



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:39 AM UTC

PDB ID : 1YWH / pdb_00001ywh
Title : crystal structure of urokinase plasminogen activator receptor
Authors : Llinas, P.; Le Du, M.H.; Gardsvoll, H.; Dano, K.; Ploug, M.; Gilquin, B.;
Stura, E.A.; Menez, A.
Deposited on : 2005-02-18
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:

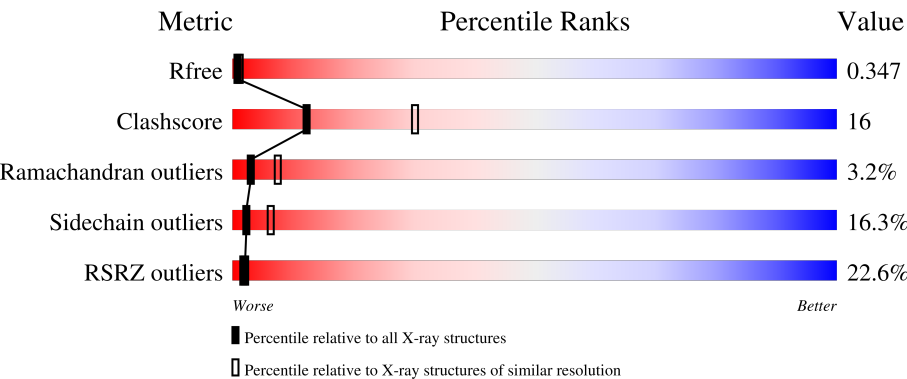
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 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	313	22% 52%25%7%14%
1	C	313	18% 52%24%6%17%
1	E	313	19% 51%26%6%16%
1	G	313	14% 50%26%7%18%
1	I	313	18% 47%29%8%16%

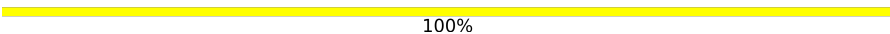
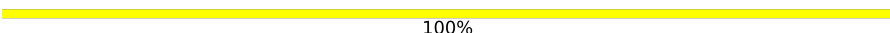
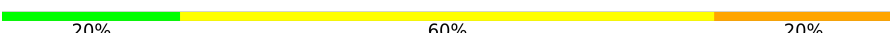
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Mol	Chain	Length	Quality of chain
1	K	313	
1	M	313	
1	O	313	
2	B	13	
2	D	13	
2	F	13	
2	H	13	
2	J	13	
2	L	13	
2	N	13	
2	P	13	
3	Q	3	
3	S	3	
3	T	3	
3	b	3	
4	R	2	
4	U	2	
4	V	2	
4	X	2	
4	Y	2	
4	a	2	
4	d	2	
4	g	2	
5	W	2	
5	f	2	

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Mol	Chain	Length	Quality of chain
6	Z	5	
6	c	5	
6	e	5	
6	h	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
3	FUC	Q	3	X	-	-	-
3	NAG	S	1	X	-	-	-
3	FUC	S	3	X	-	-	-
3	FUC	T	3	X	-	-	-
3	FUC	b	3	X	-	-	-
4	FUC	R	2	X	-	-	-
4	FUC	U	2	X	-	-	-
4	FUC	V	2	X	-	-	-
4	NAG	X	1	X	-	-	-
4	FUC	X	2	X	-	-	-
4	FUC	Y	2	X	-	-	-
4	FUC	a	2	X	-	-	-
4	FUC	d	2	X	-	-	-
4	FUC	g	2	X	-	-	-
6	NAG	Z	1	X	-	-	-
6	NAG	c	1	X	-	-	-
6	NAG	e	1	X	-	-	-
6	NAG	h	1	X	-	-	-
7	NAG	A	317	X	-	-	-
7	NAG	A	321	X	-	-	-
7	NAG	C	316	X	-	-	-
7	NAG	C	321	X	-	-	-
7	NAG	K	331	X	-	-	-
7	NAG	O	321	X	-	-	-
8	SO4	K	810	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18552 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 Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2040	1222	377	407	34			
1	C	259	Total	C	N	O	S	0	0	0
			1985	1188	368	395	34			
1	E	262	Total	C	N	O	S	0	0	0
			2006	1202	370	400	34			
1	G	258	Total	C	N	O	S	0	0	0
			1978	1186	363	395	34			
1	I	264	Total	C	N	O	S	0	0	0
			2008	1201	372	401	34			
1	K	257	Total	C	N	O	S	0	0	0
			1969	1180	363	392	34			
1	M	263	Total	C	N	O	S	0	0	0
			2016	1204	374	404	34			
1	O	258	Total	C	N	O	S	0	0	0
			1970	1180	362	394	34			

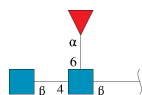
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLN	ASN	conflict	UNP Q9UMV0
C	200	GLN	ASN	conflict	UNP Q9UMV0
E	200	GLN	ASN	conflict	UNP Q9UMV0
G	200	GLN	ASN	conflict	UNP Q9UMV0
I	200	GLN	ASN	conflict	UNP Q9UMV0
K	200	GLN	ASN	conflict	UNP Q9UMV0
M	200	GLN	ASN	conflict	UNP Q9UMV0
O	200	GLN	ASN	conflict	UNP Q9UMV0

- Molecule 2 is a protein called antagonist peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	D	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	F	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	H	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	J	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	L	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	N	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	P	13	Total	C	N	O	0	0	0
			116	78	17	21			

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



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

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



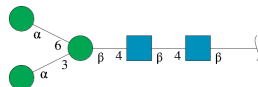
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	U	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	V	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	X	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	Y	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	a	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	d	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	g	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 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
5	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	f	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



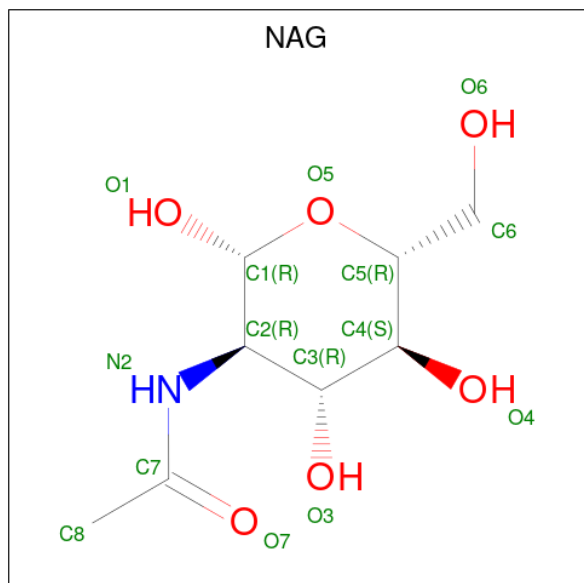
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	c	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	e	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	h	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



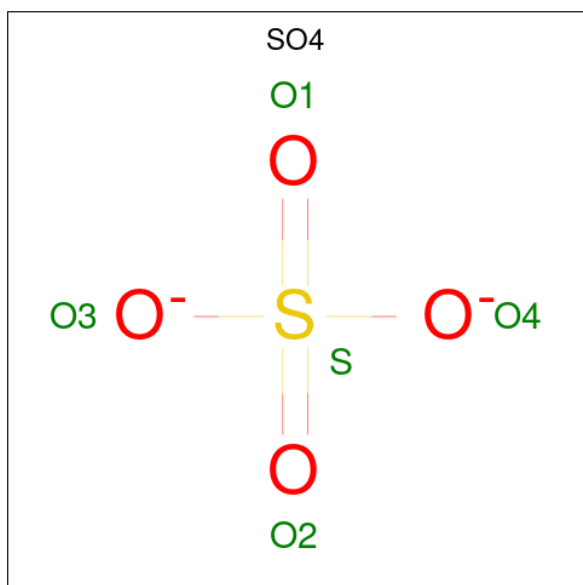
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	K	1	Total O S 5 4 1	0	0
8	K	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	O	1	Total O S 5 4 1	0	0

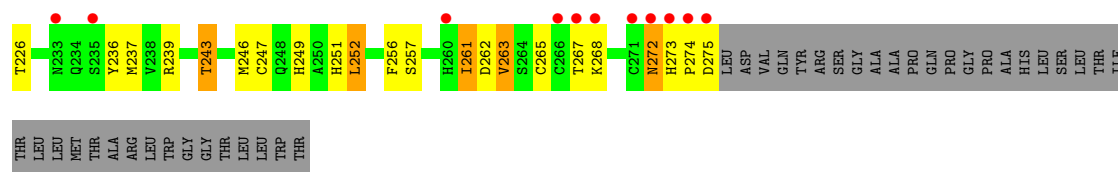
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	81	Total O 81 81	0	0
9	B	5	Total O 5 5	0	0
9	C	85	Total O 85 85	0	0
9	D	2	Total O 2 2	0	0
9	E	98	Total O 98 98	0	0
9	F	8	Total O 8 8	0	0
9	G	88	Total O 88 88	0	0

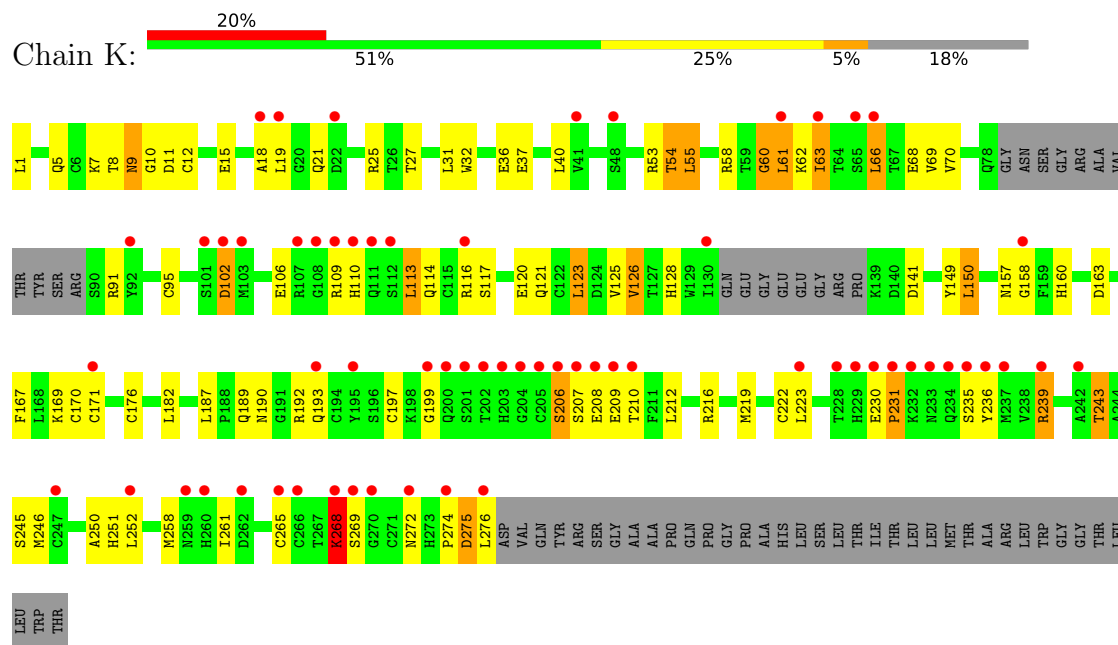
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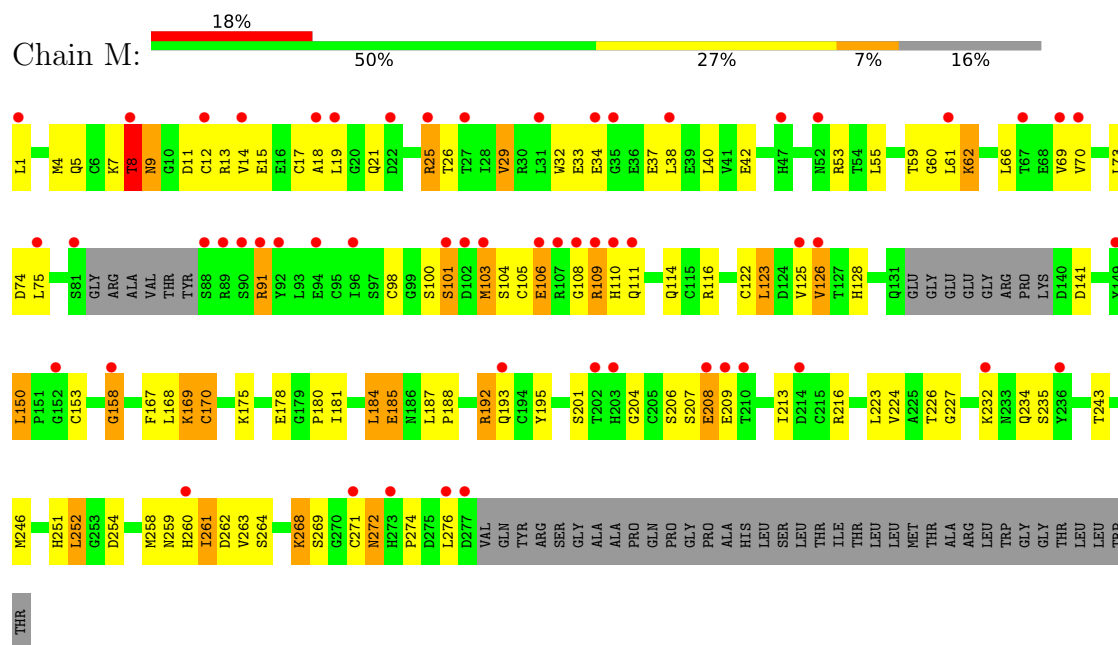
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	4	Total 4	O 4	0	0
9	I	87	Total 87	O 87	0	0
9	J	3	Total 3	O 3	0	0
9	K	83	Total 83	O 83	0	0
9	L	2	Total 2	O 2	0	0
9	M	91	Total 91	O 91	0	0
9	N	1	Total 1	O 1	0	0
9	O	106	Total 106	O 106	0	0
9	P	5	Total 5	O 5	0	0



• Molecule 1: Urokinase plasminogen activator surface receptor

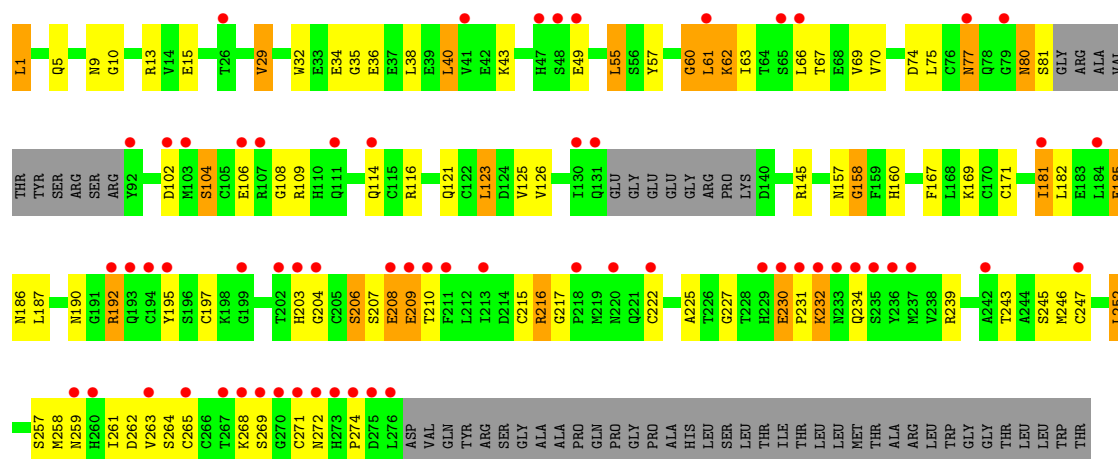


• Molecule 1: Urokinase plasminogen activator surface receptor



• Molecule 1: Urokinase plasminogen activator surface receptor





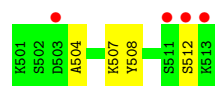
• Molecule 2: antagonist peptide



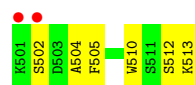
• Molecule 2: antagonist peptide



• Molecule 2: antagonist peptide



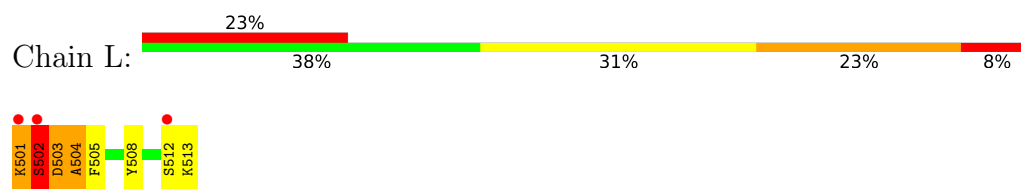
• Molecule 2: antagonist peptide



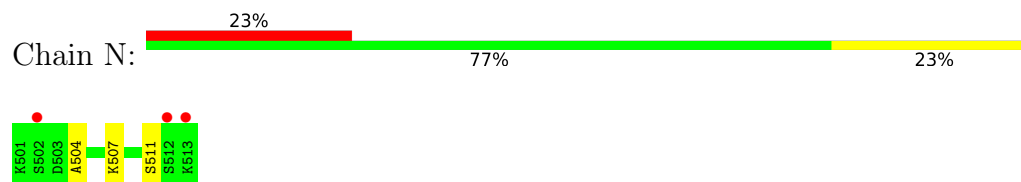
• Molecule 2: antagonist peptide



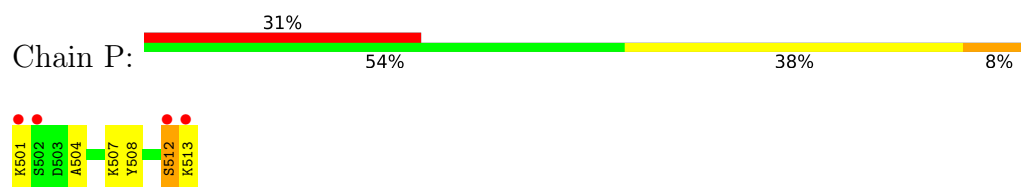
- Molecule 2: antagonist peptide



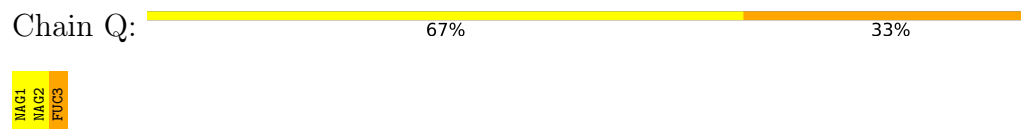
- Molecule 2: antagonist peptide



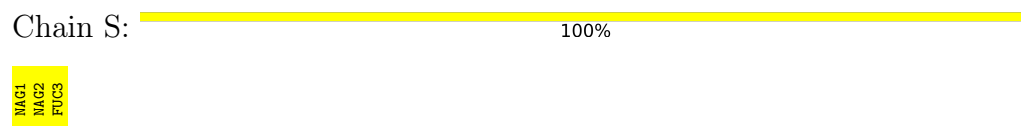
- Molecule 2: antagonist peptide



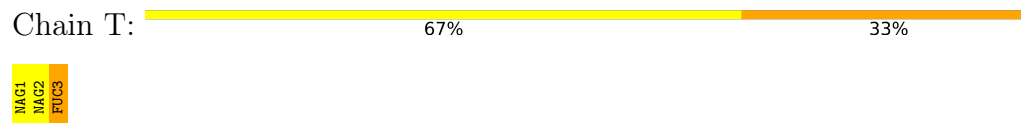
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



MAG1
MAG2
FUC3

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

Chain R:  100%

MAG1
FUC2

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

Chain U:  50% 50%

MAG1
FUC2

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

Chain V:  50% 50%

MAG1
FUC2

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

Chain X:  50% 50%

MAG1
FUC2

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

Chain Y:  100%

MAG1
FUC2

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

Chain a:  100%

MAG1
FUC2

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

Chain d:  100%

MAG1
FUC2

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

Chain g:  50% 50%

NAG1
FUC2

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

Chain W:  100%

NAG1
NAG2

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

Chain f:  100%

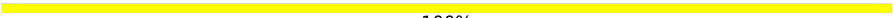
NAG1
NAG2

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

Chain Z:  20% 80%

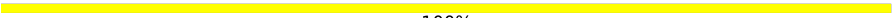
NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain c:  100%

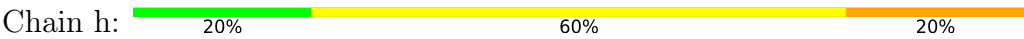
NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain e:  100%

NAG1
NAG2
BMA3
MAN4
MAN5

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.93Å 136.83Å 140.54Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	24.85 – 2.70 24.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.85-2.70) 97.1 (24.85-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.245 , 0.315 0.281 , 0.347	Depositor DCC
R_{free} test set	5335 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18552	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.00% 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, DSN, SO4, MAN, ALC, DLY, FUC, BMA

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	0.68	2/2072 (0.1%)	1.00	3/2791 (0.1%)
1	C	1.06	4/2016 (0.2%)	0.99	5/2713 (0.2%)
1	E	0.66	2/2037 (0.1%)	0.95	1/2742 (0.0%)
1	G	0.65	1/2009 (0.0%)	1.00	5/2704 (0.2%)
1	I	0.65	0/2039	0.97	3/2746 (0.1%)
1	K	0.69	1/2000 (0.1%)	0.99	2/2693 (0.1%)
1	M	0.65	0/2047	1.03	5/2755 (0.2%)
1	O	0.64	3/2001 (0.1%)	0.99	4/2695 (0.1%)
2	B	0.59	0/91	0.81	0/116
2	D	0.56	0/91	0.80	0/116
2	F	0.60	0/91	0.89	0/116
2	H	0.61	0/91	0.75	0/116
2	J	0.64	0/91	0.94	0/116
2	L	0.56	0/91	0.90	0/116
2	N	0.61	0/91	0.87	0/116
2	P	0.56	0/91	0.94	1/116 (0.9%)
All	All	0.72	13/16949 (0.1%)	0.99	29/22767 (0.1%)

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	A	0	3
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	2
All	All	0	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	273	HIS	CE1-NE2	31.57	1.64	1.32
1	C	273	HIS	CG-ND1	22.83	1.63	1.38
1	K	268	LYS	CE-NZ	11.96	1.85	1.49
1	C	273	HIS	CG-CD2	8.15	1.44	1.35
1	A	233	ASN	CG-ND2	7.91	1.49	1.33
1	A	233	ASN	CG-OD1	6.24	1.35	1.23
1	O	102	ASP	CG-OD2	5.84	1.36	1.25
1	O	62	LYS	N-CA	-5.34	1.39	1.45
1	E	259	ASN	CG-OD1	5.19	1.33	1.23
1	G	107	ARG	NE-CZ	5.10	1.38	1.33
1	E	259	ASN	CG-ND2	5.09	1.44	1.33
1	C	273	HIS	ND1-CE1	5.05	1.37	1.32
1	O	102	ASP	CG-OD1	5.05	1.34	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	HIS	ND1-CG-CD2	7.95	114.05	106.10
1	O	61	LEU	CA-C-O	7.24	125.11	119.18
1	I	138	PRO	N-CA-CB	6.93	110.53	103.25
1	C	138	PRO	N-CA-CB	6.91	110.60	103.00
1	M	158	GLY	N-CA-C	6.84	120.85	110.18
1	I	82	GLY	N-CA-C	-6.84	104.99	115.66
1	G	61	LEU	CA-C-O	6.82	124.78	119.18
1	G	209	GLU	N-CA-C	-6.69	105.27	113.50
1	O	62	LYS	N-CA-C	-6.61	99.82	110.32
1	C	273	HIS	CG-ND1-CE1	-6.37	98.47	109.30
1	M	62	LYS	N-CA-C	-6.19	99.56	109.96
1	C	77	ASN	N-CA-C	6.06	120.28	113.01
1	G	62	LYS	N-CA-C	-6.06	101.52	110.48
1	K	158	GLY	N-CA-C	6.04	119.42	110.42
1	I	19	LEU	N-CA-C	5.96	117.78	111.28
1	K	102	ASP	N-CA-C	5.92	119.52	111.17
1	A	231	PRO	N-CD-CG	-5.77	96.88	103.80
1	A	9	ASN	CB-CA-C	-5.39	99.69	110.42
1	M	192	ARG	N-CA-C	5.29	117.36	110.43
1	O	158	GLY	N-CA-C	5.23	119.24	110.56
1	G	172	ASN	N-CA-C	5.21	118.74	112.38
1	A	259	ASN	N-CA-C	5.21	119.72	112.90
1	E	158	GLY	N-CA-C	5.16	118.01	110.38
1	C	67	THR	N-CA-C	5.15	115.83	107.23
2	P	512	SER	N-CA-C	5.12	117.72	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	259	ASN	N-CA-C	5.12	119.41	112.04
1	O	209	GLU	N-CA-C	-5.06	106.62	112.89
1	G	158	GLY	N-CA-C	5.04	117.84	110.38
1	M	8	THR	N-CA-C	5.04	118.20	111.75

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Peptide
1	A	272	ASN	Peptide
1	A	61	LEU	Peptide
1	E	61	LEU	Peptide
1	G	208	GLU	Peptide
1	I	80	ASN	Peptide
1	K	102	ASP	Peptide
1	K	61	LEU	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	2040	0	1885	62	0
1	C	1985	0	1840	76	0
1	E	2006	0	1864	67	0
1	G	1978	0	1836	68	0
1	I	2008	0	1850	74	0
1	K	1969	0	1825	67	0
1	M	2016	0	1868	61	0
1	O	1970	0	1823	61	0
2	B	116	0	113	9	0
2	D	116	0	112	7	0
2	F	116	0	112	3	0
2	H	116	0	112	3	0
2	J	116	0	112	2	0
2	L	116	0	112	7	0
2	N	116	0	112	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	116	0	112	6	0
3	Q	38	0	34	0	0
3	S	38	0	34	0	0
3	T	38	0	34	0	0
3	b	38	0	34	0	0
4	R	24	0	22	0	0
4	U	24	0	22	0	0
4	V	24	0	22	0	0
4	X	24	0	22	0	0
4	Y	24	0	22	1	0
4	a	24	0	22	0	0
4	d	24	0	22	1	0
4	g	24	0	22	0	0
5	W	28	0	25	2	0
5	f	28	0	25	0	0
6	Z	61	0	52	0	0
6	c	61	0	52	0	0
6	e	61	0	52	0	0
6	h	61	0	52	1	0
7	A	28	0	26	0	0
7	C	28	0	26	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
7	I	14	0	13	0	0
7	K	28	0	26	0	0
7	M	14	0	13	0	0
7	O	14	0	13	0	0
8	A	15	0	0	1	0
8	C	15	0	0	1	0
8	E	15	0	0	0	0
8	G	20	0	0	1	0
8	I	15	0	0	1	0
8	K	10	0	0	3	0
8	M	10	0	0	1	0
8	O	5	0	0	0	0
9	A	81	0	0	2	0
9	B	5	0	0	0	0
9	C	85	0	0	1	0
9	D	2	0	0	1	0
9	E	98	0	0	4	0
9	F	8	0	0	1	0
9	G	88	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	4	0	0	0	0
9	I	87	0	0	1	0
9	J	3	0	0	0	0
9	K	83	0	0	4	0
9	L	2	0	0	1	0
9	M	91	0	0	4	0
9	N	1	0	0	0	0
9	O	106	0	0	5	0
9	P	5	0	0	1	0
All	All	18552	0	16401	530	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 16.

All (530) 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:K:268:LYS:CE	1:K:268:LYS:NZ	1.85	1.38
1:C:273:HIS:HB3	1:C:274:PRO:HD3	1.11	1.10
1:C:273:HIS:HB3	1:C:274:PRO:CD	1.86	1.05
1:C:55:LEU:HB3	1:C:66:LEU:HD23	1.35	1.04
1:G:55:LEU:HD23	1:G:123:LEU:HD12	1.46	0.97
1:M:29:VAL:HB	1:M:66:LEU:HD13	1.45	0.96
1:M:4:MET:CE	1:M:75:LEU:HD22	2.00	0.91
1:C:273:HIS:CB	1:C:274:PRO:HD3	2.01	0.90
1:G:32:TRP:CE2	1:G:62:LYS:HB3	2.06	0.90
1:G:195:TYR:H	1:G:272:ASN:HD21	1.13	0.90
1:G:198:LYS:NZ	8:G:817:SO4:O2	2.05	0.90
1:O:32:TRP:CD1	1:O:62:LYS:HB3	2.08	0.89
1:G:55:LEU:HD23	1:G:123:LEU:CD1	2.05	0.87
1:K:27:THR:HG23	1:K:68:GLU:HG2	1.53	0.87
1:E:184:LEU:HD22	1:E:216:ARG:HD3	1.55	0.87
1:C:8:THR:HG21	1:E:12:CYS:H	1.40	0.86
1:C:32:TRP:CE2	1:C:62:LYS:HB3	2.09	0.86
1:G:7:LYS:HG3	1:G:9:ASN:HD21	1.42	0.84
1:A:32:TRP:CD1	1:A:62:LYS:HB3	2.12	0.84
1:I:4:MET:H	1:I:77:ASN:HD21	1.23	0.83
1:O:9:ASN:ND2	9:O:916:HOH:O	2.11	0.83
1:C:8:THR:CG2	1:E:12:CYS:H	1.91	0.83
1:G:205:CYS:HB3	1:G:237:MET:HE2	1.60	0.83
1:E:91:ARG:NH1	1:E:116:ARG:HE	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:VAL:HB	1:M:66:LEU:CD1	2.11	0.80
2:P:508:TYR:HA	2:P:512:SER:HB3	1.63	0.80
1:I:32:TRP:CE2	1:I:62:LYS:HB3	2.17	0.80
1:C:195:TYR:H	1:C:272:ASN:HD21	1.25	0.80
1:E:32:TRP:CD1	1:E:62:LYS:HB3	2.16	0.80
1:E:54:THR:HG21	1:E:120:GLU:OE1	1.83	0.78
1:K:32:TRP:CD1	1:K:62:LYS:HB3	2.19	0.78
1:M:98:CYS:HA	1:M:103:MET:HE3	1.64	0.78
1:A:75:LEU:C	1:A:77:ASN:H	1.90	0.77
1:C:8:THR:HG21	1:E:12:CYS:N	1.99	0.77
2:F:508:TYR:HA	2:F:512:SER:HB3	1.65	0.77
2:B:508:TYR:HA	2:B:512:SER:HB3	1.67	0.77
1:I:239:ARG:HD3	1:I:272:ASN:HB3	1.67	0.75
1:C:268:LYS:H	1:C:268:LYS:HD3	1.51	0.75
1:K:157:ASN:ND2	1:K:245:SER:OG	2.20	0.75
1:M:123:LEU:HD22	1:M:170:CYS:HB3	1.69	0.75
1:M:195:TYR:H	1:M:272:ASN:HD21	1.36	0.74
1:O:29:VAL:HB	1:O:66:LEU:HD13	1.69	0.74
1:I:161:ASN:ND2	1:I:164:THR:H	1.85	0.74
1:I:123:LEU:HD22	1:I:170:CYS:HB3	1.70	0.73
1:G:274:PRO:C	1:G:276:LEU:H	1.96	0.73
1:A:275:ASP:O	1:A:276:LEU:HB2	1.88	0.73
2:J:508:TYR:CD2	2:J:512:SER:HB3	2.23	0.73
1:A:9:ASN:ND2	1:C:11:ASP:OD1	2.20	0.72
1:M:9:ASN:HD21	1:M:11:ASP:HB3	1.54	0.71
1:G:105:CYS:O	1:G:109:ARG:HG3	1.90	0.71
1:O:259:ASN:HD21	2:P:501:LYS:N	1.89	0.71
1:I:200:GLN:H	1:I:203:HIS:HD2	1.39	0.71
1:E:34:GLU:O	9:E:836:HOH:O	2.08	0.71
1:G:205:CYS:HB3	1:G:237:MET:CE	2.21	0.71
1:G:246:MET:HE1	1:G:252:LEU:HG	1.70	0.71
1:O:157:ASN:HA	1:O:243:THR:HG21	1.73	0.71
1:I:157:ASN:HA	1:I:243:THR:HG21	1.73	0.71
1:O:239:ARG:HD3	1:O:272:ASN:O	1.92	0.70
1:M:4:MET:HE3	1:M:75:LEU:HD22	1.72	0.70
1:O:195:TYR:HB2	1:O:272:ASN:HB2	1.74	0.70
1:G:126:VAL:HG13	1:G:167:PHE:HB3	1.74	0.70
1:I:200:GLN:H	1:I:203:HIS:CD2	2.10	0.70
1:C:192:ARG:HD2	1:C:220:ASN:O	1.90	0.70
1:M:188:PRO:O	1:M:216:ARG:O	2.09	0.70
1:M:4:MET:HE1	1:M:14:VAL:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:243:THR:HG22	1:K:246:MET:HG2	1.73	0.69
1:G:246:MET:CE	1:G:252:LEU:HG	2.23	0.69
8:K:810:SO4:O1	9:K:823:HOH:O	2.11	0.69
1:M:184:LEU:HD22	1:M:216:ARG:HG3	1.73	0.69
1:M:32:TRP:CE2	1:M:62:LYS:HB3	2.28	0.69
1:C:61:LEU:CA	1:O:61:LEU:CA	2.70	0.69
1:G:272:ASN:HD22	1:G:272:ASN:H	1.41	0.68
1:C:8:THR:HG22	9:E:822:HOH:O	1.91	0.68
1:E:185:GLU:CD	1:E:185:GLU:H	2.00	0.68
1:A:53:ARG:NH1	1:A:251:HIS:HB3	2.09	0.68
1:A:230:GLU:HG2	1:A:233:ASN:H	1.57	0.68
1:E:9:ASN:ND2	1:G:11:ASP:OD1	2.22	0.67
1:C:268:LYS:H	1:C:268:LYS:CD	2.06	0.67
1:C:25:ARG:NH2	1:C:42:GLU:OE1	2.25	0.67
1:O:192:ARG:HG3	1:O:269:SER:HB3	1.77	0.66
1:C:10:GLY:O	9:C:860:HOH:O	2.12	0.66
1:G:25:ARG:NH2	1:G:42:GLU:OE1	2.24	0.66
1:M:185:GLU:H	1:M:185:GLU:CD	2.04	0.65
1:I:7:LYS:NZ	9:I:834:HOH:O	2.19	0.65
1:M:246:MET:HE2	1:M:252:LEU:HG	1.77	0.65
1:I:195:TYR:HB2	1:I:272:ASN:HB2	1.78	0.65
1:C:157:ASN:HA	1:C:243:THR:HG21	1.79	0.65
1:K:109:ARG:O	1:K:110:HIS:HB2	1.97	0.65
1:M:226:THR:HG22	1:M:262:ASP:HB3	1.79	0.65
1:I:190:ASN:ND2	1:I:192:ARG:H	1.95	0.65
1:G:160:HIS:HE1	1:G:216:ARG:H	1.46	0.65
1:O:207:SER:C	1:O:209:GLU:H	2.04	0.65
1:I:273:HIS:CD2	1:I:275:ASP:H	2.16	0.64
1:G:55:LEU:CD2	1:G:123:LEU:HD12	2.26	0.64
1:A:25:ARG:HG2	1:A:46:THR:HB	1.80	0.63
1:K:66:LEU:HD23	2:L:505:PHE:CD1	2.33	0.63
1:K:197:CYS:SG	1:K:239:ARG:HD2	2.38	0.63
1:G:7:LYS:HG3	1:G:9:ASN:ND2	2.13	0.63
1:G:68:GLU:OE2	9:G:822:HOH:O	2.15	0.63
1:I:190:ASN:HD22	1:I:192:ARG:H	1.47	0.63
1:C:2:ARG:HD3	1:C:74:ASP:OD1	1.98	0.63
1:I:29:VAL:HB	1:I:66:LEU:HD13	1.80	0.63
1:M:104:SER:O	1:M:108:GLY:N	2.28	0.63
1:I:8:THR:HG22	1:K:10:GLY:O	1.99	0.63
8:A:801:SO4:O3	1:C:13:ARG:NH1	2.31	0.62
1:M:4:MET:HE2	1:M:75:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:OG1	1:A:81:SER:HB3	1.99	0.62
1:O:195:TYR:HB2	1:O:272:ASN:CB	2.28	0.62
2:L:508:TYR:HA	2:L:512:SER:HB3	1.81	0.62
1:M:25:ARG:NH1	1:M:42:GLU:OE1	2.25	0.62
1:E:43:LYS:NZ	1:E:79:GLY:H	1.98	0.61
1:I:13:ARG:HD2	8:I:804:SO4:O4	1.99	0.61
1:C:129:TRP:HZ3	1:C:140:ASP:O	1.83	0.61
1:G:60:GLY:O	1:K:61:LEU:O	2.18	0.61
1:M:25:ARG:HG2	1:M:26:THR:N	2.15	0.61
1:O:104:SER:O	1:O:108:GLY:HA3	2.01	0.61
1:O:247:CYS:HA	1:O:263:VAL:CG2	2.30	0.61
1:A:225:ALA:HB3	1:A:238:VAL:HG12	1.83	0.61
1:G:101:SER:OG	2:H:513:LYS:O	2.13	0.60
1:I:243:THR:HG22	1:I:246:MET:HG2	1.83	0.60
1:G:61:LEU:CA	1:K:61:LEU:CA	2.79	0.60
1:K:117:SER:HB2	1:K:120:GLU:HG3	1.82	0.60
1:I:116:ARG:O	1:I:117:SER:HB3	2.02	0.60
1:A:75:LEU:C	1:A:77:ASN:N	2.60	0.60
1:G:75:LEU:C	1:G:77:ASN:H	2.08	0.60
1:K:149:TYR:C	1:K:150:LEU:HD12	2.27	0.60
1:M:254:ASP:O	2:N:507:DLY:HE3	2.00	0.60
1:A:105:CYS:O	1:A:109:ARG:HG3	2.02	0.60
1:I:237:MET:HE1	1:I:239:ARG:CZ	2.32	0.59
1:A:10:GLY:O	1:G:8:THR:HG22	2.02	0.59
1:A:108:GLY:O	1:A:111:GLN:HB2	2.03	0.59
1:I:17:CYS:HB3	1:I:21:GLN:HB2	1.84	0.59
1:C:272:ASN:H	1:C:272:ASN:HD22	1.51	0.59
1:A:40:LEU:HD21	1:C:4:MET:HE1	1.85	0.58
1:C:160:HIS:CE1	1:C:241:CYS:HB2	2.38	0.58
1:K:246:MET:HE2	1:K:252:LEU:HD13	1.85	0.58
1:K:210:THR:HG21	1:K:274:PRO:HG3	1.84	0.58
1:C:9:ASN:HD22	1:C:9:ASN:H	1.49	0.58
1:A:28:ILE:HG12	1:A:41:VAL:HG22	1.86	0.58
1:C:59:THR:HG21	1:C:64:THR:OG1	2.04	0.58
1:C:226:THR:HG23	1:C:237:MET:HB3	1.85	0.58
2:D:501:LYS:HG3	1:E:13:ARG:NH2	2.19	0.58
1:E:54:THR:HG22	1:E:148:GLY:HA2	1.86	0.58
1:K:192:ARG:HH11	1:K:269:SER:HB2	1.69	0.58
1:G:225:ALA:HB3	1:G:238:VAL:HG12	1.86	0.58
1:A:205:CYS:HB3	1:A:237:MET:HE2	1.84	0.58
1:M:5:GLN:HB2	1:M:15:GLU:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLN:O	1:A:116:ARG:NH1	2.36	0.57
2:D:508:TYR:CD2	2:D:512:SER:HB3	2.39	0.57
1:E:104:SER:HB3	1:E:106:GLU:HG3	1.86	0.57
1:E:121:GLN:HB3	1:E:171:CYS:O	2.03	0.57
1:E:182:LEU:HD21	1:E:187:LEU:HD21	1.85	0.57
1:K:9:ASN:C	1:K:9:ASN:HD22	2.10	0.57
1:O:243:THR:HG23	1:O:245:SER:HB2	1.85	0.57
1:C:164:THR:HG21	8:C:818:SO4:O1	2.04	0.57
1:K:27:THR:HG23	1:K:68:GLU:CG	2.30	0.57
1:O:160:HIS:CE1	1:O:215:CYS:HA	2.38	0.57
1:C:268:LYS:HD3	1:C:268:LYS:N	2.18	0.57
1:E:34:GLU:HG3	1:E:35:GLY:H	1.69	0.57
1:I:246:MET:HE2	1:I:252:LEU:HG	1.85	0.57
1:G:251:HIS:CE1	1:G:252:LEU:HD13	2.39	0.57
2:F:507:DLY:HE3	9:F:421:HOH:O	2.03	0.57
1:G:192:ARG:HG3	1:G:220:ASN:O	2.05	0.57
1:I:207:SER:OG	1:I:274:PRO:HG3	2.05	0.57
1:K:9:ASN:HD22	1:K:10:GLY:N	2.03	0.56
1:A:195:TYR:HB2	1:A:272:ASN:HB2	1.87	0.56
1:M:246:MET:CE	1:M:252:LEU:HG	2.35	0.56
1:O:247:CYS:HA	1:O:263:VAL:HG23	1.86	0.56
1:E:105:CYS:O	1:E:109:ARG:HG3	2.05	0.56
1:K:207:SER:C	1:K:209:GLU:H	2.13	0.56
1:C:32:TRP:CD2	1:C:62:LYS:HB3	2.40	0.56
1:G:158:GLY:N	1:G:246:MET:HE3	2.21	0.56
1:M:9:ASN:ND2	1:M:11:ASP:HB3	2.20	0.56
1:E:251:HIS:HB3	9:E:908:HOH:O	2.06	0.56
1:I:216:ARG:O	1:I:219:MET:HE3	2.07	0.55
1:K:121:GLN:HB3	1:K:171:CYS:O	2.05	0.55
2:B:501:LYS:HE3	1:C:13:ARG:HH22	1.70	0.55
1:E:228:THR:HG21	1:E:233:ASN:ND2	2.22	0.55
1:A:200:GLN:HG3	1:A:203:HIS:HD2	1.70	0.55
1:A:273:HIS:HB3	1:A:274:PRO:HD3	1.88	0.55
1:O:121:GLN:HB3	1:O:171:CYS:O	2.06	0.55
1:G:274:PRO:C	1:G:276:LEU:N	2.64	0.55
1:M:1:LEU:HD13	1:M:1:LEU:O	2.06	0.55
1:E:142:ARG:HH12	2:F:512:SER:C	2.13	0.55
1:M:126:VAL:HG13	1:M:167:PHE:HB3	1.89	0.55
1:K:275:ASP:OD2	1:K:276:LEU:N	2.40	0.55
1:E:29:VAL:CG1	1:E:40:LEU:HB2	2.37	0.55
1:K:25:ARG:HD3	9:K:817:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:ARG:NH1	1:K:269:SER:HB2	2.21	0.55
1:O:239:ARG:HD2	1:O:272:ASN:HB3	1.87	0.55
1:G:160:HIS:CE1	1:G:216:ARG:H	2.25	0.54
1:O:55:LEU:HD21	1:O:57:TYR:CE2	2.43	0.54
1:O:246:MET:HE2	1:O:252:LEU:HG	1.89	0.54
1:A:106:GLU:O	1:A:107:ARG:HB3	2.06	0.54
1:M:18:ALA:HB3	1:M:21:GLN:HE21	1.72	0.54
1:C:257:SER:HA	1:E:16:GLU:OE1	2.07	0.54
1:I:14:VAL:HG21	2:P:504:ALC:HE23	1.89	0.54
1:M:32:TRP:O	1:M:33:GLU:HB2	2.07	0.54
1:E:25:ARG:HH21	1:E:42:GLU:HG2	1.72	0.54
1:K:9:ASN:HD21	1:K:11:ASP:HB3	1.73	0.54
1:O:257:SER:OG	2:P:507:DLY:NZ	2.40	0.54
1:C:60:GLY:O	1:O:61:LEU:O	2.25	0.54
1:K:192:ARG:HH12	1:K:268:LYS:NZ	2.06	0.53
1:C:199:GLY:HA2	1:C:236:TYR:CZ	2.43	0.53
1:I:47:HIS:HB3	1:I:49:GLU:OE2	2.08	0.53
2:L:513:LYS:HD2	1:M:73:LEU:HD22	1.90	0.53
1:M:73:LEU:O	1:M:74:ASP:C	2.51	0.53
1:E:43:LYS:HZ1	1:E:79:GLY:H	1.57	0.53
1:I:83:ARG:O	1:I:84:ALA:HB2	2.08	0.53
1:O:32:TRP:CG	1:O:62:LYS:HB3	2.41	0.53
1:E:142:ARG:HG3	1:E:142:ARG:HH11	1.72	0.53
1:I:195:TYR:HB3	1:I:210:THR:HG22	1.89	0.53
1:O:245:SER:HB3	1:O:252:LEU:HD23	1.90	0.53
1:G:94:GLU:CD	1:G:175:LYS:HD2	2.34	0.53
1:C:230:GLU:HB2	1:E:18:ALA:CB	2.38	0.53
1:E:53:ARG:NH2	1:E:68:GLU:OE2	2.39	0.53
1:E:15:GLU:HG2	1:E:45:CYS:SG	2.49	0.53
1:M:122:CYS:O	1:M:170:CYS:HA	2.09	0.53
1:A:9:ASN:HB3	1:A:11:ASP:H	1.73	0.52
1:M:227:GLY:HA2	1:M:260:HIS:O	2.09	0.52
1:A:126:VAL:HG13	1:A:167:PHE:HB3	1.90	0.52
1:K:160:HIS:HE1	1:K:216:ARG:H	1.57	0.52
1:C:130:ILE:O	1:C:131:GLN:HB2	2.10	0.52
1:A:124:ASP:HB3	1:A:169:LYS:HG3	1.90	0.52
1:O:55:LEU:HD23	1:O:55:LEU:C	2.34	0.52
1:M:181:ILE:HD12	1:M:181:ILE:H	1.74	0.52
2:B:501:LYS:HD3	1:C:16:GLU:HB2	1.91	0.52
1:G:189:GLN:OE1	1:G:189:GLN:N	2.39	0.52
1:G:205:CYS:CB	1:G:237:MET:HE2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HB	1:A:143:HIS:HD2	1.74	0.51
1:G:182:LEU:HD11	1:G:187:LEU:HD21	1.91	0.51
2:L:501:LYS:O	2:L:502:SER:HB2	2.10	0.51
1:A:32:TRP:CG	1:A:62:LYS:HB3	2.45	0.51
1:O:38:LEU:HD12	9:O:828:HOH:O	2.10	0.51
1:G:123:LEU:HD23	1:G:170:CYS:HB3	1.91	0.51
1:I:30:ARG:NH1	1:I:39:GLU:OE1	2.44	0.51
1:M:100:SER:O	1:M:101:SER:C	2.54	0.51
1:O:230:GLU:HG3	1:O:231:PRO:HA	1.92	0.51
1:M:5:GLN:O	1:M:12:CYS:HA	2.11	0.51
1:G:131:GLN:HG2	1:G:132:GLU:H	1.75	0.51
1:C:91:ARG:HB2	1:C:118:PRO:HB3	1.92	0.50
1:E:121:GLN:HE22	1:E:153:CYS:HB3	1.76	0.50
1:G:9:ASN:ND2	1:G:9:ASN:H	2.09	0.50
1:K:18:ALA:H	1:K:21:GLN:HE21	1.60	0.50
1:C:9:ASN:HD22	1:C:9:ASN:N	2.08	0.50
1:O:55:LEU:HD21	1:O:57:TYR:HE2	1.77	0.50
1:E:66:LEU:HD12	1:E:67:THR:N	2.27	0.50
1:G:162:ASN:HD22	5:W:1:NAG:H82	1.76	0.50
1:E:115:CYS:HB3	1:E:120:GLU:CG	2.42	0.50
1:I:29:VAL:HG13	1:I:40:LEU:HB3	1.93	0.50
1:C:200:GLN:HE21	1:C:203:HIS:HB2	1.77	0.50
1:E:110:HIS:O	1:E:111:GLN:HB2	2.10	0.50
1:K:251:HIS:HD2	9:K:823:HOH:O	1.93	0.50
1:I:25:ARG:HH22	1:I:42:GLU:CD	2.19	0.50
1:I:256:PHE:HB2	1:I:261:ILE:HD11	1.94	0.50
1:O:259:ASN:ND2	2:P:501:LYS:N	2.60	0.50
1:I:161:ASN:HD21	1:I:164:THR:H	1.58	0.50
1:I:226:THR:HG22	1:I:262:ASP:HB3	1.94	0.50
1:M:168:LEU:HD23	1:M:168:LEU:C	2.37	0.50
1:E:32:TRP:CG	1:E:62:LYS:HB3	2.46	0.49
1:I:149:TYR:O	1:I:150:LEU:HD13	2.12	0.49
1:A:230:GLU:HA	1:A:231:PRO:C	2.37	0.49
1:A:61:LEU:CA	1:I:61:LEU:CA	2.90	0.49
2:J:508:TYR:HD2	2:J:512:SER:HB3	1.76	0.49
1:O:158:GLY:N	1:O:246:MET:HE3	2.27	0.49
1:C:104:SER:OG	1:C:106:GLU:HG2	2.13	0.49
1:K:190:ASN:HB3	1:K:192:ARG:H	1.76	0.49
1:C:121:GLN:NE2	1:C:153:CYS:HB3	2.27	0.49
1:E:54:THR:CG2	1:E:120:GLU:OE1	2.59	0.49
1:K:207:SER:HA	1:K:210:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LYS:O	1:C:271:CYS:SG	2.70	0.49
1:K:192:ARG:HH12	1:K:268:LYS:HZ3	1.60	0.49
1:G:53:ARG:HG3	2:H:505:PHE:CE2	2.48	0.49
1:K:126:VAL:HG13	1:K:167:PHE:HB3	1.94	0.49
1:M:33:GLU:O	1:M:34:GLU:HB2	2.12	0.49
1:K:7:LYS:HD3	8:K:803:SO4:O4	2.12	0.49
1:O:190:ASN:HD21	1:O:217:GLY:N	2.11	0.49
1:I:108:GLY:O	1:I:111:GLN:HB2	2.12	0.49
1:I:204:GLY:O	1:I:209:GLU:HB3	2.13	0.49
1:O:158:GLY:CA	1:O:246:MET:HE3	2.42	0.49
1:C:9:ASN:H	1:C:9:ASN:ND2	2.10	0.49
1:E:22:ASP:OD2	1:E:48:SER:HA	2.12	0.49
1:K:157:ASN:HA	1:K:243:THR:HG21	1.95	0.49
1:O:29:VAL:HG13	1:O:40:LEU:HB2	1.94	0.49
1:C:4:MET:HE2	1:C:78:GLN:NE2	2.28	0.48
1:G:25:ARG:HA	1:G:69:VAL:O	2.13	0.48
1:A:60:GLY:O	1:I:61:LEU:O	2.31	0.48
1:K:63:ILE:HD11	1:K:113:LEU:HD21	1.94	0.48
1:I:247:CYS:HA	1:I:263:VAL:CG2	2.43	0.48
2:L:504:ALC:HE23	1:M:14:VAL:HG21	1.94	0.48
1:A:231:PRO:HD3	1:C:19:LEU:HB2	1.96	0.48
1:K:243:THR:HG23	1:K:245:SER:OG	2.13	0.48
1:A:51:THR:HG21	9:A:815:HOH:O	2.13	0.48
1:A:251:HIS:CE1	1:A:252:LEU:HD22	2.48	0.48
1:A:51:THR:HG22	1:A:52:ASN:N	2.29	0.48
1:A:54:THR:HG21	1:A:120:GLU:OE1	2.14	0.48
1:C:230:GLU:HB2	1:E:18:ALA:HB2	1.95	0.48
1:C:55:LEU:HB3	1:C:66:LEU:CD2	2.25	0.48
1:I:246:MET:CE	1:I:252:LEU:HG	2.43	0.48
1:O:207:SER:C	1:O:209:GLU:N	2.70	0.48
1:E:27:THR:OG1	1:E:68:GLU:HG3	2.13	0.48
1:M:8:THR:HG22	1:O:10:GLY:O	2.14	0.48
1:A:176:CYS:SG	1:A:177:ASN:N	2.79	0.48
1:K:222:CYS:HB3	1:K:272:ASN:HB3	1.95	0.48
1:O:43:LYS:NZ	9:O:879:HOH:O	2.46	0.48
1:C:185:GLU:H	1:C:185:GLU:CD	2.22	0.47
2:B:501:LYS:HB3	1:C:16:GLU:OE2	2.14	0.47
1:G:61:LEU:O	1:K:60:GLY:O	2.33	0.47
1:K:268:LYS:HD2	1:K:268:LYS:HA	1.51	0.47
1:C:27:THR:OG1	1:C:68:GLU:HG2	2.13	0.47
1:E:226:THR:C	1:E:258:MET:HE3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:GLN:HE21	1:I:114:GLN:HB2	1.56	0.47
1:A:67:THR:OG1	1:A:81:SER:CB	2.63	0.47
1:E:176:CYS:SG	1:E:177:ASN:N	2.85	0.47
1:I:203:HIS:CG	1:I:204:GLY:N	2.82	0.47
1:K:190:ASN:ND2	1:K:219:MET:O	2.47	0.47
1:O:123:LEU:O	1:O:145:ARG:HA	2.14	0.47
1:I:104:SER:O	1:I:108:GLY:HA3	2.14	0.47
1:M:251:HIS:CD2	1:M:252:LEU:HD13	2.50	0.47
1:E:54:THR:HB	1:E:149:TYR:HB3	1.96	0.47
1:E:239:ARG:NH2	1:E:274:PRO:HA	2.30	0.47
1:I:56:SER:HB2	1:I:147:CYS:HB2	1.96	0.47
1:I:273:HIS:HD2	1:I:275:ASP:H	1.59	0.47
2:N:507:DLY:O	2:N:511:SER:HB2	2.15	0.47
1:C:53:ARG:HG3	2:D:505:PHE:CE2	2.50	0.47
1:A:43:LYS:O	1:A:44:SER:HB3	2.15	0.46
1:G:21:GLN:HG2	1:G:45:CYS:HB3	1.96	0.46
1:G:60:GLY:C	1:G:62:LYS:H	2.22	0.46
1:G:218:PRO:O	1:G:243:THR:HG22	2.16	0.46
1:A:157:ASN:HD22	1:A:245:SER:CB	2.28	0.46
1:I:2:ARG:HA	1:I:15:GLU:O	2.16	0.46
1:O:5:GLN:NE2	9:O:898:HOH:O	2.48	0.46
1:G:2:ARG:HA	1:G:15:GLU:O	2.16	0.46
1:K:66:LEU:HD23	2:L:505:PHE:HD1	1.79	0.46
1:O:157:ASN:HD22	1:O:245:SER:CB	2.28	0.46
1:A:249:HIS:HB2	1:A:252:LEU:HD23	1.97	0.46
1:C:8:THR:HG23	1:E:11:ASP:HA	1.97	0.46
1:G:32:TRP:CD2	1:G:62:LYS:HB3	2.49	0.46
1:A:222:CYS:HB2	1:A:271:CYS:SG	2.56	0.46
1:G:122:CYS:O	1:G:170:CYS:HA	2.15	0.46
1:I:237:MET:HE1	1:I:239:ARG:NH2	2.30	0.46
1:E:259:ASN:O	1:E:261:ILE:N	2.48	0.46
1:G:239:ARG:NH2	1:G:274:PRO:HA	2.31	0.46
1:O:227:GLY:N	1:O:258:MET:HE2	2.31	0.46
9:O:814:HOH:O	6:h:4:MAN:H62	2.15	0.46
1:C:8:THR:CG2	1:E:12:CYS:N	2.64	0.46
1:G:276:LEU:HD11	9:G:901:HOH:O	2.15	0.46
1:O:230:GLU:HA	1:O:231:PRO:C	2.41	0.46
1:C:268:LYS:HG2	1:C:271:CYS:HB3	1.98	0.46
1:E:100:SER:O	1:E:101:SER:C	2.59	0.46
1:O:75:LEU:C	1:O:77:ASN:N	2.73	0.46
1:A:34:GLU:O	9:A:834:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD23	2:B:504:ALC:HZ2	1.97	0.45
1:K:9:ASN:ND2	1:K:11:ASP:H	2.15	0.45
1:M:272:ASN:H	1:M:272:ASN:HD22	1.63	0.45
1:C:29:VAL:HG13	1:C:66:LEU:CD1	2.46	0.45
1:C:266:CYS:HB2	1:C:268:LYS:HE2	1.98	0.45
1:K:53:ARG:HG2	1:K:68:GLU:HB2	1.97	0.45
2:L:503:ASP:HB3	9:L:745:HOH:O	2.15	0.45
1:G:255:ALA:HB2	2:H:510:TRP:CE2	2.52	0.45
1:K:123:LEU:HD22	1:K:123:LEU:HA	1.82	0.45
1:M:169:LYS:HB3	1:M:169:LYS:HE2	1.78	0.45
1:A:7:LYS:HB2	1:A:9:ASN:HB2	1.98	0.45
1:C:200:GLN:H	1:C:200:GLN:CD	2.24	0.45
1:C:8:THR:HG23	1:E:10:GLY:O	2.16	0.45
1:E:7:LYS:HB2	1:E:9:ASN:HB2	1.98	0.45
1:E:34:GLU:HG3	1:E:35:GLY:N	2.31	0.45
1:I:100:SER:O	1:I:101:SER:C	2.59	0.45
1:M:243:THR:O	1:M:246:MET:HB2	2.16	0.45
1:E:249:HIS:HB3	1:E:251:HIS:CD2	2.51	0.45
1:K:32:TRP:CG	1:K:62:LYS:HB3	2.52	0.45
1:A:33:GLU:HG2	1:C:78:GLN:O	2.16	0.45
1:E:89:ARG:N	9:E:851:HOH:O	2.49	0.45
1:G:206:SER:O	1:G:207:SER:C	2.59	0.45
1:A:175:LYS:C	1:A:177:ASN:N	2.73	0.45
1:M:158:GLY:CA	1:M:246:MET:HE3	2.47	0.45
1:M:208:GLU:HG3	1:M:209:GLU:N	2.31	0.45
1:O:195:TYR:H	1:O:272:ASN:ND2	2.15	0.45
1:A:25:ARG:HH21	1:A:42:GLU:HG2	1.83	0.45
1:C:158:GLY:H	1:C:243:THR:HG22	1.82	0.45
1:C:192:ARG:CD	1:C:220:ASN:O	2.64	0.45
1:E:34:GLU:OE1	1:E:34:GLU:HA	2.17	0.45
1:K:223:LEU:HD12	1:K:265:CYS:SG	2.57	0.45
1:M:150:LEU:HB2	1:M:153:CYS:SG	2.57	0.45
1:K:230:GLU:HA	1:K:231:PRO:HA	1.77	0.44
1:O:181:ILE:H	1:O:181:ILE:HG13	1.64	0.44
1:O:246:MET:CE	1:O:252:LEU:HG	2.46	0.44
1:E:23:LEU:HB3	1:E:70:VAL:HG22	1.99	0.44
1:I:251:HIS:CD2	1:I:252:LEU:HD13	2.52	0.44
1:M:178:GLU:HB3	9:M:823:HOH:O	2.17	0.44
1:M:261:ILE:HG22	9:M:849:HOH:O	2.15	0.44
1:O:160:HIS:CE1	1:O:216:ARG:H	2.35	0.44
2:B:504:ALC:HE12	1:C:14:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASP:OD2	1:E:73:LEU:HD23	2.18	0.44
1:I:98:CYS:SG	1:I:145:ARG:HG3	2.57	0.44
1:A:29:VAL:CG1	1:A:40:LEU:HB2	2.47	0.44
1:C:7:LYS:HB2	1:C:9:ASN:ND2	2.32	0.44
1:I:239:ARG:HD3	1:I:272:ASN:CB	2.42	0.44
1:E:115:CYS:HB3	1:E:120:GLU:HG3	1.99	0.44
1:I:83:ARG:O	1:I:84:ALA:CB	2.65	0.44
1:I:198:LYS:HG2	1:I:236:TYR:CE1	2.53	0.44
1:K:207:SER:C	1:K:209:GLU:N	2.76	0.44
1:O:158:GLY:H	1:O:243:THR:CG2	2.31	0.44
1:O:225:ALA:HA	1:O:262:ASP:O	2.17	0.44
1:O:243:THR:CG2	1:O:245:SER:HB2	2.46	0.44
1:A:128:HIS:ND1	1:A:141:ASP:OD1	2.51	0.44
1:G:122:CYS:HB3	1:G:177:ASN:CG	2.42	0.44
1:K:246:MET:HE1	1:K:252:LEU:HD22	2.00	0.44
1:G:193:GLN:CD	1:G:193:GLN:N	2.75	0.44
1:M:109:ARG:HB3	1:M:110:HIS:H	1.44	0.44
1:I:161:ASN:HD22	1:I:164:THR:H	1.64	0.44
1:K:9:ASN:HD21	1:K:11:ASP:CB	2.30	0.44
1:K:243:THR:CG2	1:K:245:SER:OG	2.66	0.44
1:E:5:GLN:O	1:E:12:CYS:HA	2.18	0.43
1:I:203:HIS:CD2	1:I:204:GLY:H	2.36	0.43
1:A:140:ASP:O	1:A:141:ASP:C	2.61	0.43
1:C:273:HIS:CB	1:C:274:PRO:CD	2.70	0.43
1:G:109:ARG:HH11	1:G:180:PRO:HA	1.83	0.43
1:A:5:GLN:O	1:A:12:CYS:HA	2.19	0.43
1:E:28:ILE:HG12	1:E:41:VAL:HG22	1.99	0.43
1:G:145:ARG:HD3	1:G:177:ASN:O	2.18	0.43
1:I:122:CYS:O	1:I:170:CYS:HA	2.19	0.43
1:I:168:LEU:C	1:I:168:LEU:HD23	2.44	0.43
1:I:190:ASN:HD22	1:I:190:ASN:C	2.26	0.43
1:G:221:GLN:NE2	1:G:244:ALA:HB2	2.34	0.43
1:K:109:ARG:O	1:K:110:HIS:CB	2.65	0.43
1:A:28:ILE:O	1:A:66:LEU:HA	2.17	0.43
1:A:101:SER:N	2:B:513:LYS:O	2.51	0.43
1:C:13:ARG:NH2	1:C:15:GLU:HA	2.34	0.43
1:O:167:PHE:HE2	1:O:169:LYS:HG3	1.83	0.43
2:B:508:TYR:CD2	2:B:512:SER:CB	3.01	0.43
1:K:55:LEU:O	1:K:66:LEU:N	2.42	0.43
1:M:223:LEU:HA	1:M:264:SER:O	2.19	0.43
1:A:75:LEU:O	1:A:77:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:834:HOH:O	4:d:1:NAG:O4	2.21	0.43
1:O:1:LEU:HD23	1:O:74:ASP:OD1	2.19	0.43
2:D:505:PHE:O	2:D:506:DSN:C	2.66	0.43
1:I:126:VAL:HA	1:I:142:ARG:O	2.18	0.43
1:K:32:TRP:CZ2	1:K:37:GLU:HG2	2.54	0.43
1:M:158:GLY:O	1:M:246:MET:HG3	2.19	0.43
1:C:158:GLY:H	1:C:243:THR:CG2	2.32	0.43
2:D:501:LYS:NZ	9:D:350:HOH:O	0.58	0.43
1:E:228:THR:OG1	1:E:259:ASN:HB2	2.19	0.43
1:G:28:ILE:HG12	1:G:41:VAL:HG22	2.01	0.43
1:I:158:GLY:CA	1:I:246:MET:HE3	2.48	0.43
1:C:167:PHE:HE2	1:C:169:LYS:HB2	1.84	0.42
1:I:208:GLU:CD	1:I:209:GLU:N	2.77	0.42
1:M:180:PRO:O	1:M:181:ILE:C	2.62	0.42
1:K:230:GLU:HG3	1:M:17:CYS:O	2.19	0.42
1:A:53:ARG:CZ	1:A:251:HIS:HB3	2.49	0.42
1:I:195:TYR:HA	1:I:211:PHE:O	2.19	0.42
1:K:54:THR:HB	1:K:149:TYR:HB3	2.01	0.42
1:A:187:LEU:O	1:A:216:ARG:HD3	2.19	0.42
1:A:200:GLN:N	1:A:203:HIS:O	2.52	0.42
1:C:222:CYS:HB2	1:C:271:CYS:SG	2.59	0.42
1:C:7:LYS:HB2	1:C:9:ASN:HD21	1.84	0.42
1:C:199:GLY:HA2	1:C:236:TYR:CE2	2.54	0.42
1:C:255:ALA:HB2	2:D:510:TRP:CE2	2.54	0.42
1:G:9:ASN:N	1:G:9:ASN:HD22	2.17	0.42
1:M:268:LYS:HE3	1:M:269:SER:H	1.84	0.42
1:E:251:HIS:CE1	1:E:252:LEU:HD13	2.55	0.42
1:K:150:LEU:HD23	1:K:251:HIS:CE1	2.55	0.42
5:W:1:NAG:H62	5:W:2:NAG:N2	2.35	0.42
1:C:272:ASN:HD22	1:C:272:ASN:N	2.13	0.42
1:G:201:SER:O	1:G:206:SER:OG	2.33	0.42
1:I:123:LEU:CD2	1:I:170:CYS:HB3	2.45	0.42
1:K:251:HIS:CD2	9:K:823:HOH:O	2.70	0.42
1:O:80:ASN:O	1:O:81:SER:C	2.63	0.42
1:O:231:PRO:O	1:O:232:LYS:C	2.63	0.42
1:O:60:GLY:C	1:O:62:LYS:H	2.28	0.42
1:A:127:THR:HG23	1:A:166:HIS:CE1	2.55	0.42
1:G:237:MET:HE1	1:G:239:ARG:NH1	2.35	0.42
1:C:73:LEU:O	1:C:74:ASP:C	2.63	0.42
1:G:252:LEU:HD12	1:G:252:LEU:HA	1.90	0.42
1:O:222:CYS:O	1:O:265:CYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:GLN:NE2	1:E:153:CYS:HB3	2.35	0.41
1:I:67:THR:HG21	1:I:84:ALA:HB1	2.01	0.41
1:A:94:GLU:HB3	1:A:174:THR:HG23	2.01	0.41
2:B:505:PHE:O	2:B:506:DSN:C	2.68	0.41
1:C:219:MET:HE2	1:C:219:MET:HB2	1.92	0.41
1:I:161:ASN:ND2	1:I:163:ASP:H	2.18	0.41
1:K:5:GLN:O	1:K:12:CYS:HA	2.19	0.41
1:K:128:HIS:CD2	1:K:141:ASP:OD1	2.73	0.41
1:O:252:LEU:HD12	1:O:252:LEU:HA	1.90	0.41
1:A:249:HIS:HB2	1:A:252:LEU:CD2	2.50	0.41
1:G:139:LYS:HD3	9:G:899:HOH:O	2.20	0.41
1:K:207:SER:O	1:K:208:GLU:HB3	2.20	0.41
1:E:126:VAL:HG13	1:E:167:PHE:HB3	2.03	0.41
1:G:145:ARG:HB3	1:G:177:ASN:ND2	2.36	0.41
1:M:116:ARG:HD3	9:M:863:HOH:O	2.21	0.41
1:I:198:LYS:HG2	1:I:236:TYR:HE1	1.85	0.41
1:M:258:MET:HG3	1:M:261:ILE:HD12	2.03	0.41
1:O:185:GLU:HG2	1:O:186:ASN:N	2.36	0.41
1:O:34:GLU:HB3	1:O:35:GLY:H	1.68	0.41
1:G:21:GLN:HG3	1:G:46:THR:C	2.45	0.41
1:K:123:LEU:CD2	1:K:170:CYS:HB3	2.50	0.41
1:K:199:GLY:HA2	1:K:236:TYR:CE2	2.55	0.41
1:M:128:HIS:HD2	1:M:141:ASP:OD1	2.03	0.41
1:M:204:GLY:O	1:M:209:GLU:HB3	2.21	0.41
1:O:75:LEU:C	1:O:77:ASN:H	2.28	0.41
4:Y:1:NAG:H2	4:Y:1:NAG:H2	1.91	0.41
1:A:142:ARG:NH2	1:A:144:LEU:HD22	2.35	0.41
1:I:247:CYS:SG	1:I:265:CYS:N	2.94	0.41
1:I:249:HIS:HB2	1:I:252:LEU:HD22	2.03	0.41
1:M:53:ARG:NH2	8:M:811:SO4:O3	2.54	0.41
1:M:223:LEU:C	1:M:223:LEU:HD23	2.46	0.41
1:O:160:HIS:HE1	1:O:215:CYS:HA	1.85	0.41
1:O:197:CYS:CB	1:O:210:THR:HG22	2.51	0.41
2:P:513:LYS:NZ	9:P:260:HOH:O	2.53	0.41
1:A:47:HIS:CD2	1:A:47:HIS:H	2.39	0.41
2:D:501:LYS:HB2	1:E:13:ARG:HH21	1.86	0.41
1:E:60:GLY:O	1:M:61:LEU:CA	2.68	0.41
1:I:208:GLU:OE1	1:I:209:GLU:HB2	2.21	0.41
1:K:250:ALA:N	8:K:810:SO4:O1	2.54	0.41
1:A:5:GLN:OE1	1:A:13:ARG:HD2	2.21	0.40
1:I:43:LYS:O	1:I:44:SER:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:268:LYS:O	1:M:271:CYS:SG	2.79	0.40
1:G:25:ARG:HH22	1:G:42:GLU:CD	2.20	0.40
1:I:239:ARG:CD	1:I:272:ASN:HB3	2.44	0.40
1:I:243:THR:O	1:I:246:MET:HB2	2.21	0.40
1:E:53:ARG:HH11	1:E:251:HIS:HB3	1.86	0.40
1:E:142:ARG:NH2	1:E:144:LEU:HG	2.35	0.40
1:E:168:LEU:C	1:E:168:LEU:HD23	2.46	0.40
1:G:182:LEU:HD13	1:G:182:LEU:HA	1.87	0.40
1:I:182:LEU:HD21	1:I:187:LEU:HD21	2.03	0.40
1:E:105:CYS:C	1:E:107:ARG:H	2.29	0.40
1:G:182:LEU:CD1	1:G:187:LEU:HD21	2.52	0.40
1:I:29:VAL:HB	1:I:66:LEU:CD1	2.50	0.40
1:K:32:TRP:CH2	1:K:37:GLU:HG2	2.56	0.40
1:K:95:CYS:O	1:K:113:LEU:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/313 (84%)	231 (88%)	16 (6%)	15 (6%)	1	2
1	C	253/313 (81%)	226 (89%)	16 (6%)	11 (4%)	2	4
1	E	256/313 (82%)	229 (90%)	22 (9%)	5 (2%)	6	16
1	G	252/313 (80%)	233 (92%)	16 (6%)	3 (1%)	10	27
1	I	258/313 (82%)	228 (88%)	23 (9%)	7 (3%)	4	10
1	K	251/313 (80%)	227 (90%)	20 (8%)	4 (2%)	7	20
1	M	257/313 (82%)	230 (90%)	15 (6%)	12 (5%)	2	3
1	O	252/313 (80%)	223 (88%)	20 (8%)	9 (4%)	2	6
2	B	8/13 (62%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	F	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	H	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	J	8/13 (62%)	7 (88%)	0	1 (12%)	0	0
2	L	8/13 (62%)	7 (88%)	0	1 (12%)	0	0
2	N	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	P	8/13 (62%)	8 (100%)	0	0	100	100
All	All	2105/2608 (81%)	1884 (90%)	153 (7%)	68 (3%)	3	7

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	A	231	PRO
1	A	276	LEU
1	C	208	GLU
1	C	273	HIS
1	E	111	GLN
1	E	259	ASN
1	I	33	GLU
1	I	101	SER
1	M	101	SER
1	O	203	HIS
1	O	206	SER
1	O	208	GLU
1	O	232	LYS
1	A	61	LEU
1	A	177	ASN
1	C	109	ARG
1	C	207	SER
1	G	275	ASP
1	I	84	ALA
1	I	208	GLU
1	K	275	ASP
1	M	91	ARG
1	M	207	SER
1	M	276	LEU
1	O	109	ARG
1	A	234	GLN
1	A	235	SER

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Mol	Chain	Res	Type
1	A	278	VAL
1	E	61	LEU
1	K	206	SER
1	M	60	GLY
1	M	105	CYS
1	M	106	GLU
1	M	208	GLU
1	M	274	PRO
1	A	90	SER
1	A	107	ARG
1	A	273	HIS
1	C	61	LEU
1	C	231	PRO
1	G	207	SER
1	I	60	GLY
1	I	117	SER
1	K	231	PRO
1	M	109	ARG
1	O	204	GLY
1	A	75	LEU
1	C	34	GLU
1	C	60	GLY
1	C	79	GLY
1	C	101	SER
1	C	107	ARG
1	I	35	GLY
1	O	106	GLU
1	A	76	CYS
1	A	233	ASN
1	E	260	HIS
2	J	502	SER
2	L	502	SER
1	M	111	GLN
1	M	206	SER
1	O	60	GLY
1	O	274	PRO
1	E	60	GLY
1	G	108	GLY
1	K	60	GLY
1	A	60	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/273 (86%)	204 (87%)	30 (13%)	4	11
1	C	229/273 (84%)	195 (85%)	34 (15%)	3	8
1	E	232/273 (85%)	194 (84%)	38 (16%)	2	6
1	G	229/273 (84%)	185 (81%)	44 (19%)	1	4
1	I	230/273 (84%)	184 (80%)	46 (20%)	1	4
1	K	228/273 (84%)	189 (83%)	39 (17%)	2	6
1	M	234/273 (86%)	193 (82%)	41 (18%)	2	5
1	O	228/273 (84%)	193 (85%)	35 (15%)	2	7
2	B	10/10 (100%)	9 (90%)	1 (10%)	7	19
2	D	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
2	H	10/10 (100%)	8 (80%)	2 (20%)	1	4
2	J	10/10 (100%)	9 (90%)	1 (10%)	7	19
2	L	10/10 (100%)	7 (70%)	3 (30%)	0	1
2	N	10/10 (100%)	10 (100%)	0	100	100
2	P	10/10 (100%)	10 (100%)	0	100	100
All	All	1924/2264 (85%)	1610 (84%)	314 (16%)	2	6

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	7	LYS
1	A	9	ASN
1	A	25	ARG
1	A	26	THR
1	A	31	LEU
1	A	33	GLU
1	A	40	LEU

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Mol	Chain	Res	Type
1	A	47	HIS
1	A	49	GLU
1	A	54	THR
1	A	55	LEU
1	A	66	LEU
1	A	77	ASN
1	A	78	GLN
1	A	125	VAL
1	A	126	VAL
1	A	141	ASP
1	A	150	LEU
1	A	164	THR
1	A	176	CYS
1	A	185	GLU
1	A	203	HIS
1	A	226	THR
1	A	234	GLN
1	A	238	VAL
1	A	252	LEU
1	A	260	HIS
1	A	266	CYS
1	A	267	THR
2	B	502	SER
1	C	1	LEU
1	C	8	THR
1	C	9	ASN
1	C	13	ARG
1	C	19	LEU
1	C	25	ARG
1	C	31	LEU
1	C	38	LEU
1	C	40	LEU
1	C	53	ARG
1	C	55	LEU
1	C	58	ARG
1	C	59	THR
1	C	65	SER
1	C	66	LEU
1	C	70	VAL
1	C	73	LEU
1	C	77	ASN
1	C	105	CYS

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Mol	Chain	Res	Type
1	C	109	ARG
1	C	125	VAL
1	C	126	VAL
1	C	140	ASP
1	C	141	ASP
1	C	185	GLU
1	C	200	GLN
1	C	202	THR
1	C	209	GLU
1	C	219	MET
1	C	238	VAL
1	C	252	LEU
1	C	263	VAL
1	C	268	LYS
1	C	272	ASN
1	E	1	LEU
1	E	9	ASN
1	E	19	LEU
1	E	21	GLN
1	E	22	ASP
1	E	25	ARG
1	E	31	LEU
1	E	38	LEU
1	E	40	LEU
1	E	53	ARG
1	E	54	THR
1	E	55	LEU
1	E	58	ARG
1	E	59	THR
1	E	91	ARG
1	E	93	LEU
1	E	106	GLU
1	E	111	GLN
1	E	112	SER
1	E	113	LEU
1	E	125	VAL
1	E	126	VAL
1	E	144	LEU
1	E	163	ASP
1	E	164	THR
1	E	171	CYS
1	E	173	THR

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Mol	Chain	Res	Type
1	E	182	LEU
1	E	183	GLU
1	E	184	LEU
1	E	185	GLU
1	E	224	VAL
1	E	229	HIS
1	E	233	ASN
1	E	238	VAL
1	E	252	LEU
1	E	257	SER
1	E	276	LEU
1	G	1	LEU
1	G	2	ARG
1	G	8	THR
1	G	9	ASN
1	G	19	LEU
1	G	25	ARG
1	G	29	VAL
1	G	31	LEU
1	G	38	LEU
1	G	40	LEU
1	G	53	ARG
1	G	55	LEU
1	G	59	THR
1	G	65	SER
1	G	67	THR
1	G	70	VAL
1	G	77	ASN
1	G	93	LEU
1	G	107	ARG
1	G	116	ARG
1	G	125	VAL
1	G	126	VAL
1	G	130	ILE
1	G	131	GLN
1	G	132	GLU
1	G	140	ASP
1	G	150	LEU
1	G	164	THR
1	G	169	LYS
1	G	182	LEU
1	G	186	ASN

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Mol	Chain	Res	Type
1	G	193	GLN
1	G	200	GLN
1	G	202	THR
1	G	203	HIS
1	G	205	CYS
1	G	210	THR
1	G	212	LEU
1	G	226	THR
1	G	234	GLN
1	G	238	VAL
1	G	252	LEU
1	G	272	ASN
1	G	276	LEU
2	H	502	SER
2	H	512	SER
1	I	1	LEU
1	I	8	THR
1	I	19	LEU
1	I	21	GLN
1	I	29	VAL
1	I	38	LEU
1	I	53	ARG
1	I	54	THR
1	I	55	LEU
1	I	59	THR
1	I	63	ILE
1	I	69	VAL
1	I	70	VAL
1	I	73	LEU
1	I	77	ASN
1	I	107	ARG
1	I	111	GLN
1	I	114	GLN
1	I	116	ARG
1	I	117	SER
1	I	119	GLU
1	I	123	LEU
1	I	125	VAL
1	I	126	VAL
1	I	127	THR
1	I	131	GLN
1	I	150	LEU

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Mol	Chain	Res	Type
1	I	161	ASN
1	I	175	LYS
1	I	182	LEU
1	I	190	ASN
1	I	193	GLN
1	I	202	THR
1	I	203	HIS
1	I	206	SER
1	I	207	SER
1	I	210	THR
1	I	224	VAL
1	I	243	THR
1	I	252	LEU
1	I	257	SER
1	I	261	ILE
1	I	263	VAL
1	I	267	THR
1	I	268	LYS
1	I	272	ASN
2	J	513	LYS
1	K	1	LEU
1	K	8	THR
1	K	9	ASN
1	K	15	GLU
1	K	19	LEU
1	K	31	LEU
1	K	36	GLU
1	K	40	LEU
1	K	54	THR
1	K	55	LEU
1	K	58	ARG
1	K	63	ILE
1	K	66	LEU
1	K	69	VAL
1	K	70	VAL
1	K	91	ARG
1	K	106	GLU
1	K	113	LEU
1	K	114	GLN
1	K	116	ARG
1	K	123	LEU
1	K	125	VAL

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Mol	Chain	Res	Type
1	K	126	VAL
1	K	150	LEU
1	K	163	ASP
1	K	169	LYS
1	K	176	CYS
1	K	182	LEU
1	K	187	LEU
1	K	189	GLN
1	K	193	GLN
1	K	206	SER
1	K	212	LEU
1	K	235	SER
1	K	239	ARG
1	K	243	THR
1	K	258	MET
1	K	261	ILE
1	K	268	LYS
2	L	501	LYS
2	L	502	SER
2	L	503	ASP
1	M	7	LYS
1	M	8	THR
1	M	9	ASN
1	M	13	ARG
1	M	19	LEU
1	M	25	ARG
1	M	29	VAL
1	M	37	GLU
1	M	38	LEU
1	M	40	LEU
1	M	55	LEU
1	M	59	THR
1	M	69	VAL
1	M	70	VAL
1	M	91	ARG
1	M	103	MET
1	M	106	GLU
1	M	114	GLN
1	M	123	LEU
1	M	125	VAL
1	M	126	VAL
1	M	150	LEU

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Mol	Chain	Res	Type
1	M	169	LYS
1	M	170	CYS
1	M	175	LYS
1	M	184	LEU
1	M	185	GLU
1	M	187	LEU
1	M	192	ARG
1	M	193	GLN
1	M	201	SER
1	M	213	ILE
1	M	224	VAL
1	M	232	LYS
1	M	234	GLN
1	M	235	SER
1	M	252	LEU
1	M	261	ILE
1	M	263	VAL
1	M	268	LYS
1	M	272	ASN
1	O	1	LEU
1	O	13	ARG
1	O	15	GLU
1	O	29	VAL
1	O	36	GLU
1	O	40	LEU
1	O	49	GLU
1	O	55	LEU
1	O	63	ILE
1	O	67	THR
1	O	69	VAL
1	O	70	VAL
1	O	77	ASN
1	O	80	ASN
1	O	104	SER
1	O	114	GLN
1	O	116	ARG
1	O	123	LEU
1	O	125	VAL
1	O	126	VAL
1	O	181	ILE
1	O	182	LEU
1	O	185	GLU

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Mol	Chain	Res	Type
1	O	187	LEU
1	O	192	ARG
1	O	206	SER
1	O	208	GLU
1	O	216	ARG
1	O	230	GLU
1	O	234	GLN
1	O	252	LEU
1	O	261	ILE
1	O	264	SER
1	O	268	LYS
1	O	271	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	HIS
1	A	78	GLN
1	A	80	ASN
1	A	111	GLN
1	A	143	HIS
1	A	157	ASN
1	A	160	HIS
1	A	200	GLN
1	A	203	HIS
1	A	233	ASN
1	A	272	ASN
1	C	9	ASN
1	C	111	GLN
1	C	114	GLN
1	C	121	GLN
1	C	143	HIS
1	C	157	ASN
1	C	186	ASN
1	C	193	GLN
1	C	200	GLN
1	C	260	HIS
1	C	272	ASN
1	E	121	GLN
1	E	128	HIS
1	E	186	ASN

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Mol	Chain	Res	Type
1	E	233	ASN
1	E	249	HIS
1	E	251	HIS
1	E	259	ASN
1	G	9	ASN
1	G	77	ASN
1	G	78	GLN
1	G	131	GLN
1	G	143	HIS
1	G	160	HIS
1	G	193	GLN
1	G	200	GLN
1	G	251	HIS
1	G	259	ASN
1	G	260	HIS
1	G	272	ASN
1	I	21	GLN
1	I	77	ASN
1	I	111	GLN
1	I	114	GLN
1	I	121	GLN
1	I	161	ASN
1	I	190	ASN
1	I	193	GLN
1	I	200	GLN
1	I	203	HIS
1	I	259	ASN
1	I	260	HIS
1	I	273	HIS
1	K	9	ASN
1	K	21	GLN
1	K	47	HIS
1	K	114	GLN
1	K	121	GLN
1	K	128	HIS
1	K	157	ASN
1	K	160	HIS
1	K	186	ASN
1	K	193	GLN
1	K	221	GLN
1	K	248	GLN
1	K	251	HIS

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Mol	Chain	Res	Type
1	K	260	HIS
1	M	9	ASN
1	M	21	GLN
1	M	80	ASN
1	M	121	GLN
1	M	128	HIS
1	M	131	GLN
1	M	157	ASN
1	M	229	HIS
1	M	234	GLN
1	M	259	ASN
1	M	272	ASN
1	O	5	GLN
1	O	9	ASN
1	O	21	GLN
1	O	77	ASN
1	O	111	GLN
1	O	157	ASN
1	O	160	HIS
1	O	189	GLN
1	O	190	ASN
1	O	200	GLN
1	O	203	HIS
1	O	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ALC	B	504	2	9,11,12	0.48	0	11,13,15	1.69	3 (27%)
2	ALC	D	504	2	9,11,12	0.59	0	11,13,15	1.52	2 (18%)
2	ALC	J	504	2	9,11,12	0.53	0	11,13,15	1.99	4 (36%)
2	ALC	P	504	2	9,11,12	0.59	0	11,13,15	0.97	0
2	ALC	F	504	2	9,11,12	0.50	0	11,13,15	1.44	2 (18%)
2	ALC	N	504	2	9,11,12	0.52	0	11,13,15	1.89	4 (36%)
2	ALC	H	504	2	9,11,12	0.60	0	11,13,15	1.84	3 (27%)
2	ALC	L	504	2	9,11,12	0.62	0	11,13,15	1.14	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALC	B	504	2	-	3/5/14/16	0/1/1/1
2	ALC	D	504	2	-	0/5/14/16	0/1/1/1
2	ALC	J	504	2	-	0/5/14/16	0/1/1/1
2	ALC	P	504	2	-	0/5/14/16	0/1/1/1
2	ALC	F	504	2	-	2/5/14/16	0/1/1/1
2	ALC	N	504	2	-	0/5/14/16	0/1/1/1
2	ALC	H	504	2	-	0/5/14/16	0/1/1/1
2	ALC	L	504	2	-	0/5/14/16	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(°)
2	H	504	ALC	CB-CG-CD1	-4.25	101.82	111.71
2	J	504	ALC	CD1-CG-CD2	3.46	117.76	109.29
2	J	504	ALC	CB-CG-CD1	-3.36	103.90	111.71
2	B	504	ALC	CG-CB-CA	3.32	118.98	114.52
2	N	504	ALC	CB-CG-CD1	-3.23	104.18	111.71
2	N	504	ALC	CD1-CG-CD2	3.15	116.99	109.29
2	L	504	ALC	CB-CA-N	-2.84	104.27	110.48
2	B	504	ALC	CB-CG-CD2	-2.83	105.13	111.71
2	D	504	ALC	CB-CG-CD1	-2.78	105.24	111.71
2	N	504	ALC	CE2-CD2-CG	2.65	117.66	112.08
2	F	504	ALC	CB-CA-N	-2.65	104.70	110.48
2	J	504	ALC	CE1-CD1-CG	2.46	117.26	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	ALC	CB-CA-N	-2.45	105.12	110.48
2	N	504	ALC	CE1-CD1-CG	2.40	117.13	112.08
2	F	504	ALC	CB-CA-C	2.39	114.67	110.99
2	D	504	ALC	CE2-CD2-CG	2.37	117.07	112.08
2	H	504	ALC	CB-CA-N	-2.19	105.69	110.48
2	H	504	ALC	CB-CG-CD2	-2.16	106.69	111.71
2	J	504	ALC	CZ-CE2-CD2	-2.07	107.16	111.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	504	ALC	O-C-CA-CB
2	F	504	ALC	C-CA-CB-CG
2	B	504	ALC	CA-CB-CG-CD1
2	B	504	ALC	CA-CB-CG-CD2
2	B	504	ALC	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	ALC	2	0
2	P	504	ALC	1	0
2	L	504	ALC	1	0

5.5 Carbohydrates ⓘ

52 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	Q	1	1,3	14,14,15	0.56	0	17,19,21	1.36	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Q	2	3	14,14,15	0.64	0	17,19,21	1.76	3 (17%)
3	FUC	Q	3	3	10,10,11	0.65	0	14,14,16	1.08	1 (7%)
4	NAG	R	1	4,1	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
4	FUC	R	2	4	10,10,11	0.58	0	14,14,16	0.73	0
3	NAG	S	1	1,3	14,14,15	0.53	0	17,19,21	2.43	4 (23%)
3	NAG	S	2	3	14,14,15	0.70	1 (7%)	17,19,21	1.49	3 (17%)
3	FUC	S	3	3	10,10,11	0.62	0	14,14,16	0.92	0
3	NAG	T	1	1,3	14,14,15	0.57	0	17,19,21	1.72	4 (23%)
3	NAG	T	2	3	14,14,15	0.58	0	17,19,21	1.39	1 (5%)
3	FUC	T	3	3	10,10,11	0.71	0	14,14,16	1.35	2 (14%)
4	NAG	U	1	4,1	14,14,15	0.57	0	17,19,21	1.84	4 (23%)
4	FUC	U	2	4	10,10,11	0.86	0	14,14,16	1.84	3 (21%)
4	NAG	V	1	4,1	14,14,15	0.55	0	17,19,21	1.66	3 (17%)
4	FUC	V	2	4	10,10,11	0.57	0	14,14,16	1.06	1 (7%)
5	NAG	W	1	1,5	14,14,15	0.67	0	17,19,21	1.06	2 (11%)
5	NAG	W	2	5	14,14,15	0.60	0	17,19,21	1.27	2 (11%)
4	NAG	X	1	4,1	14,14,15	0.58	0	17,19,21	1.50	2 (11%)
4	FUC	X	2	4	10,10,11	0.67	0	14,14,16	1.30	1 (7%)
4	NAG	Y	1	4,1	14,14,15	0.42	0	17,19,21	1.62	2 (11%)
4	FUC	Y	2	4	10,10,11	0.75	0	14,14,16	1.59	2 (14%)
6	NAG	Z	1	6,1	14,14,15	0.45	0	17,19,21	1.09	1 (5%)
6	NAG	Z	2	6	14,14,15	0.60	0	17,19,21	1.07	0
6	BMA	Z	3	6	11,11,12	0.48	0	15,15,17	2.91	5 (33%)
6	MAN	Z	4	6	11,11,12	0.62	0	15,15,17	1.90	3 (20%)
6	MAN	Z	5	6	11,11,12	0.71	0	15,15,17	1.10	1 (6%)
4	NAG	a	1	4,1	14,14,15	0.48	0	17,19,21	1.69	2 (11%)
4	FUC	a	2	4	10,10,11	0.59	0	14,14,16	1.08	0
3	NAG	b	1	1,3	14,14,15	0.62	0	17,19,21	1.57	3 (17%)
3	NAG	b	2	3	14,14,15	0.64	0	17,19,21	2.53	4 (23%)
3	FUC	b	3	3	10,10,11	0.61	0	14,14,16	0.87	0
6	NAG	c	1	6,1	14,14,15	0.66	0	17,19,21	1.61	5 (29%)
6	NAG	c	2	6	14,14,15	0.68	0	17,19,21	1.17	2 (11%)
6	BMA	c	3	6	11,11,12	0.90	1 (9%)	15,15,17	1.70	3 (20%)
6	MAN	c	4	6	11,11,12	0.73	0	15,15,17	1.83	4 (26%)
6	MAN	c	5	6	11,11,12	0.68	0	15,15,17	1.24	3 (20%)
4	NAG	d	1	4,1	14,14,15	0.42	0	17,19,21	1.90	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	d	2	4	10,10,11	0.67	0	14,14,16	0.95	1 (7%)
6	NAG	e	1	6,1	14,14,15	0.60	0	17,19,21	1.64	1 (5%)
6	NAG	e	2	6	14,14,15	0.59	0	17,19,21	1.15	1 (5%)
6	BMA	e	3	6	11,11,12	0.56	0	15,15,17	1.81	3 (20%)
6	MAN	e	4	6	11,11,12	0.76	0	15,15,17	2.52	6 (40%)
6	MAN	e	5	6	11,11,12	0.63	0	15,15,17	1.30	1 (6%)
5	NAG	f	1	1,5	14,14,15	0.68	0	17,19,21	1.31	1 (5%)
5	NAG	f	2	5	14,14,15	0.54	0	17,19,21	1.71	3 (17%)
4	NAG	g	1	4,1	14,14,15	0.52	0	17,19,21	1.32	2 (11%)
4	FUC	g	2	4	10,10,11	0.68	0	14,14,16	1.33	2 (14%)
6	NAG	h	1	6,1	14,14,15	0.68	0	17,19,21	1.79	4 (23%)
6	NAG	h	2	6	14,14,15	0.53	0	17,19,21	0.82	0
6	BMA	h	3	6	11,11,12	0.92	1 (9%)	15,15,17	1.49	2 (13%)
6	MAN	h	4	6	11,11,12	0.75	0	15,15,17	1.49	2 (13%)
6	MAN	h	5	6	11,11,12	0.62	0	15,15,17	1.73	2 (13%)

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	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	5/6/23/26	0/1/1/1
3	FUC	Q	3	3	2/2/4/5	-	0/1/1/1
4	NAG	R	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	R	2	4	2/2/4/5	-	0/1/1/1
3	NAG	S	1	1,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	FUC	S	3	3	2/2/4/5	-	0/1/1/1
3	NAG	T	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	FUC	T	3	3	2/2/4/5	-	0/1/1/1
4	NAG	U	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	U	2	4	2/2/4/5	-	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	V	2	4	2/2/4/5	-	0/1/1/1
5	NAG	W	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	3/6/23/26	0/1/1/1
4	NAG	X	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	FUC	X	2	4	2/2/4/5	-	0/1/1/1
4	NAG	Y	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	Y	2	4	2/2/4/5	-	0/1/1/1
6	NAG	Z	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	2/2/19/22	1/1/1/1
4	NAG	a	1	4,1	-	5/6/23/26	0/1/1/1
4	FUC	a	2	4	2/2/4/5	-	0/1/1/1
3	NAG	b	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	FUC	b	3	3	2/2/4/5	-	0/1/1/1
6	NAG	c	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	c	2	6	-	4/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	2/2/19/22	0/1/1/1
6	MAN	c	5	6	-	0/2/19/22	0/1/1/1
4	NAG	d	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	d	2	4	2/2/4/5	-	0/1/1/1
6	NAG	e	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	MAN	e	4	6	-	2/2/19/22	1/1/1/1
6	MAN	e	5	6	-	1/2/19/22	0/1/1/1
5	NAG	f	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	3/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	g	2	4	2/2/4/5	-	0/1/1/1
6	NAG	h	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	h	3	6	-	2/2/19/22	0/1/1/1
6	MAN	h	4	6	-	1/2/19/22	0/1/1/1
6	MAN	h	5	6	-	2/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	3	BMA	O5-C1	-2.30	1.39	1.43
6	c	3	BMA	O5-C1	-2.14	1.40	1.43
3	S	2	NAG	C1-C2	2.01	1.55	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	3	BMA	C1-O5-C5	8.96	124.20	112.19
3	b	2	NAG	C1-O5-C5	8.60	123.71	112.19
3	S	1	NAG	C1-O5-C5	7.70	122.51	112.19
6	e	4	MAN	C1-C2-C3	-6.47	100.22	109.64
6	e	1	NAG	C1-O5-C5	5.78	119.94	112.19
3	Q	2	NAG	C1-O5-C5	5.73	119.86	112.19
4	a	1	NAG	C1-O5-C5	5.63	119.74	112.19
6	Z	4	MAN	C1-C2-C3	-5.55	101.56	109.64
3	T	2	NAG	C1-O5-C5	5.08	119.00	112.19
5	f	2	NAG	C1-O5-C5	5.08	119.00	112.19
6	c	4	MAN	C1-C2-C3	-4.96	102.42	109.64
3	S	1	NAG	C4-C3-C2	4.76	117.99	111.02
4	R	1	NAG	C1-O5-C5	4.63	118.39	112.19
4	U	1	NAG	C1-O5-C5	4.55	118.28	112.19
4	X	1	NAG	C1-O5-C5	4.37	118.04	112.19
6	c	3	BMA	C1-C2-C3	4.28	115.87	109.64
4	U	2	FUC	O5-C5-C4	4.14	117.00	109.55
6	e	4	MAN	O2-C2-C1	4.13	118.67	109.22
4	Y	2	FUC	C1-C2-C3	4.12	115.64	109.64
6	h	5	MAN	C1-O5-C5	4.07	117.65	112.19
4	d	1	NAG	C1-O5-C5	4.03	117.59	112.19
6	h	5	MAN	O5-C5-C6	3.98	115.41	107.66
4	U	2	FUC	C3-C4-C5	3.97	115.85	109.81
6	e	3	BMA	C1-C2-C3	3.94	115.39	109.64
6	e	4	MAN	C1-O5-C5	-3.85	107.02	112.19
4	Y	1	NAG	C1-O5-C5	3.85	117.34	112.19
4	V	1	NAG	C1-O5-C5	3.82	117.31	112.19
6	h	4	MAN	C1-C2-C3	-3.79	104.12	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	1	NAG	C4-C3-C2	-3.74	105.54	111.02
3	b	1	NAG	O4-C4-C5	3.72	118.48	109.32
6	h	3	BMA	C1-C2-C3	3.70	115.04	109.64
6	e	3	BMA	C1-O5-C5	3.70	117.14	112.19
3	S	2	NAG	C4-C3-C2	3.69	116.43	111.02
5	W	2	NAG	C2-N2-C7	3.52	127.61	122.90
4	V	1	NAG	O5-C5-C6	3.50	114.48	107.66
4	U	1	NAG	C3-C4-C5	3.50	116.57	110.23
6	h	1	NAG	C1-O5-C5	3.45	116.81	112.19
3	T	1	NAG	C4-C3-C2	3.44	116.06	111.02
3	T	3	FUC	C1-C2-C3	3.42	114.62	109.64
6	e	2	NAG	C1-O5-C5	3.39	116.72	112.19
6	Z	1	NAG	C1-O5-C5	3.37	116.70	112.19
6	h	1	NAG	C4-C3-C2	3.36	115.94	111.02
6	h	1	NAG	C2-N2-C7	-3.35	118.41	122.90
3	T	1	NAG	O5-C1-C2	-3.35	106.10	111.29
6	c	1	NAG	C1-O5-C5	3.34	116.67	112.19
5	f	1	NAG	C1-O5-C5	3.33	116.65	112.19
6	e	5	MAN	C1-O5-C5	3.30	116.61	112.19
4	d	1	NAG	C2-N2-C7	-3.25	118.55	122.90
6	Z	3	BMA	O3-C3-C2	-3.21	103.51	110.05
6	c	3	BMA	O3-C3-C2	-3.19	103.54	110.05
6	Z	3	BMA	C3-C4-C5	3.19	116.02	110.23
4	d	1	NAG	C4-C3-C2	-3.14	106.41	111.02
4	g	2	FUC	C3-C4-C5	3.14	114.58	109.81
6	Z	4	MAN	O2-C2-C1	3.13	116.40	109.22
3	S	2	NAG	C1-O5-C5	3.12	116.37	112.19
5	W	2	NAG	C1-O5-C5	3.09	116.32	112.19
6	e	3	BMA	O3-C3-C2	-3.00	103.94	110.05
6	Z	3	BMA	C1-C2-C3	2.95	113.93	109.64
6	h	4	MAN	C3-C4-C5	2.95	115.57	110.23
3	b	2	NAG	C3-C4-C5	2.92	115.53	110.23
6	Z	3	BMA	O5-C5-C4	2.87	117.81	110.83
5	f	2	NAG	C4-C3-C2	2.85	115.20	111.02
4	U	1	NAG	O5-C5-C6	2.85	113.21	107.66
3	Q	2	NAG	O5-C1-C2	2.80	115.63	111.29
6	c	1	NAG	O5-C5-C6	2.80	113.11	107.66
4	Y	2	FUC	C2-C3-C4	2.78	115.75	110.86
4	d	1	NAG	C1-C2-N2	2.74	114.75	110.43
3	S	2	NAG	O5-C1-C2	2.70	115.47	111.29
3	b	1	NAG	C1-O5-C5	2.70	115.80	112.19
3	b	2	NAG	O5-C5-C4	2.69	117.38	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	3	FUC	C3-C4-C5	2.67	113.87	109.81
4	X	2	FUC	C1-C2-C3	-2.66	105.77	109.64
3	T	1	NAG	C1-O5-C5	2.64	115.72	112.19
4	d	1	NAG	O5-C1-C2	-2.56	107.33	111.29
6	c	2	NAG	O5-C5-C6	2.55	112.62	107.66
4	g	1	NAG	O5-C1-C2	-2.53	107.37	111.29
3	S	1	NAG	O5-C1-C2	2.52	115.19	111.29
4	V	1	NAG	C6-C5-C4	-2.52	106.84	113.02
3	Q	1	NAG	C4-C3-C2	2.51	114.69	111.02
6	c	3	BMA	C3-C4-C5	2.48	114.73	110.23
4	d	2	FUC	C1-O5-C5	2.47	118.78	112.97
4	U	1	NAG	C4-C3-C2	2.45	114.61	111.02
6	c	4	MAN	C3-C4-C5	2.41	114.60	110.23
5	f	2	NAG	C3-C4-C5	2.39	114.57	110.23
6	e	4	MAN	O5-C5-C6	2.39	112.32	107.66
4	g	1	NAG	C2-N2-C7	-2.38	119.72	122.90
6	e	4	MAN	C2-C3-C4	-2.34	106.74	110.86
6	c	5	MAN	O3-C3-C4	-2.32	104.91	110.38
6	c	4	MAN	O5-C5-C6	2.28	112.11	107.66
3	T	3	FUC	C2-C3-C4	2.28	114.86	110.86
6	h	1	NAG	C1-C2-N2	2.27	114.01	110.43
3	Q	1	NAG	C1-O5-C5	2.26	115.22	112.19
4	R	1	NAG	C2-N2-C7	-2.25	119.88	122.90
6	c	5	MAN	O6-C6-C5	-2.25	103.67	111.33
4	X	1	NAG	O5-C5-C6	2.25	112.03	107.66
5	W	1	NAG	C1-O5-C5	2.23	115.18	112.19
6	c	5	MAN	O5-C5-C6	2.20	111.95	107.66
4	V	2	FUC	C1-C2-C3	-2.20	106.44	109.64
6	c	1	NAG	C1-C2-N2	2.20	113.89	110.43
6	c	1	NAG	O7-C7-C8	-2.18	118.17	122.05
6	Z	4	MAN	C3-C4-C5	2.18	114.18	110.23
6	c	2	NAG	O4-C4-C3	-2.17	105.26	110.38
3	T	1	NAG	C8-C7-N2	2.16	119.71	116.12
6	Z	5	MAN	O2-C2-C1	2.14	114.13	109.22
3	Q	2	NAG	C4-C3-C2	2.13	114.14	111.02
6	c	1	NAG	C8-C7-N2	2.12	119.63	116.12
6	c	4	MAN	O2-C2-C1	2.12	114.07	109.22
3	Q	1	NAG	C8-C7-N2	2.12	119.63	116.12
4	a	1	NAG	C2-N2-C7	2.11	125.73	122.90
4	g	2	FUC	O5-C5-C6	2.08	111.92	107.40
5	W	1	NAG	O7-C7-C8	-2.06	118.38	122.05
3	S	1	NAG	O5-C5-C4	2.05	115.82	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2	FUC	C2-C3-C4	2.03	114.44	110.86
3	b	1	NAG	O4-C4-C3	2.03	115.16	110.38
6	e	4	MAN	O5-C5-C4	-2.02	105.91	110.83
3	b	2	NAG	O7-C7-C8	-2.01	118.47	122.05
6	h	3	BMA	O3-C3-C4	-2.00	105.65	110.38

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Q	3	FUC	C1
3	Q	3	FUC	C5
3	S	1	NAG	C1
3	S	3	FUC	C1
3	S	3	FUC	C5
3	T	3	FUC	C1
3	T	3	FUC	C5
3	b	3	FUC	C1
3	b	3	FUC	C5
4	R	2	FUC	C1
4	R	2	FUC	C5
4	U	2	FUC	C1
4	U	2	FUC	C5
4	V	2	FUC	C1
4	V	2	FUC	C5
4	X	1	NAG	C1
4	X	2	FUC	C1
4	X	2	FUC	C5
4	Y	2	FUC	C1
4	Y	2	FUC	C5
4	a	2	FUC	C1
4	a	2	FUC	C5
4	d	2	FUC	C1
4	d	2	FUC	C5
4	g	2	FUC	C1
4	g	2	FUC	C5
6	Z	1	NAG	C1
6	c	1	NAG	C1
6	e	1	NAG	C1
6	h	1	NAG	C1

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	a	1	NAG	C3-C2-N2-C7
4	a	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	f	1	NAG	C8-C7-N2-C2
5	f	1	NAG	O7-C7-N2-C2
6	c	1	NAG	C8-C7-N2-C2
6	e	1	NAG	C8-C7-N2-C2
6	e	1	NAG	O7-C7-N2-C2
6	h	1	NAG	C8-C7-N2-C2
6	h	1	NAG	O7-C7-N2-C2
4	a	1	NAG	C4-C5-C6-O6
6	c	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	R	1	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	e	4	MAN	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
6	Z	3	BMA	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
6	Z	4	MAN	O5-C5-C6-O6
6	Z	4	MAN	C4-C5-C6-O6
6	e	4	MAN	C4-C5-C6-O6
6	c	4	MAN	O5-C5-C6-O6
5	f	2	NAG	C8-C7-N2-C2
6	Z	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
6	h	1	NAG	O5-C5-C6-O6
6	Z	5	MAN	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C8-C7-N2-C2
5	f	2	NAG	O7-C7-N2-C2
6	Z	1	NAG	O7-C7-N2-C2
4	Y	1	NAG	C4-C5-C6-O6
6	c	1	NAG	C4-C5-C6-O6
6	h	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
6	Z	5	MAN	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
4	d	1	NAG	O7-C7-N2-C2
6	Z	2	NAG	C8-C7-N2-C2
6	Z	2	NAG	O7-C7-N2-C2
6	c	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	c	2	NAG	O7-C7-N2-C2
6	Z	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
6	h	5	MAN	C4-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	h	3	BMA	C4-C5-C6-O6
6	h	3	BMA	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
6	h	5	MAN	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
6	Z	3	BMA	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
6	h	4	MAN	O5-C5-C6-O6
6	c	4	MAN	C4-C5-C6-O6
6	e	5	MAN	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C1-C2-N2-C7
5	W	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	h	5	MAN	C1-C2-C3-C4-C5-O5
6	e	4	MAN	C1-C2-C3-C4-C5-O5
6	Z	5	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

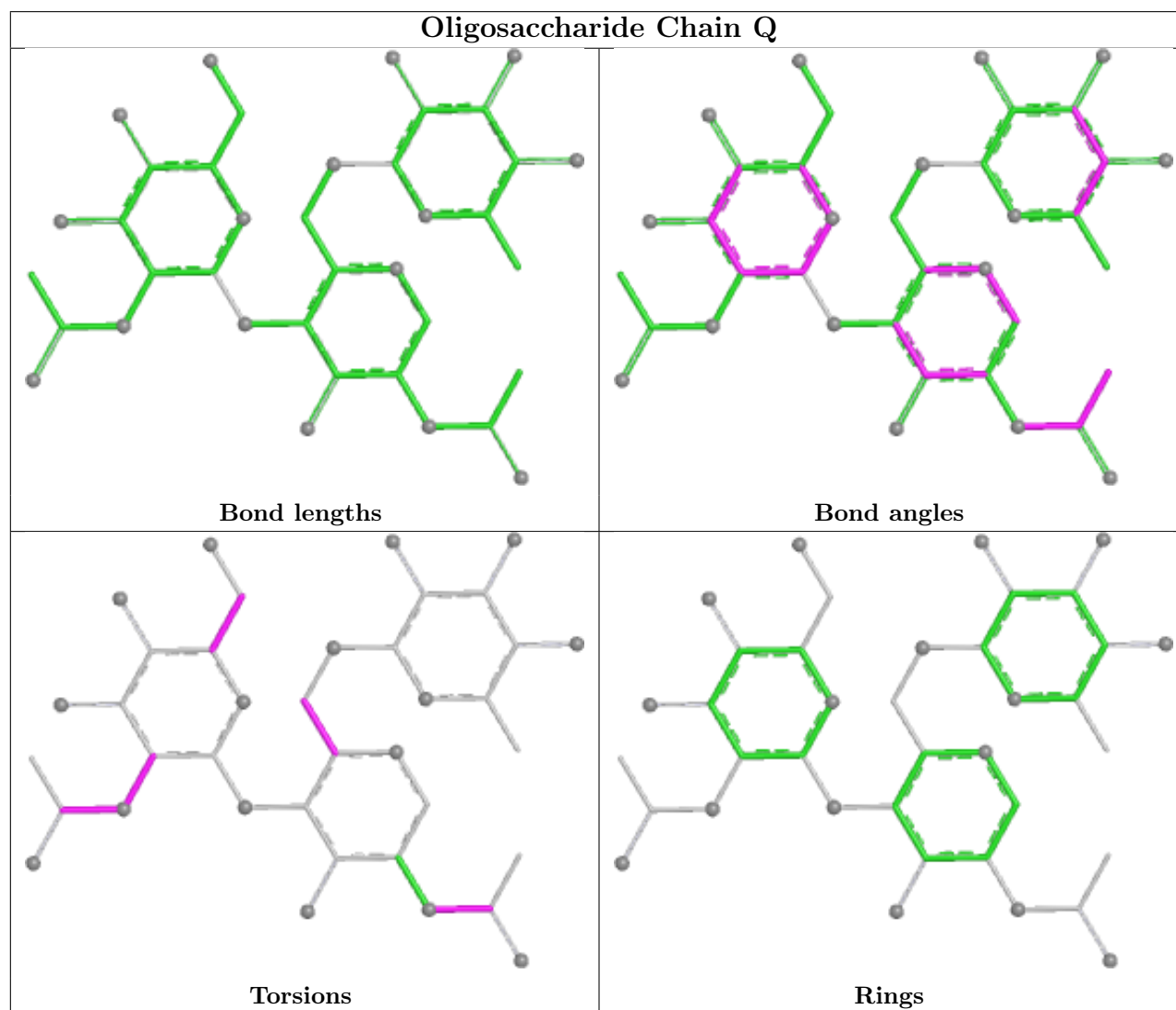
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	d	1	NAG	1	0
6	h	4	MAN	1	0

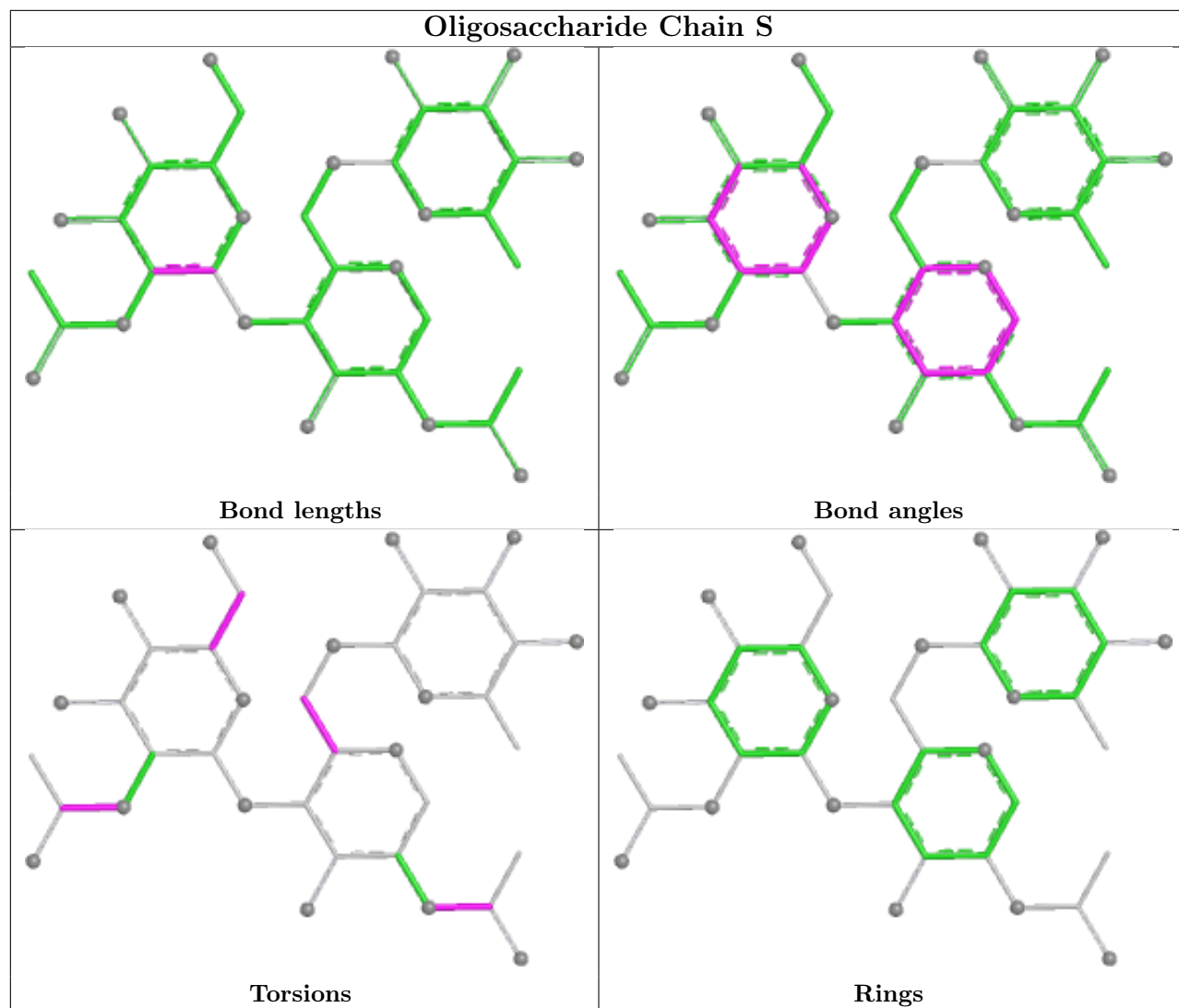
Continued on next page...

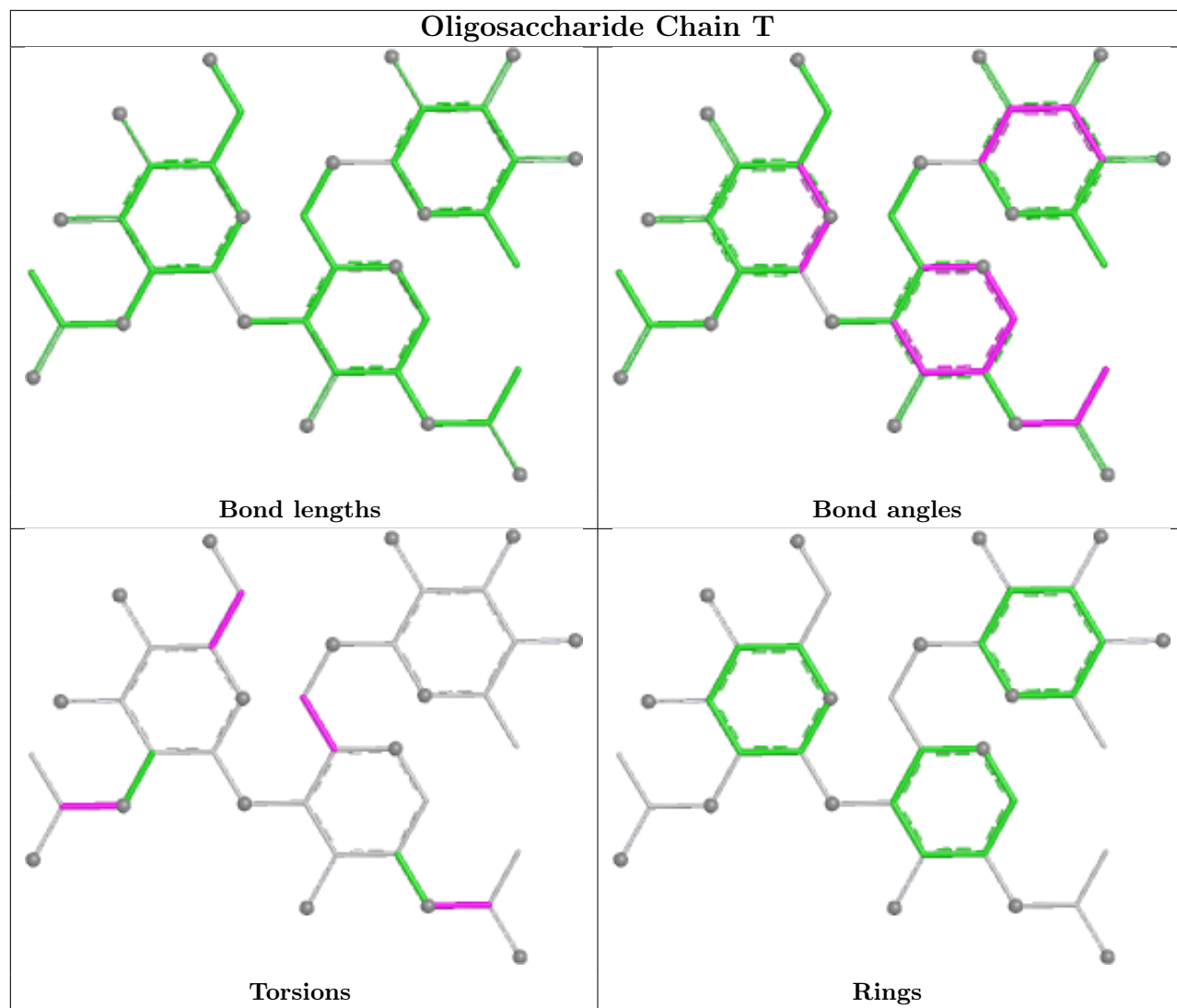
Continued from previous page...

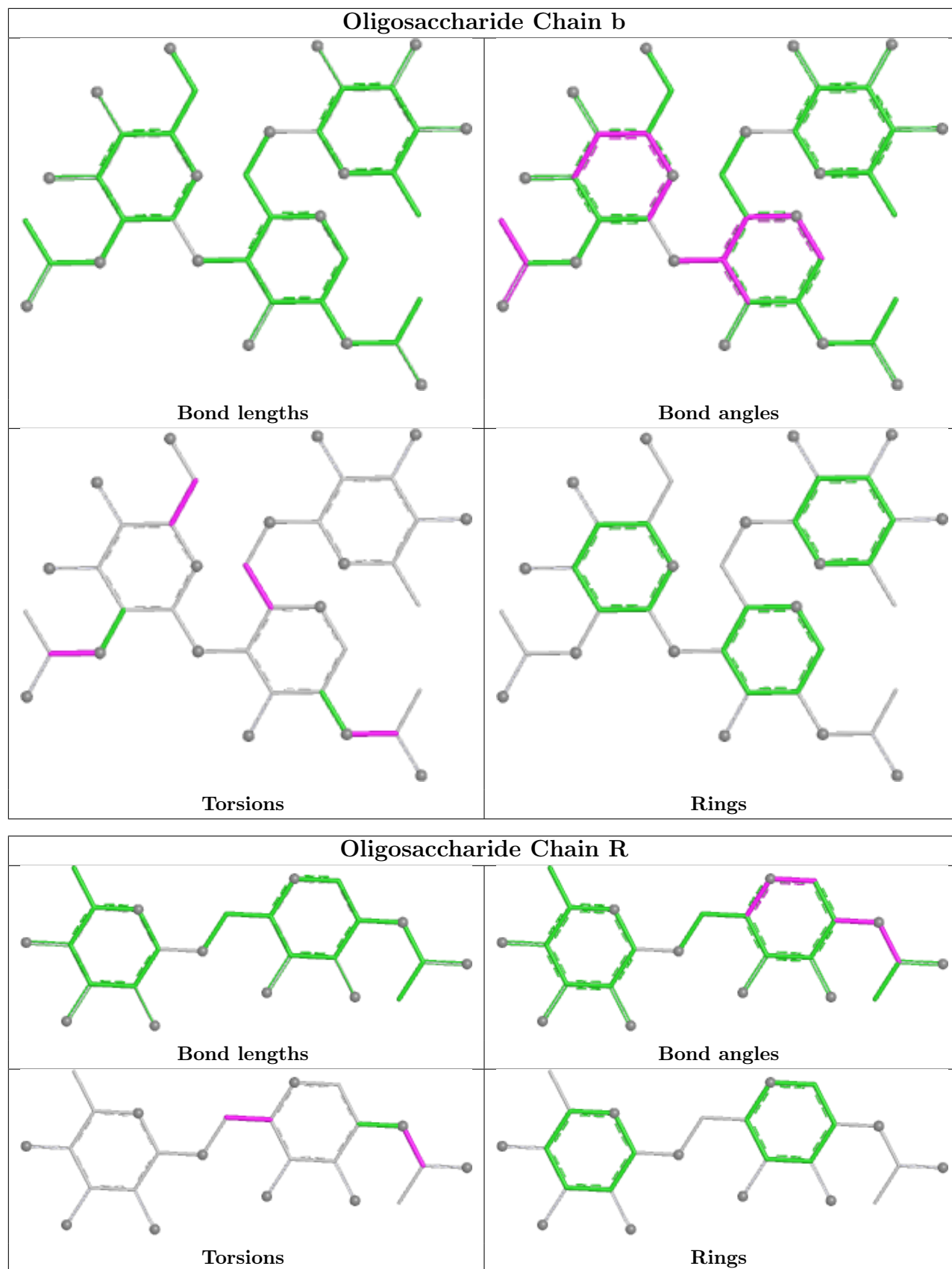
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1	NAG	1	0
5	W	1	NAG	2	0
5	W	2	NAG	1	0

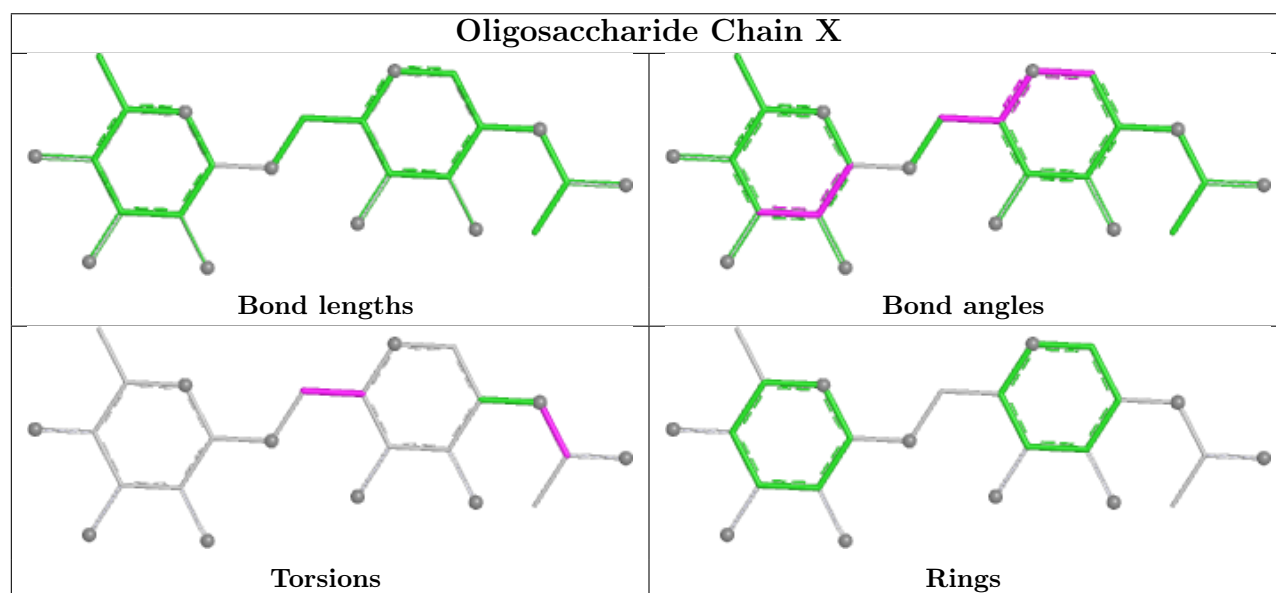
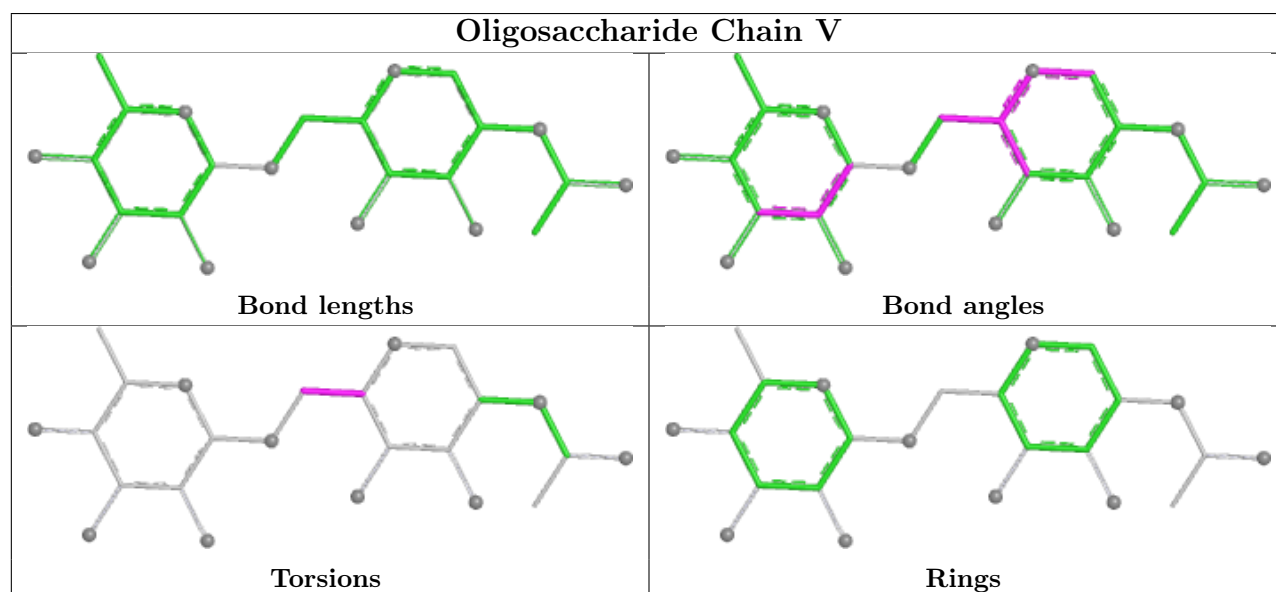
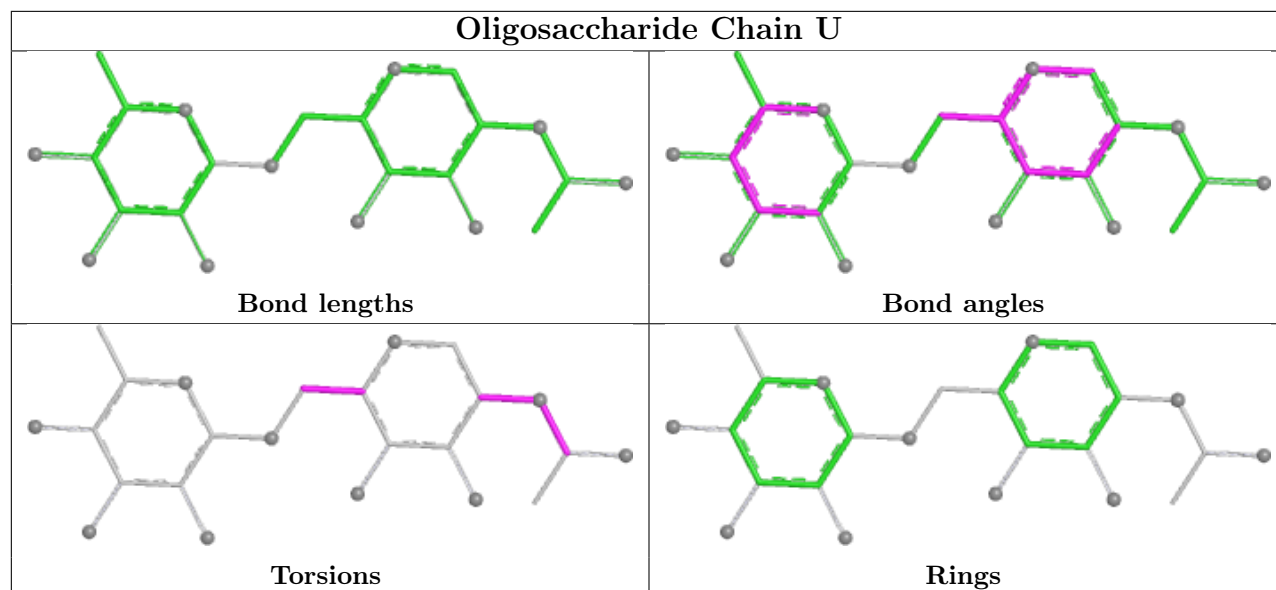
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

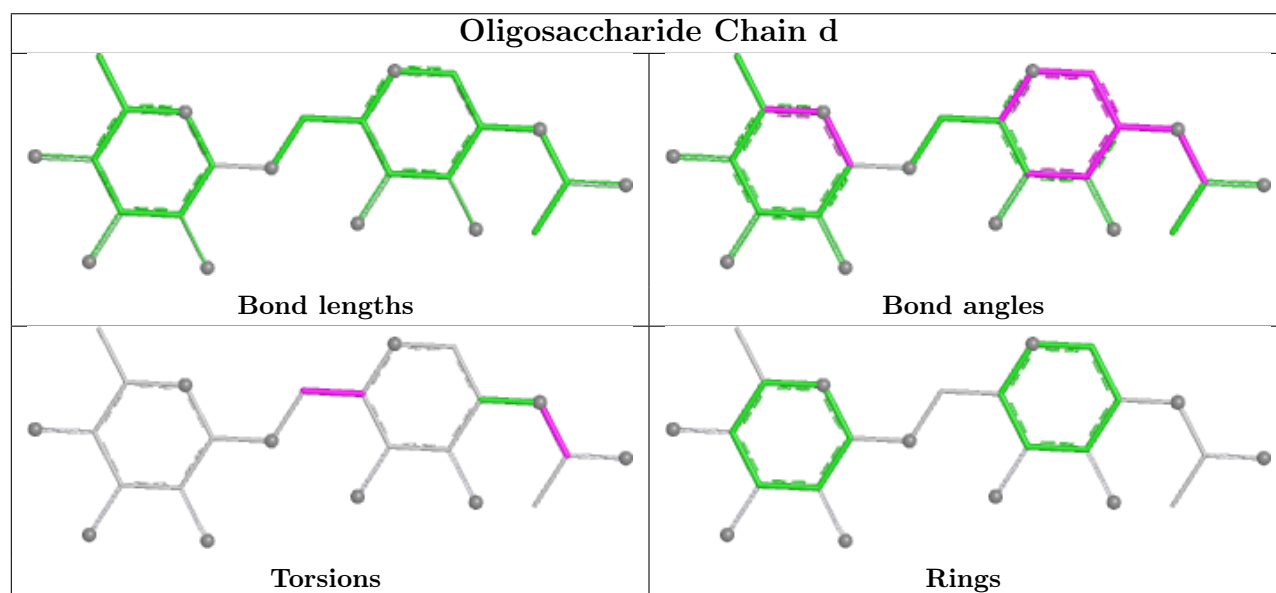
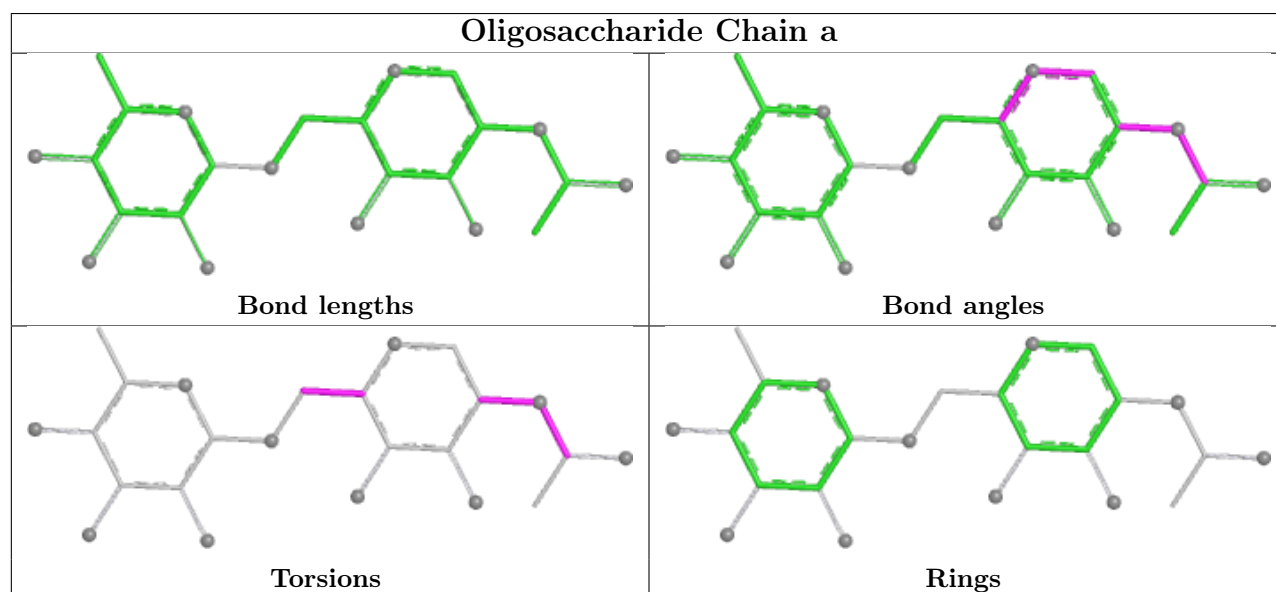
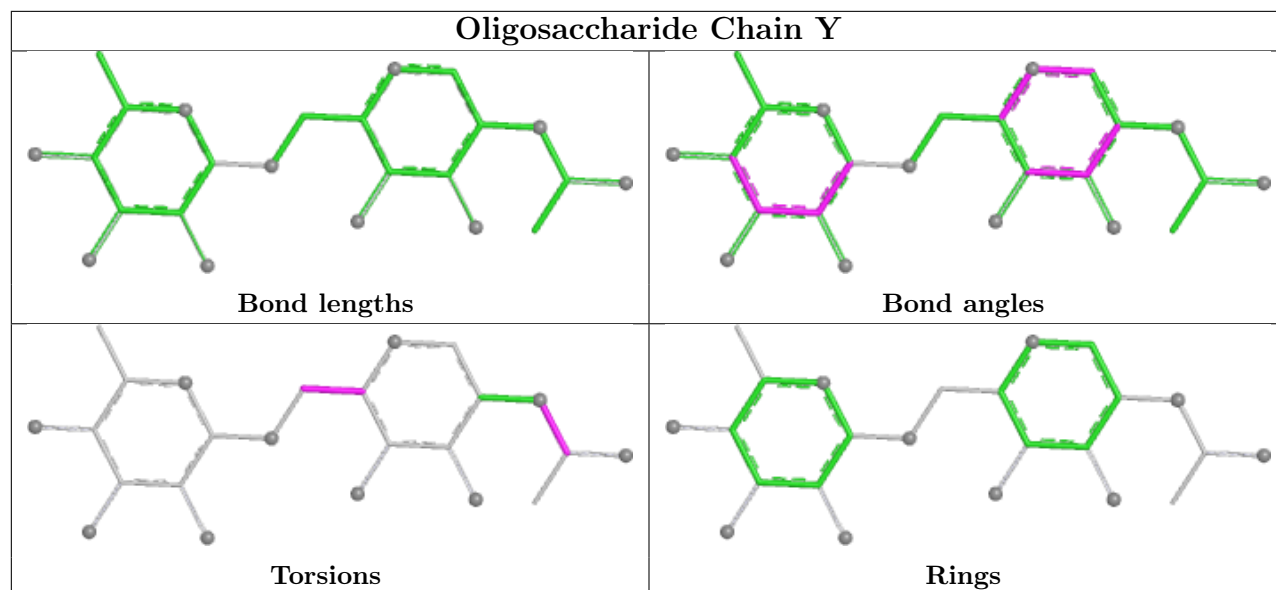


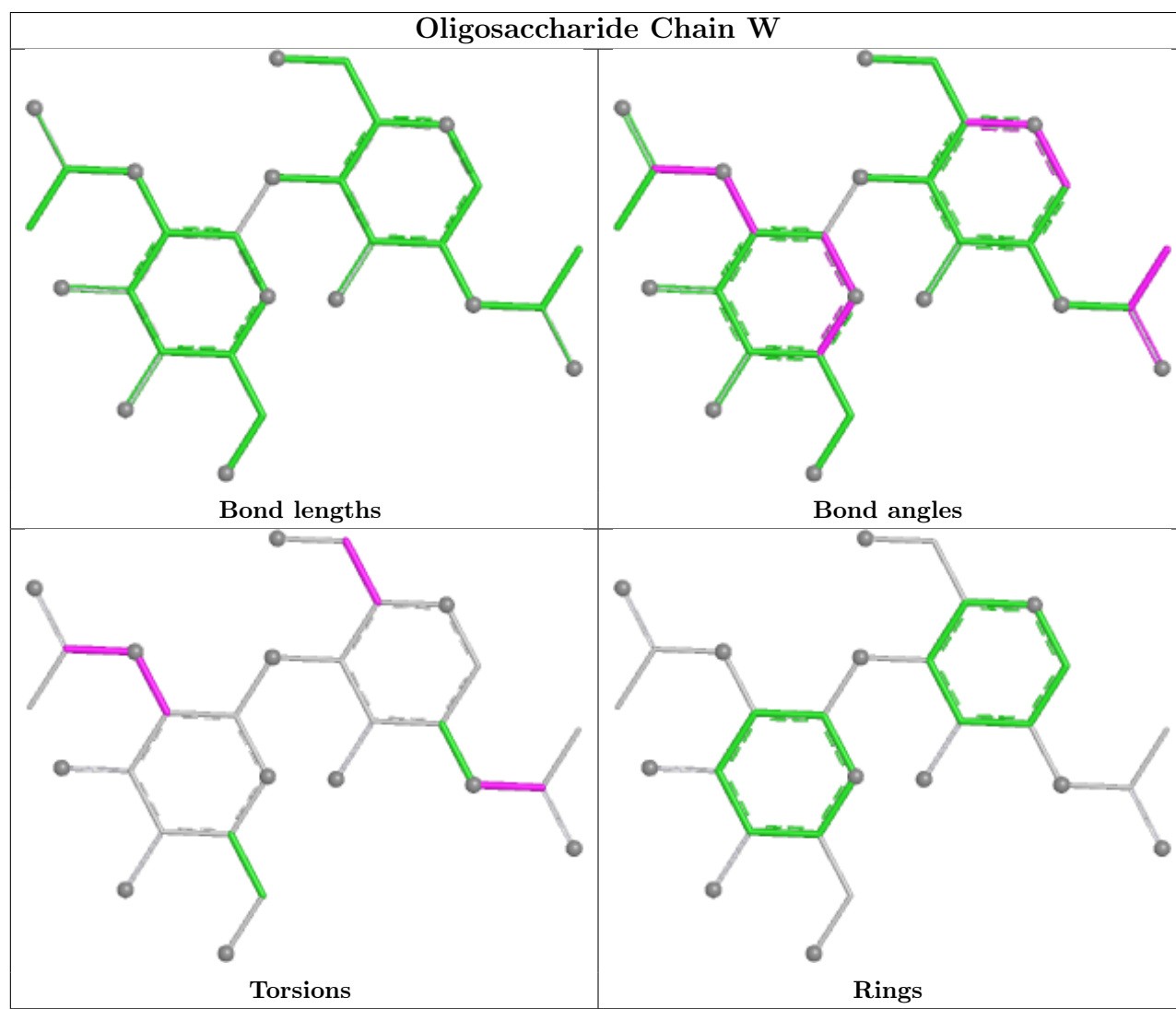
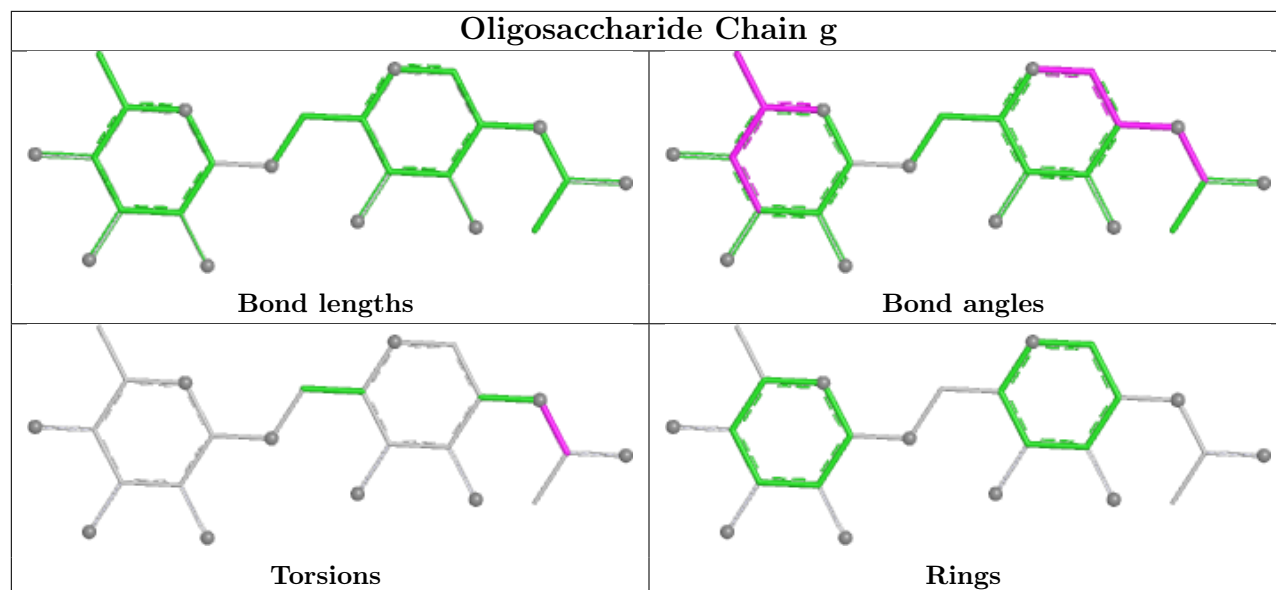


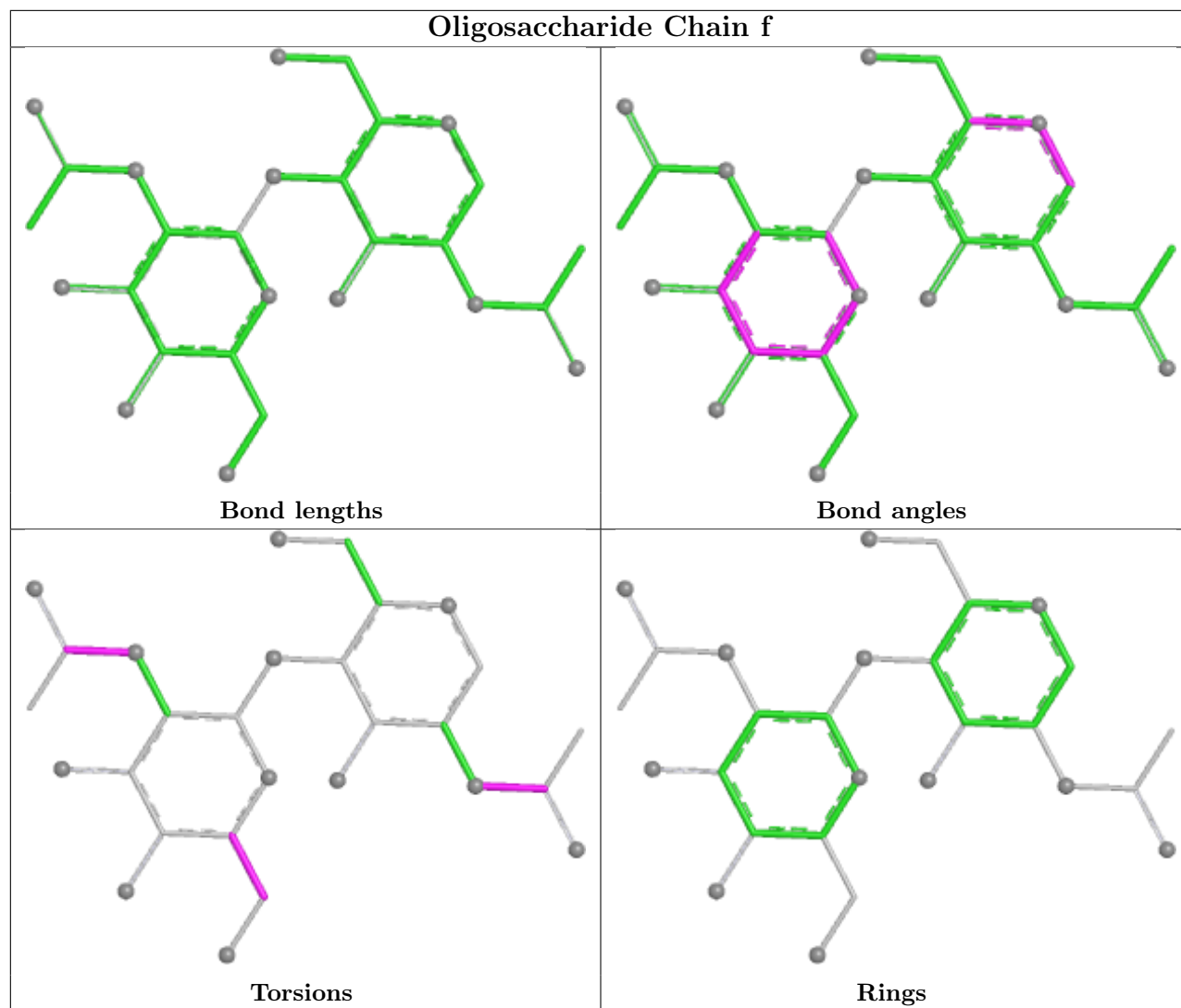


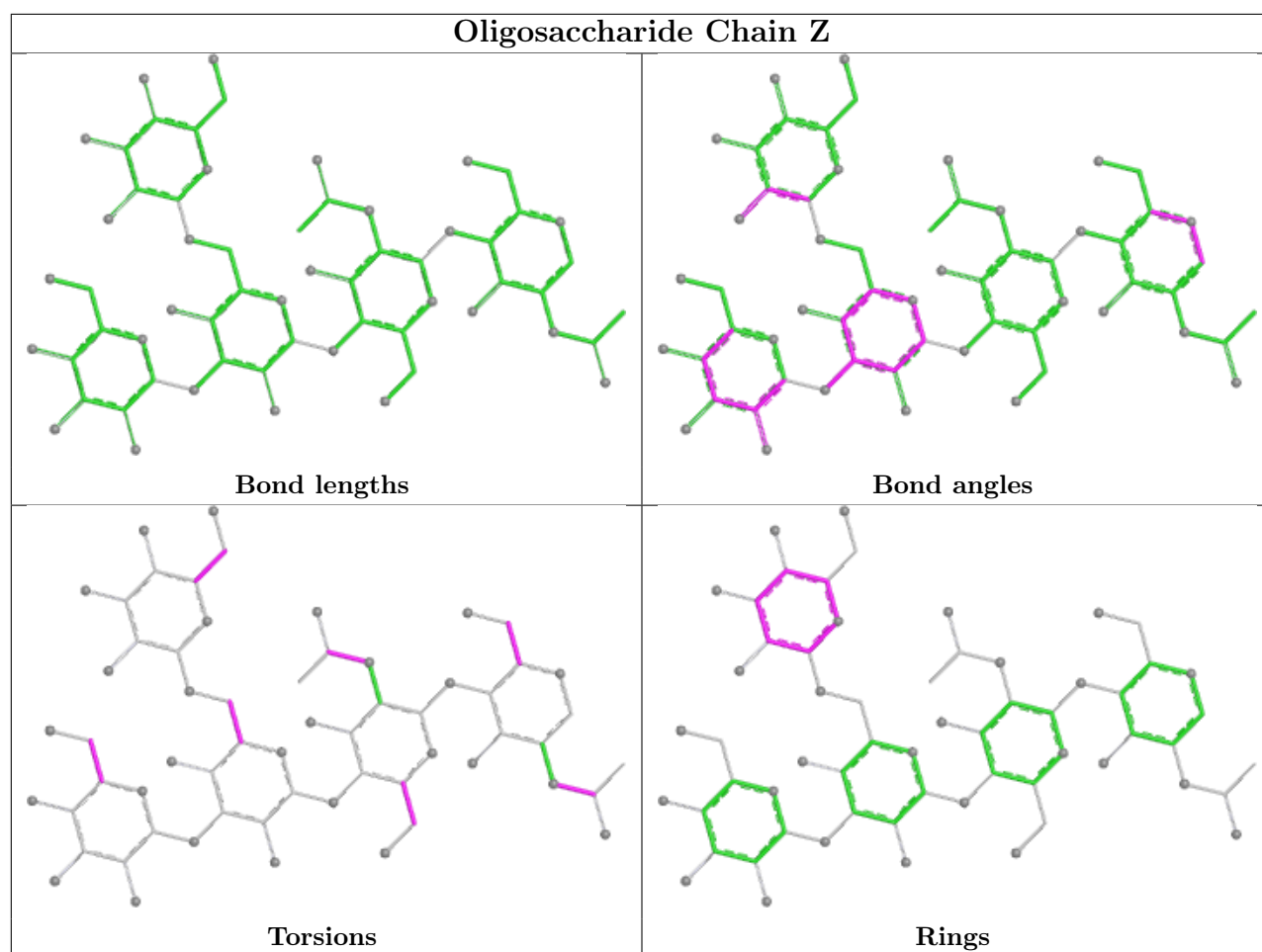


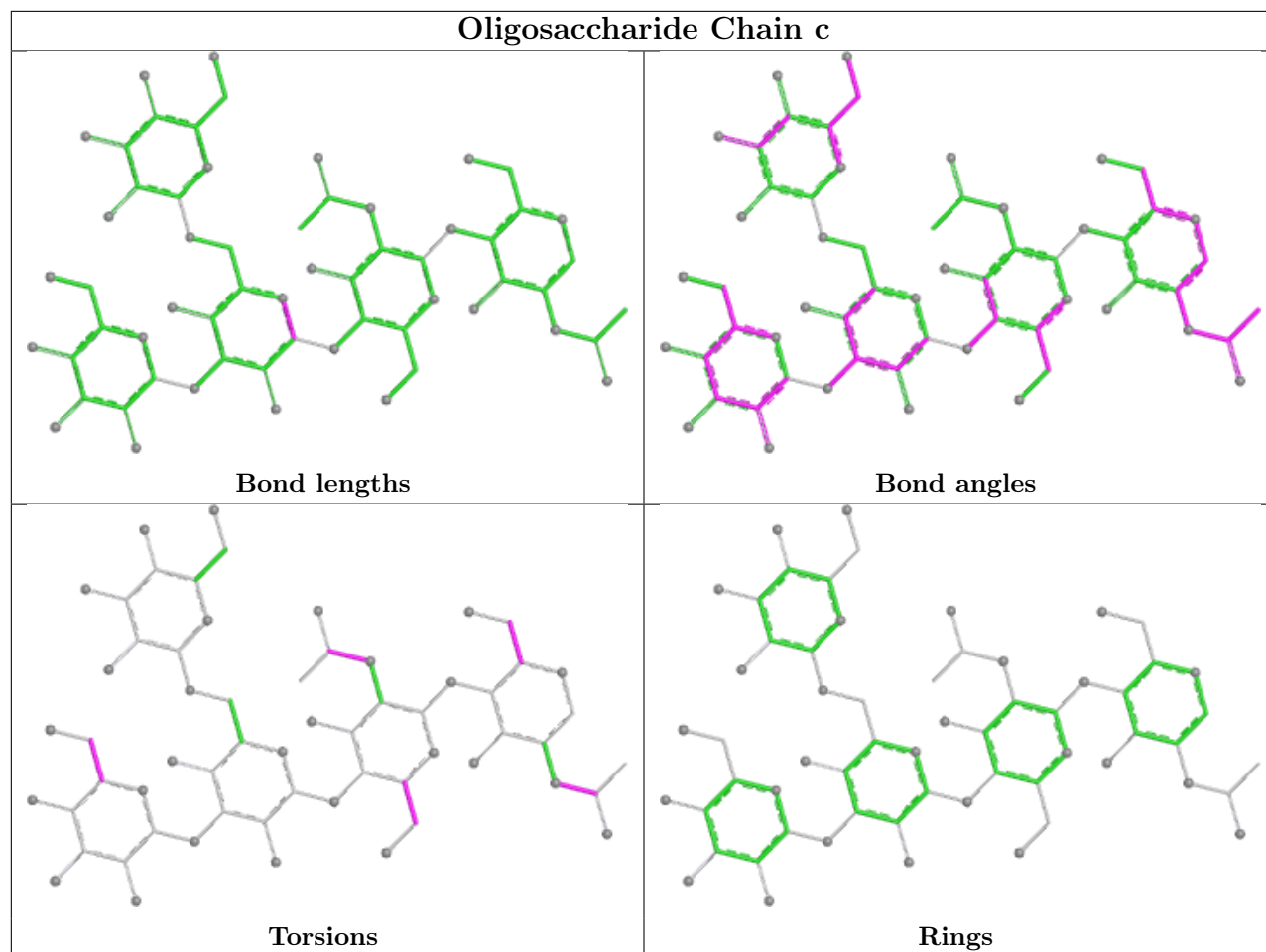


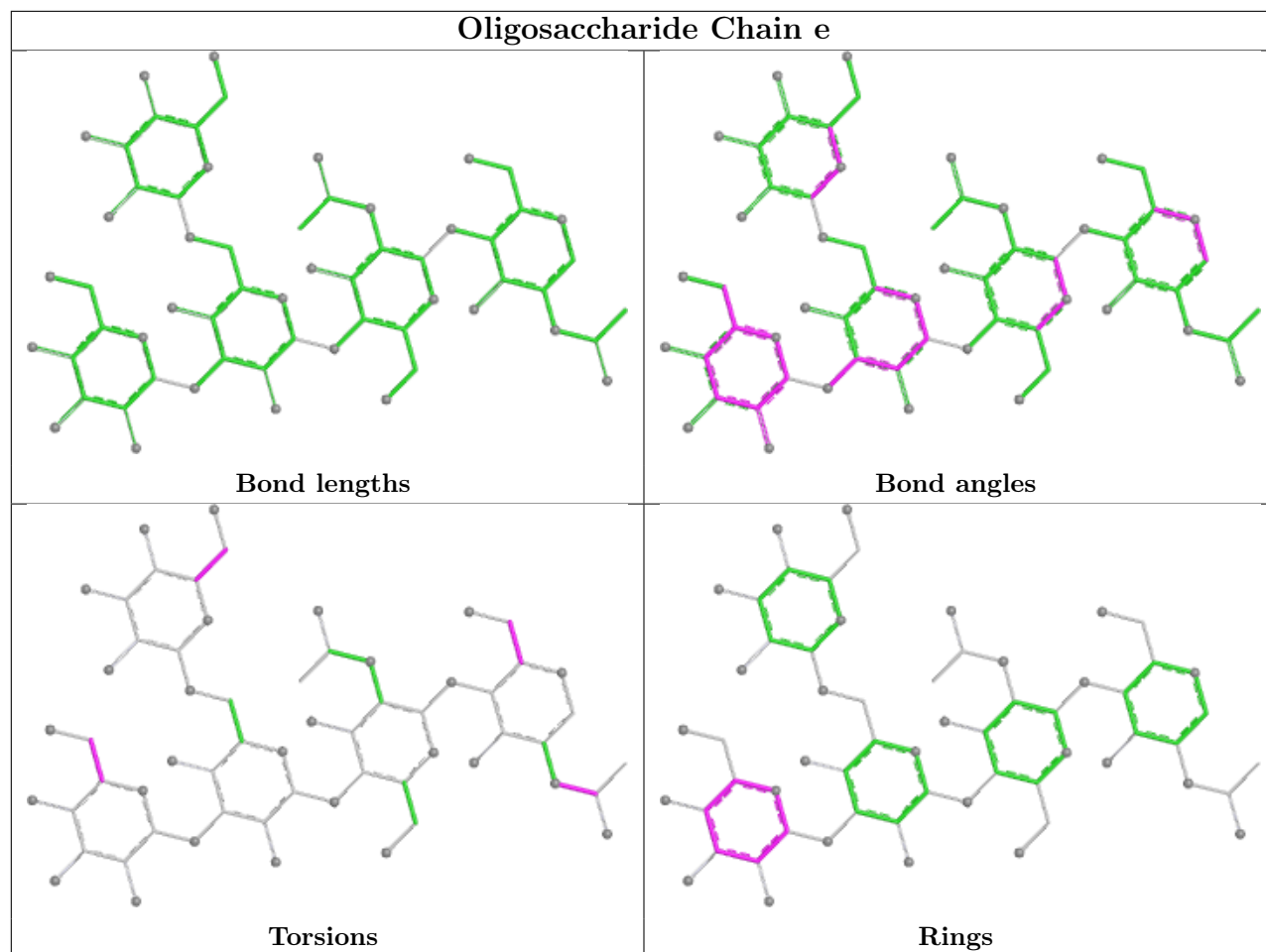


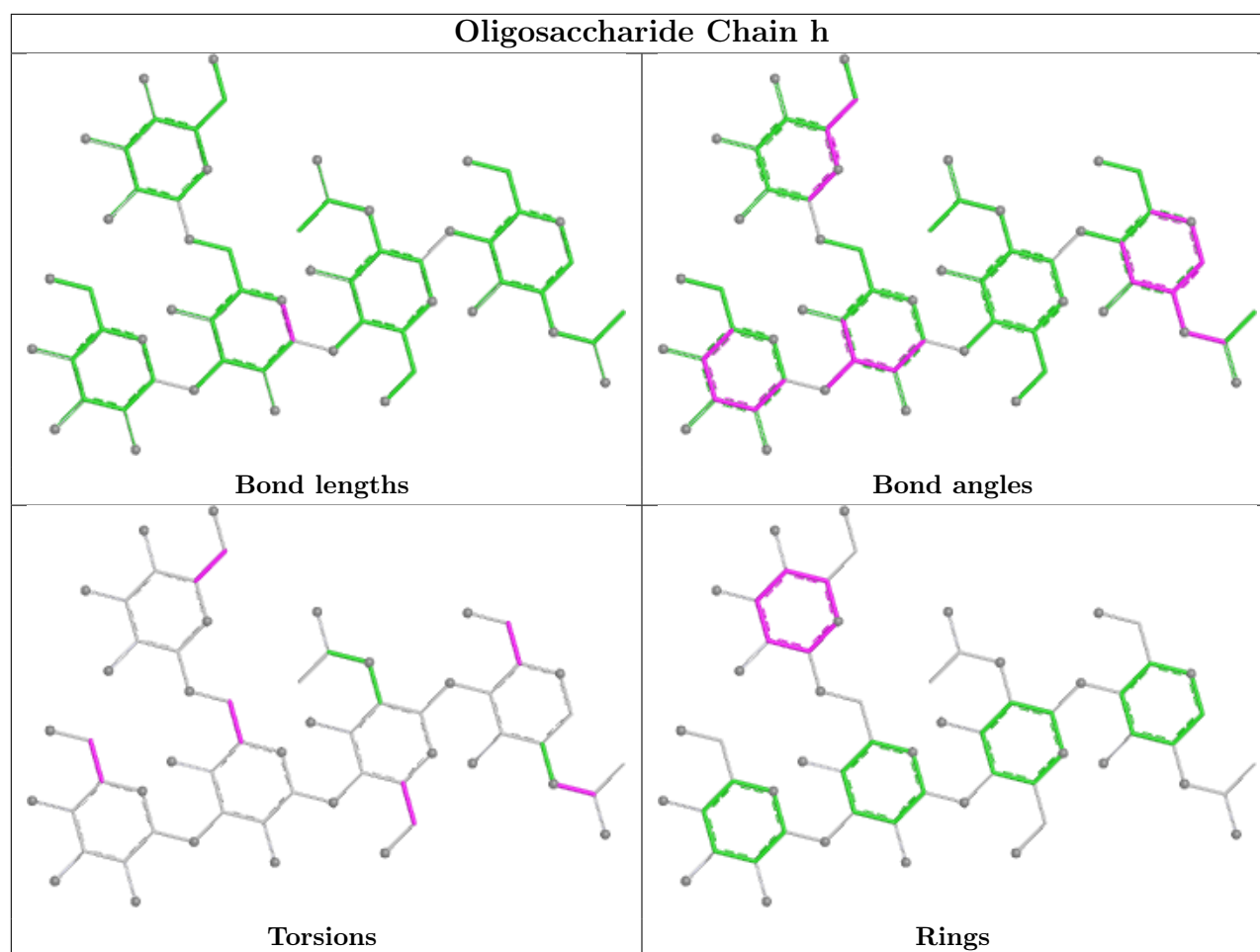












5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	M	331	1	14,14,15	0.41	0	17,19,21	1.57	1 (5%)
8	SO4	G	802	-	4,4,4	0.26	0	6,6,6	0.32	0
8	SO4	A	801	-	4,4,4	0.30	0	6,6,6	0.35	0
7	NAG	O	321	1	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
8	SO4	M	819	-	4,4,4	0.28	0	6,6,6	0.04	0
8	SO4	C	818	-	4,4,4	0.21	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	321	1	14,14,15	0.65	0	17,19,21	0.94	1 (5%)
8	SO4	E	820	-	4,4,4	0.31	0	6,6,6	0.14	0
8	SO4	I	809	-	4,4,4	0.28	0	6,6,6	0.09	0
7	NAG	K	322	1	14,14,15	0.85	0	17,19,21	1.35	2 (11%)
7	NAG	E	317	1	14,14,15	0.58	0	17,19,21	1.40	1 (5%)
8	SO4	K	803	-	4,4,4	0.27	0	6,6,6	0.17	0
8	SO4	I	821	-	4,4,4	0.26	0	6,6,6	0.14	0
7	NAG	K	331	1	14,14,15	0.54	0	17,19,21	1.63	3 (17%)
7	NAG	A	321	1	14,14,15	0.69	0	17,19,21	2.16	5 (29%)
8	SO4	C	814	-	4,4,4	0.27	0	6,6,6	0.37	0
8	SO4	I	804	-	4,4,4	0.26	0	6,6,6	0.27	0
8	SO4	M	811	-	4,4,4	0.29	0	6,6,6	0.28	0
8	SO4	A	805	-	4,4,4	0.23	0	6,6,6	0.11	0
8	SO4	G	808	-	4,4,4	0.25	0	6,6,6	0.30	0
7	NAG	I	321	1	14,14,15	0.72	1 (7%)	17,19,21	1.08	0
8	SO4	E	815	-	4,4,4	0.28	0	6,6,6	0.61	0
8	SO4	K	810	-	4,4,4	0.27	0	6,6,6	0.14	0
8	SO4	A	813	-	4,4,4	0.21	0	6,6,6	0.46	0
8	SO4	E	807	-	4,4,4	0.23	0	6,6,6	0.17	0
8	SO4	G	816	-	4,4,4	0.25	0	6,6,6	0.58	0
8	SO4	O	812	-	4,4,4	0.31	0	6,6,6	0.16	0
7	NAG	C	316	1	14,14,15	0.43	0	17,19,21	1.15	1 (5%)
8	SO4	C	806	-	4,4,4	0.24	0	6,6,6	0.29	0
7	NAG	A	317	1	14,14,15	0.48	0	17,19,21	1.69	2 (11%)
7	NAG	G	321	1	14,14,15	0.69	0	17,19,21	1.23	2 (11%)
8	SO4	G	817	-	4,4,4	0.22	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	322	1	-	5/6/23/26	0/1/1/1
7	NAG	E	317	1	-	4/6/23/26	0/1/1/1
7	NAG	M	331	1	-	4/6/23/26	0/1/1/1
7	NAG	I	321	1	-	2/6/23/26	0/1/1/1
7	NAG	O	321	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	K	331	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	321	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	317	1	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	A	321	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	G	321	1	-	5/6/23/26	0/1/1/1
7	NAG	C	316	1	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	321	NAG	C1-C2	2.17	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	321	NAG	C1-O5-C5	6.60	121.03	112.19
7	M	331	NAG	C1-O5-C5	5.85	120.02	112.19
7	A	317	NAG	C1-O5-C5	5.32	119.32	112.19
7	E	317	NAG	C1-O5-C5	3.82	117.30	112.19
7	K	331	NAG	C1-O5-C5	3.76	117.23	112.19
7	K	322	NAG	C2-N2-C7	3.42	127.48	122.90
7	K	331	NAG	C4-C3-C2	2.99	115.40	111.02
7	G	321	NAG	C3-C4-C5	2.99	115.66	110.23
7	K	322	NAG	C4-C3-C2	2.78	115.09	111.02
7	A	317	NAG	C3-C4-C5	2.73	115.19	110.23
7	K	331	NAG	C3-C4-C5	2.66	115.05	110.23
7	A	321	NAG	C1-C2-N2	2.63	114.57	110.43
7	C	316	NAG	C1-O5-C5	2.61	115.69	112.19
7	O	321	NAG	C4-C3-C2	2.47	114.63	111.02
7	A	321	NAG	C8-C7-N2	2.42	120.12	116.12
7	C	321	NAG	C2-N2-C7	2.38	126.09	122.90
7	G	321	NAG	C4-C3-C2	2.32	114.42	111.02
7	A	321	NAG	C4-C3-C2	-2.31	107.63	111.02
7	A	321	NAG	C2-N2-C7	2.06	125.66	122.90

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	317	NAG	C1
7	A	321	NAG	C1
7	C	316	NAG	C1
7	C	321	NAG	C1

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Mol	Chain	Res	Type	Atom
7	K	331	NAG	C1
7	O	321	NAG	C1

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	321	NAG	C8-C7-N2-C2
7	A	321	NAG	O7-C7-N2-C2
7	C	316	NAG	C8-C7-N2-C2
7	C	316	NAG	O7-C7-N2-C2
7	C	321	NAG	C8-C7-N2-C2
7	C	321	NAG	O7-C7-N2-C2
7	E	317	NAG	C8-C7-N2-C2
7	E	317	NAG	O7-C7-N2-C2
7	G	321	NAG	C3-C2-N2-C7
7	G	321	NAG	C8-C7-N2-C2
7	G	321	NAG	O7-C7-N2-C2
7	I	321	NAG	C8-C7-N2-C2
7	I	321	NAG	O7-C7-N2-C2
7	K	322	NAG	C3-C2-N2-C7
7	K	322	NAG	C8-C7-N2-C2
7	K	322	NAG	O7-C7-N2-C2
7	M	331	NAG	C8-C7-N2-C2
7	M	331	NAG	O7-C7-N2-C2
7	O	321	NAG	C8-C7-N2-C2
7	O	321	NAG	O7-C7-N2-C2
7	A	317	NAG	C8-C7-N2-C2
7	A	317	NAG	O7-C7-N2-C2
7	C	321	NAG	C4-C5-C6-O6
7	A	321	NAG	O5-C5-C6-O6
7	C	316	NAG	O5-C5-C6-O6
7	G	321	NAG	C4-C5-C6-O6
7	K	322	NAG	C4-C5-C6-O6
7	E	317	NAG	O5-C5-C6-O6
7	C	321	NAG	O5-C5-C6-O6
7	M	331	NAG	O5-C5-C6-O6
7	A	321	NAG	C4-C5-C6-O6
7	G	321	NAG	O5-C5-C6-O6
7	E	317	NAG	C4-C5-C6-O6
7	C	316	NAG	C4-C5-C6-O6
7	M	331	NAG	C4-C5-C6-O6
7	K	322	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	317	NAG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801	SO4	1	0
8	C	818	SO4	1	0
8	K	803	SO4	1	0
8	I	804	SO4	1	0
8	M	811	SO4	1	0
8	K	810	SO4	2	0
8	G	817	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/313 (85%)	1.58	68 (25%) 1 1	45, 57, 69, 98	0
1	C	259/313 (82%)	1.41	56 (21%) 2 2	48, 58, 66, 76	0
1	E	262/313 (83%)	1.38	61 (23%) 2 2	46, 56, 64, 72	0
1	G	258/313 (82%)	1.36	45 (17%) 4 3	46, 57, 66, 69	0
1	I	264/313 (84%)	1.43	55 (20%) 2 2	44, 58, 69, 89	0
1	K	257/313 (82%)	1.52	63 (24%) 2 1	45, 58, 67, 78	0
1	M	263/313 (84%)	1.47	56 (21%) 2 2	43, 57, 66, 83	0
1	O	258/313 (82%)	1.49	62 (24%) 2 1	47, 58, 68, 87	0
2	B	10/13 (76%)	1.86	2 (20%) 3 2	53, 60, 69, 71	0
2	D	10/13 (76%)	1.59	4 (40%) 1 0	50, 57, 64, 66	0
2	F	10/13 (76%)	2.13	4 (40%) 1 0	51, 63, 71, 71	0
2	H	10/13 (76%)	1.54	2 (20%) 3 2	52, 56, 65, 69	0
2	J	10/13 (76%)	1.62	2 (20%) 3 2	47, 54, 64, 70	0
2	L	10/13 (76%)	1.97	3 (30%) 1 1	50, 56, 72, 75	0
2	N	10/13 (76%)	1.93	3 (30%) 1 1	49, 55, 66, 71	0
2	P	10/13 (76%)	1.86	4 (40%) 1 0	52, 58, 72, 74	0
All	All	2169/2608 (83%)	1.47	490 (22%) 2 2	43, 57, 67, 98	0

All (490) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	274	PRO	7.5
1	E	231	PRO	6.5
1	A	278	VAL	6.4
1	G	202	THR	6.3
1	G	208	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
2	F	512	SER	5.9
1	K	230	GLU	5.7
1	A	138	PRO	5.5
1	O	276	LEU	5.4
1	O	233	ASN	5.4
1	O	231	PRO	5.4
1	K	208	GLU	5.3
1	A	279	GLN	5.3
1	M	61	LEU	5.3
1	I	85	VAL	5.3
1	I	61	LEU	5.2
1	K	203	HIS	5.2
1	C	61	LEU	5.1
1	G	102	ASP	5.1
1	I	33	GLU	5.0
1	M	108	GLY	5.0
1	M	90	SER	4.9
1	C	80	ASN	4.9
1	K	231	PRO	4.8
2	B	512	SER	4.8
1	A	90	SER	4.8
1	O	208	GLU	4.7
1	K	207	SER	4.7
1	A	231	PRO	4.7
2	L	502	SER	4.7
2	J	513	LYS	4.7
1	I	275	ASP	4.6
1	M	102	ASP	4.5
1	K	229	HIS	4.5
1	K	102	ASP	4.5
1	A	131	GLN	4.4
1	G	132	GLU	4.4
2	P	502	SER	4.4
1	A	81	SER	4.3
1	O	204	GLY	4.3
1	I	138	PRO	4.3
1	I	103	MET	4.2
1	G	107	ARG	4.2
1	O	202	THR	4.2
1	M	276	LEU	4.2
1	C	230	GLU	4.1
1	M	109	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	501	LYS	4.0
1	A	208	GLU	4.0
1	A	199	GLY	4.0
1	E	106	GLU	4.0
1	A	276	LEU	4.0
1	G	110	HIS	4.0
1	I	273	HIS	4.0
1	C	202	THR	4.0
1	M	107	ARG	3.9
1	O	61	LEU	3.9
1	K	202	THR	3.9
1	E	61	LEU	3.9
1	M	1	LEU	3.9
1	A	259	ASN	3.9
1	K	233	ASN	3.9
1	K	111	GLN	3.8
1	M	106	GLU	3.8
1	C	101	SER	3.8
1	K	260	HIS	3.8
1	A	270	GLY	3.8
1	A	236	TYR	3.8
1	C	139	LYS	3.8
2	L	501	LYS	3.8
1	G	61	LEU	3.8
2	D	501	LYS	3.8
1	I	137	ARG	3.8
1	O	274	PRO	3.8
1	G	234	GLN	3.7
1	E	131	GLN	3.7
1	C	102	ASP	3.7
1	A	260	HIS	3.6
1	K	276	LEU	3.6
1	M	232	LYS	3.6
1	A	229	HIS	3.6
1	C	193	GLN	3.6
1	A	61	LEU	3.6
1	A	79	GLY	3.6
1	I	84	ALA	3.6
1	I	81	SER	3.6
1	I	267	THR	3.6
1	M	19	LEU	3.6
1	G	229	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	82	GLY	3.5
1	I	209	GLU	3.5
1	A	102	ASP	3.5
1	I	108	GLY	3.5
1	O	270	GLY	3.5
1	C	207	SER	3.5
1	I	80	ASN	3.5
1	G	204	GLY	3.5
1	A	206	SER	3.5
2	L	512	SER	3.5
1	K	108	GLY	3.5
1	C	227	GLY	3.4
1	A	202	THR	3.4
1	K	266	CYS	3.4
1	A	80	ASN	3.4
1	C	109	ARG	3.4
1	K	269	SER	3.4
1	O	267	THR	3.4
1	C	138	PRO	3.4
1	K	61	LEU	3.4
1	G	140	ASP	3.4
1	I	110	HIS	3.4
1	A	234	GLN	3.3
1	K	204	GLY	3.3
1	A	103	MET	3.3
1	O	265	CYS	3.3
1	M	70	VAL	3.3
1	E	208	GLU	3.3
1	M	91	ARG	3.3
1	M	111	GLN	3.3
1	C	77	ASN	3.3
1	I	102	ASP	3.3
1	E	102	ASP	3.3
1	A	264	SER	3.3
1	K	193	GLN	3.3
1	O	77	ASN	3.3
1	I	83	ARG	3.2
1	O	275	ASP	3.2
2	B	501	LYS	3.2
1	M	110	HIS	3.2
1	O	273	HIS	3.2
1	K	234	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	3.2
1	A	272	ASN	3.2
1	E	123	LEU	3.2
1	E	108	GLY	3.2
1	O	229	HIS	3.2
1	C	108	GLY	3.2
1	G	207	SER	3.2
2	F	511	SER	3.2
1	O	92	TYR	3.2
1	I	272	ASN	3.1
1	A	273	HIS	3.1
1	C	274	PRO	3.1
2	N	502	SER	3.1
1	K	232	LYS	3.1
1	O	102	ASP	3.1
1	O	106	GLU	3.1
1	O	271	CYS	3.1
2	P	501	LYS	3.1
1	A	137	ARG	3.1
1	I	107	ARG	3.1
1	I	172	ASN	3.1
1	A	274	PRO	3.1
1	C	103	MET	3.1
1	O	130	ILE	3.0
1	K	265	CYS	3.0
1	C	206	SER	3.0
1	I	19	LEU	3.0
1	C	208	GLU	3.0
1	E	230	GLU	3.0
1	C	231	PRO	3.0
1	A	232	LYS	3.0
1	A	266	CYS	3.0
1	K	48	SER	3.0
1	E	229	HIS	3.0
1	G	106	GLU	3.0
1	M	103	MET	3.0
1	C	65	SER	3.0
1	E	47	HIS	3.0
1	G	101	SER	3.0
1	M	47	HIS	3.0
1	O	230	GLU	3.0
1	K	268	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	146	GLY	3.0
1	C	211	PHE	3.0
1	I	70	VAL	3.0
1	E	34	GLU	2.9
1	G	230	GLU	2.9
1	I	112	SER	2.9
1	K	259	ASN	2.9
1	O	210	THR	2.9
1	G	247	CYS	2.9
1	O	195	TYR	2.9
1	E	79	GLY	2.9
1	C	209	GLU	2.9
1	I	233	ASN	2.9
1	K	92	TYR	2.9
1	K	236	TYR	2.9
1	A	203	HIS	2.9
1	C	203	HIS	2.9
1	G	209	GLU	2.9
1	K	110	HIS	2.9
1	K	130	ILE	2.9
1	E	278	VAL	2.9
1	G	66	LEU	2.9
1	E	90	SER	2.8
1	M	214	ASP	2.8
1	M	92	TYR	2.8
2	F	513	LYS	2.8
1	K	210	THR	2.8
1	M	208	GLU	2.8
1	I	118	PRO	2.8
1	G	111	GLN	2.8
1	M	101	SER	2.8
1	E	242	ALA	2.8
1	I	92	TYR	2.8
1	E	107	ARG	2.8
1	A	213	ILE	2.8
1	K	242	ALA	2.8
1	E	89	ARG	2.8
1	G	78	GLN	2.7
1	A	235	SER	2.7
1	K	112	SER	2.7
1	C	226	THR	2.7
1	C	262	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	18	ALA	2.7
1	M	149	TYR	2.7
1	E	232	LYS	2.7
1	K	103	MET	2.7
2	D	502	SER	2.7
1	G	203	HIS	2.7
1	C	210	THR	2.7
1	O	263	VAL	2.7
1	E	234	GLN	2.7
2	N	513	LYS	2.7
1	C	146	GLY	2.7
1	M	35	GLY	2.7
1	O	49	GLU	2.7
1	O	192	ARG	2.7
1	K	262	ASP	2.7
2	J	501	LYS	2.7
1	O	234	GLN	2.7
1	C	130	ILE	2.7
1	G	172	ASN	2.7
1	M	209	GLU	2.7
1	M	69	VAL	2.7
1	M	277	ASP	2.7
1	I	268	LYS	2.6
1	C	92	TYR	2.6
1	A	237	MET	2.6
1	I	158	GLY	2.6
1	M	81	SER	2.6
1	O	235	SER	2.6
1	K	200	GLN	2.6
1	G	276	LEU	2.6
1	E	203	HIS	2.6
1	E	158	GLY	2.6
1	I	79	GLY	2.6
1	E	233	ASN	2.6
1	E	48	SER	2.6
2	N	512	SER	2.6
1	C	275	ASP	2.6
1	E	252	LEU	2.6
1	K	252	LEU	2.6
1	E	92	TYR	2.6
1	C	270	GLY	2.6
1	A	233	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	78	GLN	2.6
1	E	248	GLN	2.6
1	M	193	GLN	2.6
1	O	107	ARG	2.5
1	C	229	HIS	2.5
1	I	203	HIS	2.5
1	I	208	GLU	2.5
1	A	82	GLY	2.5
1	O	199	GLY	2.5
1	O	41	VAL	2.5
1	K	171	CYS	2.5
1	A	46	THR	2.5
1	M	210	THR	2.5
1	I	213	ILE	2.5
1	O	268	LYS	2.5
1	C	236	TYR	2.5
1	A	191	GLY	2.5
1	G	29	VAL	2.5
1	C	234	GLN	2.5
1	O	65	SER	2.5
1	O	269	SER	2.5
1	O	232	LYS	2.5
1	A	107	ARG	2.5
1	K	239	ARG	2.5
1	O	66	LEU	2.5
1	E	49	GLU	2.5
1	G	211	PHE	2.5
1	A	6	CYS	2.5
1	A	176	CYS	2.5
1	A	247	CYS	2.5
1	A	53	ARG	2.5
1	M	89	ARG	2.5
1	G	240	GLY	2.5
1	K	270	GLY	2.5
1	E	125	VAL	2.5
2	P	513	LYS	2.4
1	C	239	ARG	2.4
1	O	220	ASN	2.4
1	K	66	LEU	2.4
1	G	205	CYS	2.4
1	E	140	ASP	2.4
1	O	203	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	94	GLU	2.4
1	C	198	LYS	2.4
1	E	67	THR	2.4
1	I	75	LEU	2.4
1	M	96	ILE	2.4
1	O	213	ILE	2.4
1	A	271	CYS	2.4
1	C	140	ASP	2.4
1	I	34	GLU	2.4
1	O	103	MET	2.4
1	G	158	GLY	2.4
1	E	149	TYR	2.4
1	E	30	ARG	2.4
1	A	177	ASN	2.4
1	E	129	TRP	2.4
1	O	247	CYS	2.4
1	K	274	PRO	2.4
1	C	111	GLN	2.4
1	M	14	VAL	2.4
1	C	63	ILE	2.4
1	E	66	LEU	2.4
1	M	27	THR	2.4
1	E	9	ASN	2.4
1	E	65	SER	2.4
1	A	277	ASP	2.4
1	K	22	ASP	2.4
1	A	265	CYS	2.4
1	G	109	ARG	2.4
1	C	225	ALA	2.4
1	G	49	GLU	2.3
1	I	139	LYS	2.3
1	G	131	GLN	2.3
1	O	79	GLY	2.3
1	A	70	VAL	2.3
1	E	19	LEU	2.3
1	E	168	LEU	2.3
1	E	130	ILE	2.3
1	M	273	HIS	2.3
1	G	139	LYS	2.3
1	I	207	SER	2.3
1	I	214	ASP	2.3
1	G	231	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	91	ARG	2.3
1	E	20	GLY	2.3
1	M	271	CYS	2.3
1	E	23	LEU	2.3
1	E	223	LEU	2.3
1	O	211	PHE	2.3
1	O	242	ALA	2.3
1	A	226	THR	2.3
1	M	67	THR	2.3
1	M	236	TYR	2.3
1	K	237	MET	2.3
1	A	36	GLU	2.3
1	G	77	ASN	2.3
2	P	512	SER	2.3
1	E	91	ARG	2.3
1	A	125	VAL	2.3
1	K	205	CYS	2.3
1	M	12	CYS	2.3
1	C	273	HIS	2.3
1	M	8	THR	2.3
1	C	195	TYR	2.3
1	K	209	GLU	2.3
1	M	34	GLU	2.3
1	C	233	ASN	2.3
1	K	107	ARG	2.3
1	K	116	ARG	2.3
1	I	35	GLY	2.3
1	K	199	GLY	2.3
1	K	19	LEU	2.3
1	M	38	LEU	2.3
1	E	171	CYS	2.2
1	G	261	ILE	2.2
1	M	18	ALA	2.2
1	O	222	CYS	2.2
1	I	260	HIS	2.2
1	M	260	HIS	2.2
1	G	103	MET	2.2
1	I	149	TYR	2.2
1	C	259	ASN	2.2
1	E	157	ASN	2.2
1	A	140	ASP	2.2
1	K	235	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	126	VAL	2.2
1	A	211	PHE	2.2
1	I	68	GLU	2.2
1	E	25	ARG	2.2
1	O	272	ASN	2.2
1	C	204	GLY	2.2
1	K	206	SER	2.2
1	M	88	SER	2.2
1	C	106	GLU	2.2
1	I	94	GLU	2.2
1	O	218	PRO	2.2
1	A	111	GLN	2.2
1	A	22	ASP	2.2
1	A	66	LEU	2.2
1	G	19	LEU	2.2
1	G	35	GLY	2.2
1	K	158	GLY	2.2
1	K	223	LEU	2.2
2	D	511	SER	2.2
1	I	125	VAL	2.2
1	K	41	VAL	2.2
1	O	237	MET	2.2
1	E	143	HIS	2.2
1	C	243	THR	2.2
1	I	109	ARG	2.2
1	K	109	ARG	2.2
1	A	195	TYR	2.2
1	I	195	TYR	2.2
1	M	52	ASN	2.2
1	O	193	GLN	2.2
1	A	268	LYS	2.2
1	O	184	LEU	2.2
1	E	97	SER	2.2
1	A	47	HIS	2.2
1	A	130	ILE	2.2
1	G	119	GLU	2.1
1	I	106	GLU	2.1
1	O	209	GLU	2.1
1	G	194	CYS	2.1
1	O	236	TYR	2.1
1	M	22	ASP	2.1
1	A	269	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	235	SER	2.1
1	K	101	SER	2.1
2	H	502	SER	2.1
1	C	58	ARG	2.1
1	K	228	THR	2.1
1	C	131	GLN	2.1
1	I	271	CYS	2.1
1	K	247	CYS	2.1
1	O	131	GLN	2.1
1	M	158	GLY	2.1
1	G	28	ILE	2.1
1	M	203	HIS	2.1
1	O	260	HIS	2.1
1	G	69	VAL	2.1
2	F	503	ASP	2.1
1	G	206	SER	2.1
1	K	201	SER	2.1
1	O	48	SER	2.1
1	A	89	ARG	2.1
1	A	267	THR	2.1
1	O	26	THR	2.1
1	C	149	TYR	2.1
1	C	214	ASP	2.1
1	E	159	PHE	2.1
1	A	201	SER	2.1
2	D	512	SER	2.1
1	A	230	GLU	2.1
1	E	8	THR	2.1
1	E	173	THR	2.1
1	M	202	THR	2.1
1	O	114	GLN	2.1
1	I	55	LEU	2.1
1	K	272	ASN	2.1
1	C	110	HIS	2.1
1	M	152	GLY	2.1
1	O	47	HIS	2.1
1	K	63	ILE	2.1
1	M	125	VAL	2.1
1	A	275	ASP	2.0
1	E	13	ARG	2.0
1	E	53	ARG	2.0
1	I	44	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	129	TRP	2.0
1	G	26	THR	2.0
1	I	67	THR	2.0
1	M	31	LEU	2.0
1	O	111	GLN	2.0
1	E	172	ASN	2.0
1	E	220	ASN	2.0
1	O	259	ASN	2.0
1	I	146	GLY	2.0
1	O	181	ILE	2.0
1	E	6	CYS	2.0
1	G	12	CYS	2.0
1	I	266	CYS	2.0
1	O	194	CYS	2.0
1	C	44	SER	2.0
1	K	65	SER	2.0
1	M	75	LEU	2.0
1	E	110	HIS	2.0
1	C	186	ASN	2.0
1	E	77	ASN	2.0
1	A	41	VAL	2.0
1	M	25	ARG	2.0
1	K	195	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DLY	P	507	9/10	0.84	0.17	54,55,61,63	0
2	DLY	B	507	9/10	0.88	0.15	53,54,58,58	0
2	ALC	J	504	11/12	0.92	0.18	55,56,57,57	0
2	ALC	H	504	11/12	0.92	0.20	54,56,61,61	0
2	DLY	F	507	9/10	0.93	0.13	51,52,57,57	0
2	DSN	D	506	6/7	0.93	0.10	51,52,52,52	0
2	ALC	F	504	11/12	0.93	0.16	54,54,56,58	0
2	DSN	J	506	6/7	0.93	0.12	52,52,52,54	0
2	DLY	L	507	9/10	0.93	0.14	51,52,59,61	0
2	DSN	P	506	6/7	0.93	0.10	56,56,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DSN	F	506	6/7	0.93	0.14	49,50,50,50	0
2	ALC	D	504	11/12	0.94	0.15	53,54,55,56	0
2	ALC	N	504	11/12	0.94	0.16	55,56,57,58	0
2	DSN	N	506	6/7	0.94	0.13	51,51,52,53	0
2	DLY	N	507	9/10	0.94	0.17	47,50,50,51	0
2	DSN	B	506	6/7	0.94	0.09	52,54,54,54	0
2	DLY	D	507	9/10	0.94	0.16	51,52,53,53	0
2	ALC	B	504	11/12	0.95	0.15	56,57,58,60	0
2	DLY	J	507	9/10	0.95	0.15	49,50,50,51	0
2	ALC	L	504	11/12	0.96	0.14	60,61,63,63	0
2	DSN	L	506	6/7	0.96	0.09	53,54,54,55	0
2	ALC	P	504	11/12	0.96	0.18	59,60,61,63	0
2	DLY	H	507	9/10	0.96	0.13	50,50,51,51	0
2	DSN	H	506	6/7	0.96	0.09	48,50,50,50	0

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($\text{\AA}^2$)	Q<0.9
3	NAG	T	2	14/15	0.50	0.20	89,91,92,93	0
4	NAG	U	1	14/15	0.52	0.21	76,79,82,83	0
3	NAG	S	1	14/15	0.57	0.18	85,91,95,96	0
5	NAG	W	2	14/15	0.57	0.16	91,92,93,93	0
5	NAG	W	1	14/15	0.58	0.17	80,86,87,90	0
4	NAG	X	1	14/15	0.58	0.19	80,84,89,92	0
4	FUC	U	2	10/11	0.62	0.27	84,85,86,86	0
3	NAG	T	1	14/15	0.63	0.17	74,77,83,86	0
3	NAG	S	2	14/15	0.64	0.18	99,101,101,102	0
3	NAG	b	1	14/15	-	-	68,72,74,78	0
3	NAG	b	2	14/15	-	-	81,83,86,86	0
3	FUC	b	3	10/11	-	-	76,77,77,78	0
3	NAG	Q	2	14/15	0.64	0.17	83,84,86,86	0
4	FUC	X	2	10/11	0.66	0.22	94,95,96,96	0
6	MAN	Z	4	11/12	0.68	0.17	73,75,77,77	0
3	FUC	T	3	10/11	0.77	0.19	84,85,85,85	0
4	NAG	Y	1	14/15	0.79	0.14	58,61,67,71	0
4	FUC	V	2	10/11	0.79	0.20	71,73,74,75	0
3	FUC	S	3	10/11	0.80	0.16	96,97,97,98	0

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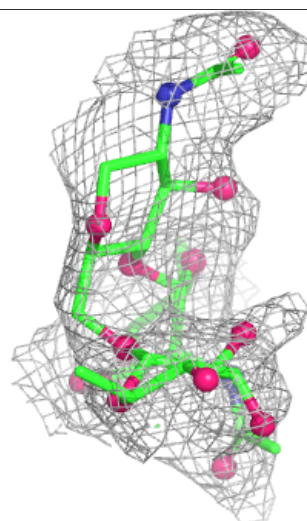
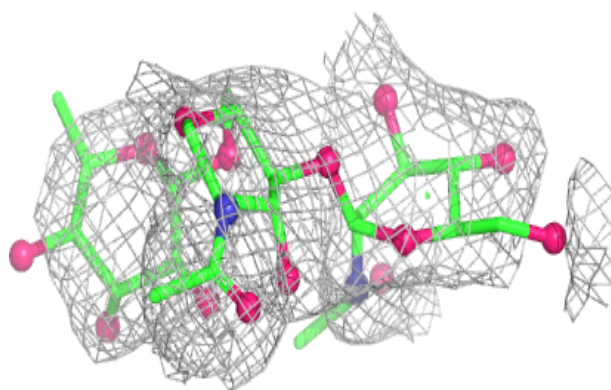
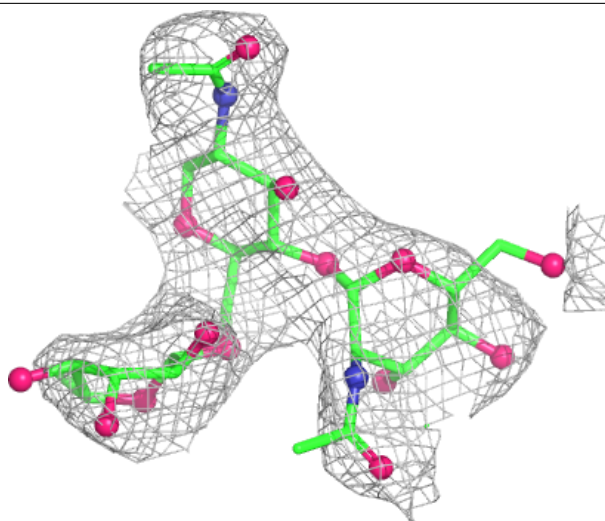
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FUC	R	2	10/11	0.83	0.15	71,72,73,73	0
3	NAG	Q	1	14/15	0.83	0.14	68,73,79,80	0
3	FUC	Q	3	10/11	0.85	0.16	81,82,82,83	0
4	NAG	a	1	14/15	-	-	76,79,81,82	0
4	FUC	a	2	10/11	-	-	83,84,84,84	0
4	NAG	d	1	14/15	-	-	57,59,61,64	0
4	FUC	d	2	10/11	-	-	66,68,69,69	0
4	NAG	g	1	14/15	-	-	63,65,67,70	0
4	FUC	g	2	10/11	-	-	71,72,73,73	0
6	NAG	Z	2	14/15	0.86	0.15	60,61,63,64	0
6	MAN	Z	5	11/12	0.86	0.14	67,68,71,72	0
5	NAG	f	1	14/15	-	-	82,86,88,92	0
5	NAG	f	2	14/15	-	-	95,96,98,99	0
4	NAG	R	1	14/15	0.87	0.12	62,65,66,68	0
6	NAG	Z	1	14/15	0.88	0.12	57,58,61,63	0
4	FUC	Y	2	10/11	0.88	0.14	73,75,76,76	0
6	BMA	Z	3	11/12	0.89	0.12	64,66,68,71	0
4	NAG	V	1	14/15	0.92	0.10	57,60,63,67	0
6	NAG	c	1	14/15	-	-	45,51,53,53	0
6	NAG	c	2	14/15	-	-	50,52,54,54	0
6	BMA	c	3	11/12	-	-	48,50,52,52	0
6	MAN	c	4	11/12	-	-	55,57,59,59	0
6	MAN	c	5	11/12	-	-	45,47,48,49	0
6	NAG	e	1	14/15	-	-	44,47,48,49	0
6	NAG	e	2	14/15	-	-	47,48,48,50	0
6	BMA	e	3	11/12	-	-	47,49,51,54	0
6	MAN	e	4	11/12	-	-	54,58,62,63	0
6	MAN	e	5	11/12	-	-	43,45,46,48	0
6	NAG	h	1	14/15	-	-	61,65,67,67	0
6	NAG	h	2	14/15	-	-	66,69,71,71	0
6	BMA	h	3	11/12	-	-	70,71,72,73	0
6	MAN	h	4	11/12	-	-	74,76,77,77	0
6	MAN	h	5	11/12	-	-	65,69,71,72	0

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

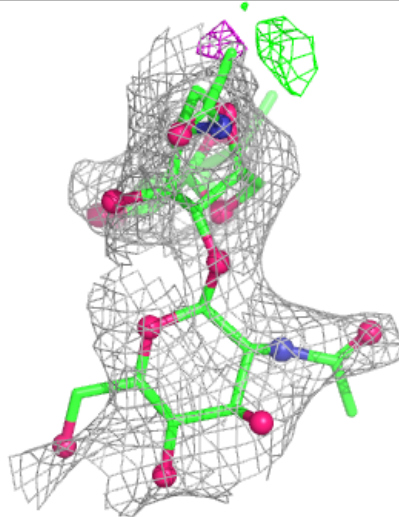
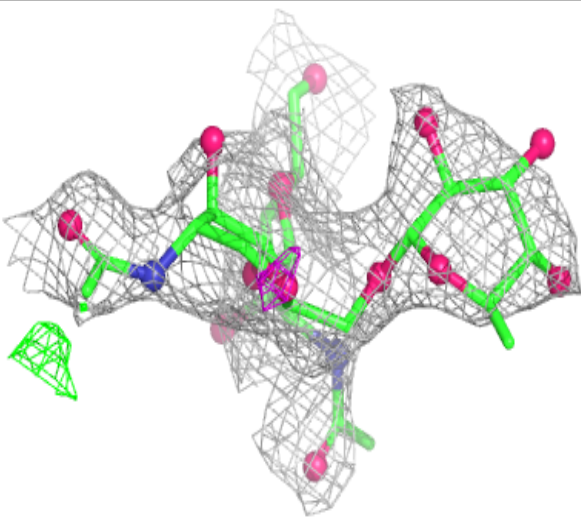
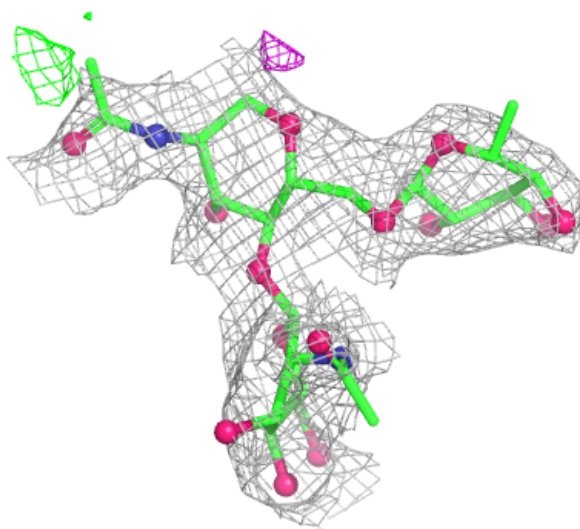
Electron density around Chain Q:

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



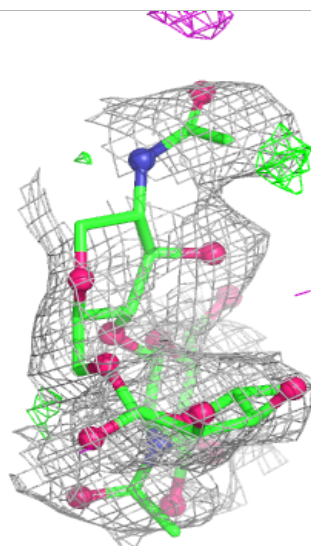
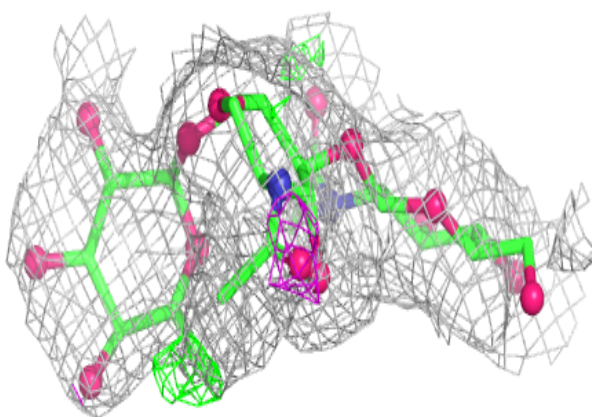
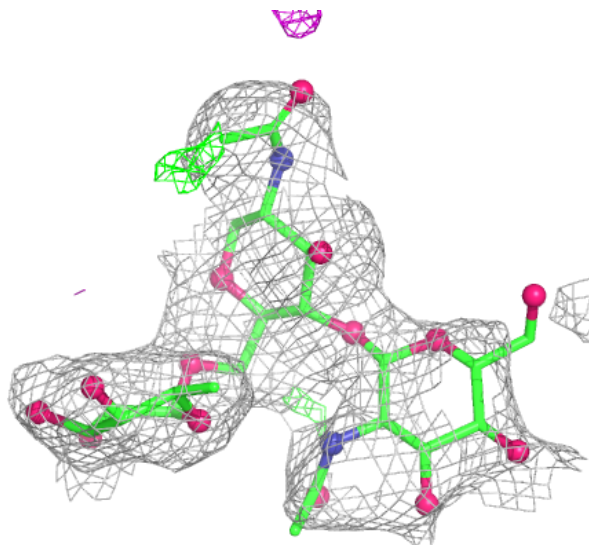
Electron density around Chain S:

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



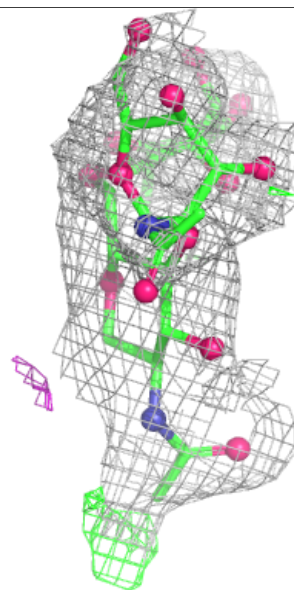
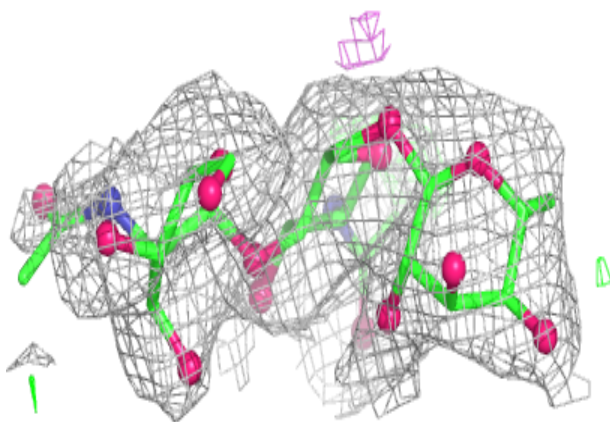
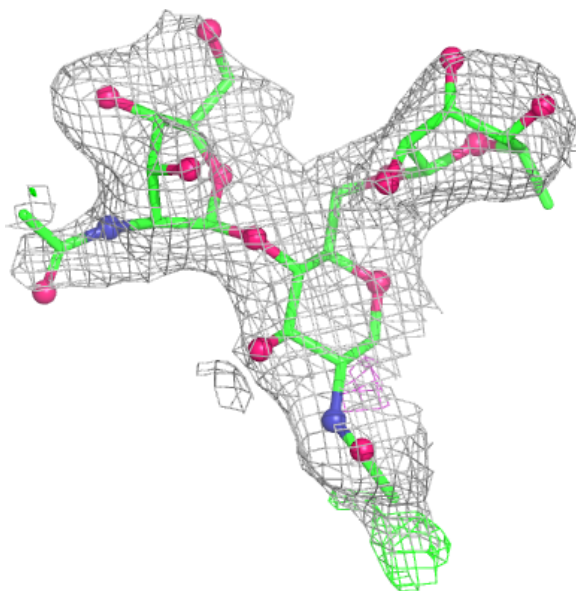
Electron density around Chain T:

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



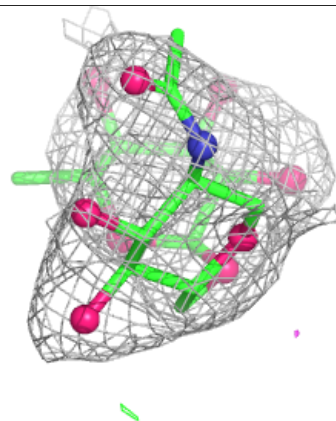
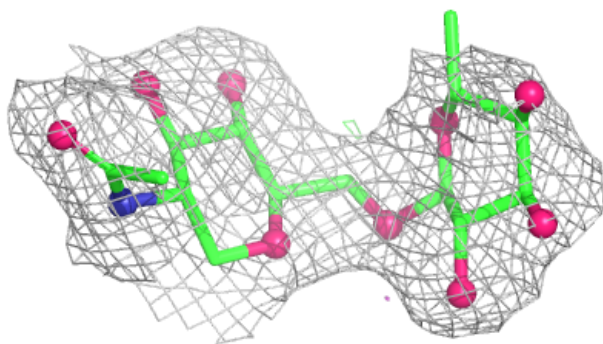
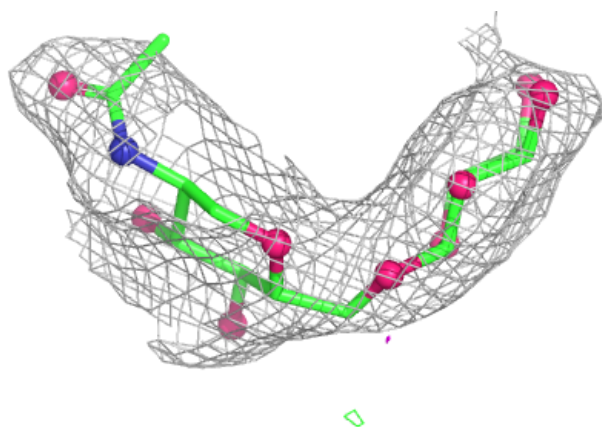
Electron density around Chain b:

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

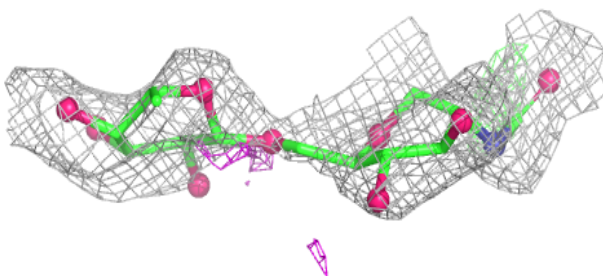
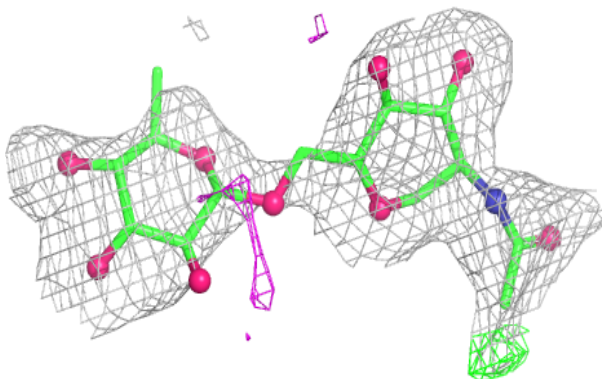


Electron density around Chain R:

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

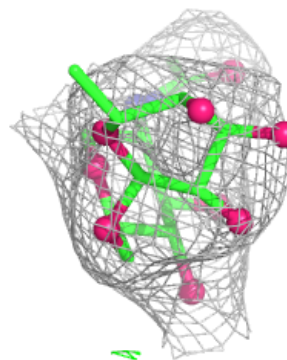
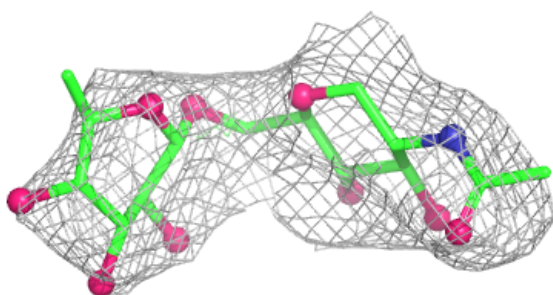
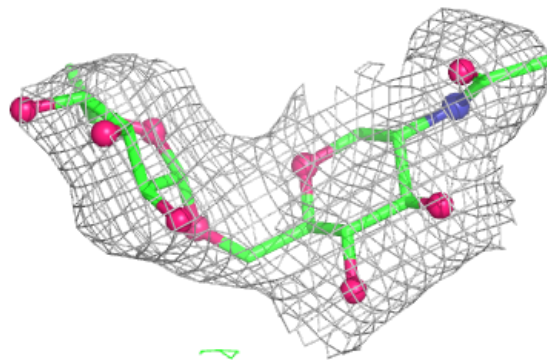
**Electron density around Chain U:**

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

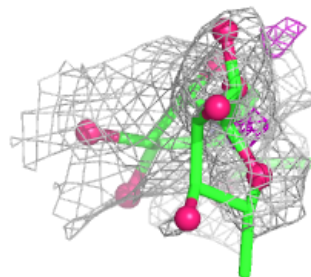
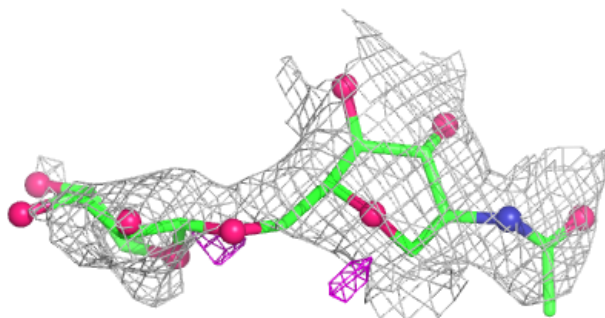
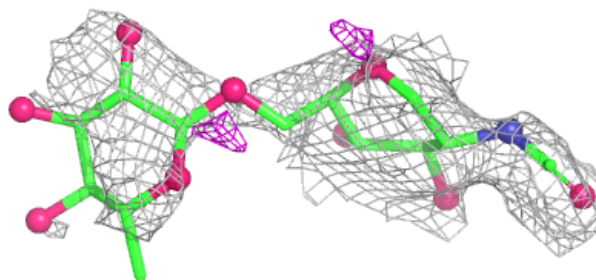


Electron density around Chain V:

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

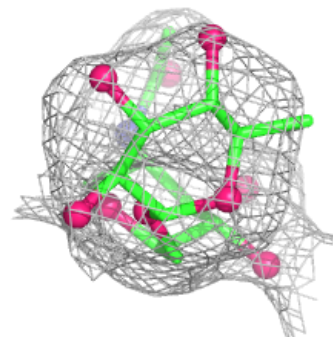
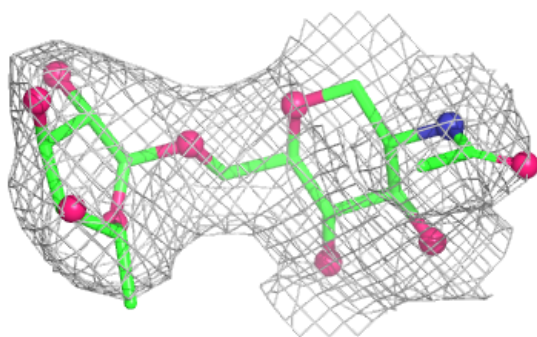
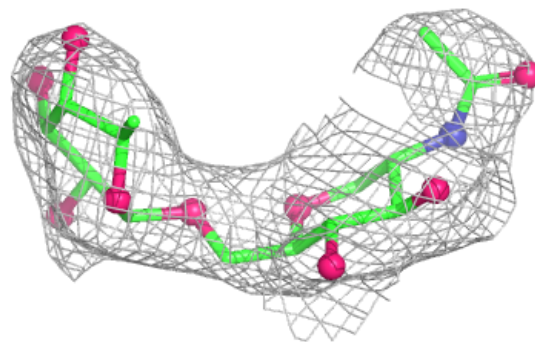
**Electron density around Chain X:**

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

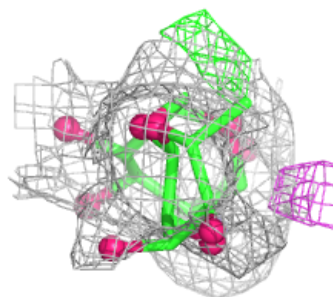
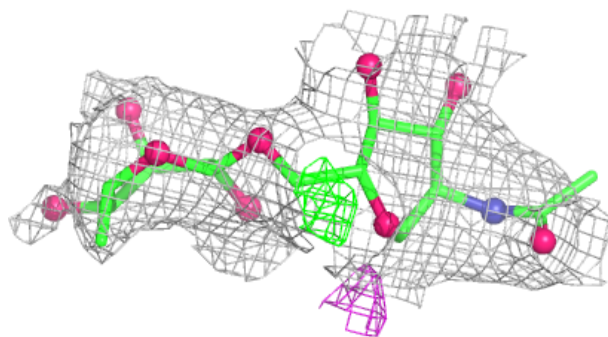
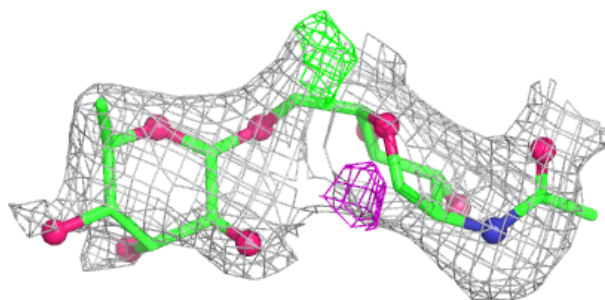


Electron density around Chain Y:

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

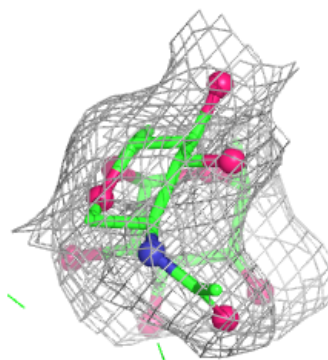
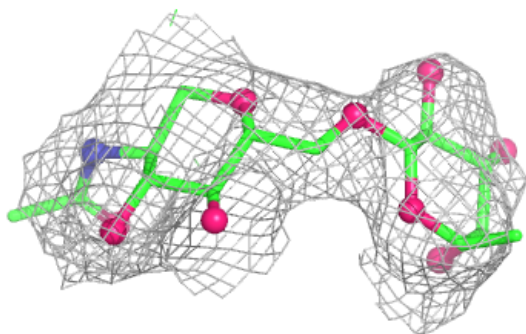
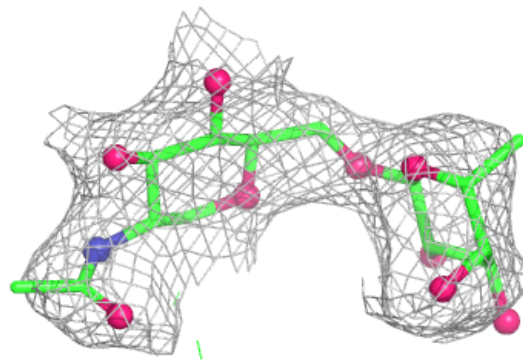
**Electron density around Chain a:**

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



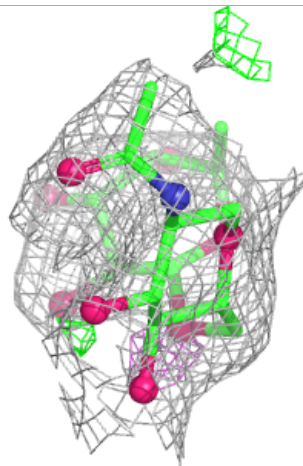
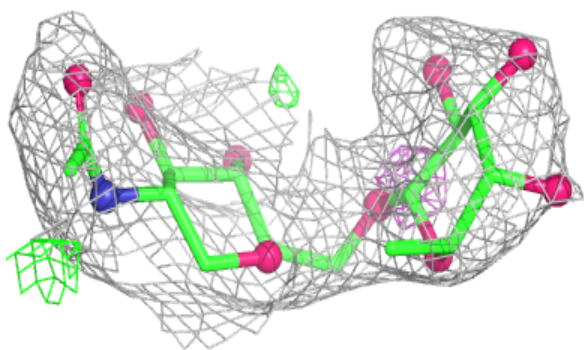
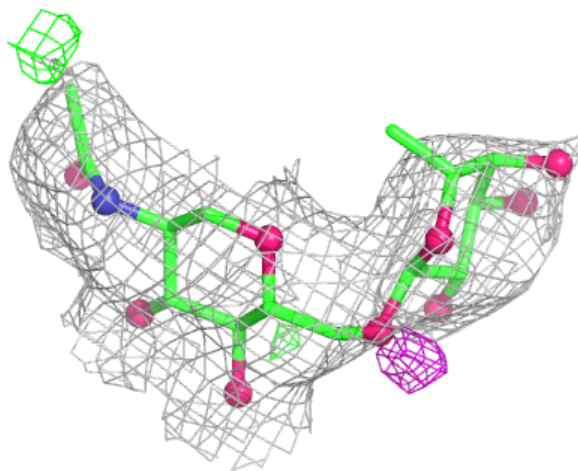
Electron density around Chain d:

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



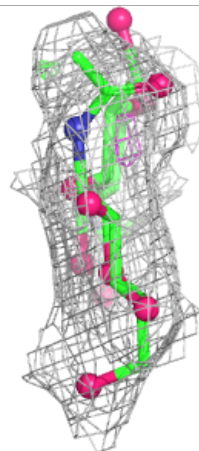
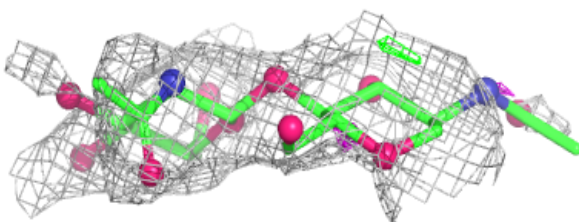
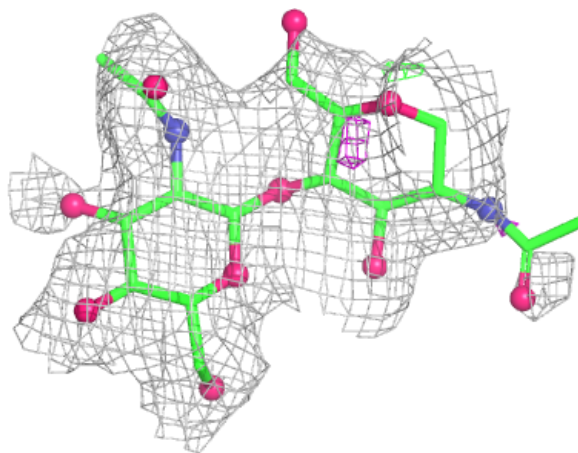
Electron density around Chain g:

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



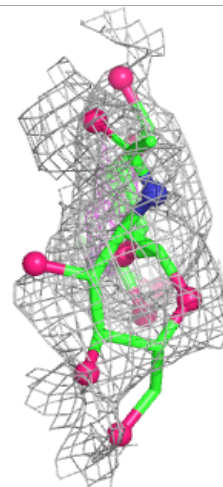
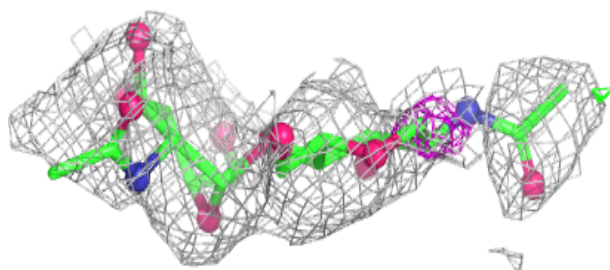
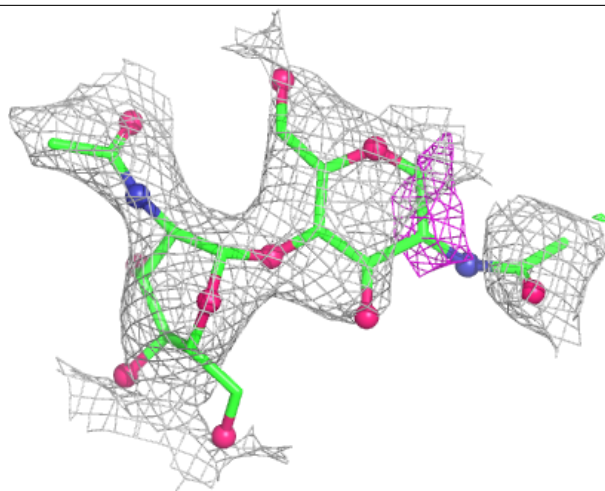
Electron density around Chain W:

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



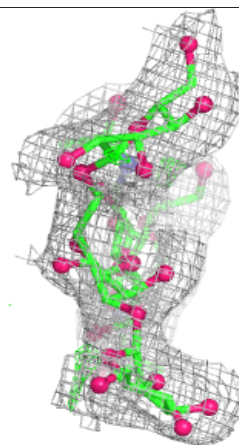
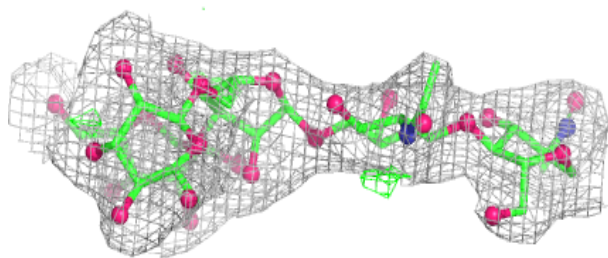
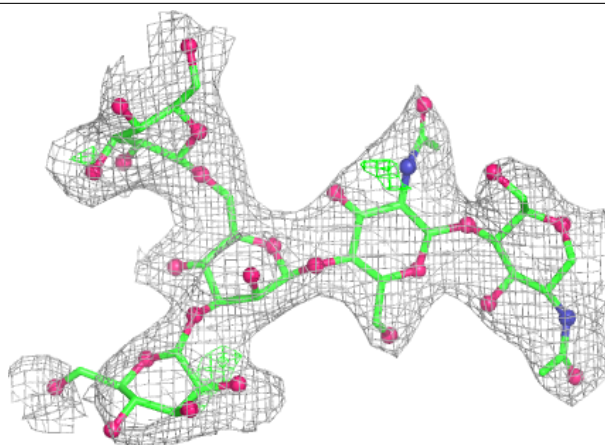
Electron density around Chain f:

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



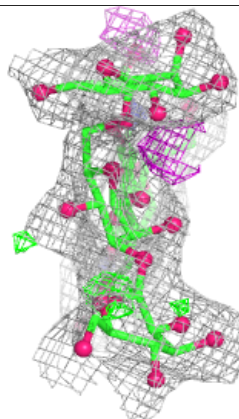
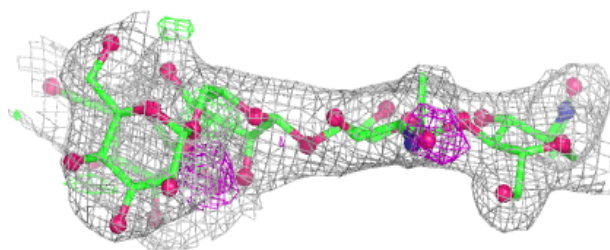
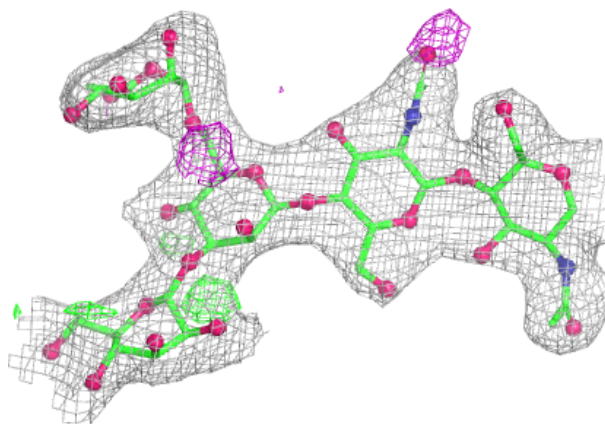
Electron density around Chain Z:

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



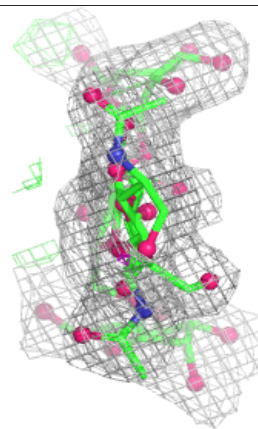
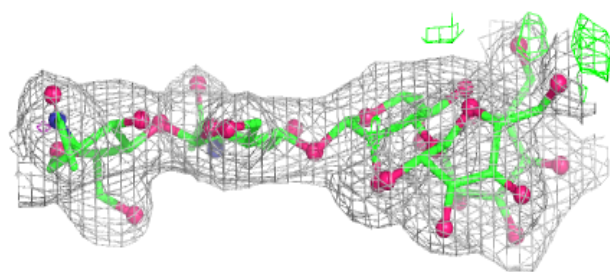
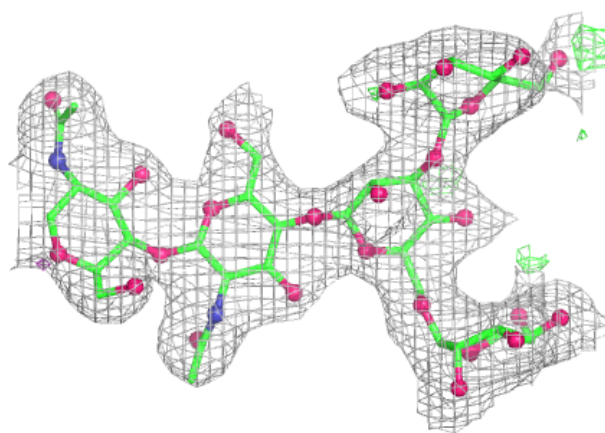
Electron density around Chain c:

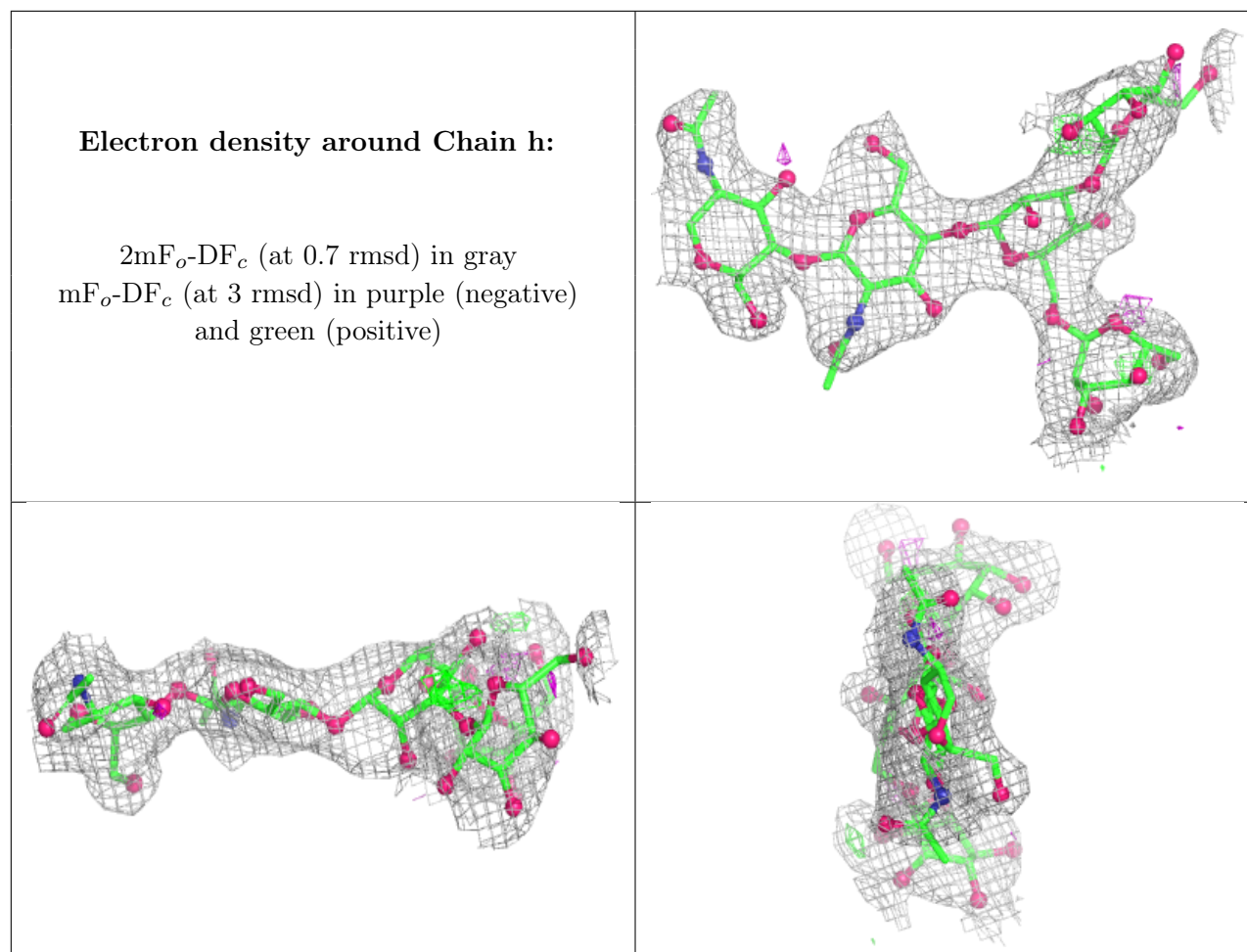
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain e:

$2mF_o - DF_c$ (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
7	NAG	A	321	14/15	0.40	0.21	75,78,80,80	0
7	NAG	K	331	14/15	0.40	0.23	84,86,88,88	0
7	NAG	K	322	14/15	0.57	0.18	76,79,80,81	0
7	NAG	G	321	14/15	0.57	0.21	76,80,82,83	0
7	NAG	I	321	14/15	0.63	0.18	76,79,80,80	0
7	NAG	C	316	14/15	0.65	0.16	77,80,84,84	0
7	NAG	E	317	14/15	0.65	0.15	72,75,80,80	0
7	NAG	A	317	14/15	0.67	0.18	78,82,85,85	0
7	NAG	C	321	14/15	0.71	0.16	78,82,83,84	0
7	NAG	O	321	14/15	0.71	0.17	78,82,82,83	0
7	NAG	M	331	14/15	0.74	0.14	72,75,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	A	805	5/5	0.85	0.19	132,132,133,133	0
8	SO4	C	806	5/5	0.86	0.16	79,80,81,81	0
8	SO4	E	807	5/5	0.89	0.21	125,125,125,125	0
8	SO4	E	820	5/5	0.89	0.22	86,87,87,87	0
8	SO4	C	814	5/5	0.90	0.15	65,67,68,69	0
8	SO4	K	810	5/5	0.90	0.13	84,85,86,86	0
8	SO4	O	812	5/5	0.90	0.17	79,79,80,80	0
8	SO4	A	801	5/5	0.91	0.10	70,70,72,72	0
8	SO4	C	818	5/5	0.92	0.15	75,75,76,77	0
8	SO4	I	821	5/5	0.92	0.22	71,72,72,73	0
8	SO4	G	816	5/5	0.93	0.11	61,62,63,63	0
8	SO4	M	819	5/5	0.93	0.20	79,79,80,80	0
8	SO4	A	813	5/5	0.93	0.10	64,66,66,67	0
8	SO4	E	815	5/5	0.94	0.10	56,57,58,58	0
8	SO4	I	804	5/5	0.94	0.11	58,58,59,60	0
8	SO4	G	802	5/5	0.94	0.09	56,57,58,58	0
8	SO4	I	809	5/5	0.95	0.11	64,65,65,65	0
8	SO4	G	817	5/5	0.95	0.12	67,69,69,70	0
8	SO4	K	803	5/5	0.95	0.07	61,61,61,62	0
8	SO4	G	808	5/5	0.96	0.10	58,58,60,60	0
8	SO4	M	811	5/5	0.97	0.06	63,63,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.