Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 03:09 am GMT

PDB ID	:	2BGN
Title	:	HIV-1 Tat protein derived N-terminal nonapeptide Trp2-Tat(1-9) bound to the active site of Dipeptidyl peptidase IV (CD26)
Authors	:	Weihofen, W.A.; Liu, J.; Reutter, W.; Saenger, W.; Fan, H.
Deposited on	:	2005-01-03
Resolution	:	3.15 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:

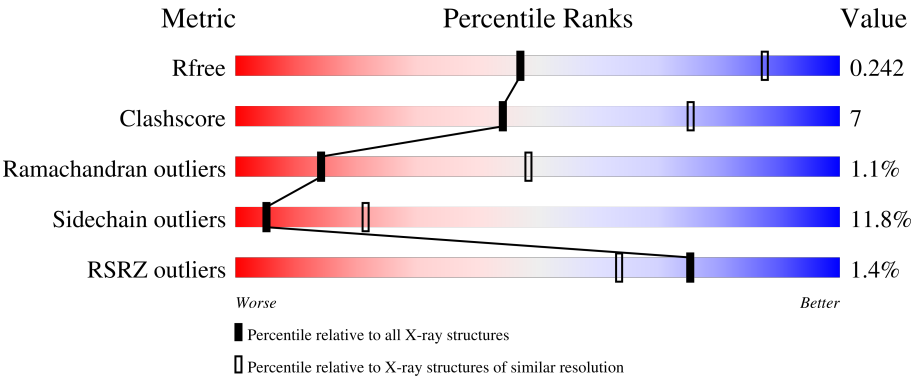
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 <=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	728	81% 16% .
1	B	728	81% 17% .
1	C	728	82% 16% .
1	D	728	80% 17% .
2	E	363	6% 63% 28% . . .

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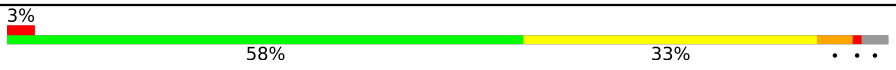
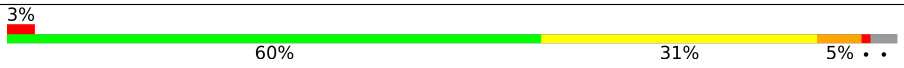
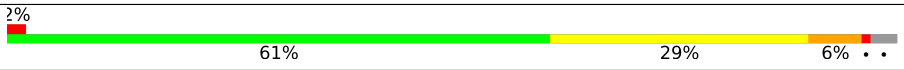
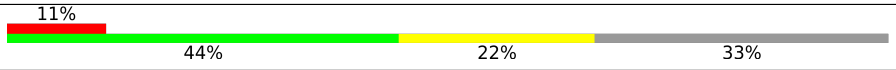
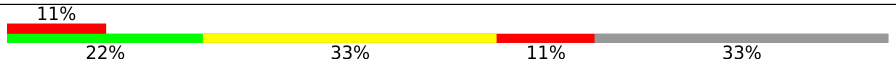
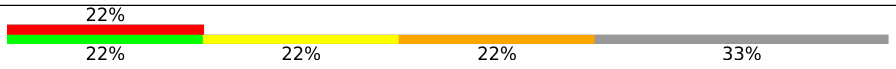
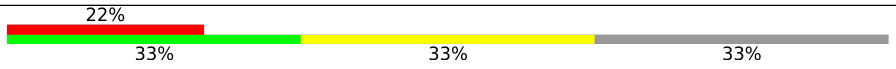
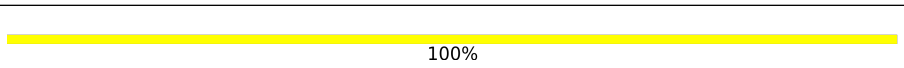
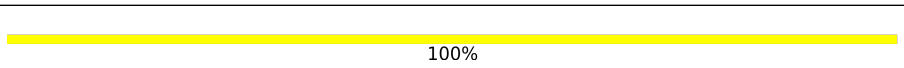
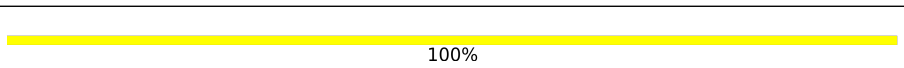
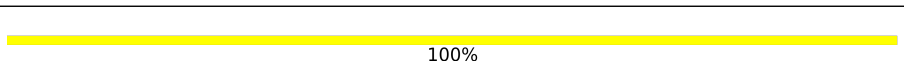
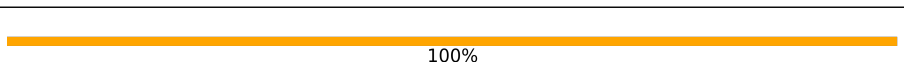
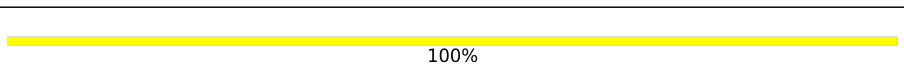
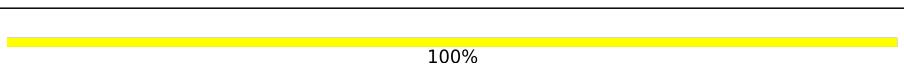
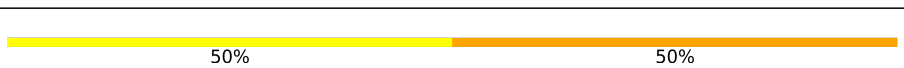
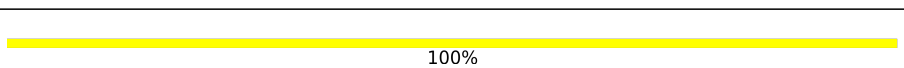
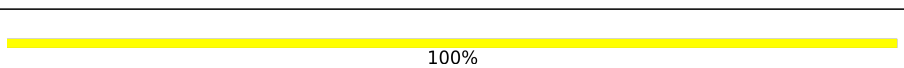
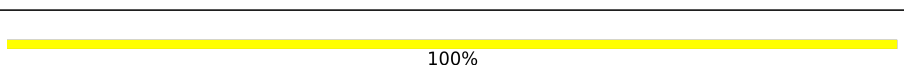
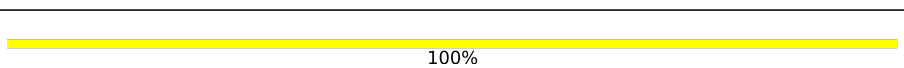
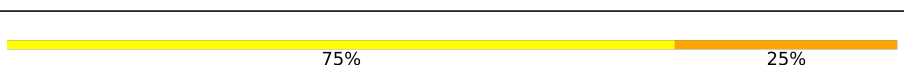
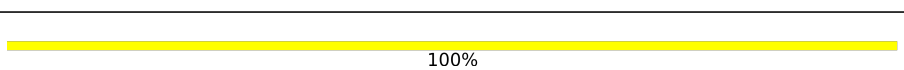
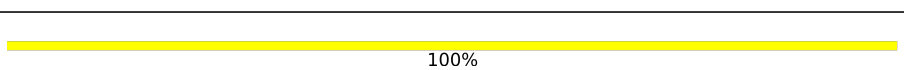
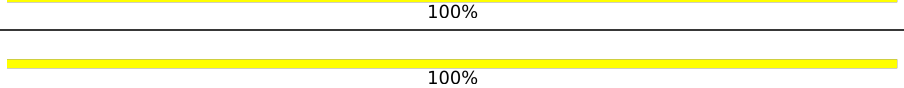
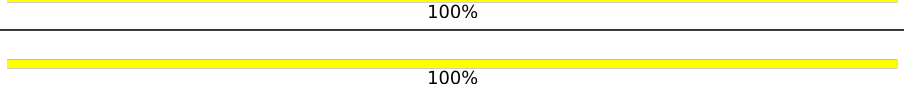
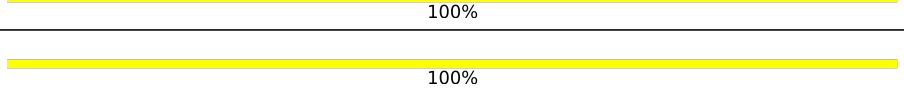
Mol	Chain	Length	Quality of chain
2	F	363	
2	G	363	
2	H	363	
3	W	9	
3	X	9	
3	Y	9	
3	Z	9	
4	I	3	
4	R	3	
5	J	2	
5	K	2	
5	M	2	
5	O	2	
5	Q	2	
5	S	2	
5	T	2	
5	V	2	
5	b	2	
5	d	2	
6	L	4	
6	P	4	
6	U	4	
6	c	4	
7	N	2	
7	a	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	R	2	-	-	-	X
5	NAG	M	2	-	-	-	X
8	NAG	A	840	X	-	-	-
8	NAG	A	860	-	-	-	X
8	NAG	B	860	X	-	-	-
8	NAG	D	860	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 36096 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 DIPEPTIDYL PEPTIDASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	C	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	D	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	F	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	G	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	H	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	ASP	ASN	conflict	UNP P56658
E	32	LYS	ARG	conflict	UNP P56658
E	33	ARG	LYS	conflict	UNP P56658
E	47	LEU	GLN	conflict	UNP P56658
E	57	THR	SER	conflict	UNP P56658
E	60	ASP	GLU	conflict	UNP P56658
E	77	ASP	GLU	conflict	UNP P56658
E	79	ILE	VAL	conflict	UNP P56658

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Chain	Residue	Modelled	Actual	Comment	Reference
E	199	GLN	LYS	variant	UNP P56658
E	246	THR	ALA	variant	UNP P56658
E	261	ILE	VAL	conflict	UNP P56658
E	279	ALA	PRO	conflict	UNP P56658
E	281	ILE	VAL	conflict	UNP P56658
E	313	LYS	ASN	conflict	UNP P56658
E	314	ASP	GLU	conflict	UNP P56658
E	352	ARG	GLY	variant	UNP P56658
F	8	ASP	ASN	conflict	UNP P56658
F	32	LYS	ARG	conflict	UNP P56658
F	33	ARG	LYS	conflict	UNP P56658
F	47	LEU	GLN	conflict	UNP P56658
F	57	THR	SER	conflict	UNP P56658
F	60	ASP	GLU	conflict	UNP P56658
F	77	ASP	GLU	conflict	UNP P56658
F	79	ILE	VAL	conflict	UNP P56658
F	199	GLN	LYS	variant	UNP P56658
F	246	THR	ALA	variant	UNP P56658
F	261	ILE	VAL	conflict	UNP P56658
F	279	ALA	PRO	conflict	UNP P56658
F	281	ILE	VAL	conflict	UNP P56658
F	313	LYS	ASN	conflict	UNP P56658
F	314	ASP	GLU	conflict	UNP P56658
F	352	ARG	GLY	variant	UNP P56658
G	8	ASP	ASN	conflict	UNP P56658
G	32	LYS	ARG	conflict	UNP P56658
G	33	ARG	LYS	conflict	UNP P56658
G	47	LEU	GLN	conflict	UNP P56658
G	57	THR	SER	conflict	UNP P56658
G	60	ASP	GLU	conflict	UNP P56658
G	77	ASP	GLU	conflict	UNP P56658
G	79	ILE	VAL	conflict	UNP P56658
G	199	GLN	LYS	variant	UNP P56658
G	246	THR	ALA	variant	UNP P56658
G	261	ILE	VAL	conflict	UNP P56658
G	279	ALA	PRO	conflict	UNP P56658
G	281	ILE	VAL	conflict	UNP P56658
G	313	LYS	ASN	conflict	UNP P56658
G	314	ASP	GLU	conflict	UNP P56658
G	352	ARG	GLY	variant	UNP P56658
H	8	ASP	ASN	conflict	UNP P56658
H	32	LYS	ARG	conflict	UNP P56658

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Chain	Residue	Modelled	Actual	Comment	Reference
H	33	ARG	LYS	conflict	UNP P56658
H	47	LEU	GLN	conflict	UNP P56658
H	57	THR	SER	conflict	UNP P56658
H	60	ASP	GLU	conflict	UNP P56658
H	77	ASP	GLU	conflict	UNP P56658
H	79	ILE	VAL	conflict	UNP P56658
H	199	GLN	LYS	variant	UNP P56658
H	246	THR	ALA	variant	UNP P56658
H	261	ILE	VAL	conflict	UNP P56658
H	279	ALA	PRO	conflict	UNP P56658
H	281	ILE	VAL	conflict	UNP P56658
H	313	LYS	ASN	conflict	UNP P56658
H	314	ASP	GLU	conflict	UNP P56658
H	352	ARG	GLY	variant	UNP P56658

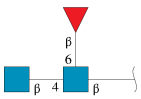
- Molecule 3 is a protein called TAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			
3	X	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			
3	Y	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			
3	Z	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	2	TRP	ASP	engineered mutation	UNP P12506
X	2	TRP	ASP	engineered mutation	UNP P12506
Y	2	TRP	ASP	engineered mutation	UNP P12506
Z	2	TRP	ASP	engineered mutation	UNP P12506

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



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

- 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	J	2	Total C N O 28 16 2 10	0	0	0
5	K	2	Total C N O 28 16 2 10	0	0	0
5	M	2	Total C N O 28 16 2 10	0	0	0
5	O	2	Total C N O 28 16 2 10	0	0	0
5	Q	2	Total C N O 28 16 2 10	0	0	0
5	S	2	Total C N O 28 16 2 10	0	0	0
5	T	2	Total C N O 28 16 2 10	0	0	0
5	V	2	Total C N O 28 16 2 10	0	0	0
5	b	2	Total C N O 28 16 2 10	0	0	0
5	d	2	Total C N O 28 16 2 10	0	0	0

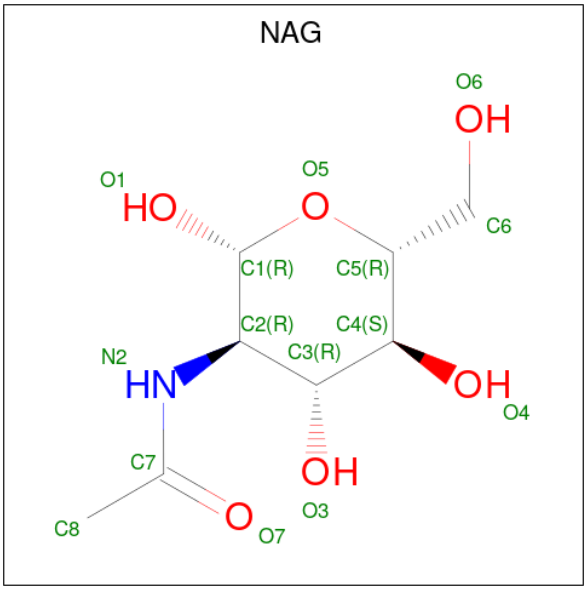
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	L	4	Total C N O 50 28 2 20	0	0	0
6	P	4	Total C N O 50 28 2 20	0	0	0
6	U	4	Total C N O 50 28 2 20	0	0	0
6	c	4	Total C N O 50 28 2 20	0	0	0

- Molecule 7 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta -D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	N	2	Total C N O 24 14 1 9	0	0	0
7	a	2	Total C N O 24 14 1 9	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

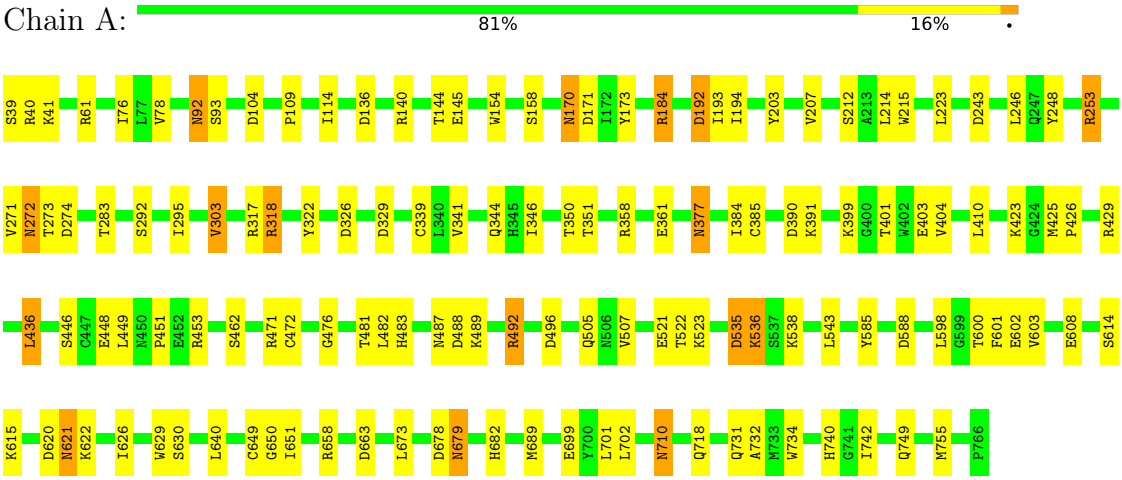
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Zn	0	0
			1	1		
9	F	1	Total	Zn	0	0
			1	1		
9	G	1	Total	Zn	0	0
			1	1		
9	H	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

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

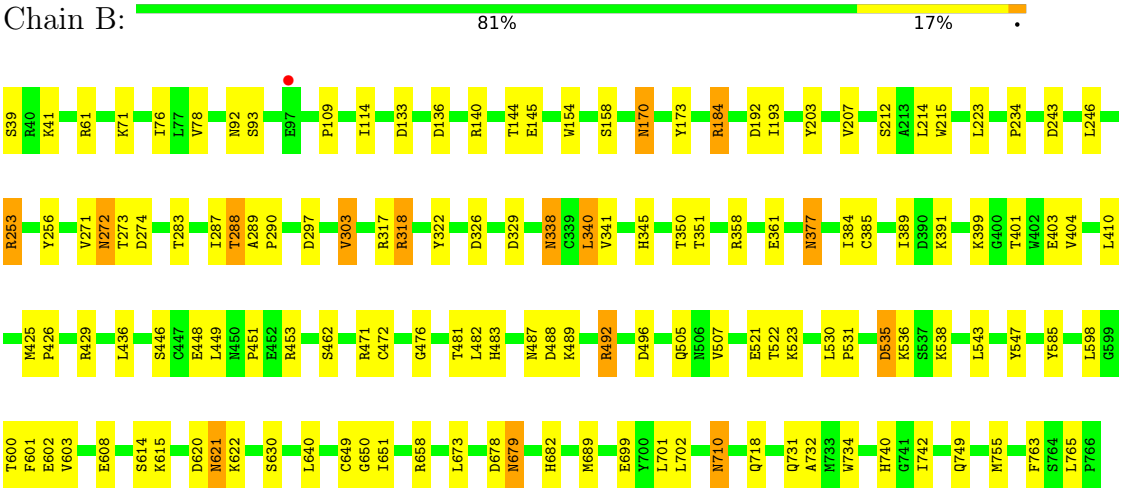
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain A:



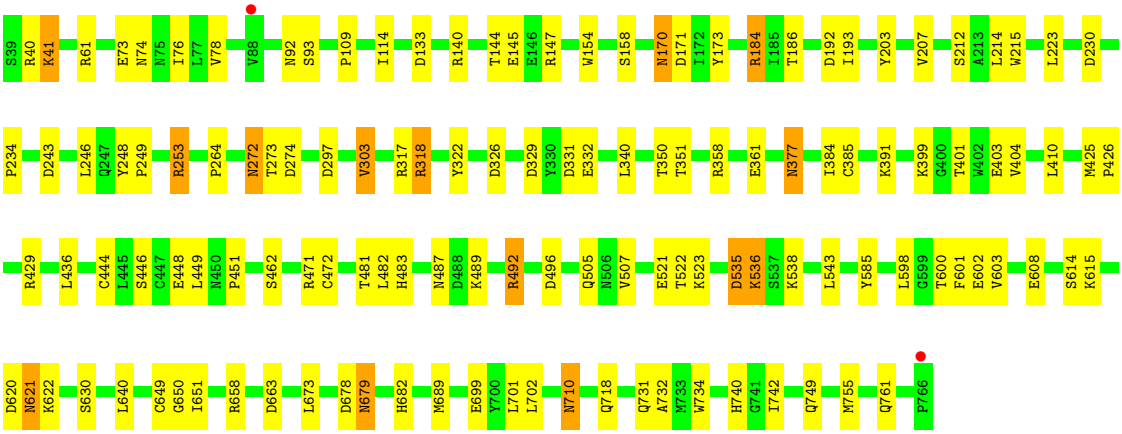
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain B:



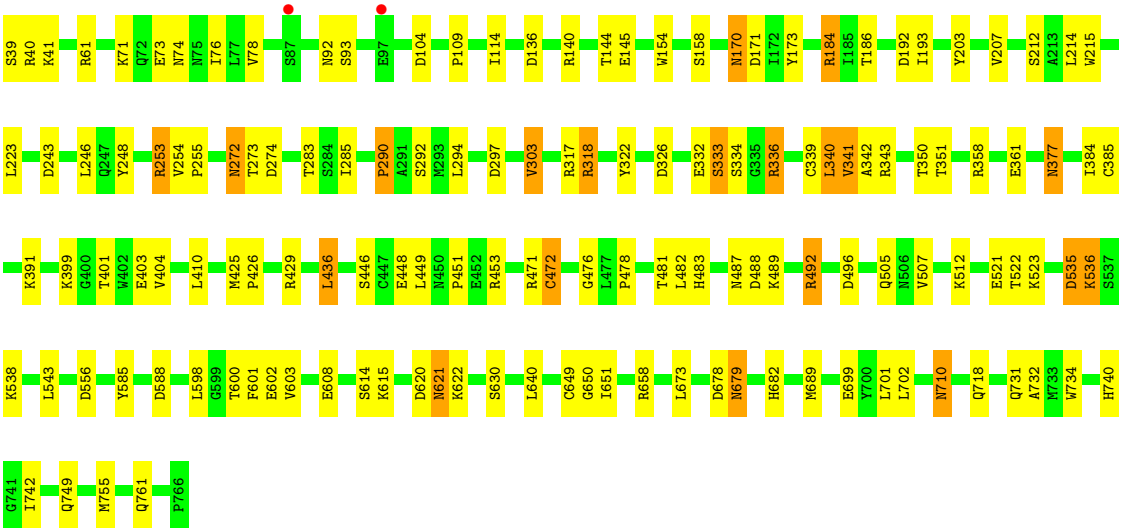
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain C:



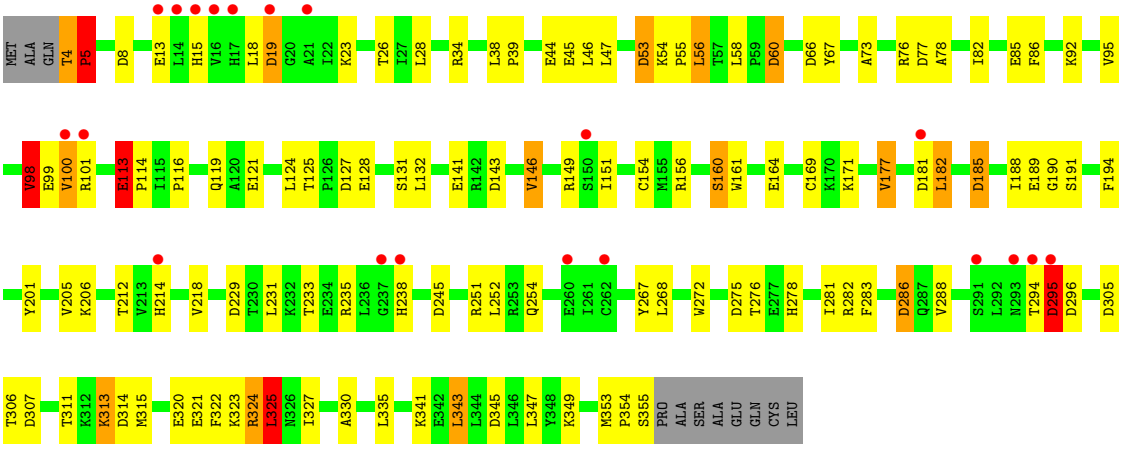
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D:



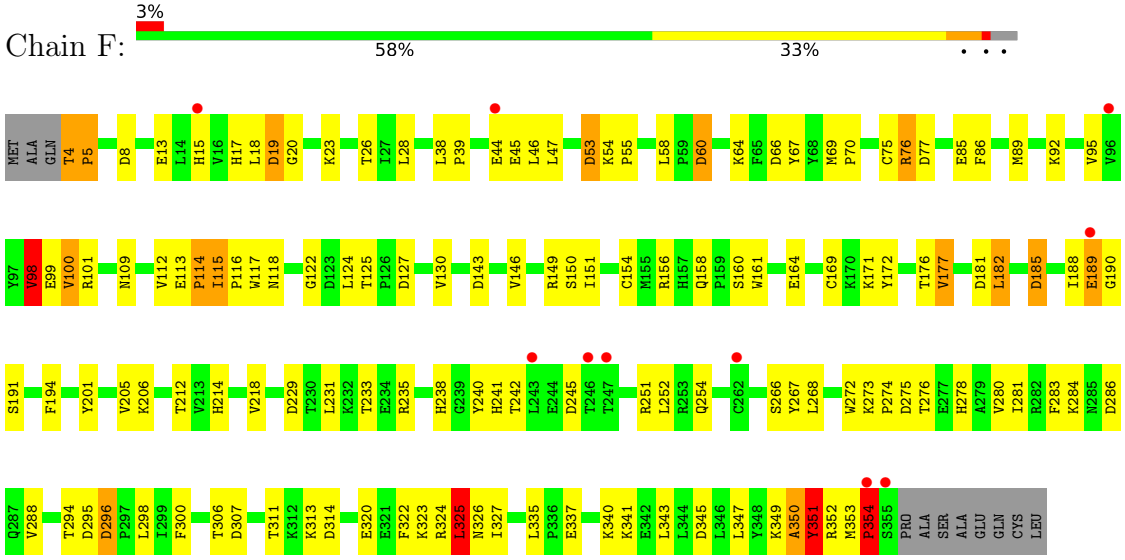
• Molecule 2: ADENOSINE DEAMINASE

Chain E:



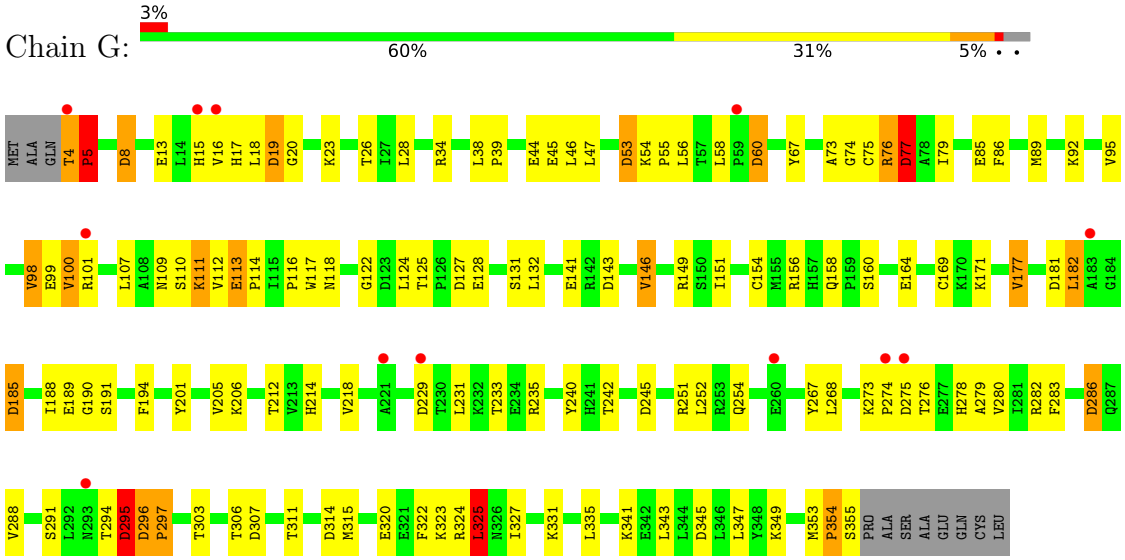
• Molecule 2: ADENOSINE DEAMINASE

Chain F:



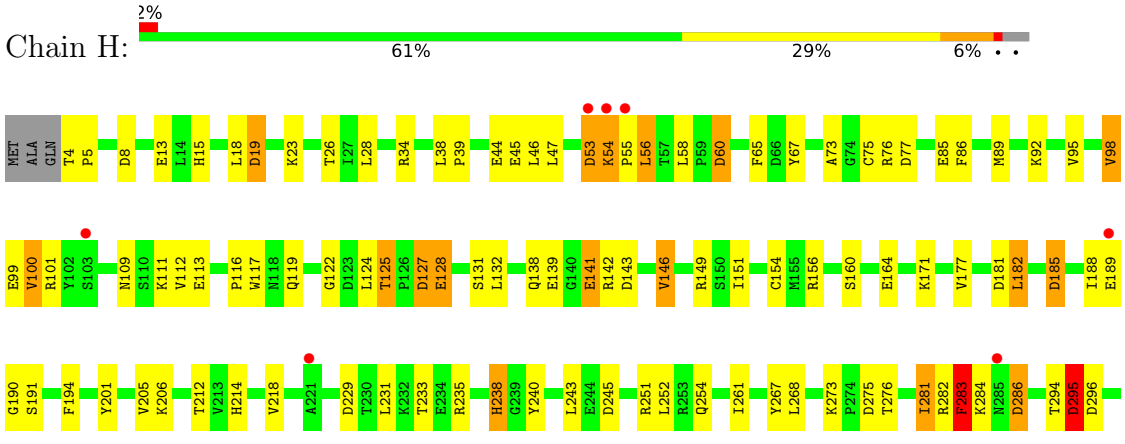
• Molecule 2: ADENOSINE DEAMINASE

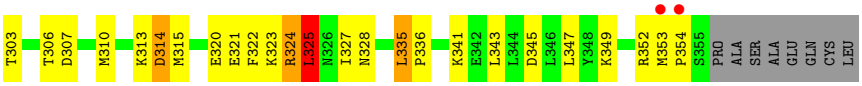
Chain G:



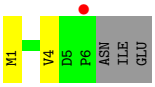
• Molecule 2: ADENOSINE DEAMINASE

Chain H:

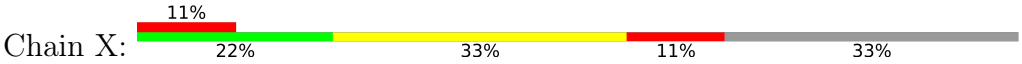


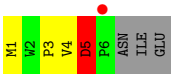


• Molecule 3: TAT PROTEIN

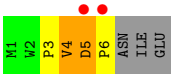


• Molecule 3: TAT PROTEIN



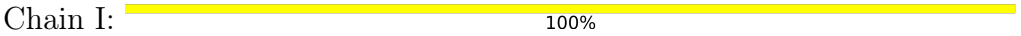


• Molecule 3: TAT PROTEIN



• Molecule 3: TAT PROTEIN

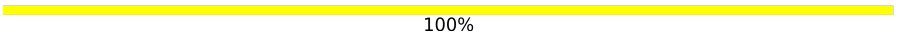
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

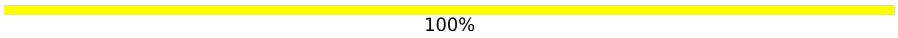
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:

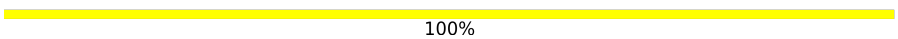


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

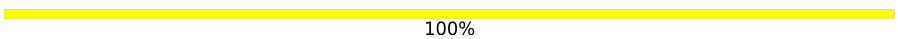
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain Q:

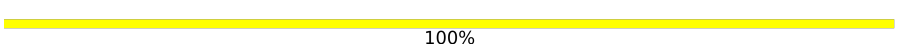


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

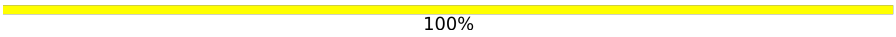
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



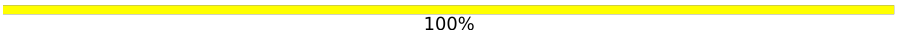
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



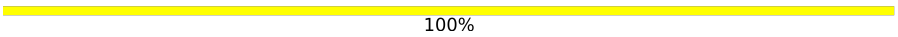
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



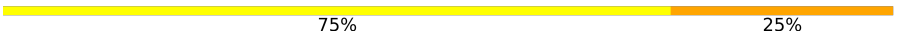
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



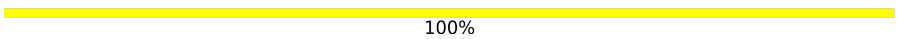
• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



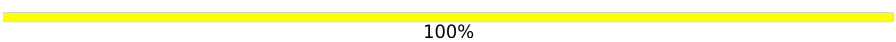
• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



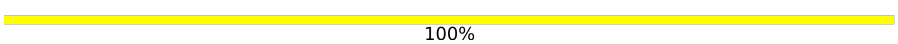
• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain c:



NAG1
NAG2
BMA3
MAN4

• Molecule 7: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%

NAG1
FUL2

• Molecule 7: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%

NAG1
FUL2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.94Å 170.27Å 239.20Å 90.00° 100.93° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 29.74 – 3.15	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-3.15) 89.6 (29.74-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.227 , 0.247 0.221 , 0.242	Depositor DCC
R_{free} test set	1925 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	36096	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, FUL, BMA, ZN, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/6135	0.85	14/8344 (0.2%)
1	B	0.44	0/6135	0.85	12/8344 (0.1%)
1	C	0.43	0/6135	0.85	11/8344 (0.1%)
1	D	0.43	0/6135	0.85	13/8344 (0.2%)
2	E	0.46	0/2874	1.01	23/3896 (0.6%)
2	F	0.65	2/2874 (0.1%)	1.16	22/3896 (0.6%)
2	G	0.47	0/2874	0.97	17/3896 (0.4%)
2	H	0.47	0/2874	0.97	17/3896 (0.4%)
3	W	0.63	0/54	0.89	0/75
3	X	0.63	0/54	1.30	1/75 (1.3%)
3	Y	0.57	0/54	1.31	1/75 (1.3%)
3	Z	0.56	0/54	0.92	0/75
All	All	0.46	2/36252 (0.0%)	0.91	131/49260 (0.3%)

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
2	E	0	1
2	F	1	1
2	H	0	1
3	X	0	1
3	Y	0	1
All	All	1	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	351	TYR	N-CA	-21.51	1.03	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	350	ALA	C-N	8.11	1.52	1.34

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	350	ALA	O-C-N	-25.49	81.92	122.70
2	F	350	ALA	CA-C-N	17.64	156.01	117.20
2	F	351	TYR	N-CA-CB	16.83	140.90	110.60
2	F	350	ALA	C-N-CA	11.19	149.68	121.70
2	F	296	ASP	CB-CG-OD2	10.62	127.85	118.30
2	E	60	ASP	CB-CG-OD2	10.28	127.55	118.30
2	G	60	ASP	CB-CG-OD2	9.90	127.22	118.30
2	H	60	ASP	CB-CG-OD2	9.78	127.11	118.30
2	G	77	ASP	CB-CG-OD2	9.69	127.02	118.30
2	E	77	ASP	CB-CG-OD2	9.56	126.91	118.30
2	F	60	ASP	CB-CG-OD2	9.24	126.62	118.30
2	F	19	ASP	CB-CG-OD2	8.74	126.17	118.30
2	G	19	ASP	CB-CG-OD2	8.73	126.16	118.30
2	E	19	ASP	CB-CG-OD2	8.67	126.10	118.30
2	H	19	ASP	CB-CG-OD2	8.66	126.09	118.30
2	E	307	ASP	CB-CG-OD2	8.63	126.06	118.30
1	C	535	ASP	CB-CG-OD2	8.58	126.02	118.30
2	F	77	ASP	CB-CG-OD2	8.39	125.85	118.30
1	A	535	ASP	CB-CG-OD2	8.30	125.77	118.30
1	B	535	ASP	CB-CG-OD2	8.19	125.67	118.30
2	H	77	ASP	CB-CG-OD2	8.11	125.60	118.30
1	A	678	ASP	CB-CG-OD2	8.09	125.58	118.30
2	F	181	ASP	CB-CG-OD2	7.83	125.35	118.30
1	D	535	ASP	CB-CG-OD2	7.82	125.34	118.30
3	X	5	ASP	CB-CG-OD2	7.75	125.28	118.30
2	E	296	ASP	CB-CG-OD2	7.73	125.26	118.30
1	D	496	ASP	CB-CG-OD2	7.67	125.20	118.30
1	C	678	ASP	CB-CG-OD2	7.66	125.19	118.30
2	H	127	ASP	CB-CG-OD2	7.64	125.17	118.30
2	G	5	PRO	N-CA-C	7.61	131.89	112.10
1	B	678	ASP	CB-CG-OD2	7.60	125.14	118.30
3	Y	5	ASP	CB-CG-OD2	7.33	124.90	118.30
2	E	181	ASP	CB-CG-OD2	7.27	124.84	118.30
2	H	181	ASP	CB-CG-OD2	7.23	124.80	118.30
2	H	245	ASP	CB-CG-OD2	7.14	124.73	118.30
2	F	245	ASP	CB-CG-OD2	7.12	124.70	118.30
2	F	143	ASP	CB-CG-OD2	7.10	124.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	8	ASP	CB-CG-OD2	7.07	124.66	118.30
2	E	143	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	496	ASP	CB-CG-OD2	6.89	124.50	118.30
2	G	181	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	496	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	620	ASP	CB-CG-OD2	6.82	124.43	118.30
2	E	314	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	496	ASP	CB-CG-OD2	6.67	124.31	118.30
2	G	245	ASP	CB-CG-OD2	6.65	124.28	118.30
1	C	620	ASP	CB-CG-OD2	6.65	124.28	118.30
2	F	307	ASP	CB-CG-OD2	6.61	124.25	118.30
1	D	678	ASP	CB-CG-OD2	6.53	124.18	118.30
2	E	295	ASP	CB-CG-OD2	6.47	124.12	118.30
2	H	307	ASP	CB-CG-OD2	6.44	124.09	118.30
2	E	305	ASP	CB-CG-OD2	6.43	124.09	118.30
2	F	325	LEU	CA-CB-CG	6.41	130.05	115.30
2	G	229	ASP	CB-CG-OD2	6.39	124.05	118.30
2	F	8	ASP	CB-CG-OD2	6.36	124.02	118.30
2	F	127	ASP	CB-CG-OD2	6.33	123.99	118.30
2	E	127	ASP	CB-CG-OD2	6.31	123.98	118.30
2	H	325	LEU	CA-CB-CG	6.30	129.79	115.30
2	E	245	ASP	CB-CG-OD2	6.27	123.94	118.30
2	E	185	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	620	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	620	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	588	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	318	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	H	53	ASP	CB-CG-OD2	6.13	123.82	118.30
2	H	8	ASP	CB-CG-OD2	6.09	123.78	118.30
2	G	143	ASP	CB-CG-OD2	6.04	123.73	118.30
1	C	297	ASP	CB-CG-OD2	6.02	123.72	118.30
2	G	307	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	329	ASP	CB-CG-OD2	5.94	123.65	118.30
2	G	8	ASP	CB-CG-OD2	5.92	123.63	118.30
2	G	286	ASP	CB-CG-OD2	5.92	123.63	118.30
2	F	229	ASP	CB-CG-OD2	5.87	123.59	118.30
1	B	243	ASP	CB-CG-OD2	5.83	123.55	118.30
2	E	53	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	243	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	171	ASP	CB-CG-OD2	5.77	123.49	118.30
2	H	335	LEU	CA-CB-CG	5.74	128.51	115.30
1	D	171	ASP	CB-CG-OD2	5.72	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	318	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	F	275	ASP	CB-CG-OD2	5.67	123.40	118.30
2	E	286	ASP	CB-CG-OD2	5.66	123.39	118.30
2	F	185	ASP	CB-CG-OD2	5.64	123.38	118.30
2	E	229	ASP	CB-CG-OD2	5.63	123.37	118.30
2	F	53	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	488	ASP	CB-CG-OD2	5.60	123.34	118.30
2	G	275	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	136	ASP	CB-CG-OD2	5.58	123.32	118.30
2	E	275	ASP	CB-CG-OD2	5.58	123.32	118.30
2	E	325	LEU	CA-CB-CG	5.58	128.13	115.30
2	H	143	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	329	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	318	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	H	229	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	133	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	318	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	136	ASP	CB-CG-OD2	5.53	123.28	118.30
2	F	66	ASP	CB-CG-OD2	5.52	123.27	118.30
2	G	314	ASP	CB-CG-OD2	5.52	123.27	118.30
2	H	296	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	104	ASP	CB-CG-OD2	5.46	123.21	118.30
2	H	275	ASP	CB-CG-OD2	5.45	123.20	118.30
2	G	127	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	243	ASP	CB-CG-OD2	5.40	123.16	118.30
2	H	185	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	336	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	171	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	390	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	289	ALA	C-N-CD	-5.30	108.93	120.60
2	G	325	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	329	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	444	CYS	CA-CB-SG	-5.28	104.50	114.00
2	E	76	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	136	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	588	ASP	CB-CG-OD2	5.23	123.01	118.30
2	G	53	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	297	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	243	ASP	CB-CG-OD2	5.17	122.95	118.30
2	E	5	PRO	N-CA-C	5.14	125.47	112.10
1	D	297	ASP	CB-CG-OD2	5.10	122.89	118.30
2	E	66	ASP	CB-CG-OD2	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	133	ASP	CB-CG-OD2	5.07	122.87	118.30
2	H	286	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	104	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	488	ASP	CB-CG-OD2	5.03	122.83	118.30
2	F	314	ASP	CB-CG-OD2	5.03	122.82	118.30
2	F	98	VAL	CB-CA-C	-5.02	101.85	111.40
1	D	488	ASP	CB-CG-OD2	5.02	122.82	118.30
2	G	185	ASP	CB-CG-OD2	5.01	122.81	118.30
2	E	98	VAL	CB-CA-C	-5.01	101.88	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	351	TYR	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	113	GLU	Peptide
2	F	350	ALA	Mainchain
2	H	113	GLU	Peptide
3	X	5	ASP	Peptide
3	Y	3	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5677	59	1
1	B	5963	0	5677	60	0
1	C	5963	0	5676	55	0
1	D	5963	0	5677	68	0
2	E	2809	0	2767	49	1
2	F	2809	0	2767	69	0
2	G	2809	0	2767	65	0
2	H	2809	0	2767	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	51	0	48	3	0
3	X	51	0	48	3	0
3	Y	51	0	48	1	0
3	Z	51	0	48	1	0
4	I	38	0	34	0	0
4	R	38	0	34	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	4	0
5	O	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	1	0
5	T	28	0	25	0	0
5	V	28	0	25	0	0
5	b	28	0	25	0	0
5	d	28	0	25	0	0
6	L	50	0	43	1	0
6	P	50	0	43	0	0
6	U	50	0	43	0	0
6	c	50	0	43	0	0
7	N	24	0	22	0	0
7	a	24	0	22	0	0
8	A	42	0	39	0	0
8	B	56	0	52	0	0
8	C	42	0	39	0	0
8	D	56	0	52	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
All	All	36096	0	34683	467	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (467) 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:A:253:ARG:HH22	1:B:253:ARG:HH22	1.09	0.94
2:E:13:GLU:OE1	2:E:294:THR:HG22	1.71	0.90
1:D:340:LEU:HD13	1:D:343:ARG:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1:NAG:O3	5:M:2:NAG:H82	1.74	0.88
2:F:283:PHE:HD2	2:F:288:VAL:HG11	1.40	0.84
1:D:340:LEU:HD12	1:D:340:LEU:H	1.45	0.80
1:B:377:ASN:C	1:B:377:ASN:HD22	1.86	0.79
2:F:109:ASN:O	2:F:122:GLY:HA2	1.82	0.79
1:C:377:ASN:C	1:C:377:ASN:HD22	1.85	0.78
1:D:377:ASN:C	1:D:377:ASN:HD22	1.88	0.77
1:A:377:ASN:C	1:A:377:ASN:HD22	1.88	0.75
2:G:283:PHE:HD1	2:G:288:VAL:HG11	1.50	0.75
2:F:283:PHE:CD2	2:F:288:VAL:HG11	2.21	0.74
2:G:110:SER:O	2:G:111:LYS:HB2	1.88	0.74
1:D:340:LEU:HD12	1:D:340:LEU:N	2.02	0.74
2:H:261:ILE:HD11	2:H:283:PHE:HE2	1.54	0.73
1:A:401:THR:O	1:A:401:THR:HG22	1.89	0.72
1:B:547:TYR:CZ	3:X:3:PRO:HD3	2.25	0.71
2:G:4:THR:N	2:G:5:PRO:HD2	2.06	0.70
2:G:20:GLY:HA3	2:G:296:ASP:HB3	1.75	0.69
1:D:401:THR:O	1:D:401:THR:HG22	1.92	0.69
1:C:401:THR:HG22	1:C:401:THR:O	1.92	0.68
1:B:401:THR:HG22	1:B:401:THR:O	1.91	0.68
2:F:240:TYR:CE2	2:F:266:SER:OG	2.45	0.68
2:G:141:GLU:HG3	2:G:146:VAL:O	1.94	0.68
2:F:240:TYR:HE2	2:F:266:SER:OG	1.75	0.68
2:H:65:PHE:HB3	2:H:117:TRP:CH2	2.29	0.67
2:F:156:ARG:HD2	2:F:185:ASP:O	1.94	0.67
1:D:340:LEU:O	1:D:342:ALA:N	2.28	0.66
2:G:283:PHE:CD1	2:G:288:VAL:HG11	2.31	0.66
1:C:734:TRP:CZ3	1:D:732:ALA:HB1	2.30	0.66
1:D:630:SER:HB3	3:Z:1:MET:SD	2.36	0.65
1:C:651:ILE:HD13	1:C:755:MET:HG2	1.79	0.65
1:A:271:VAL:HG23	1:A:283:THR:O	1.97	0.65
1:C:73:GLU:O	1:C:74:ASN:HB2	1.96	0.65
2:G:128:GLU:O	2:G:132:LEU:HD12	1.97	0.65
2:G:353:MET:HB2	2:G:354:PRO:HD2	1.78	0.65
2:H:156:ARG:HD2	2:H:185:ASP:O	1.96	0.65
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.91	0.65
3:Y:5:ASP:HB2	3:Y:6:PRO:HD2	1.79	0.64
2:G:156:ARG:HD2	2:G:185:ASP:O	1.97	0.64
1:B:272:ASN:C	1:B:272:ASN:HD22	2.01	0.64
2:F:13:GLU:OE1	2:F:294:THR:HG22	1.97	0.63
1:D:272:ASN:HD22	1:D:272:ASN:C	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:GLU:OE2	2:E:160:SER:HB2	1.98	0.63
2:E:113:GLU:HB2	2:E:161:TRP:HE1	1.63	0.63
2:F:280:VAL:HA	2:F:283:PHE:HD1	1.63	0.63
2:F:323:LYS:O	2:F:327:ILE:HG12	1.99	0.63
1:B:338:ASN:HD21	1:B:340:LEU:HD23	1.65	0.62
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.80	0.62
2:G:34:ARG:HH12	2:G:74:GLY:HA3	1.63	0.62
2:G:294:THR:HG23	2:G:297:PRO:HD3	1.81	0.62
5:M:1:NAG:O3	5:M:2:NAG:C8	2.48	0.62
2:E:156:ARG:HD2	2:E:185:ASP:O	2.01	0.61
2:E:15:HIS:CD2	2:E:295:ASP:OD1	2.52	0.61
1:D:651:ILE:HD13	1:D:755:MET:HG2	1.80	0.61
2:F:39:PRO:HG3	2:F:67:TYR:HD2	1.66	0.61
1:A:272:ASN:C	1:A:272:ASN:HD22	2.02	0.61
1:C:170:ASN:N	1:C:170:ASN:HD22	2.00	0.60
2:F:109:ASN:O	2:F:122:GLY:CA	2.49	0.60
2:G:39:PRO:HG3	2:G:67:TYR:HD2	1.66	0.60
1:B:651:ILE:HD13	1:B:755:MET:HG2	1.84	0.60
1:C:272:ASN:C	1:C:272:ASN:HD22	2.03	0.60
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.84	0.60
2:F:130:VAL:HG11	2:F:172:TYR:CD2	2.36	0.60
2:H:261:ILE:HD11	2:H:283:PHE:CE2	2.35	0.60
2:H:34:ARG:NH2	2:H:73:ALA:O	2.35	0.60
2:H:125:THR:HG23	2:H:128:GLU:HB2	1.83	0.60
2:H:39:PRO:HG3	2:H:67:TYR:HD2	1.67	0.60
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.84	0.59
1:C:253:ARG:HH22	1:D:253:ARG:HH22	1.48	0.59
1:B:345:HIS:HE1	1:B:389:ILE:O	1.85	0.59
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.84	0.59
2:F:240:TYR:HE2	2:F:266:SER:HG	1.39	0.59
2:E:283:PHE:CD1	2:E:288:VAL:HG11	2.38	0.59
1:A:170:ASN:N	1:A:170:ASN:HD22	2.01	0.59
5:M:1:NAG:HO3	5:M:2:NAG:H82	1.68	0.58
2:E:39:PRO:HG3	2:E:67:TYR:HD2	1.69	0.58
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.92	0.58
1:A:272:ASN:HD22	1:A:273:THR:N	2.02	0.58
1:D:170:ASN:N	1:D:170:ASN:HD22	2.02	0.57
2:F:278:HIS:O	2:F:281:ILE:HG22	2.04	0.57
1:B:272:ASN:HD22	1:B:273:THR:N	2.02	0.57
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.39	0.57
2:F:75:CYS:O	2:F:76:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:PRO:HG2	2:G:8:ASP:OD1	2.05	0.57
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.39	0.57
2:F:295:ASP:HB3	2:F:300:PHE:HE2	1.70	0.57
2:H:15:HIS:CD2	2:H:295:ASP:OD1	2.57	0.57
2:H:139:GLU:HG3	2:H:142:ARG:NH2	2.19	0.57
2:F:322:PHE:HA	2:F:325:LEU:HD13	1.85	0.57
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.41	0.56
2:E:272:TRP:NE1	2:E:278:HIS:HA	2.19	0.56
1:C:272:ASN:HD22	1:C:273:THR:N	2.02	0.56
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.56
1:C:710:ASN:C	1:C:710:ASN:HD22	2.09	0.56
2:E:323:LYS:O	2:E:327:ILE:HG12	2.06	0.56
2:F:114:PRO:HG3	2:F:158:GLN:NE2	2.21	0.56
2:F:191:SER:HA	2:F:194:PHE:CD2	2.41	0.56
2:G:191:SER:HA	2:G:194:PHE:CD2	2.40	0.56
1:B:170:ASN:N	1:B:170:ASN:HD22	2.04	0.55
1:D:272:ASN:HD22	1:D:273:THR:N	2.03	0.55
1:C:679:ASN:HD21	1:C:682:HIS:CD2	2.24	0.55
2:H:65:PHE:HB3	2:H:117:TRP:HH2	1.72	0.55
1:D:602:GLU:N	1:D:602:GLU:OE2	2.40	0.55
1:A:248:TYR:OH	1:B:256:TYR:O	2.18	0.55
1:B:630:SER:HB3	3:X:1:MET:SD	2.47	0.55
1:A:732:ALA:HB1	1:B:734:TRP:CZ3	2.42	0.54
1:B:602:GLU:N	1:B:602:GLU:OE2	2.39	0.54
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.42	0.54
1:D:630:SER:OG	1:D:740:HIS:NE2	2.40	0.54
1:A:710:ASN:HD22	1:A:710:ASN:C	2.11	0.54
2:F:295:ASP:HB3	2:F:300:PHE:CE2	2.42	0.54
2:E:4:THR:N	2:E:5:PRO:HD2	2.23	0.54
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.43	0.54
2:G:4:THR:N	2:G:5:PRO:CD	2.71	0.54
2:H:191:SER:HA	2:H:194:PHE:CD2	2.43	0.54
2:E:191:SER:HA	2:E:194:PHE:CD2	2.43	0.53
2:H:54:LYS:HB2	2:H:56:LEU:HD23	1.90	0.53
1:B:679:ASN:HD21	1:B:682:HIS:CD2	2.27	0.53
1:B:487:ASN:CB	1:B:489:LYS:HB2	2.39	0.53
1:A:377:ASN:C	1:A:377:ASN:ND2	2.62	0.52
1:A:401:THR:O	1:A:401:THR:CG2	2.58	0.52
2:G:73:ALA:O	2:G:107:LEU:O	2.27	0.52
2:G:113:GLU:HB2	2:G:114:PRO:CD	2.39	0.52
1:D:487:ASN:CB	1:D:489:LYS:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:TYR:OH	1:A:346:ILE:HD13	2.10	0.52
1:C:602:GLU:OE2	1:C:602:GLU:N	2.42	0.52
2:E:188:ILE:O	2:E:191:SER:OG	2.28	0.52
1:D:340:LEU:C	1:D:342:ALA:N	2.63	0.52
2:G:114:PRO:HG3	2:G:158:GLN:NE2	2.25	0.52
1:D:710:ASN:C	1:D:710:ASN:HD22	2.13	0.51
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.92	0.51
1:D:446:SER:HA	1:D:449:LEU:HG	1.92	0.51
1:B:710:ASN:C	1:B:710:ASN:HD22	2.13	0.51
1:B:341:VAL:HG12	1:B:341:VAL:O	2.11	0.51
1:C:487:ASN:CB	1:C:489:LYS:HB2	2.40	0.51
2:F:116:PRO:HB2	2:F:117:TRP:CD1	2.45	0.51
2:F:188:ILE:O	2:F:191:SER:OG	2.28	0.51
2:G:26:THR:HG21	2:G:85:GLU:OE2	2.10	0.51
1:A:629:TRP:CG	3:W:4:VAL:CG1	2.94	0.51
2:E:281:ILE:HD13	2:E:315:MET:HB2	1.92	0.51
2:G:188:ILE:O	2:G:191:SER:OG	2.29	0.51
1:A:602:GLU:N	1:A:602:GLU:OE2	2.44	0.51
1:C:446:SER:HA	1:C:449:LEU:HG	1.93	0.51
1:D:679:ASN:HD21	1:D:682:HIS:CD2	2.28	0.51
2:G:280:VAL:O	2:G:283:PHE:N	2.44	0.51
1:C:630:SER:OG	1:C:740:HIS:NE2	2.35	0.50
1:A:614:SER:HB2	1:A:621:ASN:HD22	1.77	0.50
1:A:679:ASN:HD21	1:A:682:HIS:CD2	2.29	0.50
2:H:321:GLU:OE1	2:H:324:ARG:NH2	2.44	0.50
1:B:271:VAL:HG23	1:B:283:THR:O	2.10	0.50
1:C:203:TYR:HA	1:C:207:VAL:HG13	1.92	0.50
2:H:116:PRO:O	2:H:119:GLN:HG2	2.10	0.50
2:H:281:ILE:O	2:H:284:LYS:HB3	2.11	0.50
1:A:194:ILE:HD12	6:L:1:NAG:H82	1.93	0.50
1:A:487:ASN:CB	1:A:489:LYS:HB2	2.42	0.50
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.93	0.50
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.94	0.50
2:F:4:THR:HG22	2:F:5:PRO:HD2	1.93	0.50
2:G:323:LYS:O	2:G:327:ILE:HG12	2.12	0.50
2:F:26:THR:HG21	2:F:85:GLU:OE2	2.11	0.50
2:F:322:PHE:HA	2:F:325:LEU:CD1	2.41	0.50
1:C:377:ASN:C	1:C:377:ASN:ND2	2.59	0.49
2:H:188:ILE:O	2:H:191:SER:OG	2.30	0.49
2:F:337:GLU:O	2:F:340:LYS:N	2.45	0.49
2:G:99:GLU:OE2	2:G:235:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:101:ARG:HA	2:G:151:ILE:O	2.13	0.49
2:G:116:PRO:HB2	2:G:117:TRP:CD1	2.48	0.49
1:A:446:SER:HA	1:A:449:LEU:HG	1.94	0.49
2:G:95:VAL:HG11	2:G:98:VAL:HG22	1.94	0.49
2:G:100:VAL:O	2:G:151:ILE:N	2.43	0.49
2:H:26:THR:HG21	2:H:85:GLU:OE2	2.13	0.49
1:B:614:SER:HB2	1:B:621:ASN:HD22	1.77	0.49
2:H:95:VAL:HG11	2:H:98:VAL:HG22	1.95	0.49
1:B:487:ASN:HB3	1:B:489:LYS:HB2	1.95	0.49
2:E:26:THR:HG21	2:E:85:GLU:OE2	2.12	0.49
2:F:101:ARG:HA	2:F:151:ILE:O	2.13	0.49
2:H:99:GLU:OE2	2:H:235:ARG:NH1	2.46	0.49
1:A:629:TRP:CG	3:W:4:VAL:HG11	2.48	0.49
1:C:448:GLU:HA	1:C:451:PRO:HG3	1.94	0.49
1:C:535:ASP:HB3	1:C:538:LYS:HD2	1.94	0.49
1:D:487:ASN:HB3	1:D:489:LYS:HB2	1.95	0.49
1:B:718:GLN:HA	1:B:718:GLN:NE2	2.28	0.48
2:F:95:VAL:HG11	2:F:98:VAL:HG22	1.94	0.48
1:C:147:ARG:NH2	5:S:2:NAG:H83	2.27	0.48
2:E:4:THR:N	2:E:5:PRO:CD	2.77	0.48
1:D:535:ASP:HB3	1:D:538:LYS:HD2	1.95	0.48
2:E:95:VAL:HG11	2:E:98:VAL:HG22	1.95	0.48
1:C:614:SER:HB2	1:C:621:ASN:HD22	1.77	0.48
2:H:243:LEU:HD22	2:H:282:ARG:NH2	2.29	0.48
1:D:290:PRO:O	1:D:294:LEU:HG	2.13	0.48
2:F:75:CYS:O	2:F:76:ARG:CG	2.62	0.48
1:B:446:SER:HA	1:B:449:LEU:HG	1.95	0.48
2:H:218:VAL:O	2:H:218:VAL:HG13	2.14	0.48
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.95	0.47
2:E:218:VAL:O	2:E:218:VAL:HG13	2.13	0.47
2:F:99:GLU:OE2	2:F:235:ARG:NH1	2.45	0.47
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.14	0.47
1:B:535:ASP:HB3	1:B:538:LYS:HD2	1.96	0.47
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.97	0.47
2:F:28:LEU:HD13	2:F:46:LEU:HD22	1.96	0.47
1:B:377:ASN:C	1:B:377:ASN:ND2	2.59	0.47
2:E:99:GLU:OE2	2:E:235:ARG:NH1	2.46	0.47
2:G:110:SER:O	2:G:111:LYS:CB	2.60	0.47
1:A:487:ASN:HB3	1:A:489:LYS:HB2	1.97	0.47
1:A:649:CYS:HB3	1:A:699:GLU:HB2	1.96	0.47
1:C:487:ASN:HB3	1:C:489:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:HIS:CE1	2:F:214:HIS:CE1	3.03	0.47
2:F:218:VAL:O	2:F:218:VAL:HG13	2.15	0.47
2:F:267:TYR:CD1	2:F:268:LEU:HD12	2.50	0.47
2:H:55:PRO:HG3	2:H:267:TYR:CZ	2.50	0.47
2:H:100:VAL:O	2:H:151:ILE:N	2.43	0.47
1:D:377:ASN:C	1:D:377:ASN:ND2	2.61	0.47
1:A:341:VAL:HA	1:A:344:GLN:HG3	1.97	0.47
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.80	0.47
1:B:718:GLN:CA	1:B:718:GLN:HE21	2.27	0.47
1:D:109:PRO:HG2	1:D:158:SER:O	2.15	0.47
2:E:113:GLU:HB2	2:E:114:PRO:HD2	1.97	0.47
1:A:734:TRP:CZ3	1:B:732:ALA:HB1	2.49	0.46
1:C:425:MET:HA	1:C:426:PRO:HD3	1.79	0.46
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.96	0.46
2:H:101:ARG:HA	2:H:151:ILE:O	2.14	0.46
1:A:535:ASP:HB3	1:A:538:LYS:HD2	1.97	0.46
2:G:20:GLY:CA	2:G:296:ASP:HB3	2.45	0.46
2:G:28:LEU:HD13	2:G:46:LEU:HD22	1.97	0.46
2:E:34:ARG:NH2	2:E:73:ALA:O	2.48	0.46
2:E:321:GLU:OE1	2:E:324:ARG:NH2	2.48	0.46
2:F:55:PRO:HG3	2:F:267:TYR:CZ	2.50	0.46
2:H:28:LEU:HD13	2:H:46:LEU:HD22	1.97	0.46
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.98	0.46
2:E:55:PRO:HG3	2:E:267:TYR:CZ	2.50	0.46
1:C:614:SER:HB2	1:C:621:ASN:ND2	2.31	0.46
1:D:492:ARG:HH11	1:D:492:ARG:HB3	1.81	0.46
1:D:340:LEU:O	1:D:341:VAL:C	2.53	0.46
1:D:614:SER:HB2	1:D:621:ASN:HD22	1.80	0.46
2:E:113:GLU:HG3	2:E:161:TRP:CD1	2.50	0.46
1:D:448:GLU:HA	1:D:451:PRO:HG3	1.96	0.46
1:C:92:ASN:OD1	1:C:92:ASN:N	2.48	0.46
1:A:492:ARG:HH11	1:A:492:ARG:HB3	1.81	0.46
2:H:86:PHE:CZ	2:H:100:VAL:HG13	2.51	0.46
2:H:99:GLU:HA	2:H:149:ARG:O	2.15	0.46
1:A:109:PRO:HG2	1:A:158:SER:O	2.16	0.46
1:A:215:TRP:CD2	1:A:303:VAL:HG21	2.51	0.46
1:A:192:ASP:O	1:A:193:ILE:HD13	2.16	0.45
1:A:448:GLU:HA	1:A:451:PRO:HG3	1.97	0.45
1:A:614:SER:HB2	1:A:621:ASN:ND2	2.31	0.45
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.99	0.45
2:E:322:PHE:HA	2:E:325:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:291:SER:HA	2:G:325:LEU:HD23	1.98	0.45
2:G:322:PHE:HA	2:G:325:LEU:CD1	2.47	0.45
2:H:267:TYR:CD1	2:H:268:LEU:HD12	2.51	0.45
1:A:630:SER:OG	1:A:740:HIS:NE2	2.35	0.45
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.16	0.45
1:C:401:THR:O	1:C:401:THR:CG2	2.60	0.45
2:E:28:LEU:HD13	2:E:46:LEU:HD22	1.98	0.45
2:F:15:HIS:O	2:F:294:THR:O	2.34	0.45
1:B:39:SER:O	1:B:39:SER:OG	2.33	0.45
1:B:742:ILE:O	1:B:742:ILE:HG22	2.16	0.45
2:F:17:HIS:HD2	2:F:295:ASP:O	1.99	0.45
2:H:39:PRO:HG3	2:H:67:TYR:CD2	2.50	0.45
1:D:145:GLU:OE2	1:D:145:GLU:N	2.50	0.45
2:H:294:THR:O	2:H:295:ASP:HB2	2.16	0.45
1:B:492:ARG:HH11	1:B:492:ARG:HB3	1.81	0.45
1:B:614:SER:HB2	1:B:621:ASN:ND2	2.32	0.45
1:D:336:ARG:NH1	2:H:128:GLU:HG2	2.32	0.45
2:E:267:TYR:CD1	2:E:268:LEU:HD12	2.52	0.45
1:C:332:GLU:OE1	1:C:332:GLU:HA	2.17	0.45
2:F:240:TYR:C	2:F:242:THR:H	2.19	0.45
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.90	0.45
1:B:215:TRP:CD2	1:B:303:VAL:HG21	2.52	0.45
1:B:287:ILE:C	1:B:288:THR:O	2.55	0.45
2:E:101:ARG:HA	2:E:151:ILE:O	2.17	0.45
2:G:218:VAL:O	2:G:218:VAL:HG13	2.16	0.45
2:G:280:VAL:HA	2:G:283:PHE:CD2	2.52	0.45
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.51	0.45
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.52	0.45
2:E:322:PHE:HA	2:E:325:LEU:CD1	2.47	0.45
2:G:267:TYR:CD1	2:G:268:LEU:HD12	2.51	0.45
1:B:630:SER:OG	1:B:740:HIS:NE2	2.39	0.44
1:C:192:ASP:O	1:C:193:ILE:HD13	2.17	0.44
2:F:272:TRP:NE1	2:F:278:HIS:HA	2.32	0.44
1:A:145:GLU:OE2	1:A:145:GLU:N	2.50	0.44
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.17	0.44
2:E:141:GLU:HG3	2:E:146:VAL:O	2.17	0.44
2:F:233:THR:OG1	2:F:235:ARG:O	2.32	0.44
1:A:630:SER:HB3	3:W:1:MET:SD	2.57	0.44
1:D:73:GLU:O	1:D:74:ASN:HB2	2.18	0.44
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.16	0.44
2:F:353:MET:HB2	2:F:354:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:HIS:CE1	2:G:214:HIS:CE1	3.06	0.44
2:G:23:LYS:HE2	2:G:23:LYS:HB3	1.80	0.44
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.53	0.44
2:E:86:PHE:CZ	2:E:100:VAL:HG13	2.52	0.44
2:F:267:TYR:HD1	2:F:268:LEU:HD12	1.83	0.44
2:G:99:GLU:HA	2:G:149:ARG:O	2.17	0.44
1:A:600:THR:OG1	1:A:601:PHE:N	2.50	0.44
1:B:145:GLU:N	1:B:145:GLU:OE2	2.50	0.44
1:D:215:TRP:CD2	1:D:303:VAL:HG21	2.52	0.44
1:D:317:ARG:HD2	1:D:322:TYR:HB3	2.00	0.44
1:D:333:SER:OG	1:D:334:SER:N	2.51	0.44
1:D:340:LEU:HD13	1:D:343:ARG:CD	2.36	0.44
2:E:99:GLU:HA	2:E:149:ARG:O	2.18	0.44
2:F:281:ILE:HD12	2:F:284:LYS:HD2	1.98	0.44
2:F:295:ASP:CB	2:F:300:PHE:HE2	2.31	0.44
1:A:317:ARG:HD2	1:A:322:TYR:HB3	2.00	0.44
1:B:272:ASN:C	1:B:272:ASN:ND2	2.71	0.44
1:B:600:THR:OG1	1:B:601:PHE:N	2.51	0.44
2:G:154:CYS:HB2	2:G:182:LEU:HD23	2.00	0.44
2:H:23:LYS:HE2	2:H:23:LYS:HB3	1.81	0.44
1:B:481:THR:OG1	1:B:483:HIS:HE1	2.00	0.44
2:F:86:PHE:CZ	2:F:100:VAL:HG13	2.53	0.44
2:H:15:HIS:CE1	2:H:214:HIS:CE1	3.06	0.44
2:H:322:PHE:HA	2:H:325:LEU:HD13	2.00	0.44
1:A:481:THR:OG1	1:A:483:HIS:HE1	2.00	0.43
1:B:448:GLU:HA	1:B:451:PRO:HG3	1.98	0.43
1:D:192:ASP:O	1:D:193:ILE:HD13	2.18	0.43
1:D:340:LEU:O	1:D:343:ARG:N	2.35	0.43
1:D:600:THR:OG1	1:D:601:PHE:N	2.51	0.43
2:G:76:ARG:O	2:G:79:ILE:N	2.50	0.43
1:B:92:ASN:OD1	1:B:92:ASN:N	2.51	0.43
1:B:317:ARG:HD2	1:B:322:TYR:HB3	2.00	0.43
2:G:240:TYR:C	2:G:242:THR:H	2.20	0.43
1:A:92:ASN:N	1:A:92:ASN:OD1	2.48	0.43
1:C:761:GLN:HE22	1:D:761:GLN:NE2	2.16	0.43
2:E:15:HIS:CE1	2:E:214:HIS:CE1	3.06	0.43
2:H:13:GLU:HB3	2:H:98:VAL:HG13	2.00	0.43
1:C:215:TRP:CD2	1:C:303:VAL:HG21	2.53	0.43
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.33	0.43
1:D:92:ASN:OD1	1:D:92:ASN:N	2.51	0.43
1:D:384:ILE:HG13	1:D:404:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:614:SER:HB2	1:D:621:ASN:ND2	2.33	0.43
1:D:742:ILE:O	1:D:742:ILE:HG22	2.18	0.43
2:F:156:ARG:HD2	2:F:185:ASP:C	2.38	0.43
2:G:55:PRO:HG3	2:G:267:TYR:CZ	2.53	0.43
1:A:718:GLN:NE2	1:A:718:GLN:HA	2.33	0.43
2:E:330:ALA:HB1	2:E:343:LEU:HD13	2.00	0.43
1:C:492:ARG:HB3	1:C:492:ARG:HH11	1.83	0.43
2:F:191:SER:HA	2:F:194:PHE:CE2	2.54	0.43
2:G:294:THR:HG23	2:G:297:PRO:CD	2.48	0.43
2:H:323:LYS:O	2:H:327:ILE:HG12	2.19	0.43
1:C:317:ARG:HD2	1:C:322:TYR:HB3	2.01	0.43
1:C:742:ILE:HG22	1:C:742:ILE:O	2.18	0.43
2:H:238:HIS:HB3	2:H:240:TYR:CE2	2.53	0.43
1:B:109:PRO:HG2	1:B:158:SER:O	2.18	0.43
1:C:732:ALA:HB1	1:D:734:TRP:CZ3	2.54	0.43
1:D:184:ARG:HD3	1:D:186:THR:O	2.19	0.43
2:E:113:GLU:HB2	2:E:161:TRP:NE1	2.33	0.43
1:D:336:ARG:CZ	2:H:128:GLU:HG2	2.49	0.43
2:E:13:GLU:HB3	2:E:98:VAL:HG13	2.01	0.43
2:G:86:PHE:CZ	2:G:100:VAL:HG13	2.54	0.43
2:G:113:GLU:CB	2:G:114:PRO:CD	2.96	0.43
2:H:86:PHE:O	2:H:89:MET:HG2	2.19	0.43
1:B:763:PHE:HB3	1:B:765:LEU:HD13	2.00	0.43
2:F:13:GLU:HB3	2:F:98:VAL:HG13	2.01	0.43
2:G:233:THR:OG1	2:G:235:ARG:O	2.30	0.43
1:C:536:LYS:HE2	1:C:536:LYS:HB3	1.89	0.42
1:D:401:THR:O	1:D:401:THR:CG2	2.61	0.42
2:F:169:CYS:HA	2:F:177:VAL:HG21	2.01	0.42
1:B:272:ASN:ND2	1:B:274:ASP:H	2.17	0.42
2:G:17:HIS:CD2	2:G:296:ASP:OD1	2.72	0.42
2:G:34:ARG:NH1	2:G:74:GLY:HA3	2.30	0.42
2:G:191:SER:HA	2:G:194:PHE:CE2	2.54	0.42
2:G:201:TYR:O	2:G:205:VAL:HG23	2.19	0.42
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.55	0.42
1:D:341:VAL:HG21	2:H:138:GLN:HB2	2.02	0.42
2:F:240:TYR:O	2:F:242:THR:N	2.50	0.42
1:A:272:ASN:C	1:A:272:ASN:ND2	2.72	0.42
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.01	0.42
1:B:401:THR:O	1:B:401:THR:CG2	2.60	0.42
2:F:114:PRO:O	2:F:115:ILE:C	2.57	0.42
2:G:76:ARG:O	2:G:77:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:ARG:HD2	2:H:185:ASP:C	2.39	0.42
2:H:233:THR:OG1	2:H:235:ARG:O	2.30	0.42
1:A:272:ASN:ND2	1:A:274:ASP:H	2.18	0.42
2:G:13:GLU:OE1	2:G:294:THR:HB	2.19	0.42
1:A:536:LYS:HE2	1:A:536:LYS:HB3	1.88	0.42
1:A:718:GLN:HE21	1:A:718:GLN:CA	2.32	0.42
1:D:436:LEU:HD12	1:D:436:LEU:HA	1.91	0.42
2:H:201:TYR:O	2:H:205:VAL:HG23	2.20	0.42
2:F:99:GLU:HA	2:F:149:ARG:O	2.19	0.42
2:F:283:PHE:HB3	2:F:288:VAL:CG1	2.48	0.42
1:C:600:THR:OG1	1:C:601:PHE:N	2.52	0.42
2:E:283:PHE:HB3	2:E:288:VAL:CG1	2.49	0.42
2:H:141:GLU:HA	2:H:146:VAL:O	2.19	0.42
1:B:453:ARG:HG3	1:B:476:GLY:HA3	2.01	0.42
1:D:272:ASN:C	1:D:272:ASN:ND2	2.72	0.42
2:F:39:PRO:HG3	2:F:67:TYR:CD2	2.49	0.42
2:F:100:VAL:O	2:F:151:ILE:N	2.45	0.42
2:G:156:ARG:HD2	2:G:185:ASP:C	2.40	0.42
2:G:267:TYR:HD1	2:G:268:LEU:HD12	1.85	0.42
2:G:325:LEU:C	2:G:325:LEU:HD22	2.40	0.42
2:H:109:ASN:OD1	2:H:122:GLY:HA2	2.20	0.42
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.96	0.41
1:C:230:ASP:OD1	1:C:264:PRO:HB3	2.20	0.41
1:C:272:ASN:ND2	1:C:274:ASP:H	2.17	0.41
2:E:116:PRO:O	2:E:119:GLN:HG2	2.19	0.41
2:F:86:PHE:O	2:F:89:MET:HG2	2.20	0.41
2:G:273:LYS:HA	2:G:274:PRO:HD3	1.95	0.41
2:H:154:CYS:HB2	2:H:182:LEU:HD23	2.00	0.41
1:A:425:MET:HA	1:A:426:PRO:HD3	1.81	0.41
1:C:109:PRO:HG2	1:C:158:SER:O	2.20	0.41
1:C:145:GLU:OE2	1:C:145:GLU:N	2.53	0.41
2:E:201:TYR:O	2:E:205:VAL:HG23	2.20	0.41
2:H:324:ARG:HH11	2:H:328:ASN:HD21	1.68	0.41
1:C:718:GLN:CA	1:C:718:GLN:HE21	2.32	0.41
2:E:154:CYS:HB2	2:E:182:LEU:HD23	2.02	0.41
2:F:325:LEU:HD22	2:F:326:ASN:N	2.35	0.41
1:A:626:ILE:O	1:A:650:GLY:HA2	2.21	0.41
2:E:267:TYR:HD1	2:E:268:LEU:HD12	1.86	0.41
2:F:23:LYS:HB3	2:F:23:LYS:HE2	1.81	0.41
2:G:16:VAL:HG23	2:G:295:ASP:O	2.20	0.41
2:G:169:CYS:HA	2:G:177:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:294:THR:O	2:H:295:ASP:CB	2.68	0.41
1:D:272:ASN:ND2	1:D:274:ASP:H	2.19	0.41
1:D:453:ARG:HG3	1:D:476:GLY:HA3	2.03	0.41
2:E:113:GLU:CB	2:E:114:PRO:CD	2.99	0.41
2:E:233:THR:OG1	2:E:235:ARG:O	2.32	0.41
2:G:13:GLU:HB3	2:G:98:VAL:HG13	2.02	0.41
2:G:39:PRO:HG3	2:G:67:TYR:CD2	2.50	0.41
2:E:78:ALA:O	2:E:82:ILE:HG23	2.21	0.41
2:F:150:SER:N	2:F:176:THR:O	2.29	0.41
2:H:4:THR:N	2:H:5:PRO:HD2	2.35	0.41
3:X:5:ASP:CG	3:X:5:ASP:O	2.58	0.41
1:C:248:TYR:HA	1:C:249:PRO:HD3	1.97	0.41
2:E:313:LYS:HD2	2:E:313:LYS:N	2.36	0.41
2:F:113:GLU:CB	2:F:114:PRO:HD3	2.51	0.41
2:G:86:PHE:O	2:G:89:MET:HG2	2.20	0.41
1:C:41:LYS:HB2	1:C:41:LYS:HE2	1.91	0.41
2:E:23:LYS:HE2	2:E:23:LYS:HB3	1.83	0.41
2:H:310:MET:O	2:H:314:ASP:HB2	2.21	0.41
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.55	0.41
1:A:453:ARG:HG3	1:A:476:GLY:HA3	2.03	0.41
1:B:192:ASP:O	1:B:193:ILE:HD13	2.20	0.41
1:D:254:VAL:HA	1:D:255:PRO:HD3	1.97	0.41
1:D:472:CYS:O	1:D:478:PRO:HA	2.21	0.41
2:E:169:CYS:HA	2:E:177:VAL:HG21	2.02	0.41
2:F:154:CYS:HB2	2:F:182:LEU:HD23	2.02	0.41
2:F:201:TYR:O	2:F:205:VAL:HG23	2.21	0.41
2:F:273:LYS:HA	2:F:274:PRO:HD3	1.92	0.41
2:G:109:ASN:O	2:G:122:GLY:HA2	2.21	0.41
2:H:267:TYR:HD1	2:H:268:LEU:HD12	1.85	0.41
5:M:1:NAG:O3	5:M:2:NAG:C7	2.69	0.41
1:A:384:ILE:HG13	1:A:404:VAL:HG21	2.02	0.41
1:C:331:ASP:O	1:C:332:GLU:C	2.58	0.41
2:F:20:GLY:O	2:F:298:LEU:HB3	2.21	0.41
2:F:114:PRO:HD2	2:F:161:TRP:HZ2	1.86	0.41
2:F:280:VAL:HA	2:F:283:PHE:CD1	2.51	0.41
1:A:742:ILE:HG22	1:A:742:ILE:O	2.21	0.40
1:D:512:LYS:NZ	1:D:556:ASP:O	2.49	0.40
1:D:536:LYS:HB3	1:D:536:LYS:HE2	1.88	0.40
2:E:100:VAL:O	2:E:151:ILE:N	2.47	0.40
2:G:278:HIS:ND1	2:G:279:ALA:N	2.70	0.40
1:C:184:ARG:HD3	1:C:186:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:LYS:HA	2:F:67:TYR:HD1	1.87	0.40
1:C:761:GLN:HE22	1:D:761:GLN:HE22	1.69	0.40
2:G:79:ILE:N	2:G:79:ILE:HD13	2.37	0.40
1:D:425:MET:HA	1:D:426:PRO:HD3	1.80	0.40
2:E:26:THR:HG21	2:E:85:GLU:OE1	2.21	0.40
2:E:113:GLU:CB	2:E:161:TRP:HE1	2.32	0.40
2:H:273:LYS:HE2	2:H:273:LYS:HB3	1.94	0.40
1:B:425:MET:HA	1:B:426:PRO:HD3	1.81	0.40
1:C:384:ILE:HG13	1:C:404:VAL:HG21	2.02	0.40
1:D:718:GLN:NE2	1:D:718:GLN:HA	2.37	0.40
2:F:26:THR:HG21	2:F:85:GLU:OE1	2.21	0.40
2:F:69:MET:N	2:F:70:PRO:CD	2.85	0.40
2:G:283:PHE:HB3	2:G:288:VAL:CG1	2.50	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:NZ	2:E:121:GLU:OE2[4_546]	1.77	0.43

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	726/728 (100%)	669 (92%)	55 (8%)	2 (0%)	41 73
1	B	726/728 (100%)	672 (93%)	52 (7%)	2 (0%)	41 73
1	C	726/728 (100%)	670 (92%)	55 (8%)	1 (0%)	51 83
1	D	726/728 (100%)	667 (92%)	55 (8%)	4 (1%)	25 62
2	E	350/363 (96%)	309 (88%)	34 (10%)	7 (2%)	7 34
2	F	350/363 (96%)	301 (86%)	37 (11%)	12 (3%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	350/363 (96%)	306 (87%)	34 (10%)	10 (3%)	4 25
2	H	350/363 (96%)	307 (88%)	36 (10%)	7 (2%)	7 34
3	W	4/9 (44%)	4 (100%)	0	0	100 100
3	X	4/9 (44%)	2 (50%)	2 (50%)	0	100 100
3	Y	4/9 (44%)	2 (50%)	1 (25%)	1 (25%)	0 0
3	Z	4/9 (44%)	3 (75%)	1 (25%)	0	100 100
All	All	4320/4400 (98%)	3912 (91%)	362 (8%)	46 (1%)	14 48

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	THR
1	D	341	VAL
2	E	113	GLU
2	F	351	TYR
2	F	354	PRO
2	G	5	PRO
2	G	111	LYS
2	G	354	PRO
2	H	283	PHE
2	H	354	PRO
3	Y	4	VAL
1	D	332	GLU
2	E	354	PRO
2	F	5	PRO
2	F	76	ARG
2	F	118	ASN
2	G	76	ARG
2	G	113	GLU
2	H	295	ASP
1	A	140	ARG
1	B	140	ARG
1	C	140	ARG
1	D	140	ARG
1	D	290	PRO
2	E	5	PRO
2	E	56	LEU
2	F	190	GLY
2	G	190	GLY
2	H	190	GLY

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Mol	Chain	Res	Type
2	H	238	HIS
2	E	190	GLY
2	G	77	ASP
2	G	118	ASN
2	G	295	ASP
2	E	238	HIS
2	E	295	ASP
2	F	115	ILE
2	F	238	HIS
2	F	241	HIS
2	H	336	PRO
2	F	114	PRO
2	F	189	GLU
2	F	296	ASP
2	G	297	PRO
1	A	295	ILE
2	H	353	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	653/653 (100%)	592 (91%)	61 (9%)	9 31
1	B	653/653 (100%)	594 (91%)	59 (9%)	9 32
1	C	653/653 (100%)	595 (91%)	58 (9%)	9 33
1	D	653/653 (100%)	590 (90%)	63 (10%)	8 29
2	E	307/315 (98%)	255 (83%)	52 (17%)	2 9
2	F	307/315 (98%)	260 (85%)	47 (15%)	2 12
2	G	307/315 (98%)	253 (82%)	54 (18%)	2 9
2	H	307/315 (98%)	249 (81%)	58 (19%)	1 7
3	W	6/9 (67%)	6 (100%)	0	100 100
3	X	6/9 (67%)	4 (67%)	2 (33%)	0 0
3	Y	6/9 (67%)	5 (83%)	1 (17%)	2 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Z	6/9 (67%)	4 (67%)	2 (33%)	0 0
All	All	3864/3908 (99%)	3407 (88%)	457 (12%)	5 21

All (457) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	41	LYS
1	A	61	ARG
1	A	76	ILE
1	A	78	VAL
1	A	92	ASN
1	A	93	SER
1	A	114	ILE
1	A	144	THR
1	A	170	ASN
1	A	184	ARG
1	A	214	LEU
1	A	223	LEU
1	A	246	LEU
1	A	253	ARG
1	A	272	ASN
1	A	292	SER
1	A	303	VAL
1	A	318	ARG
1	A	326	ASP
1	A	339	CYS
1	A	350	THR
1	A	351	THR
1	A	358	ARG
1	A	361	GLU
1	A	377	ASN
1	A	385	CYS
1	A	391	LYS
1	A	399	LYS
1	A	410	LEU
1	A	429	ARG
1	A	436	LEU
1	A	462	SER
1	A	471	ARG
1	A	472	CYS

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Mol	Chain	Res	Type
1	A	482	LEU
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	521	GLU
1	A	522	THR
1	A	523	LYS
1	A	536	LYS
1	A	543	LEU
1	A	598	LEU
1	A	603	VAL
1	A	608	GLU
1	A	615	LYS
1	A	621	ASN
1	A	622	LYS
1	A	658	ARG
1	A	663	ASP
1	A	673	LEU
1	A	679	ASN
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	710	ASN
1	A	731	GLN
1	A	749	GLN
1	B	41	LYS
1	B	61	ARG
1	B	71	LYS
1	B	76	ILE
1	B	78	VAL
1	B	93	SER
1	B	114	ILE
1	B	144	THR
1	B	170	ASN
1	B	184	ARG
1	B	214	LEU
1	B	223	LEU
1	B	246	LEU
1	B	253	ARG
1	B	272	ASN
1	B	290	PRO
1	B	303	VAL

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Mol	Chain	Res	Type
1	B	318	ARG
1	B	326	ASP
1	B	338	ASN
1	B	340	LEU
1	B	350	THR
1	B	351	THR
1	B	358	ARG
1	B	361	GLU
1	B	377	ASN
1	B	385	CYS
1	B	391	LYS
1	B	399	LYS
1	B	410	LEU
1	B	429	ARG
1	B	436	LEU
1	B	462	SER
1	B	471	ARG
1	B	472	CYS
1	B	482	LEU
1	B	492	ARG
1	B	505	GLN
1	B	507	VAL
1	B	521	GLU
1	B	522	THR
1	B	523	LYS
1	B	536	LYS
1	B	543	LEU
1	B	598	LEU
1	B	603	VAL
1	B	608	GLU
1	B	615	LYS
1	B	621	ASN
1	B	622	LYS
1	B	658	ARG
1	B	673	LEU
1	B	679	ASN
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	710	ASN
1	B	731	GLN
1	B	749	GLN

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Mol	Chain	Res	Type
1	C	40	ARG
1	C	41	LYS
1	C	61	ARG
1	C	76	ILE
1	C	78	VAL
1	C	93	SER
1	C	114	ILE
1	C	144	THR
1	C	170	ASN
1	C	184	ARG
1	C	214	LEU
1	C	223	LEU
1	C	246	LEU
1	C	253	ARG
1	C	272	ASN
1	C	303	VAL
1	C	318	ARG
1	C	326	ASP
1	C	340	LEU
1	C	350	THR
1	C	351	THR
1	C	358	ARG
1	C	361	GLU
1	C	377	ASN
1	C	385	CYS
1	C	391	LYS
1	C	399	LYS
1	C	410	LEU
1	C	429	ARG
1	C	436	LEU
1	C	462	SER
1	C	471	ARG
1	C	472	CYS
1	C	482	LEU
1	C	492	ARG
1	C	505	GLN
1	C	507	VAL
1	C	521	GLU
1	C	522	THR
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU

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Mol	Chain	Res	Type
1	C	598	LEU
1	C	603	VAL
1	C	608	GLU
1	C	615	LYS
1	C	621	ASN
1	C	622	LYS
1	C	658	ARG
1	C	663	ASP
1	C	673	LEU
1	C	679	ASN
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	710	ASN
1	C	731	GLN
1	C	749	GLN
1	D	39	SER
1	D	40	ARG
1	D	41	LYS
1	D	61	ARG
1	D	71	LYS
1	D	76	ILE
1	D	78	VAL
1	D	93	SER
1	D	114	ILE
1	D	144	THR
1	D	170	ASN
1	D	184	ARG
1	D	214	LEU
1	D	223	LEU
1	D	246	LEU
1	D	253	ARG
1	D	272	ASN
1	D	283	THR
1	D	285	ILE
1	D	292	SER
1	D	303	VAL
1	D	318	ARG
1	D	326	ASP
1	D	333	SER
1	D	339	CYS
1	D	340	LEU

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Mol	Chain	Res	Type
1	D	350	THR
1	D	351	THR
1	D	358	ARG
1	D	361	GLU
1	D	377	ASN
1	D	385	CYS
1	D	391	LYS
1	D	399	LYS
1	D	410	LEU
1	D	429	ARG
1	D	436	LEU
1	D	471	ARG
1	D	472	CYS
1	D	482	LEU
1	D	492	ARG
1	D	505	GLN
1	D	507	VAL
1	D	521	GLU
1	D	522	THR
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	598	LEU
1	D	603	VAL
1	D	608	GLU
1	D	615	LYS
1	D	621	ASN
1	D	622	LYS
1	D	658	ARG
1	D	673	LEU
1	D	679	ASN
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	710	ASN
1	D	731	GLN
1	D	749	GLN
2	E	4	THR
2	E	5	PRO
2	E	18	LEU
2	E	19	ASP
2	E	38	LEU

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Mol	Chain	Res	Type
2	E	44	GLU
2	E	45	GLU
2	E	47	LEU
2	E	53	ASP
2	E	54	LYS
2	E	56	LEU
2	E	58	LEU
2	E	60	ASP
2	E	92	LYS
2	E	98	VAL
2	E	100	VAL
2	E	124	LEU
2	E	125	THR
2	E	128	GLU
2	E	131	SER
2	E	132	LEU
2	E	146	VAL
2	E	160	SER
2	E	164	GLU
2	E	171	LYS
2	E	177	VAL
2	E	182	LEU
2	E	189	GLU
2	E	206	LYS
2	E	212	THR
2	E	231	LEU
2	E	251	ARG
2	E	252	LEU
2	E	254	GLN
2	E	276	THR
2	E	282	ARG
2	E	286	ASP
2	E	295	ASP
2	E	306	THR
2	E	311	THR
2	E	313	LYS
2	E	320	GLU
2	E	324	ARG
2	E	325	LEU
2	E	335	LEU
2	E	341	LYS
2	E	343	LEU

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Mol	Chain	Res	Type
2	E	345	ASP
2	E	347	LEU
2	E	349	LYS
2	E	353	MET
2	E	355	SER
2	F	4	THR
2	F	18	LEU
2	F	19	ASP
2	F	38	LEU
2	F	44	GLU
2	F	45	GLU
2	F	47	LEU
2	F	53	ASP
2	F	54	LYS
2	F	58	LEU
2	F	60	ASP
2	F	92	LYS
2	F	98	VAL
2	F	100	VAL
2	F	112	VAL
2	F	124	LEU
2	F	125	THR
2	F	146	VAL
2	F	160	SER
2	F	164	GLU
2	F	171	LYS
2	F	177	VAL
2	F	182	LEU
2	F	189	GLU
2	F	206	LYS
2	F	212	THR
2	F	231	LEU
2	F	251	ARG
2	F	252	LEU
2	F	254	GLN
2	F	276	THR
2	F	286	ASP
2	F	306	THR
2	F	311	THR
2	F	313	LYS
2	F	320	GLU
2	F	324	ARG

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Mol	Chain	Res	Type
2	F	325	LEU
2	F	335	LEU
2	F	341	LYS
2	F	343	LEU
2	F	345	ASP
2	F	347	LEU
2	F	349	LYS
2	F	351	TYR
2	F	352	ARG
2	F	354	PRO
2	G	4	THR
2	G	5	PRO
2	G	18	LEU
2	G	19	ASP
2	G	38	LEU
2	G	44	GLU
2	G	45	GLU
2	G	47	LEU
2	G	53	ASP
2	G	54	LYS
2	G	56	LEU
2	G	58	LEU
2	G	60	ASP
2	G	75	CYS
2	G	92	LYS
2	G	98	VAL
2	G	100	VAL
2	G	112	VAL
2	G	124	LEU
2	G	125	THR
2	G	131	SER
2	G	146	VAL
2	G	160	SER
2	G	164	GLU
2	G	171	LYS
2	G	177	VAL
2	G	182	LEU
2	G	189	GLU
2	G	206	LYS
2	G	212	THR
2	G	231	LEU
2	G	251	ARG

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Mol	Chain	Res	Type
2	G	252	LEU
2	G	254	GLN
2	G	276	THR
2	G	282	ARG
2	G	286	ASP
2	G	295	ASP
2	G	296	ASP
2	G	303	THR
2	G	306	THR
2	G	311	THR
2	G	315	MET
2	G	320	GLU
2	G	324	ARG
2	G	325	LEU
2	G	331	LYS
2	G	335	LEU
2	G	341	LYS
2	G	343	LEU
2	G	345	ASP
2	G	347	LEU
2	G	349	LYS
2	G	355	SER
2	H	18	LEU
2	H	19	ASP
2	H	38	LEU
2	H	44	GLU
2	H	45	GLU
2	H	47	LEU
2	H	53	ASP
2	H	54	LYS
2	H	56	LEU
2	H	58	LEU
2	H	60	ASP
2	H	75	CYS
2	H	76	ARG
2	H	92	LYS
2	H	98	VAL
2	H	100	VAL
2	H	111	LYS
2	H	112	VAL
2	H	124	LEU
2	H	125	THR

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Mol	Chain	Res	Type
2	H	127	ASP
2	H	128	GLU
2	H	131	SER
2	H	132	LEU
2	H	141	GLU
2	H	146	VAL
2	H	160	SER
2	H	164	GLU
2	H	171	LYS
2	H	177	VAL
2	H	182	LEU
2	H	189	GLU
2	H	206	LYS
2	H	212	THR
2	H	231	LEU
2	H	251	ARG
2	H	252	LEU
2	H	254	GLN
2	H	276	THR
2	H	281	ILE
2	H	283	PHE
2	H	286	ASP
2	H	295	ASP
2	H	303	THR
2	H	306	THR
2	H	313	LYS
2	H	314	ASP
2	H	315	MET
2	H	320	GLU
2	H	324	ARG
2	H	325	LEU
2	H	335	LEU
2	H	341	LYS
2	H	343	LEU
2	H	345	ASP
2	H	347	LEU
2	H	349	LYS
2	H	352	ARG
3	X	4	VAL
3	X	5	ASP
3	Y	4	VAL
3	Z	4	VAL

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Mol	Chain	Res	Type
3	Z	5	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	75	ASN
1	A	170	ASN
1	A	272	ASN
1	A	314	GLN
1	A	369	ASN
1	A	377	ASN
1	A	435	GLN
1	A	483	HIS
1	A	621	ASN
1	A	679	ASN
1	A	682	HIS
1	A	694	ASN
1	A	710	ASN
1	A	718	GLN
1	A	731	GLN
1	A	749	GLN
1	A	757	HIS
1	B	51	ASN
1	B	75	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	338	ASN
1	B	345	HIS
1	B	369	ASN
1	B	377	ASN
1	B	483	HIS
1	B	621	ASN
1	B	679	ASN
1	B	682	HIS
1	B	694	ASN
1	B	710	ASN
1	B	718	GLN
1	B	731	GLN
1	B	749	GLN

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Mol	Chain	Res	Type
1	B	757	HIS
1	B	761	GLN
1	C	51	ASN
1	C	72	GLN
1	C	75	ASN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	314	GLN
1	C	338	ASN
1	C	345	HIS
1	C	369	ASN
1	C	377	ASN
1	C	483	HIS
1	C	621	ASN
1	C	679	ASN
1	C	682	HIS
1	C	694	ASN
1	C	710	ASN
1	C	718	GLN
1	C	731	GLN
1	C	749	GLN
1	D	51	ASN
1	D	75	ASN
1	D	170	ASN
1	D	247	GLN
1	D	272	ASN
1	D	314	GLN
1	D	369	ASN
1	D	377	ASN
1	D	483	HIS
1	D	621	ASN
1	D	679	ASN
1	D	682	HIS
1	D	694	ASN
1	D	710	ASN
1	D	718	GLN
1	D	731	GLN
1	D	749	GLN
1	D	761	GLN
2	E	48	ASN
2	E	197	HIS

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Mol	Chain	Res	Type
2	E	309	GLN
2	F	48	ASN
2	F	134	ASN
2	F	197	HIS
2	F	210	HIS
2	G	48	ASN
2	G	134	ASN
2	H	48	ASN
2	H	134	ASN
2	H	197	HIS
2	H	328	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

46 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	I	1	1,4	14,14,15	0.51	0	17,19,21	1.97	3 (17%)
4	NAG	I	2	4	14,14,15	0.54	0	17,19,21	2.52	8 (47%)
4	FUL	I	3	4	10,10,11	0.61	0	14,14,16	2.32	5 (35%)
5	NAG	J	1	1,5	14,14,15	0.57	0	17,19,21	1.86	6 (35%)
5	NAG	J	2	5	14,14,15	0.66	0	17,19,21	1.77	6 (35%)
5	NAG	K	1	1,5	14,14,15	0.61	0	17,19,21	2.19	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	K	2	5	14,14,15	0.55	0	17,19,21	1.59	2 (11%)
6	NAG	L	1	1,6	14,14,15	0.75	0	17,19,21	1.70	4 (23%)
6	NAG	L	2	6	14,14,15	0.63	0	17,19,21	1.54	3 (17%)
6	BMA	L	3	6	11,11,12	0.69	0	15,15,17	2.41	4 (26%)
6	MAN	L	4	6	11,11,12	0.64	0	15,15,17	2.16	4 (26%)
5	NAG	M	1	1,5	14,14,15	0.62	0	17,19,21	1.53	3 (17%)
5	NAG	M	2	5	14,14,15	0.75	0	17,19,21	1.71	4 (23%)
7	NAG	N	1	1,7	14,14,15	0.47	0	17,19,21	2.71	5 (29%)
7	FUL	N	2	7	10,10,11	0.88	0	14,14,16	2.07	4 (28%)
5	NAG	O	1	1,5	14,14,15	0.49	0	17,19,21	2.72	7 (41%)
5	NAG	O	2	5	14,14,15	0.65	0	17,19,21	1.65	4 (23%)
6	NAG	P	1	1,6	14,14,15	0.75	0	17,19,21	2.09	6 (35%)
6	NAG	P	2	6	14,14,15	0.78	1 (7%)	17,19,21	1.20	2 (11%)
6	BMA	P	3	6	11,11,12	0.74	0	15,15,17	2.33	5 (33%)
6	MAN	P	4	6	11,11,12	0.61	0	15,15,17	1.95	2 (13%)
5	NAG	Q	1	1,5	14,14,15	0.90	0	17,19,21	2.23	7 (41%)
5	NAG	Q	2	5	14,14,15	0.47	0	17,19,21	2.09	2 (11%)
4	NAG	R	1	1,4	14,14,15	0.60	0	17,19,21	1.30	1 (5%)
4	NAG	R	2	4	14,14,15	0.54	0	17,19,21	2.24	4 (23%)
4	FUL	R	3	4	10,10,11	0.65	0	14,14,16	1.92	3 (21%)
5	NAG	S	1	1,5	14,14,15	0.72	0	17,19,21	3.08	5 (29%)
5	NAG	S	2	5	14,14,15	0.49	0	17,19,21	1.75	5 (29%)
5	NAG	T	1	1,5	14,14,15	0.46	0	17,19,21	2.39	6 (35%)
5	NAG	T	2	5	14,14,15	0.56	0	17,19,21	1.93	6 (35%)
6	NAG	U	1	1,6	14,14,15	0.70	0	17,19,21	2.43	6 (35%)
6	NAG	U	2	6	14,14,15	0.67	0	17,19,21	1.27	3 (17%)
6	BMA	U	3	6	11,11,12	0.52	0	15,15,17	1.73	3 (20%)
6	MAN	U	4	6	11,11,12	0.51	0	15,15,17	2.40	7 (46%)
5	NAG	V	1	1,5	14,14,15	0.70	0	17,19,21	2.43	6 (35%)
5	NAG	V	2	5	14,14,15	0.56	0	17,19,21	1.66	4 (23%)
7	NAG	a	1	1,7	14,14,15	0.70	1 (7%)	17,19,21	2.41	7 (41%)
7	FUL	a	2	7	10,10,11	0.93	0	14,14,16	2.72	6 (42%)
5	NAG	b	1	1,5	14,14,15	0.69	0	17,19,21	1.60	3 (17%)
5	NAG	b	2	5	14,14,15	0.73	0	17,19,21	2.03	8 (47%)
6	NAG	c	1	1,6	14,14,15	0.68	0	17,19,21	2.76	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	c	2	6	14,14,15	0.59	0	17,19,21	1.47	2 (11%)
6	BMA	c	3	6	11,11,12	0.59	0	15,15,17	2.19	6 (40%)
6	MAN	c	4	6	11,11,12	0.65	0	15,15,17	1.91	4 (26%)
5	NAG	d	1	1,5	14,14,15	0.57	0	17,19,21	2.61	6 (35%)
5	NAG	d	2	5	14,14,15	0.68	0	17,19,21	2.02	4 (23%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUL	R	3	4	-	-	0/1/1/1
5	NAG	S	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	3/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	U	2	6	-	3/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	2/2/19/22	1/1/1/1
5	NAG	V	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	V	2	5	-	3/6/23/26	0/1/1/1
7	NAG	a	1	1,7	-	5/6/23/26	0/1/1/1
7	FUL	a	2	7	-	-	0/1/1/1
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	3/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1
6	BMA	c	3	6	-	2/2/19/22	0/1/1/1
6	MAN	c	4	6	-	2/2/19/22	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	2	NAG	O5-C1	-2.11	1.40	1.43
7	a	1	NAG	C1-C2	2.07	1.55	1.52

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1	NAG	C1-O5-C5	8.90	124.25	112.19
6	c	1	NAG	C1-C2-N2	-8.78	95.49	110.49
5	S	1	NAG	C1-O5-C5	8.36	123.52	112.19
5	d	1	NAG	C1-O5-C5	7.55	122.42	112.19
5	O	1	NAG	C1-O5-C5	7.49	122.34	112.19
5	Q	2	NAG	C1-O5-C5	7.16	121.89	112.19
4	R	2	NAG	C1-O5-C5	7.00	121.67	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	3	FUL	C1-C2-C3	-6.63	101.52	109.67
5	T	1	NAG	C1-O5-C5	6.39	120.85	112.19
6	L	3	BMA	O3-C3-C2	6.28	122.02	109.99
4	I	1	NAG	O5-C5-C6	5.96	116.54	107.20
6	U	4	MAN	C1-O5-C5	5.95	120.25	112.19
4	I	2	NAG	O5-C1-C2	-5.91	101.96	111.29
7	a	1	NAG	O5-C5-C6	5.80	116.30	107.20
6	c	3	BMA	C3-C4-C5	5.52	120.08	110.24
5	S	1	NAG	C3-C4-C5	5.50	120.05	110.24
7	a	2	FUL	C1-C2-C3	-5.48	102.93	109.67
6	P	4	MAN	O5-C1-C2	-5.39	102.44	110.77
5	K	1	NAG	C1-O5-C5	5.39	119.49	112.19
4	R	3	FUL	C1-C2-C3	5.19	116.05	109.67
7	a	2	FUL	C3-C4-C5	5.19	117.85	109.77
5	K	2	NAG	C1-O5-C5	5.18	119.20	112.19
5	d	2	NAG	C8-C7-N2	5.06	124.67	116.10
5	S	1	NAG	O5-C1-C2	4.79	118.85	111.29
6	U	1	NAG	C1-C2-N2	4.70	118.52	110.49
5	V	1	NAG	C1-C2-N2	4.70	118.52	110.49
5	V	1	NAG	C1-O5-C5	4.62	118.45	112.19
6	U	1	NAG	C1-O5-C5	4.62	118.45	112.19
6	P	1	NAG	O4-C4-C5	-4.56	97.98	109.30
5	O	1	NAG	O5-C1-C2	4.50	118.39	111.29
5	T	1	NAG	O5-C1-C2	4.46	118.34	111.29
6	L	4	MAN	O5-C5-C6	4.46	114.19	107.20
5	Q	1	NAG	C2-N2-C7	4.37	129.12	122.90
6	L	4	MAN	C1-O5-C5	4.34	118.08	112.19
5	S	2	NAG	C1-O5-C5	4.30	118.02	112.19
6	L	3	BMA	O5-C5-C6	4.13	113.68	107.20
7	N	2	FUL	C3-C4-C5	4.11	116.17	109.77
5	V	2	NAG	C4-C3-C2	-4.10	105.01	111.02
4	I	2	NAG	C1-C2-N2	4.09	117.48	110.49
6	U	1	NAG	O5-C1-C2	-4.08	104.85	111.29
5	V	1	NAG	O5-C1-C2	-4.07	104.86	111.29
6	P	3	BMA	O3-C3-C2	4.05	117.75	109.99
5	b	1	NAG	C4-C3-C2	4.04	116.94	111.02
6	U	4	MAN	C1-C2-C3	-4.01	104.74	109.67
6	P	3	BMA	O3-C3-C4	4.01	119.62	110.35
5	J	2	NAG	C1-O5-C5	3.99	117.60	112.19
4	I	2	NAG	C1-O5-C5	3.98	117.59	112.19
5	d	1	NAG	C2-N2-C7	3.96	128.54	122.90
5	S	1	NAG	O4-C4-C3	3.96	119.49	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	3	BMA	O5-C5-C6	3.95	113.39	107.20
5	d	1	NAG	C3-C4-C5	3.94	117.26	110.24
6	U	3	BMA	O5-C5-C6	3.93	113.37	107.20
4	R	1	NAG	C4-C3-C2	3.75	116.52	111.02
7	a	1	NAG	C2-N2-C7	3.68	128.15	122.90
6	U	3	BMA	O5-C1-C2	-3.68	105.10	110.77
5	T	2	NAG	O5-C1-C2	-3.64	105.55	111.29
5	Q	1	NAG	C1-O5-C5	3.63	117.11	112.19
6	P	3	BMA	C1-C2-C3	-3.56	105.29	109.67
5	K	1	NAG	O5-C1-C2	-3.54	105.70	111.29
6	c	4	MAN	O2-C2-C3	3.54	117.23	110.14
7	a	2	FUL	C1-O5-C5	-3.52	104.80	112.78
6	P	1	NAG	C2-N2-C7	-3.51	117.91	122.90
5	K	1	NAG	C8-C7-N2	3.51	122.03	116.10
5	Q	1	NAG	C8-C7-N2	3.48	121.99	116.10
7	a	2	FUL	C6-C5-C4	3.47	119.49	113.07
6	P	1	NAG	C1-O5-C5	3.45	116.86	112.19
5	M	2	NAG	O5-C1-C2	-3.45	105.84	111.29
6	L	1	NAG	O5-C1-C2	-3.45	105.85	111.29
4	I	1	NAG	C3-C4-C5	-3.44	104.10	110.24
6	L	4	MAN	C1-C2-C3	3.41	113.86	109.67
6	c	4	MAN	C2-C3-C4	3.40	116.78	110.89
5	T	2	NAG	O5-C5-C6	3.40	112.53	107.20
5	J	1	NAG	C4-C3-C2	3.38	115.97	111.02
6	c	1	NAG	O4-C4-C3	-3.37	102.56	110.35
5	Q	1	NAG	O5-C5-C6	-3.35	101.96	107.20
5	b	1	NAG	C3-C4-C5	3.33	116.19	110.24
7	N	1	NAG	C2-N2-C7	-3.31	118.20	122.90
6	L	4	MAN	O3-C3-C2	3.28	116.27	109.99
5	O	2	NAG	C1-C2-N2	-3.27	104.89	110.49
5	Q	2	NAG	O5-C5-C6	3.26	112.32	107.20
6	c	4	MAN	C1-O5-C5	3.26	116.60	112.19
6	c	3	BMA	C1-O5-C5	3.25	116.60	112.19
5	d	2	NAG	O5-C5-C6	3.25	112.30	107.20
5	O	2	NAG	C4-C3-C2	3.21	115.73	111.02
5	S	1	NAG	C4-C3-C2	3.20	115.71	111.02
5	T	2	NAG	C3-C4-C5	-3.20	104.53	110.24
6	L	2	NAG	C1-O5-C5	3.20	116.52	112.19
5	M	2	NAG	C1-O5-C5	3.18	116.51	112.19
5	M	1	NAG	C1-O5-C5	3.18	116.50	112.19
5	b	2	NAG	O5-C5-C6	3.18	112.19	107.20
5	b	2	NAG	O5-C1-C2	3.18	116.30	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1	NAG	C3-C4-C5	-3.17	104.58	110.24
5	T	1	NAG	C4-C3-C2	3.17	115.66	111.02
6	L	1	NAG	C1-O5-C5	3.16	116.48	112.19
5	b	2	NAG	O7-C7-C8	-3.15	116.22	122.06
6	c	1	NAG	O7-C7-C8	3.14	127.89	122.06
7	a	1	NAG	C1-C2-N2	3.14	115.84	110.49
5	T	1	NAG	O5-C5-C4	3.13	118.44	110.83
5	O	1	NAG	O5-C5-C4	3.11	118.39	110.83
7	a	1	NAG	C4-C3-C2	-3.08	106.50	111.02
6	U	4	MAN	C2-C3-C4	-3.07	105.58	110.89
5	J	1	NAG	C1-O5-C5	3.06	116.33	112.19
7	N	2	FUL	O2-C2-C1	3.05	115.40	109.15
6	P	1	NAG	O5-C5-C6	3.05	111.98	107.20
4	I	2	NAG	C3-C4-C5	3.04	115.67	110.24
7	N	2	FUL	O3-C3-C4	3.02	117.33	110.35
6	c	2	NAG	C4-C3-C2	-3.00	106.62	111.02
7	N	2	FUL	C6-C5-C4	2.97	118.56	113.07
5	J	2	NAG	O4-C4-C5	2.95	116.63	109.30
4	I	2	NAG	O5-C5-C6	2.92	111.78	107.20
6	c	4	MAN	O5-C1-C2	-2.91	106.27	110.77
5	S	2	NAG	O5-C5-C6	2.91	111.76	107.20
5	d	2	NAG	O7-C7-C8	-2.89	116.68	122.06
6	c	2	NAG	O3-C3-C2	2.89	115.45	109.47
6	U	1	NAG	O7-C7-N2	-2.89	116.64	121.95
6	L	2	NAG	O5-C1-C2	-2.88	106.73	111.29
5	V	1	NAG	O7-C7-N2	-2.88	116.66	121.95
5	Q	1	NAG	C4-C3-C2	2.88	115.23	111.02
5	M	1	NAG	O5-C1-C2	-2.87	106.75	111.29
5	V	2	NAG	C2-N2-C7	2.87	126.99	122.90
4	I	3	FUL	O3-C3-C4	2.85	116.94	110.35
5	J	1	NAG	O4-C4-C5	-2.84	102.23	109.30
5	J	2	NAG	O7-C7-C8	-2.82	116.82	122.06
5	K	1	NAG	O5-C5-C6	-2.81	102.79	107.20
6	P	2	NAG	O4-C4-C3	-2.80	103.88	110.35
4	R	3	FUL	O5-C5-C6	2.79	113.34	107.33
7	a	2	FUL	O2-C2-C3	2.78	115.70	110.14
5	O	1	NAG	C1-C2-N2	-2.75	105.79	110.49
5	b	2	NAG	C8-C7-N2	2.74	120.74	116.10
6	U	1	NAG	O4-C4-C3	-2.73	104.04	110.35
7	a	2	FUL	O5-C1-C2	-2.73	106.56	110.77
5	V	1	NAG	O4-C4-C3	-2.73	104.05	110.35
5	V	2	NAG	O5-C5-C6	2.71	111.46	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	1	NAG	C3-C4-C5	2.71	115.07	110.24
6	L	2	NAG	C3-C4-C5	-2.70	105.42	110.24
5	M	1	NAG	C3-C4-C5	-2.68	105.46	110.24
5	T	2	NAG	C2-N2-C7	2.66	126.69	122.90
6	P	3	BMA	C6-C5-C4	2.66	119.24	113.00
7	a	1	NAG	O5-C1-C2	2.65	115.48	111.29
6	P	1	NAG	C8-C7-N2	2.65	120.58	116.10
5	d	1	NAG	O5-C5-C6	2.64	111.35	107.20
6	U	2	NAG	C2-N2-C7	-2.63	119.16	122.90
6	P	4	MAN	C1-O5-C5	2.61	115.73	112.19
5	T	2	NAG	O4-C4-C5	2.60	115.74	109.30
5	T	2	NAG	O3-C3-C2	2.58	114.81	109.47
4	R	2	NAG	C2-N2-C7	2.57	126.57	122.90
5	b	2	NAG	C1-O5-C5	2.56	115.67	112.19
7	N	1	NAG	O4-C4-C5	2.55	115.62	109.30
5	K	1	NAG	O7-C7-C8	-2.55	117.33	122.06
5	d	1	NAG	C4-C3-C2	2.53	114.72	111.02
5	J	1	NAG	C2-N2-C7	2.50	126.47	122.90
5	V	2	NAG	C1-O5-C5	2.49	115.57	112.19
5	V	1	NAG	C8-C7-N2	2.49	120.31	116.10
5	d	2	NAG	C4-C3-C2	-2.47	107.40	111.02
6	U	1	NAG	C8-C7-N2	2.47	120.28	116.10
5	O	1	NAG	O4-C4-C3	-2.47	104.65	110.35
4	I	3	FUL	O2-C2-C1	2.45	114.17	109.15
5	Q	1	NAG	C6-C5-C4	2.45	118.74	113.00
5	S	2	NAG	O7-C7-C8	-2.45	117.52	122.06
4	R	2	NAG	C4-C3-C2	2.44	114.60	111.02
6	c	3	BMA	O3-C3-C2	2.44	114.66	109.99
6	L	3	BMA	O6-C6-C5	2.43	119.62	111.29
6	U	3	BMA	O3-C3-C2	2.42	114.62	109.99
6	c	1	NAG	O5-C1-C2	2.41	115.09	111.29
5	O	1	NAG	C4-C3-C2	2.40	114.53	111.02
5	J	2	NAG	C8-C7-N2	2.39	120.15	116.10
6	c	3	BMA	C1-C2-C3	-2.39	106.72	109.67
4	I	3	FUL	O5-C1-C2	-2.36	107.13	110.77
5	J	1	NAG	O5-C1-C2	2.31	114.94	111.29
6	c	1	NAG	C8-C7-N2	-2.31	112.18	116.10
5	Q	1	NAG	O7-C7-C8	-2.31	117.78	122.06
6	U	4	MAN	O3-C3-C4	2.29	115.65	110.35
5	M	2	NAG	O5-C5-C6	2.29	110.80	107.20
6	L	1	NAG	O5-C5-C6	2.29	110.79	107.20
5	M	2	NAG	O7-C7-C8	-2.29	117.81	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	1	NAG	C6-C5-C4	2.28	118.35	113.00
4	I	2	NAG	C4-C3-C2	-2.28	107.67	111.02
6	L	1	NAG	O7-C7-C8	-2.28	117.83	122.06
4	R	2	NAG	O5-C1-C2	2.28	114.88	111.29
5	b	1	NAG	C2-N2-C7	-2.27	119.67	122.90
5	O	2	NAG	O4-C4-C5	2.27	114.92	109.30
5	b	2	NAG	C2-N2-C7	2.26	126.12	122.90
5	J	2	NAG	C1-C2-N2	2.26	114.35	110.49
5	b	2	NAG	C3-C4-C5	-2.25	106.23	110.24
5	T	1	NAG	O4-C4-C3	-2.25	105.16	110.35
7	N	1	NAG	C4-C3-C2	-2.24	107.73	111.02
6	U	2	NAG	O5-C5-C4	-2.21	105.44	110.83
5	O	2	NAG	C1-O5-C5	-2.20	109.21	112.19
4	I	2	NAG	O6-C6-C5	2.20	118.85	111.29
4	I	1	NAG	O6-C6-C5	2.20	118.83	111.29
5	d	1	NAG	O7-C7-N2	2.19	125.98	121.95
5	S	2	NAG	C8-C7-N2	2.19	119.81	116.10
6	U	4	MAN	O5-C1-C2	2.18	114.13	110.77
6	L	3	BMA	C1-C2-C3	-2.15	107.02	109.67
5	b	2	NAG	O5-C5-C4	-2.15	105.60	110.83
5	J	2	NAG	O3-C3-C4	-2.14	105.39	110.35
6	c	3	BMA	O5-C5-C6	2.13	110.54	107.20
7	a	1	NAG	O3-C3-C2	2.11	113.83	109.47
6	c	3	BMA	O4-C4-C5	-2.11	104.06	109.30
4	I	2	NAG	O3-C3-C2	2.08	113.77	109.47
6	U	4	MAN	O5-C5-C6	2.07	110.46	107.20
5	T	1	NAG	C3-C4-C5	2.07	113.93	110.24
7	a	1	NAG	O6-C6-C5	2.07	118.38	111.29
6	P	2	NAG	C4-C3-C2	-2.06	108.00	111.02
4	I	3	FUL	C3-C4-C5	2.05	112.97	109.77
5	S	2	NAG	C4-C3-C2	-2.04	108.03	111.02
6	U	2	NAG	C4-C3-C2	-2.03	108.05	111.02
6	U	4	MAN	C6-C5-C4	2.03	117.75	113.00
5	K	2	NAG	C1-C2-N2	2.02	113.94	110.49
6	P	1	NAG	C6-C5-C4	-2.02	108.28	113.00
4	R	3	FUL	O5-C1-C2	2.00	113.86	110.77

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	V	2	NAG	C3-C2-N2-C7
5	b	1	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
5	d	2	NAG	C8-C7-N2-C2
5	d	2	NAG	O7-C7-N2-C2
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	c	1	NAG	C8-C7-N2-C2
6	c	1	NAG	O7-C7-N2-C2
7	a	1	NAG	C8-C7-N2-C2
7	a	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
6	U	4	MAN	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C4-C5-C6-O6
6	U	4	MAN	C4-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C8-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
4	I	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
6	c	3	BMA	O5-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
4	R	2	NAG	O7-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	b	2	NAG	C1-C2-N2-C7
6	c	4	MAN	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
6	c	4	MAN	C4-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
6	P	4	MAN	C4-C5-C6-O6
6	c	3	BMA	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
5	V	1	NAG	C1-C2-N2-C7
6	U	1	NAG	C1-C2-N2-C7
6	P	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C1-C2-N2-C7
5	J	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	U	3	BMA	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C8-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	4	MAN	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
5	Q	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
5	T	2	NAG	C1-C2-N2-C7
5	Q	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O7-C7-N2-C2
6	U	3	BMA	C4-C5-C6-O6
5	M	2	NAG	O7-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
5	d	2	NAG	C1-C2-N2-C7
5	O	1	NAG	C3-C2-N2-C7
6	U	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
7	a	1	NAG	C1-C2-N2-C7
6	c	2	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6

All (1) ring outliers are listed below:

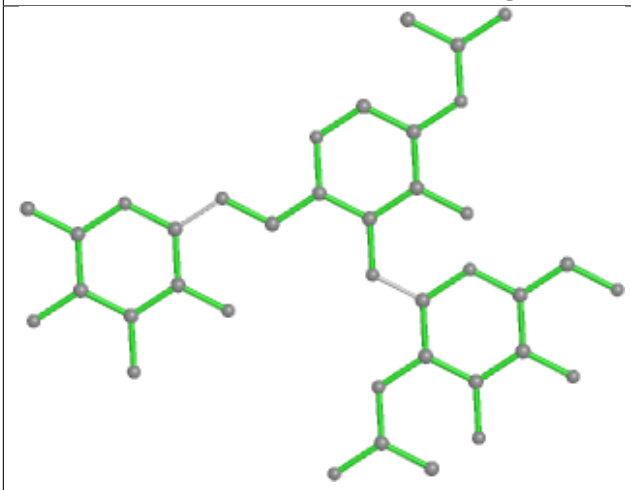
Mol	Chain	Res	Type	Atoms
6	U	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 6 short contacts:

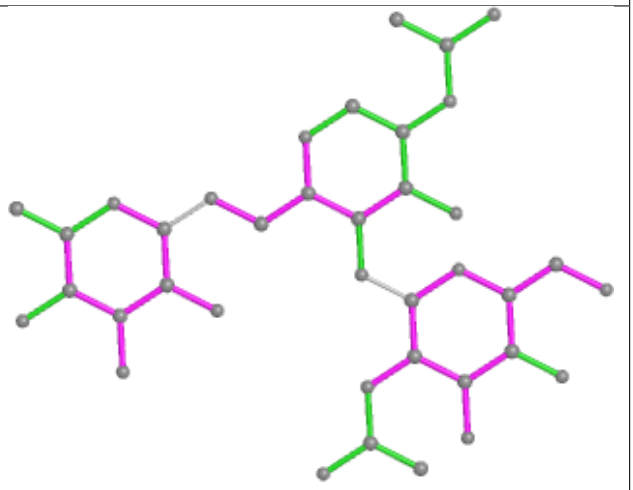
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	2	NAG	4	0
6	L	1	NAG	1	0
5	M	1	NAG	4	0
5	S	2	NAG	1	0

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

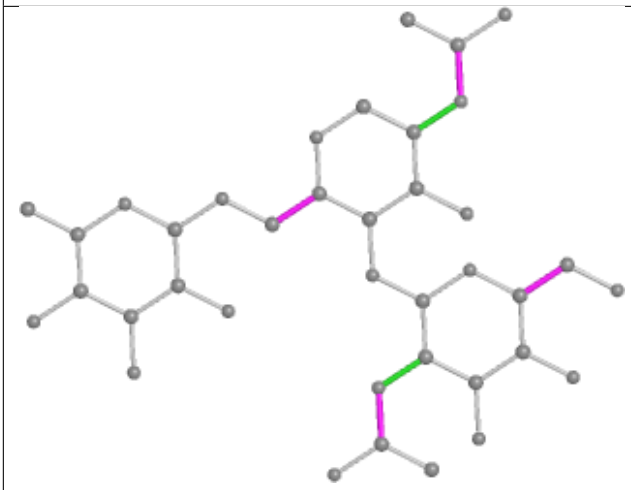
Oligosaccharide Chain I



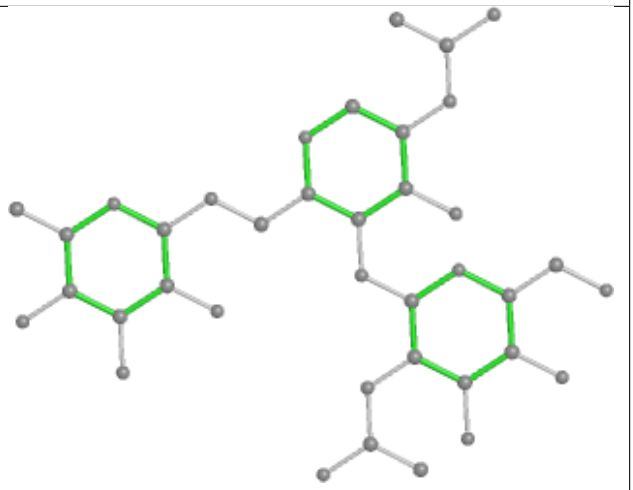
Bond lengths



Bond angles

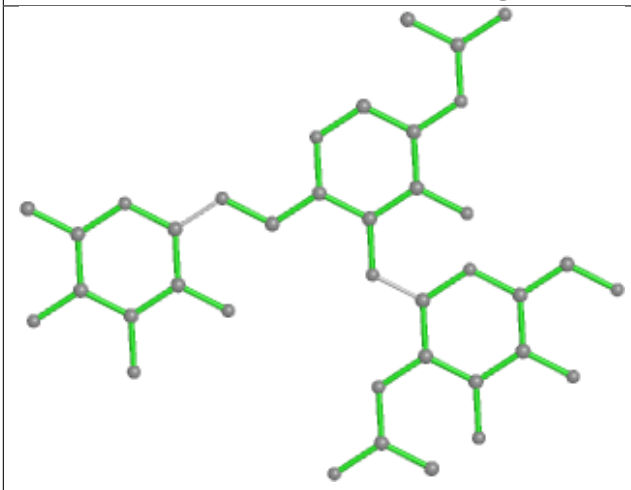


Torsions

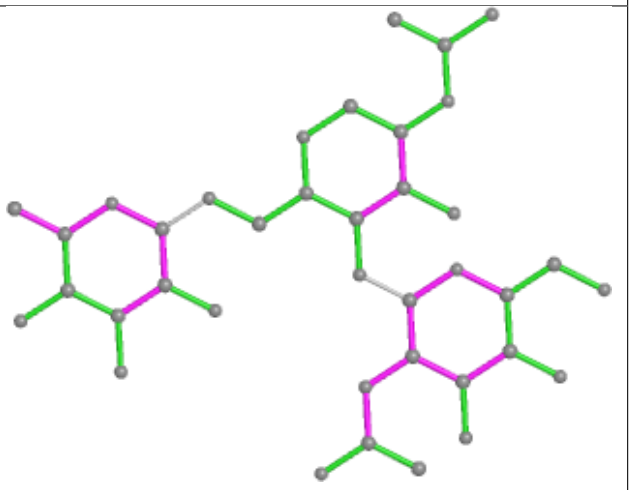


Rings

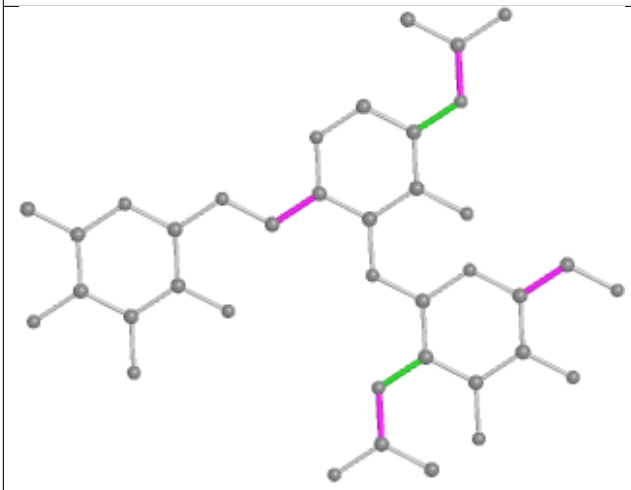
Oligosaccharide Chain R



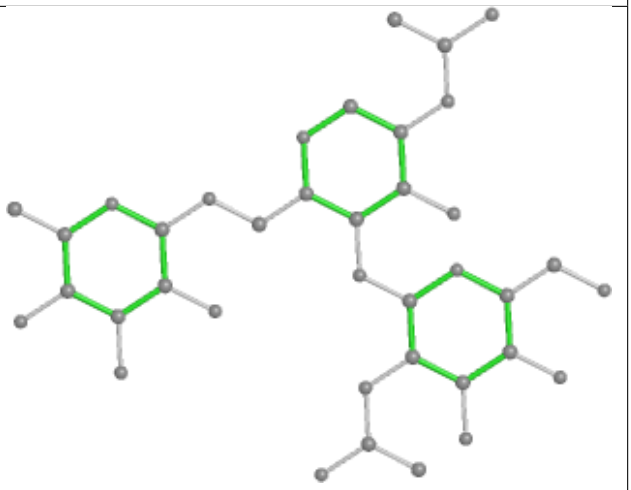
Bond lengths



Bond angles

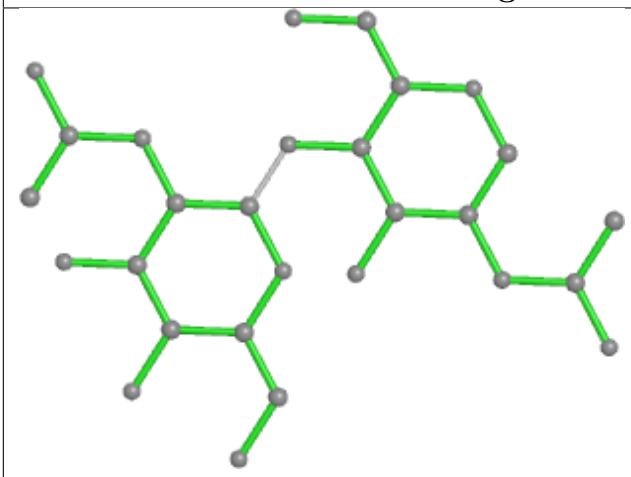


Torsions



Rings

Oligosaccharide Chain J



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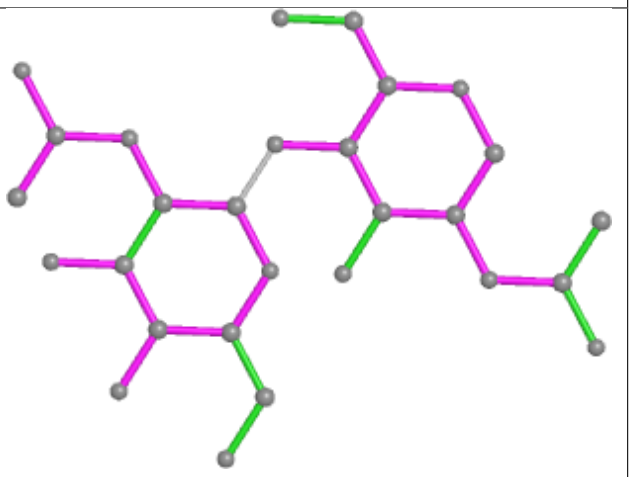

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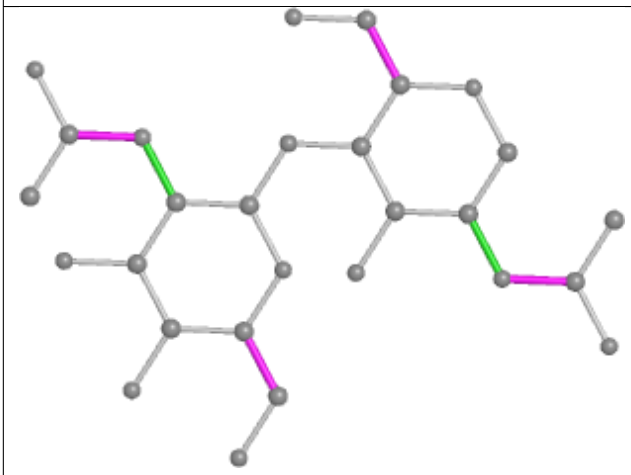

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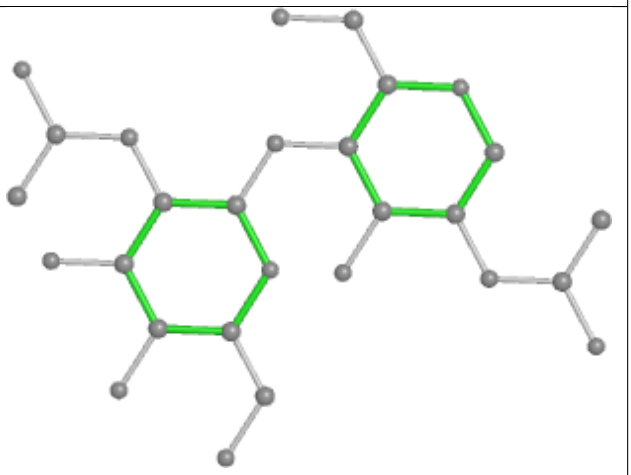
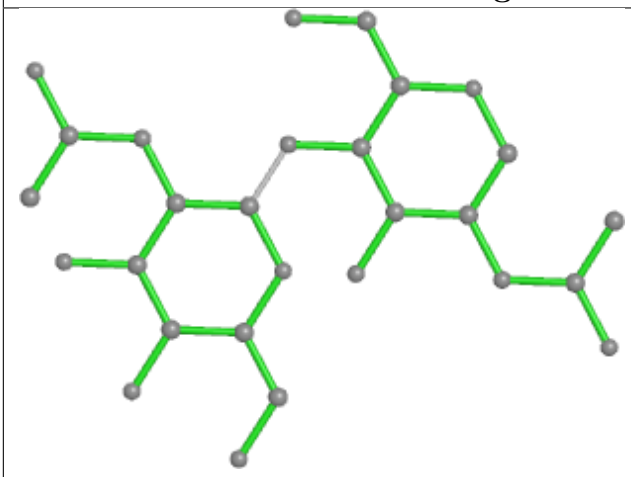


Rings

Oligosaccharide Chain K



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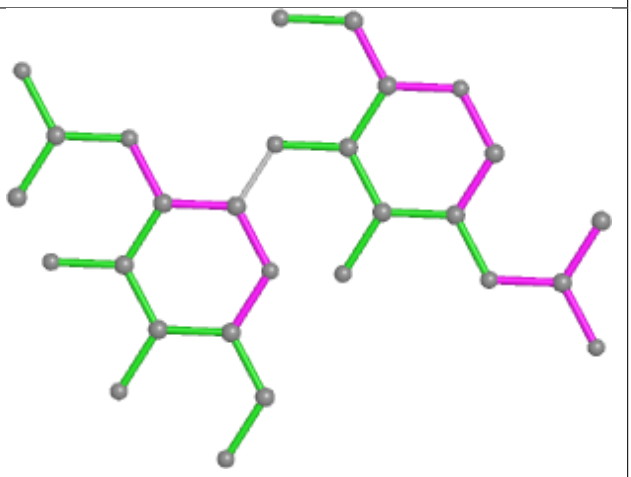
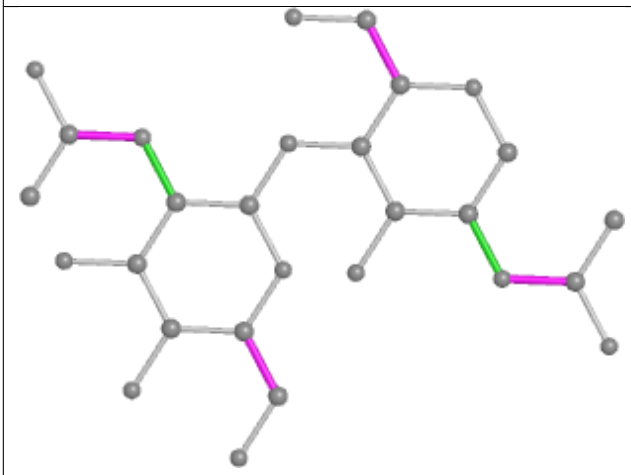


Bond angles



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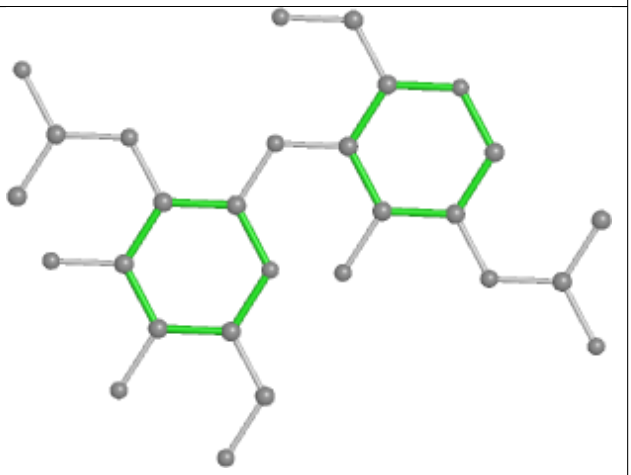
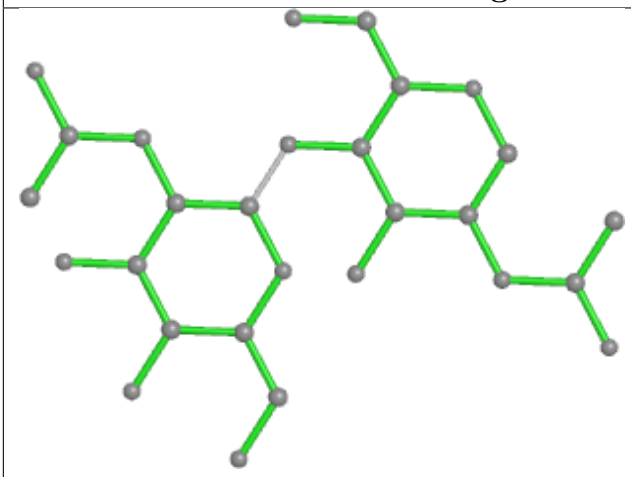


Rings

Oligosaccharide Chain M



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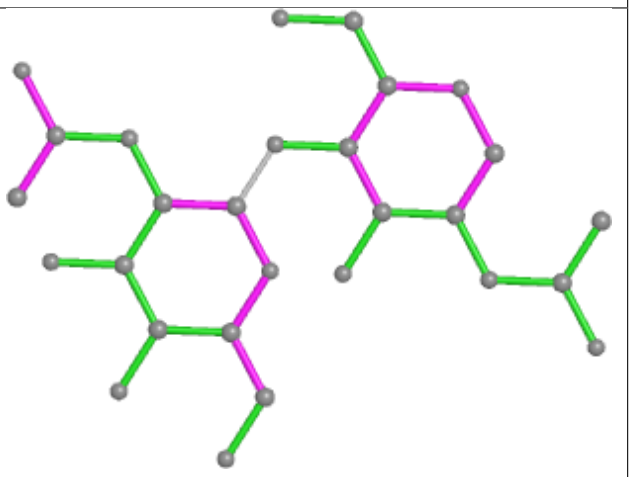
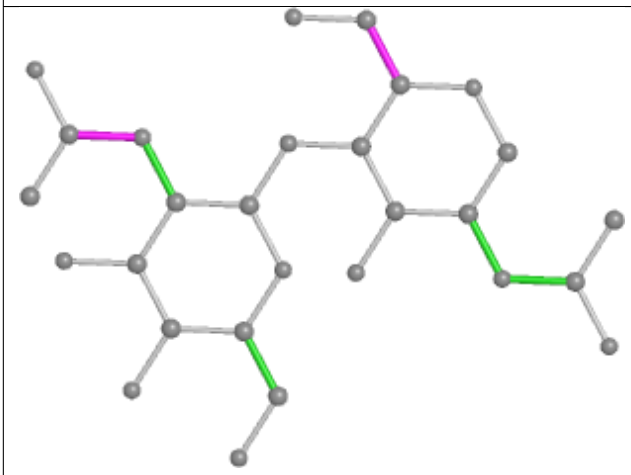


Bond angles



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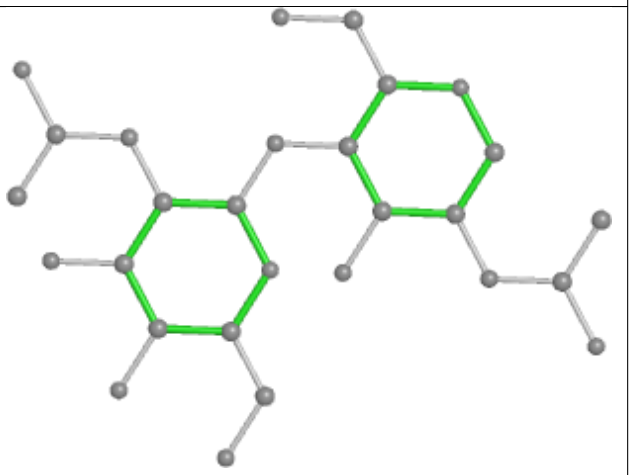
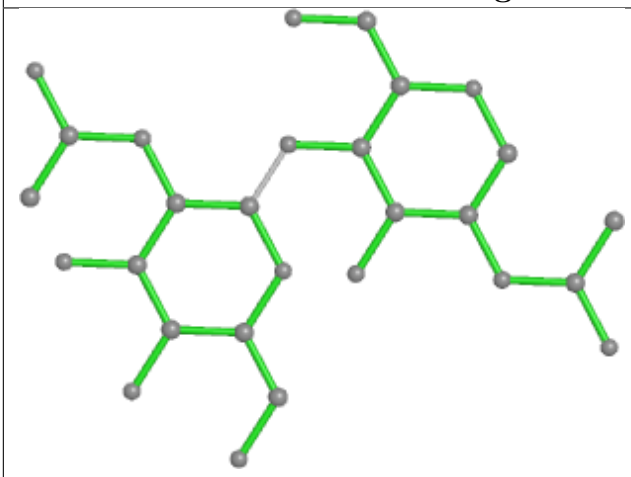


Rings

Oligosaccharide Chain O



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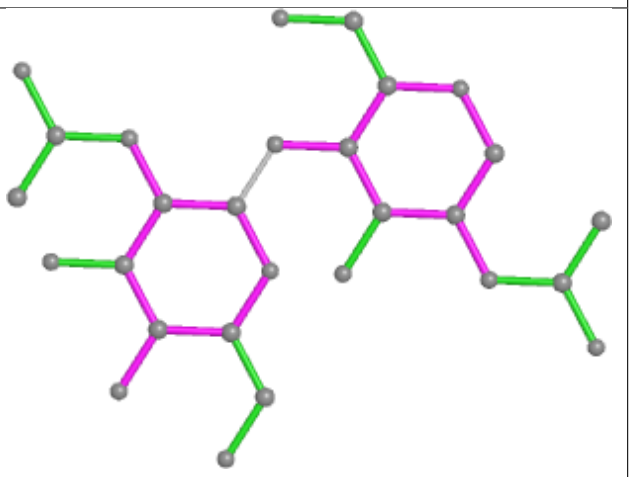

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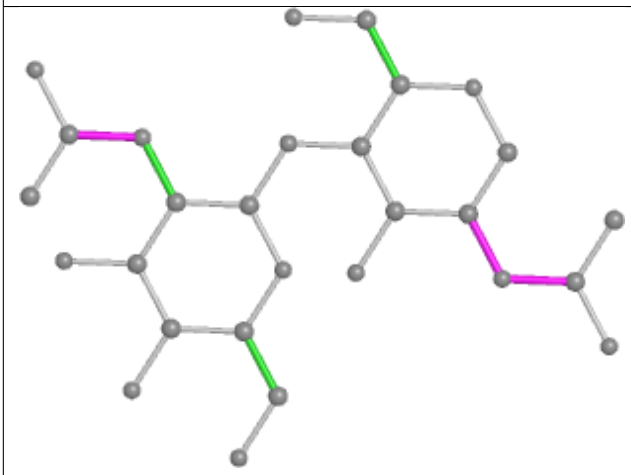

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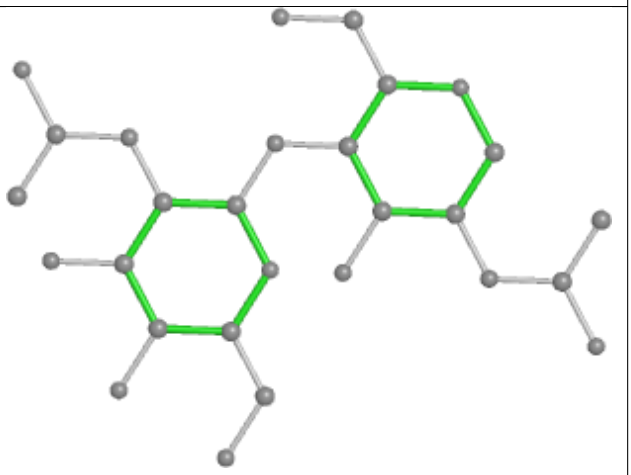
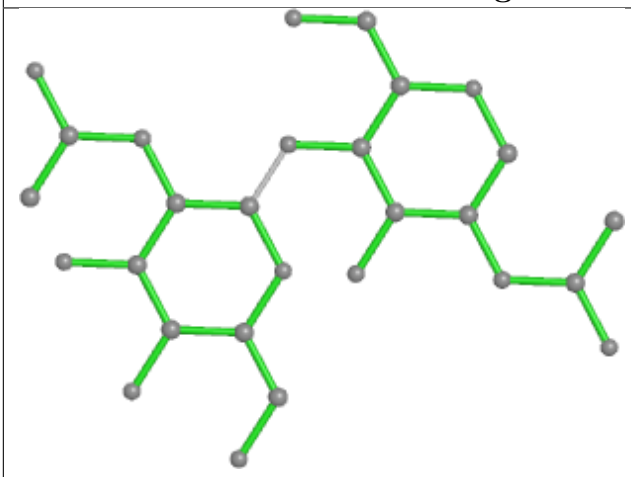


Rings

Oligosaccharide Chain Q



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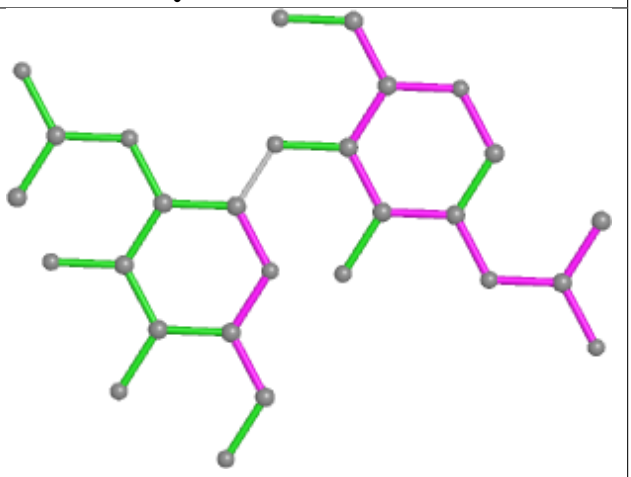

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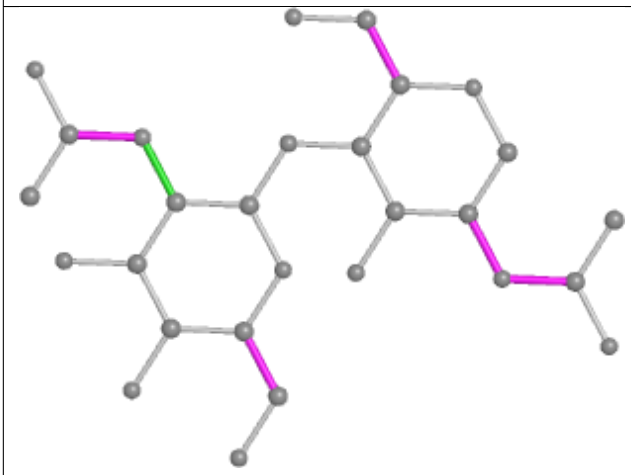

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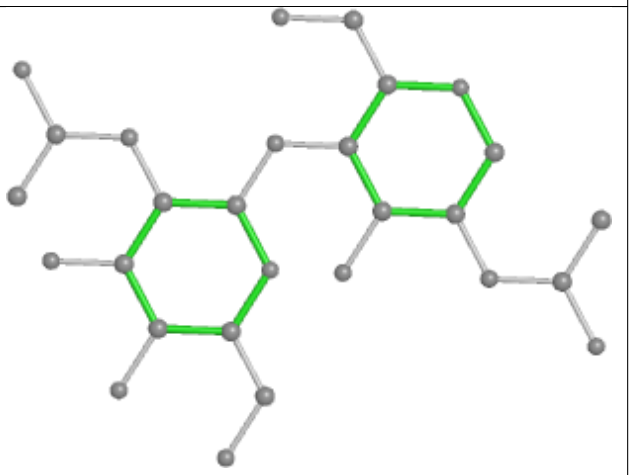
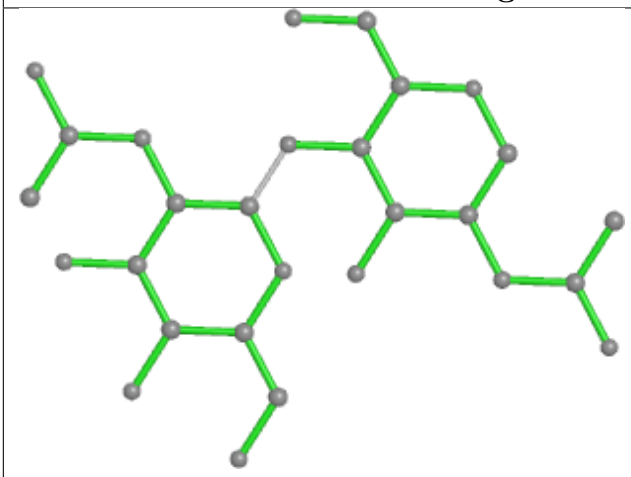


Rings

Oligosaccharide Chain S



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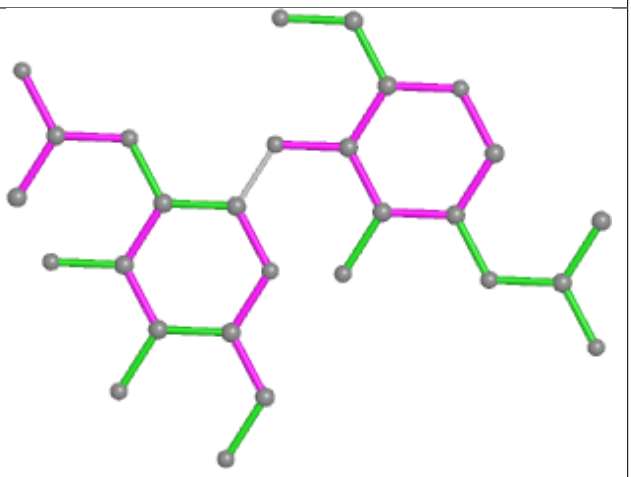

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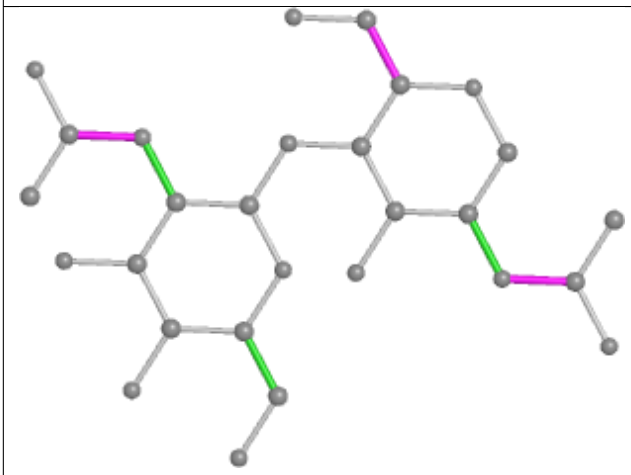

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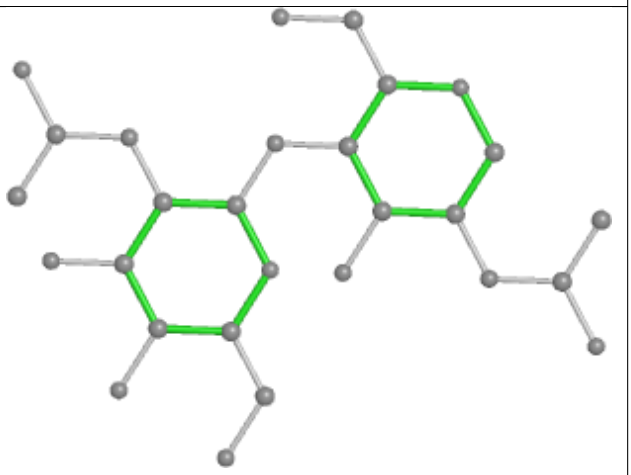
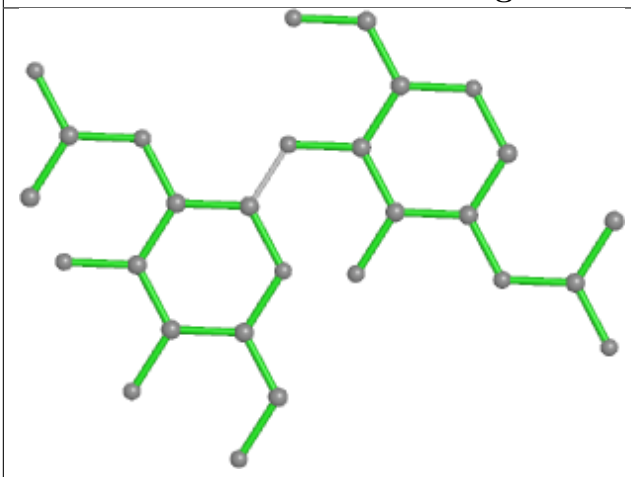


Rings

Oligosaccharide Chain T



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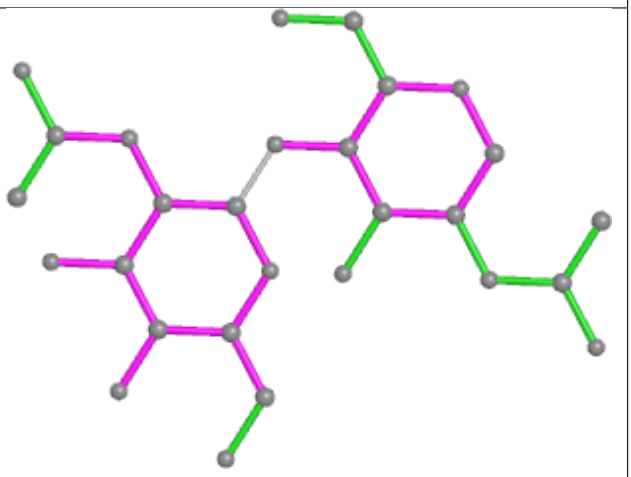

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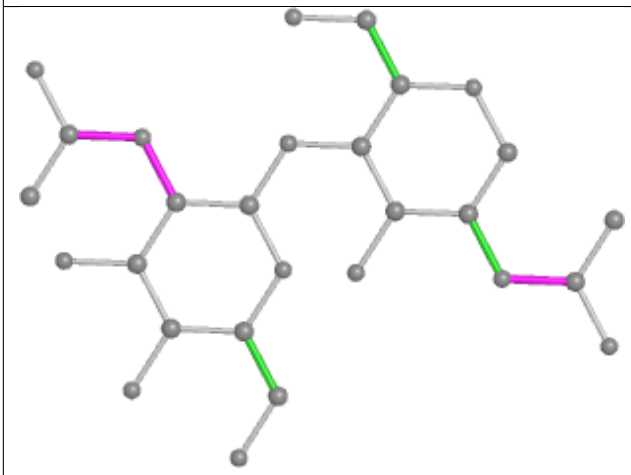

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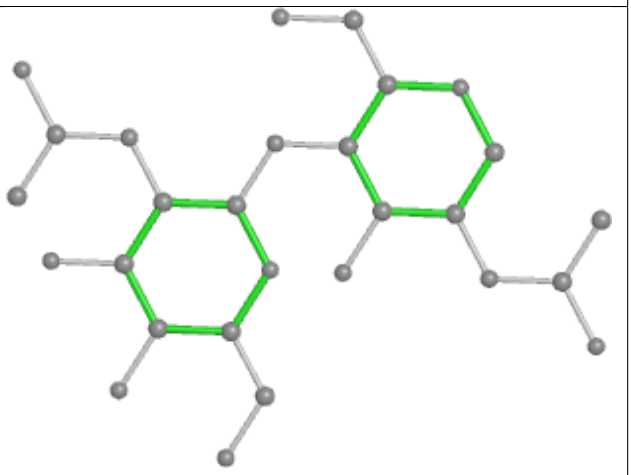
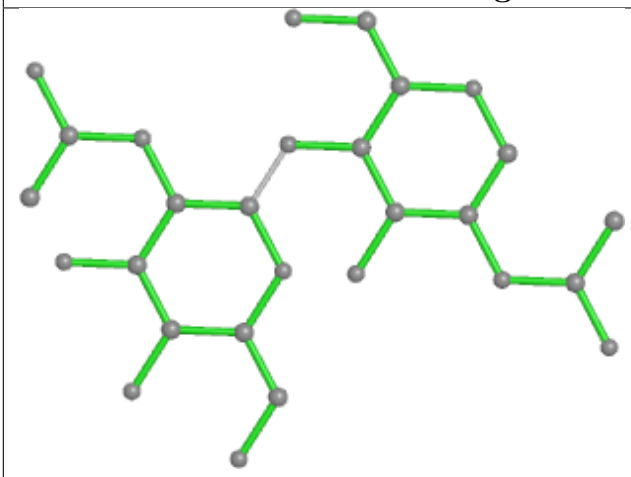


Rings

Oligosaccharide Chain V



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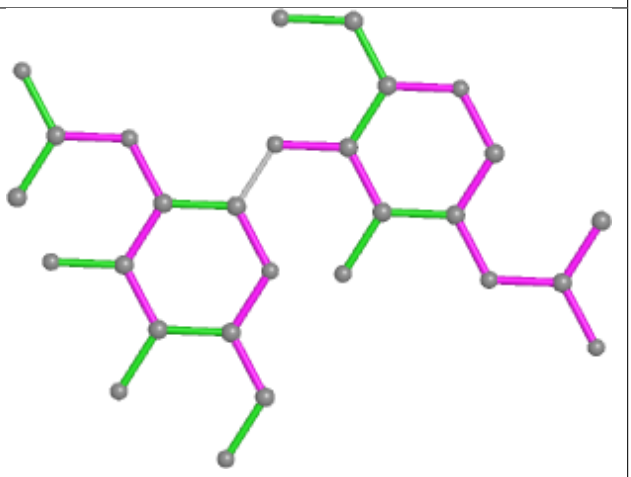

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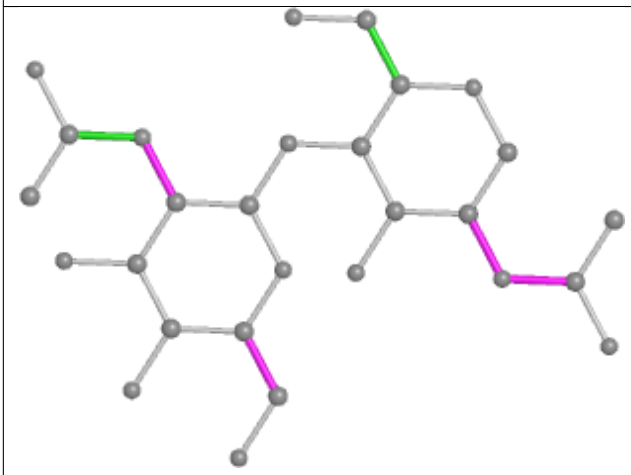

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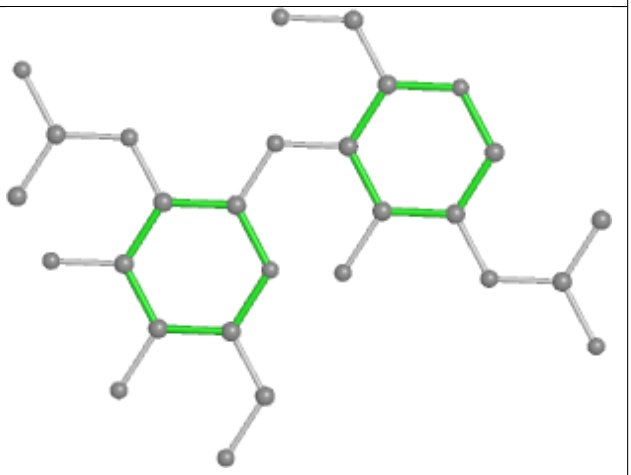
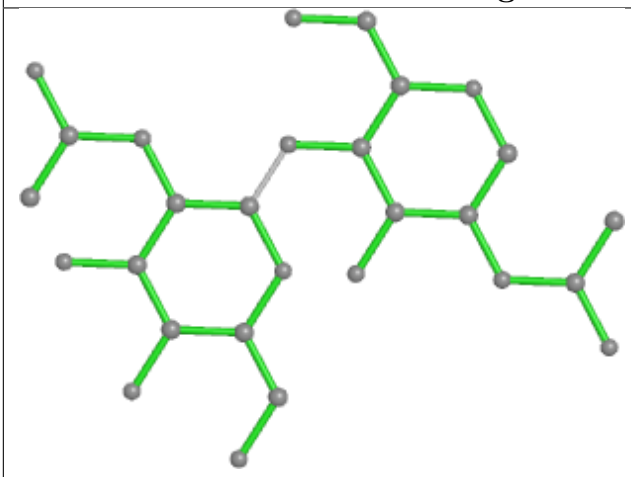


Rings

Oligosaccharide Chain b



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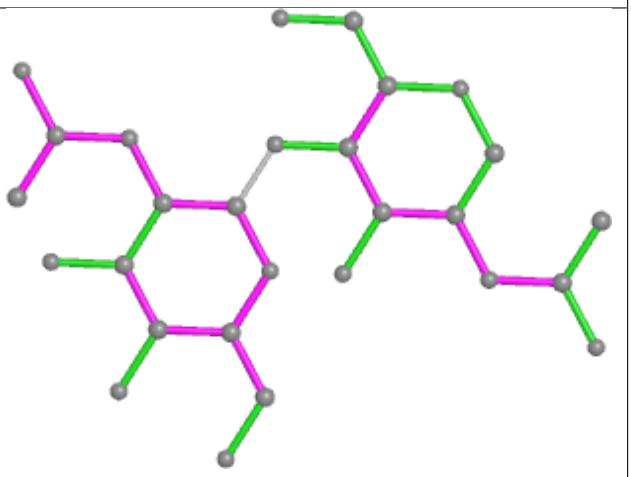

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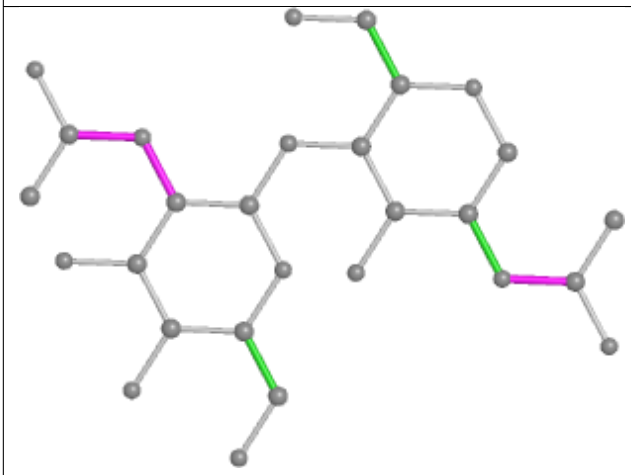

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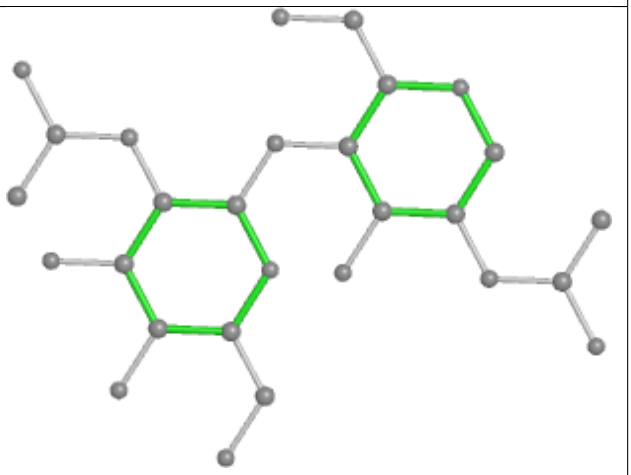
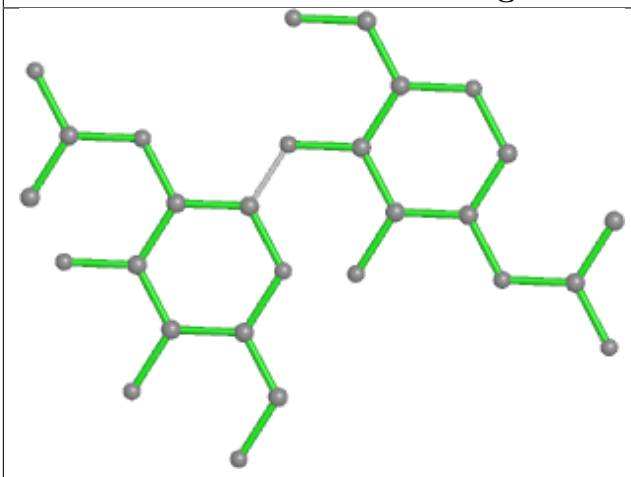


Rings

Oligosaccharide Chain d



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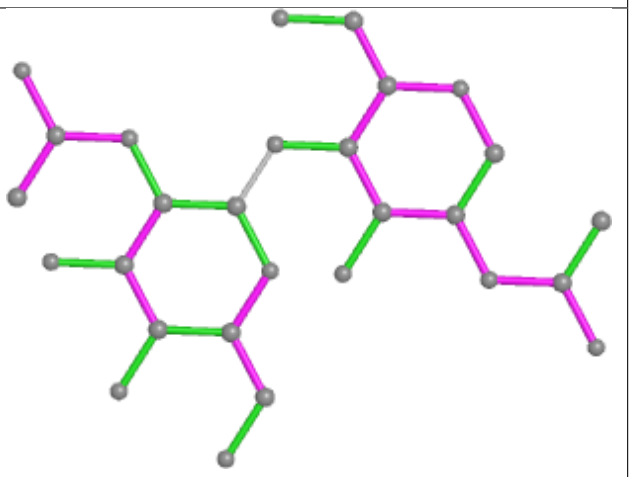
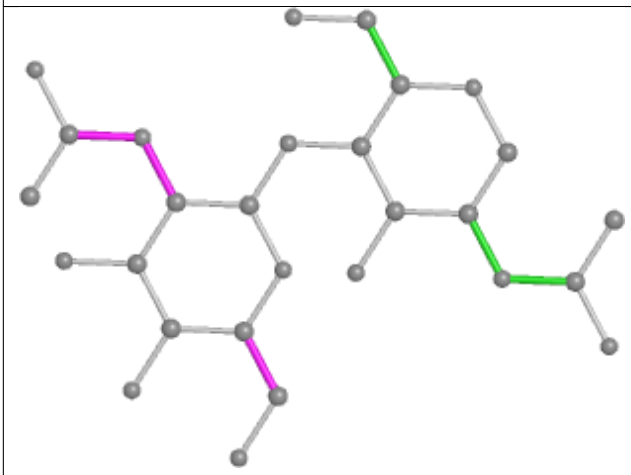


Bond angles



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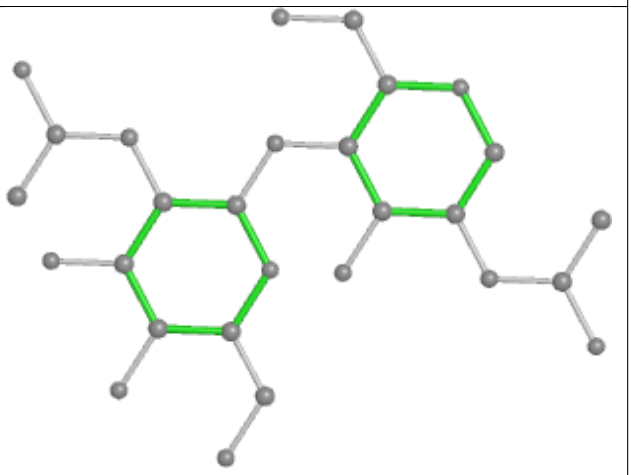
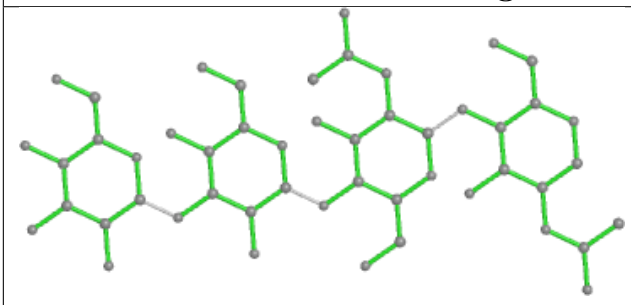


Rings

Oligosaccharide Chain L



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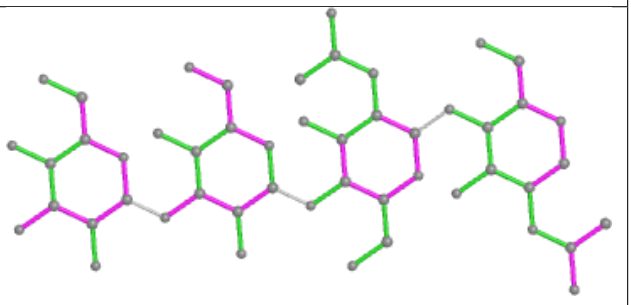
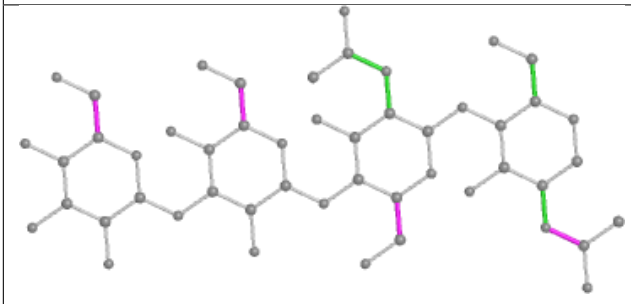


Bond angles



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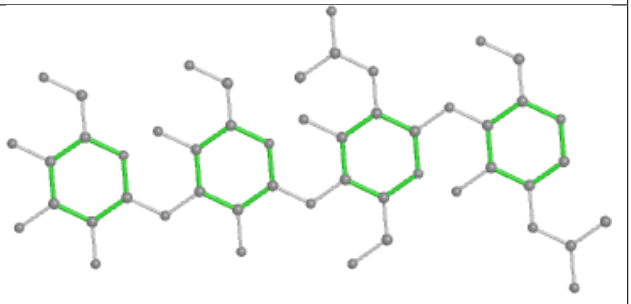
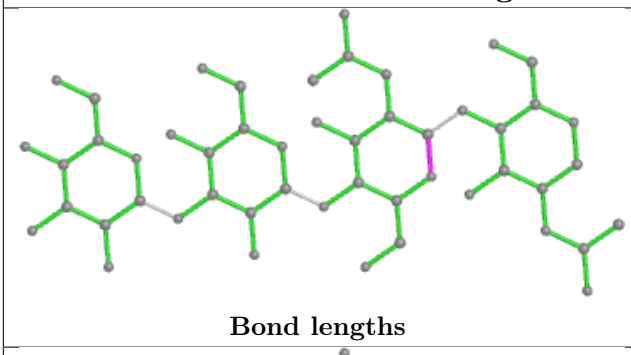


Rings

Oligosaccharide Chain P



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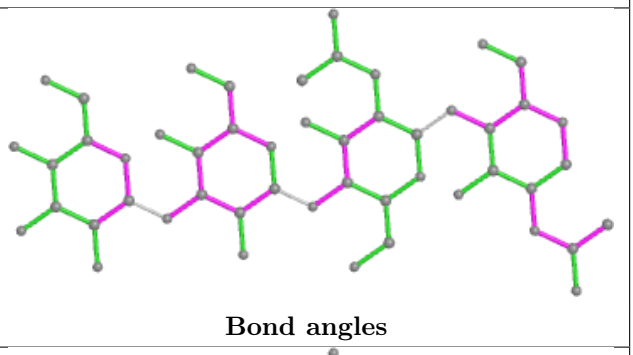
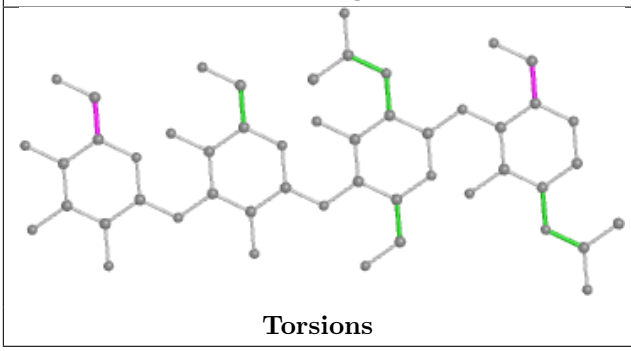


Bond angles



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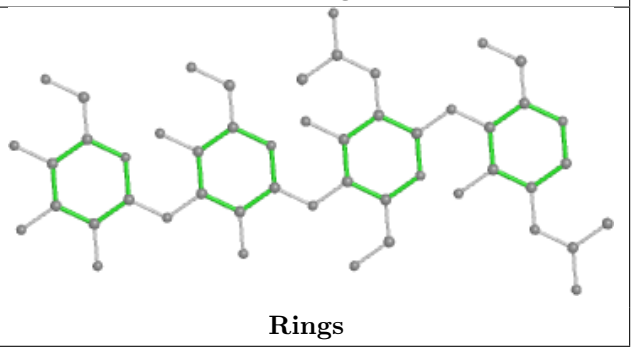
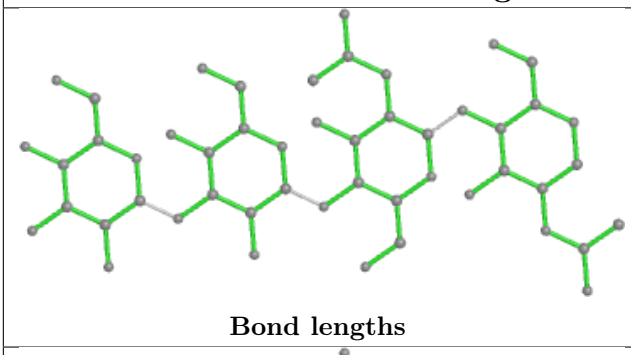


Rings

Oligosaccharide Chain U



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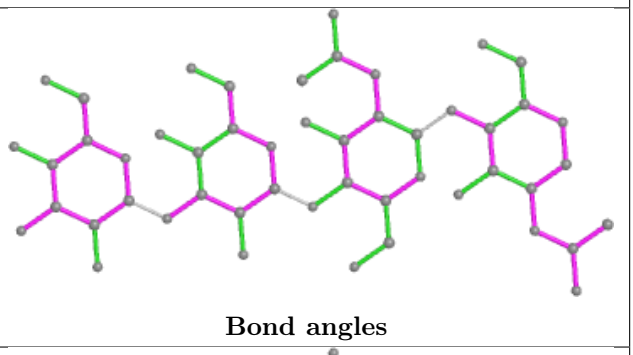
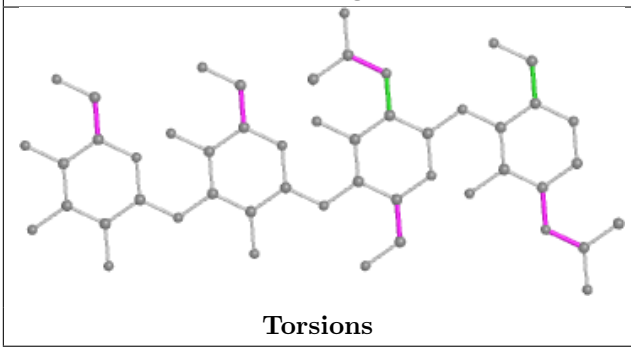


Bond angles



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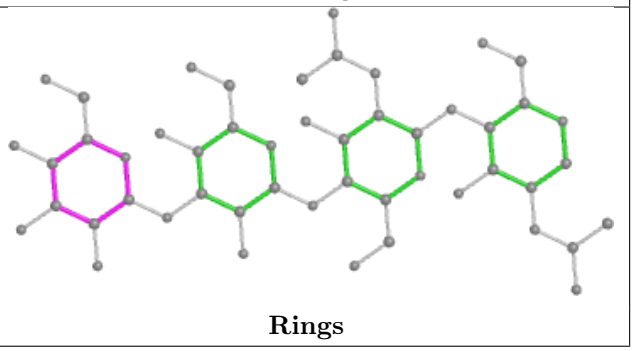
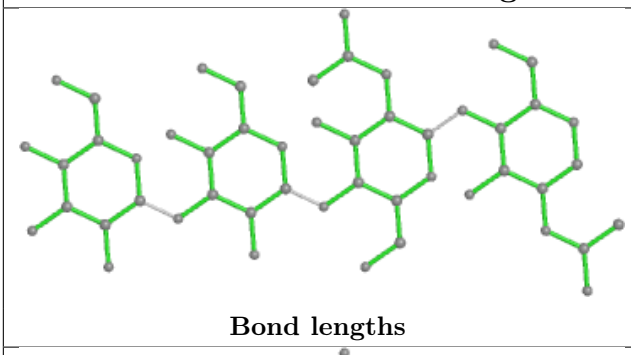
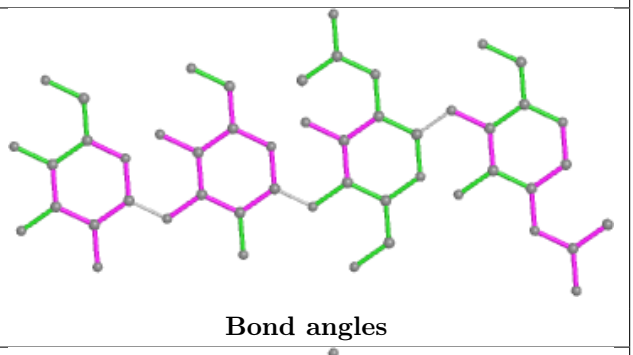


Rings

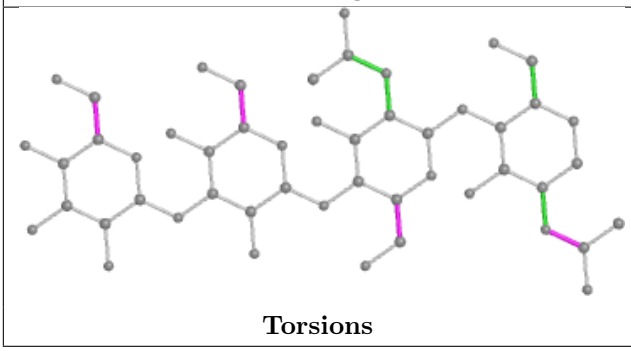
Oligosaccharide Chain c



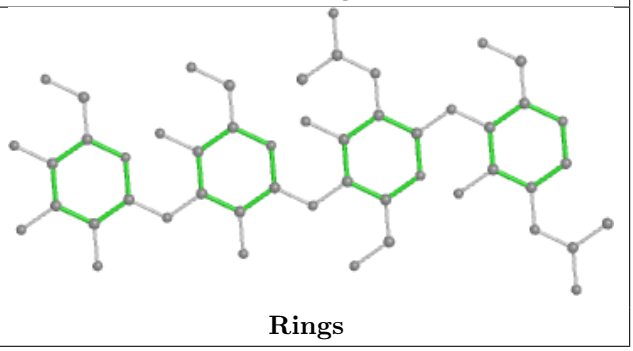
Bond lengths



Bond angles

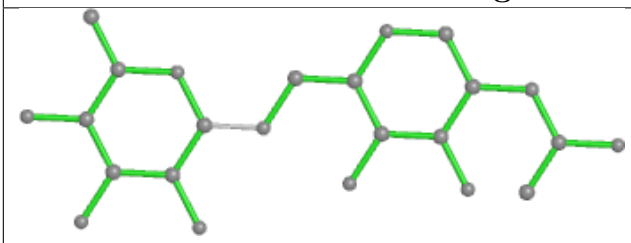


Torsions

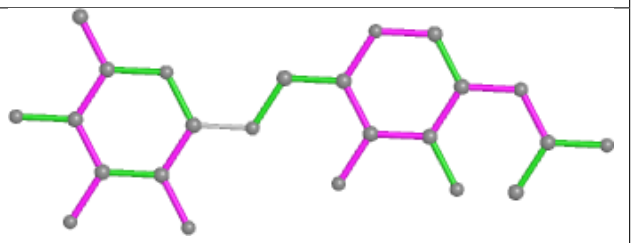


Rings

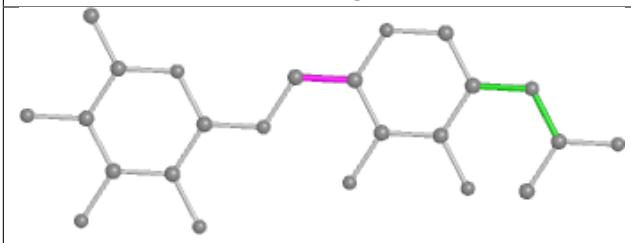
Oligosaccharide Chain N



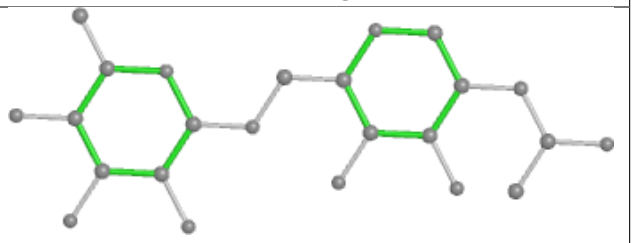
Bond lengths



Bond angles

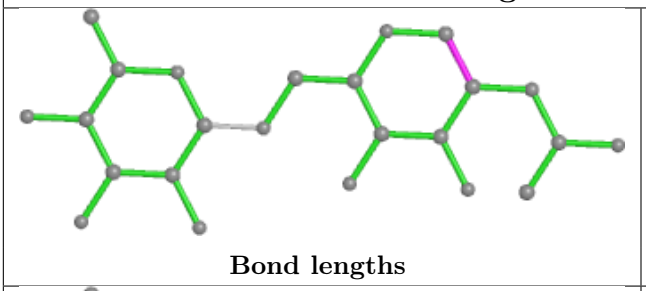


Torsions

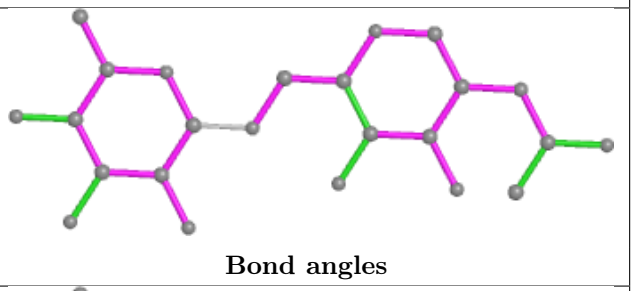


Rings

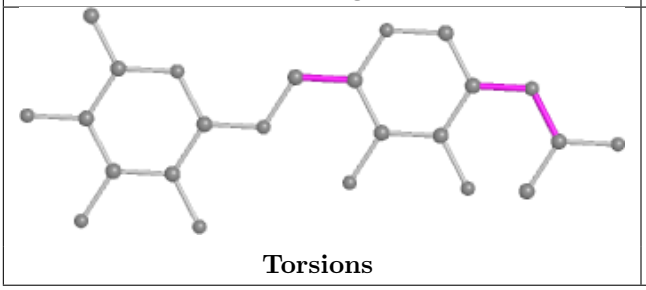
Oligosaccharide Chain a



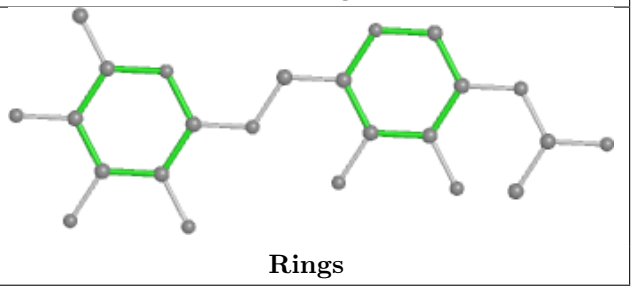
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	B	870	1	14,14,15	0.44	0	17,19,21	1.92	3 (17%)
8	NAG	A	840	1	14,14,15	0.88	1 (7%)	17,19,21	2.71	6 (35%)
8	NAG	D	870	1	14,14,15	0.64	0	17,19,21	1.81	5 (29%)
8	NAG	D	840	1	14,14,15	0.88	0	17,19,21	3.02	6 (35%)
8	NAG	C	860	1	14,14,15	0.89	0	17,19,21	3.36	7 (41%)
8	NAG	B	810	1	14,14,15	0.67	0	17,19,21	2.35	6 (35%)
8	NAG	D	860	1	14,14,15	0.66	0	17,19,21	2.51	8 (47%)
8	NAG	C	870	1	14,14,15	0.53	0	17,19,21	1.53	4 (23%)
8	NAG	A	860	1	14,14,15	0.77	0	17,19,21	2.44	7 (41%)
8	NAG	B	860	1	14,14,15	0.70	0	17,19,21	2.08	6 (35%)
8	NAG	A	870	1	14,14,15	0.50	0	17,19,21	2.18	2 (11%)
8	NAG	B	840	1	14,14,15	0.66	0	17,19,21	3.01	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	D	810	1	14,14,15	0.66	0	17,19,21	2.25	6 (35%)
8	NAG	C	840	1	14,14,15	0.79	1 (7%)	17,19,21	1.64	5 (29%)

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
8	NAG	B	870	1	-	4/6/23/26	0/1/1/1
8	NAG	A	840	1	1/1/5/7	6/6/23/26	0/1/1/1
8	NAG	D	870	1	-	5/6/23/26	0/1/1/1
8	NAG	D	840	1	-	4/6/23/26	0/1/1/1
8	NAG	C	860	1	-	5/6/23/26	0/1/1/1
8	NAG	D	860	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	870	1	-	4/6/23/26	0/1/1/1
8	NAG	B	860	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	A	860	1	-	4/6/23/26	0/1/1/1
8	NAG	A	870	1	-	4/6/23/26	0/1/1/1
8	NAG	B	810	1	-	1/6/23/26	0/1/1/1
8	NAG	B	840	1	-	6/6/23/26	0/1/1/1
8	NAG	D	810	1	-	2/6/23/26	0/1/1/1
8	NAG	C	840	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	840	NAG	C1-C2	2.51	1.56	1.52
8	C	840	NAG	C1-C2	2.02	1.55	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	840	NAG	C1-O5-C5	9.26	124.74	112.19
8	B	840	NAG	C1-O5-C5	8.87	124.21	112.19
8	C	860	NAG	C1-O5-C5	8.48	123.68	112.19
8	A	870	NAG	C1-O5-C5	7.48	122.33	112.19
8	C	860	NAG	O5-C1-C2	6.16	121.02	111.29
8	D	860	NAG	C1-O5-C5	6.10	120.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	810	NAG	O5-C5-C6	5.78	116.26	107.20
8	B	870	NAG	C1-O5-C5	5.44	119.56	112.19
8	C	860	NAG	C3-C4-C5	5.33	119.74	110.24
8	A	860	NAG	C2-N2-C7	5.11	130.18	122.90
8	C	860	NAG	C2-N2-C7	4.77	129.70	122.90
8	D	810	NAG	C1-O5-C5	4.75	118.63	112.19
8	A	840	NAG	O4-C4-C5	4.74	121.07	109.30
8	B	860	NAG	C2-N2-C7	4.73	129.64	122.90
8	D	840	NAG	O4-C4-C5	4.62	120.76	109.30
8	A	840	NAG	O3-C3-C2	4.60	118.98	109.47
8	D	870	NAG	C4-C3-C2	4.45	117.54	111.02
8	A	840	NAG	C1-O5-C5	4.43	118.19	112.19
8	A	840	NAG	O3-C3-C4	-4.37	100.24	110.35
8	D	810	NAG	O5-C1-C2	4.36	118.18	111.29
8	A	860	NAG	O5-C5-C6	4.32	113.97	107.20
8	A	860	NAG	C1-C2-N2	4.18	117.63	110.49
8	A	840	NAG	O5-C5-C6	4.04	113.53	107.20
8	D	860	NAG	C3-C4-C5	3.94	117.27	110.24
8	D	840	NAG	O3-C3-C2	3.90	117.53	109.47
8	A	840	NAG	O5-C1-C2	-3.74	105.38	111.29
8	B	840	NAG	O7-C7-N2	3.70	128.76	121.95
8	B	840	NAG	O4-C4-C5	3.56	118.14	109.30
8	B	840	NAG	C2-N2-C7	3.52	127.92	122.90
8	B	810	NAG	C6-C5-C4	-3.51	104.78	113.00
8	B	860	NAG	O7-C7-C8	-3.47	115.62	122.06
8	B	840	NAG	O3-C3-C4	-3.42	102.44	110.35
8	D	840	NAG	C2-N2-C7	3.38	127.71	122.90
8	D	810	NAG	O7-C7-C8	-3.37	115.80	122.06
8	C	870	NAG	O5-C1-C2	3.23	116.38	111.29
8	B	870	NAG	C3-C4-C5	3.16	115.87	110.24
8	B	810	NAG	C1-O5-C5	3.11	116.41	112.19
8	A	860	NAG	C1-O5-C5	2.96	116.20	112.19
8	C	840	NAG	C4-C3-C2	2.93	115.31	111.02
8	D	870	NAG	C1-O5-C5	2.85	116.05	112.19
8	B	860	NAG	C1-C2-N2	2.84	115.33	110.49
8	D	860	NAG	C4-C3-C2	2.82	115.15	111.02
8	C	840	NAG	C1-C2-N2	2.81	115.28	110.49
8	D	810	NAG	C1-C2-N2	2.73	115.15	110.49
8	C	860	NAG	O5-C5-C4	2.72	117.46	110.83
8	D	860	NAG	C8-C7-N2	2.69	120.66	116.10
8	B	810	NAG	O4-C4-C5	2.68	115.94	109.30
8	D	860	NAG	C1-C2-N2	-2.66	105.94	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	870	NAG	O5-C1-C2	-2.64	107.11	111.29
8	C	870	NAG	C2-N2-C7	-2.60	119.20	122.90
8	D	860	NAG	O3-C3-C2	2.59	114.83	109.47
8	D	810	NAG	C8-C7-N2	2.55	120.41	116.10
8	A	870	NAG	C4-C3-C2	-2.54	107.29	111.02
8	D	870	NAG	C3-C4-C5	2.53	114.75	110.24
8	A	860	NAG	O3-C3-C2	2.52	114.68	109.47
8	A	860	NAG	O3-C3-C4	-2.50	104.56	110.35
8	D	810	NAG	O4-C4-C3	2.49	116.12	110.35
8	C	870	NAG	O5-C5-C6	2.47	111.08	107.20
8	C	840	NAG	C2-N2-C7	2.45	126.39	122.90
8	C	840	NAG	O4-C4-C5	2.42	115.32	109.30
8	B	840	NAG	O5-C5-C4	2.39	116.64	110.83
8	B	860	NAG	O3-C3-C2	2.34	114.31	109.47
8	D	870	NAG	C8-C7-N2	2.34	120.06	116.10
8	D	870	NAG	C2-N2-C7	2.31	126.19	122.90
8	D	860	NAG	O5-C5-C6	2.31	110.82	107.20
8	C	870	NAG	C1-O5-C5	2.30	115.31	112.19
8	D	840	NAG	C1-C2-N2	2.30	114.42	110.49
8	D	860	NAG	O7-C7-C8	-2.30	117.79	122.06
8	B	860	NAG	O7-C7-N2	2.21	126.01	121.95
8	C	860	NAG	O3-C3-C2	2.20	114.02	109.47
8	C	840	NAG	C1-O5-C5	2.20	115.17	112.19
8	B	810	NAG	C4-C3-C2	2.19	114.23	111.02
8	C	860	NAG	C6-C5-C4	2.19	118.13	113.00
8	A	860	NAG	O4-C4-C3	-2.18	105.31	110.35
8	B	860	NAG	C1-O5-C5	2.12	115.07	112.19
8	B	840	NAG	C8-C7-N2	-2.12	112.52	116.10
8	B	810	NAG	C1-C2-N2	-2.09	106.92	110.49
8	D	840	NAG	O3-C3-C4	-2.00	105.72	110.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	840	NAG	C5
8	B	860	NAG	C1
8	D	860	NAG	C1

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	840	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	A	860	NAG	C1-C2-N2-C7
8	A	860	NAG	O7-C7-N2-C2
8	A	870	NAG	C8-C7-N2-C2
8	A	870	NAG	O7-C7-N2-C2
8	B	840	NAG	O7-C7-N2-C2
8	B	860	NAG	C8-C7-N2-C2
8	B	860	NAG	O7-C7-N2-C2
8	B	870	NAG	C8-C7-N2-C2
8	B	870	NAG	O7-C7-N2-C2
8	C	860	NAG	C3-C2-N2-C7
8	C	870	NAG	C8-C7-N2-C2
8	C	870	NAG	O7-C7-N2-C2
8	D	840	NAG	C1-C2-N2-C7
8	D	840	NAG	C8-C7-N2-C2
8	D	840	NAG	O7-C7-N2-C2
8	D	860	NAG	C3-C2-N2-C7
8	D	860	NAG	C8-C7-N2-C2
8	D	860	NAG	O7-C7-N2-C2
8	D	870	NAG	C8-C7-N2-C2
8	D	870	NAG	O7-C7-N2-C2
8	A	870	NAG	C4-C5-C6-O6
8	A	840	NAG	C8-C7-N2-C2
8	A	840	NAG	O7-C7-N2-C2
8	A	860	NAG	C8-C7-N2-C2
8	B	840	NAG	C8-C7-N2-C2
8	C	870	NAG	O5-C5-C6-O6
8	A	870	NAG	O5-C5-C6-O6
8	B	840	NAG	C4-C5-C6-O6
8	C	870	NAG	C4-C5-C6-O6
8	A	840	NAG	O5-C5-C6-O6
8	D	870	NAG	C1-C2-N2-C7
8	B	870	NAG	C4-C5-C6-O6
8	A	840	NAG	C4-C5-C6-O6
8	C	860	NAG	C4-C5-C6-O6
8	C	860	NAG	C8-C7-N2-C2
8	C	860	NAG	O7-C7-N2-C2
8	D	810	NAG	C8-C7-N2-C2
8	D	810	NAG	O7-C7-N2-C2
8	B	840	NAG	C1-C2-N2-C7
8	B	840	NAG	O5-C5-C6-O6
8	B	870	NAG	O5-C5-C6-O6
8	D	870	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	810	NAG	O5-C5-C6-O6
8	D	870	NAG	O5-C5-C6-O6
8	C	860	NAG	O5-C5-C6-O6
8	D	840	NAG	O5-C5-C6-O6
8	D	860	NAG	C4-C5-C6-O6
8	B	860	NAG	C3-C2-N2-C7
8	A	840	NAG	C1-C2-N2-C7
8	A	860	NAG	C4-C5-C6-O6
8	B	840	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	728/728 (100%)	-0.35	0 100 100	38, 57, 86, 106	0
1	B	728/728 (100%)	-0.32	1 (0%) 95 95	36, 57, 86, 106	0
1	C	728/728 (100%)	-0.41	2 (0%) 94 92	38, 57, 86, 106	0
1	D	728/728 (100%)	-0.42	2 (0%) 94 92	38, 58, 87, 106	0
2	E	352/363 (96%)	0.19	20 (5%) 23 12	40, 82, 90, 93	0
2	F	352/363 (96%)	0.19	10 (2%) 53 36	67, 83, 91, 100	0
2	G	352/363 (96%)	0.18	12 (3%) 45 28	71, 84, 92, 95	0
2	H	352/363 (96%)	0.21	9 (2%) 56 40	65, 83, 91, 104	0
3	W	6/9 (66%)	0.68	1 (16%) 1 1	72, 82, 94, 95	0
3	X	6/9 (66%)	0.83	1 (16%) 1 1	64, 73, 82, 85	0
3	Y	6/9 (66%)	0.89	2 (33%) 0 0	84, 92, 99, 100	0
3	Z	6/9 (66%)	0.93	2 (33%) 0 0	86, 92, 99, 100	0
All	All	4344/4400 (98%)	-0.18	62 (1%) 75 63	36, 67, 90, 106	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	354	PRO	4.0
2	E	15	HIS	3.8
2	E	17	HIS	3.7
2	E	262	CYS	3.7
2	E	16	VAL	3.7
2	E	293	ASN	3.6
2	E	101	ARG	3.6
2	G	15	HIS	3.6
2	E	294	THR	3.4
2	H	53	ASP	3.3
3	Z	5	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
3	Y	5	ASP	3.2
2	F	243	LEU	3.2
3	X	6	PRO	3.1
2	H	353	MET	3.0
2	E	237	GLY	3.0
2	G	275	ASP	3.0
2	E	295	ASP	2.9
1	C	766	PRO	2.9
2	F	262	CYS	2.9
2	E	291	SER	2.8
3	W	6	PRO	2.8
2	F	246	THR	2.8
3	Z	6	PRO	2.7
2	E	181	ASP	2.7
2	F	44	GLU	2.7
2	G	4	THR	2.6
2	G	293	ASN	2.6
2	F	354	PRO	2.6
1	B	97	GLU	2.5
2	E	100	VAL	2.4
2	F	189	GLU	2.4
2	H	54	LYS	2.3
2	H	221	ALA	2.3
2	E	19	ASP	2.3
2	G	274	PRO	2.3
2	G	229	ASP	2.3
2	F	96	VAL	2.3
2	H	189	GLU	2.3
2	G	16	VAL	2.3
2	H	103	SER	2.3
2	G	101	ARG	2.2
2	E	238	HIS	2.2
2	E	21	ALA	2.2
2	H	285	ASN	2.2
2	E	214	HIS	2.1
2	G	260	GLU	2.1
1	C	88	VAL	2.1
2	F	355	SER	2.1
2	E	13	GLU	2.1
2	F	247	THR	2.1
2	E	14	LEU	2.1
2	G	59	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	Y	6	PRO	2.1
2	E	260	GLU	2.1
2	E	150	SER	2.1
2	F	15	HIS	2.1
2	G	183	ALA	2.0
2	G	221	ALA	2.0
2	H	55	PRO	2.0
1	D	87	SER	2.0
1	D	97	GLU	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	R	2	14/15	0.73	0.41	110,111,111,112	0
5	NAG	V	2	14/15	0.76	0.31	99,102,106,107	0
5	NAG	M	2	14/15	0.79	0.42	86,88,90,90	0
4	NAG	I	2	14/15	0.80	0.36	97,102,103,104	0
5	NAG	d	2	14/15	0.80	0.37	98,99,100,101	0
7	NAG	N	1	14/15	0.80	0.25	80,86,88,89	0
5	NAG	J	2	14/15	0.81	0.36	92,93,96,96	0
5	NAG	S	1	14/15	0.81	0.33	91,96,99,104	0
5	NAG	S	2	14/15	0.81	0.43	106,107,108,109	0
4	FUL	I	3	10/11	0.82	0.32	98,99,99,100	0
6	MAN	c	4	11/12	0.84	0.29	91,93,93,94	0
4	FUL	R	3	10/11	0.85	0.33	106,106,107,107	0
6	BMA	L	3	11/12	0.85	0.22	74,76,77,79	0
7	FUL	N	2	10/11	0.85	0.37	78,83,83,83	0
7	FUL	a	2	10/11	0.85	0.29	107,109,110,111	0
5	NAG	O	2	14/15	0.86	0.33	67,76,78,81	0
5	NAG	b	2	14/15	0.86	0.38	84,87,89,90	0
5	NAG	J	1	14/15	0.87	0.25	77,82,85,90	0
5	NAG	K	2	14/15	0.87	0.32	82,86,87,87	0

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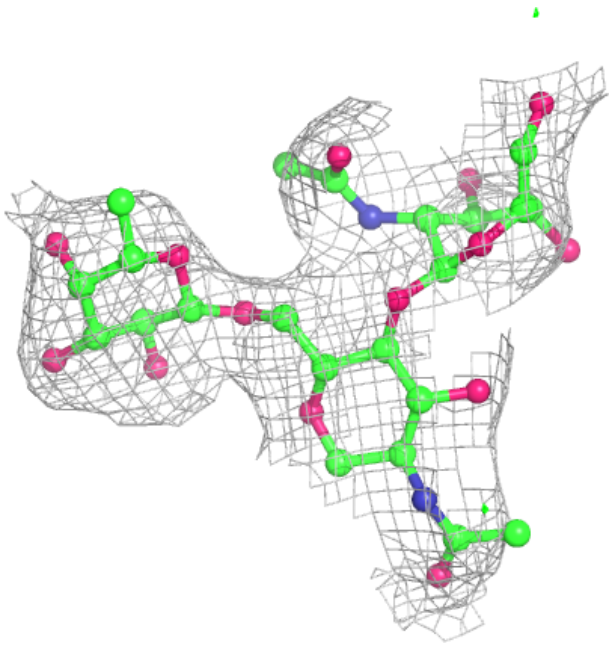
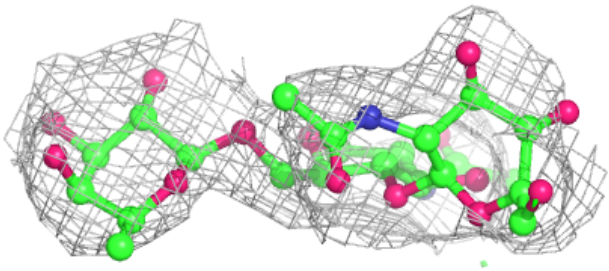
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	M	1	14/15	0.87	0.30	73,76,80,84	0
5	NAG	Q	1	14/15	0.88	0.29	75,82,86,86	0
7	NAG	a	1	14/15	0.88	0.21	100,102,103,103	0
5	NAG	d	1	14/15	0.88	0.27	75,80,82,83	0
6	MAN	P	4	11/12	0.89	0.17	68,69,72,73	0
6	BMA	c	3	11/12	0.89	0.21	84,87,89,92	0
5	NAG	T	2	14/15	0.89	0.31	91,93,94,94	0
5	NAG	V	1	14/15	0.89	0.26	71,75,78,79	0
4	NAG	I	1	14/15	0.89	0.29	92,95,99,100	0
5	NAG	b	1	14/15	0.89	0.29	78,82,83,85	0
6	MAN	L	4	11/12	0.89	0.31	82,84,85,85	0
5	NAG	Q	2	14/15	0.90	0.32	87,88,89,89	0
6	MAN	U	4	11/12	0.90	0.23	91,92,94,95	0
6	BMA	U	3	11/12	0.91	0.26	85,88,89,90	0
6	NAG	U	2	14/15	0.91	0.20	66,69,74,80	0
4	NAG	R	1	14/15	0.92	0.26	99,102,105,108	0
5	NAG	K	1	14/15	0.93	0.24	77,81,83,84	0
6	BMA	P	3	11/12	0.93	0.16	57,60,61,64	0
5	NAG	T	1	14/15	0.93	0.32	79,83,85,88	0
5	NAG	O	1	14/15	0.94	0.30	70,71,72,74	0
6	NAG	c	1	14/15	0.94	0.18	55,60,62,67	0
6	NAG	c	2	14/15	0.94	0.24	68,74,79,83	0
6	NAG	P	2	14/15	0.95	0.23	42,45,51,52	0
6	NAG	L	2	14/15	0.95	0.20	58,60,63,68	0
6	NAG	U	1	14/15	0.96	0.12	46,52,58,61	0
6	NAG	P	1	14/15	0.96	0.13	38,39,42,43	0
6	NAG	L	1	14/15	0.96	0.13	44,47,52,54	0

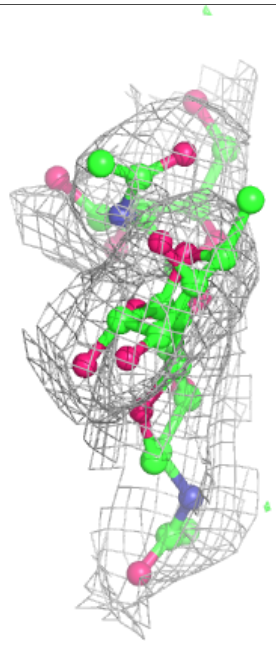
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

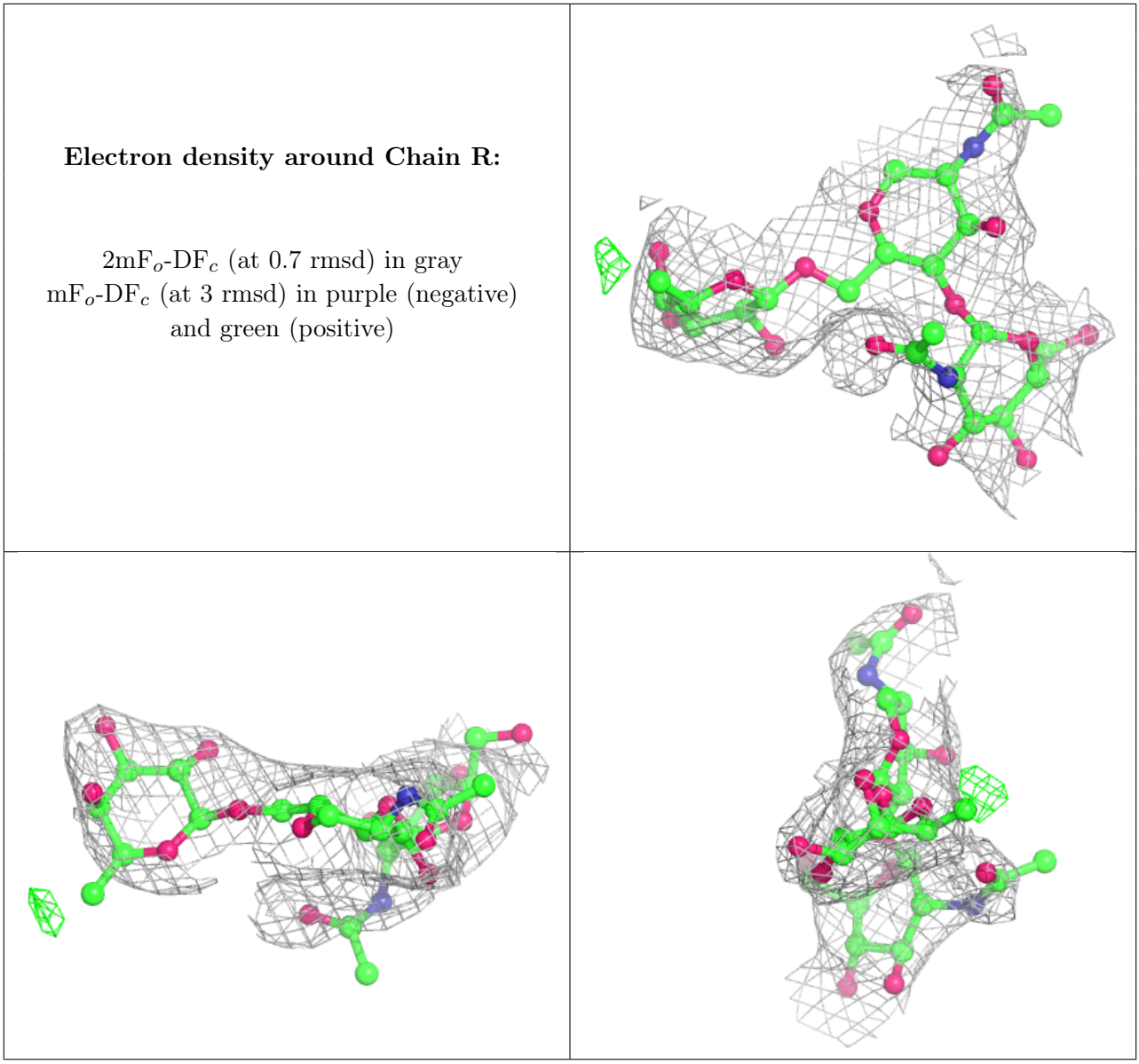






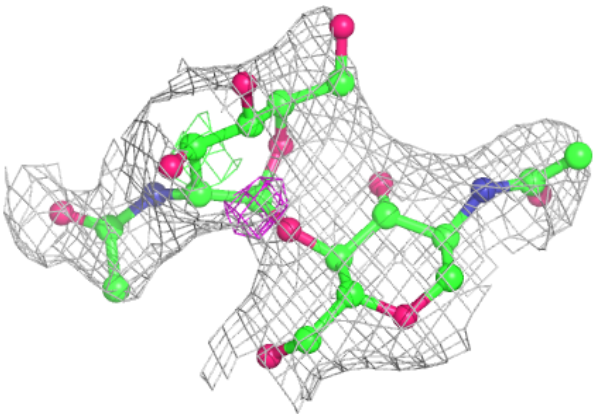
Electron density around Chain R:

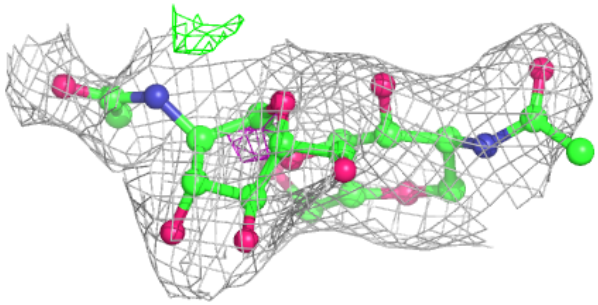
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

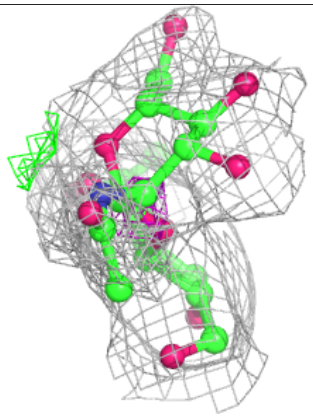


Electron density around Chain J:

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

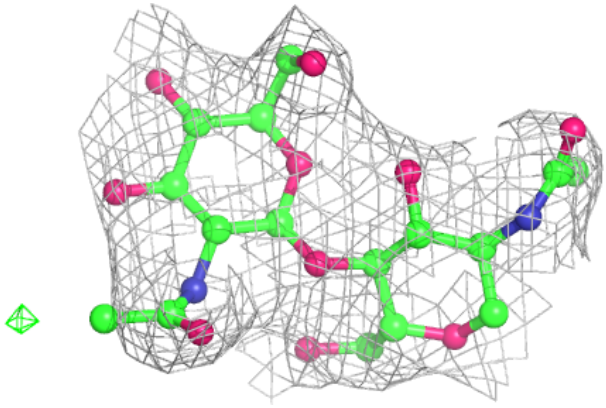


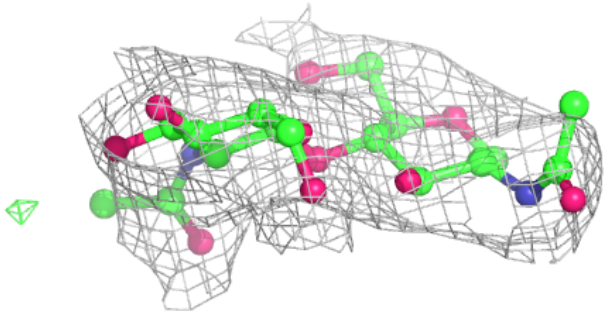


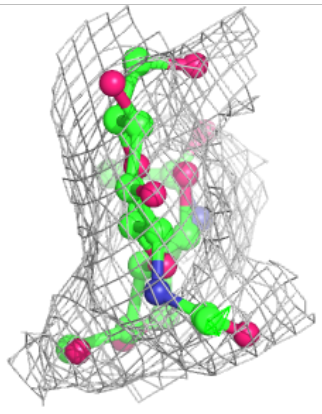


Electron density around Chain K:

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

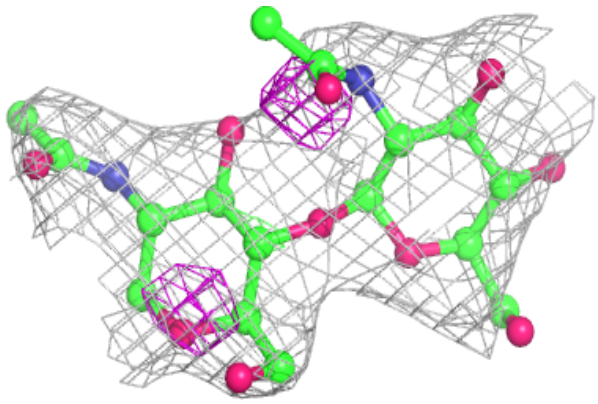


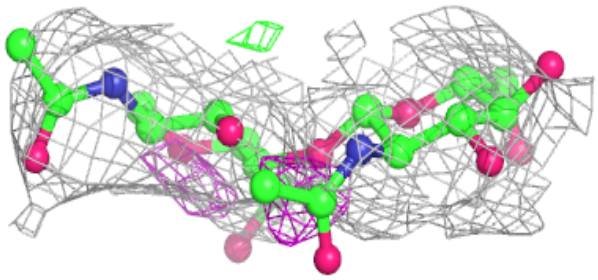


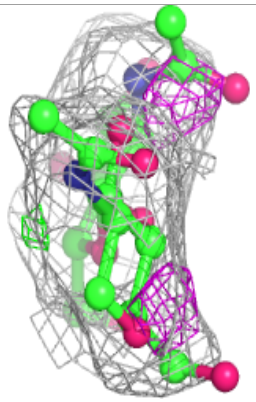


Electron density around Chain M:

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

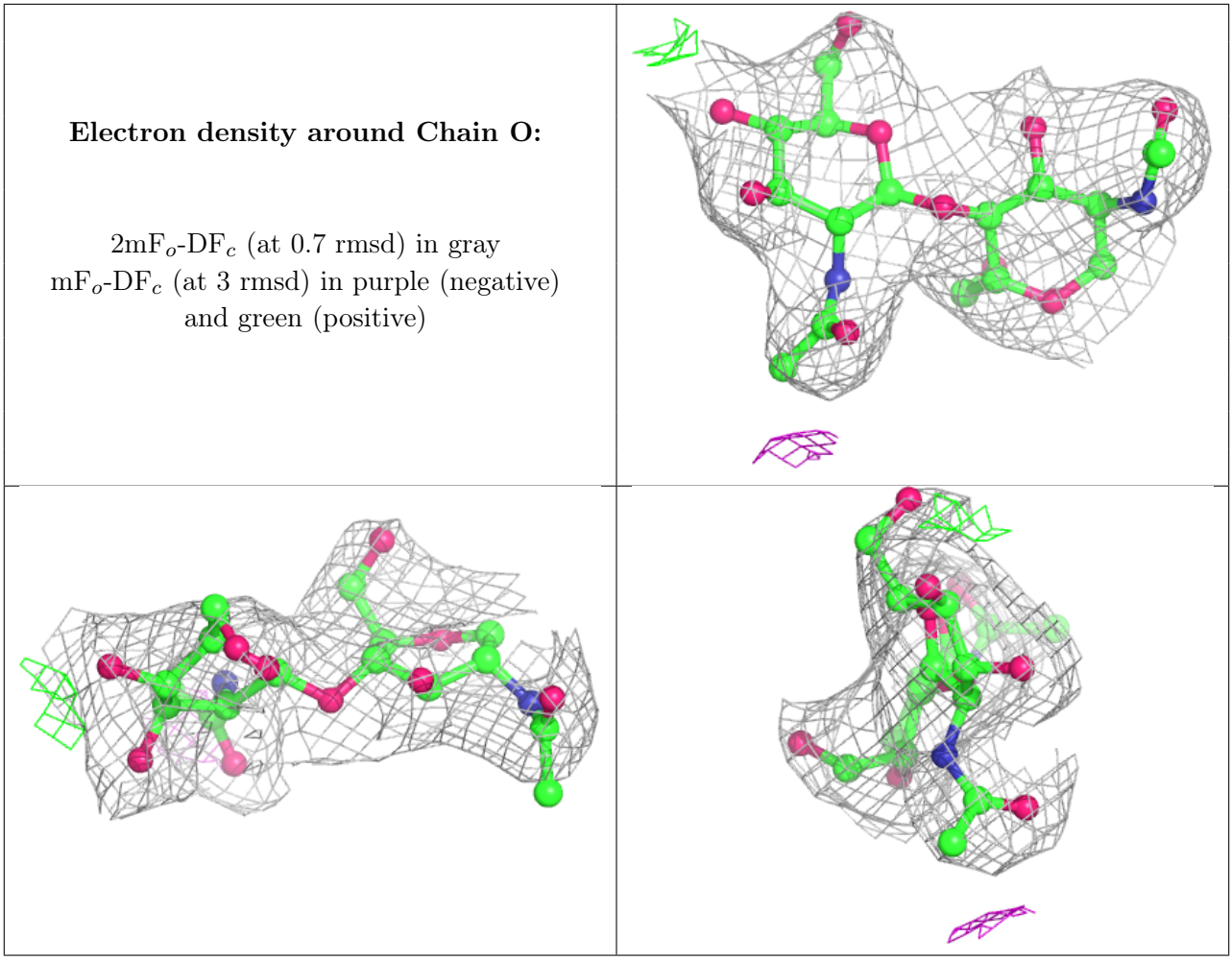






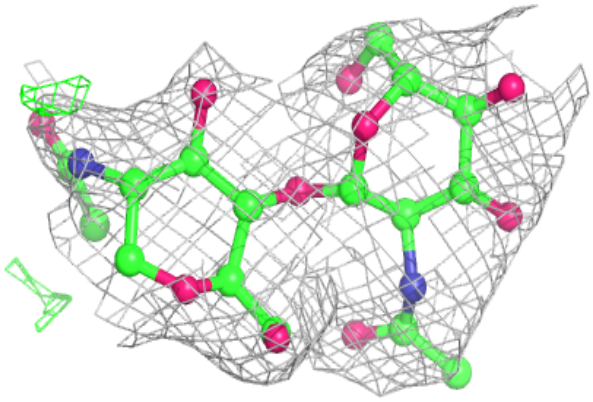
Electron density around Chain O:

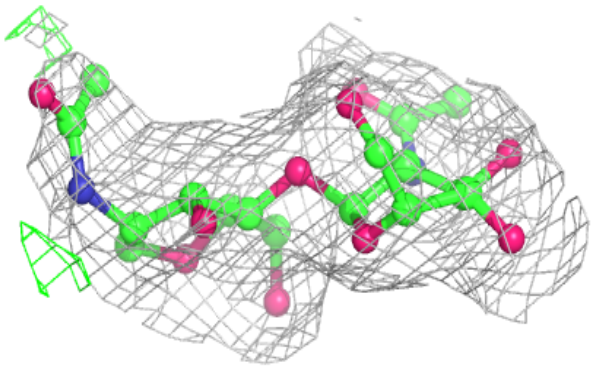
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

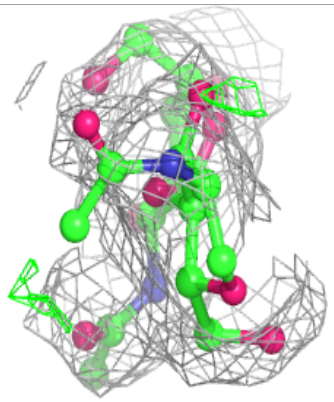


Electron density around Chain Q:

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

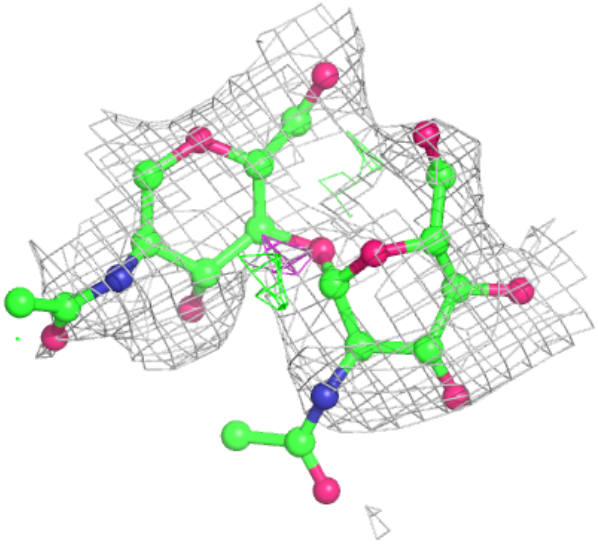


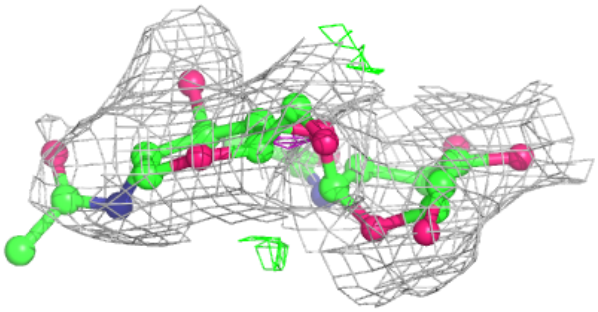


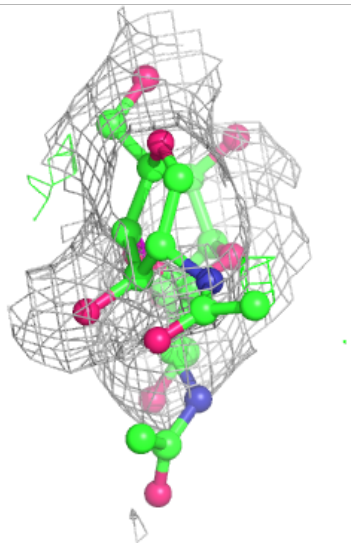


Electron density around Chain S:

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

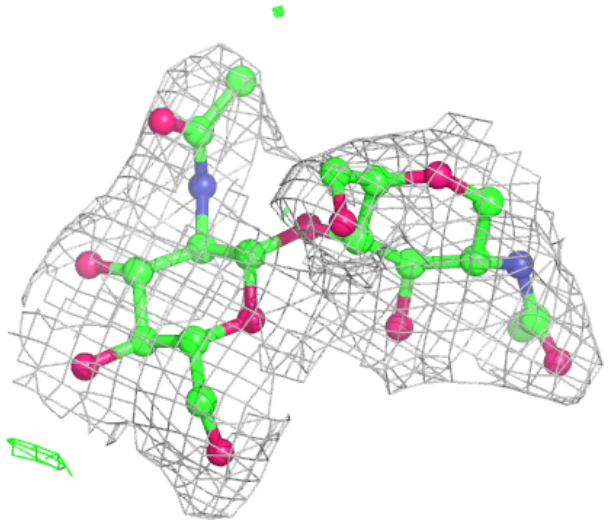


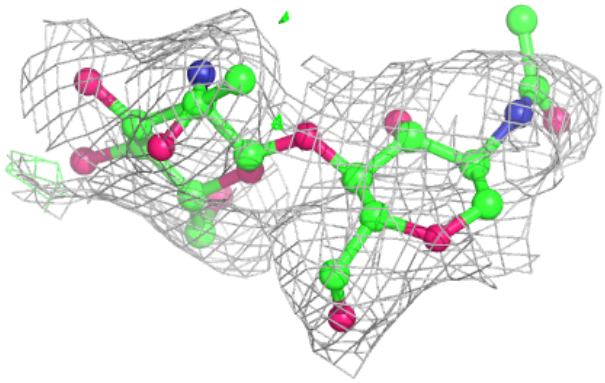


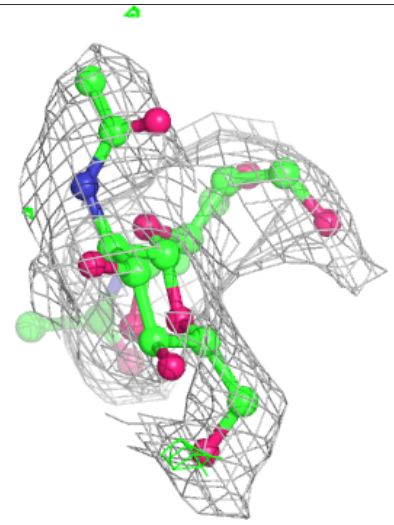


Electron density around Chain T:

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

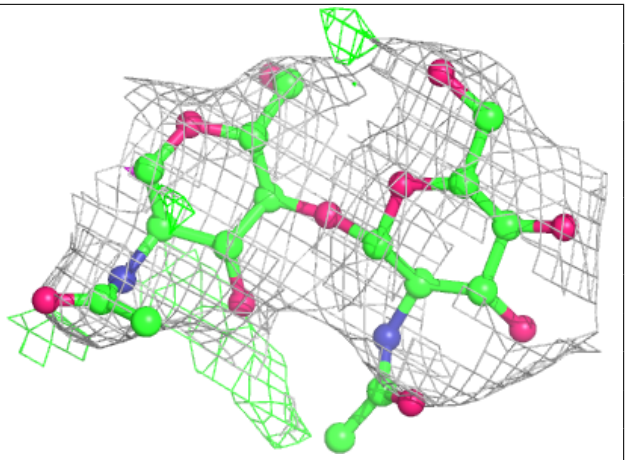


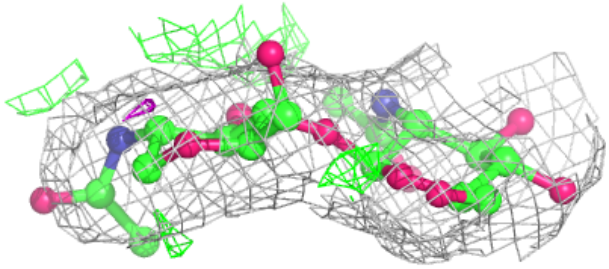


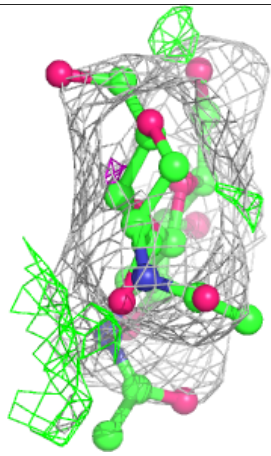


Electron density around Chain V:

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

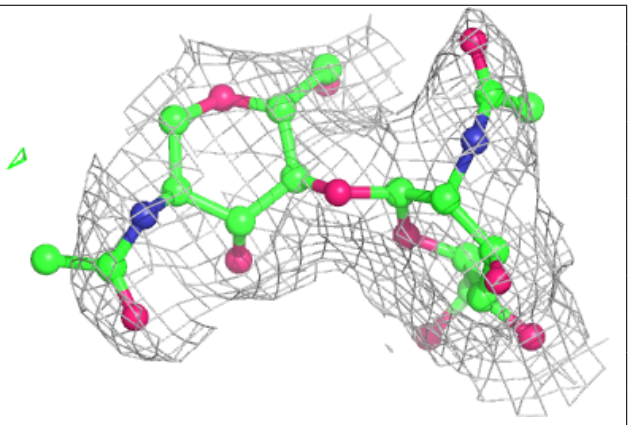


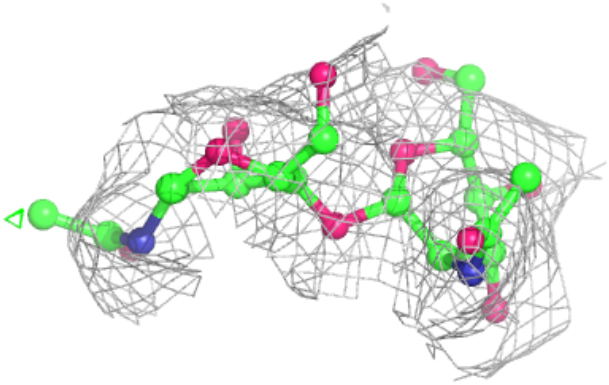


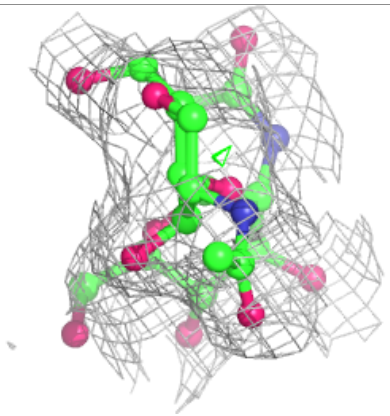


Electron density around Chain b:

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

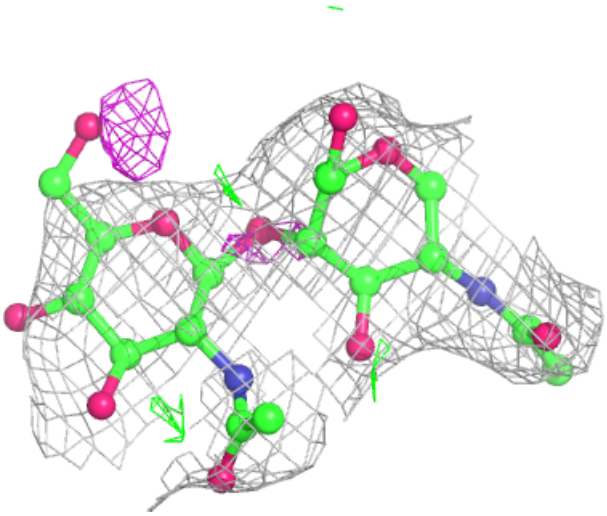


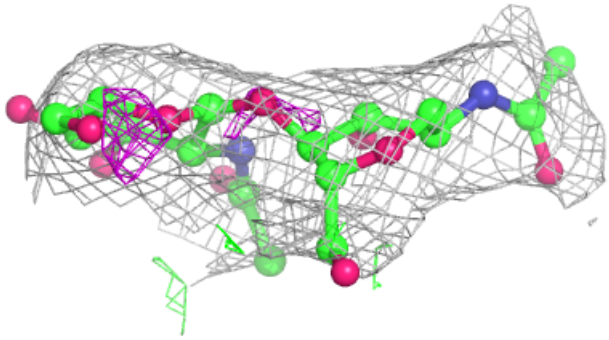


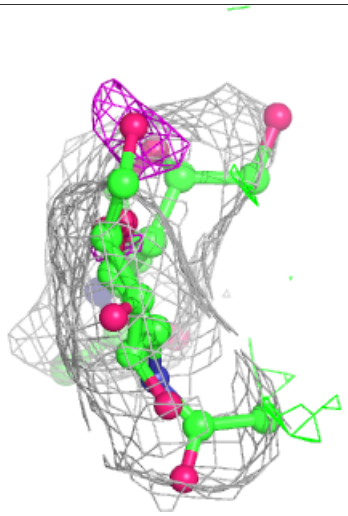


Electron density around Chain d:

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

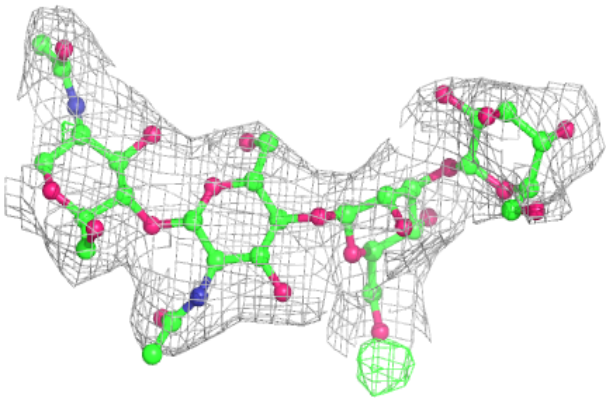


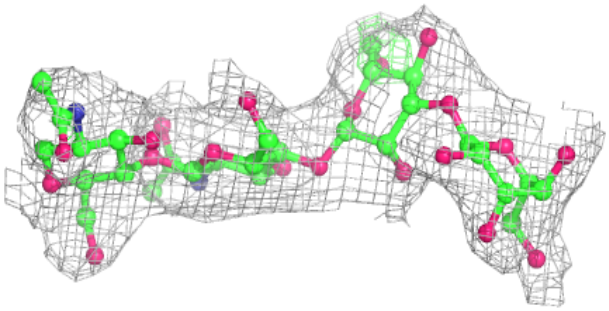


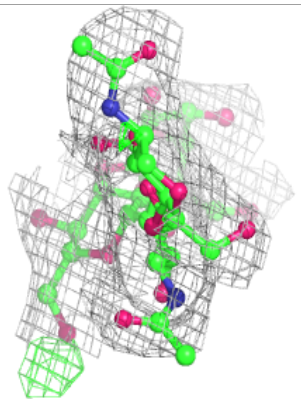


Electron density around Chain L:

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

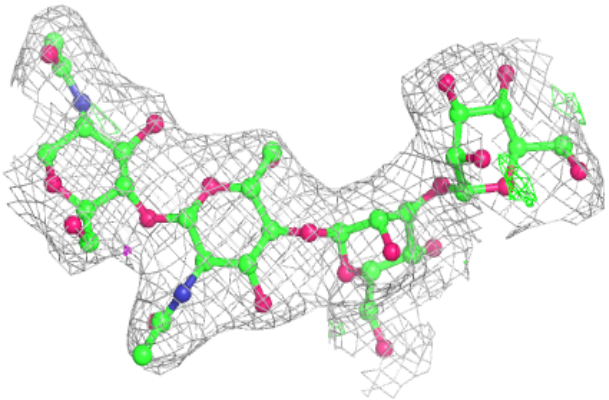


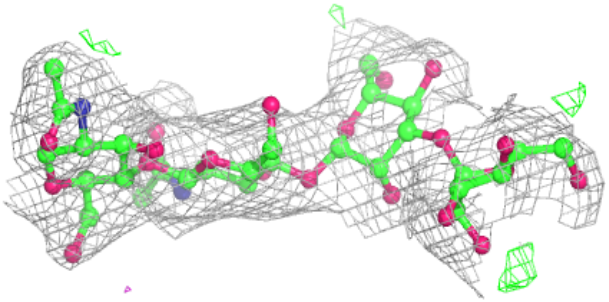


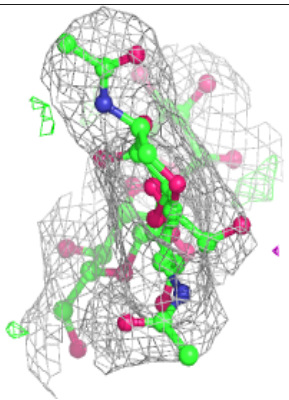


Electron density around Chain P:

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

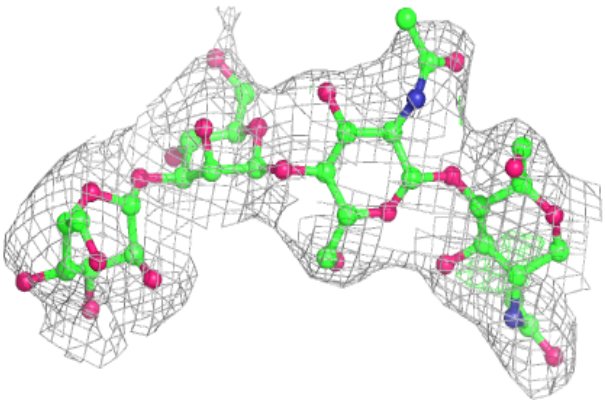


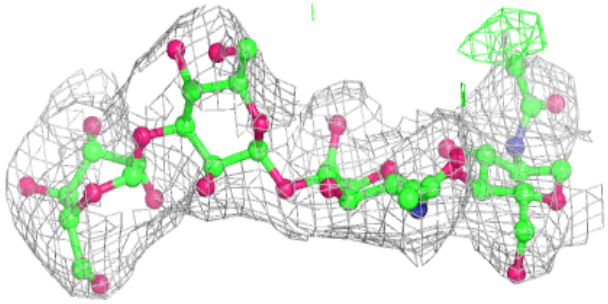


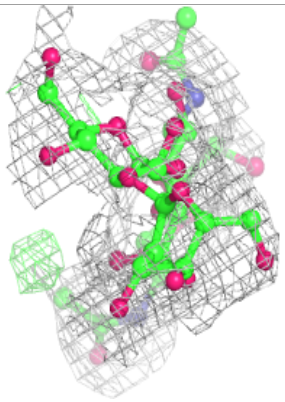


Electron density around Chain U:

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

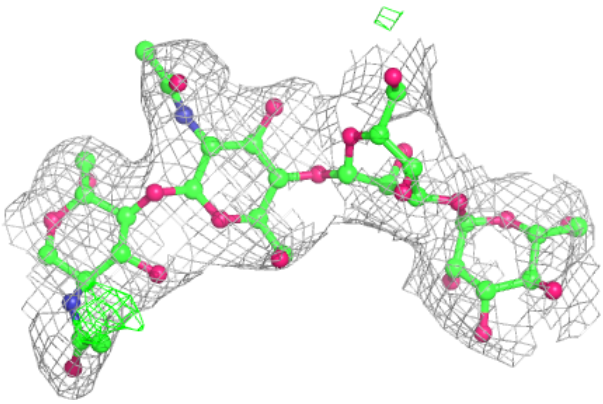


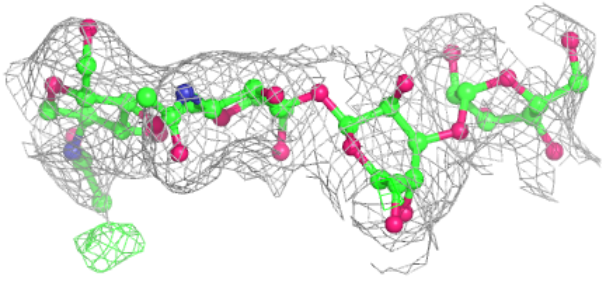


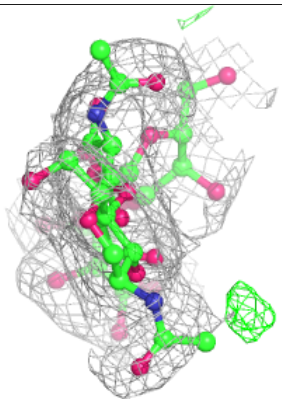


Electron density around Chain c:

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

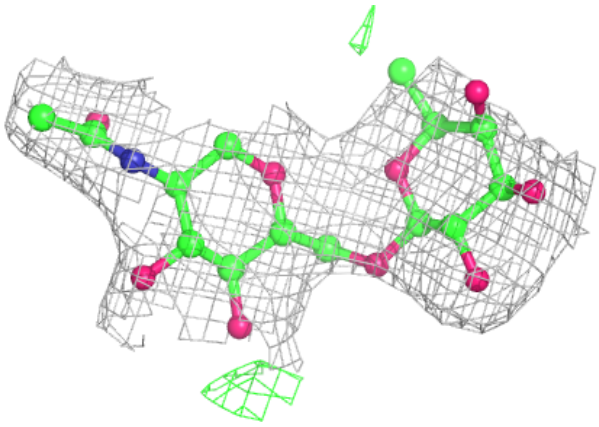


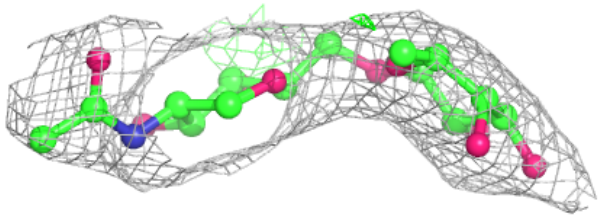


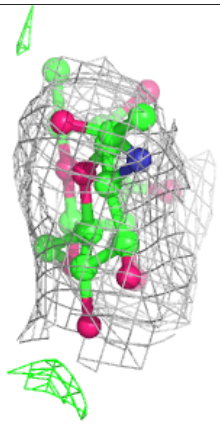


Electron density around Chain N:

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

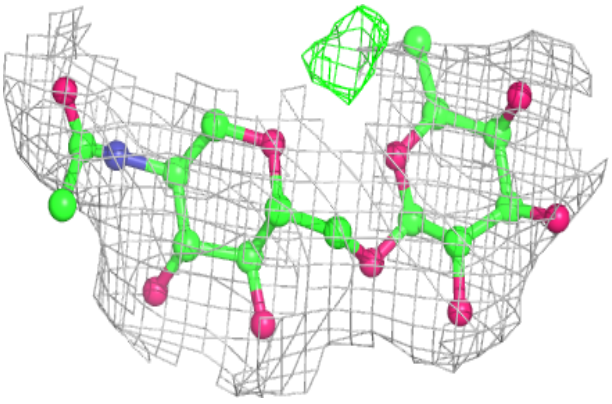


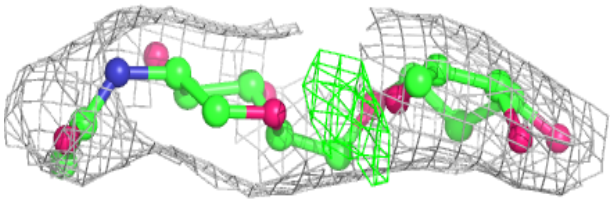


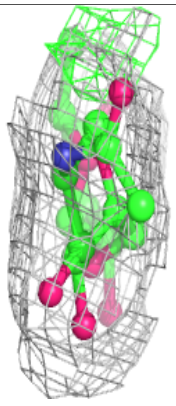


Electron density around Chain a:

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







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, 95^{th} 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
8	NAG	A	860	14/15	0.72	0.44	89,92,96,97	0
8	NAG	C	870	14/15	0.78	0.32	101,104,106,106	0
8	NAG	D	860	14/15	0.79	0.33	87,89,90,91	0
8	NAG	B	860	14/15	0.80	0.38	84,90,93,93	0
8	NAG	C	860	14/15	0.81	0.36	92,94,95,96	0
8	NAG	D	870	14/15	0.83	0.28	101,103,104,104	0
8	NAG	B	810	14/15	0.84	0.24	74,82,85,85	0
8	NAG	D	810	14/15	0.84	0.29	90,94,95,96	0
8	NAG	B	870	14/15	0.86	0.23	98,102,103,103	0
9	ZN	F	501	1/1	0.86	0.24	83,83,83,83	0
8	NAG	B	840	14/15	0.87	0.17	61,64,66,67	0
8	NAG	C	840	14/15	0.88	0.31	70,72,76,76	0
8	NAG	A	840	14/15	0.88	0.22	69,71,72,72	0
8	NAG	D	840	14/15	0.88	0.19	64,67,69,69	0
8	NAG	A	870	14/15	0.91	0.23	93,97,99,99	0
9	ZN	G	501	1/1	0.95	0.23	85,85,85,85	0
9	ZN	H	501	1/1	0.95	0.20	83,83,83,83	0
9	ZN	E	501	1/1	0.97	0.34	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.