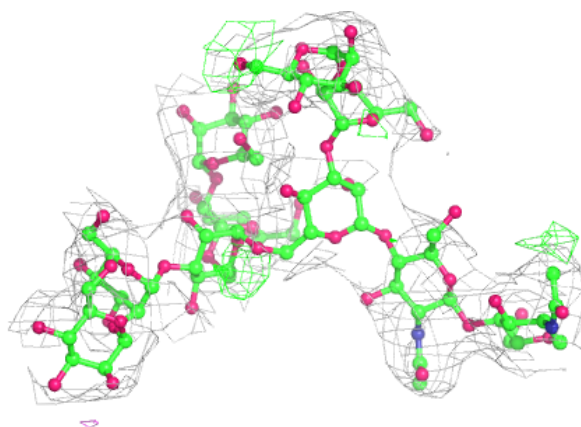
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	E	6	11/12	0.95	0.22	59,67,75,75	0
3	NAG	L	2	14/15	0.95	0.18	77,92,102,109	0
3	BMA	E	3	11/12	0.96	0.22	89,98,100,106	0
3	MAN	E	5	11/12	0.97	0.18	63,67,69,72	0

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.



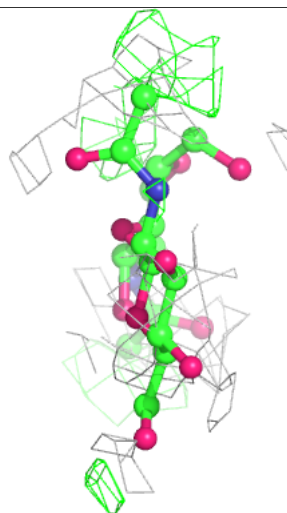
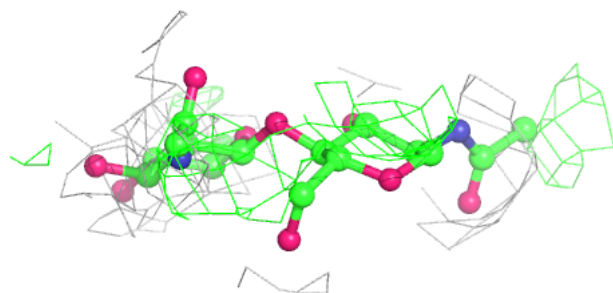
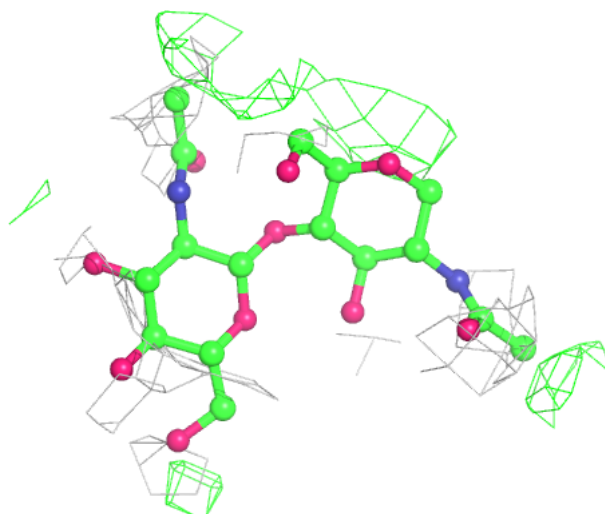
Electron density around Chain L:

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



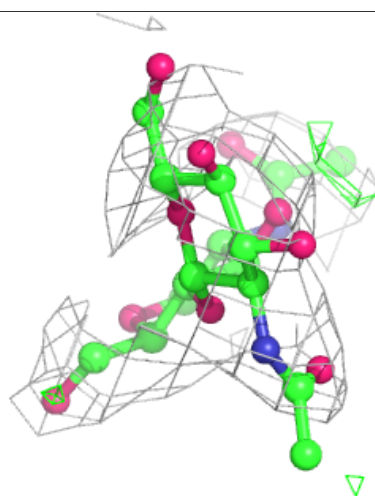
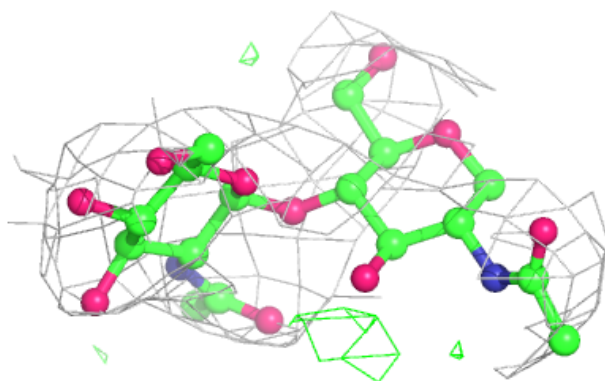
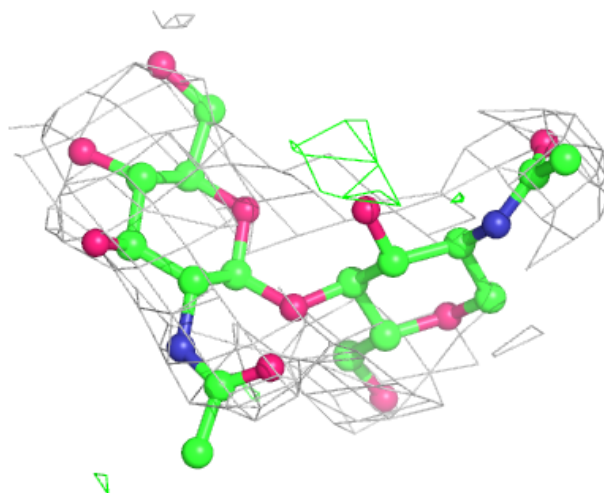
Electron density around Chain F:

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



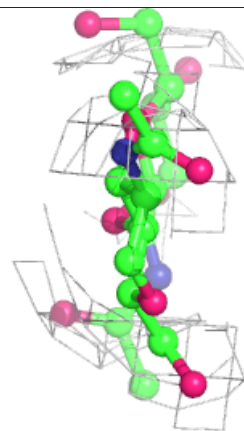
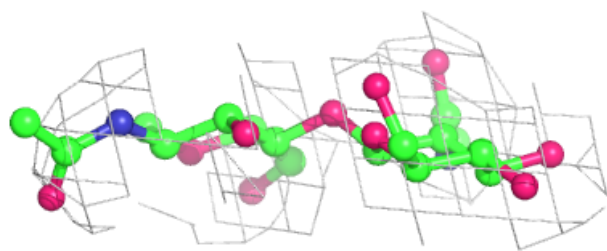
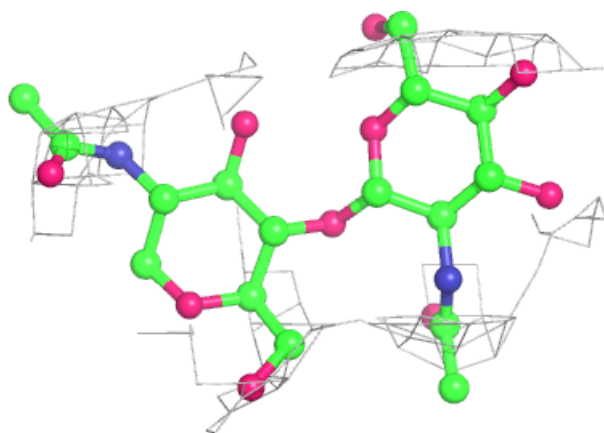
Electron density around Chain G:

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



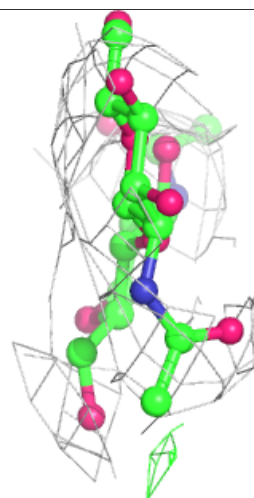
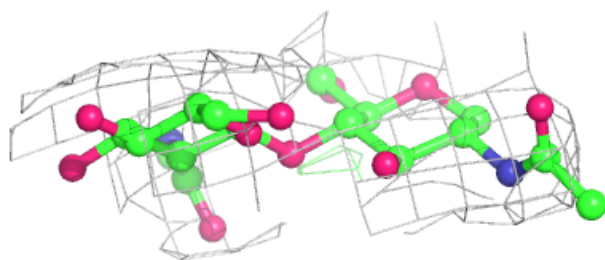
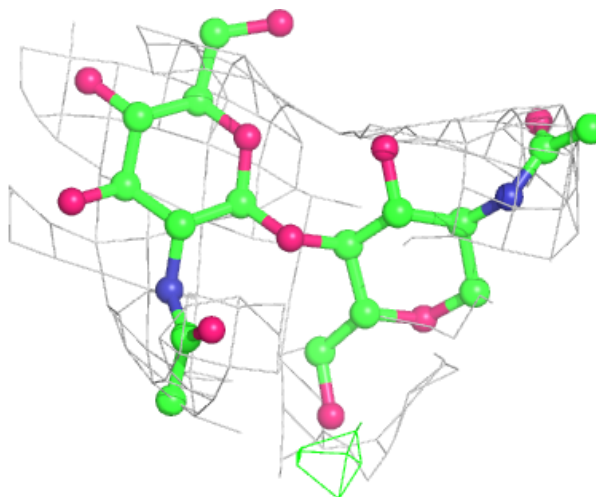
Electron density around Chain J:

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



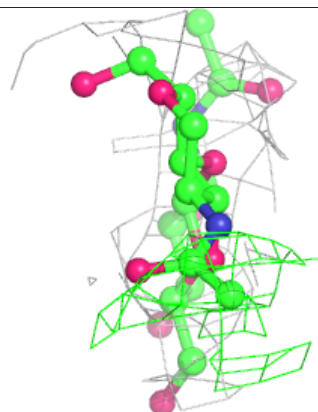
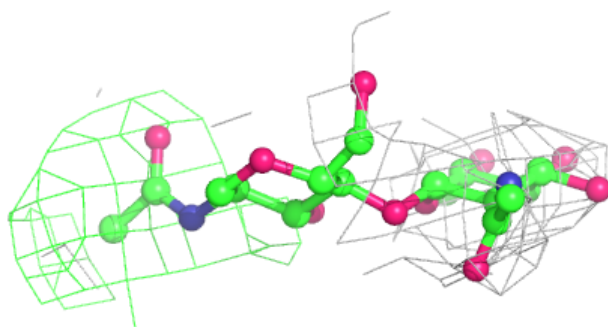
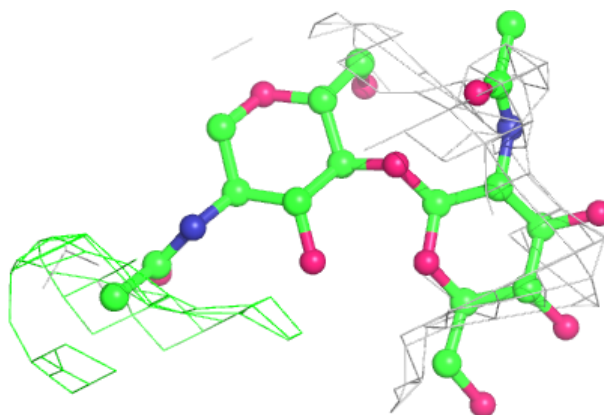
Electron density around Chain K:

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



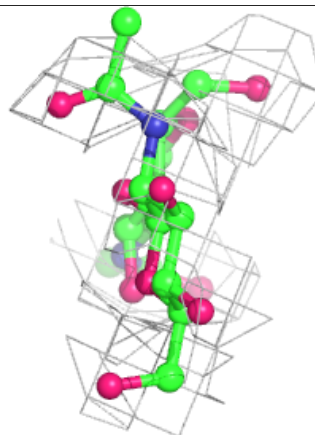
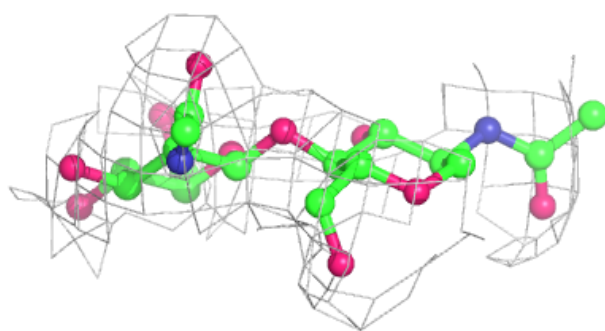
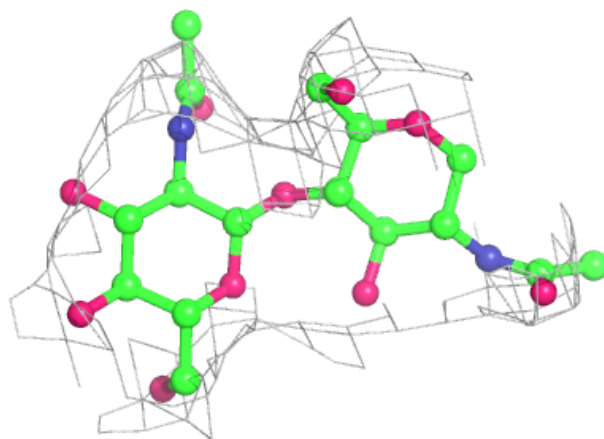
Electron density around Chain M:

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

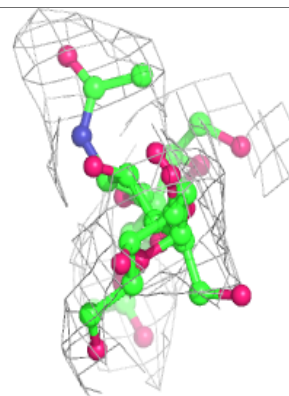
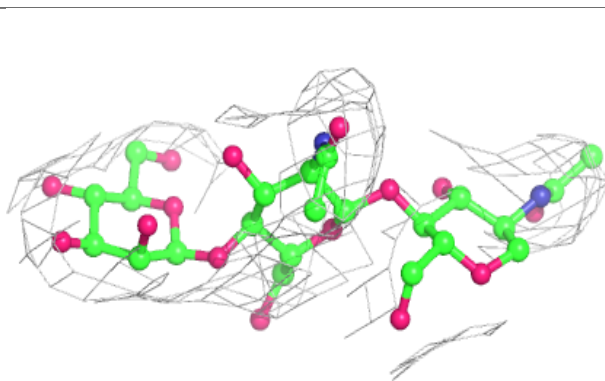
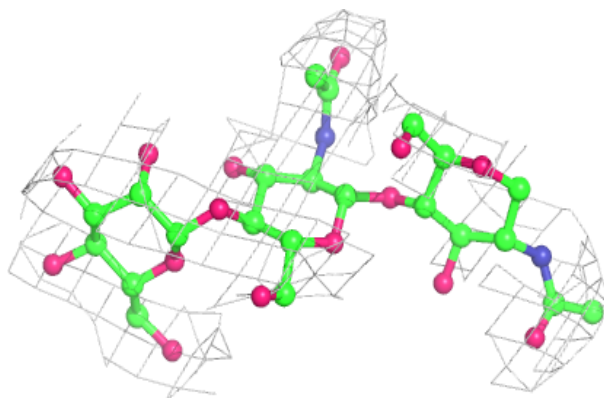


Electron density around Chain Q:

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

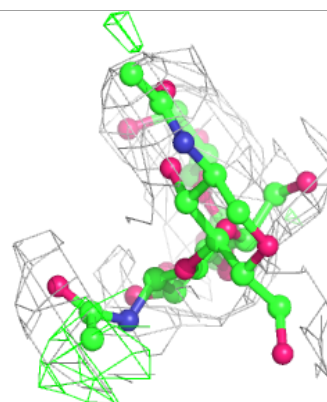
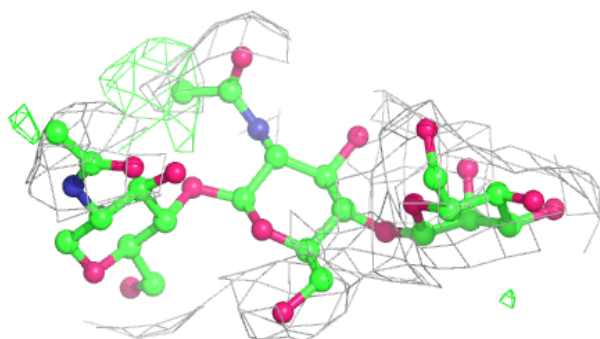
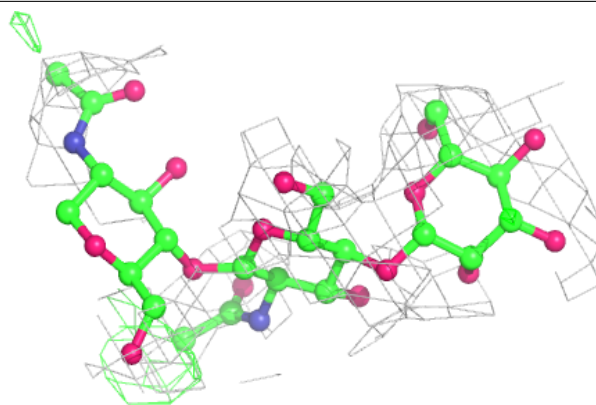
**Electron density around Chain H:**

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

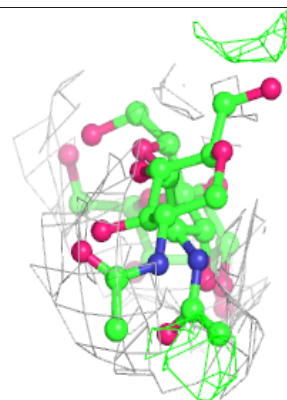
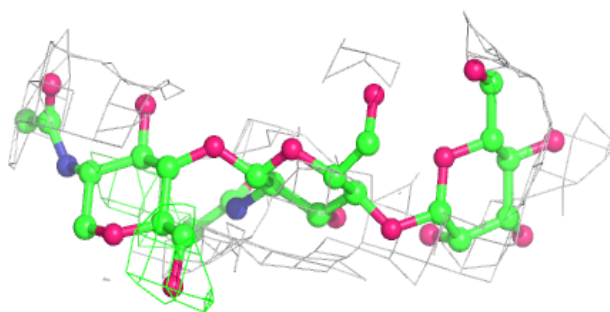
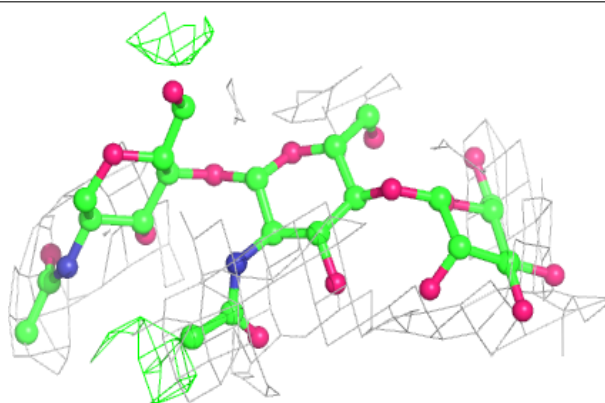


Electron density around Chain N:

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

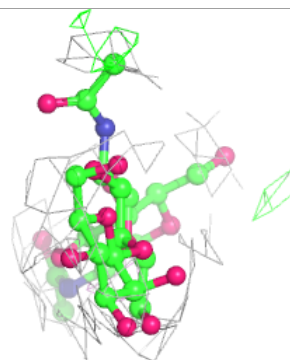
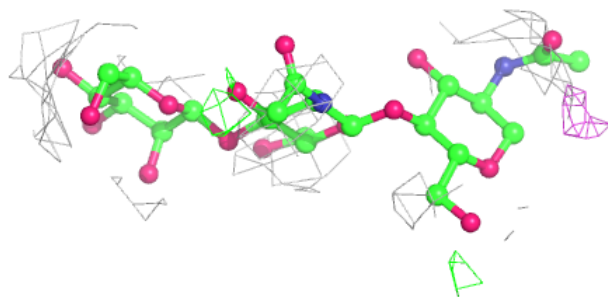
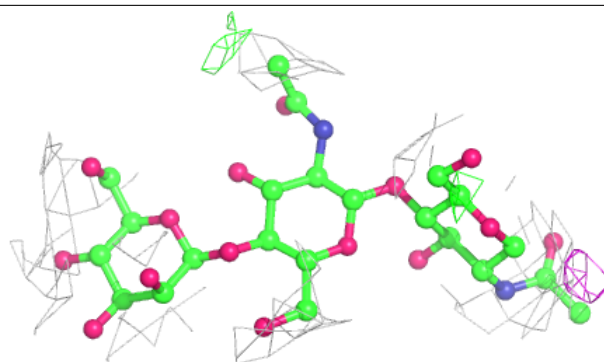
**Electron density around Chain O:**

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



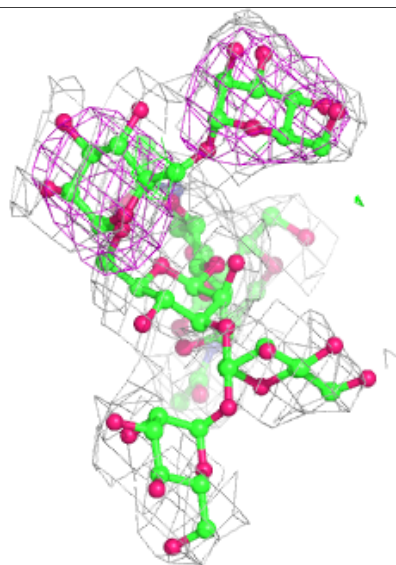
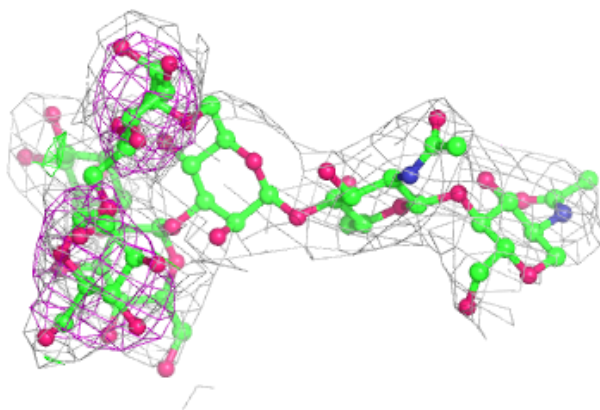
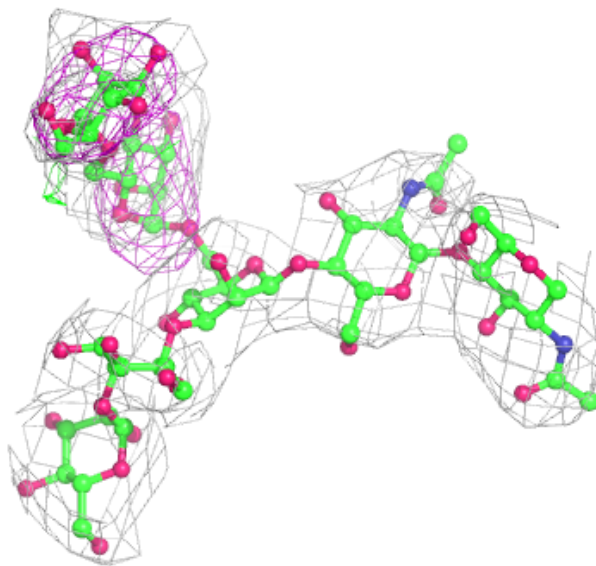
Electron density around Chain R:

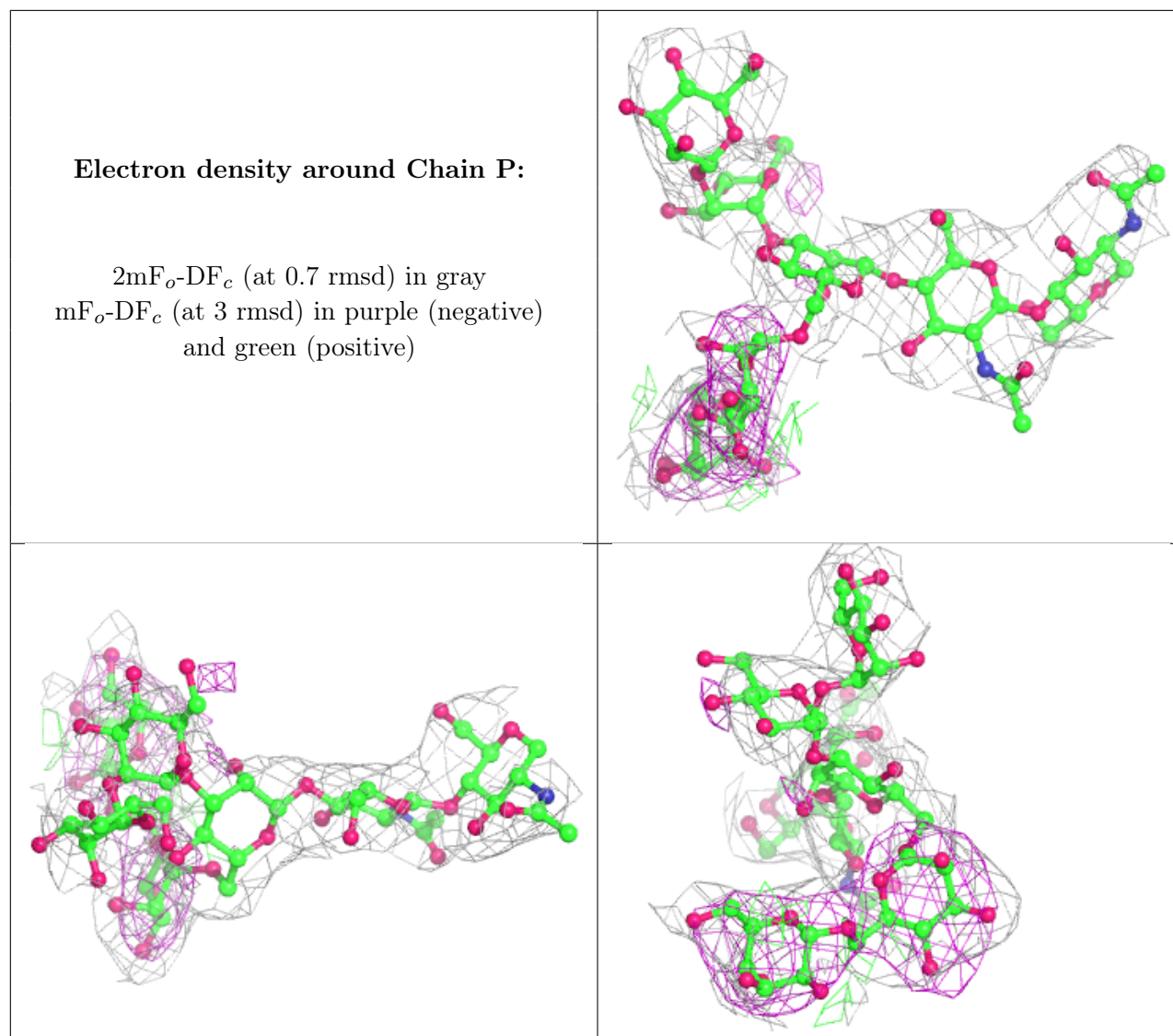
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





6.4 Ligands [i](#)

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
7	NAG	D	1003	14/15	0.27	0.69	167,179,186,189	0
7	NAG	C	1003	14/15	0.61	0.35	141,154,157,160	0
7	NAG	D	1002	14/15	0.64	0.33	149,158,161,168	0
7	NAG	D	1001	14/15	0.65	0.67	127,142,151,152	0
7	NAG	C	1002	14/15	0.74	0.19	95,122,130,132	0
7	NAG	C	1001	14/15	0.86	0.19	99,116,123,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.