



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 4D69 / pdb_00004d69
Title : SOYBEAN AGGLUTININ FROM GLYCINE MAX IN COMPLEX WITH THE ANTIGEN Tn
Authors : Madariaga, D.; Martinez-Saez, N.; Somovilla, V.J.; Coelho, H.; Valero-Gonzalez, J.; Castro-Lopez, J.; Asensio, J.L.; Jimenez-Barbero, J.; Busto, J.H.; Avenoza, A.; Marcelo, F.; Hurtado-Guerrero, R.; Corzana, F.; Peregrina, J.M.
Deposited on : 2014-11-10
Resolution : 2.70 Å(reported)

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

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

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:

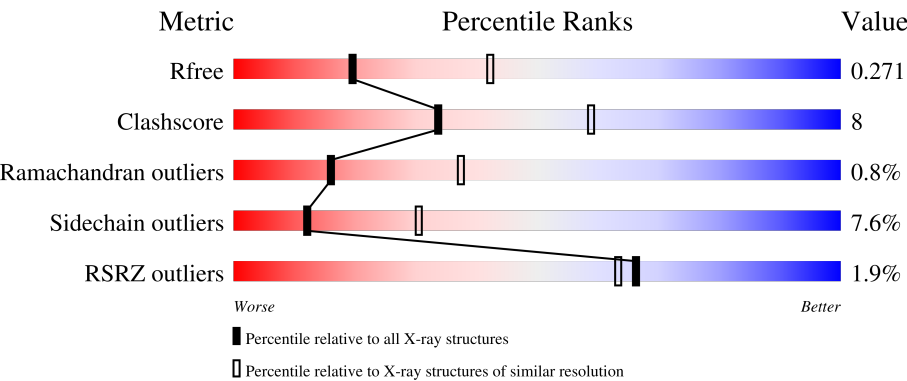
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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 2.70 Å.

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



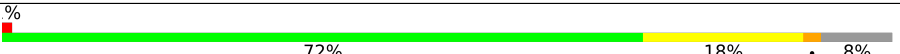
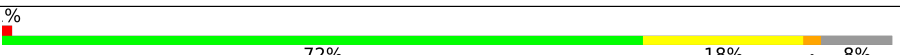
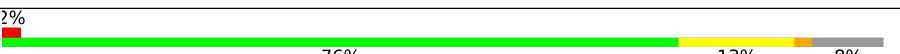
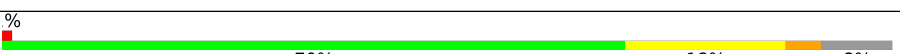
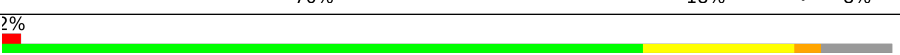
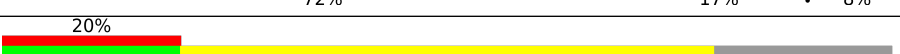
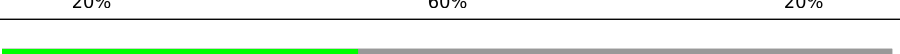
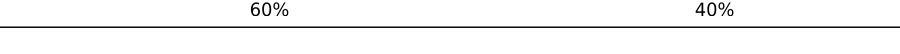
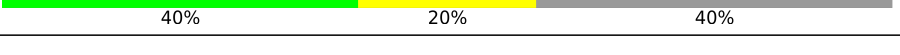
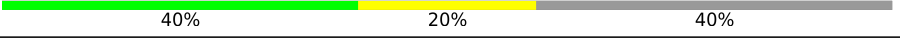
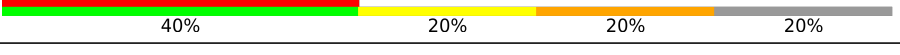
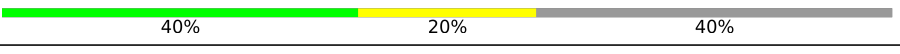
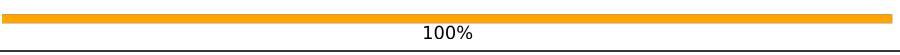
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	253	3% 74%14%•8%
1	B	253	% 74%15%•8%
1	C	253	4% 72%18%•9%
1	D	253	% 79%11%•8%

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Mol	Chain	Length	Quality of chain
1	E	253	
1	F	253	
1	G	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	253	
2	O	5	
2	P	5	
2	Q	5	
2	R	5	
2	S	5	
2	T	5	
2	U	5	
2	V	5	
2	W	5	
2	X	5	
2	Y	5	
2	Z	5	
3	M	2	
3	N	2	
3	a	2	
3	b	2	
3	c	2	

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Mol	Chain	Length	Quality of chain
3	d	2	 50%50%
3	e	2	 50%50%
3	f	2	 50%50%
3	g	2	 50%50%
3	h	2	 50%50%
3	i	2	 100%
3	j	2	 50%50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A2G	J	1235	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22512 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1809	1157	301	350	1			
1	B	232	Total	C	N	O	S	0	0	0
			1793	1148	297	347	1			
1	C	231	Total	C	N	O	S	0	0	0
			1790	1147	298	344	1			
1	D	234	Total	C	N	O	S	0	0	0
			1809	1157	301	350	1			
1	E	231	Total	C	N	O	S	0	0	0
			1790	1147	298	344	1			
1	F	234	Total	C	N	O	S	0	0	0
			1809	1157	301	350	1			
1	G	233	Total	C	N	O	S	0	0	0
			1803	1154	300	348	1			
1	H	232	Total	C	N	O	S	0	1	0
			1805	1156	300	348	1			
1	I	234	Total	C	N	O	S	0	0	0
			1809	1157	301	350	1			
1	J	232	Total	C	N	O	S	0	0	0
			1797	1151	299	346	1			
1	K	232	Total	C	N	O	S	0	1	0
			1805	1156	300	348	1			
1	L	232	Total	C	N	O	S	0	0	0
			1799	1152	299	347	1			

- Molecule 2 is a protein called SHORT ANTIGEN PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	4	Total	C	N	O	0	0	0
			33	19	7	7			
2	P	2	Total	C	N	O	0	0	0
			15	8	2	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	2	Total	C	N	O	0	0	0
			15	8	2	5			
2	R	3	Total	C	N	O	0	0	0
			26	14	6	6			
2	S	1	Total	C	N	O	0	0	0
			7	4	1	2			
2	T	2	Total	C	N	O	0	0	0
			15	8	2	5			
2	U	3	Total	C	N	O	0	0	0
			22	13	3	6			
2	V	3	Total	C	N	O	0	0	0
			26	14	6	6			
2	W	2	Total	C	N	O	0	0	0
			15	8	2	5			
2	X	4	Total	C	N	O	0	0	0
			33	19	7	7			
2	Y	3	Total	C	N	O	0	0	0
			26	14	6	6			
2	Z	2	Total	C	N	O	0	0	0
			15	8	2	5			

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



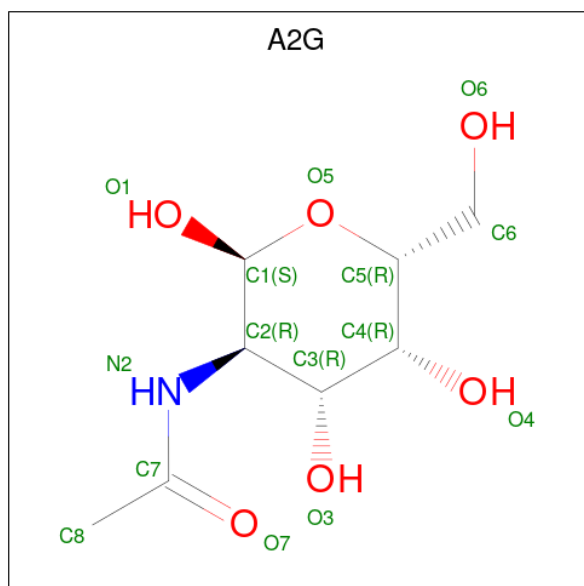
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	g	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	h	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	i	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	j	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mn	0	0
			2	2		
5	B	2	Total	Mn	0	0
			2	2		
5	C	2	Total	Mn	0	0
			2	2		
5	D	2	Total	Mn	0	0
			2	2		
5	E	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		
5	G	2	Total	Mn	0	0
			2	2		
5	H	2	Total	Mn	0	0
			2	2		
5	I	2	Total	Mn	0	0
			2	2		
5	J	2	Total	Mn	0	0
			2	2		
5	K	2	Total	Mn	0	0
			2	2		
5	L	2	Total	Mn	0	0
			2	2		

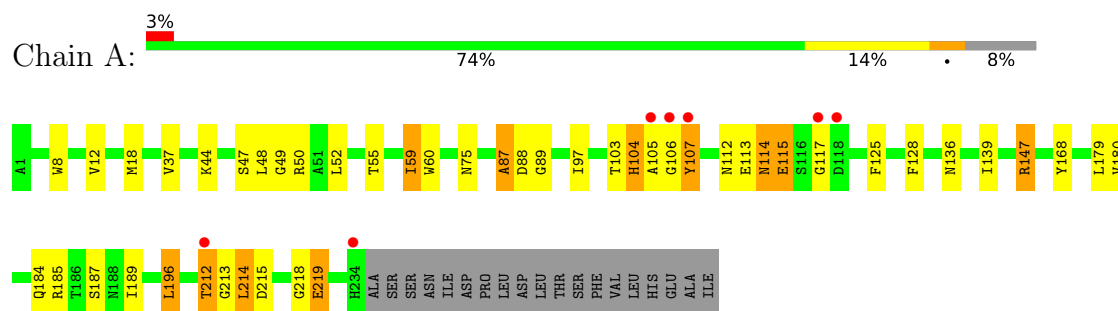
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total O 11 11	0	0
6	B	7	Total O 7 7	0	0
6	C	9	Total O 9 9	0	0
6	D	16	Total O 16 16	0	0
6	E	11	Total O 11 11	0	0
6	F	10	Total O 10 10	0	0
6	G	7	Total O 7 7	0	0
6	H	11	Total O 11 11	0	0
6	I	12	Total O 12 12	0	0
6	J	5	Total O 5 5	0	0
6	K	7	Total O 7 7	0	0
6	L	12	Total O 12 12	0	0

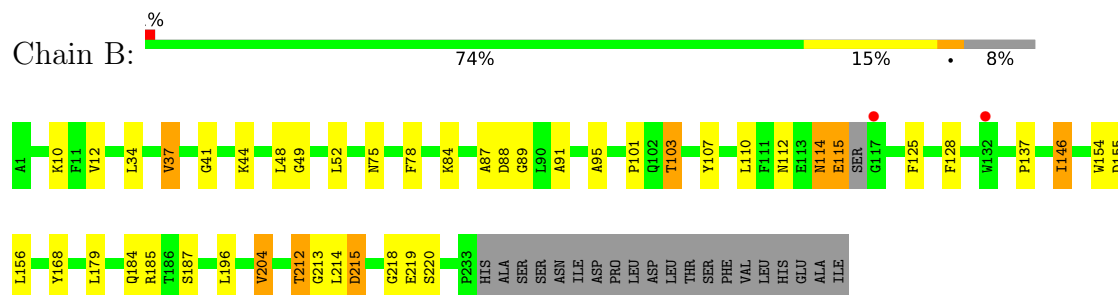
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

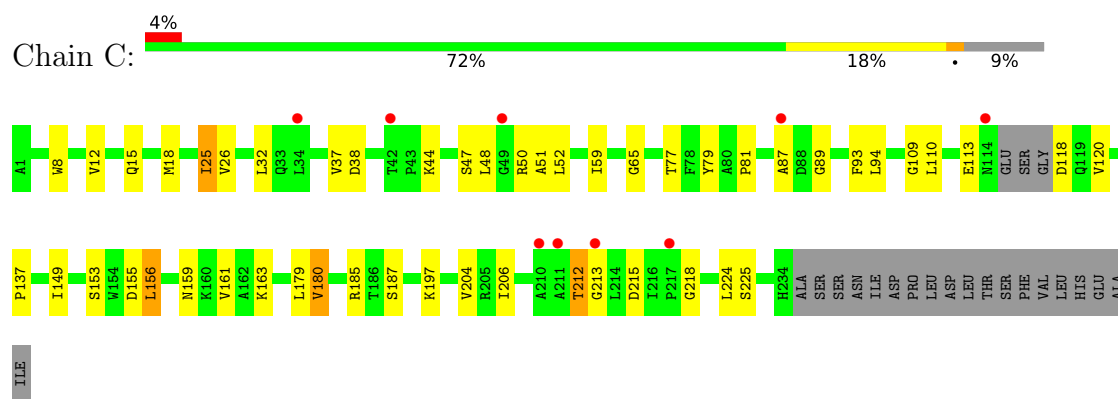
• Molecule 1: LECTIN



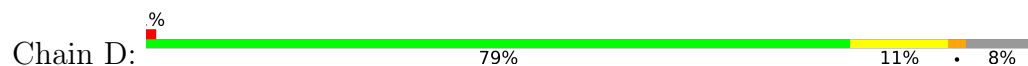
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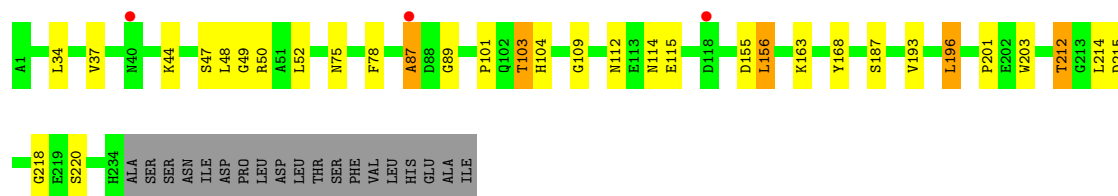


• Molecule 1: LECTIN

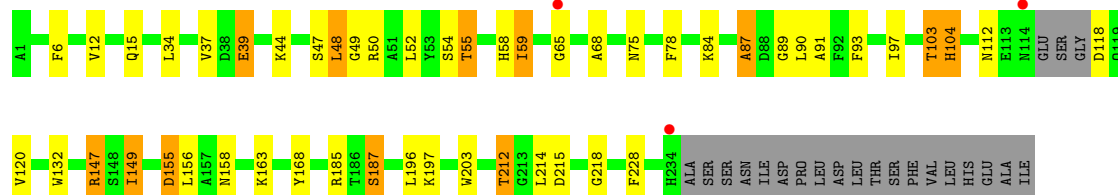


• Molecule 1: LECTIN

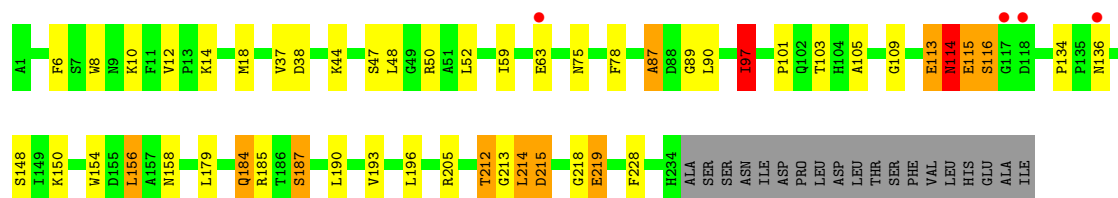




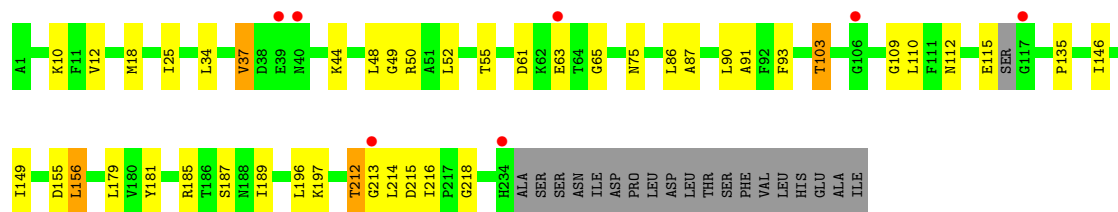
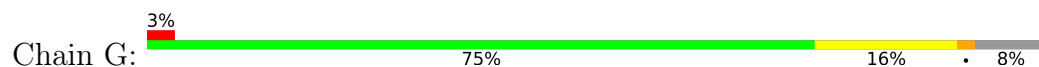
• Molecule 1: LECTIN



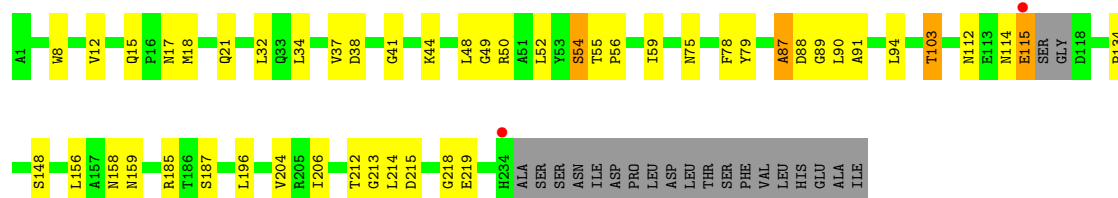
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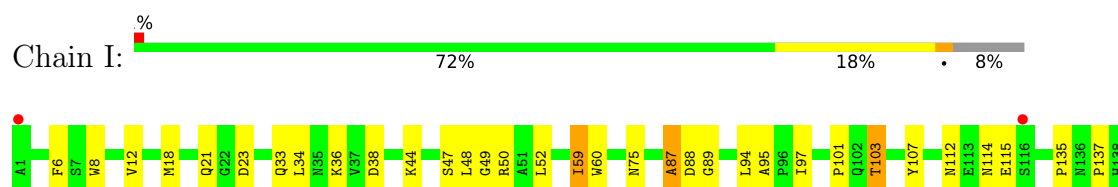
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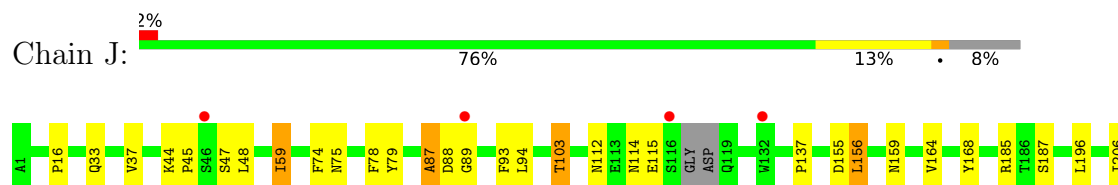
• Molecule 1: LECTIN



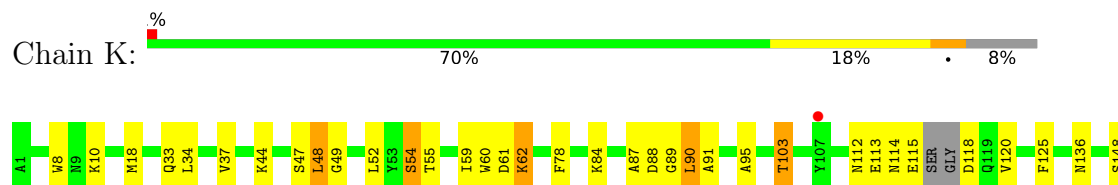
• Molecule 1: LECTIN



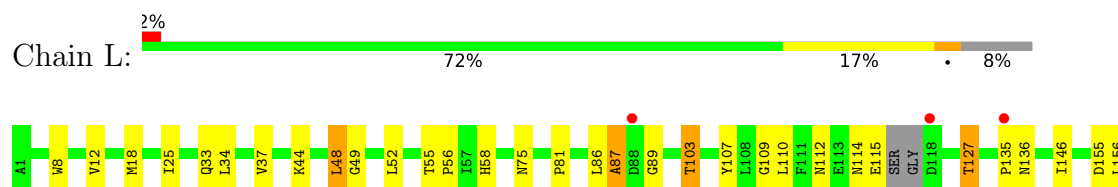
- Molecule 1: LECTIN



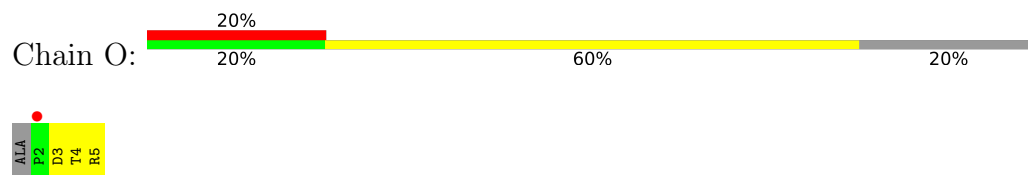
- Molecule 1: LECTIN



- Molecule 1: LECTIN

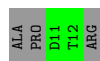


- Molecule 2: SHORT ANTIGEN PEPTIDE



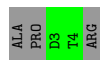
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain P:  40% 60%



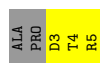
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain Q:  40% 60%



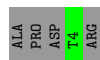
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain R:  60% 40%



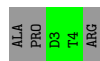
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain S:  20% 80%

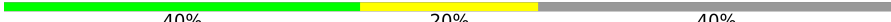


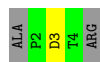
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain T:  40% 60%

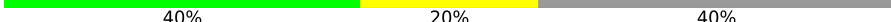


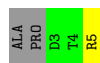
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain U:  40% 20% 40%



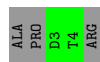
- Molecule 2: SHORT ANTIGEN PEPTIDE

Chain V:  40% 20% 40%

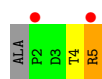


- Molecule 2: SHORT ANTIGEN PEPTIDE

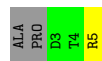
Chain W:  40% 60%



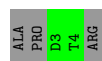
- Molecule 2: SHORT ANTIGEN PEPTIDE



- Molecule 2: SHORT ANTIGEN PEPTIDE



- Molecule 2: SHORT ANTIGEN PEPTIDE



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



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



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



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



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

Chain c:  50% 50%

MAG1
MAG2

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

Chain d:  50% 50%

MAG1
MAG2

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

Chain e:  50% 50%

MAG1
MAG2

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

Chain f:  50% 50%

MAG1
MAG2

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

Chain g:  50% 50%

MAG1
MAG2

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

Chain h:  50% 50%

MAG1
MAG2

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

Chain i:  100%

MAG1
MAG2

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

Chain j:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	114.23Å 114.23Å 202.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	202.89 – 2.70 98.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (202.89-2.70) 99.7 (98.93-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.230 , 0.274 0.233 , 0.271	Depositor DCC
R_{free} test set	2232 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.037 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22512	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, A2G, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	1/1858 (0.1%)	0.93	6/2540 (0.2%)
1	B	0.75	0/1840	0.93	3/2514 (0.1%)
1	C	0.82	0/1838	0.95	2/2512 (0.1%)
1	D	0.80	0/1858	0.93	2/2540 (0.1%)
1	E	1.01	2/1838 (0.1%)	1.11	7/2512 (0.3%)
1	F	0.83	0/1858	1.00	6/2540 (0.2%)
1	G	0.79	0/1851	0.91	1/2529 (0.0%)
1	H	0.95	2/1856 (0.1%)	1.03	7/2536 (0.3%)
1	I	0.82	0/1858	0.94	4/2540 (0.2%)
1	J	0.74	0/1845	0.92	4/2521 (0.2%)
1	K	1.07	2/1856 (0.1%)	0.97	5/2536 (0.2%)
1	L	0.81	0/1847	1.03	6/2524 (0.2%)
2	O	0.91	0/33	1.08	0/43
2	P	0.74	0/14	0.55	0/18
2	Q	1.02	0/14	0.46	0/18
2	R	0.89	0/25	1.03	0/32
2	S	0.92	0/6	0.56	0/7
2	T	1.07	0/14	0.65	0/18
2	U	0.92	0/22	0.79	0/29
2	V	0.81	0/25	0.66	0/32
2	W	0.90	0/14	0.80	0/18
2	X	0.59	0/33	1.29	0/43
2	Y	0.89	0/25	0.76	0/32
2	Z	0.72	0/14	1.03	0/18
All	All	0.86	7/22442 (0.0%)	0.97	53/30652 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
1	K	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	54	SER	C-N	-27.75	0.89	1.33
1	E	54	SER	C-N	-23.17	0.95	1.33
1	H	55	THR	C-N	-19.81	1.08	1.33
1	H	54	SER	C-N	-10.59	0.95	1.33
1	E	55	THR	C-N	-6.03	1.25	1.33
1	K	55	THR	C-N	-5.98	1.25	1.33
1	A	55	THR	C-N	5.01	1.40	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	SER	CA-C-N	18.75	147.67	121.61
1	E	54	SER	C-N-CA	18.75	147.67	121.61
1	L	135	PRO	N-CA-C	16.58	146.63	112.47
1	H	55	THR	O-C-N	-12.91	100.42	121.59
1	L	136	ASN	N-CA-CB	-12.83	87.53	110.37
1	E	54	SER	O-C-N	-12.64	108.94	122.09
1	B	115	GLU	CB-CA-C	-10.10	90.92	110.10
1	K	54	SER	O-C-N	-9.74	111.79	122.12
1	B	115	GLU	N-CA-C	-8.29	87.80	111.00
1	K	54	SER	CA-C-N	7.98	134.28	121.83
1	K	54	SER	C-N-CA	7.98	134.28	121.83
1	C	89	GLY	N-CA-C	7.73	120.87	110.43
1	F	89	GLY	N-CA-C	7.69	120.81	110.43
1	A	104	HIS	N-CA-C	7.62	121.19	112.57
1	J	89	GLY	N-CA-C	7.49	120.55	110.43
1	F	134	PRO	CA-C-N	-7.14	113.31	120.31
1	F	134	PRO	C-N-CA	-7.14	113.31	120.31
1	K	89	GLY	N-CA-C	7.10	120.01	110.43
1	H	55	THR	CA-C-N	7.02	127.58	120.14
1	H	55	THR	C-N-CA	7.02	127.58	120.14
1	H	89	GLY	N-CA-C	6.96	120.42	110.46
1	E	55	THR	O-C-N	6.84	127.65	121.35
1	D	89	GLY	N-CA-C	6.81	120.55	110.60
1	L	89	GLY	N-CA-C	6.59	119.33	110.43
1	B	89	GLY	N-CA-C	6.54	120.15	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	89	GLY	N-CA-C	6.45	120.01	110.60
1	I	87	ALA	N-CA-C	6.40	118.20	109.11
1	L	232	LEU	CA-C-N	6.23	127.63	119.84
1	L	232	LEU	C-N-CA	6.23	127.63	119.84
1	A	89	GLY	N-CA-C	6.09	119.49	110.60
1	A	55	THR	CA-C-N	-6.09	113.70	119.85
1	A	55	THR	C-N-CA	-6.09	113.70	119.85
1	I	89	GLY	N-CA-C	6.04	118.58	110.43
1	D	87	ALA	N-CA-C	5.91	117.50	109.11
1	F	87	ALA	N-CA-C	5.89	117.47	109.11
1	E	87	ALA	N-CA-C	5.75	117.28	109.11
1	J	216	ILE	CA-C-N	-5.62	112.82	119.84
1	J	216	ILE	C-N-CA	-5.62	112.82	119.84
1	H	87	ALA	N-CA-C	5.61	117.07	109.11
1	J	87	ALA	N-CA-C	5.51	117.64	107.73
1	H	134	PRO	CA-C-N	-5.34	114.75	120.03
1	H	134	PRO	C-N-CA	-5.34	114.75	120.03
1	E	93	PHE	N-CA-C	5.33	116.38	108.60
1	C	161	VAL	CB-CA-C	-5.20	105.00	111.08
1	F	115	GLU	N-CA-C	-5.17	105.83	111.82
1	F	97	ILE	CB-CA-C	-5.15	102.84	111.29
1	I	181	TYR	CA-C-N	-5.12	113.64	119.28
1	I	181	TYR	C-N-CA	-5.12	113.64	119.28
1	G	93	PHE	N-CA-C	5.10	116.59	108.79
1	A	87	ALA	N-CA-C	5.07	116.31	109.11
1	L	87	ALA	N-CA-C	5.07	116.31	109.11
1	A	107	TYR	N-CA-C	-5.05	106.71	112.92
1	K	55	THR	O-C-N	-5.01	115.80	121.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	54	SER	Mainchain,Peptide
1	K	54	SER	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1767	34	0
1	B	1793	0	1754	26	0
1	C	1790	0	1752	35	0
1	D	1809	0	1767	19	0
1	E	1790	0	1751	26	1
1	F	1809	0	1767	39	0
1	G	1803	0	1761	19	1
1	H	1805	0	1765	24	0
1	I	1809	0	1767	32	0
1	J	1797	0	1759	30	0
1	K	1805	0	1765	32	0
1	L	1799	0	1758	23	0
2	O	33	0	30	2	0
2	P	15	0	9	0	0
2	Q	15	0	9	0	0
2	R	26	0	22	1	0
2	S	7	0	5	0	0
2	T	15	0	9	0	0
2	U	22	0	17	0	0
2	V	26	0	22	1	0
2	W	15	0	9	0	0
2	X	33	0	30	10	0
2	Y	26	0	22	1	0
2	Z	15	0	9	0	0
3	M	28	0	25	3	0
3	N	28	0	25	1	0
3	a	28	0	25	2	0
3	b	28	0	25	1	0
3	c	28	0	25	1	0
3	d	28	0	25	1	0
3	e	28	0	25	1	0
3	f	28	0	25	1	0
3	g	28	0	25	1	0
3	h	28	0	25	1	0
3	i	28	0	25	1	0
3	j	28	0	25	1	0
4	A	14	0	12	2	0
4	B	14	0	12	2	0
4	C	14	0	12	0	0
4	D	14	0	12	0	0
4	E	14	0	12	0	0
4	F	14	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	14	0	12	0	0
4	H	14	0	12	0	0
4	I	14	0	12	0	0
4	J	14	0	12	9	0
4	K	14	0	12	0	0
4	L	14	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0
5	K	2	0	0	0	0
5	L	2	0	0	0	0
6	A	11	0	0	0	0
6	B	7	0	0	1	0
6	C	9	0	0	0	0
6	D	16	0	0	0	0
6	E	11	0	0	0	0
6	F	10	0	0	0	0
6	G	7	0	0	0	0
6	H	11	0	0	1	0
6	I	12	0	0	1	0
6	J	5	0	0	1	0
6	K	7	0	0	1	0
6	L	12	0	0	1	0
All	All	22512	0	21770	339	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:ASN:OD1	1:F:116:SER:N	1.74	1.20
1:F:87:ALA:HB2	1:F:218:GLY:HA3	1.25	1.16
1:J:87:ALA:HB2	1:J:218:GLY:HA3	1.21	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:ILE:HG12	4:J:1235:A2G:C6	1.83	1.09
1:A:87:ALA:HB2	1:A:218:GLY:HA3	1.35	1.08
1:H:87:ALA:HB2	1:H:218:GLY:HA3	1.37	1.06
1:C:87:ALA:HB2	1:C:218:GLY:HA3	1.33	1.05
1:L:87:ALA:HB2	1:L:218:GLY:HA3	1.37	1.05
1:D:87:ALA:HB2	1:D:218:GLY:HA3	1.36	1.04
1:G:87:ALA:HB2	1:G:218:GLY:HA3	1.39	1.04
1:B:87:ALA:HB2	1:B:218:GLY:HA3	1.40	1.04
1:E:87:ALA:HB2	1:E:218:GLY:HA3	1.35	1.03
1:J:216:ILE:HD11	4:J:1235:A2G:H14	1.41	0.99
1:I:87:ALA:HB2	1:I:218:GLY:HA3	1.47	0.96
1:A:105:ALA:O	1:A:107:TYR:N	2.00	0.93
1:J:216:ILE:CD1	4:J:1235:A2G:H14	1.96	0.93
1:K:87:ALA:HB2	1:K:218:GLY:HA3	1.52	0.91
1:J:216:ILE:CG1	4:J:1235:A2G:C6	2.52	0.88
1:F:44:LYS:O	1:F:212:THR:HG21	1.76	0.85
1:K:44:LYS:O	1:K:212:THR:HG21	1.79	0.83
1:J:44:LYS:O	1:J:212:THR:HG21	1.81	0.81
1:F:113:GLU:N	1:F:113:GLU:OE1	2.12	0.81
1:G:44:LYS:O	1:G:212:THR:HG21	1.81	0.80
1:H:44:LYS:O	1:H:212:THR:HG21	1.81	0.80
1:A:8:TRP:HZ2	1:A:18:MET:HE1	1.47	0.79
1:A:136:ASN:OD1	1:G:149:ILE:HB	1.82	0.79
1:B:114:ASN:O	1:B:115:GLU:C	2.25	0.79
1:D:44:LYS:O	1:D:212:THR:HG21	1.84	0.77
1:J:216:ILE:HG12	4:J:1235:A2G:H6	1.66	0.77
4:F:1239:A2G:H8A	2:X:5:ARG:HG3	1.67	0.77
1:J:216:ILE:CG1	4:J:1235:A2G:H14	2.12	0.77
1:L:44:LYS:O	1:L:212:THR:HG21	1.86	0.76
1:I:44:LYS:O	1:I:212:THR:HG21	1.88	0.74
1:G:75:ASN:HD21	3:e:1:NAG:H83	1.52	0.73
1:A:75:ASN:HD21	3:M:1:NAG:H83	1.55	0.72
1:B:75:ASN:HD21	3:N:1:NAG:H83	1.55	0.71
1:F:114:ASN:OD1	1:F:115:GLU:N	2.23	0.71
1:F:8:TRP:CZ2	1:F:18:MET:HE1	2.25	0.70
1:J:215:ASP:OD1	1:J:215:ASP:N	2.22	0.70
1:B:88:ASP:HA	6:B:2003:HOH:O	1.90	0.70
1:C:44:LYS:O	1:C:212:THR:HG21	1.91	0.69
1:H:75:ASN:HD21	3:f:1:NAG:H83	1.58	0.69
1:J:87:ALA:CB	1:J:218:GLY:HA3	2.12	0.68
1:A:8:TRP:CZ2	1:A:18:MET:HE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ALA:CB	1:C:218:GLY:HA3	2.18	0.68
1:F:8:TRP:CH2	1:F:18:MET:HE1	2.29	0.67
1:C:8:TRP:HZ2	1:C:18:MET:HE1	1.60	0.66
1:E:44:LYS:O	1:E:212:THR:HG21	1.96	0.66
1:A:44:LYS:O	1:A:212:THR:HG21	1.96	0.66
1:C:87:ALA:HB1	1:C:213:GLY:N	2.11	0.66
1:G:87:ALA:HB1	1:G:213:GLY:N	2.11	0.66
1:B:44:LYS:O	1:B:212:THR:HG21	1.97	0.65
1:J:79:TYR:HD1	1:J:159:ASN:HD21	1.45	0.65
1:F:59:ILE:HG23	1:F:196:LEU:HD23	1.78	0.64
1:J:45:PRO:HB3	1:J:214:LEU:O	1.99	0.63
1:K:48:LEU:C	1:K:48:LEU:HD23	2.23	0.63
1:A:48:LEU:C	1:A:48:LEU:HD23	2.24	0.62
1:J:75:ASN:HD21	3:h:1:NAG:H83	1.65	0.62
1:K:87:ALA:HB1	1:K:213:GLY:N	2.14	0.61
3:a:1:NAG:H82	3:a:1:NAG:O3	1.99	0.61
1:F:87:ALA:CB	1:F:218:GLY:HA3	2.17	0.61
1:K:90:LEU:HD23	1:K:90:LEU:C	2.25	0.61
1:D:48:LEU:HD11	1:D:109:GLY:CA	2.31	0.61
1:E:75:ASN:HD21	3:c:1:NAG:H83	1.66	0.61
1:I:75:ASN:HD21	3:g:1:NAG:H83	1.66	0.61
1:J:216:ILE:HG12	4:J:1235:A2G:O6	2.00	0.60
1:B:87:ALA:HB1	1:B:213:GLY:N	2.16	0.60
1:J:74:PHE:CZ	1:J:164:VAL:HG11	2.37	0.60
1:L:8:TRP:HZ2	1:L:18:MET:HE1	1.66	0.60
1:I:137:PRO:HG2	1:I:156:LEU:HD11	1.84	0.60
1:H:8:TRP:HZ2	1:H:18:MET:HE1	1.66	0.59
1:E:39:GLU:N	1:E:39:GLU:CD	2.60	0.59
1:C:77:THR:HG23	1:C:224:LEU:HD11	1.85	0.59
1:I:50:ARG:HD2	1:I:101:PRO:HG3	1.86	0.58
1:G:87:ALA:CB	1:G:218:GLY:HA3	2.25	0.58
1:C:79:TYR:HD1	1:C:159:ASN:HD21	1.52	0.58
1:F:48:LEU:HD11	1:F:109:GLY:HA3	1.86	0.58
1:E:78:PHE:CE1	1:E:158:ASN:HA	2.39	0.58
1:F:78:PHE:CE1	1:F:158:ASN:HA	2.39	0.58
1:C:137:PRO:HG2	1:C:156:LEU:HD11	1.85	0.57
1:H:88:ASP:HA	6:H:2009:HOH:O	2.03	0.57
1:I:139:ILE:HG13	1:I:154:TRP:HB2	1.85	0.57
1:E:48:LEU:C	1:E:48:LEU:HD23	2.29	0.57
1:E:155:ASP:OD1	1:G:135:PRO:HG3	2.05	0.57
1:K:61:ASP:HB2	1:K:232:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:OD2	1:A:105:ALA:HB1	2.05	0.57
1:J:137:PRO:HG2	1:J:156:LEU:HD11	1.85	0.57
1:A:103:THR:OG1	1:A:112:ASN:ND2	2.38	0.56
1:A:48:LEU:HD23	1:A:49:GLY:N	2.20	0.56
1:C:59:ILE:HG12	1:C:204:VAL:HG22	1.87	0.56
1:H:8:TRP:CZ2	1:H:18:MET:HE1	2.39	0.56
1:K:88:ASP:HA	6:K:2005:HOH:O	2.05	0.56
1:A:179:LEU:HD23	1:A:180:VAL:N	2.21	0.56
1:E:149:ILE:HB	1:F:136:ASN:OD1	2.05	0.56
1:F:114:ASN:HD21	1:F:116:SER:C	2.14	0.56
1:H:12:VAL:O	1:H:15:GLN:HG2	2.05	0.56
1:I:6:PHE:CE2	1:I:228:PHE:HB3	2.41	0.56
1:C:8:TRP:CZ2	1:C:18:MET:HE1	2.40	0.56
1:G:179:LEU:HD21	1:G:181:TYR:CE2	2.41	0.56
1:A:107:TYR:N	1:A:107:TYR:CD1	2.73	0.56
1:G:48:LEU:HD11	1:G:109:GLY:HA3	1.87	0.56
1:D:48:LEU:HD11	1:D:109:GLY:HA3	1.88	0.55
1:B:114:ASN:HA	2:V:5:ARG:HG2	1.88	0.55
1:B:125:PHE:CE2	1:B:179:LEU:HD12	2.41	0.55
2:X:4:THR:O	2:X:5:ARG:O	2.24	0.55
1:I:94:LEU:HG	1:I:206:ILE:HG22	1.88	0.54
1:K:8:TRP:HZ2	1:K:18:MET:HE1	1.72	0.54
1:L:75:ASN:HD21	3:j:1:NAG:H83	1.73	0.54
1:F:8:TRP:CZ2	1:F:18:MET:CE	2.91	0.54
1:C:15:GLN:OE1	1:C:18:MET:HE2	2.07	0.54
1:L:110:LEU:HD21	1:L:209:SER:HB2	1.90	0.54
2:X:5:ARG:HH11	2:X:5:ARG:CG	2.19	0.54
4:F:1239:A2G:H8A	2:X:5:ARG:CG	2.36	0.54
1:K:47:SER:H	1:K:212:THR:HG22	1.73	0.54
1:L:179:LEU:HD23	1:L:180:VAL:N	2.23	0.54
1:J:87:ALA:HB1	1:J:213:GLY:N	2.23	0.53
1:F:113:GLU:HB3	2:X:5:ARG:HH21	1.73	0.53
1:A:48:LEU:HD12	1:A:104:HIS:HA	1.90	0.53
1:F:48:LEU:HD11	1:F:109:GLY:CA	2.38	0.53
1:C:25:ILE:HD12	1:C:26:VAL:C	2.35	0.52
1:C:137:PRO:CG	1:C:156:LEU:HD11	2.39	0.52
1:E:6:PHE:CE1	1:E:228:PHE:HB3	2.45	0.52
1:L:58:HIS:HB2	1:L:203:TRP:CH2	2.44	0.52
1:L:87:ALA:HB1	1:L:213:GLY:N	2.25	0.52
1:B:91:ALA:HB3	1:B:110:LEU:HD11	1.91	0.52
1:C:113:GLU:O	1:G:37:VAL:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:HD21	3:b:1:NAG:H83	1.74	0.51
2:X:5:ARG:HG2	2:X:5:ARG:NH1	2.25	0.51
1:K:168:TYR:CE2	1:K:196:LEU:HD22	2.46	0.51
1:H:21:GLN:HB2	1:H:50:ARG:HB2	1.93	0.51
1:K:154:TRP:CE2	1:K:156:LEU:HD23	2.46	0.51
1:I:59:ILE:HG22	1:I:60:TRP:HD1	1.76	0.50
3:i:1:NAG:H61	3:i:2:NAG:C1	2.42	0.50
1:B:107:TYR:HA	1:B:146:ILE:HD13	1.93	0.50
1:J:216:ILE:CD1	4:J:1235:A2G:C6	2.77	0.50
2:R:3:ASP:OD1	2:R:4:THR:N	2.44	0.50
1:F:97:ILE:HG23	1:F:205:ARG:NH1	2.27	0.50
1:J:88:ASP:HA	6:J:2003:HOH:O	2.11	0.50
1:K:48:LEU:C	1:K:48:LEU:CD2	2.84	0.50
1:K:90:LEU:HD23	1:K:91:ALA:N	2.27	0.50
1:C:149:ILE:HD12	1:K:136:ASN:OD1	2.10	0.50
3:M:2:NAG:H2	3:M:2:NAG:H61	1.92	0.50
1:D:78:PHE:CZ	1:D:156:LEU:HD22	2.47	0.50
1:K:179:LEU:HD23	1:K:180:VAL:N	2.26	0.50
1:A:97:ILE:HD12	1:A:97:ILE:H	1.77	0.49
1:D:50:ARG:HD2	1:D:101:PRO:HG3	1.94	0.49
1:E:90:LEU:HG	1:E:91:ALA:N	2.27	0.49
2:O:3:ASP:OD1	2:O:4:THR:N	2.45	0.49
1:A:179:LEU:HD23	1:A:179:LEU:C	2.38	0.49
1:H:103:THR:OG1	1:H:112:ASN:ND2	2.46	0.49
1:A:147:ARG:HG3	1:A:147:ARG:O	2.12	0.49
1:E:48:LEU:HD12	1:E:104:HIS:HB3	1.93	0.49
1:K:60:TRP:HZ3	1:K:62:LYS:HG2	1.78	0.49
1:F:115:GLU:O	1:F:116:SER:HB3	2.13	0.48
1:L:81:PRO:HD2	1:L:218:GLY:O	2.13	0.48
1:B:87:ALA:CB	1:B:218:GLY:HA3	2.27	0.48
1:B:128:PHE:CE1	4:B:1234:A2G:H3	2.48	0.48
1:B:168:TYR:CE2	1:B:196:LEU:HD22	2.48	0.48
1:A:59:ILE:HG22	1:A:60:TRP:HD1	1.79	0.48
1:F:47:SER:H	1:F:212:THR:HG22	1.78	0.48
1:F:59:ILE:CG2	1:F:196:LEU:HD23	2.44	0.48
1:B:215:ASP:OD1	4:B:1234:A2G:O6	2.31	0.48
1:F:115:GLU:O	1:F:116:SER:CB	2.62	0.48
1:H:94:LEU:HG	1:H:206:ILE:HG22	1.94	0.48
1:B:103:THR:OG1	1:B:112:ASN:ND2	2.47	0.47
1:C:48:LEU:HD11	1:C:109:GLY:HA3	1.95	0.47
1:G:103:THR:OG1	1:G:112:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:SER:N	1:K:212:THR:HG22	2.29	0.47
1:K:113:GLU:OE1	2:Y:5:ARG:NH1	2.46	0.47
1:D:48:LEU:HD23	1:D:48:LEU:C	2.40	0.47
1:E:59:ILE:HD13	1:E:68:ALA:HB3	1.97	0.47
1:A:87:ALA:HB1	1:A:213:GLY:N	2.30	0.47
1:E:34:LEU:O	1:E:49:GLY:HA3	2.15	0.47
1:F:75:ASN:HD21	3:d:1:NAG:H83	1.80	0.47
1:F:150:LYS:HG2	1:F:190:LEU:HD11	1.96	0.47
1:J:214:LEU:HB3	1:J:215:ASP:OD1	2.15	0.47
1:K:48:LEU:HD23	1:K:49:GLY:N	2.30	0.47
1:I:21:GLN:HB2	1:I:50:ARG:HB2	1.97	0.47
1:E:103:THR:OG1	1:E:112:ASN:ND2	2.47	0.47
1:J:93:PHE:C	1:J:94:LEU:HD12	2.40	0.47
1:K:8:TRP:CZ2	1:K:18:MET:HE1	2.50	0.47
1:B:78:PHE:HB2	1:B:220:SER:O	2.15	0.47
1:C:110:LEU:HD22	1:C:120:VAL:HG11	1.97	0.47
1:H:90:LEU:HG	1:H:91:ALA:N	2.30	0.47
1:J:103:THR:OG1	1:J:112:ASN:ND2	2.48	0.47
1:C:59:ILE:CG1	1:C:204:VAL:HG22	2.45	0.46
1:F:50:ARG:HD2	1:F:101:PRO:HG3	1.96	0.46
1:C:38:ASP:N	1:C:44:LYS:HE2	2.30	0.46
1:D:47:SER:H	1:D:212:THR:CG2	2.29	0.46
1:A:48:LEU:C	1:A:48:LEU:CD2	2.88	0.46
1:I:95:ALA:O	1:I:204:VAL:HB	2.14	0.46
1:I:103:THR:HB	1:I:107:TYR:HB2	1.97	0.46
1:K:47:SER:H	1:K:212:THR:CG2	2.28	0.46
1:D:47:SER:N	1:D:212:THR:HG22	2.31	0.46
1:H:87:ALA:HB1	1:H:213:GLY:N	2.31	0.46
1:I:103:THR:OG1	1:I:112:ASN:ND2	2.48	0.46
1:I:23:ASP:CG	1:I:36:LYS:HG2	2.41	0.46
1:B:95:ALA:O	1:B:204:VAL:HB	2.16	0.45
1:C:32:LEU:HD11	1:C:51:ALA:CB	2.46	0.45
1:C:94:LEU:HG	1:C:206:ILE:HG22	1.96	0.45
1:D:47:SER:H	1:D:212:THR:HG22	1.81	0.45
1:E:132:TRP:HB2	1:E:147:ARG:HG2	1.97	0.45
1:H:59:ILE:HG12	1:H:204:VAL:HG22	1.97	0.45
1:F:179:LEU:C	1:F:179:LEU:HD23	2.41	0.45
1:H:34:LEU:O	1:H:49:GLY:HA3	2.16	0.45
1:K:78:PHE:CE1	1:K:158:ASN:HA	2.51	0.45
1:D:34:LEU:O	1:D:49:GLY:HA3	2.15	0.45
1:F:215:ASP:OD1	4:F:1239:A2G:O6	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:LEU:HD11	1:L:109:GLY:HA3	1.97	0.45
1:F:47:SER:N	1:F:212:THR:HG22	2.32	0.45
2:X:4:THR:C	2:X:5:ARG:O	2.59	0.45
1:C:137:PRO:HG2	1:C:156:LEU:CD1	2.47	0.45
1:I:152:THR:HB	1:I:190:LEU:HD13	1.97	0.45
1:A:168:TYR:CE2	1:A:196:LEU:HD22	2.52	0.45
1:L:146:ILE:O	6:L:2006:HOH:O	2.20	0.45
1:I:34:LEU:O	1:I:49:GLY:HA3	2.17	0.45
1:A:87:ALA:HB3	1:A:219:GLU:H	1.81	0.45
1:H:79:TYR:HD1	1:H:159:ASN:HD21	1.65	0.45
1:B:154:TRP:CE2	1:B:156:LEU:HD23	2.52	0.44
1:E:58:HIS:HB2	1:E:203:TRP:CH2	2.51	0.44
1:L:48:LEU:CD1	1:L:109:GLY:HA3	2.46	0.44
1:K:103:THR:OG1	1:K:112:ASN:ND2	2.47	0.44
1:J:216:ILE:CG1	4:J:1235:A2G:H6	2.36	0.44
1:A:189:ILE:HG23	1:E:187:SER:HB2	1.99	0.44
1:C:81:PRO:HD2	1:C:218:GLY:O	2.17	0.44
1:C:93:PHE:CG	1:C:110:LEU:HD21	2.52	0.44
1:I:59:ILE:HD13	1:I:59:ILE:HA	1.90	0.44
1:J:114:ASN:O	1:J:115:GLU:C	2.61	0.44
1:D:103:THR:OG1	1:D:112:ASN:ND2	2.47	0.44
1:G:34:LEU:O	1:G:49:GLY:HA3	2.18	0.44
1:G:65:GLY:O	1:G:197:LYS:HE3	2.18	0.44
1:J:168:TYR:CE2	1:J:196:LEU:HD22	2.52	0.44
1:K:150:LYS:HG2	1:K:190:LEU:HD11	1.98	0.44
1:E:47:SER:H	1:E:212:THR:CG2	2.31	0.44
1:I:88:ASP:HA	6:I:2004:HOH:O	2.18	0.44
1:L:168:TYR:CE2	1:L:196:LEU:HD22	2.53	0.44
1:C:32:LEU:HD11	1:C:51:ALA:HB2	1.99	0.43
1:H:18:MET:HE2	1:H:18:MET:HB2	1.78	0.43
1:H:59:ILE:CG1	1:H:204:VAL:HG22	2.47	0.43
1:L:103:THR:OG1	1:L:112:ASN:ND2	2.47	0.43
2:O:4:THR:O	2:O:5:ARG:HG3	2.17	0.43
1:A:75:ASN:HD21	3:M:1:NAG:C8	2.28	0.43
1:A:136:ASN:OD1	1:G:149:ILE:CB	2.60	0.43
1:C:47:SER:H	1:C:212:THR:HG22	1.83	0.43
2:X:5:ARG:HH11	2:X:5:ARG:HG2	1.83	0.43
4:F:1239:A2G:H8A	2:X:5:ARG:HD2	2.00	0.43
1:C:118:ASP:CB	1:C:120:VAL:HG23	2.48	0.43
1:C:225:SER:HB3	3:a:1:NAG:O6	2.19	0.43
4:F:1239:A2G:C8	2:X:5:ARG:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PRO:CG	1:B:156:LEU:HD11	2.49	0.43
1:E:39:GLU:CD	1:E:39:GLU:H	2.25	0.43
1:I:189:ILE:HG23	1:K:187:SER:HB2	2.01	0.43
1:L:34:LEU:O	1:L:49:GLY:HA3	2.18	0.43
1:A:105:ALA:C	1:A:107:TYR:N	2.72	0.43
1:A:128:PHE:CE2	4:A:1235:A2G:H3	2.53	0.43
1:C:179:LEU:HD23	1:C:180:VAL:N	2.33	0.43
1:D:87:ALA:CB	1:D:218:GLY:HA3	2.27	0.43
1:D:168:TYR:CE2	1:D:196:LEU:HD22	2.54	0.43
1:A:184:GLN:NE2	1:F:184:GLN:NE2	2.66	0.43
1:B:179:LEU:C	1:B:179:LEU:HD23	2.43	0.43
1:C:47:SER:N	1:C:212:THR:HG22	2.34	0.43
1:I:47:SER:N	1:I:212:THR:HG22	2.33	0.43
1:G:91:ALA:HB3	1:G:110:LEU:HD11	2.01	0.43
1:G:146:ILE:O	1:G:146:ILE:HG13	2.17	0.43
1:I:48:LEU:HG	1:I:49:GLY:N	2.33	0.43
1:A:125:PHE:CE1	1:A:139:ILE:HG23	2.54	0.42
1:A:214:LEU:HD12	4:A:1235:A2G:H2	2.01	0.42
1:C:65:GLY:O	1:C:197:LYS:CE	2.66	0.42
1:D:114:ASN:O	1:D:115:GLU:C	2.62	0.42
1:I:114:ASN:O	1:I:115:GLU:C	2.61	0.42
1:I:47:SER:H	1:I:212:THR:CG2	2.32	0.42
1:L:55:THR:HA	1:L:56:PRO:HD3	1.96	0.42
1:J:78:PHE:HB2	1:J:220:SER:O	2.20	0.42
1:E:48:LEU:C	1:E:48:LEU:CD2	2.93	0.42
1:E:65:GLY:O	1:E:197:LYS:CE	2.68	0.42
1:H:78:PHE:CE1	1:H:158:ASN:HA	2.55	0.42
1:D:48:LEU:HD11	1:D:109:GLY:HA2	2.01	0.42
1:F:78:PHE:HB2	1:F:219:GLU:HG3	2.02	0.42
1:K:95:ALA:HB2	1:K:120:VAL:HG22	2.02	0.42
1:E:118:ASP:HB2	1:E:120:VAL:HG23	2.02	0.42
1:A:184:GLN:HE22	1:F:184:GLN:HE22	1.67	0.42
1:E:12:VAL:HG13	1:E:15:GLN:HB3	2.02	0.42
1:L:179:LEU:HD23	1:L:179:LEU:C	2.45	0.42
1:F:187:SER:HB2	1:G:189:ILE:HG23	2.02	0.42
1:B:101:PRO:O	1:L:114:ASN:CB	2.68	0.41
1:I:6:PHE:CD1	1:I:6:PHE:C	2.98	0.41
1:K:118:ASP:CB	1:K:120:VAL:HG23	2.50	0.41
1:L:86:LEU:HB3	1:L:127:THR:HB	2.02	0.41
1:H:56:PRO:HG2	1:J:16:PRO:HB2	2.02	0.41
1:I:8:TRP:CZ2	1:I:18:MET:HE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:SER:H	1:I:212:THR:HG22	1.84	0.41
1:L:103:THR:HB	1:L:107:TYR:HB2	2.02	0.41
1:C:179:LEU:HD23	1:C:179:LEU:C	2.45	0.41
1:E:168:TYR:CZ	1:E:196:LEU:HD13	2.55	0.41
1:K:34:LEU:O	1:K:49:GLY:HA3	2.20	0.41
1:I:38:ASP:HB3	1:I:44:LYS:HE2	2.02	0.41
1:A:87:ALA:CB	1:A:218:GLY:HA3	2.26	0.41
1:B:48:LEU:C	1:B:48:LEU:HD23	2.45	0.41
1:F:47:SER:H	1:F:212:THR:CG2	2.33	0.41
1:F:87:ALA:HB1	1:F:213:GLY:N	2.36	0.41
1:G:61:ASP:OD2	1:G:63:GLU:HB2	2.21	0.41
1:H:32:LEU:HD21	1:H:34:LEU:HD21	2.02	0.41
1:I:87:ALA:HB1	1:I:212:THR:HA	2.02	0.41
1:C:47:SER:H	1:C:212:THR:CG2	2.32	0.41
1:I:38:ASP:OD1	1:I:38:ASP:C	2.63	0.41
1:L:18:MET:HE2	1:L:18:MET:HB2	1.92	0.41
1:A:47:SER:N	1:A:212:THR:HG22	2.35	0.41
1:F:105:ALA:CB	1:F:214:LEU:HD12	2.51	0.41
1:J:59:ILE:HD13	1:J:59:ILE:HA	1.83	0.41
1:K:125:PHE:CE1	1:K:179:LEU:HD12	2.56	0.41
1:C:137:PRO:HB3	1:C:156:LEU:HD21	2.02	0.41
1:E:47:SER:N	1:E:212:THR:HG22	2.36	0.41
1:F:87:ALA:HB3	1:F:219:GLU:H	1.85	0.41
1:H:114:ASN:O	1:H:115:GLU:C	2.64	0.41
1:I:185:ARG:CD	1:I:185:ARG:N	2.84	0.41
1:J:94:LEU:HG	1:J:206:ILE:HG22	2.03	0.41
1:L:87:ALA:HB3	1:L:219:GLU:H	1.86	0.41
1:B:34:LEU:O	1:B:49:GLY:HA3	2.20	0.41
1:G:86:LEU:HD13	1:G:156:LEU:HD11	2.02	0.41
1:H:38:ASP:OD1	1:H:38:ASP:C	2.64	0.41
1:J:47:SER:N	1:J:212:THR:HG22	2.36	0.41
1:K:154:TRP:CE2	1:K:156:LEU:CD2	3.04	0.41
1:A:114:ASN:O	1:A:115:GLU:C	2.64	0.40
1:E:149:ILE:CB	1:F:136:ASN:OD1	2.69	0.40
1:K:62:LYS:HB2	1:K:202:GLU:CD	2.46	0.40
1:C:153:SER:OG	1:I:135:PRO:CG	2.69	0.40
1:H:37:VAL:HG13	1:H:41:GLY:C	2.46	0.40
1:K:114:ASN:O	1:K:115:GLU:C	2.64	0.40
1:B:48:LEU:HD21	1:B:101:PRO:HB3	2.04	0.40
1:F:6:PHE:CE2	1:F:228:PHE:HB3	2.57	0.40
1:F:154:TRP:CD2	1:F:156:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:114:ASN:O	1:L:115:GLU:C	2.65	0.40
1:B:37:VAL:HG13	1:B:41:GLY:C	2.47	0.40
1:B:87:ALA:HB3	1:B:219:GLU:H	1.86	0.40
1:D:78:PHE:HB2	1:D:220:SER:O	2.22	0.40
1:D:201:PRO:HG2	1:D:203:TRP:O	2.20	0.40
1:F:38:ASP:OD1	1:F:38:ASP:C	2.64	0.40
1:H:15:GLN:HB2	1:H:17:ASN:OD1	2.21	0.40
1:I:21:GLN:OE1	1:I:50:ARG:HD3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:THR:OG1	1:G:55:THR:OG1[3_655]	1.63	0.57

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/253 (92%)	217 (94%)	13 (6%)	2 (1%)	14	35
1	B	228/253 (90%)	217 (95%)	11 (5%)	0	100	100
1	C	227/253 (90%)	216 (95%)	10 (4%)	1 (0%)	30	54
1	D	232/253 (92%)	217 (94%)	14 (6%)	1 (0%)	30	54
1	E	227/253 (90%)	215 (95%)	10 (4%)	2 (1%)	14	35
1	F	232/253 (92%)	218 (94%)	10 (4%)	4 (2%)	7	19
1	G	229/253 (90%)	213 (93%)	15 (7%)	1 (0%)	30	54
1	H	229/253 (90%)	216 (94%)	12 (5%)	1 (0%)	30	54
1	I	232/253 (92%)	216 (93%)	14 (6%)	2 (1%)	14	35
1	J	228/253 (90%)	215 (94%)	10 (4%)	3 (1%)	9	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	229/253 (90%)	218 (95%)	10 (4%)	1 (0%)	30	54
1	L	228/253 (90%)	214 (94%)	12 (5%)	2 (1%)	14	35
2	O	2/5 (40%)	2 (100%)	0	0	100	100
2	R	1/5 (20%)	0	1 (100%)	0	100	100
2	U	1/5 (20%)	0	0	1 (100%)	0	0
2	V	1/5 (20%)	1 (100%)	0	0	100	100
2	X	2/5 (40%)	2 (100%)	0	0	100	100
2	Y	1/5 (20%)	0	1 (100%)	0	100	100
All	All	2761/3066 (90%)	2597 (94%)	143 (5%)	21 (1%)	16	37

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	114	ASN
1	J	214	LEU
1	A	106	GLY
1	F	116	SER
1	G	156	LEU
1	H	156	LEU
1	J	217	PRO
1	L	156	LEU
1	E	156	LEU
1	K	156	LEU
1	C	156	LEU
1	D	156	LEU
1	F	156	LEU
1	I	156	LEU
1	L	233	PRO
2	U	3	ASP
1	J	156	LEU
1	A	117	GLY
1	E	97	ILE
1	I	97	ILE
1	F	97	ILE

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/219 (92%)	186 (92%)	16 (8%)	11	28
1	B	200/219 (91%)	184 (92%)	16 (8%)	11	28
1	C	200/219 (91%)	188 (94%)	12 (6%)	17	41
1	D	202/219 (92%)	190 (94%)	12 (6%)	18	42
1	E	200/219 (91%)	182 (91%)	18 (9%)	9	23
1	F	202/219 (92%)	183 (91%)	19 (9%)	8	21
1	G	201/219 (92%)	183 (91%)	18 (9%)	9	23
1	H	202/219 (92%)	191 (95%)	11 (5%)	20	45
1	I	202/219 (92%)	189 (94%)	13 (6%)	16	38
1	J	201/219 (92%)	190 (94%)	11 (6%)	19	45
1	K	202/219 (92%)	180 (89%)	22 (11%)	6	16
1	L	201/219 (92%)	184 (92%)	17 (8%)	10	25
2	O	4/4 (100%)	4 (100%)	0	100	100
2	P	2/4 (50%)	2 (100%)	0	100	100
2	Q	2/4 (50%)	2 (100%)	0	100	100
2	R	3/4 (75%)	2 (67%)	1 (33%)	0	1
2	S	1/4 (25%)	1 (100%)	0	100	100
2	T	2/4 (50%)	2 (100%)	0	100	100
2	U	3/4 (75%)	3 (100%)	0	100	100
2	V	3/4 (75%)	3 (100%)	0	100	100
2	W	2/4 (50%)	2 (100%)	0	100	100
2	X	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	Y	3/4 (75%)	3 (100%)	0	100	100
2	Z	2/4 (50%)	2 (100%)	0	100	100
All	All	2446/2676 (91%)	2259 (92%)	187 (8%)	12	30

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL

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Mol	Chain	Res	Type
1	A	37	VAL
1	A	50	ARG
1	A	52	LEU
1	A	59	ILE
1	A	113	GLU
1	A	114	ASN
1	A	115	GLU
1	A	147	ARG
1	A	185	ARG
1	A	187	SER
1	A	196	LEU
1	A	212	THR
1	A	214	LEU
1	A	215	ASP
1	A	219	GLU
1	B	10	LYS
1	B	12	VAL
1	B	37	VAL
1	B	52	LEU
1	B	84	LYS
1	B	103	THR
1	B	114	ASN
1	B	146	ILE
1	B	155	ASP
1	B	184	GLN
1	B	185	ARG
1	B	187	SER
1	B	204	VAL
1	B	212	THR
1	B	214	LEU
1	B	215	ASP
1	C	12	VAL
1	C	25	ILE
1	C	37	VAL
1	C	50	ARG
1	C	52	LEU
1	C	155	ASP
1	C	163	LYS
1	C	180	VAL
1	C	185	ARG
1	C	187	SER
1	C	212	THR

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Mol	Chain	Res	Type
1	C	215	ASP
1	D	37	VAL
1	D	52	LEU
1	D	103	THR
1	D	104	HIS
1	D	155	ASP
1	D	163	LYS
1	D	187	SER
1	D	193	VAL
1	D	196	LEU
1	D	212	THR
1	D	214	LEU
1	D	215	ASP
1	E	37	VAL
1	E	39	GLU
1	E	48	LEU
1	E	50	ARG
1	E	52	LEU
1	E	59	ILE
1	E	84	LYS
1	E	103	THR
1	E	104	HIS
1	E	147	ARG
1	E	149	ILE
1	E	155	ASP
1	E	163	LYS
1	E	185	ARG
1	E	187	SER
1	E	212	THR
1	E	214	LEU
1	E	215	ASP
1	F	10	LYS
1	F	12	VAL
1	F	14	LYS
1	F	37	VAL
1	F	52	LEU
1	F	63	GLU
1	F	90	LEU
1	F	103	THR
1	F	113	GLU
1	F	114	ASN
1	F	148	SER

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Mol	Chain	Res	Type
1	F	184	GLN
1	F	185	ARG
1	F	187	SER
1	F	193	VAL
1	F	212	THR
1	F	214	LEU
1	F	215	ASP
1	F	219	GLU
1	G	10	LYS
1	G	12	VAL
1	G	18	MET
1	G	25	ILE
1	G	37	VAL
1	G	50	ARG
1	G	52	LEU
1	G	90	LEU
1	G	103	THR
1	G	115	GLU
1	G	155	ASP
1	G	185	ARG
1	G	187	SER
1	G	196	LEU
1	G	212	THR
1	G	214	LEU
1	G	215	ASP
1	G	216	ILE
1	H	48	LEU
1	H	52	LEU
1	H	103	THR
1	H	115	GLU
1	H	148	SER
1	H	185	ARG
1	H	187	SER
1	H	196	LEU
1	H	214	LEU
1	H	215	ASP
1	H	219	GLU
1	I	12	VAL
1	I	33	GLN
1	I	52	LEU
1	I	59	ILE
1	I	103	THR

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Mol	Chain	Res	Type
1	I	155	ASP
1	I	185	ARG
1	I	187	SER
1	I	193	VAL
1	I	212	THR
1	I	214	LEU
1	I	215	ASP
1	I	232	LEU
1	J	33	GLN
1	J	37	VAL
1	J	48	LEU
1	J	59	ILE
1	J	103	THR
1	J	155	ASP
1	J	185	ARG
1	J	187	SER
1	J	214	LEU
1	J	215	ASP
1	J	234	HIS
1	K	10	LYS
1	K	33	GLN
1	K	37	VAL
1	K	48	LEU
1	K	52	LEU
1	K	59	ILE
1	K	62	LYS
1	K	84	LYS
1	K	90	LEU
1	K	103	THR
1	K	148	SER
1	K	163	LYS
1	K	180	VAL
1	K	184[A]	GLN
1	K	184[B]	GLN
1	K	185	ARG
1	K	187	SER
1	K	193	VAL
1	K	196	LEU
1	K	212	THR
1	K	214	LEU
1	K	215	ASP
1	L	12	VAL

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Mol	Chain	Res	Type
1	L	25	ILE
1	L	33	GLN
1	L	37	VAL
1	L	48	LEU
1	L	52	LEU
1	L	103	THR
1	L	127	THR
1	L	155	ASP
1	L	187	SER
1	L	193	VAL
1	L	196	LEU
1	L	212	THR
1	L	214	LEU
1	L	215	ASP
1	L	219	GLU
1	L	234	HIS
2	R	5	ARG
2	X	5	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	112	ASN
1	A	144	ASN
1	A	184	GLN
1	B	102	GLN
1	B	112	ASN
1	B	144	ASN
1	B	184	GLN
1	C	102	GLN
1	C	112	ASN
1	C	119	GLN
1	C	159	ASN
1	C	184	GLN
1	D	102	GLN
1	D	112	ASN
1	D	144	ASN
1	D	184	GLN
1	E	102	GLN
1	E	112	ASN
1	E	136	ASN

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Mol	Chain	Res	Type
1	E	144	ASN
1	E	184	GLN
1	F	102	GLN
1	F	130	ASN
1	F	144	ASN
1	F	184	GLN
1	G	102	GLN
1	G	112	ASN
1	G	144	ASN
1	G	159	ASN
1	G	184	GLN
1	H	102	GLN
1	H	112	ASN
1	H	144	ASN
1	H	159	ASN
1	I	102	GLN
1	I	144	ASN
1	I	159	ASN
1	I	184	GLN
1	I	234	HIS
1	J	102	GLN
1	J	112	ASN
1	J	144	ASN
1	J	159	ASN
1	J	234	HIS
1	K	102	GLN
1	K	112	ASN
1	K	144	ASN
1	L	33	GLN
1	L	144	ASN
1	L	159	ASN
1	L	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	M	1	3,1	14,14,15	0.55	0	17,19,21	2.26	6 (35%)
3	NAG	M	2	3	14,14,15	0.58	0	17,19,21	1.48	1 (5%)
3	NAG	N	1	3,1	14,14,15	0.67	0	17,19,21	2.29	5 (29%)
3	NAG	N	2	3	14,14,15	0.50	0	17,19,21	1.31	2 (11%)
3	NAG	a	1	3,1	14,14,15	0.53	0	17,19,21	2.03	5 (29%)
3	NAG	a	2	3	14,14,15	0.63	0	17,19,21	2.37	4 (23%)
3	NAG	b	1	3,1	14,14,15	1.08	2 (14%)	17,19,21	2.26	10 (58%)
3	NAG	b	2	3	14,14,15	0.75	0	17,19,21	3.38	8 (47%)
3	NAG	c	1	3,1	14,14,15	0.54	0	17,19,21	1.98	6 (35%)
3	NAG	c	2	3	14,14,15	0.73	0	17,19,21	1.51	3 (17%)
3	NAG	d	1	3,1	14,14,15	0.60	0	17,19,21	2.39	6 (35%)
3	NAG	d	2	3	14,14,15	0.64	0	17,19,21	2.74	6 (35%)
3	NAG	e	1	3,1	14,14,15	0.71	0	17,19,21	2.16	5 (29%)
3	NAG	e	2	3	14,14,15	0.79	1 (7%)	17,19,21	1.77	4 (23%)
3	NAG	f	1	3,1	14,14,15	0.61	0	17,19,21	2.22	5 (29%)
3	NAG	f	2	3	14,14,15	0.93	0	17,19,21	2.35	6 (35%)
3	NAG	g	1	3,1	14,14,15	0.78	1 (7%)	17,19,21	2.05	6 (35%)
3	NAG	g	2	3	14,14,15	0.47	0	17,19,21	2.06	4 (23%)
3	NAG	h	1	3,1	14,14,15	1.13	1 (7%)	17,19,21	2.24	7 (41%)
3	NAG	h	2	3	14,14,15	0.79	1 (7%)	17,19,21	2.54	3 (17%)
3	NAG	i	1	3,1	14,14,15	0.80	0	17,19,21	2.01	5 (29%)
3	NAG	i	2	3	14,14,15	0.61	0	17,19,21	2.09	4 (23%)
3	NAG	j	1	3,1	14,14,15	0.93	1 (7%)	17,19,21	2.32	5 (29%)
3	NAG	j	2	3	14,14,15	0.89	1 (7%)	17,19,21	1.84	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	3/6/23/26	0/1/1/1
3	NAG	d	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1	NAG	C1-C2	3.08	1.56	1.52
3	b	1	NAG	C4-C5	2.58	1.58	1.53
3	b	1	NAG	C1-C2	2.46	1.55	1.52
3	e	2	NAG	C1-C2	2.35	1.55	1.52
3	h	2	NAG	C1-C2	2.27	1.55	1.52
3	j	1	NAG	C1-C2	2.22	1.55	1.52
3	g	1	NAG	C1-C2	2.18	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	2	NAG	C4-C5	2.04	1.57	1.53

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	2	NAG	C1-O5-C5	9.86	125.39	112.19
3	h	2	NAG	C1-O5-C5	9.11	124.40	112.19
3	d	2	NAG	C1-O5-C5	7.97	122.87	112.19
3	a	2	NAG	C1-O5-C5	7.39	122.09	112.19
3	f	2	NAG	C1-O5-C5	7.08	121.68	112.19
3	g	2	NAG	C1-O5-C5	6.70	121.17	112.19
3	j	1	NAG	C8-C7-N2	6.07	126.18	116.12
3	N	1	NAG	O5-C1-C2	-5.91	102.14	111.29
3	b	2	NAG	C1-C2-N2	-5.83	101.25	110.43
3	e	1	NAG	C1-O5-C5	5.36	119.36	112.19
3	i	2	NAG	C1-O5-C5	5.25	119.23	112.19
3	M	2	NAG	C1-O5-C5	5.16	119.11	112.19
3	e	2	NAG	C1-O5-C5	5.15	119.09	112.19
3	M	1	NAG	C8-C7-N2	4.95	124.32	116.12
3	j	2	NAG	C1-O5-C5	4.80	118.62	112.19
3	M	1	NAG	O5-C1-C2	-4.74	103.96	111.29
3	i	1	NAG	C8-C7-N2	4.69	123.89	116.12
3	f	1	NAG	O5-C1-C2	-4.65	104.10	111.29
3	c	1	NAG	O5-C1-C2	-4.63	104.13	111.29
3	h	1	NAG	C2-N2-C7	4.62	129.09	122.90
3	d	1	NAG	C2-N2-C7	4.60	129.07	122.90
3	d	1	NAG	C8-C7-N2	4.58	123.71	116.12
3	d	1	NAG	O5-C1-C2	-4.54	104.27	111.29
3	a	1	NAG	C1-O5-C5	4.49	118.21	112.19
3	b	1	NAG	C8-C7-N2	4.49	123.56	116.12
3	f	1	NAG	C8-C7-N2	4.24	123.15	116.12
3	N	1	NAG	C2-N2-C7	4.10	128.40	122.90
3	g	1	NAG	C8-C7-N2	4.07	122.88	116.12
3	j	1	NAG	O7-C7-C8	-4.05	114.84	122.05
3	d	2	NAG	O5-C5-C4	3.95	120.44	110.83
3	a	1	NAG	C8-C7-N2	3.92	122.62	116.12
3	e	1	NAG	C2-N2-C7	3.88	128.10	122.90
3	i	2	NAG	C2-N2-C7	3.88	128.09	122.90
3	M	1	NAG	O7-C7-C8	-3.81	115.28	122.05
3	d	2	NAG	C1-C2-N2	-3.73	104.55	110.43
3	j	2	NAG	O4-C4-C5	3.71	118.46	109.32
3	b	2	NAG	O5-C5-C4	3.62	119.63	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	2	NAG	C4-C3-C2	3.62	116.32	111.02
3	h	1	NAG	C8-C7-N2	3.53	121.97	116.12
3	g	1	NAG	O5-C1-C2	-3.45	105.95	111.29
3	i	1	NAG	O7-C7-C8	-3.40	115.99	122.05
3	i	2	NAG	O7-C7-N2	3.39	127.97	121.98
3	N	1	NAG	C8-C7-N2	3.37	121.70	116.12
3	c	1	NAG	C8-C7-N2	3.32	121.63	116.12
3	h	2	NAG	O5-C5-C4	3.30	118.86	110.83
3	a	2	NAG	C3-C4-C5	3.27	116.17	110.23
3	e	1	NAG	C8-C7-N2	3.21	121.44	116.12
3	f	1	NAG	C1-C2-N2	3.19	115.45	110.43
3	h	1	NAG	O7-C7-C8	-3.15	116.45	122.05
3	i	2	NAG	O7-C7-C8	-3.13	116.47	122.05
3	a	1	NAG	O7-C7-C8	-3.13	116.48	122.05
3	e	1	NAG	O5-C1-C2	-3.11	106.48	111.29
3	b	1	NAG	O4-C4-C5	3.07	116.89	109.32
3	j	1	NAG	O5-C1-C2	-2.99	106.67	111.29
3	d	1	NAG	O7-C7-N2	-2.98	116.72	121.98
3	c	2	NAG	C1-O5-C5	2.94	116.13	112.19
3	i	1	NAG	O5-C1-C2	-2.93	106.76	111.29
3	j	1	NAG	C2-N2-C7	2.93	126.82	122.90
3	M	1	NAG	C1-C2-N2	2.91	115.02	110.43
3	f	1	NAG	O4-C4-C5	2.89	116.44	109.32
3	h	1	NAG	O5-C1-C2	-2.89	106.82	111.29
3	f	1	NAG	O7-C7-C8	-2.89	116.91	122.05
3	h	1	NAG	C1-O5-C5	2.89	116.05	112.19
3	f	2	NAG	C2-N2-C7	2.86	126.73	122.90
3	i	1	NAG	O4-C4-C5	2.80	116.23	109.32
3	d	1	NAG	O4-C4-C5	2.79	116.18	109.32
3	b	1	NAG	O7-C7-C8	-2.77	117.13	122.05
3	b	2	NAG	C3-C4-C5	2.76	115.24	110.23
3	b	1	NAG	C3-C4-C5	-2.75	105.25	110.23
3	c	1	NAG	O7-C7-C8	-2.72	117.20	122.05
3	c	2	NAG	O5-C1-C2	-2.71	107.10	111.29
3	d	2	NAG	O5-C1-C2	2.68	115.43	111.29
3	e	2	NAG	C1-C2-N2	2.66	114.63	110.43
3	b	2	NAG	O3-C3-C2	-2.63	103.94	109.40
3	M	1	NAG	C2-N2-C7	2.62	126.41	122.90
3	g	1	NAG	O4-C4-C5	2.61	115.75	109.32
3	a	2	NAG	O5-C1-C2	2.60	115.31	111.29
3	h	1	NAG	C4-C3-C2	2.59	114.81	111.02
3	f	2	NAG	O7-C7-C8	-2.58	117.47	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	1	NAG	O5-C1-C2	-2.57	107.32	111.29
3	b	1	NAG	O4-C4-C3	-2.56	104.33	110.38
3	N	1	NAG	O7-C7-C8	-2.54	117.53	122.05
3	d	2	NAG	C2-N2-C7	2.53	126.29	122.90
3	c	2	NAG	C1-C2-N2	2.50	114.37	110.43
3	g	2	NAG	C2-N2-C7	2.49	126.24	122.90
3	b	2	NAG	C8-C7-N2	-2.49	111.99	116.12
3	i	1	NAG	C1-O5-C5	2.46	115.49	112.19
3	c	1	NAG	O3-C3-C2	-2.46	104.28	109.40
3	f	2	NAG	O7-C7-N2	2.45	126.32	121.98
3	f	2	NAG	O5-C5-C4	2.44	116.77	110.83
3	b	1	NAG	C2-N2-C7	2.44	126.17	122.90
3	g	1	NAG	O7-C7-N2	-2.44	117.67	121.98
3	b	1	NAG	O6-C6-C5	-2.43	103.06	111.33
3	f	2	NAG	O4-C4-C3	2.43	116.11	110.38
3	a	1	NAG	C6-C5-C4	-2.42	107.08	113.02
3	g	2	NAG	O7-C7-C8	-2.41	117.77	122.05
3	N	1	NAG	O3-C3-C2	2.38	114.35	109.40
3	c	1	NAG	C2-N2-C7	2.37	126.08	122.90
3	d	1	NAG	O4-C4-C3	-2.35	104.83	110.38
3	d	2	NAG	O6-C6-C5	-2.33	103.40	111.33
3	a	2	NAG	O7-C7-C8	-2.30	117.97	122.05
3	N	2	NAG	O5-C1-C2	-2.29	107.74	111.29
3	h	2	NAG	O4-C4-C5	2.29	114.96	109.32
3	g	1	NAG	O4-C4-C3	-2.29	104.99	110.38
3	j	2	NAG	O5-C5-C4	2.26	116.33	110.83
3	b	2	NAG	O5-C1-C2	2.21	114.71	111.29
3	a	1	NAG	C2-N2-C7	2.21	125.86	122.90
3	e	2	NAG	O7-C7-C8	-2.17	118.20	122.05
3	b	1	NAG	O5-C5-C6	-2.16	103.46	107.66
3	b	1	NAG	C1-O5-C5	2.15	115.06	112.19
3	j	1	NAG	C1-O5-C5	2.14	115.05	112.19
3	c	1	NAG	C6-C5-C4	-2.13	107.79	113.02
3	h	1	NAG	O3-C3-C2	-2.08	105.08	109.40
3	M	1	NAG	C3-C4-C5	-2.06	106.50	110.23
3	e	1	NAG	O5-C5-C4	2.04	115.79	110.83
3	g	2	NAG	O7-C7-N2	2.01	125.54	121.98
3	N	2	NAG	C3-C4-C5	-2.01	106.58	110.23
3	g	1	NAG	C1-O5-C5	2.00	114.87	112.19
3	e	2	NAG	O4-C4-C5	2.00	114.25	109.32

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	d	2	NAG	O5-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	i	1	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	c	1	NAG	C8-C7-N2-C2
3	c	1	NAG	O7-C7-N2-C2
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	e	1	NAG	C8-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
3	f	1	NAG	C8-C7-N2-C2
3	f	1	NAG	O7-C7-N2-C2
3	g	1	NAG	C8-C7-N2-C2
3	g	1	NAG	O7-C7-N2-C2
3	h	1	NAG	C8-C7-N2-C2
3	h	1	NAG	O7-C7-N2-C2
3	i	1	NAG	C8-C7-N2-C2
3	i	1	NAG	O7-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6

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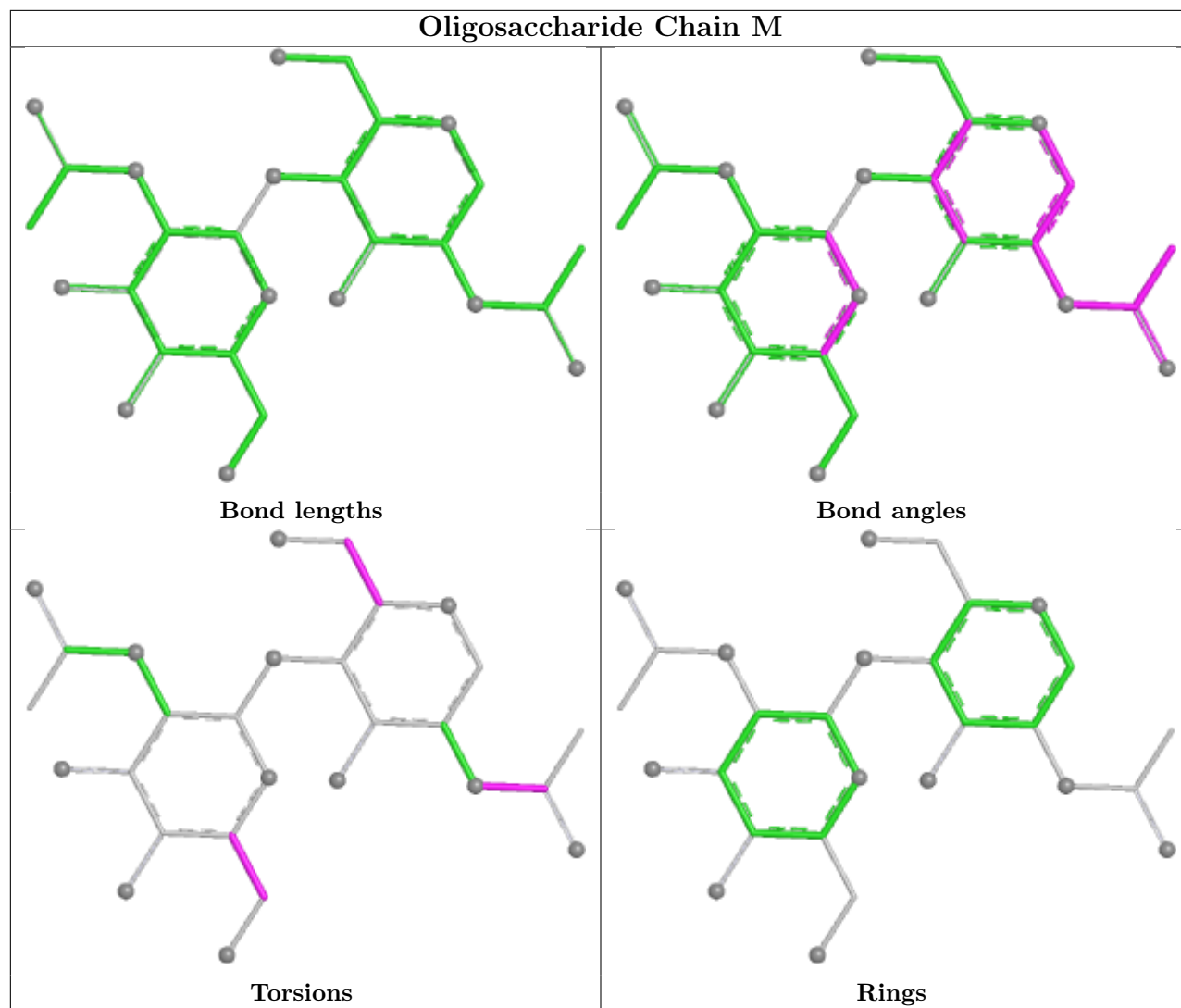
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	b	1	NAG	C1-C2-N2-C7
3	c	2	NAG	C1-C2-N2-C7
3	a	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6

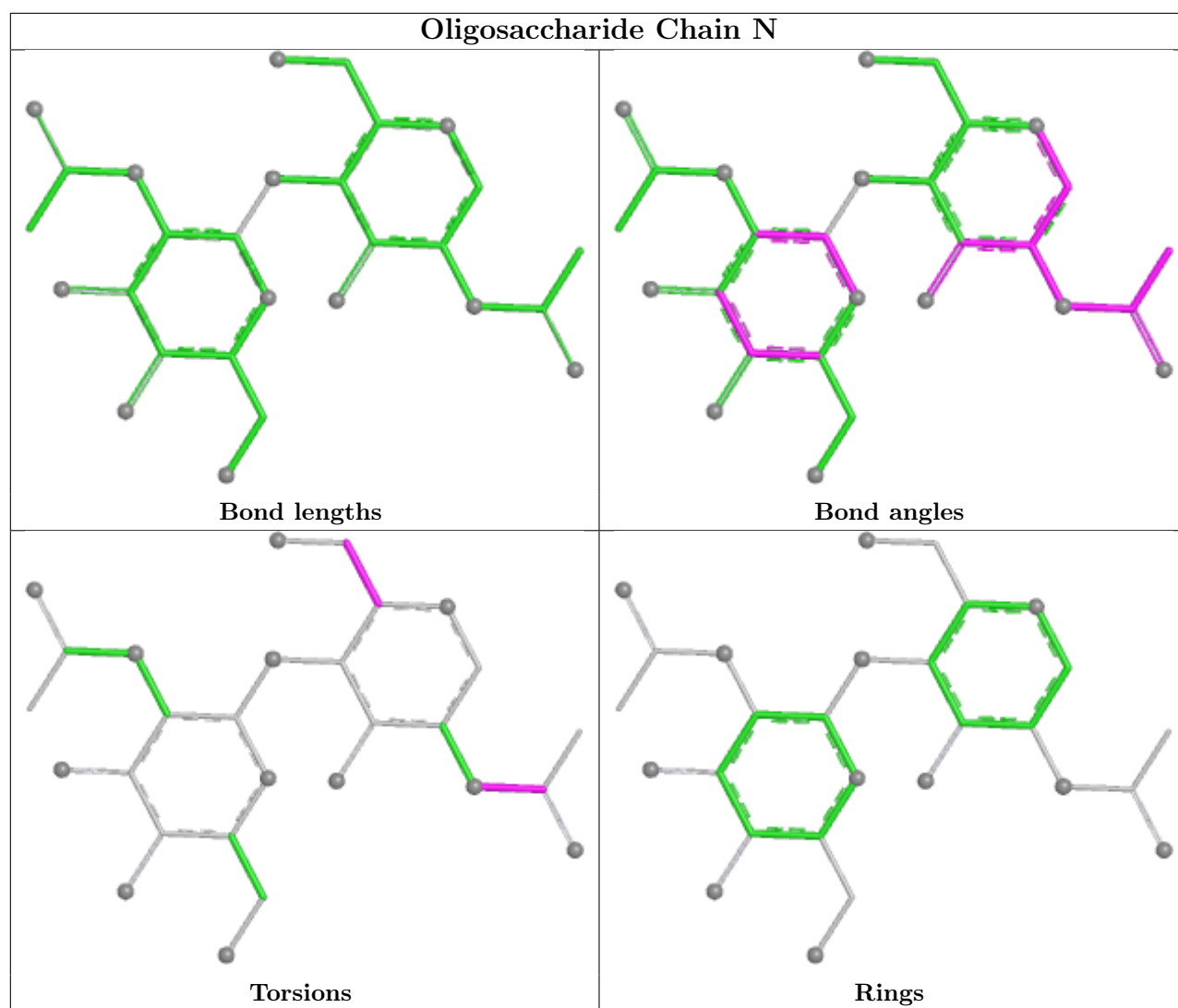
There are no ring outliers.

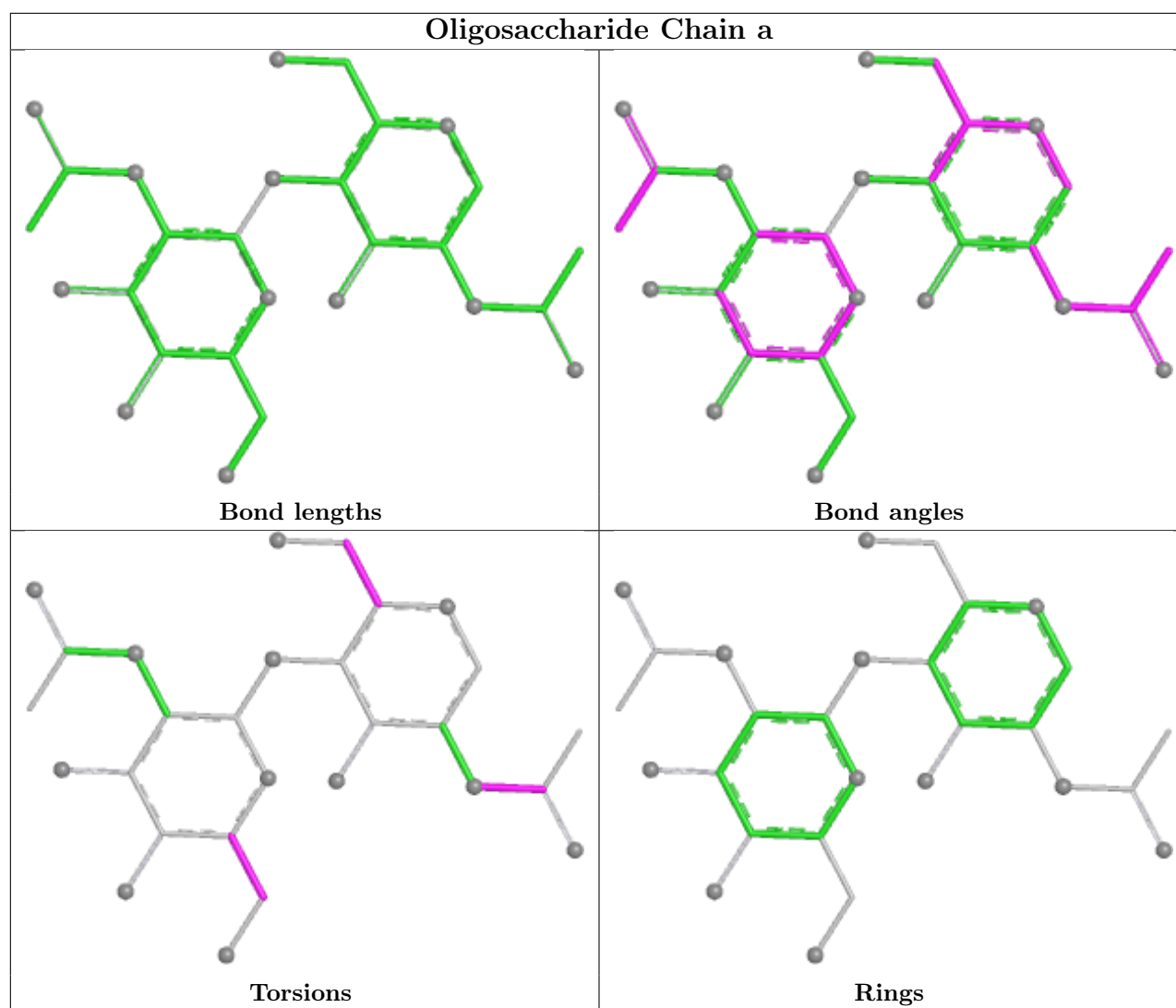
14 monomers are involved in 15 short contacts:

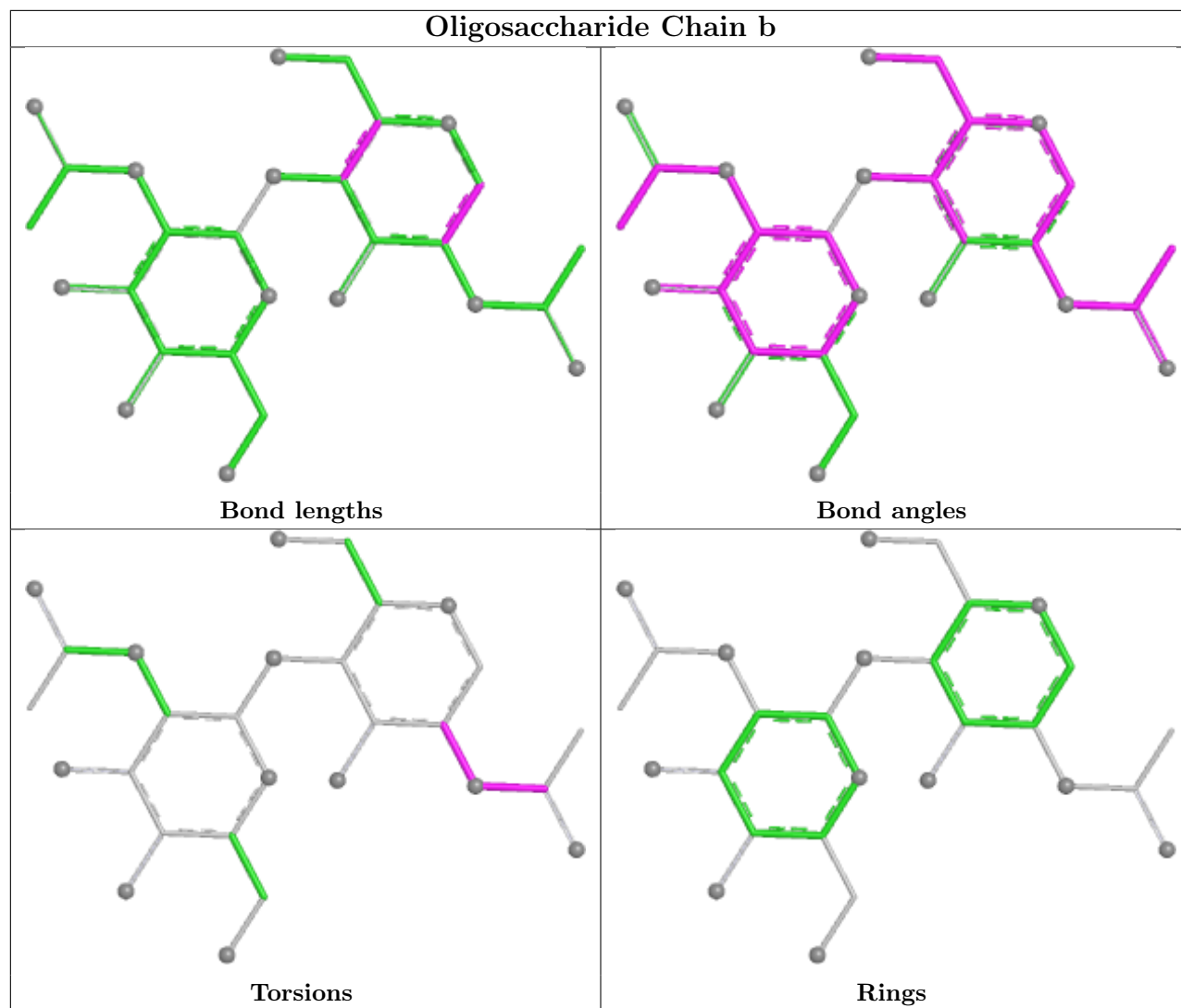
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	i	1	NAG	1	0
3	d	1	NAG	1	0
3	b	1	NAG	1	0
3	M	2	NAG	1	0
3	M	1	NAG	2	0
3	c	1	NAG	1	0
3	f	1	NAG	1	0
3	e	1	NAG	1	0
3	j	1	NAG	1	0
3	h	1	NAG	1	0
3	g	1	NAG	1	0
3	a	1	NAG	2	0
3	N	1	NAG	1	0
3	i	2	NAG	1	0

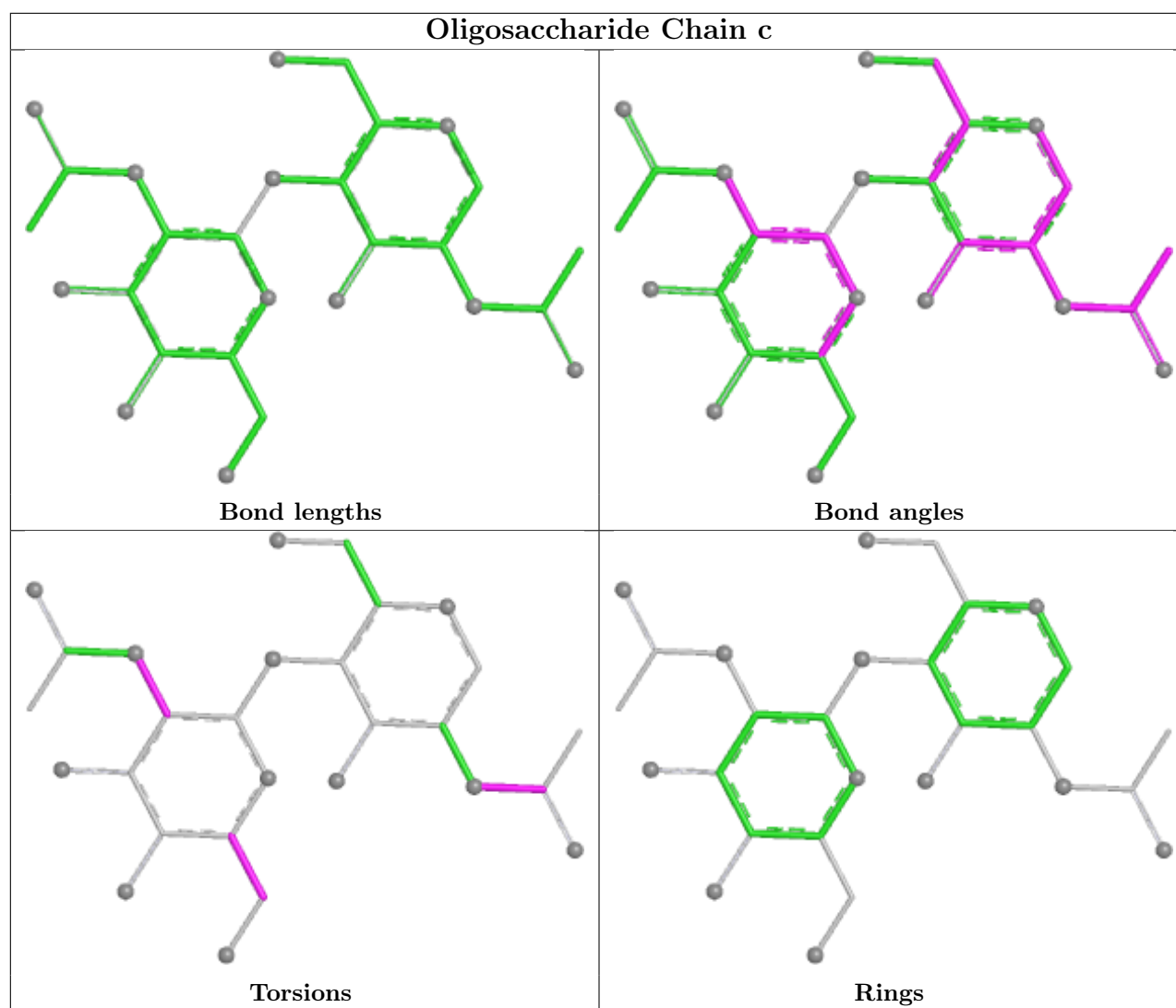
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

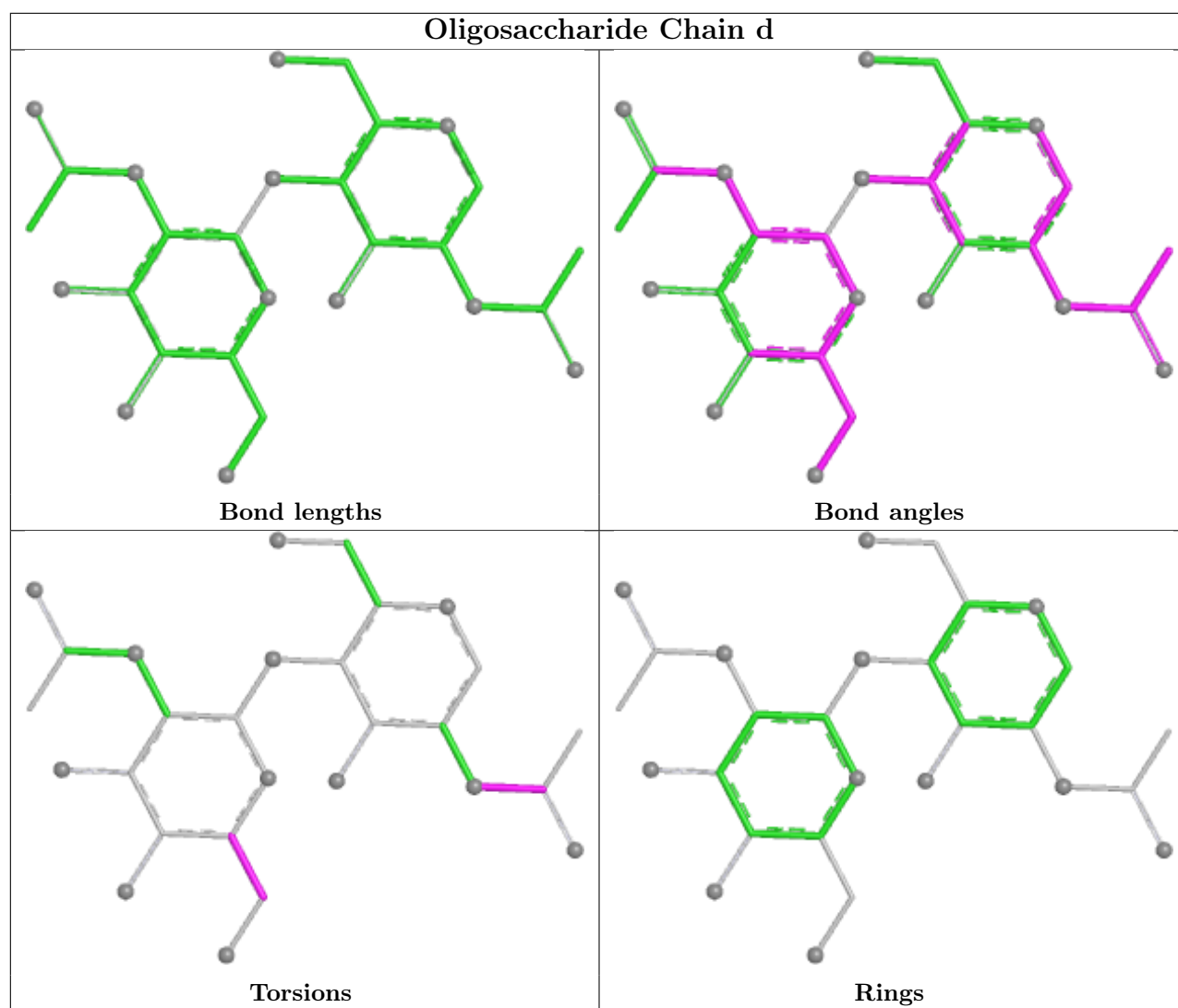


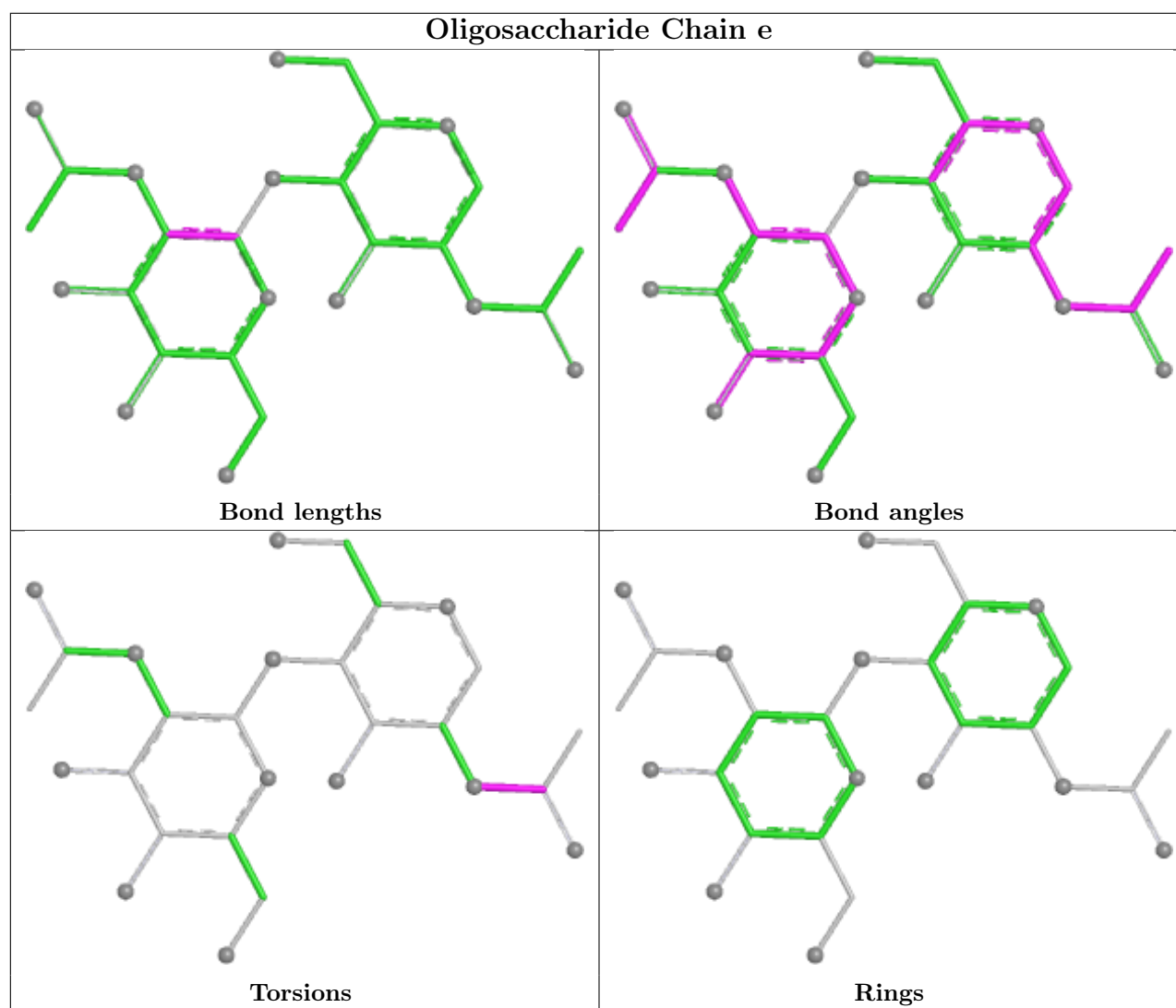


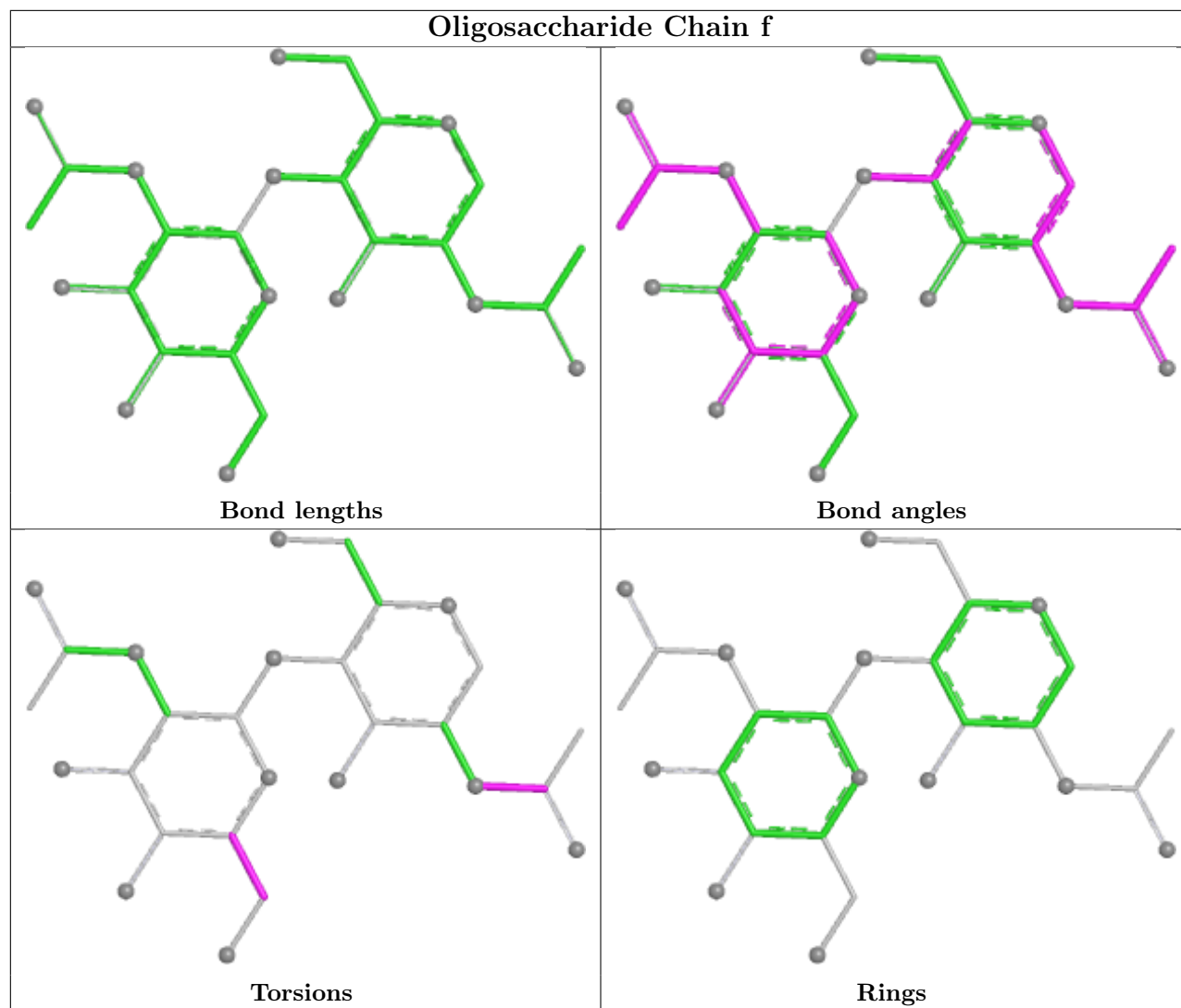


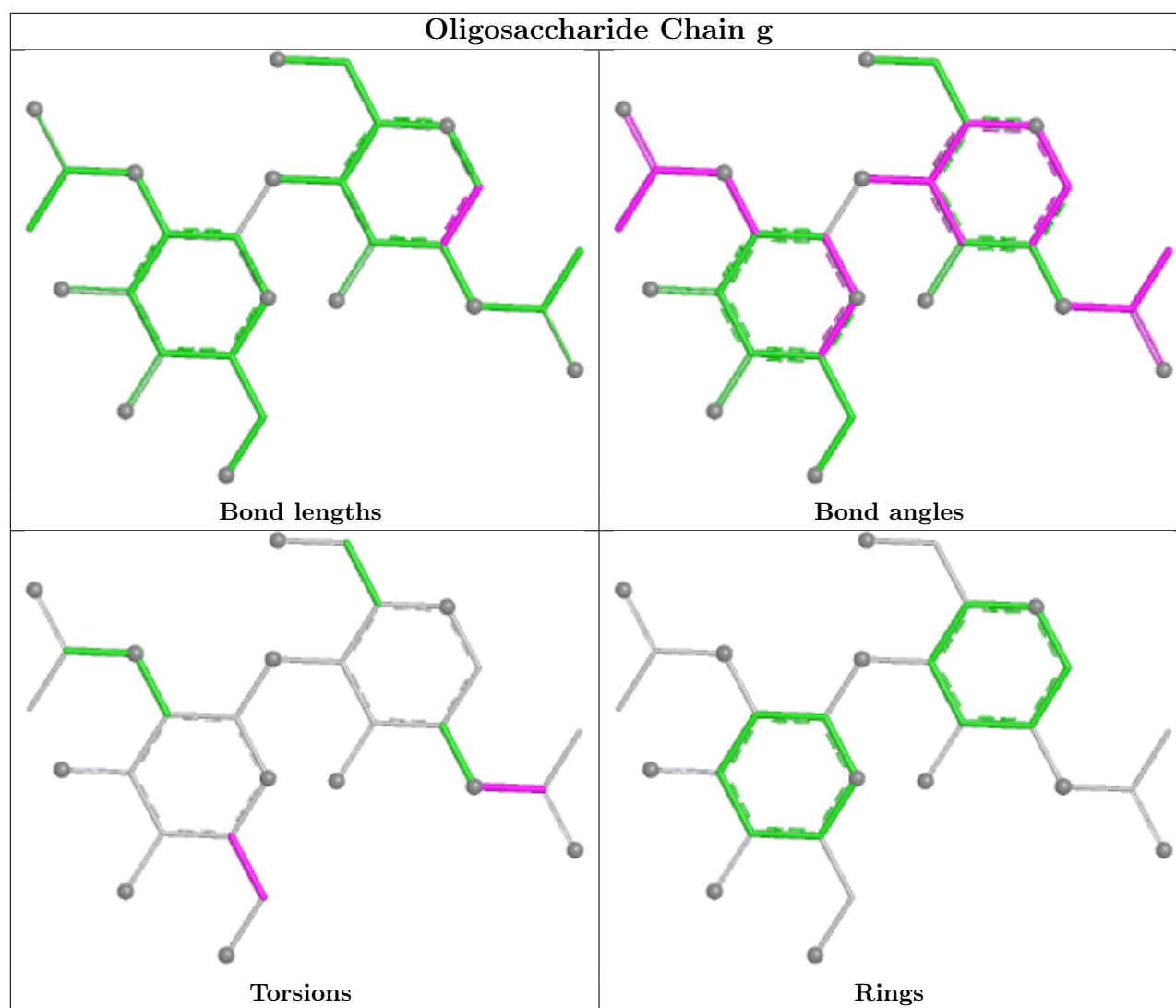


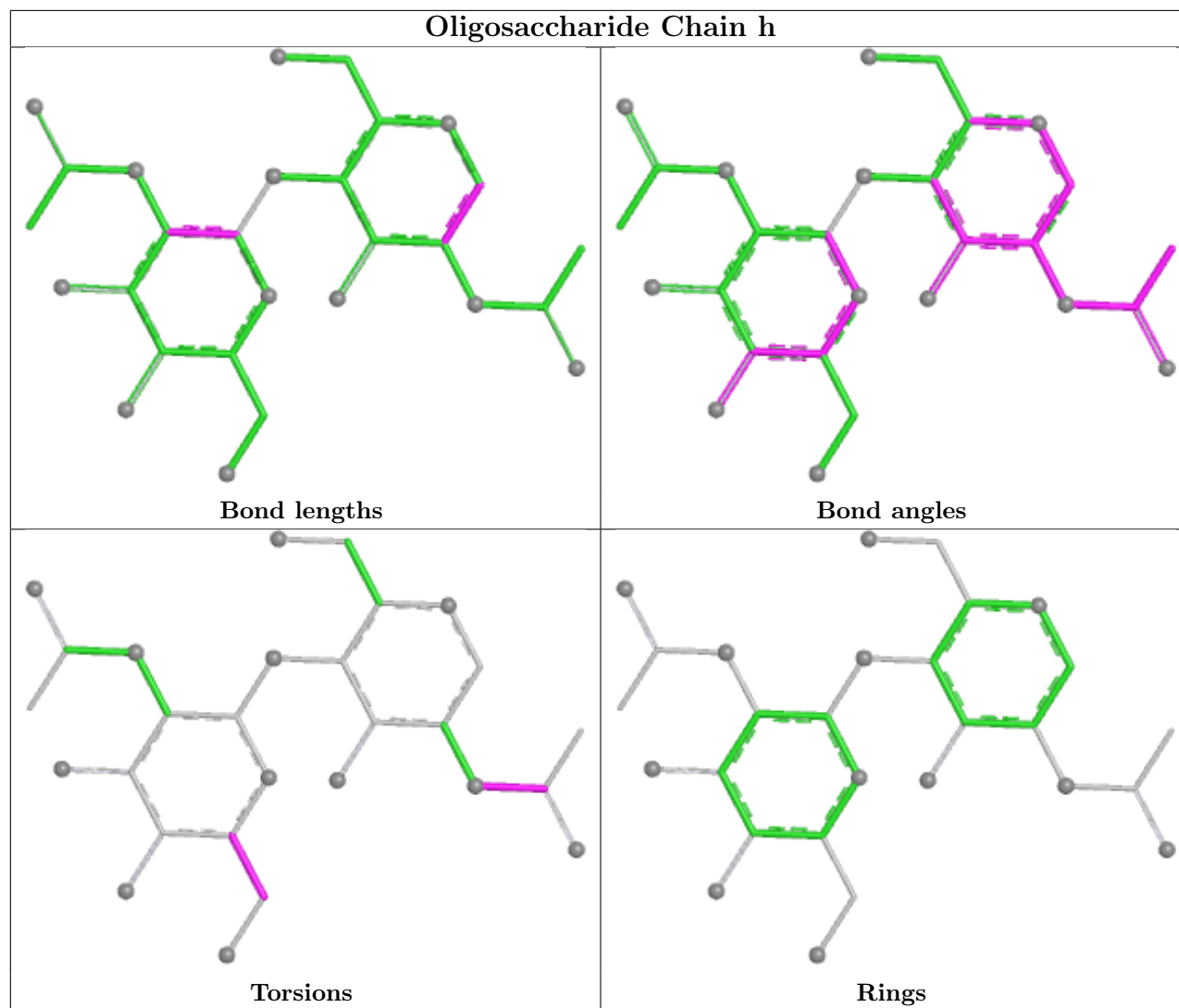


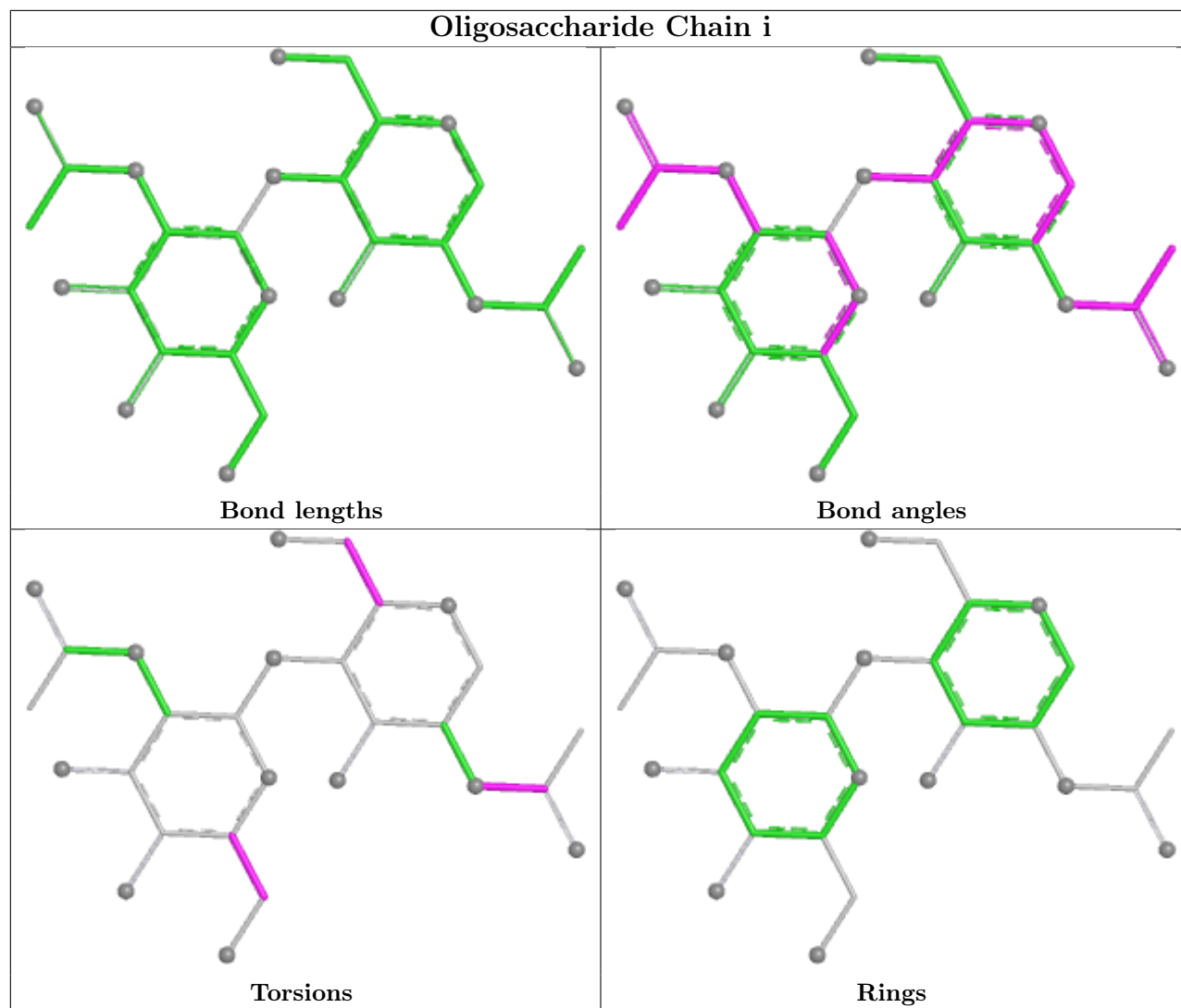


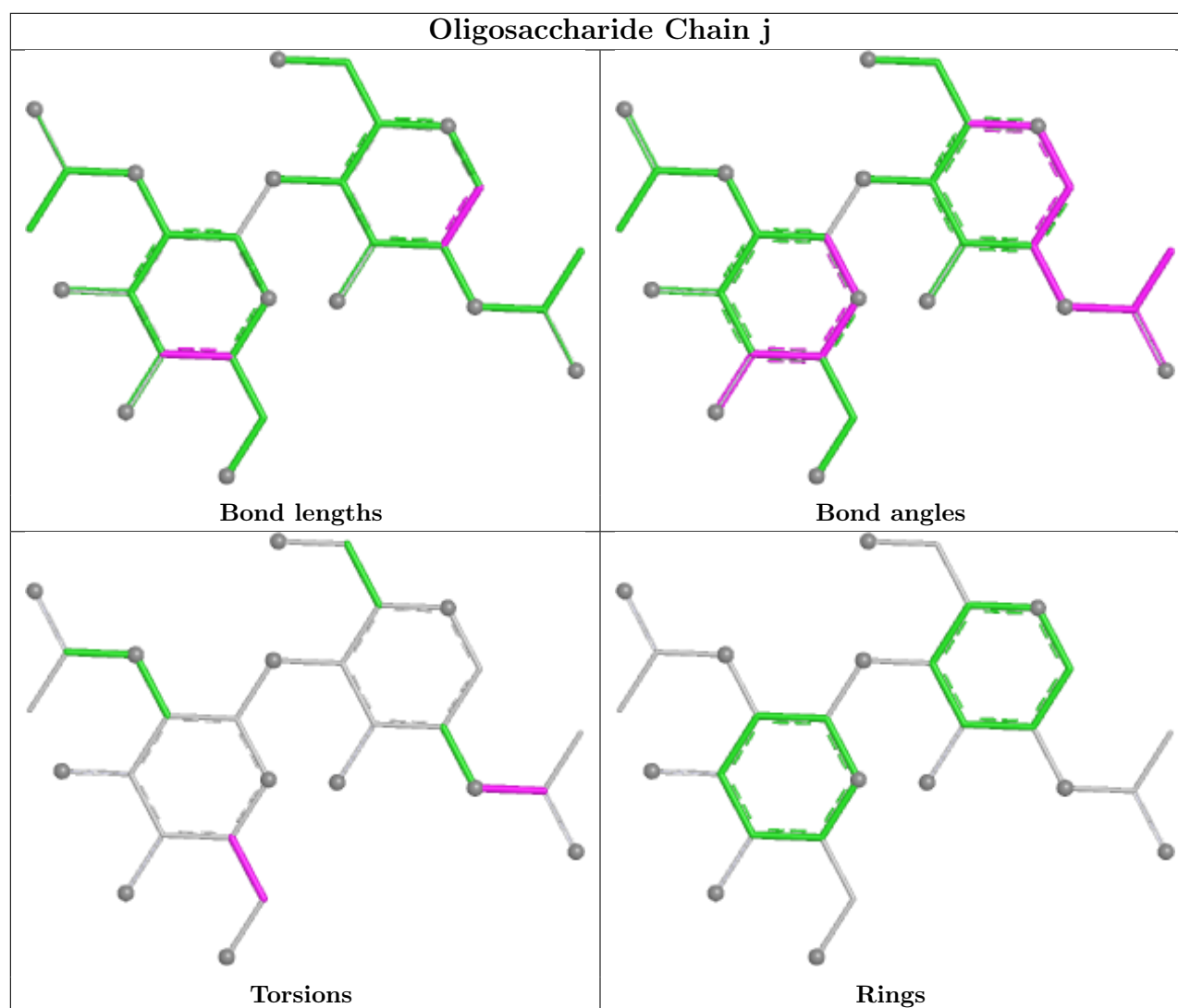












5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

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	A2G	C	1235	2	14,14,15	0.70	0	17,19,21	1.63	3 (17%)
4	A2G	A	1235	2	14,14,15	0.73	0	17,19,21	1.34	1 (5%)
4	A2G	K	1235	2	14,14,15	0.68	0	17,19,21	1.19	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2G	B	1234	2	14,14,15	0.46	0	17,19,21	1.35	3 (17%)
4	A2G	D	1235	2	14,14,15	0.41	0	17,19,21	0.88	0
4	A2G	H	1235	2	14,14,15	0.60	0	17,19,21	1.25	2 (11%)
4	A2G	J	1235	2	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
4	A2G	I	1235	2	14,14,15	0.27	0	17,19,21	1.25	1 (5%)
4	A2G	G	1235	2	14,14,15	0.48	0	17,19,21	1.14	1 (5%)
4	A2G	L	1235	2	14,14,15	0.29	0	17,19,21	0.82	0
4	A2G	F	1239	2	14,14,15	0.52	0	17,19,21	1.73	4 (23%)
4	A2G	E	1235	2	14,14,15	0.38	0	17,19,21	0.97	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	A2G	C	1235	2	-	1/6/23/26	0/1/1/1
4	A2G	A	1235	2	-	1/6/23/26	0/1/1/1
4	A2G	K	1235	2	-	0/6/23/26	0/1/1/1
4	A2G	B	1234	2	-	2/6/23/26	0/1/1/1
4	A2G	D	1235	2	-	0/6/23/26	0/1/1/1
4	A2G	H	1235	2	-	0/6/23/26	0/1/1/1
4	A2G	J	1235	2	-	0/6/23/26	0/1/1/1
4	A2G	I	1235	2	-	0/6/23/26	0/1/1/1
4	A2G	G	1235	2	-	1/6/23/26	0/1/1/1
4	A2G	L	1235	2	-	0/6/23/26	0/1/1/1
4	A2G	F	1239	2	-	0/6/23/26	0/1/1/1
4	A2G	E	1235	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1239	A2G	C1-O5-C5	4.25	117.88	112.19
4	C	1235	A2G	C2-N2-C7	4.18	128.51	122.90
4	I	1235	A2G	C1-O5-C5	4.14	117.73	112.19
4	A	1235	A2G	C1-O5-C5	3.86	117.36	112.19
4	J	1235	A2G	O5-C1-C2	-3.40	106.04	111.29
4	B	1234	A2G	O5-C1-C2	-3.12	106.46	111.29
4	K	1235	A2G	O4-C4-C5	3.03	116.79	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1235	A2G	O4-C4-C3	-2.98	103.35	110.38
4	F	1239	A2G	C6-C5-C4	-2.97	105.74	113.02
4	F	1239	A2G	C2-N2-C7	-2.53	119.52	122.90
4	B	1234	A2G	C1-C2-N2	2.52	114.40	110.43
4	C	1235	A2G	O7-C7-N2	2.47	126.35	121.98
4	K	1235	A2G	O4-C4-C3	-2.44	104.63	110.38
4	F	1239	A2G	O7-C7-C8	-2.29	117.97	122.05
4	C	1235	A2G	C1-O5-C5	2.29	115.25	112.19
4	H	1235	A2G	O5-C1-C2	-2.18	107.91	111.29
4	B	1234	A2G	O5-C5-C6	2.14	111.83	107.66
4	E	1235	A2G	O6-C6-C5	-2.10	104.20	111.33
4	G	1235	A2G	O7-C7-C8	-2.06	118.39	122.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1234	A2G	O5-C5-C6-O6
4	B	1234	A2G	C4-C5-C6-O6
4	A	1235	A2G	C4-C5-C6-O6
4	C	1235	A2G	C4-C5-C6-O6
4	G	1235	A2G	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1235	A2G	2	0
4	B	1234	A2G	2	0
4	J	1235	A2G	9	0
4	F	1239	A2G	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	2
1	E	1
1	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	55:THR	C	56:PRO	N	1.08
1	H	54:SER	C	55:THR	N	0.96
1	E	54:SER	C	55:THR	N	0.95
1	K	54:SER	C	55:THR	N	0.89

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/253 (92%)	0.19	7 (2%) 52 49	43, 56, 98, 127	0
1	B	232/253 (91%)	0.13	2 (0%) 81 80	44, 56, 83, 111	0
1	C	231/253 (91%)	0.67	9 (3%) 43 39	47, 61, 85, 118	0
1	D	234/253 (92%)	0.04	3 (1%) 75 73	44, 49, 63, 87	0
1	E	231/253 (91%)	-0.01	3 (1%) 75 73	44, 49, 65, 83	0
1	F	234/253 (92%)	0.01	4 (1%) 69 67	44, 49, 64, 107	0
1	G	233/253 (92%)	0.05	7 (3%) 52 49	43, 50, 76, 116	0
1	H	232/253 (91%)	-0.00	2 (0%) 81 80	29, 50, 66, 116	1 (0%)
1	I	234/253 (92%)	-0.02	2 (0%) 81 80	43, 49, 61, 85	0
1	J	232/253 (91%)	0.26	5 (2%) 62 59	42, 66, 108, 141	0
1	K	232/253 (91%)	-0.02	2 (0%) 81 80	30, 49, 70, 113	1 (0%)
1	L	232/253 (91%)	0.06	4 (1%) 69 67	44, 51, 75, 125	0
2	O	4/5 (80%)	0.54	1 (25%) 2 1	47, 50, 73, 77	0
2	P	2/5 (40%)	0.48	0 100 100	77, 77, 77, 86	0
2	Q	2/5 (40%)	0.98	0 100 100	72, 72, 72, 81	0
2	R	3/5 (60%)	0.05	0 100 100	76, 76, 76, 82	0
2	S	1/5 (20%)	1.43	0 100 100	71, 71, 71, 71	0
2	T	2/5 (40%)	0.44	0 100 100	63, 63, 63, 63	0
2	U	3/5 (60%)	0.33	0 100 100	61, 61, 62, 82	0
2	V	3/5 (60%)	0.82	0 100 100	71, 71, 73, 98	0
2	W	2/5 (40%)	0.85	0 100 100	70, 70, 70, 70	0
2	X	4/5 (80%)	1.87	2 (50%) 0 0	65, 71, 73, 91	0
2	Y	3/5 (60%)	0.39	0 100 100	50, 50, 55, 75	0
2	Z	2/5 (40%)	0.09	0 100 100	61, 61, 61, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2822/3096 (91%)	0.12	53 (1%) 66 63	29, 51, 83, 141	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	GLY	3.6
1	F	118	ASP	3.1
2	X	2	PRO	3.0
1	H	115	GLU	3.0
1	L	88	ASP	2.9
1	J	46	SER	2.9
1	G	40	ASN	2.9
1	J	116	SER	2.8
1	F	63	GLU	2.8
1	A	106	GLY	2.8
1	L	135	PRO	2.7
1	J	218	GLY	2.7
1	G	39	GLU	2.7
1	L	212	THR	2.7
1	A	117	GLY	2.6
1	C	211	ALA	2.6
1	A	234	HIS	2.5
1	G	117	GLY	2.5
1	C	114	ASN	2.5
1	A	105	ALA	2.5
1	C	213	GLY	2.5
1	C	49	GLY	2.4
1	I	1	ALA	2.4
1	E	234	HIS	2.3
1	F	136	ASN	2.3
1	G	63	GLU	2.3
1	L	118	ASP	2.3
1	C	210	ALA	2.3
2	O	2	PRO	2.2
1	E	65	GLY	2.2
1	G	234	HIS	2.2
1	D	118	ASP	2.2
1	H	234	HIS	2.2
1	A	107	TYR	2.2
1	K	107	TYR	2.2
1	C	217	PRO	2.2
1	C	34	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	132	TRP	2.2
1	E	114	ASN	2.1
1	C	87	ALA	2.1
1	D	40	ASN	2.1
1	A	118	ASP	2.1
1	I	116	SER	2.1
2	X	5	ARG	2.1
1	J	89	GLY	2.1
1	D	87	ALA	2.1
1	B	132	TRP	2.1
1	A	212	THR	2.1
1	G	213	GLY	2.1
1	K	234	HIS	2.0
1	C	42	THR	2.0
1	F	117	GLY	2.0
1	G	106	GLY	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.

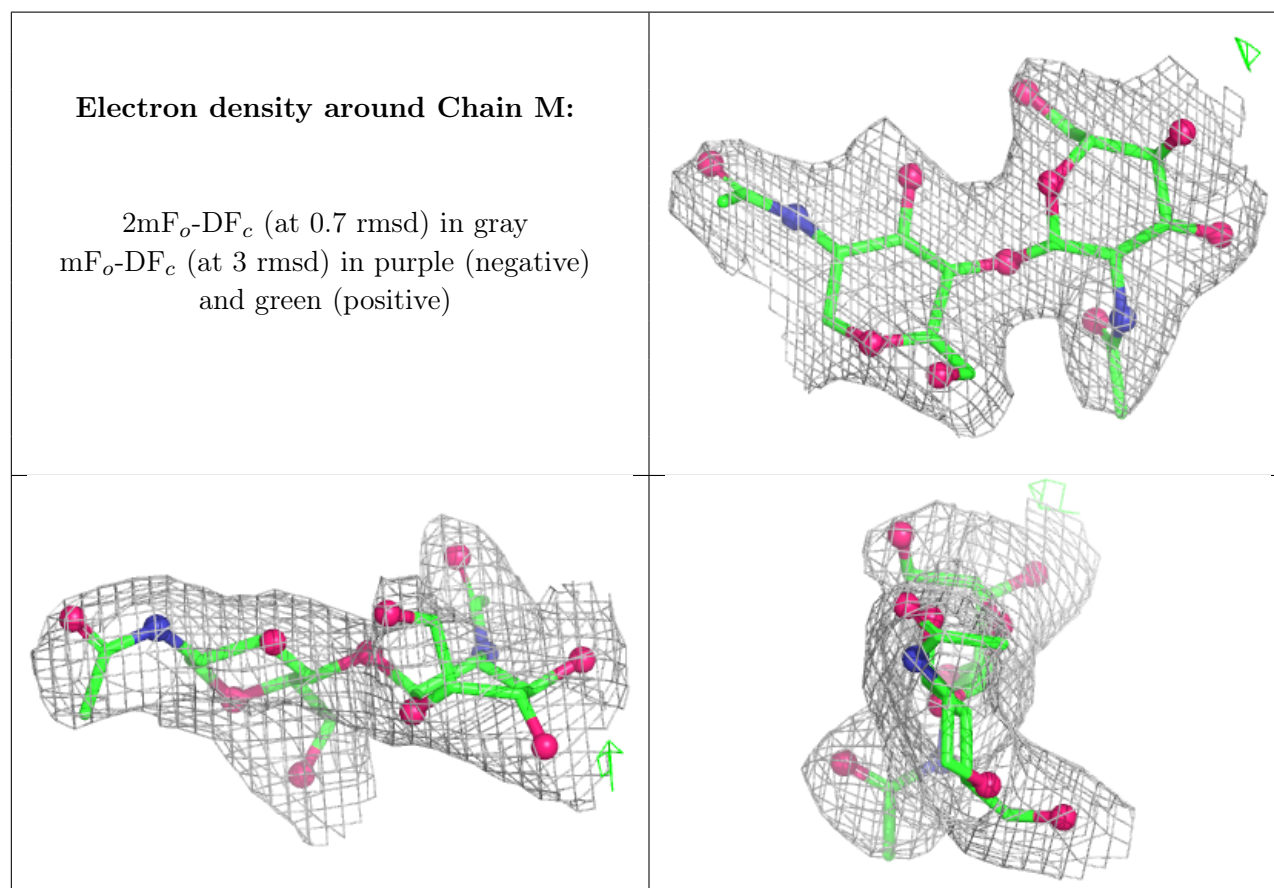
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	M	1	14/15	-	-	29,39,46,48	0
3	NAG	M	2	14/15	-	-	52,57,59,59	0
3	NAG	N	1	14/15	-	-	29,45,50,50	0
3	NAG	N	2	14/15	-	-	50,58,63,67	0
3	NAG	a	1	14/15	-	-	44,60,77,79	0
3	NAG	a	2	14/15	-	-	61,69,90,91	0
3	NAG	b	1	14/15	-	-	24,39,51,52	0
3	NAG	b	2	14/15	-	-	44,58,64,75	0
3	NAG	c	1	14/15	-	-	21,32,46,50	0
3	NAG	c	2	14/15	-	-	42,47,54,67	0
3	NAG	d	1	14/15	-	-	23,33,36,40	0
3	NAG	d	2	14/15	-	-	44,48,55,60	0

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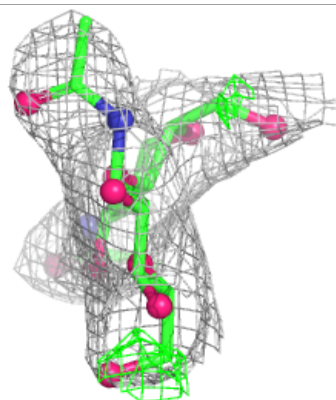
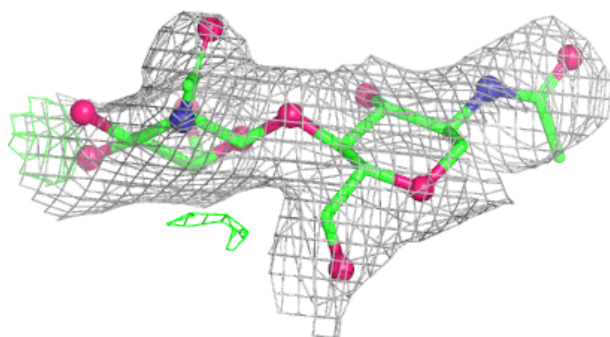
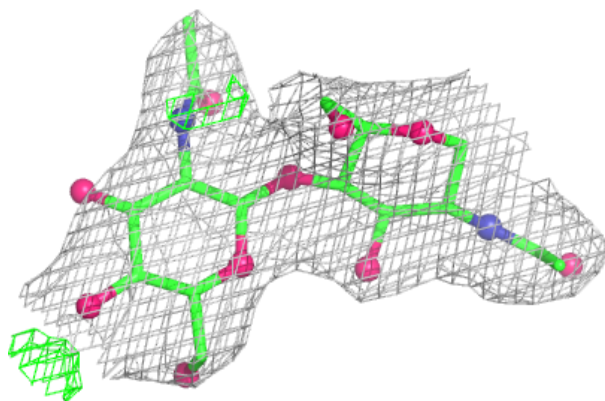
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	e	1	14/15	-	-	28,41,44,46	0
3	NAG	e	2	14/15	-	-	49,55,64,65	0
3	NAG	f	1	14/15	-	-	23,35,39,41	0
3	NAG	f	2	14/15	-	-	41,50,58,59	0
3	NAG	g	1	14/15	-	-	29,41,52,53	0
3	NAG	g	2	14/15	-	-	58,65,75,76	0
3	NAG	h	1	14/15	-	-	32,44,50,50	0
3	NAG	h	2	14/15	-	-	50,59,71,73	0
3	NAG	i	1	14/15	-	-	31,50,63,71	0
3	NAG	i	2	14/15	-	-	45,65,74,75	0
3	NAG	j	1	14/15	-	-	23,33,43,50	0
3	NAG	j	2	14/15	-	-	47,53,64,66	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.

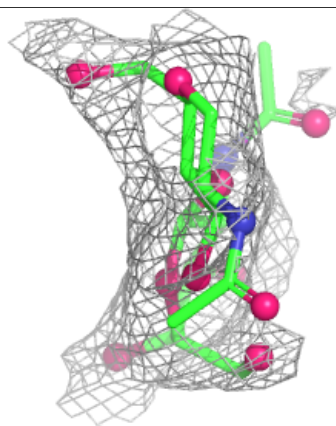
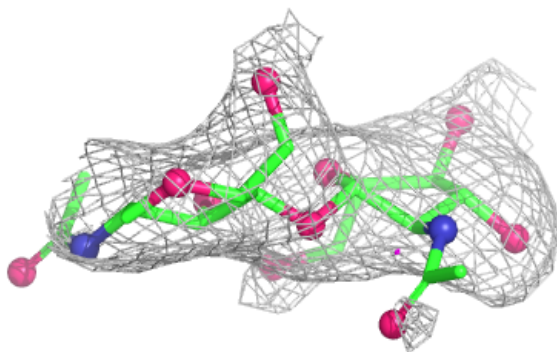
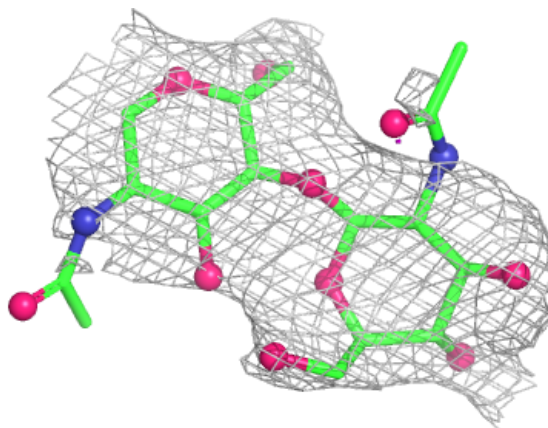


Electron density around Chain N:

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

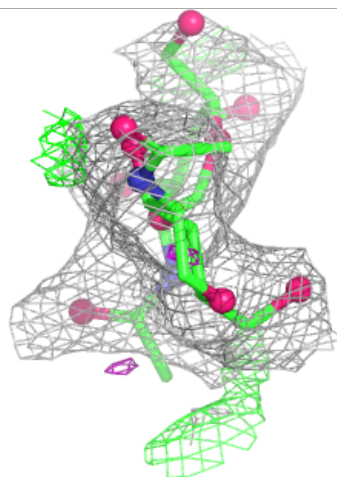
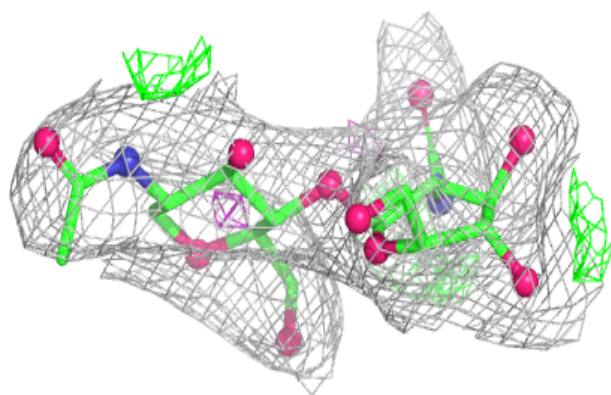
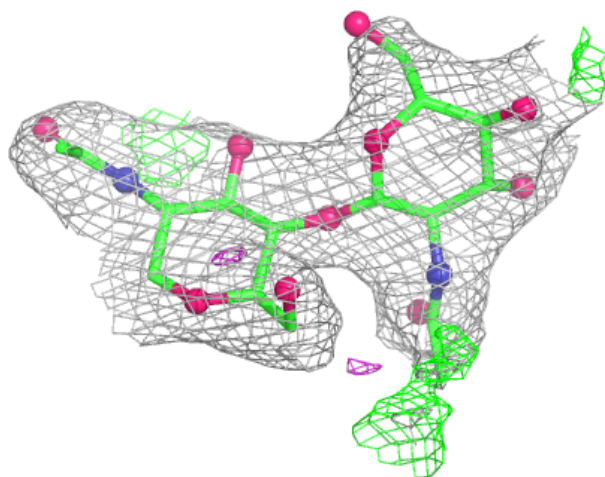
**Electron density around Chain a:**

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



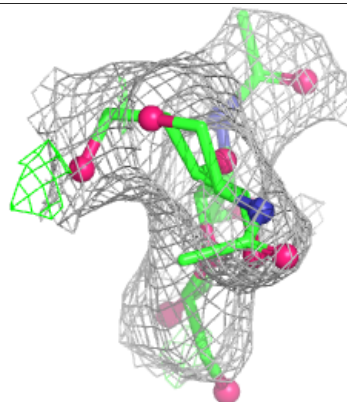
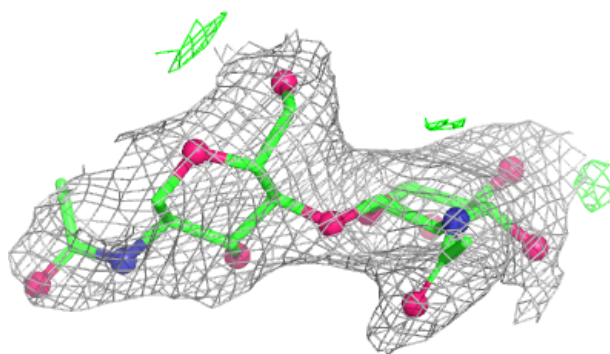
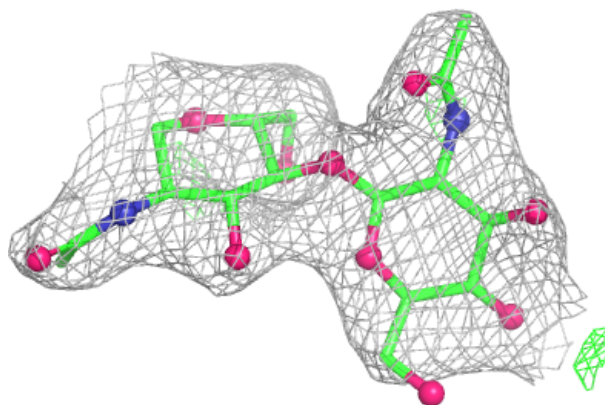
Electron density around Chain b:

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

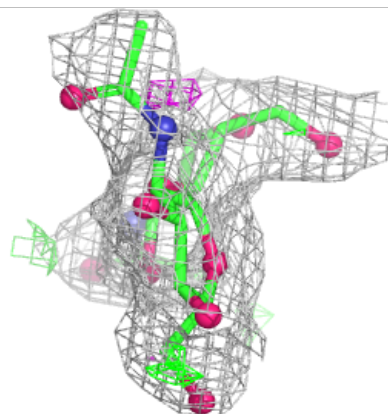
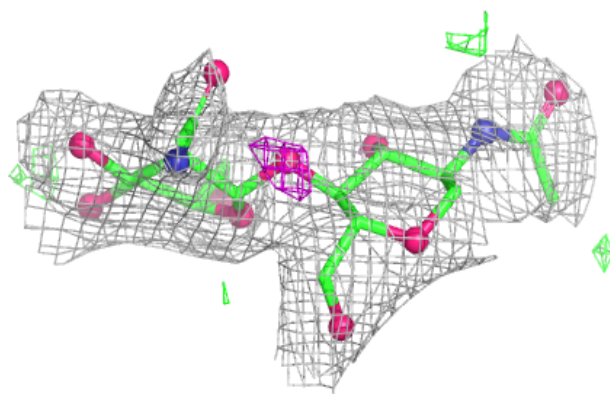
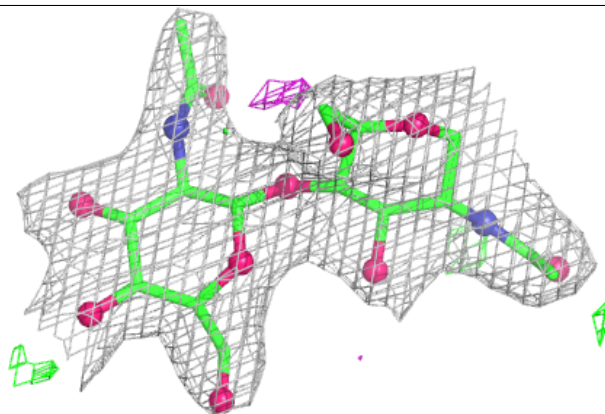


Electron density around Chain c:

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

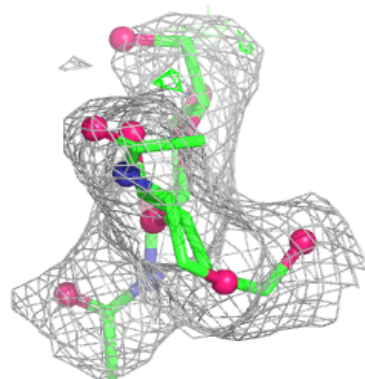
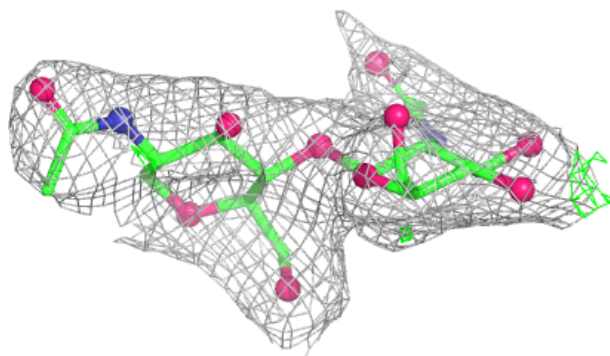
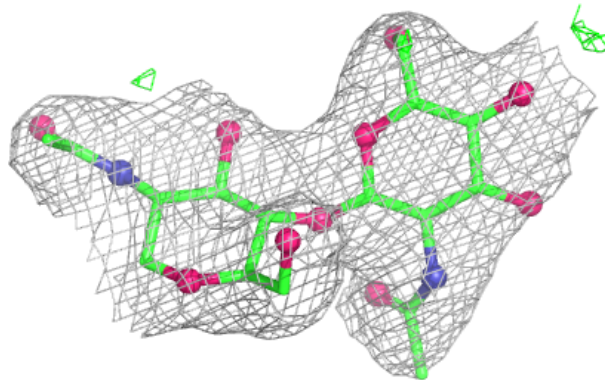
**Electron density around Chain d:**

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

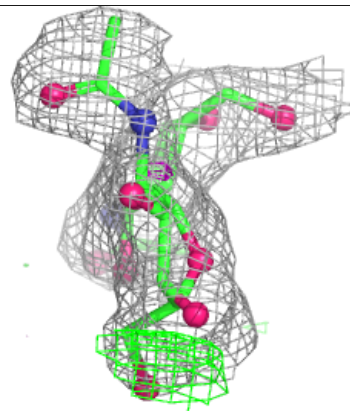
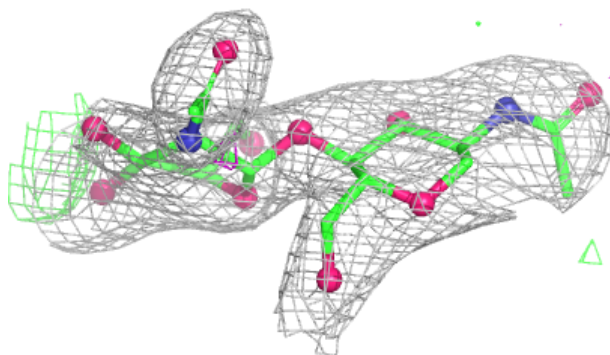
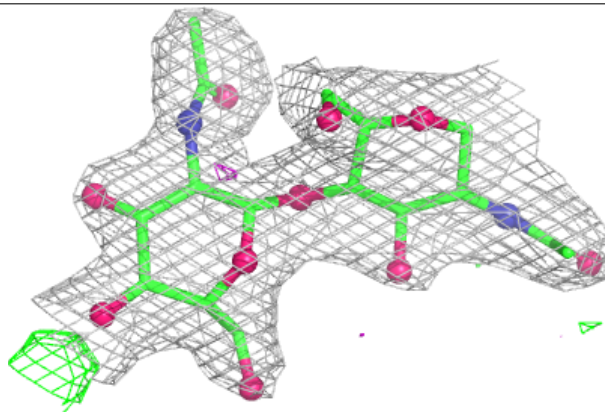


Electron density around Chain e:

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

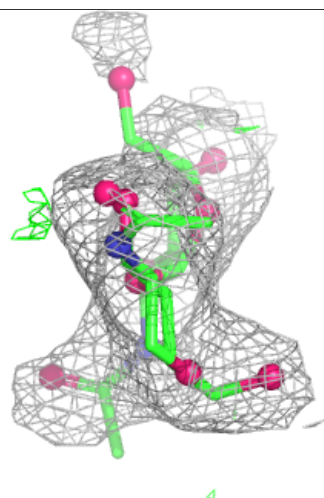
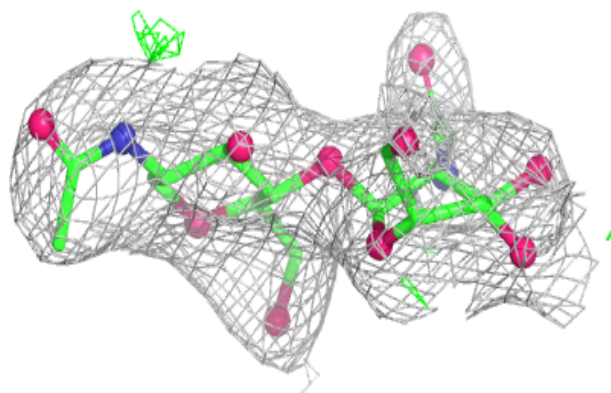
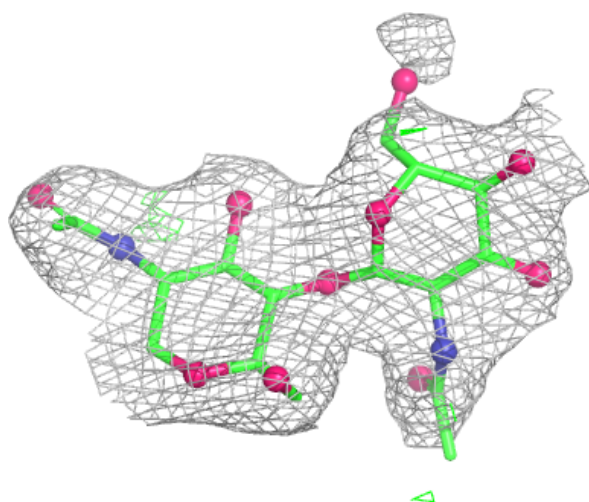
**Electron density around Chain f:**

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



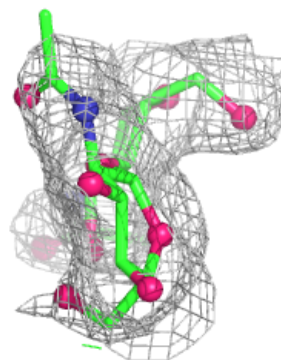
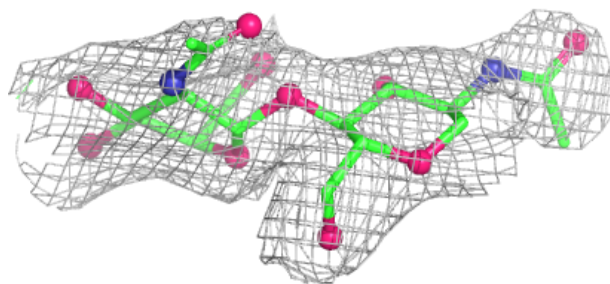
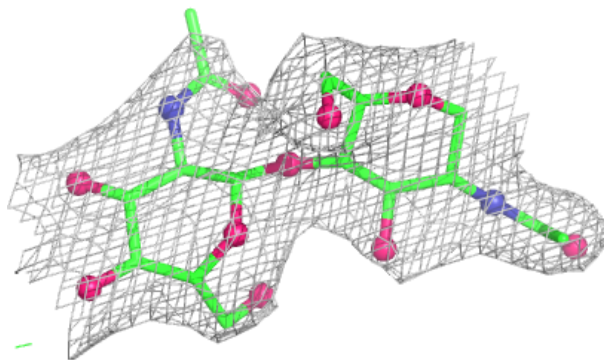
Electron density around Chain g:

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

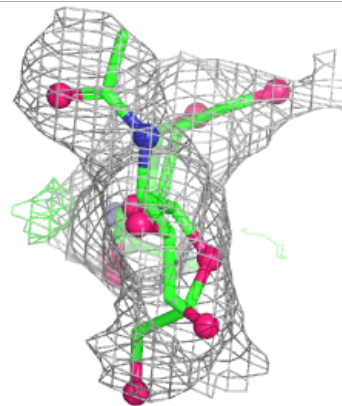
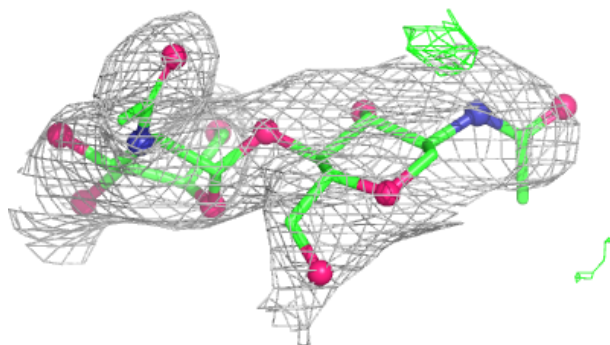
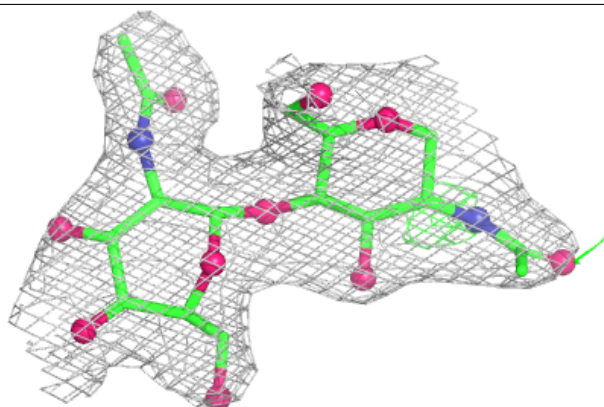


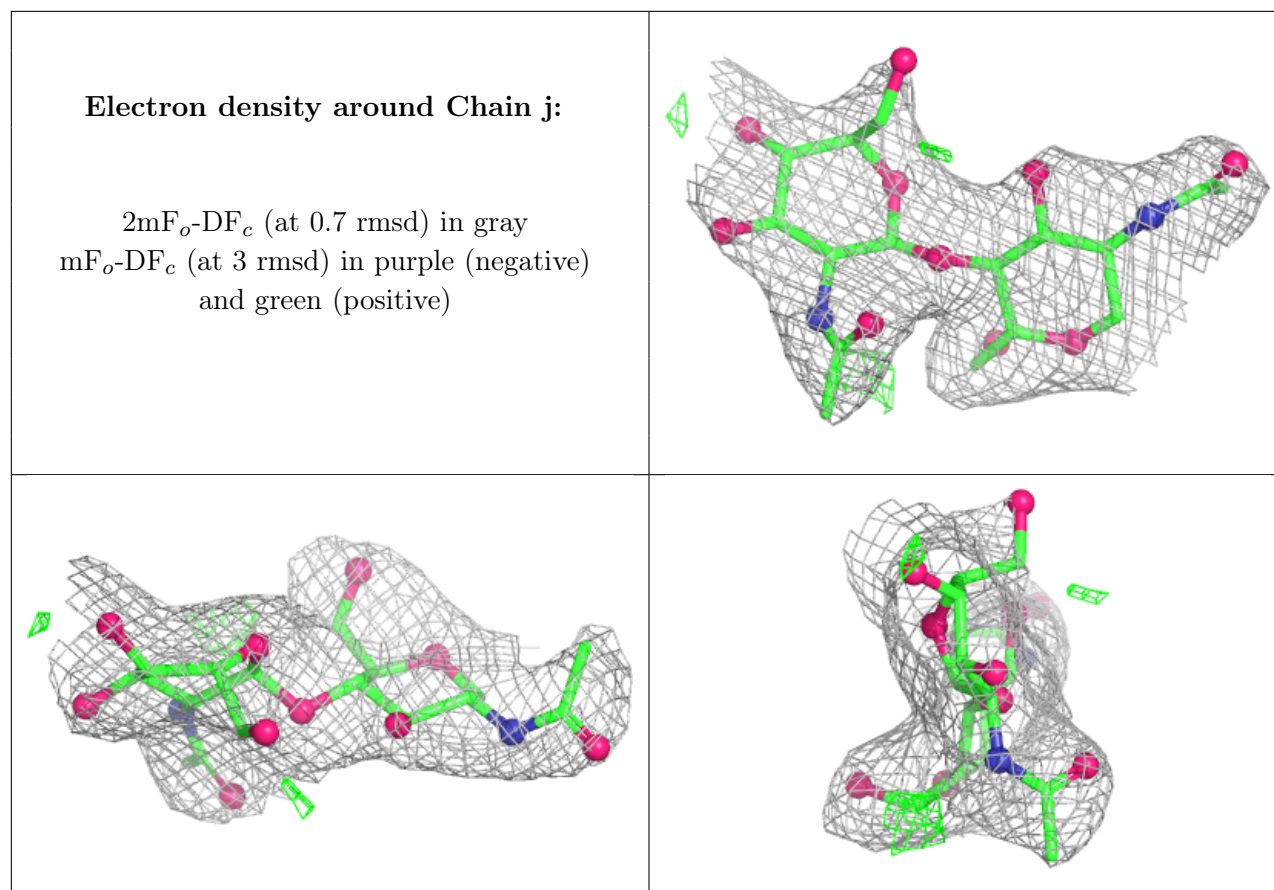
Electron density around Chain h:

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

**Electron density around Chain i:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A2G	C	1235	14/15	0.75	0.13	59,74,79,81	0
4	A2G	J	1235	14/15	0.79	0.13	57,72,78,79	0
4	A2G	A	1235	14/15	0.83	0.11	53,69,74,74	0
5	MN	A	1237	1/1	0.85	0.09	86,86,86,86	0
4	A2G	B	1234	14/15	0.86	0.09	47,52,59,60	0
4	A2G	G	1235	14/15	0.88	0.09	48,58,61,63	0
4	A2G	I	1235	14/15	0.90	0.10	26,29,32,32	0
5	MN	G	1237	1/1	0.90	0.07	66,66,66,66	0
5	MN	F	1238	1/1	0.91	0.06	67,67,67,67	0
4	A2G	H	1235	14/15	0.91	0.11	41,44,49,52	0
4	A2G	F	1239	14/15	0.92	0.07	34,39,42,44	0
4	A2G	D	1235	14/15	0.92	0.08	33,39,42,46	0
4	A2G	L	1235	14/15	0.93	0.07	40,46,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A2G	K	1235	14/15	0.93	0.08	33,40,50,57	0
5	MN	C	1236	1/1	0.94	0.05	65,65,65,65	0
5	MN	H	1237	1/1	0.94	0.08	55,55,55,55	0
5	MN	L	1237	1/1	0.94	0.06	75,75,75,75	0
4	A2G	E	1235	14/15	0.95	0.06	34,40,45,50	0
5	MN	J	1236	1/1	0.95	0.07	63,63,63,63	0
5	MN	A	1236	1/1	0.95	0.05	61,61,61,61	0
5	MN	B	1235	1/1	0.96	0.04	55,55,55,55	0
5	MN	C	1237	1/1	0.96	0.05	65,65,65,65	0
5	MN	E	1237	1/1	0.96	0.05	60,60,60,60	0
5	MN	J	1237	1/1	0.96	0.06	76,76,76,76	0
5	MN	K	1237	1/1	0.96	0.05	65,65,65,65	0
5	MN	B	1236	1/1	0.96	0.05	60,60,60,60	0
5	MN	G	1236	1/1	0.97	0.04	59,59,59,59	0
5	MN	E	1236	1/1	0.98	0.04	44,44,44,44	0
5	MN	H	1236	1/1	0.98	0.03	41,41,41,41	0
5	MN	D	1237	1/1	0.98	0.03	55,55,55,55	0
5	MN	I	1236	1/1	0.98	0.04	43,43,43,43	0
5	MN	F	1237	1/1	0.99	0.03	49,49,49,49	0
5	MN	L	1236	1/1	0.99	0.03	53,53,53,53	0
5	MN	K	1236	1/1	0.99	0.03	43,43,43,43	0
5	MN	D	1236	1/1	1.00	0.04	37,37,37,37	0
5	MN	I	1237	1/1	1.00	0.05	46,46,46,46	0

6.5 Other polymers

There are no such residues in this entry.