



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:13 PM UTC

PDB ID : 3CIY / pdb_00003ciy
Title : Mouse Toll-like receptor 3 ectodomain complexed with double-stranded RNA
Authors : Liu, L.; Botos, I.; Wang, Y.; Leonard, J.N.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on : 2008-03-12
Resolution : 3.41 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

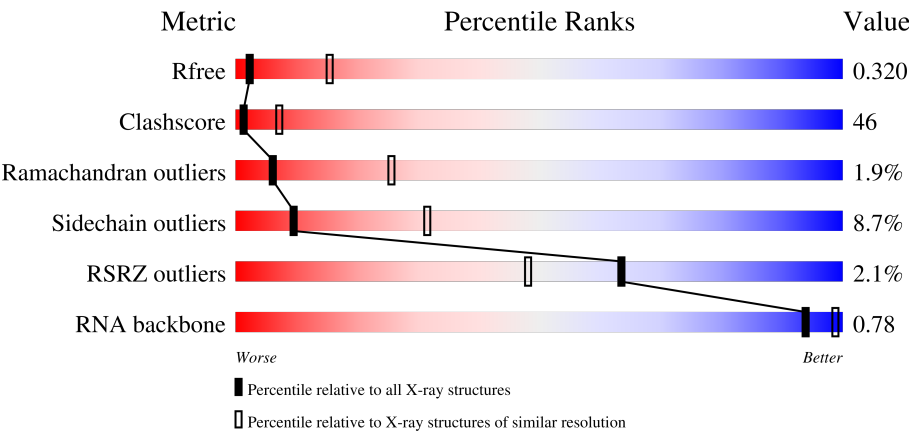
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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.



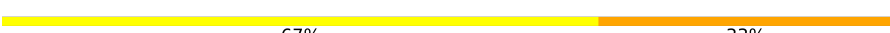
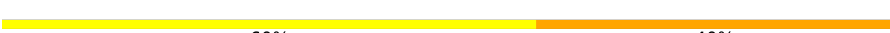
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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	C	46	48%52%
2	D	46	2% 37%63%
3	A	697	2% 32%54%8%5%
3	B	697	2% 31%56%8%

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Mol	Chain	Length	Quality of chain
4	E	2	
4	H	2	
4	L	2	
4	O	2	
5	F	3	
6	G	3	
7	I	5	
8	J	3	
8	Q	3	
9	K	2	
9	R	2	
10	M	3	
11	N	3	
12	P	5	

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
12	NAG	P	1	X	-	-	-
13	NAG	A	724	X	-	-	-
7	NAG	I	1	X	-	-	-
8	NAG	J	1	X	-	-	-
8	NAG	Q	1	X	-	-	-
9	NAG	K	1	X	-	-	-
9	NAG	R	1	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13194 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 RNA chain called 46-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	46	Total	C	N	O	P	0	0	0
			978	439	176	318	45			

- Molecule 2 is a RNA chain called 46-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	46	Total	C	N	O	P	0	0	0
			968	435	166	322	45			

- Molecule 3 is a protein called Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	661	Total	C	N	O	S	0	0	0
			5310	3392	905	999	14			
3	B	668	Total	C	N	O	S	0	0	0
			5360	3422	914	1010	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	ASN	-	expression tag	UNP Q99MB1
A	705	LEU	-	expression tag	UNP Q99MB1
A	706	TYR	-	expression tag	UNP Q99MB1
A	707	PHE	-	expression tag	UNP Q99MB1
A	708	GLN	-	expression tag	UNP Q99MB1
A	709	GLY	-	expression tag	UNP Q99MB1
A	710	HIS	-	expression tag	UNP Q99MB1
A	711	HIS	-	expression tag	UNP Q99MB1
A	712	HIS	-	expression tag	UNP Q99MB1
A	713	HIS	-	expression tag	UNP Q99MB1
A	714	HIS	-	expression tag	UNP Q99MB1
A	715	HIS	-	expression tag	UNP Q99MB1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	716	TRP	-	expression tag	UNP Q99MB1
A	717	SER	-	expression tag	UNP Q99MB1
A	718	HIS	-	expression tag	UNP Q99MB1
A	719	PRO	-	expression tag	UNP Q99MB1
A	720	GLN	-	expression tag	UNP Q99MB1
A	721	PHE	-	expression tag	UNP Q99MB1
A	722	GLU	-	expression tag	UNP Q99MB1
A	723	LYS	-	expression tag	UNP Q99MB1
B	704	ASN	-	expression tag	UNP Q99MB1
B	705	LEU	-	expression tag	UNP Q99MB1
B	706	TYR	-	expression tag	UNP Q99MB1
B	707	PHE	-	expression tag	UNP Q99MB1
B	708	GLN	-	expression tag	UNP Q99MB1
B	709	GLY	-	expression tag	UNP Q99MB1
B	710	HIS	-	expression tag	UNP Q99MB1
B	711	HIS	-	expression tag	UNP Q99MB1
B	712	HIS	-	expression tag	UNP Q99MB1
B	713	HIS	-	expression tag	UNP Q99MB1
B	714	HIS	-	expression tag	UNP Q99MB1
B	715	HIS	-	expression tag	UNP Q99MB1
B	716	TRP	-	expression tag	UNP Q99MB1
B	717	SER	-	expression tag	UNP Q99MB1
B	718	HIS	-	expression tag	UNP Q99MB1
B	719	PRO	-	expression tag	UNP Q99MB1
B	720	GLN	-	expression tag	UNP Q99MB1
B	721	PHE	-	expression tag	UNP Q99MB1
B	722	GLU	-	expression tag	UNP Q99MB1
B	723	LYS	-	expression tag	UNP Q99MB1

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



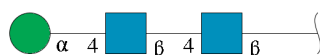
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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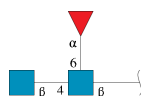
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



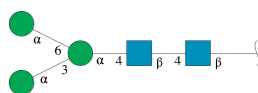
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



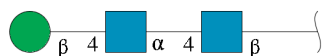
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



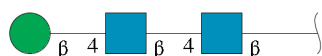
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



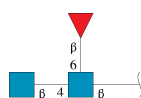
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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.



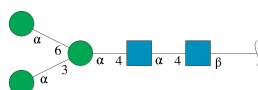
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



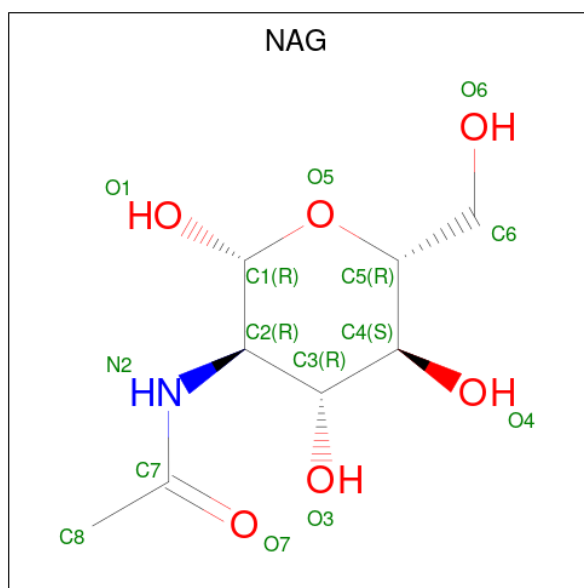
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	N	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



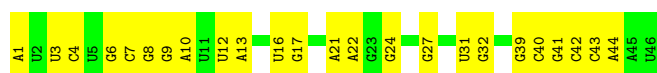
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			14	8	1	5		
13	A	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

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

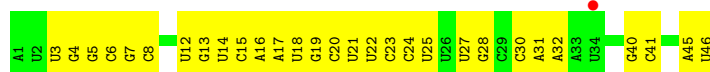
• Molecule 1: 46-MER

Chain C: 



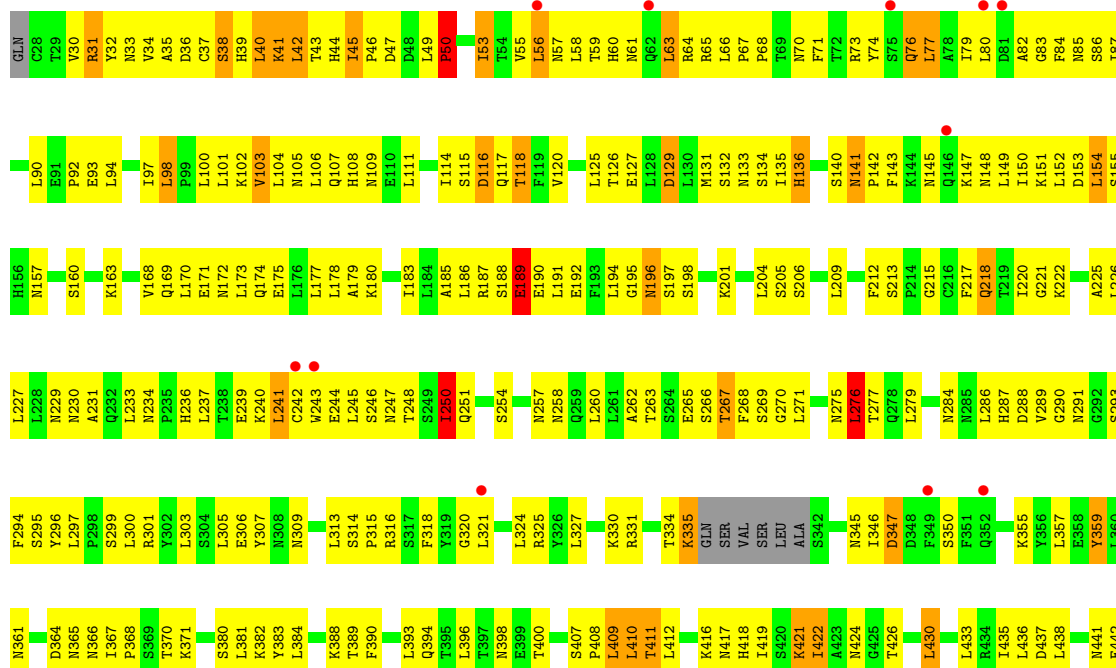
• Molecule 2: 46-MER

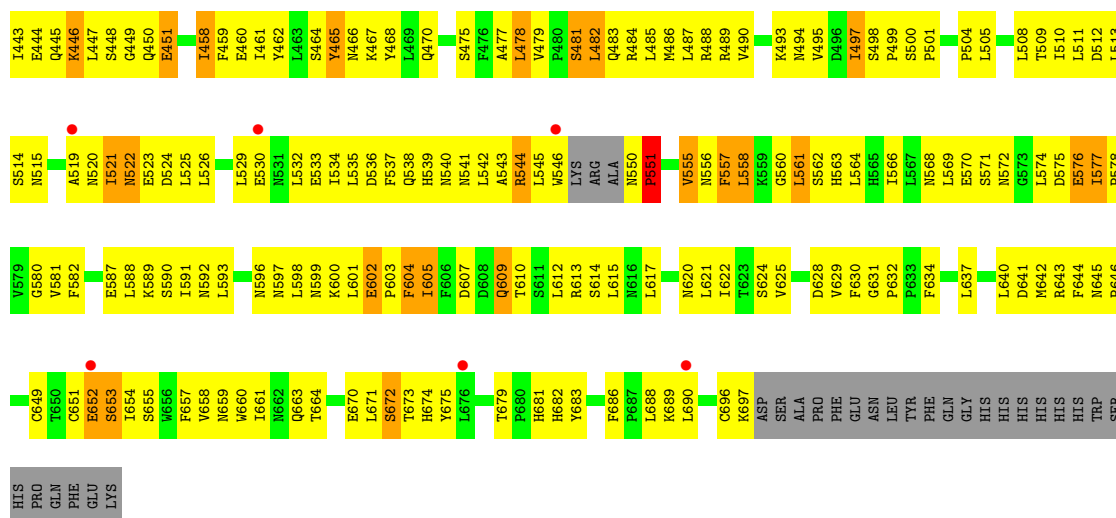
Chain D: 



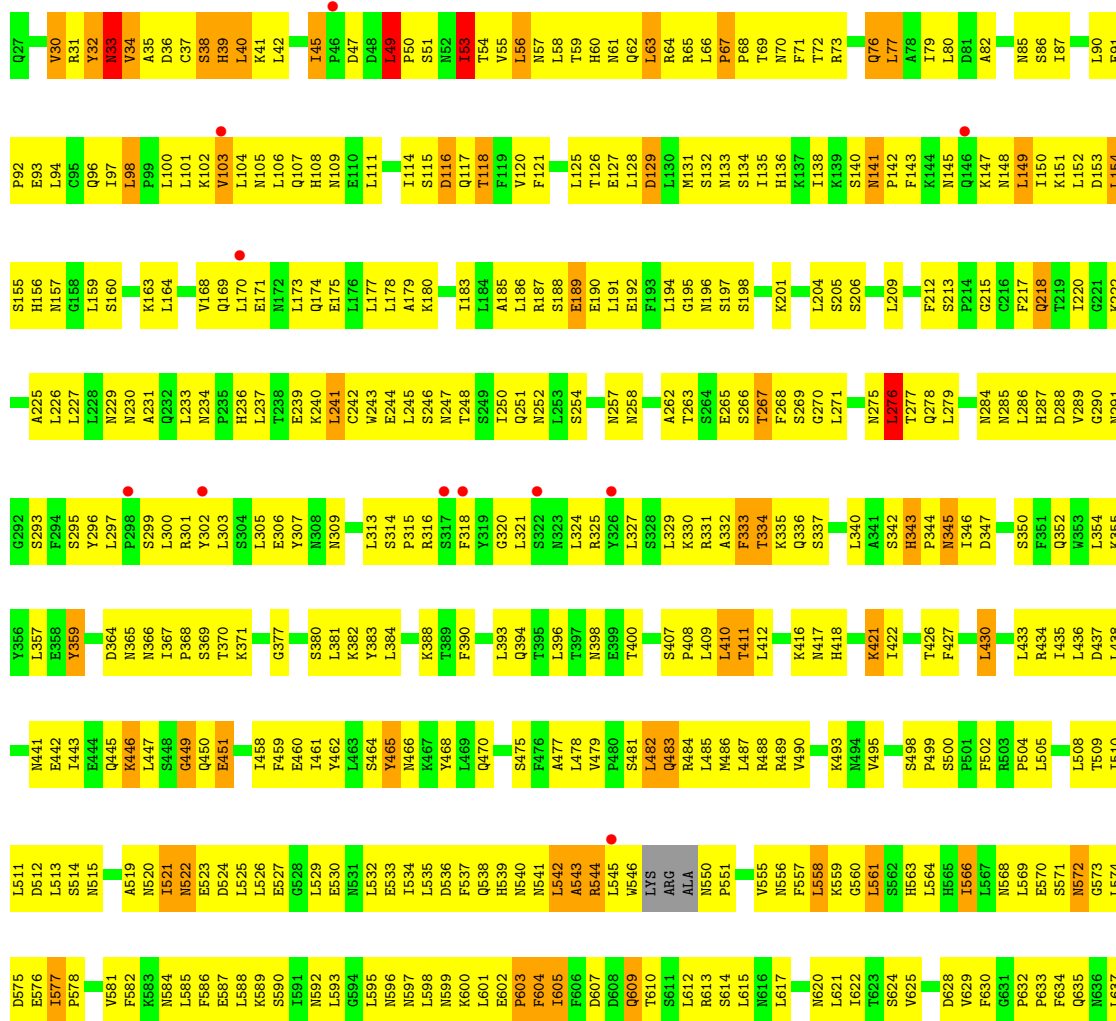
• Molecule 3: Toll-like receptor 3

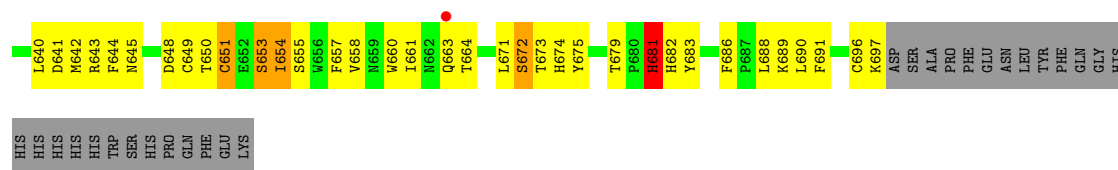
Chain A: 





• Molecule 3: Toll-like receptor 3





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

Chain E:  50%



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

Chain H:  100%



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

Chain L:  100%



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

Chain O:  50%



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

Chain F:  33%



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

Chain G:  67%



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain J:



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

Chain Q:



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

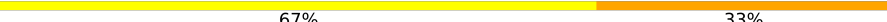


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

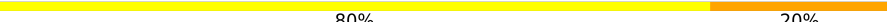


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  67% 33%

MAG1
MAG2
FUL3

- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  80% 20%

MAG1
NDG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.85Å 225.88Å 259.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 3.41 47.29 – 3.41	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.29-3.41) 97.5 (47.29-3.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.288 , 0.333 0.307 , 0.320	Depositor DCC
R_{free} test set	2355 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	119.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 95.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13194	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: BMA, FUL, FUC, NDG, 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	C	0.34	0/1094	0.53	0/1703
2	D	0.34	0/1080	0.54	0/1679
3	A	0.56	2/5421 (0.0%)	1.04	35/7360 (0.5%)
3	B	0.56	4/5472 (0.1%)	1.04	38/7431 (0.5%)
All	All	0.53	6/13067 (0.0%)	0.97	73/18173 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	53	ILE	CA-CB	9.55	1.67	1.54
3	A	189	GLU	N-CA	8.50	1.57	1.46
3	A	189	GLU	CA-C	7.91	1.61	1.52
3	B	333	PHE	N-CA	6.01	1.53	1.46
3	B	33	ASN	N-CA	5.43	1.53	1.46
3	B	53	ILE	CA-C	5.08	1.59	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	50	PRO	CB-CA-C	-9.13	99.54	111.23
3	A	276	LEU	N-CA-C	8.97	123.36	108.73
3	B	276	LEU	N-CA-C	8.33	122.44	108.20
3	B	543	ALA	N-CA-C	7.92	120.68	111.02
3	A	495	VAL	N-CA-C	-7.73	105.48	112.90
3	B	136	HIS	N-CA-C	7.42	119.36	111.28
3	A	41	LYS	N-CA-C	-7.35	102.83	112.24
3	B	495	VAL	N-CA-C	-7.31	105.88	112.90
3	B	542	LEU	N-CA-C	-7.29	104.41	112.72
3	A	542	LEU	N-CA-C	-7.12	104.52	112.57
3	A	50	PRO	N-CA-C	7.06	122.43	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	118	THR	N-CA-C	6.87	119.64	111.33
3	A	196	ASN	N-CA-C	-6.81	103.55	112.41
3	A	141	ASN	CA-C-N	6.80	127.36	119.47
3	A	141	ASN	C-N-CA	6.80	127.36	119.47
3	A	118	THR	N-CA-C	6.75	119.50	111.33
3	B	141	ASN	CA-C-N	6.74	127.29	119.47
3	B	141	ASN	C-N-CA	6.74	127.29	119.47
3	A	663	GLN	N-CA-C	6.74	120.81	112.59
3	B	663	GLN	N-CA-C	6.57	120.60	112.59
3	B	188	SER	N-CA-C	-6.54	105.41	113.19
3	B	196	ASN	N-CA-C	-6.29	104.23	112.41
3	A	580	GLY	N-CA-C	6.26	122.62	113.48
3	B	343	HIS	CA-C-N	6.25	126.22	119.78
3	B	343	HIS	C-N-CA	6.25	126.22	119.78
3	B	250	ILE	N-CA-C	6.23	117.08	109.30
3	A	250	ILE	N-CA-C	6.22	117.08	109.30
3	A	188	SER	N-CA-C	-6.21	105.80	113.19
3	B	33	ASN	N-CA-C	6.17	122.14	113.56
3	B	77	LEU	N-CA-C	6.15	119.28	110.24
3	B	39	HIS	N-CA-C	-6.02	97.98	110.80
3	A	558	LEU	N-CA-C	6.00	119.70	111.54
3	A	160	SER	N-CA-C	-5.96	105.97	113.72
3	A	610	THR	N-CA-C	-5.90	105.67	112.92
3	B	674	HIS	N-CA-C	5.84	119.17	112.97
3	B	34	VAL	N-CA-C	-5.81	97.65	106.42
3	A	602	GLU	N-CA-C	-5.81	100.96	109.50
3	A	77	LEU	N-CA-C	5.77	118.72	110.24
3	A	103	VAL	N-CA-C	5.76	116.15	107.80
3	A	136	HIS	N-CA-C	5.72	118.28	111.71
3	B	558	LEU	N-CA-C	5.64	119.21	111.54
3	B	632	PRO	N-CA-C	5.64	117.58	110.70
3	B	334	THR	N-CA-C	5.63	117.56	110.24
3	A	632	PRO	N-CA-C	5.62	117.56	110.70
3	B	160	SER	N-CA-C	-5.62	106.42	113.72
3	A	482	LEU	N-CA-C	5.61	118.46	110.10
3	A	602	GLU	CB-CA-C	5.55	118.83	109.67
3	B	482	LEU	N-CA-C	5.55	118.29	109.96
3	B	610	THR	N-CA-C	-5.54	106.11	112.92
3	B	672	SER	N-CA-C	5.47	117.32	111.36
3	A	129	ASP	N-CA-C	5.45	117.41	108.52
3	A	674	HIS	N-CA-C	5.43	118.72	112.97
3	A	590	SER	N-CA-C	5.43	117.27	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	PHE	N-CA-CB	-5.37	102.99	110.29
3	B	653	SER	N-CA-C	5.36	122.22	110.80
3	A	576	GLU	CA-C-N	-5.35	118.96	122.60
3	A	576	GLU	C-N-CA	-5.35	118.96	122.60
3	B	129	ASP	N-CA-C	5.35	117.23	108.52
3	A	560	GLY	N-CA-C	5.34	125.83	113.18
3	B	590	SER	N-CA-C	5.31	117.08	108.26
3	B	332	ALA	N-CA-C	5.30	119.85	113.17
3	B	103	VAL	N-CA-C	5.22	115.38	107.80
3	A	653	SER	N-CA-C	5.22	121.92	110.80
3	B	681	HIS	N-CA-C	5.21	119.97	111.37
3	A	652	GLU	N-CA-C	-5.21	106.18	112.54
3	B	72	THR	N-CA-C	-5.18	107.51	113.88
3	B	149	LEU	N-CA-C	5.17	116.74	108.41
3	B	560	GLY	N-CA-C	5.12	125.32	113.18
3	A	63	LEU	N-CA-C	5.12	116.75	108.41
3	B	483	GLN	N-CA-C	-5.11	106.14	112.93
3	B	49	LEU	N-CA-C	5.09	121.05	109.81
3	A	672	SER	N-CA-C	5.09	116.91	111.36
3	B	63	LEU	N-CA-C	5.04	116.62	108.41

There are no chirality outliers.

There are no planarity outliers.

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	C	978	0	496	29	0
2	D	968	0	494	33	0
3	A	5310	0	5311	538	0
3	B	5360	0	5363	546	0
4	E	28	0	24	4	0
4	H	28	0	24	5	0
4	L	28	0	24	5	0
4	O	28	0	24	3	0
5	F	39	0	34	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	38	0	34	4	0
7	I	61	0	52	6	0
8	J	39	0	33	6	0
8	Q	39	0	33	6	0
9	K	28	0	25	3	0
9	R	28	0	25	2	0
10	M	39	0	34	3	0
11	N	38	0	34	1	0
12	P	61	0	51	1	0
13	A	28	0	26	2	0
13	B	28	0	26	1	0
All	All	13194	0	12167	1159	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 46.

All (1159) 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)
3:B:650:THR:O	3:B:654:ILE:HD12	1.41	1.21
3:A:605:ILE:HD11	3:A:629:VAL:HG13	1.19	1.13
3:B:450:GLN:HG3	8:Q:1:NAG:H62	1.29	1.12
3:A:536:ASP:HB3	3:A:538:GLN:HE22	1.20	1.06
3:B:108:HIS:HA	3:B:132:SER:HB2	1.32	1.06
3:A:108:HIS:HA	3:A:132:SER:HB2	1.32	1.06
3:A:277:THR:HG21	4:E:1:NAG:H82	1.37	1.05
3:A:56:LEU:HD11	3:A:58:LEU:HG	1.38	1.05
3:B:605:ILE:HD11	3:B:629:VAL:HG13	1.07	1.05
3:B:536:ASP:HB3	3:B:538:GLN:HE22	1.23	1.00
3:B:468:TYR:HE1	3:B:470:GLN:HB2	1.29	0.97
3:B:650:THR:O	3:B:654:ILE:CD1	2.13	0.97
3:B:605:ILE:HD13	3:B:605:ILE:H	1.31	0.95
3:B:68:PRO:HB2	3:B:93:GLU:HB2	1.48	0.95
3:B:33:ASN:HA	3:B:53:ILE:HB	1.47	0.94
3:A:521:ILE:HD11	3:A:525:LEU:HB3	1.50	0.94
3:A:468:TYR:HE1	3:A:470:GLN:HB2	1.33	0.94
3:A:545:LEU:HD12	3:A:555:VAL:HG21	1.48	0.93
3:A:68:PRO:HB2	3:A:93:GLU:HB2	1.52	0.92
3:B:605:ILE:CD1	3:B:629:VAL:HG13	1.97	0.92
3:B:56:LEU:HD11	3:B:58:LEU:HG	1.49	0.91
3:B:33:ASN:HD22	3:B:33:ASN:N	1.65	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:90:LEU:HD11	3:B:94:LEU:HD22	1.52	0.91
3:A:133:ASN:H	3:A:157:ASN:ND2	1.70	0.90
3:A:577:ILE:HD13	3:A:605:ILE:HG21	1.53	0.90
3:A:31:ARG:HE	3:A:31:ARG:HA	1.34	0.90
3:A:605:ILE:CD1	3:A:629:VAL:HG13	2.02	0.90
3:B:521:ILE:HD11	3:B:525:LEU:HB3	1.55	0.89
3:B:450:GLN:CG	8:Q:1:NAG:H62	2.02	0.88
3:A:396:LEU:HB2	3:A:422:ILE:HD12	1.55	0.88
3:A:575:ASP:HA	3:A:597:ASN:O	1.73	0.88
3:B:599:ASN:HB3	3:B:621:LEU:O	1.74	0.87
3:A:536:ASP:CB	3:A:538:GLN:HE22	1.87	0.87
3:B:577:ILE:HD13	3:B:605:ILE:HG21	1.57	0.87
3:B:40:LEU:HB2	3:B:61:ASN:HD21	1.40	0.86
3:A:550:ASN:CB	3:A:551:PRO:HD2	2.05	0.86
3:B:269:SER:HA	3:B:296:TYR:CD1	2.11	0.86
1:C:41:G:O2'	1:C:42:C:H5'	1.76	0.86
3:B:488:ARG:HG3	3:B:514:SER:OG	1.75	0.86
3:A:605:ILE:HD13	3:A:605:ILE:H	1.40	0.85
3:B:654:ILE:HD13	3:B:655:SER:N	1.90	0.85
3:B:33:ASN:HA	3:B:53:ILE:CB	2.06	0.85
3:B:575:ASP:HA	3:B:597:ASN:O	1.76	0.85
3:A:488:ARG:HG3	3:A:514:SER:OG	1.76	0.84
3:B:396:LEU:HD12	3:B:422:ILE:HG12	1.59	0.84
3:B:334:THR:HG22	3:B:344:PRO:HB3	1.59	0.84
3:B:55:VAL:HG22	3:B:79:ILE:HG12	1.58	0.83
3:B:80:LEU:HD21	3:B:104:LEU:HD12	1.60	0.83
3:A:300:LEU:HD23	3:A:324:LEU:HD13	1.59	0.83
3:B:654:ILE:O	3:B:658:VAL:HG23	1.78	0.83
3:A:90:LEU:HD11	3:A:94:LEU:HD22	1.59	0.83
3:A:234:ASN:HB3	3:A:237:LEU:HD13	1.60	0.83
3:B:133:ASN:H	3:B:157:ASN:ND2	1.75	0.83
3:A:55:VAL:HG22	3:A:79:ILE:HG12	1.58	0.83
3:A:141:ASN:HB3	3:A:169:GLN:HE22	1.43	0.83
3:A:114:ILE:HD11	3:A:118:THR:HB	1.61	0.83
3:B:536:ASP:CB	3:B:538:GLN:HE22	1.92	0.82
3:B:482:LEU:HB2	3:B:505:LEU:HD22	1.61	0.81
3:B:141:ASN:HB3	3:B:169:GLN:HE22	1.43	0.81
3:A:47:ASP:HB2	3:A:73:ARG:HD3	1.61	0.81
3:A:461:ILE:HD12	3:A:482:LEU:HD11	1.61	0.81
3:A:609:GLN:H	3:A:609:GLN:NE2	1.77	0.81
3:A:37:CYS:HB3	3:A:40:LEU:HD21	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:500:SER:HB2	3:B:525:LEU:HA	1.62	0.80
3:B:38:SER:C	3:B:40:LEU:HD13	2.06	0.80
3:B:42:LEU:H	3:B:61:ASN:HD22	1.28	0.80
3:A:40:LEU:HD22	3:A:42:LEU:HD12	1.63	0.80
3:B:31:ARG:C	3:B:32:TYR:HD1	1.89	0.80
3:B:49:LEU:HD22	3:B:73:ARG:HH21	1.47	0.80
3:B:561:LEU:H	3:B:561:LEU:HD12	1.47	0.80
3:A:578:PRO:HG2	3:A:581:VAL:HG11	1.64	0.80
3:A:561:LEU:HD12	3:A:561:LEU:H	1.45	0.79
3:A:35:ALA:HB3	3:A:56:LEU:HA	1.65	0.79
3:B:578:PRO:HG2	3:B:581:VAL:HG11	1.62	0.79
3:B:279:LEU:HB3	3:B:300:LEU:HD11	1.63	0.79
3:B:543:ALA:HB2	3:B:573:GLY:HA3	1.64	0.79
3:B:234:ASN:HB3	3:B:237:LEU:HD13	1.65	0.78
3:B:49:LEU:HD13	3:B:73:ARG:HH22	1.48	0.78
3:A:269:SER:HA	3:A:296:TYR:CD1	2.18	0.78
3:B:300:LEU:HD23	3:B:324:LEU:HD13	1.66	0.78
3:A:56:LEU:CD1	3:A:58:LEU:HG	2.11	0.78
3:A:481:SER:HA	9:K:1:NAG:H83	1.65	0.78
3:A:80:LEU:HD21	3:A:104:LEU:HD12	1.64	0.78
3:B:268:PHE:HB3	3:B:271:LEU:HD23	1.66	0.78
3:B:49:LEU:HD13	3:B:73:ARG:NH2	2.00	0.77
3:B:367:ILE:HD12	3:B:367:ILE:H	1.49	0.77
3:A:63:LEU:HB2	3:A:85:ASN:HB3	1.67	0.77
3:A:133:ASN:H	3:A:157:ASN:HD21	1.32	0.77
3:B:398:ASN:ND2	4:O:1:NAG:H62	1.99	0.77
3:A:279:LEU:HB3	3:A:300:LEU:HD11	1.66	0.77
3:A:393:LEU:HD21	3:A:396:LEU:HD23	1.65	0.77
3:B:150:ILE:CG2	3:B:174:GLN:HB2	2.13	0.77
9:R:1:NAG:O3	9:R:2:NAG:H61	1.85	0.76
3:B:90:LEU:HD11	3:B:94:LEU:CD2	2.15	0.76
3:A:268:PHE:HB3	3:A:271:LEU:HD23	1.66	0.76
3:B:609:GLN:H	3:B:609:GLN:NE2	1.83	0.76
3:A:599:ASN:HB3	3:A:621:LEU:O	1.85	0.76
3:A:482:LEU:HB2	3:A:505:LEU:HD22	1.68	0.76
3:B:127:GLU:HG3	3:B:151:LYS:HB2	1.67	0.75
3:B:393:LEU:HD21	3:B:396:LEU:HD23	1.68	0.75
3:A:500:SER:HB2	3:A:525:LEU:HA	1.67	0.75
3:A:367:ILE:HD12	3:A:367:ILE:H	1.51	0.75
3:B:287:HIS:HA	3:B:309:ASN:O	1.86	0.75
3:B:605:ILE:HD11	3:B:629:VAL:CG1	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:598:LEU:HB2	3:A:620:ASN:HD22	1.51	0.74
3:B:147:LYS:HE2	3:B:147:LYS:HA	1.68	0.74
3:B:651:CYS:HB3	3:B:655:SER:OG	1.88	0.74
3:A:42:LEU:HB2	3:A:61:ASN:HD22	1.53	0.74
3:A:120:VAL:HA	3:A:145:ASN:ND2	2.03	0.74
8:J:2:NDG:H4	8:J:3:BMA:O2	1.88	0.74
3:A:90:LEU:HD11	3:A:94:LEU:CD2	2.18	0.74
3:A:115:SER:O	3:A:118:THR:HG22	1.87	0.74
3:A:550:ASN:HB2	3:A:551:PRO:HD2	1.68	0.74
1:C:39:G:H2'	1:C:40:C:H6	1.51	0.74
3:A:104:LEU:HG	3:A:106:LEU:HD13	1.70	0.74
3:A:398:ASN:ND2	4:H:1:NAG:H61	2.03	0.74
3:B:578:PRO:HG2	3:B:581:VAL:CG1	2.17	0.73
3:A:49:LEU:HB3	3:A:50:PRO:HD2	1.70	0.73
3:B:605:ILE:H	3:B:605:ILE:CD1	1.99	0.73
3:A:421:LYS:C	3:A:422:ILE:HD13	2.12	0.73
3:A:521:ILE:HD11	3:A:525:LEU:CB	2.19	0.73
3:B:30:VAL:HA	3:B:35:ALA:HA	1.69	0.73
3:B:63:LEU:HB2	3:B:85:ASN:HB3	1.69	0.73
3:B:521:ILE:HD11	3:B:525:LEU:CB	2.18	0.73
3:A:127:GLU:HG3	3:A:151:LYS:HB2	1.70	0.73
3:B:265:GLU:HA	3:B:293:SER:HA	1.70	0.73
3:A:40:LEU:N	3:A:40:LEU:HD12	2.03	0.73
3:A:168:VAL:HG13	3:A:195:GLY:H	1.52	0.73
3:B:120:VAL:HA	3:B:145:ASN:ND2	2.02	0.73
3:B:66:LEU:HB3	3:B:94:LEU:HD21	1.70	0.72
3:B:56:LEU:CD1	3:B:58:LEU:HG	2.17	0.72
3:A:334:THR:HG22	3:A:335:LYS:H	1.54	0.72
3:A:396:LEU:HD12	3:A:422:ILE:CD1	2.19	0.72
3:A:419:ILE:CG2	3:A:422:ILE:HD11	2.19	0.72
3:A:446:LYS:HB3	3:A:470:GLN:HB3	1.71	0.72
3:A:620:ASN:HB2	3:A:645:ASN:HD21	1.54	0.72
2:D:21:U:O2	3:A:541:ASN:ND2	2.22	0.72
3:B:605:ILE:HD13	3:B:605:ILE:N	2.02	0.72
3:A:150:ILE:CG2	3:A:174:GLN:HB2	2.18	0.71
3:A:246:SER:O	3:A:248:THR:HG23	1.90	0.71
3:B:300:LEU:HD21	3:B:303:LEU:HB2	1.70	0.71
3:B:620:ASN:HB2	3:B:645:ASN:HD21	1.54	0.71
3:A:605:ILE:CD1	3:A:605:ILE:H	2.04	0.71
3:B:262:ALA:CB	3:B:288:ASP:HB2	2.21	0.71
3:A:287:HIS:HA	3:A:309:ASN:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:654:ILE:O	3:A:658:VAL:HG23	1.89	0.71
3:A:49:LEU:HB3	3:A:50:PRO:CD	2.21	0.71
3:A:243:TRP:CD1	3:A:270:GLY:HA2	2.26	0.71
3:B:243:TRP:CD1	3:B:270:GLY:HA2	2.26	0.71
3:B:104:LEU:HG	3:B:106:LEU:HD13	1.71	0.71
3:A:605:ILE:HD13	3:A:605:ILE:N	2.06	0.70
3:A:265:GLU:HA	3:A:293:SER:HA	1.73	0.70
4:E:1:NAG:H2	4:E:1:NAG:H61	1.73	0.70
3:B:168:VAL:HG13	3:B:195:GLY:H	1.55	0.70
3:B:660:TRP:O	3:B:664:THR:HG22	1.91	0.70
3:A:300:LEU:HD21	3:A:303:LEU:HB2	1.73	0.70
3:B:325:ARG:C	3:B:357:LEU:HD12	2.15	0.70
3:A:42:LEU:HB2	3:A:61:ASN:ND2	2.05	0.70
3:B:446:LYS:HB3	3:B:470:GLN:HB3	1.74	0.70
3:B:313:LEU:HD12	3:B:346:ILE:HG21	1.72	0.70
3:A:150:ILE:HD13	3:A:172:ASN:O	1.92	0.70
3:B:201:LYS:HA	3:B:225:ALA:HB3	1.72	0.70
3:A:66:LEU:HB3	3:A:94:LEU:HD21	1.72	0.69
3:A:526:LEU:HD23	3:A:529:LEU:HD12	1.73	0.69
3:A:535:LEU:HD11	3:A:537:PHE:CE2	2.27	0.69
3:B:185:ALA:C	3:B:186:LEU:HD12	2.17	0.69
3:A:550:ASN:HB3	3:A:551:PRO:HD2	1.73	0.69
3:A:622:ILE:H	3:A:645:ASN:HD22	1.37	0.69
3:A:511:LEU:HD23	3:A:512:ASP:N	2.08	0.69
9:K:1:NAG:O4	9:K:2:NAG:H61	1.93	0.69
3:A:430:LEU:HD23	3:A:433:LEU:HD22	1.75	0.68
3:A:557:PHE:HD2	3:A:558:LEU:HG	1.57	0.68
3:B:313:LEU:HB2	3:B:346:ILE:HG22	1.75	0.68
6:G:1:NAG:O3	6:G:2:NAG:H2	1.93	0.68
2:D:45:A:H2'	2:D:46:U:C6	2.28	0.68
3:B:38:SER:O	3:B:40:LEU:HD13	1.94	0.68
3:B:215:GLY:HA2	3:B:218:GLN:HG2	1.76	0.68
3:B:461:ILE:HD12	3:B:482:LEU:HD11	1.76	0.68
3:A:34:VAL:HG12	3:A:55:VAL:HB	1.76	0.68
3:B:93:GLU:O	3:B:97:ILE:HG12	1.94	0.68
3:B:526:LEU:HD23	3:B:529:LEU:HD12	1.76	0.68
3:A:68:PRO:O	3:A:97:ILE:HG13	1.94	0.68
3:B:295:SER:HA	3:B:320:GLY:HA3	1.74	0.68
3:A:150:ILE:HG23	3:A:174:GLN:HB2	1.74	0.67
3:A:93:GLU:O	3:A:97:ILE:HG12	1.93	0.67
3:B:68:PRO:HA	3:B:94:LEU:HG	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:133:ASN:H	3:B:157:ASN:HD21	1.41	0.67
3:A:201:LYS:HA	3:A:225:ALA:HB3	1.74	0.67
3:A:147:LYS:HA	3:A:147:LYS:HE2	1.75	0.67
3:B:34:VAL:HA	3:B:55:VAL:HB	1.74	0.67
3:B:116:ASP:HA	3:B:142:PRO:HA	1.77	0.67
3:B:150:ILE:HG23	3:B:174:GLN:HB2	1.73	0.67
3:B:542:LEU:H	3:B:572:ASN:ND2	1.92	0.67
3:B:546:TRP:HB3	3:B:578:PRO:HD3	1.77	0.67
3:B:49:LEU:HD22	3:B:73:ARG:NH2	2.09	0.67
3:B:598:LEU:HB2	3:B:620:ASN:HD22	1.60	0.67
3:B:34:VAL:HG23	3:B:34:VAL:O	1.94	0.67
3:B:607:ASP:N	3:B:609:GLN:HE22	1.92	0.67
3:A:536:ASP:HB3	3:A:538:GLN:NE2	2.02	0.66
3:B:68:PRO:O	3:B:97:ILE:HG13	1.95	0.66
3:A:143:PHE:C	3:A:145:ASN:H	1.99	0.66
3:A:185:ALA:C	3:A:186:LEU:HD12	2.19	0.66
3:B:31:ARG:C	3:B:32:TYR:CD1	2.72	0.66
3:A:313:LEU:HB2	3:A:346:ILE:HG22	1.77	0.66
3:A:578:PRO:HG2	3:A:581:VAL:CG1	2.25	0.66
3:B:68:PRO:CB	3:B:93:GLU:HB2	2.24	0.66
3:A:541:ASN:OD1	3:A:541:ASN:O	2.13	0.66
3:A:40:LEU:HD13	3:A:61:ASN:HD21	1.60	0.66
3:A:624:SER:HB3	3:A:653:SER:HB3	1.75	0.66
3:B:291:ASN:OD1	3:B:316:ARG:HB3	1.95	0.66
3:B:593:LEU:HB2	3:B:617:LEU:HD23	1.75	0.66
3:A:295:SER:HA	3:A:320:GLY:HA3	1.78	0.66
3:B:557:PHE:HD2	3:B:558:LEU:HG	1.61	0.66
3:B:622:ILE:H	3:B:645:ASN:HD22	1.44	0.66
3:A:275:ASN:HD21	5:F:1:NAG:C6	2.10	0.65
3:B:115:SER:O	3:B:118:THR:HG22	1.96	0.65
3:B:180:LYS:HA	3:B:206:SER:HB2	1.76	0.65
3:A:215:GLY:HA2	3:A:218:GLN:HG2	1.77	0.65
3:B:624:SER:HB3	3:B:653:SER:HB3	1.77	0.65
3:A:419:ILE:HG21	3:A:422:ILE:HD11	1.76	0.65
3:B:33:ASN:CA	3:B:53:ILE:HB	2.22	0.65
3:A:660:TRP:O	3:A:664:THR:HG22	1.95	0.65
3:B:275:ASN:ND2	10:M:1:NAG:H61	2.11	0.65
3:B:325:ARG:HA	3:B:357:LEU:HA	1.79	0.65
3:A:180:LYS:HA	3:A:206:SER:HB2	1.77	0.65
3:A:596:ASN:O	3:A:620:ASN:HA	1.96	0.65
3:A:607:ASP:N	3:A:609:GLN:HE22	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:ASN:O	3:A:569:LEU:HD12	1.96	0.65
3:B:187:ARG:O	3:B:191:LEU:HD23	1.97	0.65
3:A:511:LEU:HD21	3:A:513:LEU:HG	1.78	0.65
3:B:55:VAL:HG13	3:B:79:ILE:HG13	1.79	0.65
1:C:12:U:H2'	1:C:13:A:H8	1.61	0.65
3:A:468:TYR:OH	3:A:493:LYS:HD3	1.97	0.65
3:B:624:SER:HB3	3:B:653:SER:CB	2.27	0.65
3:A:68:PRO:CB	3:A:93:GLU:HB2	2.26	0.64
3:B:150:ILE:O	3:B:173:LEU:HD12	1.97	0.64
3:B:231:ALA:HB3	3:B:233:LEU:HD11	1.79	0.64
3:B:533:GLU:HB2	3:B:534:ILE:HD12	1.79	0.64
3:A:624:SER:HB3	3:A:653:SER:CB	2.27	0.64
3:B:94:LEU:HD12	3:B:94:LEU:H	1.62	0.64
3:B:596:ASN:O	3:B:620:ASN:HA	1.97	0.64
3:B:297:LEU:HD13	3:B:300:LEU:HD13	1.80	0.64
3:A:458:ILE:HD13	3:A:458:ILE:C	2.23	0.64
3:B:252:ASN:HD22	4:L:1:NAG:H61	1.60	0.64
3:A:94:LEU:HD12	3:A:94:LEU:H	1.62	0.64
3:B:545:LEU:O	3:B:546:TRP:HD1	1.80	0.64
3:A:68:PRO:HA	3:A:94:LEU:HG	1.79	0.64
3:A:187:ARG:O	3:A:191:LEU:HD23	1.98	0.64
3:A:325:ARG:C	3:A:357:LEU:HD12	2.23	0.64
3:B:654:ILE:HD11	3:B:691:PHE:CE1	2.33	0.64
3:A:107:GLN:HB2	3:A:131:MET:HB3	1.78	0.64
3:A:533:GLU:HA	3:A:564:LEU:HA	1.80	0.64
3:A:97:ILE:HB	3:A:98:LEU:HD22	1.79	0.64
3:B:483:GLN:O	3:B:508:LEU:HD12	1.98	0.64
3:A:55:VAL:HG13	3:A:79:ILE:HG13	1.78	0.63
3:B:45:ILE:HG23	3:B:45:ILE:O	1.96	0.63
3:B:143:PHE:C	3:B:145:ASN:H	2.06	0.63
3:A:484:ARG:HG2	3:A:510:ILE:HB	1.79	0.63
3:B:33:ASN:N	3:B:33:ASN:ND2	2.37	0.63
3:A:150:ILE:O	3:A:173:LEU:HD12	1.99	0.63
3:A:511:LEU:CD2	3:A:513:LEU:HG	2.28	0.63
4:H:1:NAG:H83	4:H:1:NAG:O3	1.97	0.63
3:B:102:LYS:O	3:B:125:LEU:HD12	1.98	0.63
1:C:27:G:H4'	3:A:519:ALA:HB1	1.81	0.63
3:A:194:LEU:HB3	3:A:197:SER:HB2	1.78	0.63
3:A:538:GLN:NE2	3:A:538:GLN:H	1.96	0.63
3:B:198:SER:OG	3:B:222:LYS:HB2	1.98	0.63
3:B:286:LEU:HD21	3:B:289:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:33:ASN:O	3:A:53:ILE:HB	1.99	0.63
3:B:53:ILE:O	3:B:76:GLN:HB3	1.98	0.63
3:B:541:ASN:OD1	3:B:541:ASN:O	2.15	0.63
3:A:42:LEU:H	3:A:61:ASN:HD22	1.47	0.63
3:A:59:THR:HG22	3:A:60:HIS:CD2	2.34	0.63
3:B:246:SER:O	3:B:248:THR:HG23	1.99	0.63
3:A:300:LEU:CD2	3:A:324:LEU:HD13	2.28	0.63
3:A:550:ASN:CB	3:A:551:PRO:CD	2.76	0.63
3:A:561:LEU:HD22	3:A:564:LEU:HD12	1.79	0.63
3:B:568:ASN:O	3:B:569:LEU:HD12	1.99	0.63
3:A:545:LEU:HD12	3:A:555:VAL:CG2	2.25	0.62
3:B:97:ILE:HB	3:B:98:LEU:HD22	1.81	0.62
3:A:231:ALA:HB3	3:A:233:LEU:HD11	1.79	0.62
3:B:443:ILE:H	3:B:466:ASN:HD22	1.45	0.62
3:B:500:SER:OG	3:B:525:LEU:HD12	1.98	0.62
3:B:696:CYS:O	3:B:697:LYS:HG2	1.99	0.62
3:A:577:ILE:HD11	3:A:601:LEU:CD1	2.29	0.62
3:A:607:ASP:H	3:A:609:GLN:HE22	1.46	0.62
3:B:138:ILE:HD12	3:B:159:LEU:HD11	1.79	0.62
3:A:640:LEU:HD21	3:A:642:MET:HE2	1.81	0.62
3:A:535:LEU:HD11	3:A:537:PHE:HE2	1.62	0.62
3:B:68:PRO:HB2	3:B:93:GLU:CB	2.27	0.62
3:A:44:HIS:O	3:A:46:PRO:HD3	1.98	0.62
3:A:589:LYS:O	3:A:612:LEU:HD12	1.99	0.62
3:B:50:PRO:O	3:B:53:ILE:HD12	2.00	0.62
3:B:37:CYS:HB3	3:B:40:LEU:HD22	1.80	0.62
3:A:116:ASP:HA	3:A:142:PRO:HA	1.81	0.62
3:A:262:ALA:CB	3:A:288:ASP:HB2	2.30	0.62
3:A:458:ILE:HD11	3:A:461:ILE:HG13	1.81	0.62
3:B:509:THR:O	3:B:532:LEU:HD22	1.99	0.62
3:B:607:ASP:H	3:B:609:GLN:HE22	1.48	0.62
3:A:533:GLU:HB2	3:A:534:ILE:HD12	1.82	0.61
3:B:577:ILE:HD11	3:B:601:LEU:CD1	2.29	0.61
1:C:39:G:H2'	1:C:40:C:C6	2.33	0.61
3:A:32:TYR:HD1	3:A:32:TYR:H	1.46	0.61
3:B:194:LEU:HB3	3:B:197:SER:HB2	1.82	0.61
3:B:300:LEU:HD22	3:B:321:LEU:HD22	1.81	0.61
3:B:242:CYS:HA	3:B:245:LEU:HD12	1.81	0.61
3:A:325:ARG:HA	3:A:357:LEU:HA	1.81	0.61
3:A:612:LEU:HD21	3:A:615:LEU:HD13	1.83	0.61
3:B:262:ALA:HB1	3:B:288:ASP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:570:GLU:HB2	3:B:592:ASN:ND2	2.15	0.61
3:A:114:ILE:HG12	3:A:118:THR:HG21	1.83	0.61
3:A:564:LEU:C	3:A:564:LEU:HD23	2.26	0.61
3:B:314:SER:HB2	3:B:315:PRO:HD2	1.82	0.61
3:B:37:CYS:HB3	3:B:40:LEU:CD2	2.30	0.61
3:A:511:LEU:HD23	3:A:511:LEU:C	2.25	0.61
3:A:521:ILE:HG13	3:A:525:LEU:HD22	1.82	0.61
3:B:484:ARG:HG2	3:B:510:ILE:HB	1.83	0.61
3:B:536:ASP:HB3	3:B:538:GLN:NE2	2.06	0.61
3:B:522:ASN:C	3:B:522:ASN:HD22	2.08	0.61
3:B:535:LEU:HD11	3:B:537:PHE:CE2	2.35	0.61
3:B:675:TYR:O	3:B:688:LEU:HB2	2.01	0.61
3:A:212:PHE:H	3:A:240:LYS:NZ	1.99	0.61
3:B:468:TYR:OH	3:B:493:LYS:HD3	2.01	0.61
3:B:561:LEU:HD22	3:B:564:LEU:HD12	1.82	0.61
3:B:153:ASP:HA	3:B:177:LEU:HB2	1.83	0.60
3:A:313:LEU:HD12	3:A:346:ILE:HG21	1.83	0.60
3:B:215:GLY:HA2	3:B:218:GLN:CG	2.30	0.60
3:A:242:CYS:HA	3:A:245:LEU:HD12	1.83	0.60
3:B:521:ILE:HG13	3:B:525:LEU:HD22	1.83	0.60
3:A:140:SER:C	3:A:142:PRO:HD3	2.27	0.60
3:B:107:GLN:HB2	3:B:131:MET:HB3	1.83	0.60
3:B:279:LEU:CB	3:B:300:LEU:HD11	2.31	0.60
3:A:63:LEU:HB3	3:A:87:ILE:HD11	1.84	0.60
3:A:250:ILE:HD13	3:A:250:ILE:C	2.26	0.60
3:B:212:PHE:H	3:B:240:LYS:NZ	1.99	0.60
3:B:538:GLN:NE2	3:B:538:GLN:H	2.00	0.60
3:B:630:PHE:HB3	3:B:634:PHE:CE1	2.37	0.60
3:A:494:ASN:O	3:A:497:ILE:HD12	2.00	0.60
3:B:334:THR:O	3:B:344:PRO:HG3	2.00	0.60
3:A:675:TYR:O	3:A:688:LEU:HB2	2.02	0.60
3:B:535:LEU:HD11	3:B:537:PHE:HE2	1.67	0.60
2:D:23:C:OP1	3:A:539:HIS:HB3	2.01	0.60
3:A:68:PRO:HB2	3:A:93:GLU:CB	2.30	0.60
3:A:102:LYS:O	3:A:125:LEU:HD12	2.02	0.60
3:A:458:ILE:HD13	3:A:459:PHE:N	2.16	0.60
3:B:511:LEU:HD23	3:B:512:ASP:N	2.15	0.60
3:B:36:ASP:HA	3:B:57:ASN:HB3	1.83	0.60
3:B:65:ARG:O	3:B:67:PRO:HD3	2.02	0.60
3:B:64:ARG:HG2	3:B:65:ARG:HD2	1.83	0.60
3:A:42:LEU:HD11	3:A:46:PRO:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:365:ASN:HB3	3:A:367:ILE:HD12	1.83	0.59
3:B:329:LEU:HD13	3:B:333:PHE:CZ	2.37	0.59
3:B:577:ILE:HD12	3:B:577:ILE:O	2.02	0.59
3:B:61:ASN:O	3:B:85:ASN:OD1	2.21	0.59
3:B:430:LEU:HD23	3:B:433:LEU:HD22	1.83	0.59
3:A:321:LEU:HD13	3:A:324:LEU:HD22	1.85	0.59
3:B:468:TYR:CE1	3:B:470:GLN:HB2	2.21	0.59
3:B:511:LEU:HD21	3:B:513:LEU:HG	1.83	0.59
3:B:640:LEU:HG	3:B:641:ASP:N	2.17	0.59
3:B:63:LEU:O	3:B:86:SER:O	2.19	0.59
1:C:16:U:H4'	7:I:5:MAN:O2	2.02	0.59
3:A:334:THR:C	3:A:335:LYS:HD3	2.27	0.59
3:A:520:ASN:HB3	3:A:544:ARG:HH12	1.66	0.59
3:B:49:LEU:O	3:B:51:SER:N	2.34	0.59
3:B:252:ASN:ND2	4:L:1:NAG:H61	2.18	0.59
3:B:597:ASN:HA	3:B:621:LEU:HD13	1.85	0.59
1:C:12:U:H2'	1:C:13:A:C8	2.38	0.59
3:A:103:VAL:HG22	3:A:127:GLU:HB3	1.83	0.59
3:A:396:LEU:HD12	3:A:422:ILE:HD12	1.84	0.59
3:B:334:THR:CG2	3:B:344:PRO:HB3	2.32	0.59
3:B:486:MET:C	3:B:487:LEU:HD22	2.28	0.59
3:B:178:LEU:O	3:B:204:LEU:HA	2.02	0.59
3:B:107:GLN:HA	3:B:131:MET:H	1.67	0.58
3:A:63:LEU:O	3:A:86:SER:O	2.20	0.58
3:A:488:ARG:O	3:A:490:VAL:HG13	2.04	0.58
3:A:599:ASN:OD1	3:A:600:LYS:HG3	2.04	0.58
3:A:314:SER:HB2	3:A:315:PRO:HD2	1.85	0.58
3:A:520:ASN:HB3	3:A:544:ARG:NH1	2.19	0.58
3:A:393:LEU:O	3:A:393:LEU:HD23	2.03	0.58
3:A:45:ILE:O	3:A:45:ILE:HG23	2.03	0.58
3:A:215:GLY:HA2	3:A:218:GLN:CG	2.33	0.58
3:A:509:THR:O	3:A:532:LEU:HD22	2.03	0.58
3:A:640:LEU:HG	3:A:641:ASP:N	2.17	0.58
3:A:53:ILE:O	3:A:76:GLN:HB3	2.03	0.58
3:B:152:LEU:O	3:B:152:LEU:HD13	2.03	0.58
3:A:71:PHE:HE2	3:A:94:LEU:HD23	1.69	0.58
3:A:79:ILE:HB	3:A:103:VAL:HB	1.84	0.58
3:A:153:ASP:HA	3:A:177:LEU:HB2	1.85	0.58
3:B:34:VAL:HG12	3:B:55:VAL:HB	1.86	0.58
3:B:336:GLN:HG3	3:B:343:HIS:HB3	1.86	0.58
3:B:488:ARG:O	3:B:490:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:56:LEU:HD11	3:A:58:LEU:CG	2.25	0.58
3:A:315:PRO:HA	3:A:350:SER:HA	1.85	0.58
4:H:2:NDG:H2	4:H:2:NDG:H6C2	1.85	0.58
3:A:71:PHE:O	3:A:97:ILE:HG22	2.04	0.58
3:A:79:ILE:CG2	3:A:103:VAL:HB	2.34	0.58
3:A:396:LEU:CB	3:A:422:ILE:HD12	2.32	0.58
3:B:313:LEU:HD12	3:B:346:ILE:CG2	2.34	0.58
3:A:300:LEU:HD22	3:A:321:LEU:HD22	1.86	0.57
3:A:521:ILE:HD13	3:A:522:ASN:O	2.04	0.57
3:A:598:LEU:HB2	3:A:620:ASN:ND2	2.18	0.57
3:B:511:LEU:CD2	3:B:513:LEU:HG	2.34	0.57
3:A:306:GLU:HG2	3:A:330:LYS:HB3	1.86	0.57
3:A:451:GLU:CD	3:A:451:GLU:H	2.10	0.57
3:A:640:LEU:HD21	3:A:642:MET:CE	2.34	0.57
3:B:459:PHE:CE1	3:B:483:GLN:HG3	2.39	0.57
3:A:297:LEU:HD13	3:A:300:LEU:HD13	1.87	0.57
3:B:33:ASN:C	3:B:53:ILE:HB	2.29	0.57
3:B:315:PRO:HA	3:B:350:SER:HA	1.84	0.57
1:C:21:A:C1'	3:B:541:ASN:HB2	2.34	0.57
3:A:534:ILE:HG23	3:A:566:ILE:HG23	1.86	0.57
3:B:212:PHE:H	3:B:240:LYS:HZ1	1.52	0.57
3:B:577:ILE:CD1	3:B:605:ILE:HG21	2.33	0.57
3:A:481:SER:HA	9:K:1:NAG:C8	2.34	0.57
3:B:329:LEU:HD13	3:B:333:PHE:HZ	1.70	0.57
3:B:566:ILE:C	3:B:566:ILE:HD13	2.29	0.57
3:A:80:LEU:HD23	3:A:80:LEU:H	1.69	0.57
3:A:107:GLN:HA	3:A:131:MET:H	1.69	0.57
3:B:520:ASN:HB3	3:B:544:ARG:NH1	2.20	0.57
3:A:306:GLU:HB3	3:A:307:TYR:HD1	1.70	0.57
3:B:79:ILE:HB	3:B:103:VAL:HB	1.85	0.57
3:B:114:ILE:HD11	3:B:118:THR:CB	2.35	0.57
3:B:520:ASN:HB3	3:B:544:ARG:HH12	1.69	0.57
3:B:654:ILE:HD13	3:B:654:ILE:C	2.28	0.57
3:B:108:HIS:H	3:B:132:SER:H	1.52	0.57
3:B:482:LEU:HB2	3:B:505:LEU:CD2	2.33	0.57
3:B:511:LEU:HD23	3:B:511:LEU:C	2.29	0.57
1:C:24:G:N2	2:D:24:C:C2	2.73	0.57
3:A:65:ARG:O	3:A:67:PRO:HD3	2.05	0.57
3:A:483:GLN:O	3:A:508:LEU:HD12	2.04	0.57
3:B:343:HIS:O	3:B:343:HIS:ND1	2.38	0.57
3:B:422:ILE:H	3:B:445:GLN:NE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:563:HIS:HA	3:B:587:GLU:OE2	2.05	0.57
3:B:640:LEU:HD21	3:B:642:MET:HE2	1.87	0.57
3:A:109:ASN:O	3:A:132:SER:O	2.23	0.56
3:A:522:ASN:C	3:A:522:ASN:HD22	2.12	0.56
3:A:545:LEU:O	3:A:546:TRP:HD1	1.87	0.56
3:B:101:LEU:HD22	3:B:125:LEU:HD13	1.85	0.56
3:B:109:ASN:O	3:B:132:SER:O	2.23	0.56
3:A:108:HIS:H	3:A:132:SER:H	1.51	0.56
1:C:1:A:N6	2:D:45:A:N6	2.52	0.56
3:A:597:ASN:HA	3:A:621:LEU:HD13	1.87	0.56
3:B:103:VAL:HG22	3:B:127:GLU:HB3	1.85	0.56
3:B:109:ASN:O	3:B:133:ASN:HA	2.06	0.56
3:B:126:THR:HA	3:B:149:LEU:HA	1.86	0.56
3:A:388:LYS:HA	3:A:416:LYS:O	2.06	0.56
3:B:388:LYS:HA	3:B:416:LYS:O	2.05	0.56
3:A:421:LYS:HG2	3:A:445:GLN:NE2	2.21	0.56
3:B:365:ASN:HB3	3:B:367:ILE:HD12	1.86	0.56
3:A:168:VAL:HG13	3:A:195:GLY:N	2.20	0.56
3:A:485:LEU:HG	3:A:487:LEU:CD2	2.36	0.56
3:A:178:LEU:O	3:A:204:LEU:HA	2.06	0.56
3:B:233:LEU:HD13	3:B:258:ASN:OD1	2.04	0.56
3:B:306:GLU:HG2	3:B:330:LYS:HB3	1.87	0.56
3:B:570:GLU:HB2	3:B:592:ASN:HD21	1.70	0.56
3:A:126:THR:HA	3:A:148:ASN:O	2.06	0.56
3:A:443:ILE:H	3:A:466:ASN:HD22	1.53	0.56
3:A:500:SER:OG	3:A:525:LEU:HD12	2.06	0.56
3:B:451:GLU:CD	3:B:451:GLU:H	2.13	0.56
3:B:521:ILE:HD13	3:B:522:ASN:O	2.05	0.56
3:B:588:LEU:C	3:B:588:LEU:HD23	2.31	0.56
3:A:577:ILE:HD12	3:A:577:ILE:O	2.06	0.55
3:A:630:PHE:HB3	3:A:634:PHE:CE1	2.40	0.55
3:A:63:LEU:HB3	3:A:87:ILE:CD1	2.36	0.55
3:B:321:LEU:HD13	3:B:324:LEU:HD22	1.88	0.55
3:A:37:CYS:HB3	3:A:40:LEU:HD11	1.87	0.55
3:A:335:LYS:HZ2	3:A:335:LYS:N	2.04	0.55
3:B:79:ILE:CG2	3:B:103:VAL:HB	2.36	0.55
3:B:589:LYS:O	3:B:612:LEU:HD12	2.06	0.55
3:A:143:PHE:C	3:A:145:ASN:N	2.64	0.55
3:A:540:ASN:O	3:A:541:ASN:C	2.50	0.55
3:A:550:ASN:HB3	3:A:551:PRO:CD	2.35	0.55
3:A:643:ARG:O	3:A:644:PHE:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:393:LEU:HD23	3:B:393:LEU:O	2.06	0.55
3:A:497:ILE:HD11	3:A:501:PRO:HD3	1.88	0.55
3:A:603:PRO:O	3:A:604:PHE:HB2	2.05	0.55
3:B:252:ASN:HD22	4:L:1:NAG:C6	2.19	0.55
3:B:577:ILE:HD11	3:B:601:LEU:HD12	1.86	0.55
3:B:276:LEU:O	3:B:300:LEU:HA	2.06	0.55
3:B:484:ARG:HG3	3:B:484:ARG:HH11	1.70	0.55
3:A:424:ASN:CG	8:J:1:NAG:N2	2.65	0.55
3:A:593:LEU:HB2	3:A:617:LEU:HD23	1.89	0.55
3:B:32:TYR:CD1	3:B:32:TYR:N	2.73	0.55
3:A:64:ARG:HG2	3:A:65:ARG:HD2	1.89	0.55
3:A:141:ASN:CB	3:A:169:GLN:HE22	2.16	0.55
3:A:696:CYS:O	3:A:697:LYS:HB3	2.07	0.55
3:B:275:ASN:ND2	10:M:1:NAG:C6	2.69	0.55
3:A:126:THR:HA	3:A:149:LEU:HA	1.89	0.54
3:B:114:ILE:HG12	3:B:118:THR:HG21	1.88	0.54
3:A:101:LEU:HD22	3:A:125:LEU:HD13	1.88	0.54
3:A:109:ASN:O	3:A:133:ASN:HA	2.06	0.54
3:A:313:LEU:HD13	3:A:318:PHE:HE1	1.72	0.54
3:B:359:TYR:C	3:B:359:TYR:CD2	2.85	0.54
3:A:180:LYS:H	3:A:206:SER:HB2	1.72	0.54
3:A:538:GLN:HG3	3:A:568:ASN:OD1	2.07	0.54
3:B:131:MET:O	3:B:155:SER:O	2.24	0.54
3:B:239:GLU:HA	3:B:267:THR:O	2.07	0.54
3:A:233:LEU:HD13	3:A:258:ASN:OD1	2.07	0.54
3:B:564:LEU:C	3:B:564:LEU:HD23	2.33	0.54
3:B:33:ASN:O	3:B:55:VAL:N	2.39	0.54
6:G:1:NAG:H5	6:G:3:FUC:O5	2.06	0.54
1:C:43:C:H2'	1:C:44:A:C8	2.43	0.54
3:A:187:ARG:HD3	3:A:189:GLU:OE1	2.07	0.54
3:A:462:TYR:HD1	3:A:486:MET:HG3	1.72	0.54
3:B:603:PRO:O	3:B:604:PHE:HB2	2.06	0.54
3:A:198:SER:OG	3:A:222:LYS:HB2	2.07	0.54
3:A:484:ARG:HG3	3:A:484:ARG:HH11	1.73	0.54
3:B:168:VAL:HG13	3:B:195:GLY:N	2.22	0.54
3:A:36:ASP:HA	3:A:57:ASN:HB3	1.90	0.54
3:B:140:SER:C	3:B:142:PRO:HD3	2.33	0.54
3:A:449:GLY:HA2	3:A:475:SER:O	2.08	0.54
3:A:486:MET:C	3:A:487:LEU:HD22	2.33	0.54
3:A:689:LYS:HG3	3:A:690:LEU:N	2.23	0.53
3:B:198:SER:HG	3:B:222:LYS:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:641:ASP:OD2	3:B:643:ARG:HG2	2.08	0.53
3:A:262:ALA:HB1	3:A:288:ASP:HB2	1.90	0.53
3:B:82:ALA:O	3:B:105:ASN:O	2.26	0.53
3:A:550:ASN:O	3:A:551:PRO:C	2.49	0.53
3:B:126:THR:HA	3:B:148:ASN:O	2.07	0.53
3:B:443:ILE:N	3:B:466:ASN:HD22	2.06	0.53
3:A:80:LEU:HD21	3:A:104:LEU:HA	1.89	0.53
3:A:163:LYS:HB2	3:A:190:GLU:HB2	1.89	0.53
3:A:577:ILE:HD11	3:A:601:LEU:HD13	1.89	0.53
3:A:276:LEU:O	3:A:300:LEU:HA	2.08	0.53
3:A:609:GLN:NE2	3:A:609:GLN:N	2.54	0.53
3:B:68:PRO:HB3	3:B:94:LEU:CD1	2.38	0.53
3:B:212:PHE:CD2	3:B:241:LEU:HB2	2.43	0.53
3:B:295:SER:HA	3:B:320:GLY:CA	2.38	0.53
3:B:435:ILE:HG13	3:B:460:GLU:HG2	1.91	0.53
1:C:16:U:H2'	1:C:17:G:H8	1.72	0.53
3:A:180:LYS:HA	3:A:206:SER:CB	2.38	0.53
3:A:291:ASN:OD1	3:A:316:ARG:HB3	2.09	0.53
3:A:615:LEU:HB3	3:A:640:LEU:HD12	1.90	0.53
3:B:80:LEU:H	3:B:80:LEU:HD23	1.74	0.53
3:A:279:LEU:CB	3:A:300:LEU:HD11	2.37	0.53
3:B:59:THR:HG22	3:B:60:HIS:CD2	2.43	0.53
3:B:212:PHE:CE2	3:B:241:LEU:HB2	2.44	0.53
3:B:370:THR:OG1	3:B:400:THR:HG23	2.08	0.53
3:B:464:SER:O	3:B:465:TYR:HB2	2.08	0.53
3:B:612:LEU:HD21	3:B:615:LEU:HD13	1.90	0.53
3:A:151:LYS:HG2	3:A:175:GLU:OE1	2.08	0.53
3:A:297:LEU:C	3:A:299:SER:H	2.16	0.53
3:A:410:LEU:HD12	3:A:410:LEU:N	2.24	0.53
3:B:56:LEU:HD11	3:B:58:LEU:CG	2.32	0.53
3:B:163:LYS:HB2	3:B:190:GLU:HB2	1.91	0.53
3:A:436:LEU:HD21	3:A:438:LEU:HG	1.92	0.52
3:A:534:ILE:HG13	3:A:566:ILE:CG2	2.38	0.52
3:B:180:LYS:H	3:B:206:SER:HB2	1.74	0.52
3:B:485:LEU:HG	3:B:487:LEU:CD2	2.39	0.52
3:B:689:LYS:HG3	3:B:690:LEU:N	2.25	0.52
3:B:331:ARG:NH2	3:B:335:LYS:HE2	2.24	0.52
3:A:80:LEU:HD23	3:A:80:LEU:N	2.25	0.52
3:A:114:ILE:CG1	3:A:118:THR:HG21	2.39	0.52
3:A:359:TYR:C	3:A:359:TYR:CD2	2.88	0.52
3:B:73:ARG:HG3	3:B:73:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:205:SER:OG	3:B:229:ASN:HB2	2.09	0.52
3:B:421:LYS:HG2	3:B:445:GLN:NE2	2.24	0.52
3:B:449:GLY:H	3:B:475:SER:HA	1.75	0.52
3:B:643:ARG:O	3:B:644:PHE:HB2	2.08	0.52
3:A:534:ILE:HG13	3:A:566:ILE:HG22	1.92	0.52
3:A:61:ASN:O	3:A:85:ASN:OD1	2.28	0.52
3:A:234:ASN:CB	3:A:237:LEU:HD13	2.37	0.52
3:A:275:ASN:ND2	5:F:1:NAG:H61	2.24	0.52
3:B:40:LEU:HB2	3:B:61:ASN:ND2	2.19	0.52
7:I:1:NAG:C6	7:I:2:NAG:HN2	2.23	0.52
3:A:555:VAL:O	3:A:557:PHE:N	2.41	0.52
3:A:602:GLU:O	3:A:605:ILE:HG23	2.09	0.52
3:B:35:ALA:O	3:B:56:LEU:HA	2.10	0.52
3:A:582:PHE:HB3	3:A:609:GLN:OE1	2.10	0.52
3:B:534:ILE:HD12	3:B:534:ILE:N	2.25	0.52
1:C:22:A:H5"	3:B:539:HIS:HB3	1.92	0.52
3:A:422:ILE:H	3:A:445:GLN:NE2	2.07	0.52
3:A:458:ILE:CD1	3:A:461:ILE:HG13	2.39	0.52
3:B:502:PHE:CD2	3:B:525:LEU:HD11	2.45	0.52
3:B:71:PHE:O	3:B:97:ILE:HG22	2.10	0.51
3:A:40:LEU:N	3:A:40:LEU:CD1	2.72	0.51
3:B:39:HIS:HA	3:B:60:HIS:O	2.10	0.51
3:B:151:LYS:HG2	3:B:175:GLU:OE1	2.10	0.51
3:A:525:LEU:O	3:A:526:LEU:HB2	2.08	0.51
3:B:80:LEU:HD21	3:B:104:LEU:CD1	2.36	0.51
3:B:180:LYS:HA	3:B:206:SER:CB	2.40	0.51
3:B:241:LEU:HD12	3:B:241:LEU:O	2.10	0.51
3:B:336:GLN:N	3:B:366:ASN:OD1	2.43	0.51
3:B:477:ALA:HA	3:B:504:PRO:HG3	1.92	0.51
3:B:521:ILE:HD12	3:B:557:PHE:CE1	2.45	0.51
3:A:150:ILE:HD12	3:A:174:GLN:HE21	1.75	0.51
3:A:180:LYS:CA	3:A:206:SER:HB2	2.39	0.51
3:A:398:ASN:ND2	4:H:1:NAG:C6	2.71	0.51
3:B:180:LYS:CA	3:B:206:SER:HB2	2.39	0.51
3:B:534:ILE:HG13	3:B:566:ILE:CG2	2.40	0.51
3:B:337:SER:OG	3:B:342:SER:HB2	2.10	0.51
3:B:436:LEU:HD21	3:B:438:LEU:HG	1.92	0.51
3:B:654:ILE:HD12	3:B:654:ILE:H	1.76	0.51
3:A:32:TYR:O	3:A:33:ASN:HB3	2.10	0.51
3:A:53:ILE:HG12	3:A:77:LEU:HD23	1.92	0.51
3:B:92:PRO:HB3	3:B:117:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:105:ASN:HA	3:A:129:ASP:HB3	1.92	0.51
3:A:286:LEU:HD21	3:A:289:VAL:HG22	1.93	0.51
3:A:570:GLU:HB2	3:A:592:ASN:ND2	2.25	0.51
3:B:138:ILE:CD1	3:B:159:LEU:HD11	2.41	0.51
1:C:3:U:H2'	1:C:4:C:H6	1.76	0.51
1:C:16:U:H2'	1:C:17:G:C8	2.46	0.51
3:A:410:LEU:N	3:A:410:LEU:CD1	2.74	0.51
3:A:577:ILE:HD11	3:A:601:LEU:HD12	1.92	0.51
3:A:250:ILE:HD12	3:A:276:LEU:HD21	1.93	0.51
3:B:449:GLY:HA2	3:B:475:SER:O	2.11	0.51
3:B:526:LEU:HA	3:B:529:LEU:CD1	2.40	0.51
3:B:126:THR:HG22	3:B:148:ASN:HB3	1.92	0.50
3:B:409:LEU:C	3:B:410:LEU:HD12	2.37	0.50
3:A:275:ASN:ND2	5:F:1:NAG:C6	2.73	0.50
3:A:421:LYS:O	3:A:422:ILE:HD13	2.10	0.50
3:A:534:ILE:HD12	3:A:534:ILE:N	2.26	0.50
3:B:35:ALA:N	3:B:55:VAL:O	2.38	0.50
3:B:450:GLN:HG3	8:Q:1:NAG:C6	2.21	0.50
3:B:489:ARG:HA	3:B:515:ASN:O	2.11	0.50
3:B:671:LEU:HA	3:B:675:TYR:CD1	2.46	0.50
3:A:601:LEU:N	3:A:601:LEU:HD22	2.26	0.50
3:A:641:ASP:OD2	3:A:643:ARG:HG2	2.11	0.50
3:B:297:LEU:C	3:B:299:SER:H	2.18	0.50
3:A:489:ARG:HA	3:A:515:ASN:O	2.11	0.50
3:A:558:LEU:CA	3:A:561:LEU:HD11	2.41	0.50
3:B:540:ASN:O	3:B:541:ASN:C	2.54	0.50
1:C:16:U:H4'	7:I:5:MAN:O3	2.12	0.50
3:A:111:LEU:O	3:A:135:ILE:HG12	2.12	0.50
3:A:295:SER:HA	3:A:320:GLY:CA	2.41	0.50
3:A:331:ARG:HA	3:A:364:ASP:O	2.10	0.50
3:B:147:LYS:NZ	3:B:171:GLU:HG2	2.26	0.50
3:B:266:SER:HA	3:B:269:SER:HB3	1.93	0.50
3:B:366:ASN:O	3:B:367:ILE:C	2.53	0.50
3:B:521:ILE:HG21	3:B:557:PHE:HE1	1.76	0.50
2:D:7:G:H2'	2:D:8:C:H6	1.77	0.50
3:B:33:ASN:CB	3:B:53:ILE:HA	2.41	0.50
3:B:651:CYS:HB3	3:B:655:SER:HG	1.74	0.50
3:A:30:VAL:HG12	3:A:30:VAL:O	2.12	0.50
3:A:301:ARG:C	3:A:324:LEU:HD12	2.37	0.50
3:A:177:LEU:HD12	3:A:177:LEU:N	2.26	0.50
3:A:231:ALA:HB3	3:A:233:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:266:SER:HA	3:A:269:SER:HB3	1.93	0.50
3:A:393:LEU:HD21	3:A:396:LEU:CD2	2.38	0.50
3:A:468:TYR:CE1	3:A:470:GLN:HB2	2.26	0.50
3:A:568:ASN:C	3:A:569:LEU:HD12	2.36	0.50
3:B:306:GLU:HB3	3:B:307:TYR:HD1	1.74	0.50
3:B:510:ILE:HG12	3:B:534:ILE:HD13	1.93	0.50
3:A:92:PRO:HB3	3:A:117:GLN:O	2.12	0.50
3:A:131:MET:O	3:A:155:SER:O	2.28	0.50
3:A:558:LEU:C	3:A:561:LEU:HD11	2.36	0.50
3:B:87:ILE:HD12	3:B:109:ASN:ND2	2.26	0.50
3:B:111:LEU:O	3:B:135:ILE:HG12	2.11	0.50
3:B:239:GLU:HG3	3:B:266:SER:O	2.12	0.50
3:B:615:LEU:HB3	3:B:640:LEU:HD12	1.93	0.50
3:A:563:HIS:HA	3:A:587:GLU:OE2	2.12	0.49
3:B:599:ASN:OD1	3:B:600:LYS:HG3	2.12	0.49
3:A:152:LEU:HD13	3:A:152:LEU:O	2.12	0.49
3:A:526:LEU:HD23	3:A:529:LEU:CD1	2.39	0.49
3:B:300:LEU:CD2	3:B:324:LEU:HD13	2.37	0.49
3:B:324:LEU:HD21	3:B:327:LEU:HD13	1.93	0.49
3:B:557:PHE:CD2	3:B:558:LEU:HG	2.45	0.49
3:B:500:SER:CB	3:B:525:LEU:HA	2.37	0.49
13:B:724:NAG:O3	13:B:724:NAG:H83	2.11	0.49
3:A:147:LYS:NZ	3:A:171:GLU:HG2	2.27	0.49
3:A:437:ASP:OD2	3:A:462:TYR:HD2	1.94	0.49
3:B:231:ALA:HB3	3:B:233:LEU:CD1	2.43	0.49
3:B:258:ASN:HB2	3:B:284:ASN:OD1	2.12	0.49
3:B:269:SER:HA	3:B:296:TYR:CE1	2.47	0.49
1:C:8:G:H2'	1:C:9:G:H8	1.77	0.49
3:A:47:ASP:OD1	3:A:47:ASP:O	2.31	0.49
3:A:417:ASN:O	3:A:418:HIS:HB2	2.11	0.49
3:A:477:ALA:HA	3:A:504:PRO:HG3	1.94	0.49
3:B:138:ILE:HD13	3:B:164:LEU:CD2	2.42	0.49
3:B:177:LEU:N	3:B:177:LEU:HD12	2.28	0.49
3:B:234:ASN:ND2	3:B:236:HIS:H	2.09	0.49
3:B:484:ARG:HG3	3:B:484:ARG:NH1	2.26	0.49
3:B:532:LEU:HD11	3:B:535:LEU:HB2	1.94	0.49
1:C:7:C:OP1	3:A:39:HIS:HB3	2.12	0.49
3:B:114:ILE:HD11	3:B:118:THR:OG1	2.12	0.49
3:B:187:ARG:HA	3:B:213:SER:HB3	1.95	0.49
3:A:66:LEU:O	3:A:68:PRO:HD3	2.13	0.49
3:A:67:PRO:HB2	3:A:70:ASN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:532:LEU:C	3:A:532:LEU:HD13	2.37	0.49
3:B:45:ILE:O	3:B:45:ILE:CG2	2.61	0.49
3:B:412:LEU:HD22	3:B:430:LEU:HD21	1.93	0.49
3:B:141:ASN:CB	3:B:169:GLN:HE22	2.20	0.49
3:B:577:ILE:HD11	3:B:601:LEU:HD13	1.95	0.49
4:O:1:NAG:H3	4:O:2:NDG:O5	2.12	0.49
3:A:56:LEU:HD13	3:A:56:LEU:C	2.38	0.49
3:A:94:LEU:O	3:A:98:LEU:HD23	2.12	0.49
3:A:189:GLU:O	3:A:192:GLU:HG2	2.13	0.49
3:A:409:LEU:C	3:A:410:LEU:HD12	2.38	0.49
3:B:53:ILE:HG12	3:B:77:LEU:HD23	1.94	0.49
3:B:80:LEU:HD21	3:B:104:LEU:HA	1.95	0.49
3:B:252:ASN:ND2	4:L:1:NAG:C6	2.76	0.49
3:B:526:LEU:HA	3:B:529:LEU:HD11	1.94	0.49
3:B:331:ARG:HA	3:B:364:ASP:O	2.11	0.49
3:B:383:TYR:HD2	3:B:411:THR:OG1	1.96	0.49
3:A:443:ILE:N	3:A:466:ASN:HD22	2.11	0.48
3:A:464:SER:O	3:A:465:TYR:HB2	2.12	0.48
3:A:484:ARG:HG3	3:A:484:ARG:NH1	2.28	0.48
3:A:537:PHE:CZ	3:A:557:PHE:HZ	2.31	0.48
3:B:251:GLN:O	3:B:276:LEU:HD13	2.12	0.48
3:B:437:ASP:OD2	3:B:462:TYR:HD2	1.96	0.48
3:B:526:LEU:HD23	3:B:529:LEU:CD1	2.41	0.48
3:B:649:CYS:HB2	3:B:683:TYR:HB3	1.94	0.48
3:A:334:THR:O	3:A:335:LYS:HD3	2.13	0.48
3:B:77:LEU:O	3:B:100:LEU:O	2.31	0.48
3:B:243:TRP:CD1	3:B:270:GLY:CA	2.96	0.48
3:A:77:LEU:O	3:A:100:LEU:O	2.32	0.48
3:A:613:ARG:C	3:A:637:LEU:HD12	2.38	0.48
3:B:114:ILE:CD1	3:B:118:THR:HG21	2.42	0.48
1:C:43:C:H2'	1:C:44:A:H8	1.79	0.48
3:A:37:CYS:HB3	3:A:40:LEU:CD2	2.40	0.48
3:B:187:ARG:HG3	3:B:187:ARG:HH11	1.78	0.48
3:A:226:LEU:HD12	3:A:227:LEU:H	1.78	0.48
3:A:239:GLU:HA	3:A:267:THR:O	2.13	0.48
3:B:179:ALA:HB1	3:B:205:SER:HB2	1.95	0.48
3:B:190:GLU:HG3	3:B:191:LEU:HD22	1.95	0.48
3:B:578:PRO:CG	3:B:581:VAL:HG11	2.40	0.48
2:D:5:G:H2'	2:D:6:C:O4'	2.12	0.48
3:A:53:ILE:HG12	3:A:77:LEU:CD2	2.44	0.48
3:A:79:ILE:CB	3:A:103:VAL:HB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:105:ASN:O	3:B:106:LEU:HD12	2.13	0.48
1:C:31:U:H2'	1:C:32:G:C8	2.48	0.48
3:A:150:ILE:HD12	3:A:174:GLN:NE2	2.28	0.48
3:A:588:LEU:C	3:A:588:LEU:HD23	2.38	0.48
3:B:169:GLN:HG3	3:B:170:LEU:CD2	2.43	0.48
3:B:301:ARG:C	3:B:324:LEU:HD12	2.39	0.48
3:B:390:PHE:CD2	3:B:393:LEU:HD13	2.49	0.48
3:B:602:GLU:O	3:B:603:PRO:C	2.55	0.48
4:E:1:NAG:H61	4:E:1:NAG:C2	2.42	0.48
3:A:39:HIS:C	3:A:40:LEU:HD12	2.39	0.48
3:A:73:ARG:HG3	3:A:73:ARG:HH11	1.78	0.48
3:B:53:ILE:HG12	3:B:77:LEU:CD2	2.44	0.48
3:B:68:PRO:HB3	3:B:94:LEU:HD12	1.96	0.48
3:B:331:ARG:HH22	3:B:335:LYS:CE	2.26	0.48
3:B:31:ARG:HA	3:B:31:ARG:HD3	1.72	0.48
3:B:393:LEU:HD21	3:B:396:LEU:CD2	2.42	0.48
3:B:542:LEU:H	3:B:572:ASN:HD22	1.60	0.48
3:A:169:GLN:HG3	3:A:170:LEU:CD2	2.44	0.48
3:A:243:TRP:CD1	3:A:270:GLY:CA	2.95	0.48
3:A:366:ASN:O	3:A:367:ILE:C	2.56	0.48
3:B:550:ASN:N	3:B:551:PRO:CD	2.77	0.48
3:A:187:ARG:HA	3:A:213:SER:HB3	1.95	0.47
3:A:196:ASN:HD22	13:A:1961:NAG:H4	1.79	0.47
3:A:396:LEU:HB3	3:A:426:THR:HG21	1.96	0.47
3:A:459:PHE:CE1	3:A:483:GLN:HG3	2.48	0.47
2:D:13:G:O2'	2:D:14:U:H5'	2.13	0.47
3:A:250:ILE:HD13	3:A:251:GLN:N	2.29	0.47
3:A:306:GLU:HB3	3:A:307:TYR:CD1	2.47	0.47
3:A:447:LEU:HD23	3:A:451:GLU:HG3	1.96	0.47
3:A:479:VAL:HG23	3:A:479:VAL:O	2.15	0.47
3:A:510:ILE:HG12	3:A:534:ILE:HD13	1.96	0.47
3:A:530:GLU:HG3	3:A:530:GLU:O	2.13	0.47
3:B:558:LEU:C	3:B:561:LEU:HD11	2.39	0.47
3:B:558:LEU:CA	3:B:561:LEU:HD11	2.44	0.47
3:A:234:ASN:ND2	3:A:236:HIS:H	2.13	0.47
3:B:143:PHE:C	3:B:145:ASN:N	2.69	0.47
3:B:441:ASN:O	3:B:466:ASN:HA	2.14	0.47
3:B:534:ILE:HG23	3:B:566:ILE:HG23	1.96	0.47
3:B:613:ARG:C	3:B:637:LEU:HD12	2.40	0.47
2:D:6:C:N3	2:D:7:G:N7	2.61	0.47
3:A:217:PHE:HB2	3:A:244:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:SER:CB	3:A:525:LEU:HA	2.43	0.47
1:C:21:A:O4'	3:B:541:ASN:HB2	2.13	0.47
3:A:212:PHE:H	3:A:240:LYS:HZ1	1.61	0.47
3:A:446:LYS:HD3	3:A:470:GLN:NE2	2.29	0.47
3:A:570:GLU:HB2	3:A:592:ASN:HD21	1.80	0.47
3:B:593:LEU:HB2	3:B:617:LEU:CD2	2.45	0.47
3:A:59:THR:HG22	3:A:60:HIS:CG	2.50	0.47
3:A:133:ASN:O	3:A:134:SER:C	2.57	0.47
3:A:347:ASP:HA	3:A:371:LYS:NZ	2.29	0.47
3:B:459:PHE:CE2	3:B:484:ARG:NH1	2.83	0.47
3:A:68:PRO:HB3	3:A:94:LEU:CD1	2.45	0.47
3:A:126:THR:HG22	3:A:148:ASN:HB3	1.96	0.47
3:A:187:ARG:C	3:A:189:GLU:H	2.21	0.47
3:A:205:SER:OG	3:A:229:ASN:HB2	2.14	0.47
3:A:227:LEU:HD23	3:A:254:SER:HB3	1.97	0.47
3:A:561:LEU:HB2	3:A:564:LEU:HB2	1.97	0.47
3:B:80:LEU:HD23	3:B:80:LEU:N	2.30	0.47
3:B:485:LEU:HG	3:B:487:LEU:HD21	1.97	0.47
1:C:22:A:OP1	3:B:539:HIS:HB3	2.15	0.47
2:D:28:G:H4'	3:B:519:ALA:HB1	1.97	0.47
3:A:82:ALA:O	3:A:105:ASN:O	2.33	0.47
3:B:105:ASN:HA	3:B:129:ASP:HB3	1.96	0.47
3:B:187:ARG:C	3:B:189:GLU:H	2.22	0.47
3:A:42:LEU:HD23	3:A:43:THR:H	1.80	0.47
3:A:206:SER:HA	3:A:230:ASN:O	2.15	0.47
3:A:239:GLU:HG3	3:A:266:SER:O	2.15	0.47
3:A:324:LEU:HD21	3:A:327:LEU:HD13	1.96	0.47
3:B:226:LEU:HD12	3:B:227:LEU:H	1.79	0.47
3:B:417:ASN:O	3:B:418:HIS:HB2	2.14	0.47
3:A:180:LYS:N	3:A:206:SER:HB2	2.30	0.47
3:A:671:LEU:HA	3:A:675:TYR:CD1	2.50	0.47
3:B:654:ILE:CD1	3:B:655:SER:N	2.73	0.47
3:A:190:GLU:HG3	3:A:191:LEU:HD22	1.95	0.46
3:A:365:ASN:HB3	3:A:367:ILE:CD1	2.45	0.46
3:A:458:ILE:C	3:A:458:ILE:CD1	2.88	0.46
3:A:603:PRO:O	3:A:604:PHE:CB	2.63	0.46
3:B:67:PRO:HB2	3:B:70:ASN:HB2	1.97	0.46
3:B:92:PRO:HG2	3:B:117:GLN:HB3	1.97	0.46
3:B:357:LEU:O	3:B:380:SER:HB2	2.15	0.46
3:B:640:LEU:HD21	3:B:642:MET:CE	2.44	0.46
2:D:20:C:O2'	2:D:21:U:H5'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:53:ILE:HD11	3:A:74:TYR:CD2	2.50	0.46
3:A:412:LEU:HD22	3:A:430:LEU:HD21	1.97	0.46
3:A:458:ILE:HD12	3:A:482:LEU:HD21	1.98	0.46
3:B:217:PHE:HB2	3:B:244:GLU:O	2.16	0.46
8:J:1:NAG:O3	8:J:1:NAG:C7	2.62	0.46
3:A:67:PRO:HB3	13:A:724:NAG:H82	1.97	0.46
3:A:80:LEU:CD2	3:A:104:LEU:HA	2.45	0.46
3:A:92:PRO:HG2	3:A:117:GLN:HB3	1.97	0.46
3:A:275:ASN:HD21	5:F:1:NAG:H61	1.78	0.46
3:A:309:ASN:OD1	3:A:334:THR:HG23	2.15	0.46
3:A:557:PHE:CD2	3:A:558:LEU:HG	2.46	0.46
3:A:696:CYS:O	3:A:697:LYS:CB	2.63	0.46
3:B:79:ILE:CB	3:B:103:VAL:HB	2.45	0.46
3:B:313:LEU:CB	3:B:346:ILE:HG22	2.43	0.46
3:B:410:LEU:HD12	3:B:410:LEU:N	2.31	0.46
6:G:1:NAG:O3	6:G:1:NAG:H83	2.16	0.46
1:C:41:G:C2'	1:C:42:C:H5'	2.44	0.46
3:A:80:LEU:HD21	3:A:104:LEU:CD1	2.39	0.46
3:A:31:ARG:HE	3:A:31:ARG:CA	2.15	0.46
3:A:40:LEU:HD13	3:A:61:ASN:ND2	2.29	0.46
3:B:383:TYR:HD2	3:B:411:THR:HG1	1.63	0.46
1:C:3:U:H2'	1:C:4:C:C6	2.50	0.46
2:D:24:C:H2'	2:D:25:U:H6	1.81	0.46
3:A:179:ALA:HB1	3:A:205:SER:HB2	1.98	0.46
3:A:301:ARG:O	3:A:324:LEU:HD12	2.16	0.46
3:A:436:LEU:HD23	3:A:436:LEU:C	2.40	0.46
3:B:169:GLN:HG3	3:B:170:LEU:HD23	1.97	0.46
3:B:347:ASP:HA	3:B:371:LYS:NZ	2.31	0.46
3:B:409:LEU:O	3:B:433:LEU:HA	2.16	0.46
8:Q:1:NAG:O4	8:Q:2:NDG:H8C1	2.15	0.46
1:C:6:G:O2'	1:C:7:C:H5'	2.16	0.46
2:D:18:U:H2'	2:D:19:G:C8	2.51	0.46
3:A:105:ASN:O	3:A:106:LEU:HD12	2.16	0.46
3:A:382:LYS:HA	3:A:408:PRO:O	2.15	0.46
3:A:651:CYS:HA	3:A:655:SER:OG	2.15	0.46
3:B:133:ASN:O	3:B:134:SER:C	2.57	0.46
3:B:525:LEU:O	3:B:526:LEU:HB2	2.15	0.46
3:B:575:ASP:OD2	3:B:575:ASP:C	2.59	0.46
3:B:654:ILE:CD1	3:B:654:ILE:C	2.89	0.46
3:A:277:THR:HG21	4:E:1:NAG:C8	2.25	0.46
3:A:357:LEU:O	3:A:380:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:532:LEU:HD11	3:A:535:LEU:HB2	1.98	0.46
3:A:73:ARG:HG3	3:A:73:ARG:NH1	2.31	0.46
3:A:458:ILE:HD12	3:A:482:LEU:CD2	2.46	0.46
3:A:521:ILE:CD1	3:A:522:ASN:O	2.64	0.46
3:B:227:LEU:HD23	3:B:254:SER:HB3	1.97	0.46
2:D:31:A:O2'	2:D:32:A:H5'	2.15	0.45
3:A:37:CYS:C	3:A:40:LEU:HD11	2.41	0.45
3:B:154:LEU:O	3:B:178:LEU:HD23	2.16	0.45
3:B:180:LYS:N	3:B:206:SER:HB2	2.31	0.45
3:B:183:ILE:O	3:B:209:LEU:HD23	2.16	0.45
3:B:462:TYR:HD1	3:B:486:MET:HG3	1.81	0.45
3:B:534:ILE:HG13	3:B:566:ILE:HG22	1.97	0.45
3:B:73:ARG:HG3	3:B:73:ARG:NH1	2.31	0.45
3:B:277:THR:HG22	3:B:278:GLN:N	2.31	0.45
3:B:484:ARG:HG2	3:B:510:ILE:HD12	1.97	0.45
3:B:545:LEU:HD12	3:B:555:VAL:HG21	1.99	0.45
3:B:47:ASP:O	3:B:73:ARG:HD3	2.17	0.45
3:B:306:GLU:HB3	3:B:307:TYR:CD1	2.51	0.45
3:B:410:LEU:N	3:B:410:LEU:CD1	2.79	0.45
3:B:578:PRO:HG2	3:B:581:VAL:HG13	1.98	0.45
2:D:7:G:H2'	2:D:8:C:C6	2.51	0.45
3:A:114:ILE:HD11	3:A:118:THR:CB	2.40	0.45
3:A:183:ILE:O	3:A:209:LEU:HD23	2.17	0.45
3:A:577:ILE:CD1	3:A:605:ILE:HG21	2.35	0.45
3:A:614:SER:HA	3:A:637:LEU:HD11	1.98	0.45
3:B:49:LEU:HA	3:B:73:ARG:NH2	2.31	0.45
3:B:92:PRO:HG3	3:B:117:GLN:C	2.41	0.45
3:B:543:ALA:HB2	3:B:573:GLY:CA	2.42	0.45
3:B:561:LEU:HB2	3:B:564:LEU:HB2	1.97	0.45
2:D:22:U:H2'	2:D:23:C:C6	2.51	0.45
3:A:79:ILE:HG22	3:A:103:VAL:HB	1.99	0.45
3:A:201:LYS:NZ	3:A:227:LEU:HD11	2.32	0.45
3:A:263:THR:HG23	3:A:286:LEU:HD11	1.98	0.45
3:A:497:ILE:HD13	3:A:497:ILE:N	2.32	0.45
3:B:106:LEU:HD23	3:B:111:LEU:HD11	1.98	0.45
3:B:187:ARG:C	3:B:189:GLU:N	2.75	0.45
3:B:187:ARG:HD3	3:B:189:GLU:OE1	2.17	0.45
3:B:239:GLU:HG3	3:B:267:THR:HA	1.98	0.45
3:B:302:TYR:CE2	4:L:2:NDG:H8C3	2.52	0.45
3:B:352:GLN:HA	3:B:377:GLY:HA3	1.98	0.45
3:B:396:LEU:HB3	3:B:426:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:2:NDG:H4	8:Q:3:BMA:O2	2.16	0.45
3:A:34:VAL:HG12	3:A:55:VAL:CB	2.45	0.45
3:A:526:LEU:HA	3:A:529:LEU:HD11	1.97	0.45
3:B:530:GLU:O	3:B:530:GLU:HG3	2.16	0.45
3:A:37:CYS:CB	3:A:40:LEU:HD11	2.47	0.45
3:A:154:LEU:O	3:A:178:LEU:HD23	2.17	0.45
3:A:187:ARG:C	3:A:189:GLU:N	2.74	0.45
3:A:444:GLU:O	3:A:444:GLU:HG2	2.16	0.45
3:A:449:GLY:H	3:A:475:SER:HA	1.81	0.45
3:A:497:ILE:CD1	3:A:497:ILE:H	2.29	0.45
3:B:71:PHE:HE2	3:B:94:LEU:HD23	1.81	0.45
3:B:434:ARG:O	3:B:459:PHE:N	2.46	0.45
3:B:614:SER:HA	3:B:637:LEU:HD11	1.98	0.45
1:C:9:G:O2'	1:C:10:A:H5'	2.16	0.45
2:D:7:G:O2'	2:D:8:C:H5'	2.16	0.45
2:D:15:C:H2'	2:D:16:A:H8	1.82	0.45
3:A:246:SER:C	3:A:248:THR:N	2.74	0.45
3:A:409:LEU:O	3:A:433:LEU:HA	2.17	0.45
3:A:625:VAL:HB	3:A:657:PHE:HB2	1.97	0.45
10:M:1:NAG:H83	10:M:1:NAG:H3	1.99	0.45
3:A:212:PHE:CE2	3:A:241:LEU:HB2	2.53	0.45
3:A:526:LEU:HA	3:A:529:LEU:CD1	2.46	0.45
3:B:150:ILE:HG23	3:B:174:GLN:CB	2.44	0.45
2:D:18:U:H2'	2:D:19:G:H8	1.82	0.44
3:A:212:PHE:CD2	3:A:241:LEU:HB2	2.53	0.44
3:B:263:THR:HG23	3:B:286:LEU:HD11	2.00	0.44
3:B:410:LEU:C	3:B:433:LEU:HD12	2.43	0.44
2:D:17:A:C6	2:D:18:U:C4	3.05	0.44
3:A:461:ILE:HG22	3:A:461:ILE:O	2.16	0.44
3:A:498:SER:HA	3:A:499:PRO:C	2.42	0.44
3:A:538:GLN:H	3:A:538:GLN:CD	2.24	0.44
2:D:30:C:H2'	2:D:31:A:H8	1.82	0.44
3:A:169:GLN:HG3	3:A:170:LEU:HD23	1.99	0.44
3:A:390:PHE:CD2	3:A:393:LEU:HD13	2.52	0.44
3:B:321:LEU:O	3:B:354:LEU:HD23	2.17	0.44
3:B:434:ARG:O	3:B:458:ILE:HD12	2.17	0.44
3:B:532:LEU:HD13	3:B:532:LEU:C	2.41	0.44
3:B:601:LEU:N	3:B:601:LEU:HD22	2.32	0.44
3:A:140:SER:OG	3:A:141:ASN:N	2.50	0.44
3:A:313:LEU:HD12	3:A:346:ILE:CG2	2.46	0.44
3:A:383:TYR:HD2	3:A:411:THR:OG1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:301:ARG:O	3:B:324:LEU:HD12	2.16	0.44
11:N:2:NAG:O7	11:N:3:FUL:H63	2.17	0.44
2:D:23:C:H2'	2:D:24:C:C6	2.52	0.44
3:A:220:ILE:O	3:A:221:GLY:C	2.60	0.44
3:A:241:LEU:O	3:A:241:LEU:HD12	2.17	0.44
3:B:217:PHE:HD1	3:B:220:ILE:HD12	1.82	0.44
3:B:603:PRO:O	3:B:604:PHE:CB	2.65	0.44
5:F:1:NAG:H4	5:F:2:NAG:N2	2.32	0.44
2:D:23:C:H5''	3:A:539:HIS:HB3	1.99	0.44
3:A:40:LEU:CD1	3:A:61:ASN:HD21	2.28	0.44
3:B:384:LEU:O	3:B:412:LEU:HA	2.17	0.44
3:B:609:GLN:NE2	3:B:609:GLN:N	2.59	0.44
3:A:80:LEU:HD23	3:A:103:VAL:O	2.17	0.44
3:A:260:LEU:C	3:A:262:ALA:N	2.76	0.44
3:A:422:ILE:HD13	3:A:422:ILE:N	2.30	0.44
3:A:424:ASN:CG	8:J:1:NAG:HN2	2.26	0.44
3:A:497:ILE:HD13	3:A:497:ILE:H	1.83	0.44
3:B:62:GLN:C	3:B:63:LEU:HD12	2.43	0.44
3:B:114:ILE:CG1	3:B:118:THR:HG21	2.47	0.44
3:B:284:ASN:O	3:B:285:ASN:C	2.60	0.44
3:B:437:ASP:OD2	3:B:437:ASP:C	2.61	0.44
3:A:194:LEU:HD12	3:A:220:ILE:HD12	1.99	0.44
3:A:313:LEU:CB	3:A:346:ILE:HG22	2.47	0.44
3:A:410:LEU:C	3:A:433:LEU:HD12	2.43	0.44
3:A:570:GLU:O	3:A:571:SER:C	2.61	0.44
9:R:2:NAG:O3	9:R:2:NAG:H83	2.17	0.44
1:C:21:A:H1'	3:B:541:ASN:HB2	1.99	0.44
3:A:31:ARG:HA	3:A:31:ARG:NE	2.17	0.44
3:A:92:PRO:HG3	3:A:117:GLN:C	2.42	0.44
3:A:649:CYS:HB2	3:A:683:TYR:HB3	1.99	0.44
3:B:345:ASN:HD21	3:B:371:LYS:HZ1	1.66	0.44
3:A:126:THR:HG22	3:A:148:ASN:O	2.18	0.43
3:B:33:ASN:HA	3:B:53:ILE:CG2	2.48	0.43
3:A:625:VAL:HG11	3:A:657:PHE:CD1	2.53	0.43
3:B:80:LEU:CD2	3:B:104:LEU:HA	2.48	0.43
3:B:246:SER:C	3:B:248:THR:N	2.76	0.43
3:B:523:GLU:O	3:B:524:ASP:C	2.61	0.43
3:A:482:LEU:HB2	3:A:505:LEU:CD2	2.41	0.43
3:A:605:ILE:HD11	3:A:629:VAL:CG1	2.14	0.43
3:B:55:VAL:HG12	3:B:56:LEU:N	2.34	0.43
3:B:135:ILE:N	3:B:157:ASN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:331:ARG:NH2	3:B:335:LYS:CE	2.81	0.43
3:B:599:ASN:O	3:B:601:LEU:HD22	2.18	0.43
3:A:194:LEU:HD12	3:A:220:ILE:CD1	2.48	0.43
3:A:419:ILE:HG22	3:A:422:ILE:HD11	2.00	0.43
3:A:437:ASP:OD2	3:A:437:ASP:C	2.61	0.43
3:B:33:ASN:O	3:B:54:THR:N	2.39	0.43
3:B:50:PRO:O	3:B:53:ILE:HG23	2.18	0.43
3:B:56:LEU:C	3:B:56:LEU:HD13	2.43	0.43
3:B:333:PHE:CD2	3:B:367:ILE:HD11	2.53	0.43
3:B:359:TYR:HD2	3:B:359:TYR:O	2.01	0.43
3:B:538:GLN:H	3:B:538:GLN:CD	2.26	0.43
3:A:485:LEU:HG	3:A:487:LEU:HD21	2.00	0.43
3:A:575:ASP:C	3:A:575:ASP:OD2	2.61	0.43
3:B:233:LEU:HD12	3:B:233:LEU:N	2.32	0.43
3:B:568:ASN:C	3:B:569:LEU:HD12	2.43	0.43
2:D:24:C:O2'	2:D:25:U:H5'	2.19	0.43
3:A:42:LEU:HD22	3:A:44:HIS:O	2.19	0.43
3:A:114:ILE:HG13	3:A:115:SER:N	2.34	0.43
3:A:187:ARG:HG3	3:A:187:ARG:HH11	1.83	0.43
3:B:102:LYS:C	3:B:125:LEU:HD12	2.44	0.43
3:B:313:LEU:HD13	3:B:318:PHE:HE1	1.83	0.43
3:B:555:VAL:O	3:B:557:PHE:N	2.42	0.43
7:I:1:NAG:H62	7:I:2:NAG:HN2	1.83	0.43
3:B:262:ALA:HB2	3:B:288:ASP:HB2	1.98	0.43
3:B:571:SER:HA	3:B:595:LEU:O	2.19	0.43
3:B:651:CYS:HA	3:B:655:SER:OG	2.19	0.43
2:D:14:U:O2'	2:D:15:C:H5'	2.18	0.43
3:A:134:SER:HB2	3:A:136:HIS:CE1	2.53	0.43
3:A:450:GLN:HG3	8:J:1:NAG:H5	1.99	0.43
3:B:230:ASN:HA	3:B:257:ASN:O	2.19	0.43
3:B:263:THR:HG23	3:B:286:LEU:CD1	2.49	0.43
3:B:345:ASN:ND2	3:B:371:LYS:NZ	2.67	0.43
3:B:410:LEU:O	3:B:433:LEU:HD12	2.19	0.43
2:D:40:G:H2'	2:D:41:C:C6	2.54	0.43
3:A:45:ILE:O	3:A:45:ILE:CG2	2.64	0.43
3:A:246:SER:C	3:A:248:THR:H	2.27	0.43
3:A:652:GLU:OE1	3:B:681:HIS:HB3	2.19	0.43
3:B:59:THR:HG22	3:B:60:HIS:CG	2.54	0.43
3:B:582:PHE:HA	3:B:585:LEU:HD12	2.01	0.43
3:B:602:GLU:O	3:B:605:ILE:HG23	2.19	0.43
8:Q:1:NAG:H5	8:Q:2:NDG:H8C1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:90:LEU:HG	3:A:94:LEU:HD13	2.00	0.42
3:A:544:ARG:H	3:A:544:ARG:HG3	1.51	0.42
3:A:575:ASP:OD2	3:A:576:GLU:N	2.52	0.42
3:B:521:ILE:HD13	3:B:521:ILE:C	2.44	0.42
3:B:527:GLU:HG3	3:B:559:LYS:NZ	2.33	0.42
3:B:609:GLN:N	3:B:609:GLN:CD	2.77	0.42
3:B:630:PHE:O	3:B:634:PHE:CD1	2.72	0.42
3:B:651:CYS:O	3:B:655:SER:HB2	2.18	0.42
2:D:3:U:H2'	2:D:4:G:O4'	2.19	0.42
3:A:294:PHE:C	3:A:296:TYR:H	2.27	0.42
3:A:359:TYR:C	3:A:359:TYR:HD2	2.26	0.42
3:A:441:ASN:O	3:A:466:ASN:HA	2.19	0.42
3:B:126:THR:HG22	3:B:148:ASN:O	2.18	0.42
3:B:382:LYS:HA	3:B:408:PRO:O	2.19	0.42
3:B:436:LEU:C	3:B:436:LEU:HD23	2.44	0.42
7:I:1:NAG:H61	7:I:2:NAG:HN2	1.83	0.42
3:A:511:LEU:CD2	3:A:511:LEU:C	2.92	0.42
3:A:536:ASP:CA	3:A:538:GLN:HE22	2.32	0.42
3:A:599:ASN:OD1	3:A:600:LYS:N	2.52	0.42
3:B:66:LEU:O	3:B:68:PRO:HD3	2.19	0.42
3:B:365:ASN:HB3	3:B:367:ILE:CD1	2.48	0.42
3:B:575:ASP:OD2	3:B:576:GLU:N	2.53	0.42
3:A:384:LEU:O	3:A:412:LEU:HA	2.20	0.42
3:A:521:ILE:HD13	3:A:521:ILE:C	2.44	0.42
3:B:42:LEU:O	3:B:62:GLN:O	2.37	0.42
3:B:147:LYS:HZ3	3:B:171:GLU:HG2	1.84	0.42
3:B:169:GLN:O	3:B:170:LEU:HB2	2.20	0.42
3:B:661:ILE:CG2	3:B:671:LEU:HD21	2.49	0.42
2:D:27:U:H2'	2:D:28:G:C8	2.55	0.42
3:A:53:ILE:HD11	3:A:74:TYR:HD2	1.85	0.42
3:A:396:LEU:CG	3:A:422:ILE:HD12	2.50	0.42
3:A:497:ILE:CD1	3:A:501:PRO:HD3	2.49	0.42
3:A:535:LEU:HD11	3:A:537:PHE:CD2	2.53	0.42
3:B:234:ASN:HD22	3:B:236:HIS:H	1.67	0.42
5:F:1:NAG:H4	5:F:2:NAG:HN2	1.85	0.42
3:A:609:GLN:H	3:A:609:GLN:HE21	1.61	0.42
3:B:201:LYS:NZ	3:B:227:LEU:HD11	2.34	0.42
3:B:206:SER:HA	3:B:230:ASN:O	2.20	0.42
3:B:243:TRP:O	3:B:246:SER:HB2	2.20	0.42
3:B:382:LYS:HB2	3:B:410:LEU:HD13	2.00	0.42
3:B:427:PHE:CZ	3:B:436:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:449:GLY:N	3:B:475:SER:HA	2.34	0.42
3:B:479:VAL:HG23	3:B:479:VAL:O	2.20	0.42
3:B:502:PHE:CE2	3:B:525:LEU:HD11	2.54	0.42
3:B:537:PHE:CZ	3:B:557:PHE:HZ	2.38	0.42
3:A:598:LEU:O	3:A:622:ILE:HG12	2.20	0.42
3:B:91:GLU:HB3	3:B:93:GLU:HG2	2.02	0.42
3:A:169:GLN:O	3:A:170:LEU:HB2	2.20	0.42
3:A:260:LEU:C	3:A:262:ALA:H	2.27	0.42
3:A:643:ARG:NH1	3:A:670:GLU:OE1	2.53	0.42
3:B:96:GLN:HB3	3:B:121:PHE:CG	2.55	0.42
3:A:116:ASP:O	3:A:120:VAL:HG23	2.19	0.42
3:A:246:SER:O	3:A:248:THR:N	2.53	0.42
3:A:370:THR:OG1	3:A:400:THR:HG23	2.20	0.42
3:B:126:THR:C	3:B:149:LEU:HD12	2.45	0.42
3:B:488:ARG:O	3:B:489:ARG:C	2.63	0.42
3:B:498:SER:HA	3:B:499:PRO:C	2.44	0.42
1:C:16:U:C4'	7:I:5:MAN:O3	2.67	0.42
3:A:106:LEU:HD23	3:A:111:LEU:HD11	2.01	0.41
3:A:140:SER:O	3:A:142:PRO:HD3	2.19	0.41
3:A:294:PHE:C	3:A:296:TYR:N	2.74	0.41
3:A:382:LYS:HB2	3:A:410:LEU:HD13	2.02	0.41
3:A:599:ASN:O	3:A:601:LEU:HD22	2.20	0.41
3:A:643:ARG:HG3	3:A:644:PHE:CD2	2.55	0.41
3:B:192:GLU:C	3:B:194:LEU:H	2.26	0.41
3:B:297:LEU:HB3	3:B:300:LEU:HB2	2.01	0.41
3:B:433:LEU:HD21	3:B:436:LEU:HB2	2.01	0.41
4:H:2:NDG:H6C2	4:H:2:NDG:C2	2.50	0.41
3:A:38:SER:O	3:A:60:HIS:HB2	2.20	0.41
3:A:458:ILE:HD13	3:A:459:PHE:C	2.44	0.41
3:B:116:ASP:CA	3:B:142:PRO:HA	2.48	0.41
3:B:598:LEU:HB2	3:B:620:ASN:ND2	2.30	0.41
3:A:147:LYS:HZ3	3:A:171:GLU:HG2	1.84	0.41
3:A:177:LEU:N	3:A:177:LEU:CD1	2.83	0.41
3:A:239:GLU:HG3	3:A:267:THR:HA	2.02	0.41
3:A:250:ILE:C	3:A:250:ILE:CD1	2.91	0.41
3:A:689:LYS:CG	3:A:690:LEU:N	2.83	0.41
3:B:67:PRO:HA	3:B:68:PRO:HD2	1.91	0.41
3:B:128:LEU:N	3:B:149:LEU:HD11	2.36	0.41
3:B:658:VAL:O	3:B:661:ILE:HB	2.20	0.41
6:G:2:NAG:H3	6:G:2:NAG:H82	2.01	0.41
3:B:234:ASN:CB	3:B:237:LEU:HD13	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:A:H4'	12:P:5:MAN:H62	2.03	0.41
3:A:361:ASN:OD1	3:A:361:ASN:C	2.63	0.41
3:A:478:LEU:HD23	3:A:478:LEU:O	2.20	0.41
3:A:546:TRP:HB3	3:A:578:PRO:HD3	2.02	0.41
3:A:645:ASN:HA	3:A:646:PRO:HD3	1.90	0.41
3:B:359:TYR:C	3:B:359:TYR:HD2	2.26	0.41
3:B:584:ASN:HA	3:B:586:PHE:CE2	2.55	0.41
2:D:12:U:H2'	2:D:13:G:H8	1.85	0.41
3:A:297:LEU:C	3:A:299:SER:N	2.79	0.41
3:B:33:ASN:HB3	3:B:53:ILE:HA	2.03	0.41
3:B:284:ASN:C	3:B:286:LEU:N	2.76	0.41
3:B:612:LEU:HD23	3:B:633:PRO:HB2	2.03	0.41
3:B:657:PHE:O	3:B:658:VAL:C	2.64	0.41
3:A:234:ASN:HD22	3:A:236:HIS:H	1.69	0.41
3:A:523:GLU:O	3:A:524:ASP:C	2.63	0.41
3:B:521:ILE:CD1	3:B:522:ASN:O	2.68	0.41
3:A:435:ILE:HG12	3:A:460:GLU:HG2	2.03	0.41
3:A:620:ASN:HB2	3:A:645:ASN:ND2	2.29	0.41
3:B:39:HIS:O	3:B:40:LEU:HD12	2.20	0.41
3:B:337:SER:HB3	3:B:340:LEU:HB2	2.01	0.41
3:B:369:SER:OG	3:B:370:THR:N	2.54	0.41
1:C:31:U:H2'	1:C:32:G:H8	1.86	0.41
2:D:20:C:H2'	2:D:21:U:H6	1.86	0.41
3:A:68:PRO:HB3	3:A:94:LEU:HD12	2.03	0.41
3:A:83:GLY:O	3:A:84:PHE:HB2	2.20	0.41
3:A:389:THR:O	3:A:389:THR:HG22	2.20	0.41
3:A:602:GLU:OE2	3:A:602:GLU:HA	2.19	0.41
3:A:661:ILE:CG2	3:A:671:LEU:HD21	2.50	0.41
3:B:37:CYS:HB2	3:B:57:ASN:O	2.20	0.41
3:B:233:LEU:CD1	3:B:233:LEU:N	2.83	0.41
3:B:625:VAL:HB	3:B:657:PHE:HB2	2.03	0.41
8:J:1:NAG:O3	8:J:2:NDG:C1	2.69	0.41
2:D:30:C:H2'	2:D:31:A:C8	2.55	0.41
3:B:40:LEU:CB	3:B:61:ASN:HD21	2.21	0.41
3:B:79:ILE:HG22	3:B:103:VAL:HB	2.03	0.41
3:B:96:GLN:HB3	3:B:121:PHE:CD2	2.56	0.41
3:B:131:MET:O	3:B:156:HIS:HB3	2.21	0.41
3:B:570:GLU:O	3:B:571:SER:C	2.63	0.41
3:B:582:PHE:HB3	3:B:609:GLN:OE1	2.21	0.41
3:B:620:ASN:HB3	3:B:621:LEU:H	1.76	0.41
3:A:263:THR:HG23	3:A:286:LEU:CD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:309:ASN:OD1	3:A:334:THR:HA	2.21	0.40
3:B:189:GLU:O	3:B:192:GLU:HG2	2.21	0.40
3:B:331:ARG:HH22	3:B:335:LYS:HD3	1.86	0.40
3:B:521:ILE:HD12	3:B:557:PHE:HE1	1.86	0.40
2:D:19:G:H2'	2:D:20:C:C6	2.55	0.40
3:A:168:VAL:HG11	3:A:195:GLY:HA3	2.02	0.40
3:A:493:LYS:O	3:A:494:ASN:HB2	2.21	0.40
3:B:66:LEU:HD23	3:B:66:LEU:HA	1.92	0.40
3:B:94:LEU:O	3:B:98:LEU:HD23	2.21	0.40
3:B:187:ARG:HB2	3:B:190:GLU:HG2	2.03	0.40
3:B:447:LEU:HD23	3:B:451:GLU:HG3	2.02	0.40
3:A:102:LYS:C	3:A:125:LEU:HD12	2.45	0.40
3:A:197:SER:O	3:A:221:GLY:HA3	2.21	0.40
3:A:230:ASN:HA	3:A:257:ASN:O	2.21	0.40
3:A:396:LEU:CD1	3:A:422:ILE:HD12	2.50	0.40
3:A:564:LEU:O	3:A:588:LEU:HA	2.21	0.40
3:A:659:ASN:O	3:A:660:TRP:C	2.63	0.40
3:B:140:SER:OG	3:B:141:ASN:N	2.50	0.40
4:O:1:NAG:H3	4:O:1:NAG:H83	2.03	0.40
3:A:284:ASN:C	3:A:286:LEU:N	2.76	0.40
3:A:410:LEU:O	3:A:433:LEU:HD12	2.22	0.40
3:A:541:ASN:C	3:A:543:ALA:H	2.29	0.40
3:A:561:LEU:O	3:A:562:SER:C	2.64	0.40
3:A:652:GLU:CD	3:B:681:HIS:HB3	2.46	0.40
3:B:422:ILE:CD1	3:B:438:LEU:HD13	2.52	0.40
3:B:648:ASP:O	3:B:654:ILE:HG23	2.22	0.40
3:A:297:LEU:HB3	3:A:300:LEU:HB2	2.03	0.40
3:A:591:ILE:HB	3:A:615:LEU:HD12	2.01	0.40
3:B:69:THR:C	3:B:71:PHE:H	2.29	0.40
3:B:114:ILE:HD11	3:B:118:THR:HG21	2.02	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	
3	A	655/697 (94%)	527 (80%)	117 (18%)	11 (2%)	7	27
3	B	664/697 (95%)	537 (81%)	113 (17%)	14 (2%)	5	24
All	All	1319/1394 (95%)	1064 (81%)	230 (17%)	25 (2%)	6	26

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	551	PRO
3	A	247	ASN
3	A	290	GLY
3	A	38	SER
3	A	267	THR
3	A	465	TYR
3	A	556	ASN
3	B	38	SER
3	B	247	ASN
3	B	465	TYR
3	B	556	ASN
3	B	604	PHE
3	A	555	VAL
3	A	604	PHE
3	B	30	VAL
3	B	49	LEU
3	B	267	THR
3	B	635	GLN
3	B	603	PRO
3	A	368	PRO
3	B	290	GLY
3	B	67	PRO
3	B	368	PRO
3	A	631	GLY
3	B	449	GLY

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	619/651 (95%)	561 (91%)	58 (9%)	8	28
3	B	625/651 (96%)	575 (92%)	50 (8%)	11	35
All	All	1244/1302 (96%)	1136 (91%)	108 (9%)	9	31

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	31	ARG
3	A	40	LEU
3	A	41	LYS
3	A	42	LEU
3	A	45	ILE
3	A	50	PRO
3	A	53	ILE
3	A	56	LEU
3	A	76	GLN
3	A	98	LEU
3	A	116	ASP
3	A	154	LEU
3	A	189	GLU
3	A	218	GLN
3	A	241	LEU
3	A	250	ILE
3	A	276	LEU
3	A	305	LEU
3	A	335	LYS
3	A	345	ASN
3	A	347	ASP
3	A	355	LYS
3	A	359	TYR
3	A	381	LEU
3	A	394	GLN
3	A	407	SER
3	A	409	LEU
3	A	410	LEU
3	A	411	THR
3	A	421	LYS
3	A	422	ILE
3	A	430	LEU
3	A	442	GLU
3	A	446	LYS

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Mol	Chain	Res	Type
3	A	448	SER
3	A	451	GLU
3	A	458	ILE
3	A	467	LYS
3	A	478	LEU
3	A	481	SER
3	A	497	ILE
3	A	521	ILE
3	A	522	ASN
3	A	544	ARG
3	A	551	PRO
3	A	561	LEU
3	A	572	ASN
3	A	574	LEU
3	A	577	ILE
3	A	605	ILE
3	A	609	GLN
3	A	628	ASP
3	A	672	SER
3	A	673	THR
3	A	679	THR
3	A	681	HIS
3	A	682	HIS
3	A	686	PHE
3	B	32	TYR
3	B	33	ASN
3	B	40	LEU
3	B	41	LYS
3	B	45	ILE
3	B	53	ILE
3	B	56	LEU
3	B	76	GLN
3	B	98	LEU
3	B	116	ASP
3	B	154	LEU
3	B	189	GLU
3	B	218	GLN
3	B	241	LEU
3	B	276	LEU
3	B	305	LEU
3	B	345	ASN
3	B	355	LYS

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Mol	Chain	Res	Type
3	B	359	TYR
3	B	381	LEU
3	B	394	GLN
3	B	407	SER
3	B	410	LEU
3	B	411	THR
3	B	421	LYS
3	B	430	LEU
3	B	442	GLU
3	B	446	LYS
3	B	451	GLU
3	B	478	LEU
3	B	481	SER
3	B	521	ILE
3	B	522	ASN
3	B	544	ARG
3	B	561	LEU
3	B	566	ILE
3	B	572	ASN
3	B	574	LEU
3	B	577	ILE
3	B	605	ILE
3	B	609	GLN
3	B	628	ASP
3	B	651	CYS
3	B	654	ILE
3	B	672	SER
3	B	673	THR
3	B	679	THR
3	B	681	HIS
3	B	682	HIS
3	B	686	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	61	ASN
3	A	76	GLN
3	A	85	ASN
3	A	113	GLN
3	A	145	ASN
3	A	146	GLN

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Mol	Chain	Res	Type
3	A	157	ASN
3	A	169	GLN
3	A	174	GLN
3	A	218	GLN
3	A	230	ASN
3	A	234	ASN
3	A	257	ASN
3	A	278	GLN
3	A	345	ASN
3	A	394	GLN
3	A	418	HIS
3	A	445	GLN
3	A	450	GLN
3	A	466	ASN
3	A	470	GLN
3	A	483	GLN
3	A	494	ASN
3	A	517	ASN
3	A	538	GLN
3	A	541	ASN
3	A	556	ASN
3	A	572	ASN
3	A	609	GLN
3	A	620	ASN
3	A	638	ASN
3	A	645	ASN
3	A	674	HIS
3	A	681	HIS
3	B	33	ASN
3	B	60	HIS
3	B	61	ASN
3	B	76	GLN
3	B	85	ASN
3	B	107	GLN
3	B	113	GLN
3	B	145	ASN
3	B	146	GLN
3	B	157	ASN
3	B	169	GLN
3	B	218	GLN
3	B	230	ASN
3	B	234	ASN

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Mol	Chain	Res	Type
3	B	251	GLN
3	B	257	ASN
3	B	278	GLN
3	B	336	GLN
3	B	345	ASN
3	B	394	GLN
3	B	418	HIS
3	B	445	GLN
3	B	450	GLN
3	B	466	ASN
3	B	470	GLN
3	B	483	GLN
3	B	494	ASN
3	B	517	ASN
3	B	522	ASN
3	B	538	GLN
3	B	539	HIS
3	B	541	ASN
3	B	556	ASN
3	B	572	ASN
3	B	609	GLN
3	B	618	GLN
3	B	620	ASN
3	B	638	ASN
3	B	645	ASN
3	B	674	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	45/46 (97%)	0	0
2	D	45/46 (97%)	0	0
All	All	90/92 (97%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

40 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	$\# Z > 2$
4	NAG	E	1	3,4	14,14,15	1.02	1 (7%)	17,19,21	0.86	0
4	NDG	E	2	4	14,14,15	0.96	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	F	1	3,5	14,14,15	0.89	0	17,19,21	1.00	1 (5%)
5	NAG	F	2	5	14,14,15	0.85	1 (7%)	17,19,21	0.68	0
5	MAN	F	3	5	11,11,12	0.89	0	15,15,17	0.75	1 (6%)
6	NAG	G	1	3,6	14,14,15	0.93	0	17,19,21	0.86	0
6	NAG	G	2	6	14,14,15	0.92	1 (7%)	17,19,21	0.57	0
6	FUC	G	3	6	10,10,11	0.80	0	14,14,16	0.48	0
4	NAG	H	1	3,4	14,14,15	1.14	1 (7%)	17,19,21	0.86	0
4	NDG	H	2	4	14,14,15	1.02	1 (7%)	17,19,21	0.88	1 (5%)
7	NAG	I	1	3,7	14,14,15	0.53	0	17,19,21	1.21	2 (11%)
7	NAG	I	2	7	14,14,15	0.80	0	17,19,21	0.83	0
7	MAN	I	3	7	11,11,12	1.12	1 (9%)	15,15,17	0.86	0
7	MAN	I	4	7	11,11,12	0.88	0	15,15,17	0.75	1 (6%)
7	MAN	I	5	7	11,11,12	0.91	0	15,15,17	1.06	1 (6%)
8	NAG	J	1	3,8	14,14,15	1.05	1 (7%)	17,19,21	0.85	0
8	NDG	J	2	8	14,14,15	0.83	0	17,19,21	0.75	0
8	BMA	J	3	8	11,11,12	0.69	0	15,15,17	0.37	0
9	NAG	K	1	3,9	14,14,15	0.57	0	17,19,21	1.09	2 (11%)
9	NAG	K	2	9	14,14,15	0.86	1 (7%)	17,19,21	0.87	0
4	NAG	L	1	3,4	14,14,15	1.12	1 (7%)	17,19,21	1.22	1 (5%)
4	NDG	L	2	4	14,14,15	1.07	1 (7%)	17,19,21	0.86	0
10	NAG	M	1	3,10	14,14,15	1.09	0	17,19,21	1.22	2 (11%)
10	NAG	M	2	10	14,14,15	0.84	0	17,19,21	0.58	0
10	BMA	M	3	10	11,11,12	0.94	0	15,15,17	0.80	1 (6%)
11	NAG	N	1	3,11	14,14,15	1.02	1 (7%)	17,19,21	0.74	0
11	NAG	N	2	11	14,14,15	0.93	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FUL	N	3	11	10,10,11	0.71	0	14,14,16	0.60	0
4	NAG	O	1	3,4	14,14,15	0.83	0	17,19,21	0.80	0
4	NDG	O	2	4	14,14,15	0.94	1 (7%)	17,19,21	0.94	1 (5%)
12	NAG	P	1	3,12	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
12	NDG	P	2	12	14,14,15	1.11	0	17,19,21	1.20	2 (11%)
12	MAN	P	3	12	11,11,12	1.24	1 (9%)	15,15,17	0.92	1 (6%)
12	MAN	P	4	12	11,11,12	0.85	0	15,15,17	0.80	1 (6%)
12	MAN	P	5	12	11,11,12	0.85	0	15,15,17	0.98	2 (13%)
8	NAG	Q	1	3,8	14,14,15	0.98	0	17,19,21	0.88	1 (5%)
8	NDG	Q	2	8	14,14,15	1.11	1 (7%)	17,19,21	0.71	0
8	BMA	Q	3	8	11,11,12	0.90	0	15,15,17	0.31	0
9	NAG	R	1	3,9	14,14,15	1.31	1 (7%)	17,19,21	0.83	0
9	NAG	R	2	9	14,14,15	1.22	2 (14%)	17,19,21	1.15	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	2	NAG	C1-C2	3.23	1.56	1.52
8	J	1	NAG	C1-C2	3.16	1.56	1.52
4	H	1	NAG	C1-C2	3.03	1.56	1.52
11	N	1	NAG	C1-C2	2.96	1.56	1.52
9	R	1	NAG	C1-C2	2.78	1.56	1.52
4	L	2	NDG	C1-C2	2.76	1.56	1.52
8	Q	2	NDG	C1-C2	2.70	1.56	1.52
4	L	1	NAG	C1-C2	2.63	1.55	1.52
7	I	3	MAN	C2-C3	2.49	1.56	1.52
6	G	2	NAG	C1-C2	2.39	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NDG	C1-C2	2.38	1.55	1.52
4	H	2	NDG	C1-C2	2.34	1.55	1.52
4	E	1	NAG	C1-C2	2.27	1.55	1.52
12	P	3	MAN	C2-C3	2.27	1.56	1.52
5	F	2	NAG	C1-C2	2.19	1.55	1.52
9	K	2	NAG	C1-C2	2.14	1.55	1.52
9	R	2	NAG	O5-C5	2.13	1.47	1.43
4	O	2	NDG	C1-C2	2.08	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	5	MAN	C1-O5-C5	3.53	116.92	112.19
9	R	2	NAG	C1-O5-C5	3.51	116.89	112.19
12	P	1	NAG	C2-N2-C7	-3.37	118.38	122.90
10	M	1	NAG	C3-C4-C5	3.23	116.09	110.23
12	P	2	NDG	C2-N2-C7	-3.17	118.65	122.90
11	N	2	NAG	C4-C3-C2	3.09	115.54	111.02
7	I	1	NAG	C4-C3-C2	-3.02	106.60	111.02
12	P	3	MAN	C1-C2-C3	2.81	113.74	109.64
4	O	2	NDG	C1-O5-C5	2.81	115.95	112.19
7	I	1	NAG	C2-N2-C7	-2.80	119.15	122.90
12	P	2	NDG	C4-C3-C2	-2.76	106.98	111.02
9	K	1	NAG	C4-C3-C2	-2.75	106.99	111.02
4	L	1	NAG	C4-C3-C2	2.64	114.89	111.02
9	K	1	NAG	C2-N2-C7	-2.60	119.41	122.90
8	Q	1	NAG	C2-N2-C7	-2.53	119.51	122.90
12	P	5	MAN	C1-C2-C3	2.52	113.32	109.64
4	H	2	NDG	C1-O5-C5	2.51	115.55	112.19
12	P	5	MAN	C1-O5-C5	2.50	115.53	112.19
12	P	4	MAN	C1-O5-C5	2.43	115.44	112.19
10	M	3	BMA	C1-C2-C3	2.38	113.11	109.64
5	F	1	NAG	C3-C4-C5	2.29	114.38	110.23
10	M	1	NAG	C4-C3-C2	2.29	114.37	111.02
5	F	3	MAN	C1-O5-C5	2.24	115.19	112.19
7	I	4	MAN	C1-O5-C5	2.20	115.14	112.19
4	E	2	NDG	C1-O5-C5	2.05	114.93	112.19

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	I	1	NAG	C1

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Mol	Chain	Res	Type	Atom
8	J	1	NAG	C1
8	Q	1	NAG	C1
9	K	1	NAG	C1
9	R	1	NAG	C1
12	P	1	NAG	C1

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NDG	C8-C7-N2-C2
4	E	2	NDG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NDG	C8-C7-N2-C2
4	H	2	NDG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	L	2	NDG	C8-C7-N2-C2
4	L	2	NDG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	O	2	NDG	C8-C7-N2-C2
4	O	2	NDG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
6	G	1	NAG	C8-C7-N2-C2
6	G	1	NAG	O7-C7-N2-C2
6	G	2	NAG	C1-C2-N2-C7
6	G	2	NAG	C8-C7-N2-C2
6	G	2	NAG	O7-C7-N2-C2
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
7	I	2	NAG	C3-C2-N2-C7
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
8	J	1	NAG	C3-C2-N2-C7
8	J	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	J	1	NAG	O7-C7-N2-C2
8	J	2	NDG	C8-C7-N2-C2
8	J	2	NDG	O7-C7-N2-C2
8	Q	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O7-C7-N2-C2
8	Q	2	NDG	C3-C2-N2-C7
8	Q	2	NDG	C8-C7-N2-C2
8	Q	2	NDG	O7-C7-N2-C2
9	K	1	NAG	C8-C7-N2-C2
9	K	1	NAG	O7-C7-N2-C2
9	K	2	NAG	C8-C7-N2-C2
9	K	2	NAG	O7-C7-N2-C2
9	R	2	NAG	C8-C7-N2-C2
9	R	2	NAG	O7-C7-N2-C2
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
10	M	2	NAG	C8-C7-N2-C2
10	M	2	NAG	O7-C7-N2-C2
11	N	1	NAG	C8-C7-N2-C2
11	N	1	NAG	O7-C7-N2-C2
12	P	1	NAG	C8-C7-N2-C2
12	P	1	NAG	O7-C7-N2-C2
12	P	2	NDG	O7-C7-N2-C2
12	P	2	NDG	C8-C7-N2-C2
7	I	4	MAN	C4-C5-C6-O6
8	Q	1	NAG	C4-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
12	P	4	MAN	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
12	P	4	MAN	C4-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
10	M	1	NAG	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	F	3	MAN	O5-C5-C6-O6
4	O	2	NDG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	3	MAN	C4-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
4	O	2	NDG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
12	P	3	MAN	C4-C5-C6-O6
7	I	3	MAN	C4-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
4	E	2	NDG	C4-C5-C6-O6
10	M	3	BMA	C4-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
8	J	3	BMA	O5-C5-C6-O6
12	P	2	NDG	O5-C5-C6-O6
7	I	3	MAN	O5-C5-C6-O6
11	N	2	NAG	C8-C7-N2-C2
10	M	3	BMA	O5-C5-C6-O6
12	P	3	MAN	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
4	E	2	NDG	O5-C5-C6-O6
11	N	2	NAG	O7-C7-N2-C2
4	H	2	NDG	O5-C5-C6-O6
12	P	5	MAN	O5-C5-C6-O6
4	H	2	NDG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	H	2	NDG	C1-C2-N2-C7
8	J	3	BMA	C4-C5-C6-O6
8	Q	1	NAG	C3-C2-N2-C7
9	R	2	NAG	C3-C2-N2-C7
10	M	1	NAG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
12	P	2	NDG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	Q	3	BMA	C4-C5-C6-O6
11	N	2	NAG	C4-C5-C6-O6
7	I	5	MAN	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	3	MAN	C1-C2-C3-C4-C5-O5
12	P	4	MAN	C1-C2-C3-C4-C5-O5

29 monomers are involved in 55 short contacts:

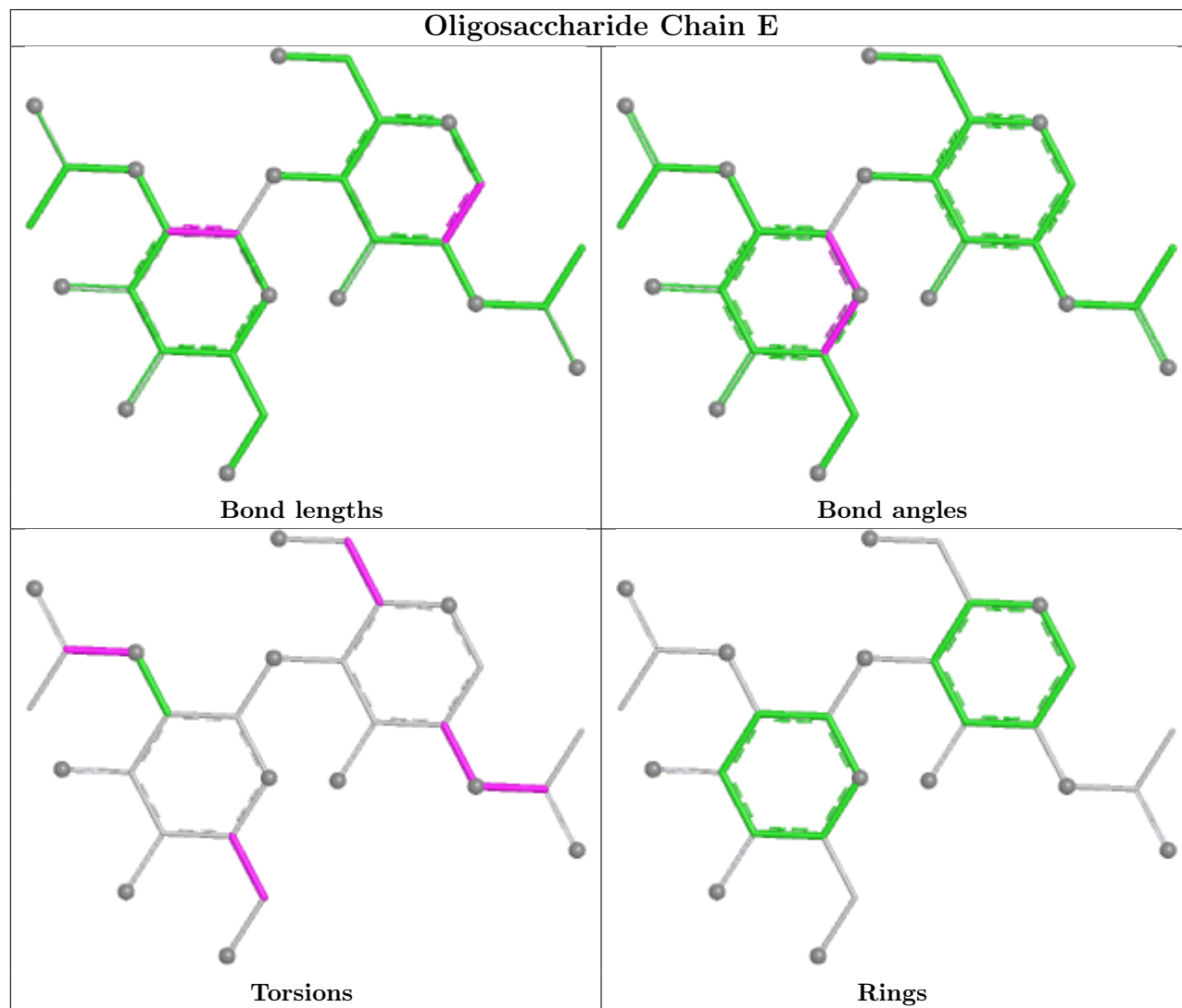
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	1	NAG	1	0
8	J	2	NDG	2	0
7	I	2	NAG	3	0
4	H	2	NDG	2	0
6	G	2	NAG	2	0
11	N	3	FUL	1	0
6	G	3	FUC	1	0
5	F	1	NAG	6	0
8	Q	1	NAG	5	0
6	G	1	NAG	3	0
7	I	5	MAN	3	0
8	Q	2	NDG	3	0
9	K	1	NAG	3	0
4	O	2	NDG	1	0
10	M	1	NAG	3	0
4	H	1	NAG	3	0
11	N	2	NAG	1	0
5	F	2	NAG	2	0
4	L	2	NDG	1	0
8	Q	3	BMA	1	0
9	R	2	NAG	2	0
7	I	1	NAG	3	0
4	O	1	NAG	3	0
9	K	2	NAG	1	0
4	L	1	NAG	4	0
8	J	1	NAG	5	0
4	E	1	NAG	4	0
12	P	5	MAN	1	0

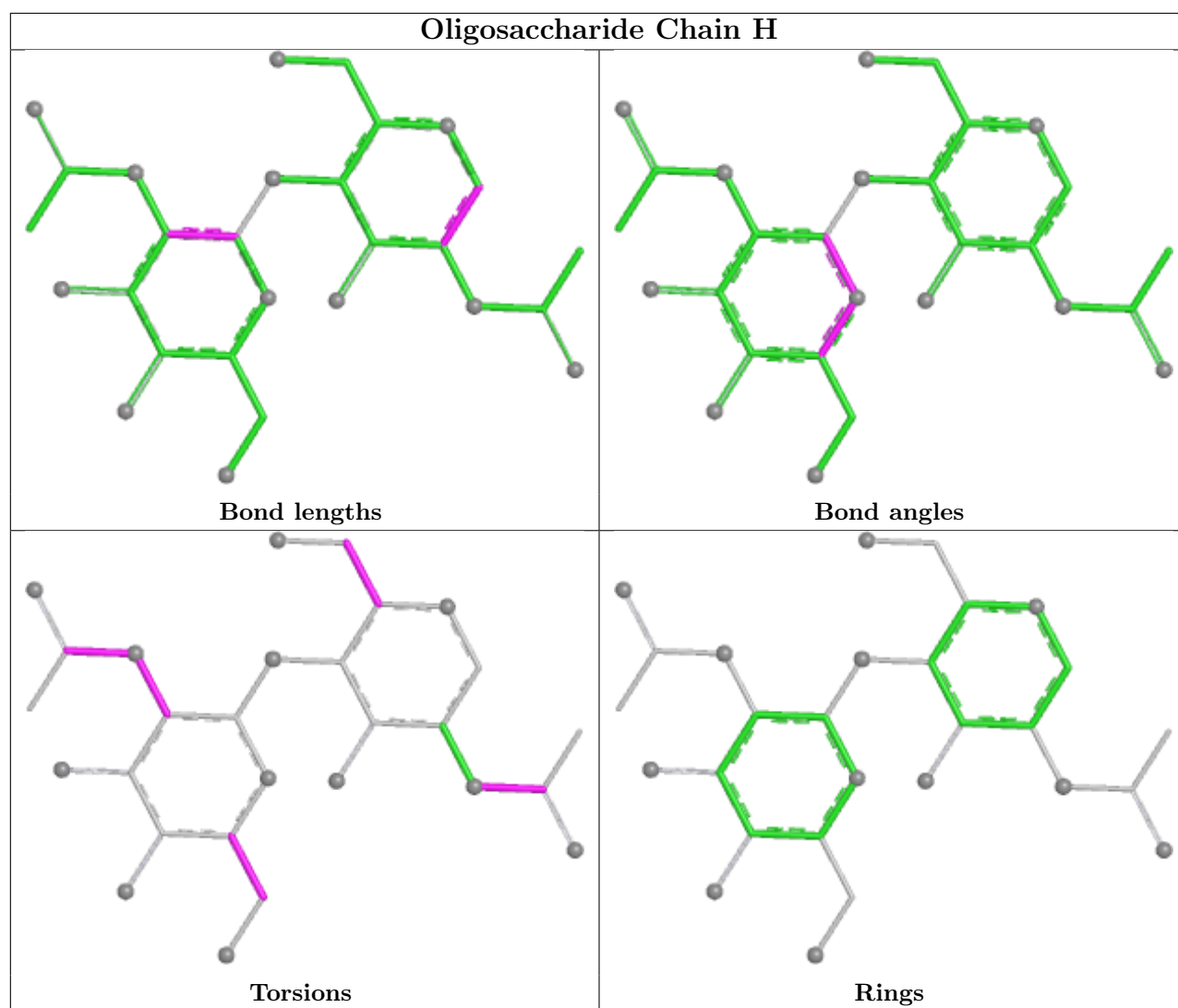
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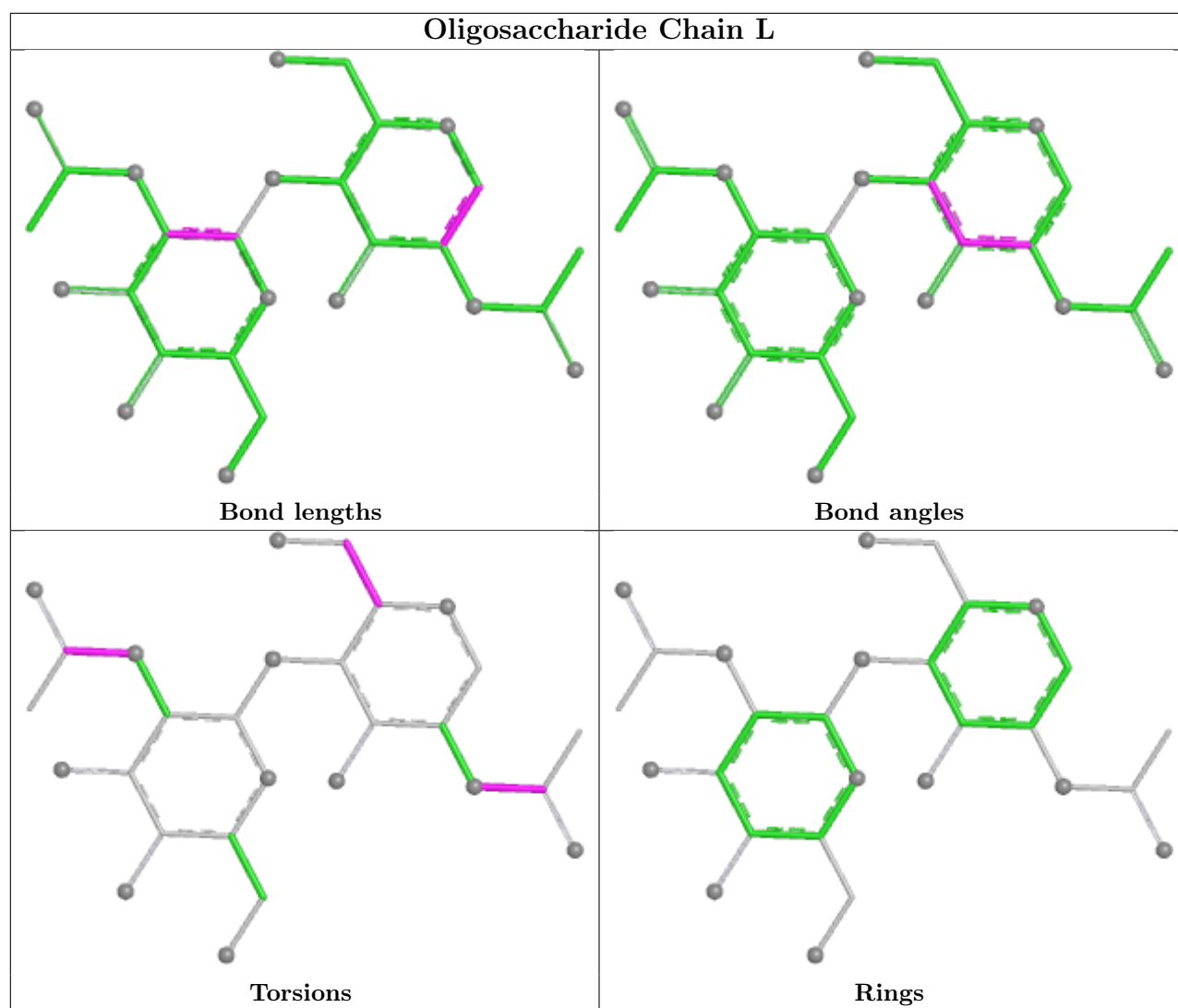
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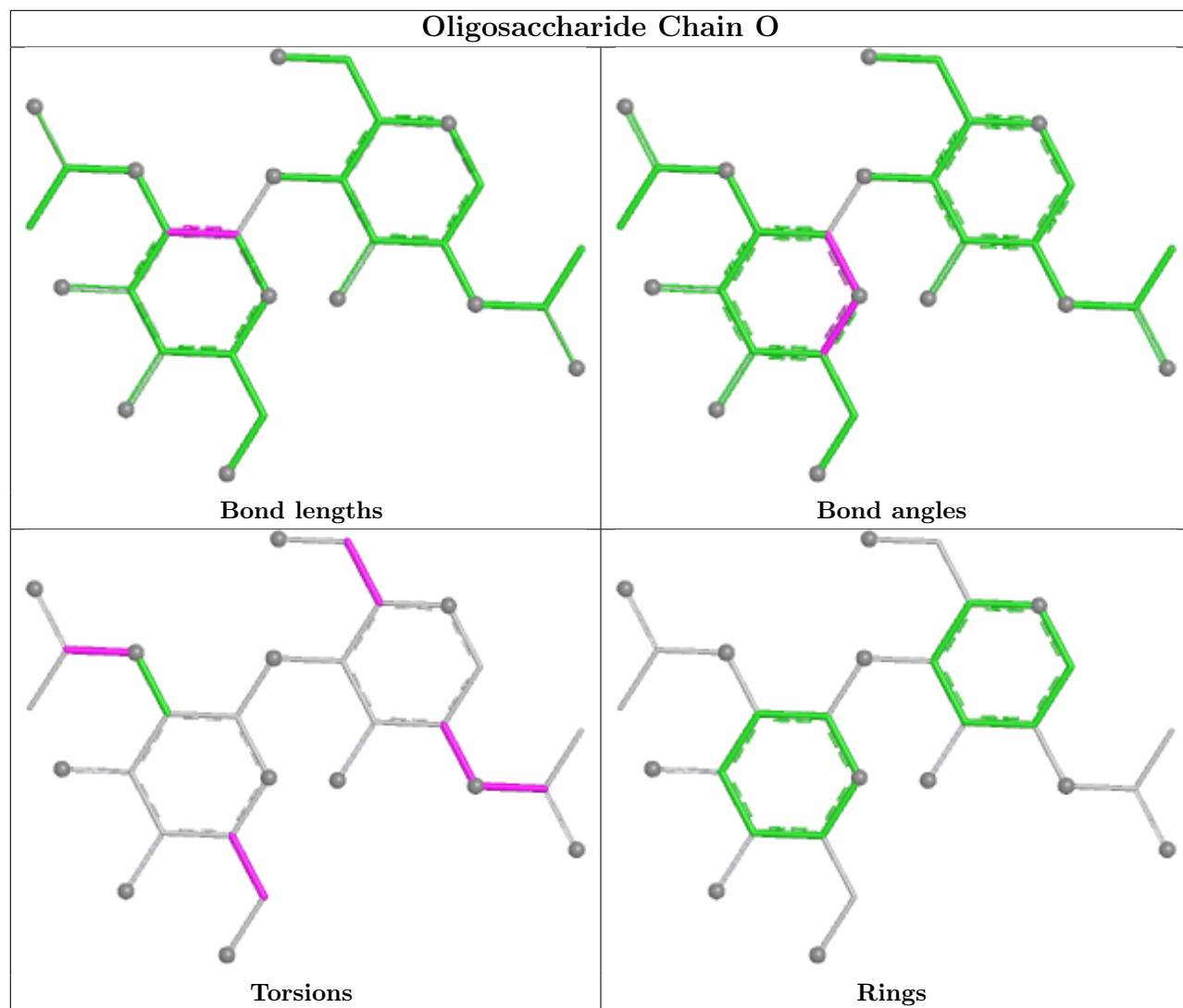
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	3	BMA	1	0

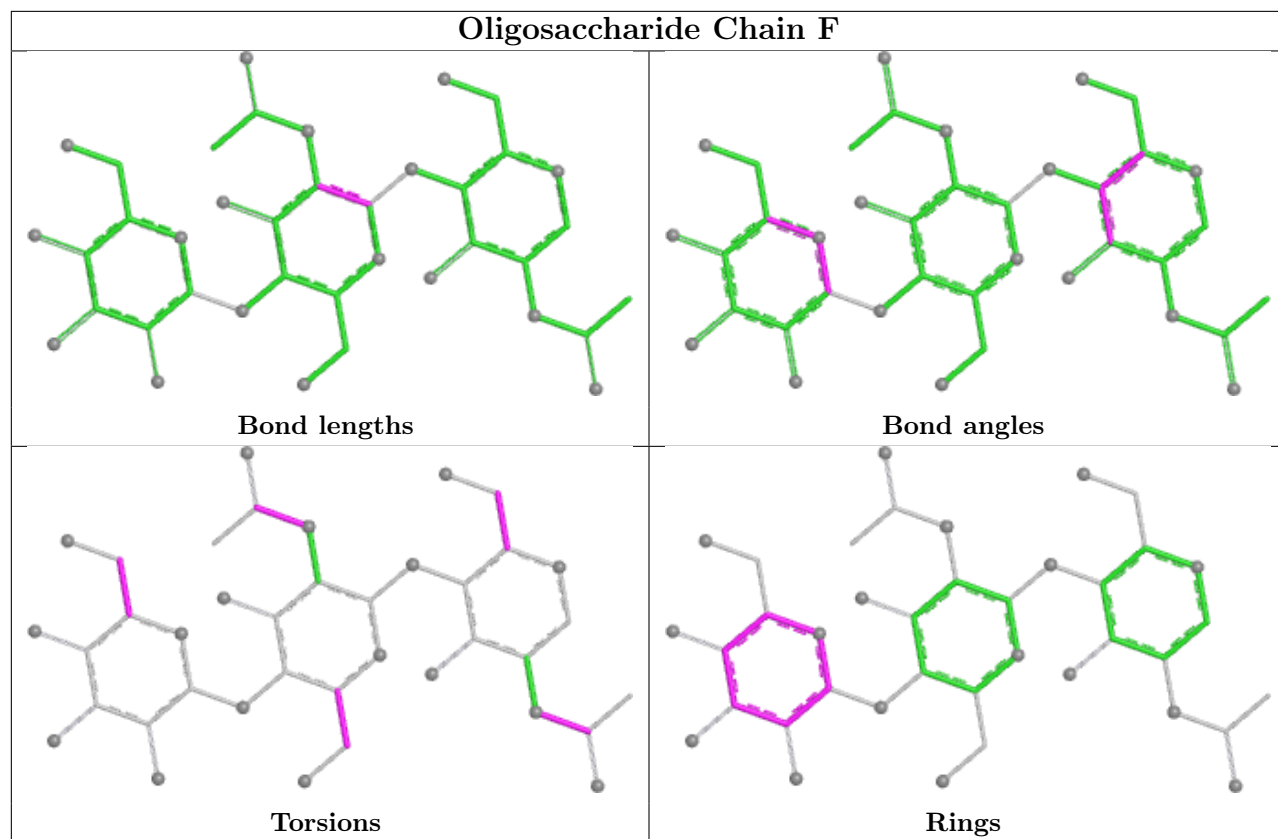
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

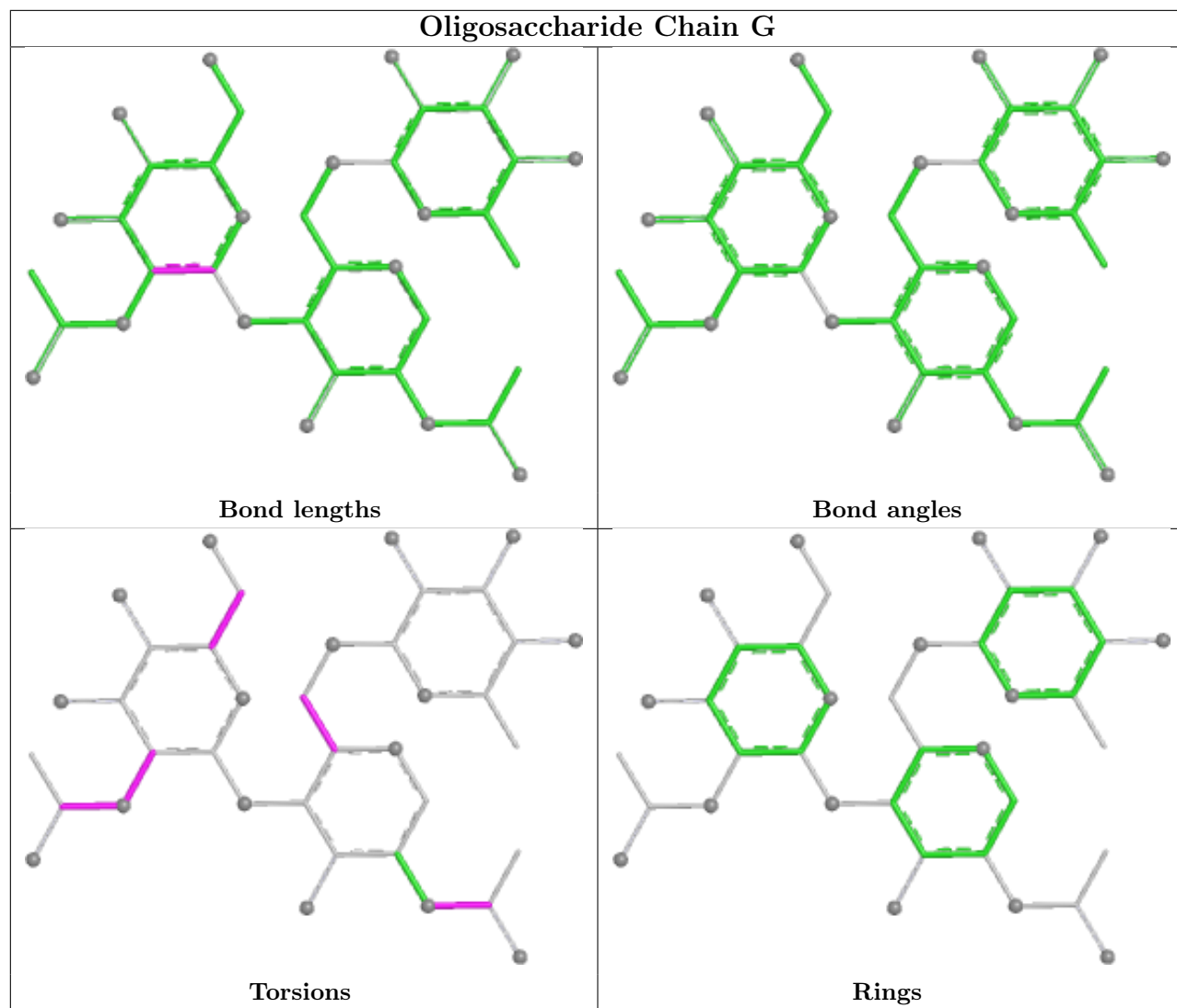




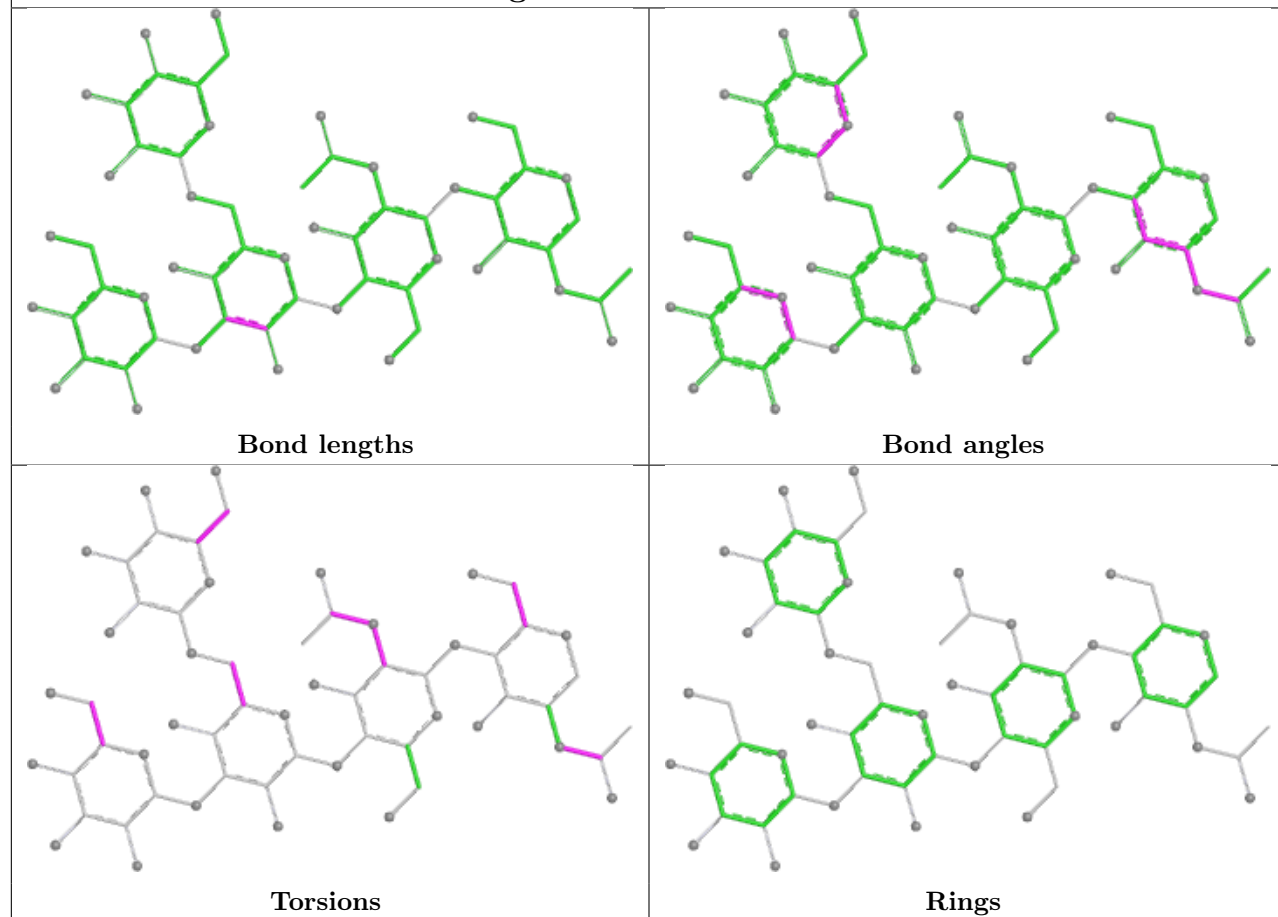




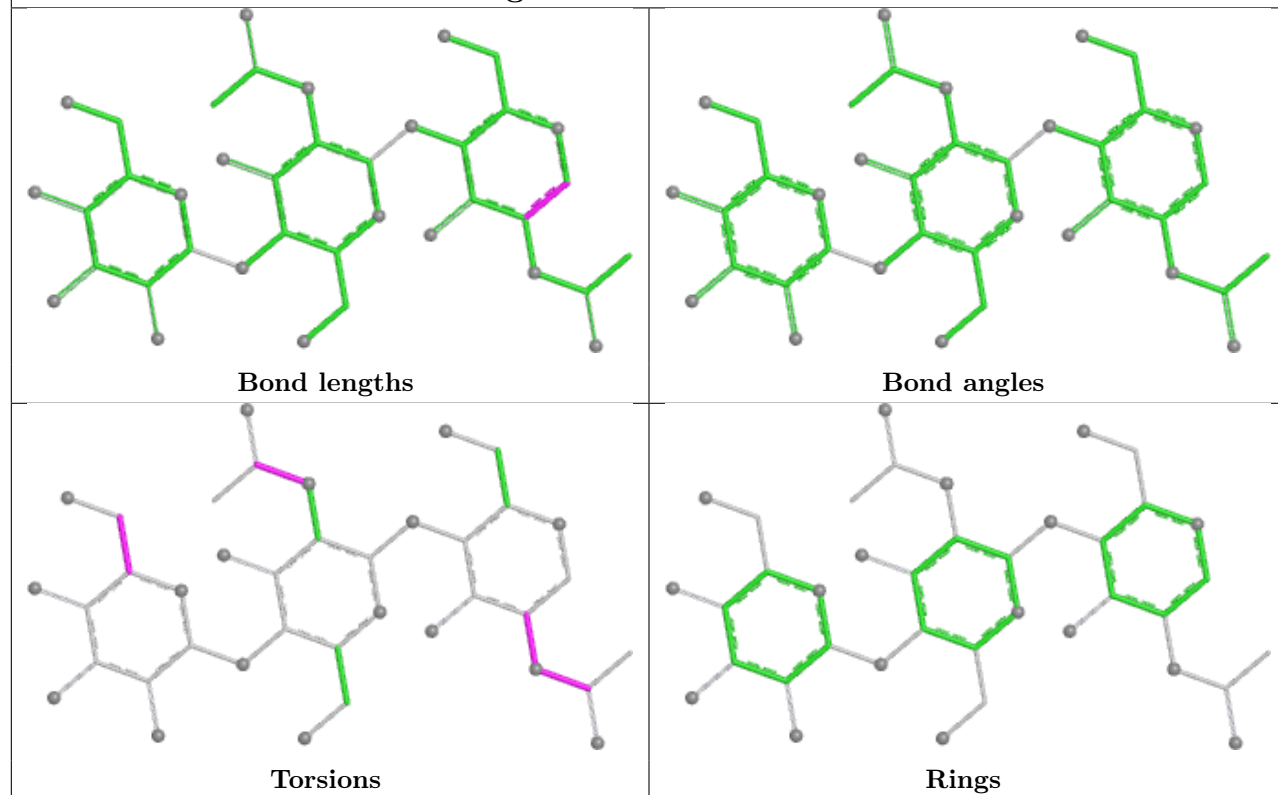


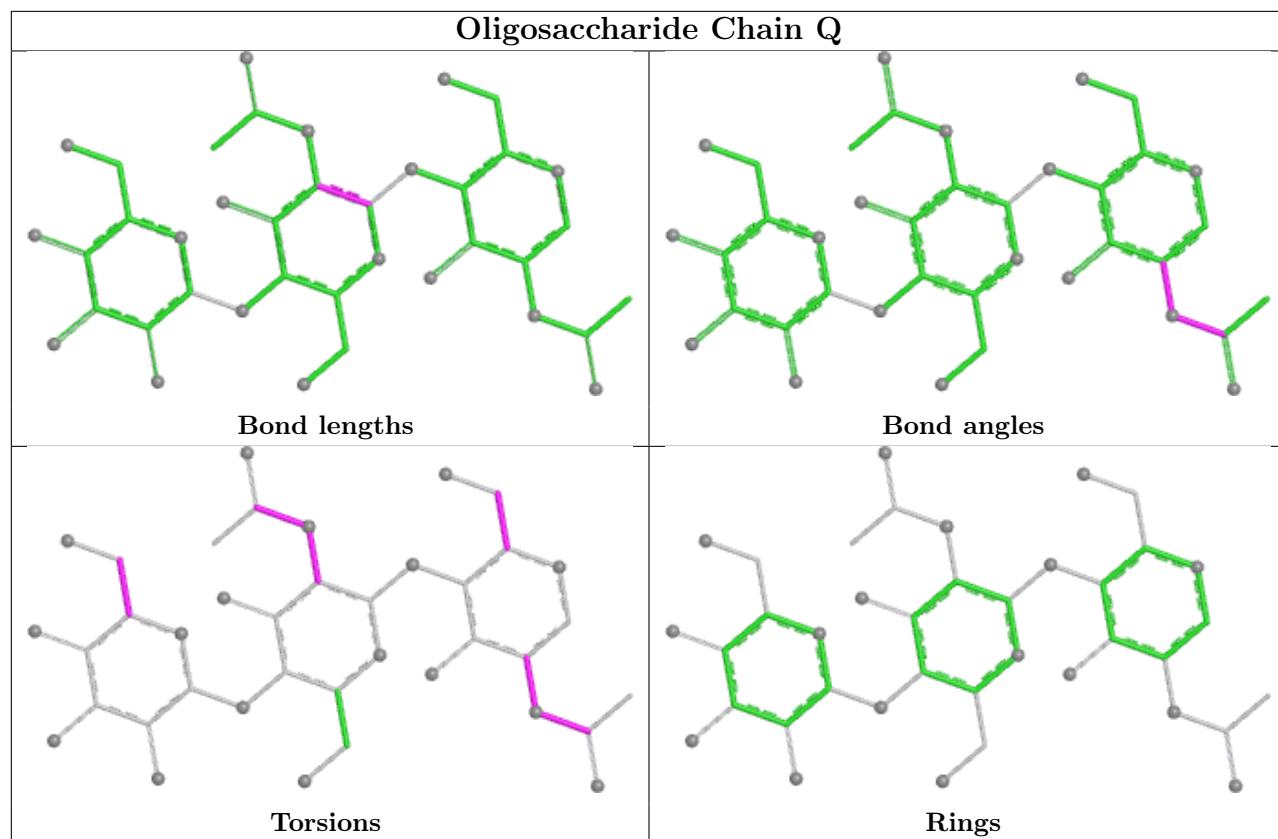


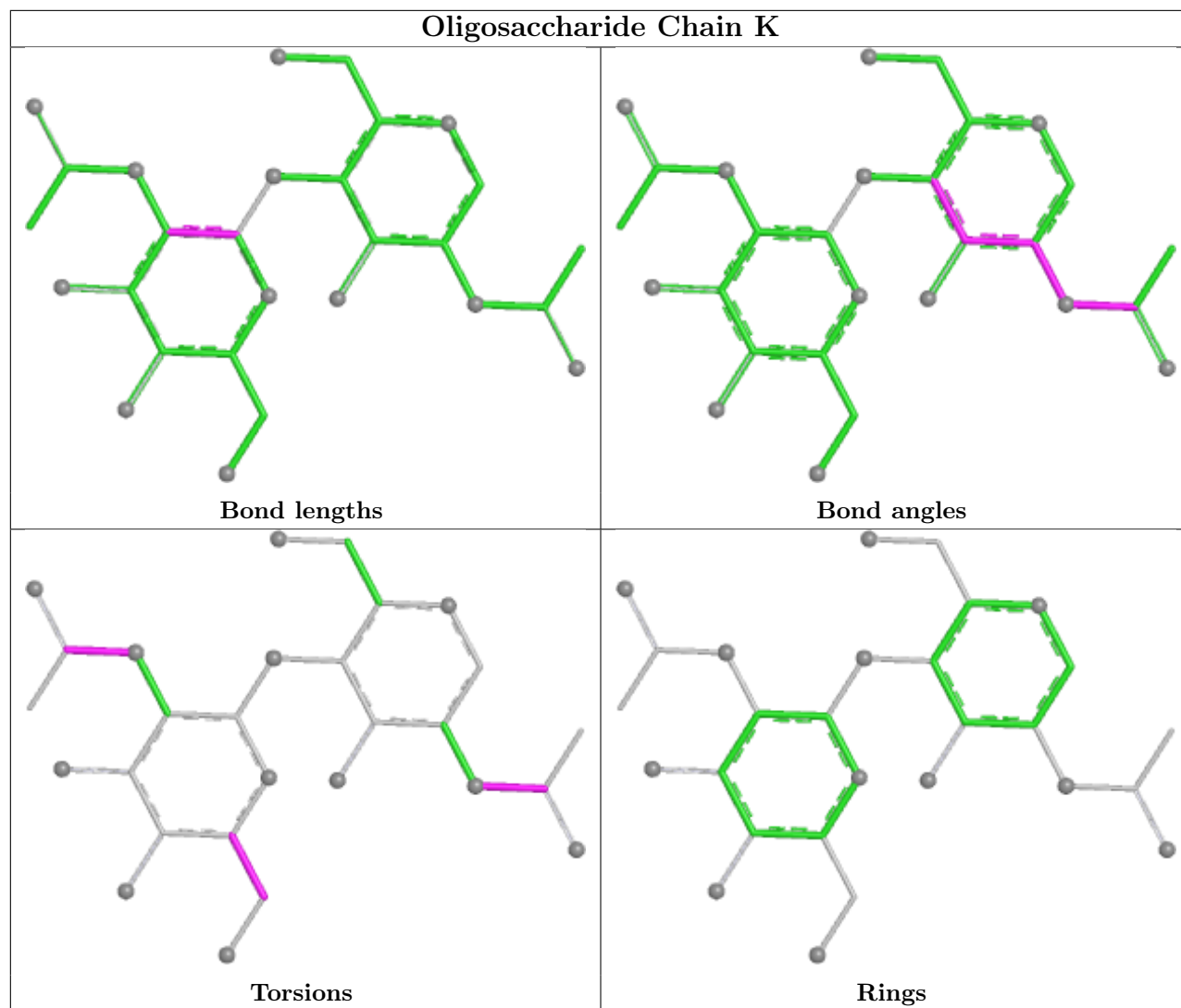
Oligosaccharide Chain I

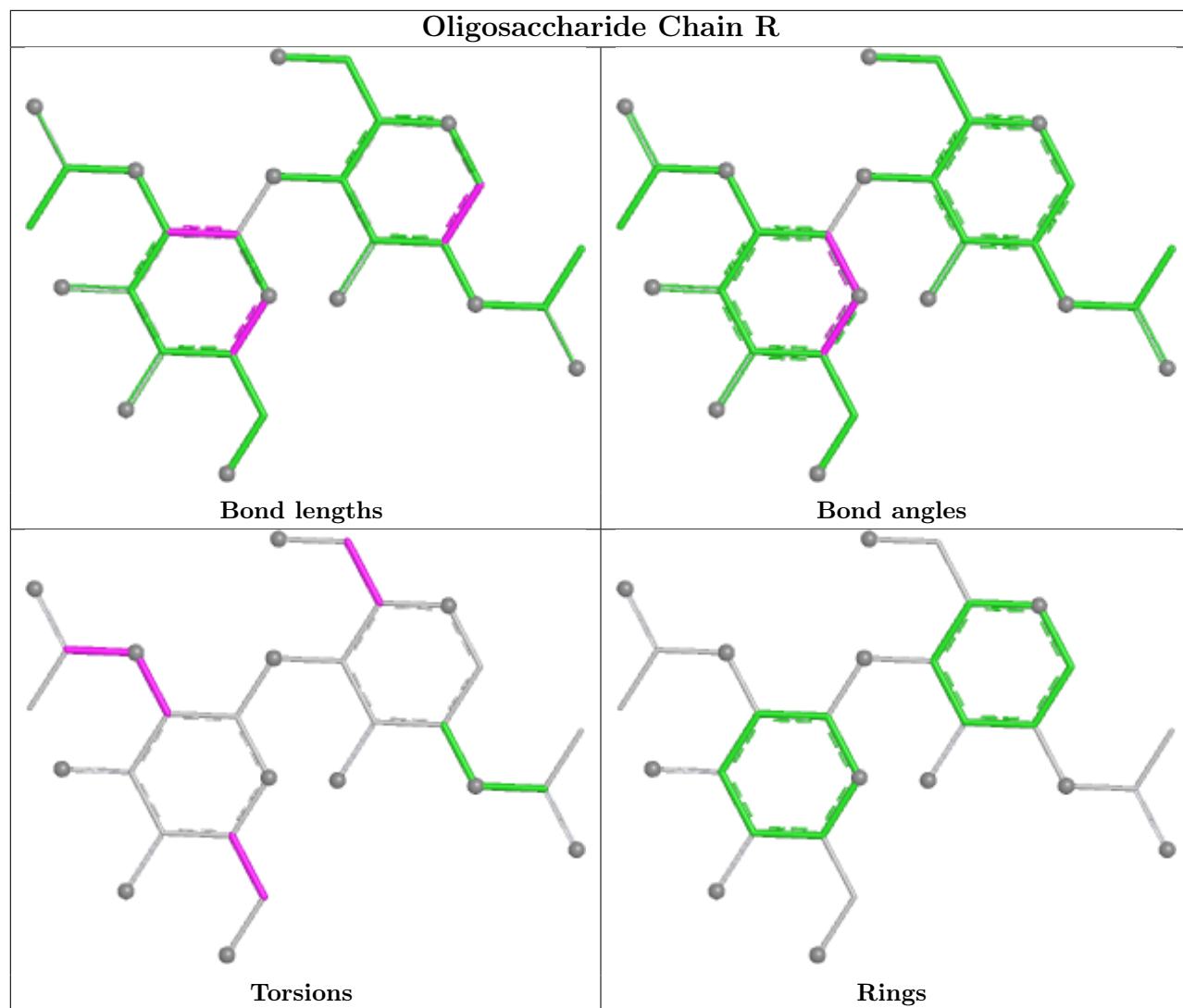


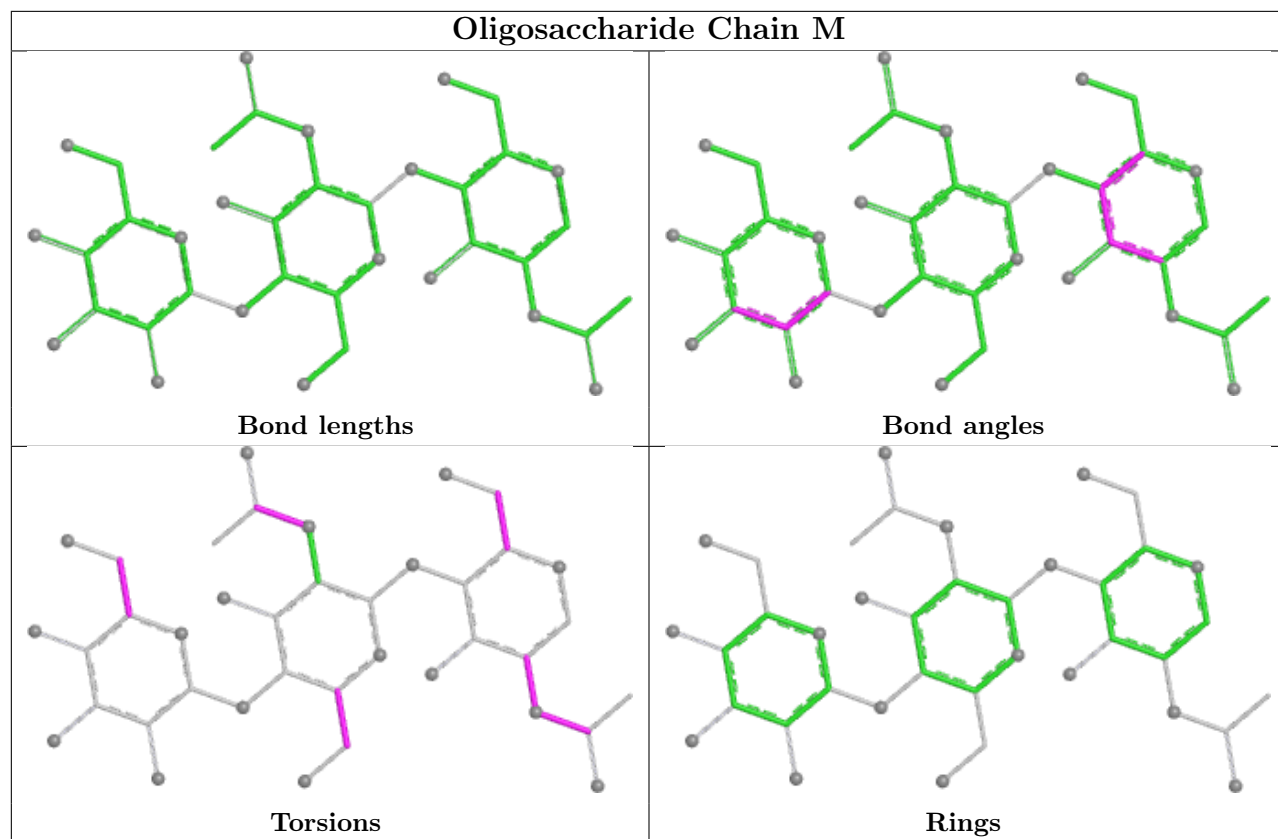
Oligosaccharide Chain J

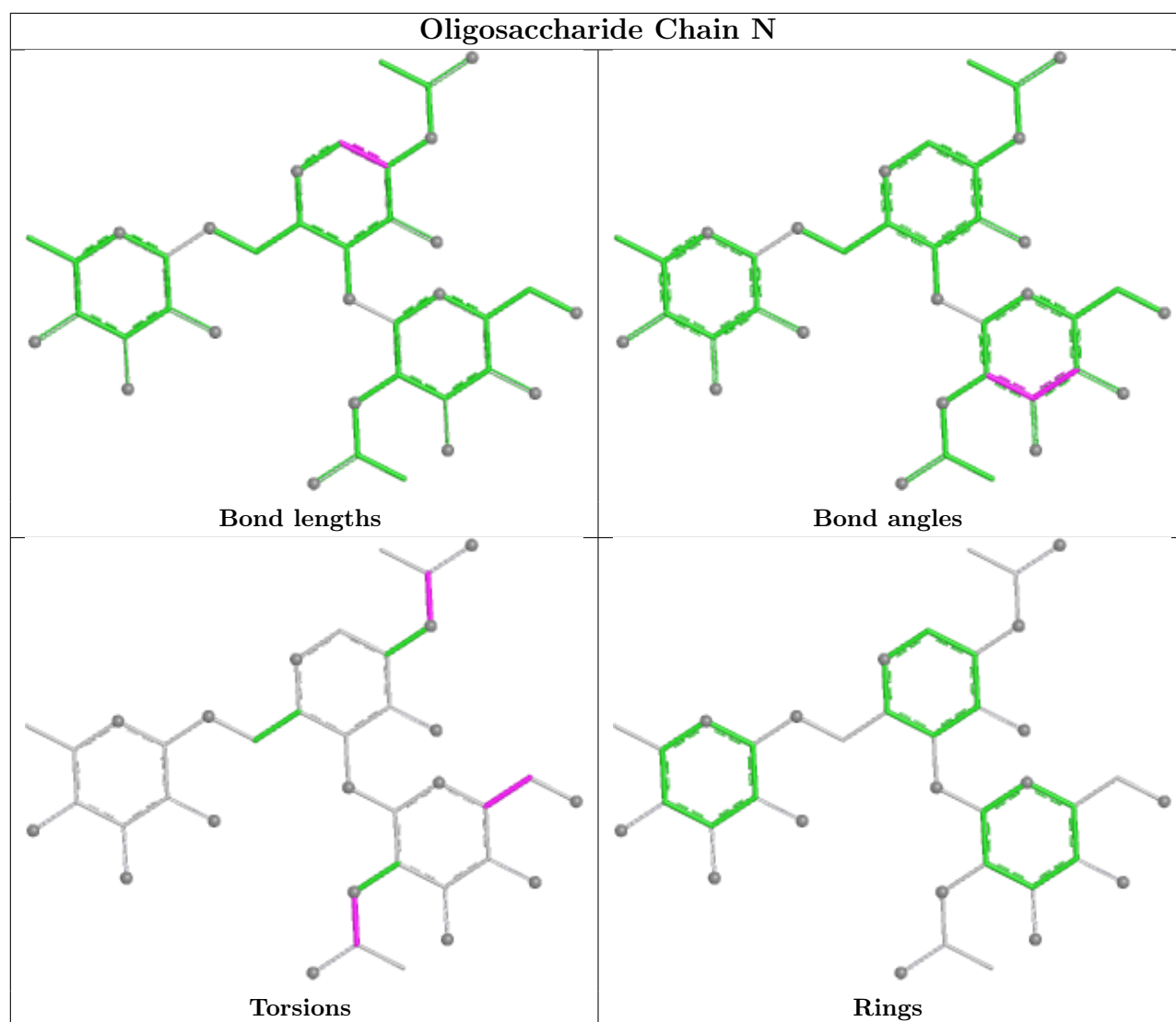


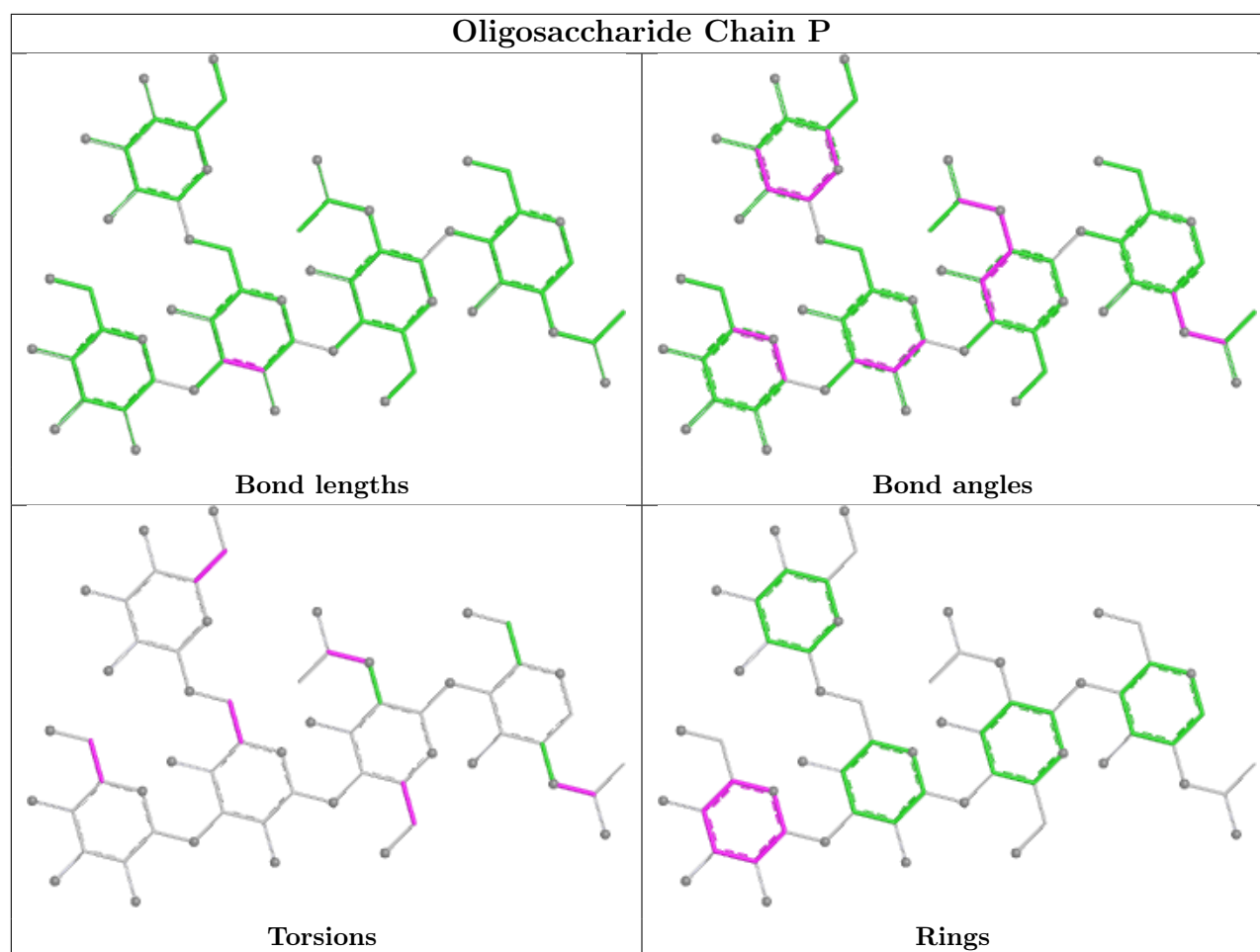












5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
13	NAG	A	724	3	14,14,15	0.92	1 (7%)	17,19,21	0.84	0
13	NAG	B	724	3	14,14,15	0.87	1 (7%)	17,19,21	0.64	0
13	NAG	B	1961	3	14,14,15	1.26	1 (7%)	17,19,21	0.83	1 (5%)
13	NAG	A	1961	3	14,14,15	1.02	0	17,19,21	0.95	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	724	3	1/1/5/7	4/6/23/26	0/1/1/1
13	NAG	B	724	3	-	4/6/23/26	0/1/1/1
13	NAG	B	1961	3	-	4/6/23/26	0/1/1/1
13	NAG	A	1961	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1961	NAG	C1-C2	3.62	1.57	1.52
13	B	724	NAG	C1-C2	2.50	1.55	1.52
13	A	724	NAG	C1-C2	2.34	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1961	NAG	C1-O5-C5	2.75	115.87	112.19
13	B	1961	NAG	C1-O5-C5	2.33	115.31	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	724	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	724	NAG	C8-C7-N2-C2
13	A	724	NAG	O7-C7-N2-C2
13	A	1961	NAG	C8-C7-N2-C2
13	A	1961	NAG	O7-C7-N2-C2
13	B	724	NAG	C8-C7-N2-C2
13	B	724	NAG	O7-C7-N2-C2
13	B	1961	NAG	C8-C7-N2-C2
13	B	1961	NAG	O7-C7-N2-C2
13	B	1961	NAG	O5-C5-C6-O6
13	A	724	NAG	O5-C5-C6-O6
13	A	724	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	B	1961	NAG	C4-C5-C6-O6
13	B	724	NAG	O5-C5-C6-O6
13	B	724	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	724	NAG	1	0
13	B	724	NAG	1	0
13	A	1961	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	C	46/46 (100%)	-0.06	0 100 100	167, 194, 197, 197	0
2	D	46/46 (100%)	-0.02	1 (2%) 62 47	164, 193, 197, 197	0
3	A	661/697 (94%)	0.03	17 (2%) 57 42	108, 144, 182, 191	0
3	B	668/697 (95%)	-0.03	12 (1%) 67 53	109, 144, 179, 189	0
All	All	1421/1486 (95%)	-0.00	30 (2%) 63 48	108, 145, 188, 197	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	80	LEU	4.1
3	B	302	TYR	3.4
3	A	519	ALA	3.3
3	B	663	GLN	3.2
3	A	56	LEU	3.2
3	A	352	GLN	3.2
3	A	652	GLU	3.1
3	B	322	SER	2.8
3	A	242	CYS	2.8
3	A	676	LEU	2.7
3	B	170	LEU	2.7
3	A	243	TRP	2.6
3	B	298	PRO	2.6
3	B	146	GLN	2.6
3	B	103	VAL	2.6
2	D	34	U	2.5
3	B	326	TYR	2.5
3	A	75	SER	2.5
3	A	530	GLU	2.4
3	A	62	GLN	2.4
3	B	318	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	546	TRP	2.2
3	A	690	LEU	2.1
3	A	146	GLN	2.1
3	A	349	PHE	2.1
3	A	321	LEU	2.1
3	B	46	PRO	2.1
3	B	317	SER	2.0
3	A	81	ASP	2.0
3	B	545	LEU	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
9	NAG	R	2	14/15	0.12	0.12	197,197,197,197	0
8	BMA	J	3	11/12	0.20	0.13	186,187,187,187	0
7	MAN	I	5	11/12	0.21	0.19	186,187,187,188	0
11	NAG	N	2	14/15	0.34	0.11	176,179,180,180	0
4	NAG	L	1	14/15	0.38	0.15	173,177,179,183	0
12	MAN	P	4	11/12	0.38	0.09	188,189,190,190	0
10	BMA	M	3	11/12	0.39	0.09	191,193,193,194	0
4	NDG	H	2	14/15	0.41	0.09	184,185,187,188	0
7	MAN	I	4	11/12	0.42	0.11	188,190,191,192	0
10	NAG	M	2	14/15	0.45	0.09	183,184,188,190	0
12	MAN	P	5	11/12	0.47	0.15	185,187,187,188	0
8	BMA	Q	3	11/12	0.51	0.10	190,191,192,192	0
10	NAG	M	1	14/15	0.55	0.12	173,176,179,182	0
4	NDG	L	2	14/15	0.56	0.11	186,188,188,188	0
6	NAG	G	2	14/15	0.59	0.10	179,180,180,180	0
8	NAG	Q	1	14/15	0.63	0.10	168,171,174,177	0
12	MAN	P	3	11/12	0.65	0.11	180,182,186,187	0
7	NAG	I	2	14/15	0.66	0.11	159,162,167,172	0
4	NDG	O	2	14/15	0.68	0.11	172,175,177,177	0

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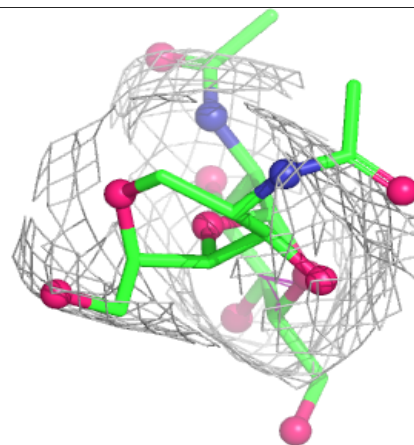
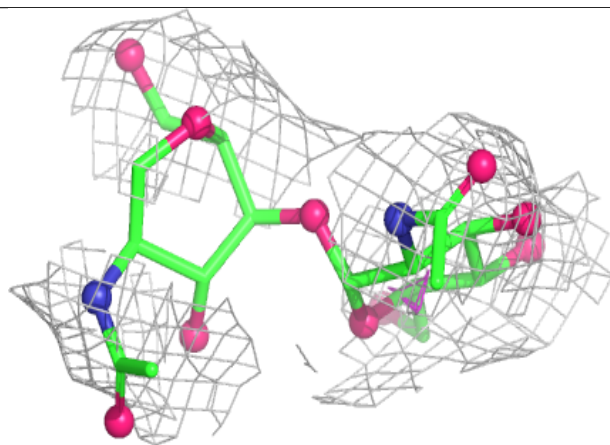
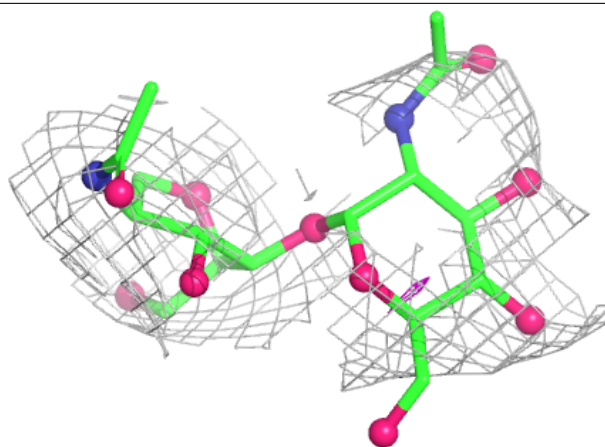
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	O	1	14/15	0.68	0.09	163,167,168,171	0
4	NAG	H	1	14/15	0.69	0.11	168,171,176,180	0
4	NDG	E	2	14/15	0.72	0.07	181,182,182,183	0
9	NAG	K	2	14/15	0.73	0.09	170,172,174,174	0
6	FUC	G	3	10/11	0.74	0.14	189,190,191,191	0
5	MAN	F	3	11/12	0.74	0.09	192,195,196,197	0
7	MAN	I	3	11/12	0.75	0.12	177,180,185,185	0
9	NAG	R	1	14/15	0.76	0.09	160,162,163,163	0
11	FUL	N	3	10/11	0.77	0.13	191,192,192,192	0
8	NAG	J	1	14/15	0.78	0.10	169,173,174,176	0
4	NAG	E	1	14/15	0.78	0.09	171,175,177,179	0
12	NDG	P	2	14/15	0.78	0.12	158,165,169,175	0
8	NDG	J	2	14/15	0.79	0.12	180,182,184,186	0
5	NAG	F	2	14/15	0.79	0.07	183,185,188,191	0
11	NAG	N	1	14/15	0.79	0.12	169,171,173,176	0
6	NAG	G	1	14/15	0.81	0.12	172,176,178,178	0
8	NDG	Q	2	14/15	0.84	0.08	177,181,184,188	0
9	NAG	K	1	14/15	0.86	0.08	160,164,165,168	0
5	NAG	F	1	14/15	0.86	0.07	167,172,176,180	0
7	NAG	I	1	14/15	0.93	0.12	140,145,147,152	0
12	NAG	P	1	14/15	0.94	0.14	141,144,149,155	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.

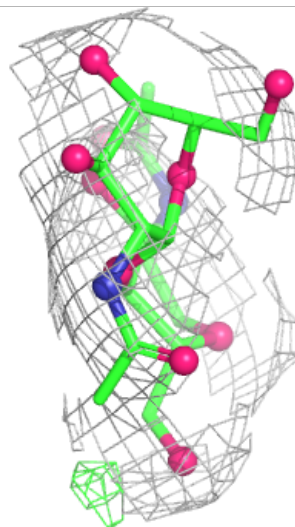
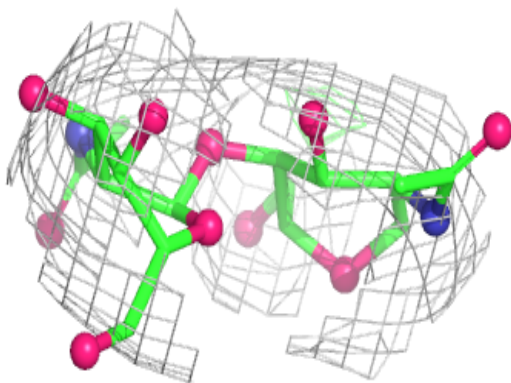
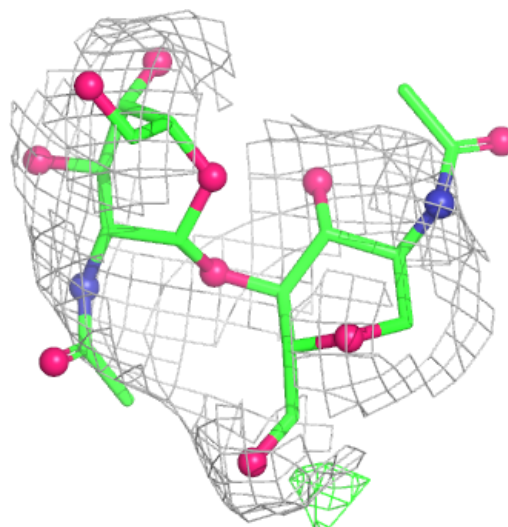
Electron density around Chain E:

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



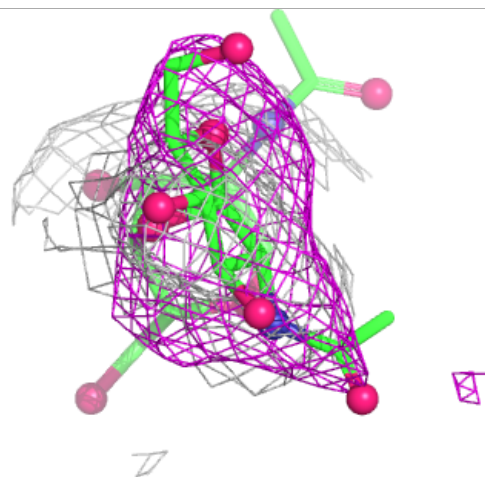
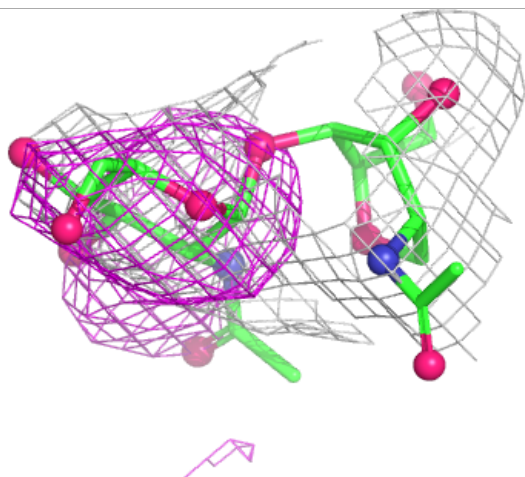
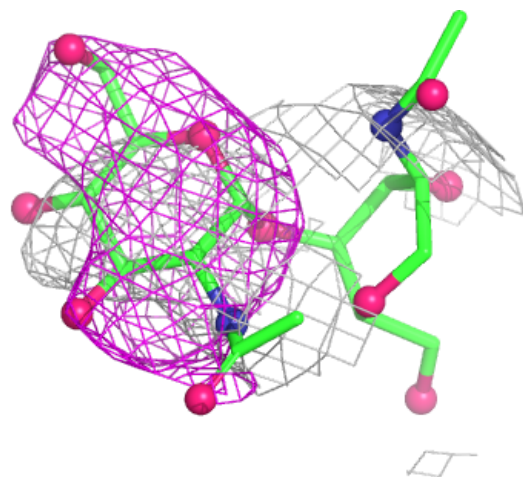
Electron density around Chain H:

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



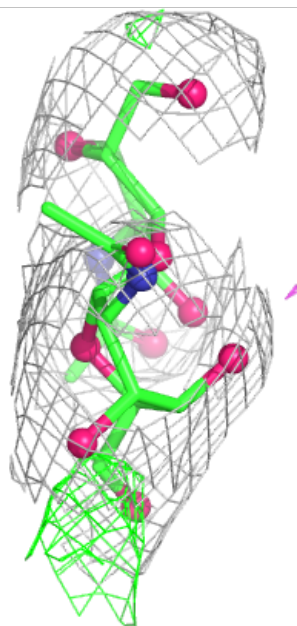
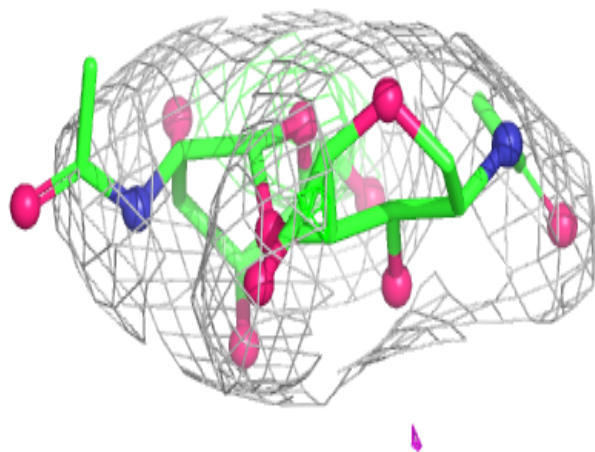
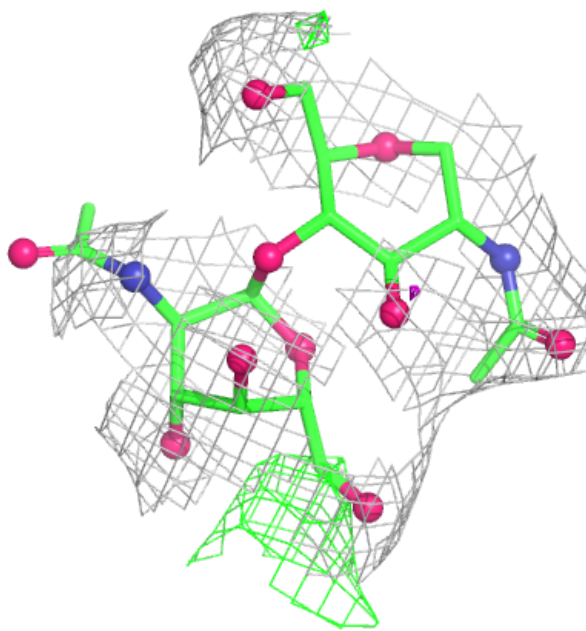
Electron density around Chain L:

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



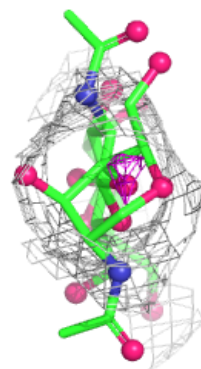
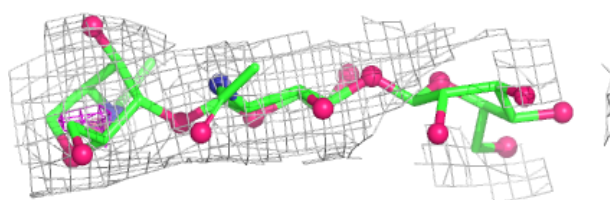
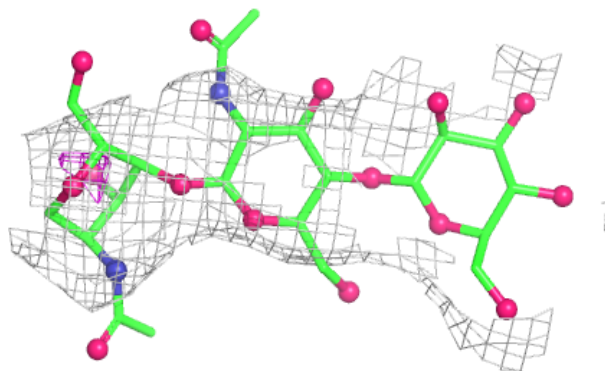
Electron density around Chain O:

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



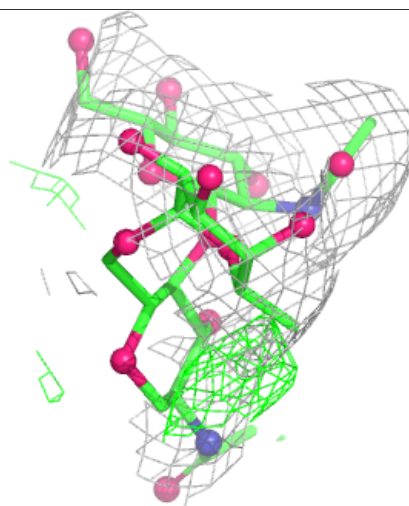
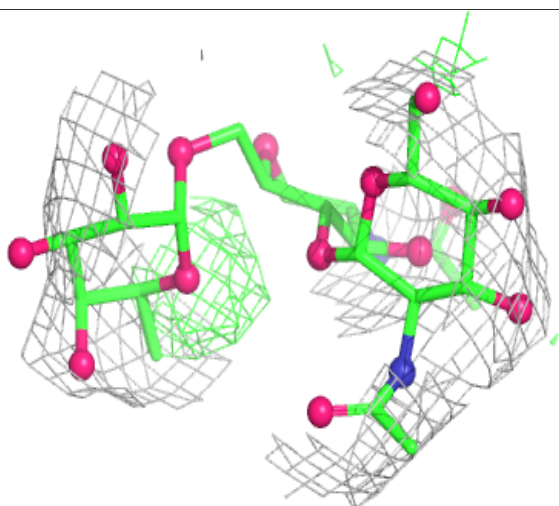
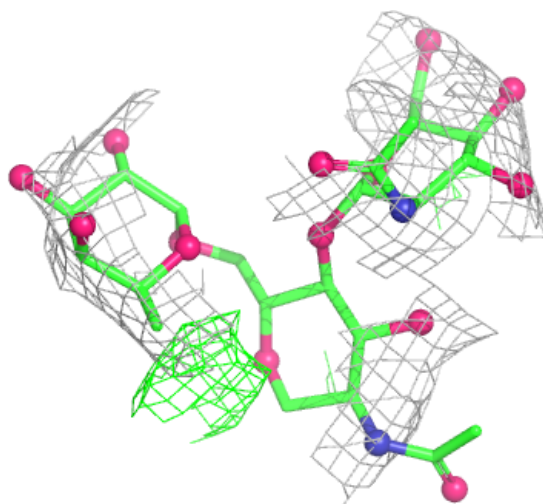
Electron density around Chain F:

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



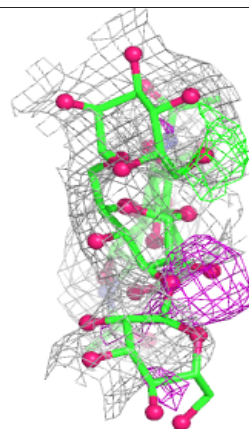
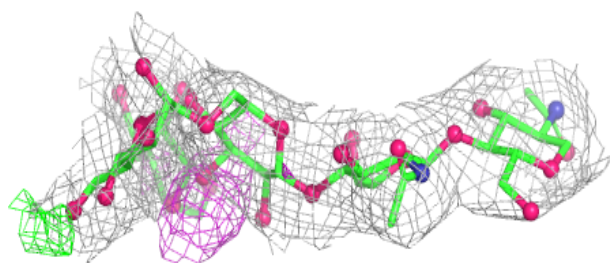
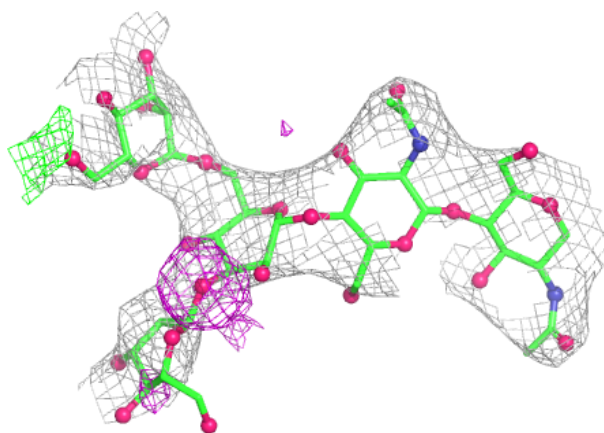
Electron density around Chain G:

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

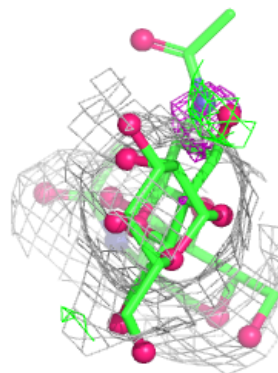
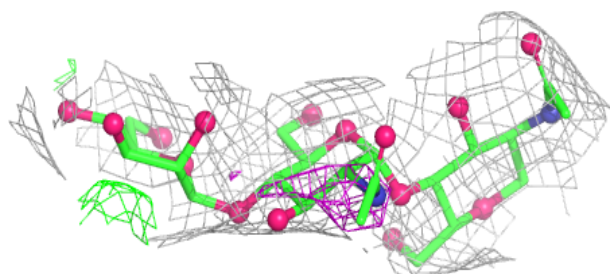
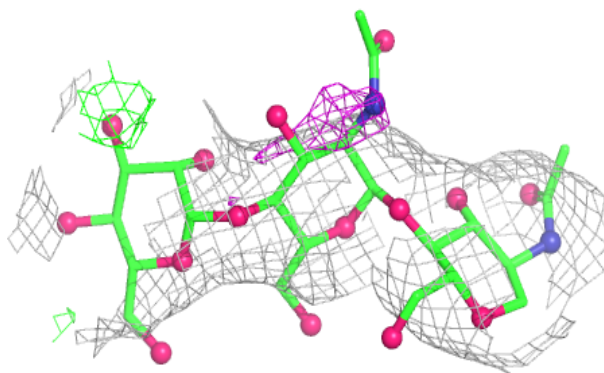


Electron density around Chain I:

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

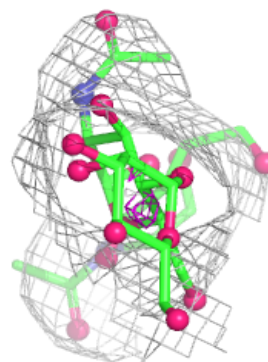
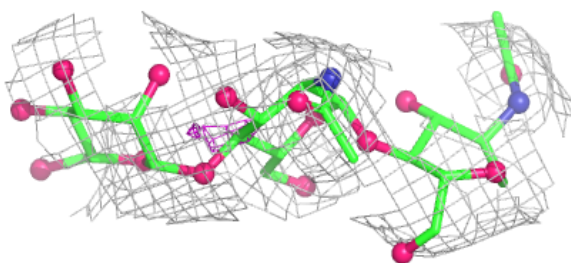
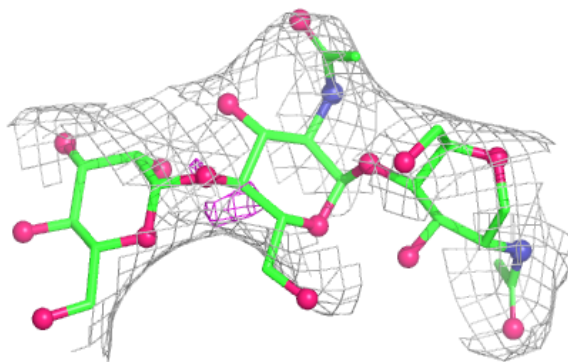
**Electron density around Chain J:**

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

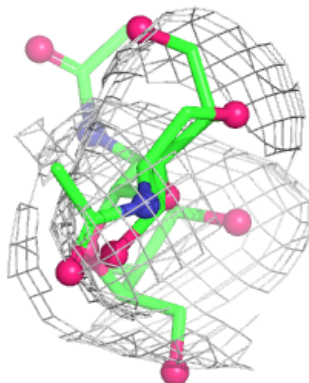
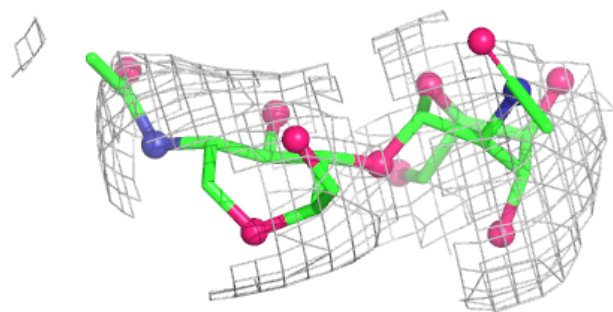
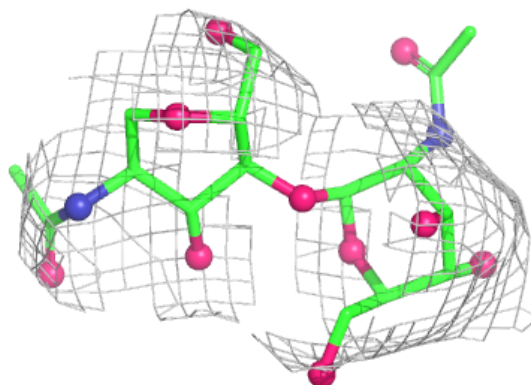


Electron density around Chain Q:

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

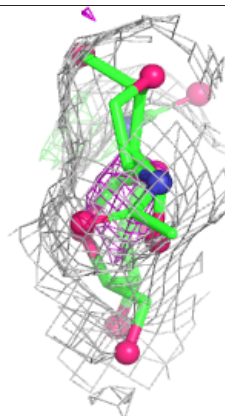
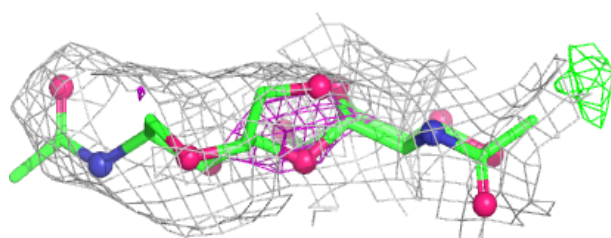
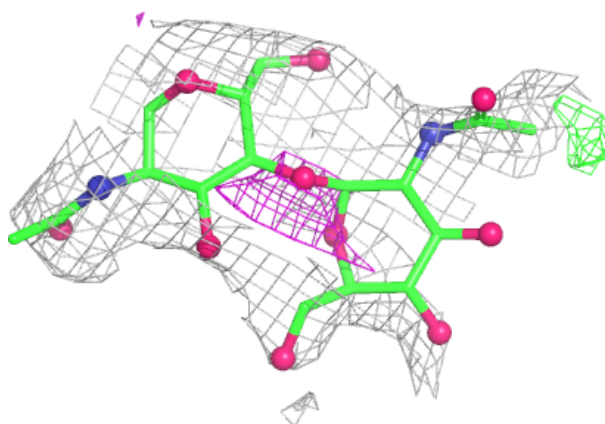
**Electron density around Chain K:**

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

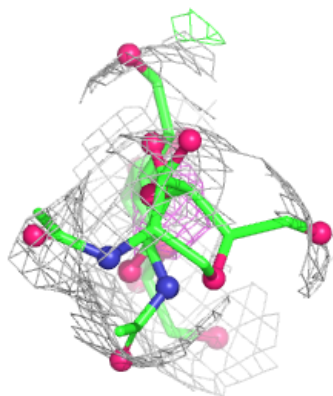
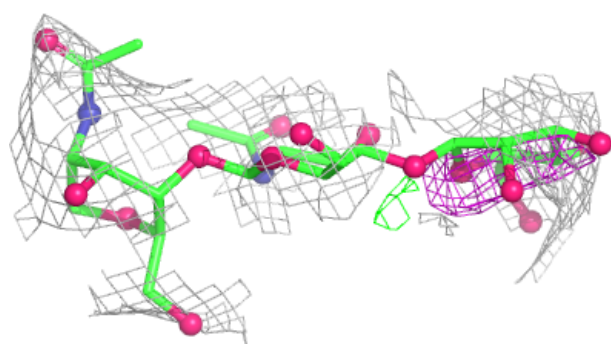
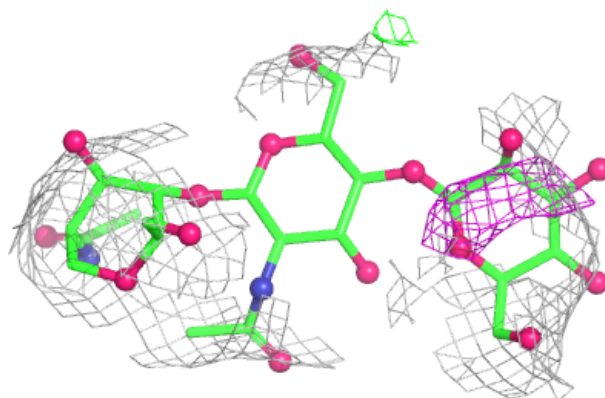


Electron density around Chain R:

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

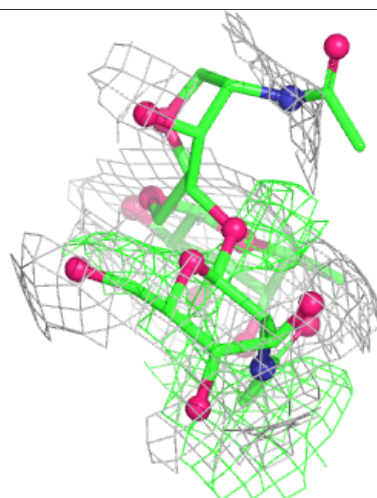
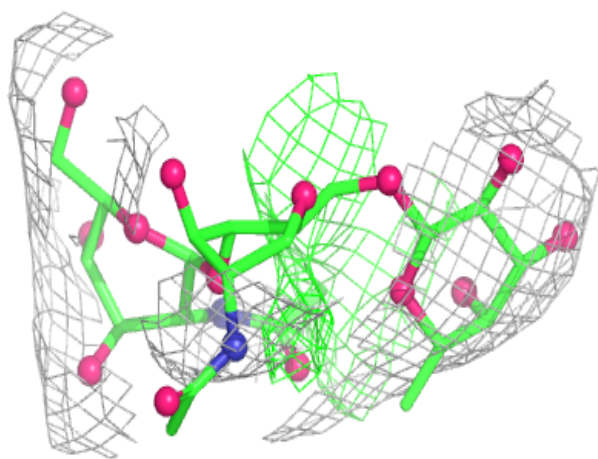
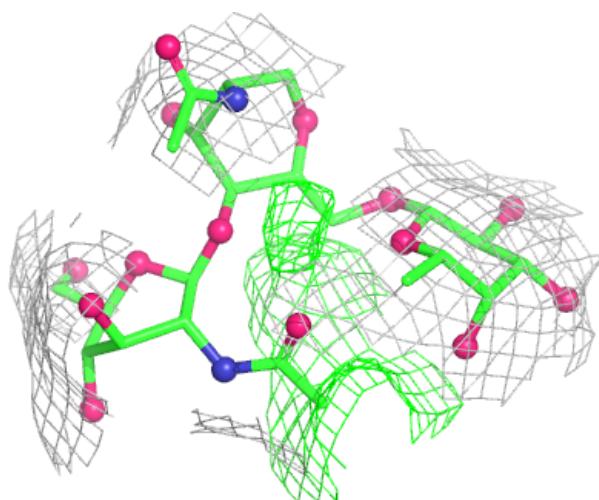
**Electron density around Chain M:**

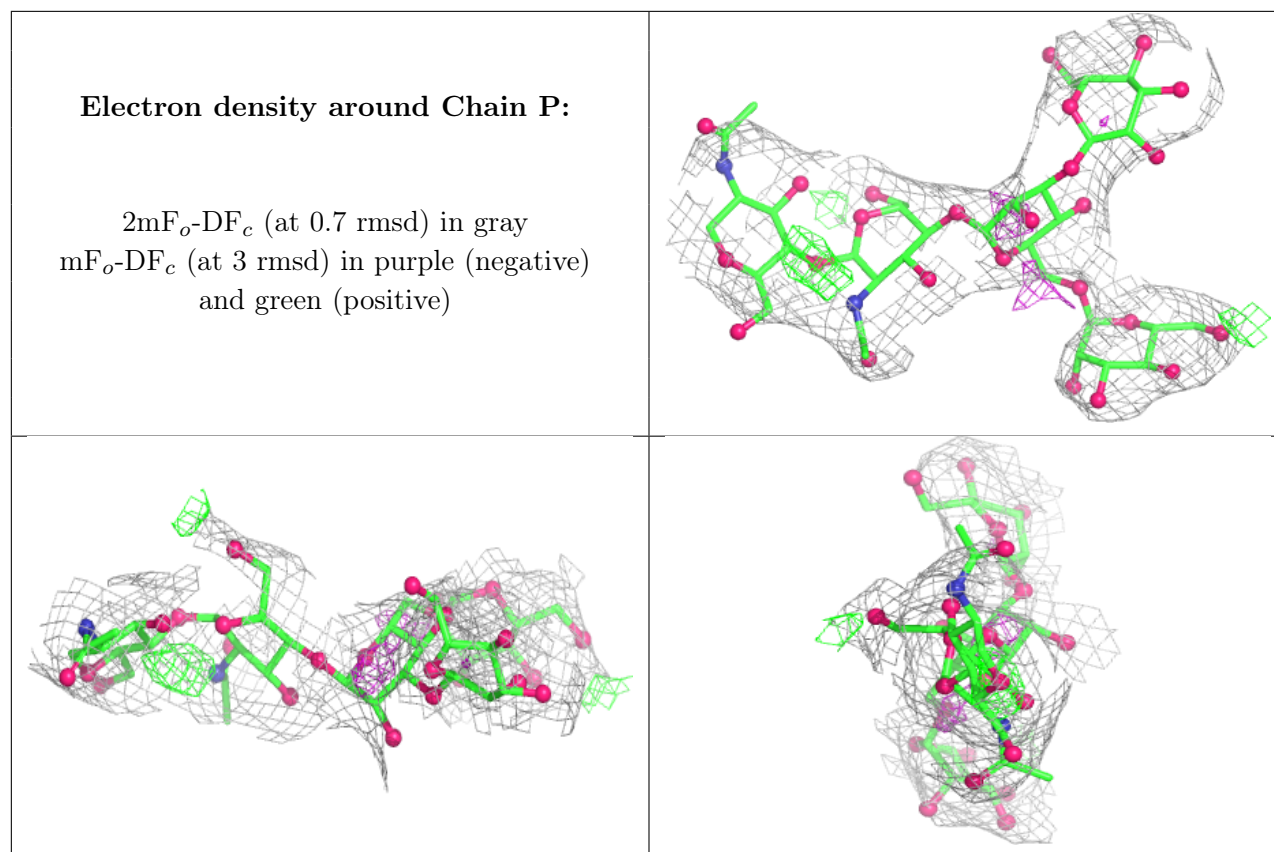
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
13	NAG	A	724	14/15	0.27	0.10	196,197,197,197	0
13	NAG	A	1961	14/15	0.46	0.10	182,186,187,187	0
13	NAG	B	724	14/15	0.62	0.10	189,190,190,190	0
13	NAG	B	1961	14/15	0.70	0.08	181,183,184,184	0

6.5 Other polymers [i](#)

There are no such residues in this entry.