



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:14 AM UTC

PDB ID : 6LKS / pdb_00006lks
Title : Effects of zinc ion on oligomerization and pH stability of influenza virus hemagglutinin
Authors : Seok, J.; Kim, K.
Deposited on : 2019-12-20
Resolution : 3.24 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

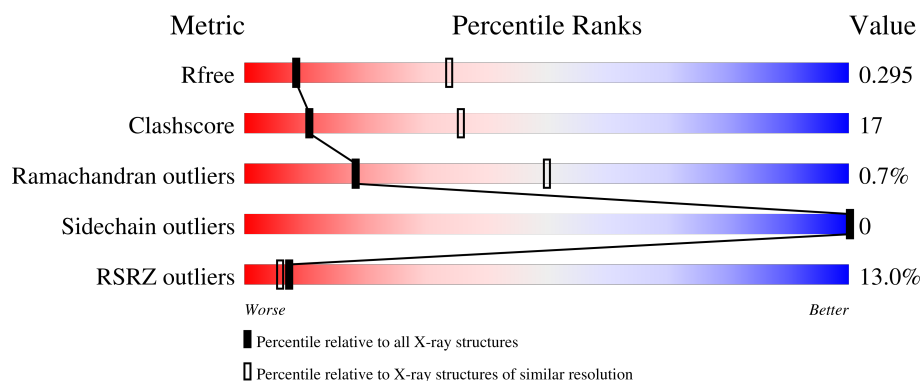
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	330	8% 59% 38% ..
1	C	330	9% 67% 30% .
1	E	330	5% 62% 34% .
1	G	330	3% 60% 36% ..
1	I	330	7% 63% 32% ..

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Mol	Chain	Length	Quality of chain
1	K	330	
2	B	183	
2	D	183	
2	F	183	
2	H	183	
2	J	183	
2	L	183	
3	M	6	
3	S	6	
3	V	6	
4	N	5	
4	P	5	
5	O	4	
5	Q	4	
5	R	4	
5	T	4	
5	U	4	
5	X	4	
6	W	3	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24413 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	A	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	C	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	E	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	G	320	Total	C	N	O	S	0	0	0
			2507	1585	435	476	11			
1	I	320	Total	C	N	O	S	0	0	0
			2507	1585	435	476	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	ALA	-	expression tag	UNP A7LI25
K	-2	ASP	-	expression tag	UNP A7LI25
K	-1	PRO	-	expression tag	UNP A7LI25
K	0	GLY	-	expression tag	UNP A7LI25
K	116	ILE	MET	conflict	UNP A7LI25
A	-3	ALA	-	expression tag	UNP A7LI25
A	-2	ASP	-	expression tag	UNP A7LI25
A	-1	PRO	-	expression tag	UNP A7LI25
A	0	GLY	-	expression tag	UNP A7LI25
A	116	ILE	MET	conflict	UNP A7LI25
C	-3	ALA	-	expression tag	UNP A7LI25
C	-2	ASP	-	expression tag	UNP A7LI25
C	-1	PRO	-	expression tag	UNP A7LI25
C	0	GLY	-	expression tag	UNP A7LI25
C	116	ILE	MET	conflict	UNP A7LI25
E	-3	ALA	-	expression tag	UNP A7LI25
E	-2	ASP	-	expression tag	UNP A7LI25

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP A7LI25
E	0	GLY	-	expression tag	UNP A7LI25
E	116	ILE	MET	conflict	UNP A7LI25
G	-3	ALA	-	expression tag	UNP A7LI25
G	-2	ASP	-	expression tag	UNP A7LI25
G	-1	PRO	-	expression tag	UNP A7LI25
G	0	GLY	-	expression tag	UNP A7LI25
G	116	ILE	MET	conflict	UNP A7LI25
I	-3	ALA	-	expression tag	UNP A7LI25
I	-2	ASP	-	expression tag	UNP A7LI25
I	-1	PRO	-	expression tag	UNP A7LI25
I	0	GLY	-	expression tag	UNP A7LI25
I	116	ILE	MET	conflict	UNP A7LI25

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	B	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	D	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	F	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	H	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	J	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	VAL	ILE	conflict	UNP A7LI25
L	169	SER	ASN	conflict	UNP A7LI25
L	177	SER	-	expression tag	UNP A7LI25
L	178	GLY	-	expression tag	UNP A7LI25
L	179	ARG	-	expression tag	UNP A7LI25
L	180	LEU	-	expression tag	UNP A7LI25
L	181	VAL	-	expression tag	UNP A7LI25
L	182	PRO	-	expression tag	UNP A7LI25
L	183	ARG	-	expression tag	UNP A7LI25

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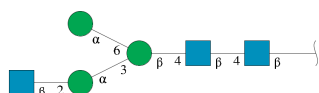
Chain	Residue	Modelled	Actual	Comment	Reference
B	91	VAL	ILE	conflict	UNP A7LI25
B	169	SER	ASN	conflict	UNP A7LI25
B	177	SER	-	expression tag	UNP A7LI25
B	178	GLY	-	expression tag	UNP A7LI25
B	179	ARG	-	expression tag	UNP A7LI25
B	180	LEU	-	expression tag	UNP A7LI25
B	181	VAL	-	expression tag	UNP A7LI25
B	182	PRO	-	expression tag	UNP A7LI25
B	183	ARG	-	expression tag	UNP A7LI25
D	91	VAL	ILE	conflict	UNP A7LI25
D	169	SER	ASN	conflict	UNP A7LI25
D	177	SER	-	expression tag	UNP A7LI25
D	178	GLY	-	expression tag	UNP A7LI25
D	179	ARG	-	expression tag	UNP A7LI25
D	180	LEU	-	expression tag	UNP A7LI25
D	181	VAL	-	expression tag	UNP A7LI25
D	182	PRO	-	expression tag	UNP A7LI25
D	183	ARG	-	expression tag	UNP A7LI25
F	91	VAL	ILE	conflict	UNP A7LI25
F	169	SER	ASN	conflict	UNP A7LI25
F	177	SER	-	expression tag	UNP A7LI25
F	178	GLY	-	expression tag	UNP A7LI25
F	179	ARG	-	expression tag	UNP A7LI25
F	180	LEU	-	expression tag	UNP A7LI25
F	181	VAL	-	expression tag	UNP A7LI25
F	182	PRO	-	expression tag	UNP A7LI25
F	183	ARG	-	expression tag	UNP A7LI25
H	91	VAL	ILE	conflict	UNP A7LI25
H	169	SER	ASN	conflict	UNP A7LI25
H	177	SER	-	expression tag	UNP A7LI25
H	178	GLY	-	expression tag	UNP A7LI25
H	179	ARG	-	expression tag	UNP A7LI25
H	180	LEU	-	expression tag	UNP A7LI25
H	181	VAL	-	expression tag	UNP A7LI25
H	182	PRO	-	expression tag	UNP A7LI25
H	183	ARG	-	expression tag	UNP A7LI25
J	91	VAL	ILE	conflict	UNP A7LI25
J	169	SER	ASN	conflict	UNP A7LI25
J	177	SER	-	expression tag	UNP A7LI25
J	178	GLY	-	expression tag	UNP A7LI25
J	179	ARG	-	expression tag	UNP A7LI25
J	180	LEU	-	expression tag	UNP A7LI25

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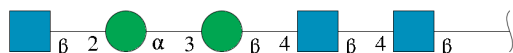
Chain	Residue	Modelled	Actual	Comment	Reference
J	181	VAL	-	expression tag	UNP A7LI25
J	182	PRO	-	expression tag	UNP A7LI25
J	183	ARG	-	expression tag	UNP A7LI25

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	0	0	0
			75	42	3	30			
3	S	6	Total	C	N	O	0	0	0
			75	42	3	30			
3	V	6	Total	C	N	O	0	0	0
			75	42	3	30			

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



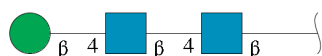
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	5	Total	C	N	O	0	0	0
			64	36	3	25			
4	P	5	Total	C	N	O	0	0	0
			64	36	3	25			

- Molecule 5 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.



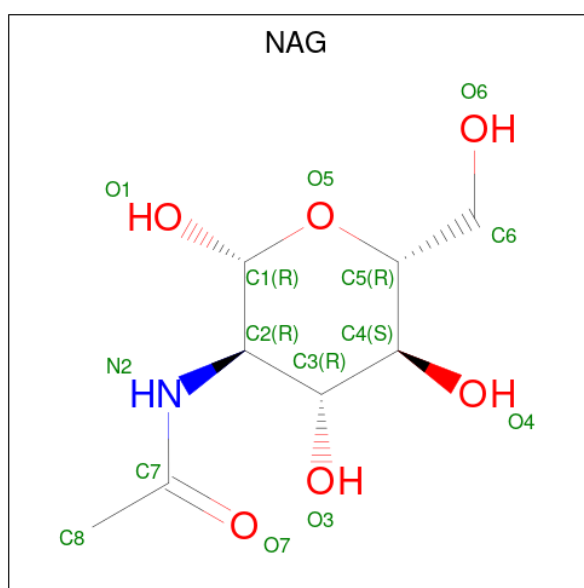
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	U	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total Zn 1 1	0	0
8	G	1	Total Zn 1 1	0	0
8	I	1	Total Zn 1 1	0	0

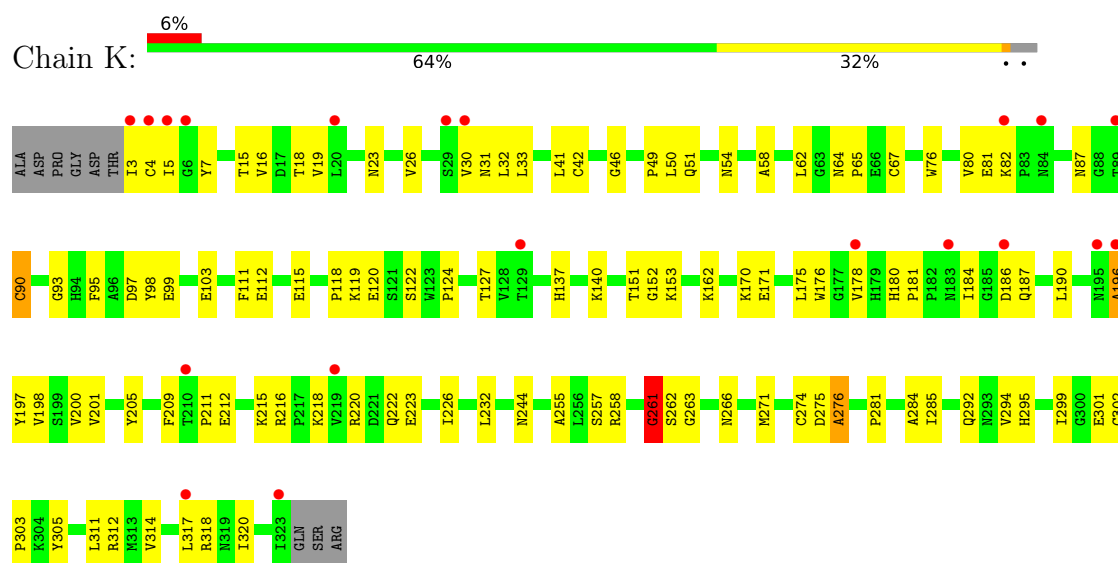
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	61	Total O 61 61	0	0
9	L	19	Total O 19 19	0	0
9	A	71	Total O 71 71	0	0
9	B	7	Total O 7 7	0	0
9	C	61	Total O 61 61	0	0
9	D	13	Total O 13 13	0	0
9	E	42	Total O 42 42	0	0
9	F	17	Total O 17 17	0	0
9	G	44	Total O 44 44	0	0
9	H	16	Total O 16 16	0	0
9	I	61	Total O 61 61	0	0
9	J	16	Total O 16 16	0	0

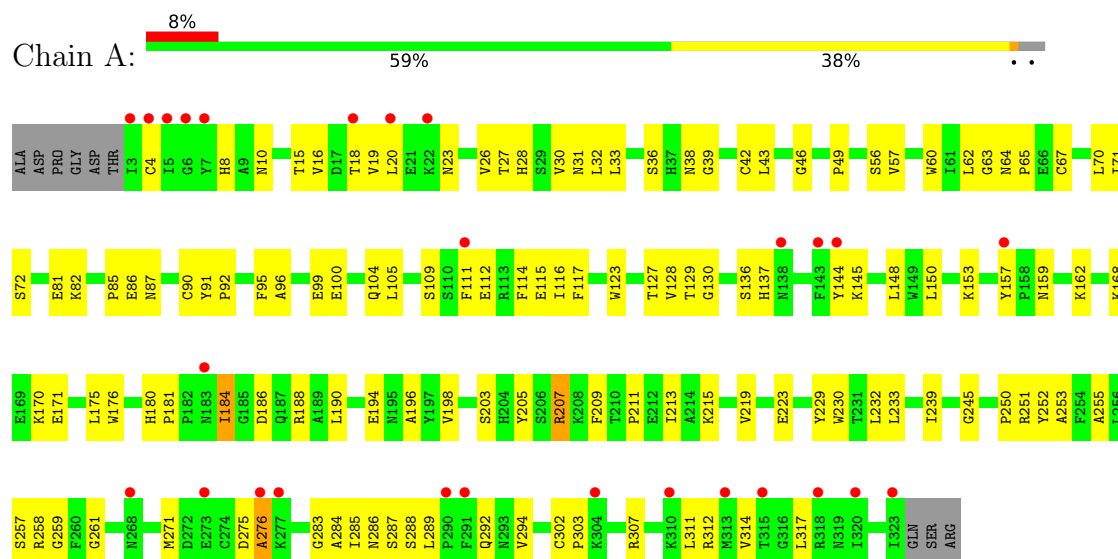
3 Residue-property plots

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

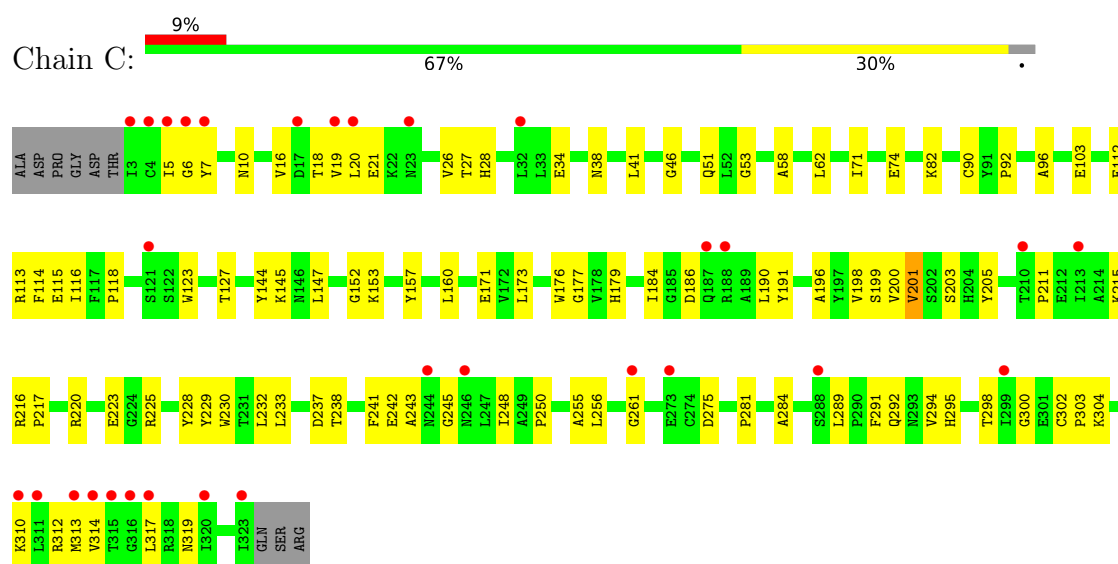
- Molecule 1: Hemagglutinin HA1 chain



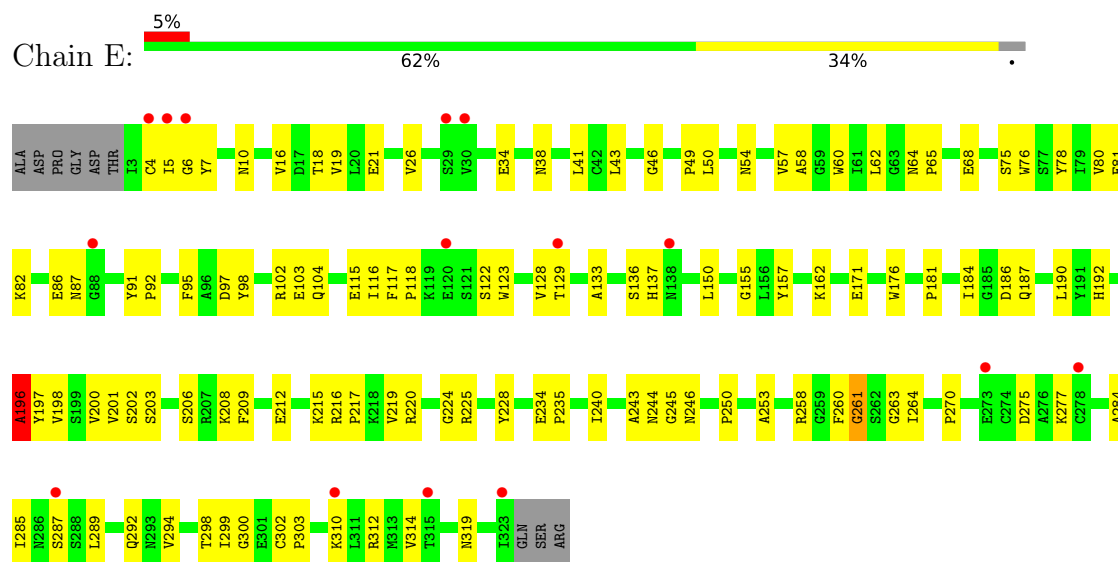
- Molecule 1: Hemagglutinin HA1 chain



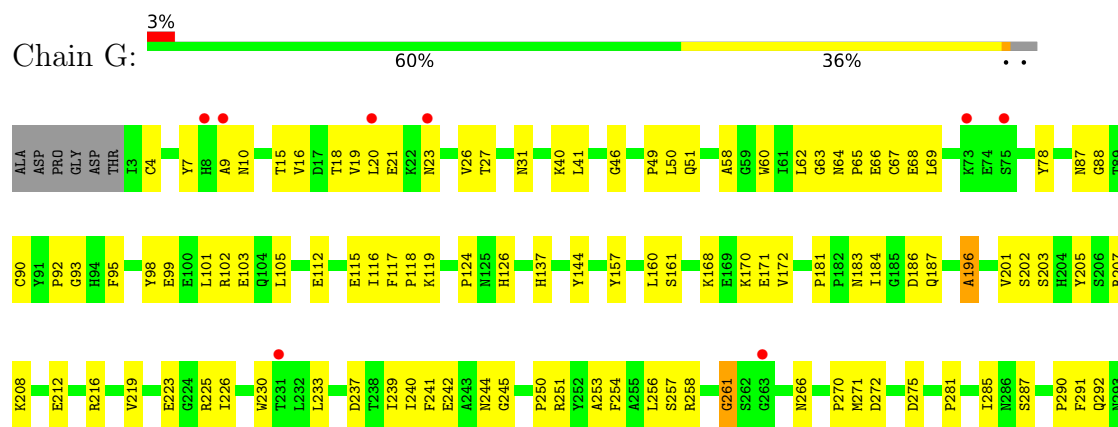
- Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

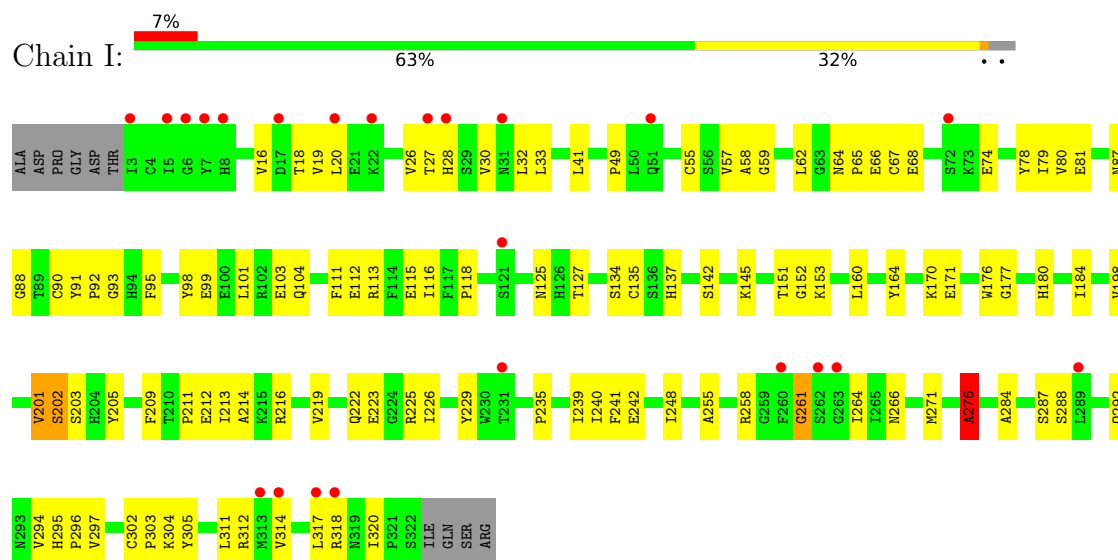


• Molecule 1: Hemagglutinin HA1 chain

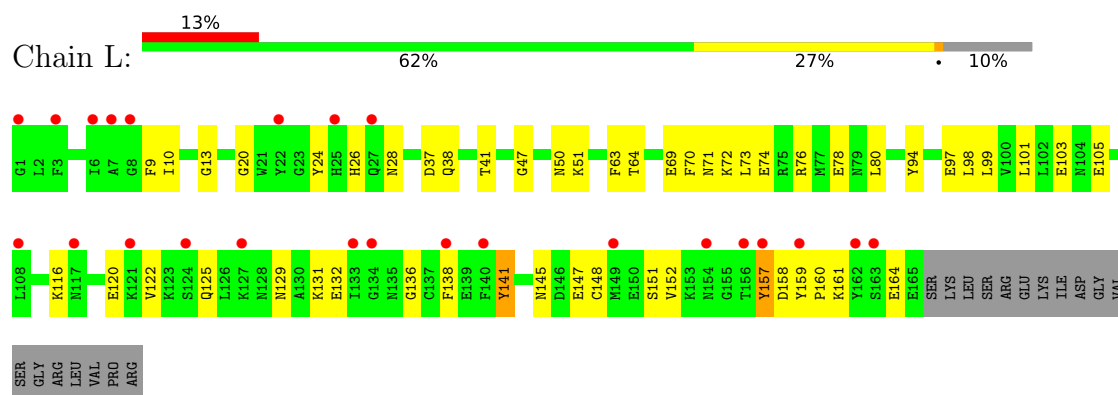




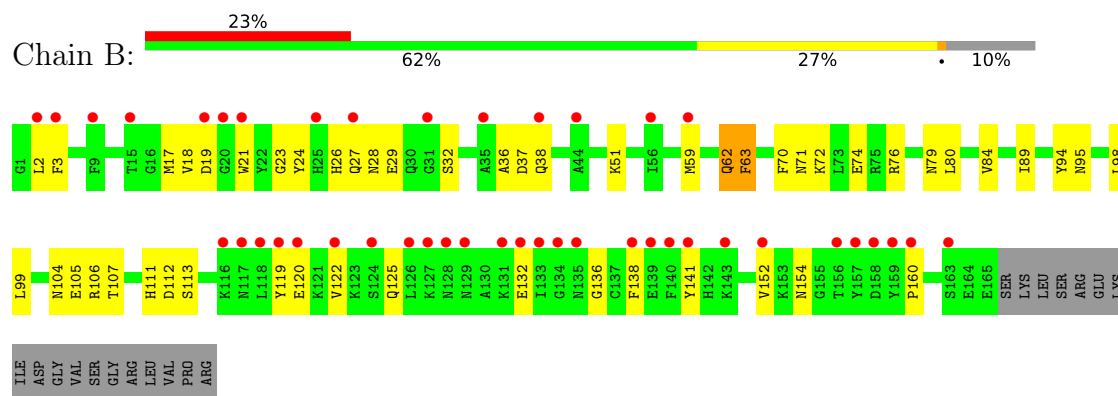
• Molecule 1: Hemagglutinin HA1 chain



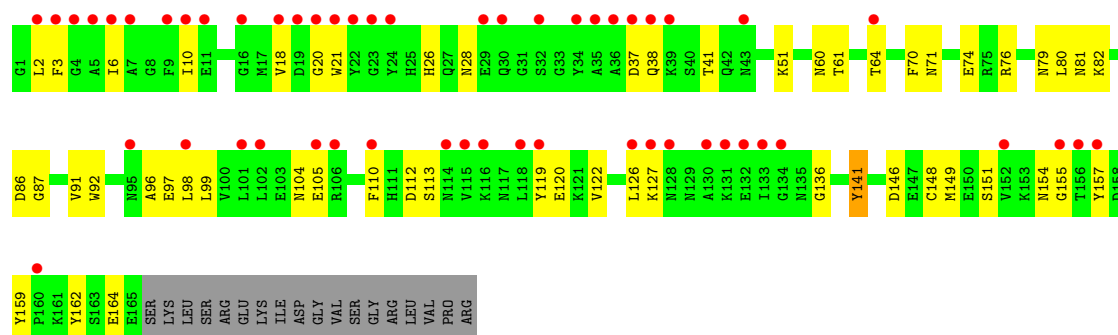
• Molecule 2: Hemagglutinin HA2 chain



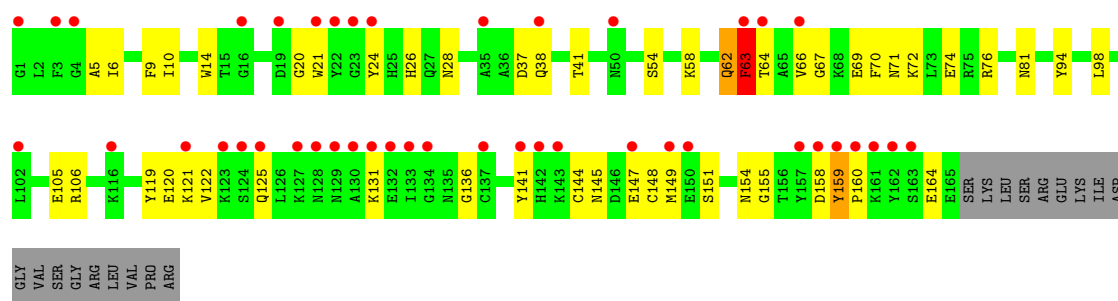
• Molecule 2: Hemagglutinin HA2 chain



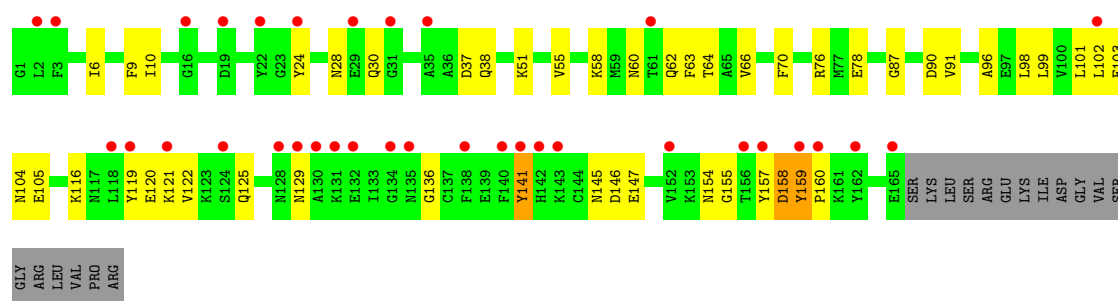
• Molecule 2: Hemagglutinin HA2 chain



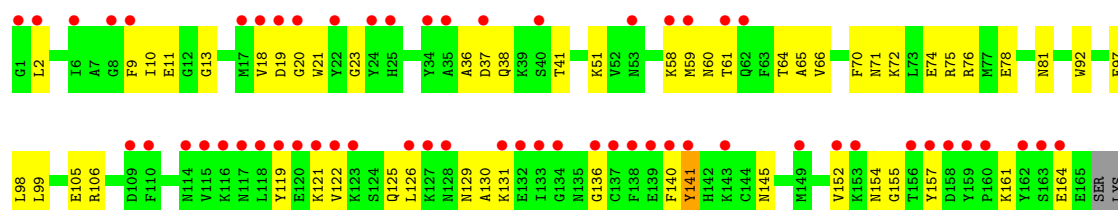
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



LEU
SER
ARG
GLU
LYS
TLE
ASP
GLY
VAL
SER
GLY
ARG
LEU
VAL
PRO
ARG

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

Chain M:  17% 83%

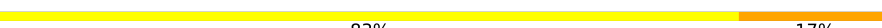
NAG1
NAG2
BMA3
MAN4
NAG5
MAN6

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

Chain S:  50% 50%

NAG1
NAG2
BMA3
MAN4
NAG5
MAN6

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

Chain V:  83% 17%

NAG1
NAG2
BMA3
MAN4
NAG5
MAN6

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

Chain N:  40% 60%

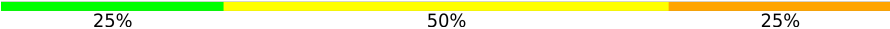
NAG1
NAG2
BMA3
MAN4
NAG5

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

Chain P:  60% 40%

NAG1
NAG2
BMA3
MAN4
NAG5

- Molecule 5: 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 O:  25% 50% 25%



- Molecule 5: 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 Q:  50% 50%



- Molecule 5: 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 R:  50% 50%

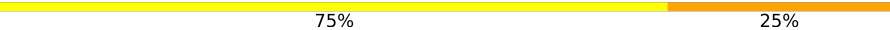


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%

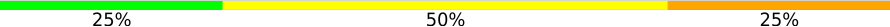


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  75% 25%



- Molecule 5: 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 X:  25% 50% 25%



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

Chain W:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.71Å 124.27Å 214.53Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	48.75 – 3.24 48.75 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.75-3.24) 94.7 (48.75-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.265 , 0.295 0.265 , 0.295	Depositor DCC
R_{free} test set	1999 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.550	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24413	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6117e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/2581	1.02	4/3512 (0.1%)
1	C	0.58	0/2581	0.96	3/3512 (0.1%)
1	E	0.57	0/2581	1.01	5/3512 (0.1%)
1	G	0.57	0/2573	0.99	5/3501 (0.1%)
1	I	0.58	0/2573	1.00	6/3501 (0.2%)
1	K	0.57	0/2581	0.97	5/3512 (0.1%)
2	B	0.40	0/1352	0.92	2/1819 (0.1%)
2	D	0.37	0/1352	0.89	2/1819 (0.1%)
2	F	0.45	0/1352	0.94	6/1819 (0.3%)
2	H	0.44	0/1352	0.96	4/1819 (0.2%)
2	J	0.42	0/1352	0.94	3/1819 (0.2%)
2	L	0.46	0/1352	0.98	3/1819 (0.2%)
All	All	0.53	0/23582	0.97	48/31964 (0.2%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	276	ALA	N-CA-C	7.10	120.29	110.35
2	L	158	ASP	N-CA-C	-6.99	98.28	109.39
2	H	158	ASP	N-CA-C	-6.70	98.74	109.39
2	F	159	TYR	N-CA-C	6.65	122.60	113.16
2	F	158	ASP	N-CA-C	-6.62	98.86	109.39
1	A	276	ALA	N-CA-C	6.35	124.33	110.80
2	B	141	TYR	N-CA-C	-6.24	105.15	112.89
1	G	261	GLY	N-CA-C	6.19	127.84	113.18
2	L	141	TYR	N-CA-C	-6.12	104.52	112.23
1	A	184	ILE	N-CA-C	-5.91	104.28	112.50
2	B	152	VAL	N-CA-C	-5.85	104.44	113.16
1	K	261	GLY	N-CA-C	5.79	126.91	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	184	ILE	N-CA-C	-5.75	104.50	112.50
1	K	111	PHE	CB-CA-C	-5.72	99.49	110.24
2	H	157	TYR	N-CA-C	5.69	119.37	110.32
1	I	276	ALA	N-CA-C	5.65	122.83	110.80
2	J	141	TYR	N-CA-C	-5.64	105.89	112.89
2	F	5	ALA	N-CA-C	5.64	117.29	111.03
1	I	111	PHE	CB-CA-C	-5.62	99.68	110.24
1	G	287	SER	N-CA-C	5.62	117.24	109.15
1	I	184	ILE	N-CA-C	-5.60	104.72	112.50
1	E	261	GLY	N-CA-C	5.46	122.86	115.32
2	L	157	TYR	N-CA-C	5.45	118.54	110.48
2	F	67	GLY	CA-C-N	-5.44	113.69	122.23
2	F	67	GLY	C-N-CA	-5.44	113.69	122.23
1	C	310	LYS	N-CA-C	5.43	119.28	111.02
1	E	86	GLU	CA-C-N	-5.43	115.05	121.90
1	E	86	GLU	C-N-CA	-5.43	115.05	121.90
2	H	141	TYR	N-CA-C	-5.41	105.41	112.23
1	A	207	ARG	CA-CB-CG	5.38	124.86	114.10
1	E	196	ALA	N-CA-C	5.38	122.26	110.80
1	G	124	PRO	N-CA-C	-5.31	103.21	111.13
2	D	18	VAL	N-CA-C	-5.28	102.38	108.82
1	C	201	VAL	N-CA-C	5.23	115.57	107.78
2	H	159	TYR	N-CA-C	5.20	120.67	113.45
1	E	310	LYS	N-CA-C	5.17	118.87	111.02
1	K	124	PRO	N-CA-C	-5.16	104.00	111.22
1	C	184	ILE	N-CA-C	-5.13	105.36	112.50
2	D	141	TYR	N-CA-C	-5.12	106.54	112.89
1	K	184	ILE	N-CA-C	-5.11	105.40	112.50
2	J	152	VAL	N-CA-C	-5.10	105.56	113.16
1	A	111	PHE	CB-CA-C	-5.07	100.71	110.24
2	F	63	PHE	N-CA-CB	5.06	119.04	110.49
1	G	310	LYS	N-CA-C	5.03	121.52	110.80
2	J	157	TYR	N-CA-C	5.03	117.92	110.48
1	I	202	SER	N-CA-C	-5.03	102.05	109.94
1	I	201	VAL	CA-C-N	5.01	132.35	122.73
1	I	201	VAL	C-N-CA	5.01	132.35	122.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2515	0	2435	109	0
1	C	2515	0	2440	87	0
1	E	2515	0	2437	107	1
1	G	2507	0	2427	111	0
1	I	2507	0	2427	102	1
1	K	2515	0	2439	92	0
2	B	1325	0	1246	49	0
2	D	1325	0	1246	50	0
2	F	1325	0	1246	53	0
2	H	1325	0	1246	47	0
2	J	1325	0	1246	53	0
2	L	1325	0	1246	51	0
3	M	75	0	64	5	0
3	S	75	0	64	2	0
3	V	75	0	64	5	0
4	N	64	0	55	6	0
4	P	64	0	55	4	0
5	O	50	0	43	1	0
5	Q	50	0	43	0	0
5	R	50	0	43	3	0
5	T	50	0	43	2	0
5	U	50	0	43	1	0
5	X	50	0	43	4	0
6	W	39	0	34	1	0
7	A	70	0	65	4	0
7	C	14	0	13	1	0
7	E	56	0	52	0	0
7	G	42	0	39	1	0
7	I	42	0	39	1	0
7	K	42	0	39	1	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
9	A	71	0	0	4	0
9	B	7	0	0	1	0
9	C	61	0	0	4	0
9	D	13	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	42	0	0	3	0
9	F	17	0	0	1	0
9	G	44	0	0	1	0
9	H	16	0	0	0	0
9	I	61	0	0	3	0
9	J	16	0	0	0	0
9	K	61	0	0	4	0
9	L	19	0	0	1	0
All	All	24413	0	22922	783	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 17.

All (783) 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:G:310:LYS:HB3	1:G:312:ARG:HD3	1.41	1.02
1:E:19:VAL:HG12	2:F:105:GLU:HG3	1.36	1.01
2:J:71:ASN:HB3	2:J:74:GLU:HG3	1.41	1.00
1:K:87:ASN:HD22	4:N:1:NAG:H83	1.30	0.96
1:I:202:SER:HB3	1:I:205:TYR:HB3	1.53	0.88
1:K:19:VAL:HG12	2:L:105:GLU:HG3	1.56	0.87
1:E:68:GLU:OE1	1:E:137:HIS:CE1	2.28	0.86
1:C:300:GLY:H	2:D:64:THR:HG22	1.38	0.86
1:I:292:GLN:HB3	1:I:303:PRO:HG2	1.56	0.85
2:D:98:LEU:HD21	2:J:99:LEU:HD13	1.57	0.84
1:E:19:VAL:HG12	2:F:105:GLU:CG	2.08	0.83
2:L:71:ASN:OD1	2:L:72:LYS:N	2.13	0.82
1:E:19:VAL:CG1	2:F:105:GLU:HG3	2.10	0.82
1:E:68:GLU:OE1	1:E:137:HIS:NE2	2.13	0.81
2:J:71:ASN:OD1	2:J:72:LYS:N	2.14	0.81
5:R:1:NAG:H62	5:R:2:NAG:HN2	1.46	0.80
1:I:87:ASN:HD22	5:X:1:NAG:H83	1.45	0.80
1:A:16:VAL:HG21	1:A:314:VAL:HG13	1.62	0.80
1:E:58:ALA:HB2	1:E:98:TYR:HE1	1.45	0.80
2:F:76:ARG:HG3	1:G:103:GLU:HG3	1.64	0.80
1:G:21:GLU:OE1	1:G:318:ARG:NH2	2.16	0.79
1:A:26:VAL:HG21	1:A:314:VAL:HG11	1.63	0.79
1:G:171:GLU:OE1	1:G:258:ARG:NH1	2.16	0.79
1:A:65:PRO:HB2	1:A:137:HIS:HB2	1.63	0.79
1:K:16:VAL:HG11	1:K:314:VAL:HG13	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:OG1	2:B:105:GLU:HG2	1.83	0.78
1:E:64:ASN:HD22	1:E:87:ASN:HB3	1.49	0.77
1:A:112:GLU:HB3	1:A:255:ALA:HB3	1.66	0.76
1:G:95:PHE:HB3	1:G:98:TYR:HB2	1.68	0.76
2:D:76:ARG:HG3	1:I:103:GLU:HG3	1.69	0.75
1:K:103:GLU:HG3	2:H:76:ARG:HG3	1.68	0.75
1:I:134:SER:OG	1:I:222:GLN:HG2	1.86	0.75
1:A:198:VAL:HB	1:A:209:PHE:HB2	1.69	0.74
1:C:176:TRP:HB3	1:C:250:PRO:HG3	1.67	0.74
2:L:76:ARG:HG3	1:E:103:GLU:HG3	1.68	0.74
1:K:42:CYS:SG	1:K:274:CYS:HB2	2.29	0.73
1:K:292:GLN:HB3	1:K:303:PRO:HG2	1.72	0.72
1:G:212:GLU:O	1:G:216:ARG:NH2	2.21	0.72
1:G:49:PRO:HD2	1:G:271:MET:HE1	1.71	0.72
1:K:54:ASN:OD1	1:K:82:LYS:NZ	2.21	0.72
1:I:112:GLU:HB3	1:I:255:ALA:HB3	1.71	0.72
1:E:299:ILE:HA	2:F:64:THR:HG22	1.72	0.72
2:F:71:ASN:ND2	2:F:74:GLU:OE2	2.22	0.72
1:K:65:PRO:HB2	1:K:137:HIS:HB2	1.72	0.71
2:F:72:LYS:HG3	9:F:209:HOH:O	1.91	0.71
1:G:87:ASN:HD22	3:V:1:NAG:H83	1.56	0.71
1:E:220:ARG:NH2	5:T:1:NAG:O7	2.24	0.70
1:A:100:GLU:HG2	2:J:76:ARG:HE	1.56	0.70
1:K:93:GLY:HA3	1:K:226:ILE:O	1.92	0.70
2:B:28:ASN:ND2	2:B:29:GLU:OE2	2.25	0.70
1:G:299:ILE:HA	2:H:64:THR:HG22	1.74	0.70
3:S:5:NAG:O7	3:S:5:NAG:O3	2.07	0.70
1:E:261:GLY:O	2:F:64:THR:HG21	1.91	0.70
1:C:19:VAL:HG22	2:J:51:LYS:HG2	1.73	0.69
1:E:171:GLU:OE1	1:E:258:ARG:NH1	2.25	0.69
2:F:37:ASP:OD1	2:F:38:GLN:N	2.25	0.69
1:G:90:CYS:HB3	3:V:1:NAG:H81	1.75	0.69
1:I:16:VAL:HG22	1:I:312:ARG:HG2	1.75	0.69
1:E:58:ALA:HB2	1:E:98:TYR:CE1	2.26	0.68
1:I:59:GLY:HA3	1:I:88:GLY:HA2	1.75	0.68
2:F:125:GLN:NE2	2:F:154:ASN:O	2.26	0.68
1:C:123:TRP:HZ3	1:C:160:LEU:HD21	1.58	0.68
1:C:304:LYS:HE2	2:D:92:TRP:CD1	2.29	0.68
1:K:302:CYS:SG	1:K:303:PRO:HD2	2.34	0.67
1:C:46:GLY:N	1:C:275:ASP:OD1	2.28	0.67
1:K:197:TYR:CD1	1:K:244:ASN:HB2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:THR:OG1	1:E:302:CYS:SG	2.52	0.67
1:E:298:THR:HG21	2:F:62:GLN:HG2	1.75	0.67
1:G:93:GLY:HA3	1:G:226:ILE:O	1.94	0.67
2:B:113:SER:OG	2:J:2:LEU:O	2.12	0.67
1:G:307:ARG:NH2	2:H:90:ASP:OD1	2.20	0.67
1:A:8:HIS:NE2	1:A:10:ASN:OD1	2.28	0.67
1:E:18:THR:HG22	1:E:21:GLU:O	1.96	0.66
1:A:116:ILE:HD13	1:A:253:ALA:HB2	1.76	0.66
1:I:171:GLU:OE1	1:I:258:ARG:NH1	2.28	0.66
2:L:141:TYR:HB2	2:L:164:GLU:HG3	1.78	0.66
1:K:46:GLY:N	1:K:275:ASP:OD1	2.27	0.66
1:K:49:PRO:HD2	1:K:271:MET:HE1	1.76	0.66
2:D:71:ASN:HB3	2:D:74:GLU:HG3	1.75	0.66
1:I:216:ARG:O	1:I:223:GLU:HG3	1.95	0.66
1:C:19:VAL:HG12	2:D:105:GLU:HG3	1.77	0.66
2:D:76:ARG:NH1	2:J:74:GLU:OE1	2.29	0.65
1:I:18:THR:HG23	1:I:20:LEU:H	1.60	0.65
2:B:76:ARG:CG	1:C:103:GLU:HG3	2.27	0.65
2:L:71:ASN:HB3	2:L:74:GLU:CD	2.21	0.65
1:K:171:GLU:OE1	1:K:258:ARG:NH1	2.29	0.65
2:B:99:LEU:HD13	2:J:98:LEU:HD21	1.79	0.65
2:B:76:ARG:NH2	2:D:74:GLU:OE1	2.27	0.65
1:E:128:VAL:HG12	1:E:150:LEU:HD22	1.78	0.65
1:I:176:TRP:CE2	1:I:229:TYR:HB2	2.32	0.65
2:L:101:LEU:HD11	2:F:54:SER:OG	1.96	0.65
1:A:100:GLU:OE2	2:J:75:ARG:N	2.30	0.65
1:K:26:VAL:HG21	1:K:314:VAL:HG11	1.79	0.64
1:C:16:VAL:HG11	1:C:314:VAL:HG13	1.79	0.64
1:C:115:GLU:HG2	1:C:118:PRO:HA	1.79	0.64
1:I:65:PRO:HB2	1:I:137:HIS:HB2	1.79	0.64
1:I:115:GLU:CD	1:I:118:PRO:HA	2.22	0.64
2:D:97:GLU:HB3	2:J:58:LYS:HE3	1.80	0.64
1:G:40:LYS:HD2	1:G:272:ASP:OD2	1.97	0.64
1:I:104:GLN:OE1	1:I:258:ARG:NH2	2.31	0.64
1:G:302:CYS:SG	1:G:303:PRO:HD2	2.37	0.64
2:B:2:LEU:O	2:D:113:SER:OG	2.08	0.64
1:E:300:GLY:H	2:F:64:THR:HG23	1.63	0.64
1:K:299:ILE:HA	2:L:64:THR:HG22	1.80	0.64
2:F:145:ASN:ND2	2:F:147:GLU:OE1	2.31	0.64
2:H:37:ASP:OD1	2:H:38:GLN:N	2.31	0.64
1:G:16:VAL:HG11	1:G:314:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:28:ASN:HD21	2:L:145:ASN:HA	1.63	0.63
1:C:114:PHE:CE2	1:C:116:ILE:HG22	2.32	0.63
1:E:16:VAL:HG11	1:E:314:VAL:HG13	1.80	0.63
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.62	0.63
2:H:121:LYS:O	2:H:125:GLN:HG3	1.98	0.63
2:L:105:GLU:HB3	2:F:106:ARG:HH22	1.62	0.63
1:G:202:SER:HB3	1:G:205:TYR:HB3	1.80	0.63
1:G:64:ASN:HD22	1:G:87:ASN:HB3	1.62	0.63
1:I:58:ALA:HB2	1:I:98:TYR:CE1	2.33	0.63
1:C:18:THR:HG23	1:C:20:LEU:H	1.64	0.62
2:B:29:GLU:OE2	2:B:29:GLU:N	2.30	0.62
1:I:16:VAL:HG11	1:I:314:VAL:HG13	1.81	0.62
1:K:196:ALA:HA	1:K:244:ASN:HB3	1.81	0.62
1:A:19:VAL:HG12	2:B:105:GLU:HG3	1.81	0.62
1:G:19:VAL:O	1:G:20:LEU:HG	1.99	0.62
1:I:59:GLY:CA	1:I:88:GLY:HA2	2.30	0.62
1:E:43:LEU:HD23	1:E:46:GLY:O	2.00	0.62
1:E:197:TYR:CD1	1:E:244:ASN:HB2	2.34	0.62
1:K:103:GLU:HG3	2:H:76:ARG:CG	2.29	0.62
1:E:157:TYR:CZ	1:E:245:GLY:HA2	2.35	0.62
1:K:64:ASN:HD21	4:N:1:NAG:C8	2.13	0.62
2:F:20:GLY:HA2	2:F:41:THR:HG21	1.82	0.62
2:L:120:GLU:C	2:L:122:VAL:H	2.07	0.61
1:A:96:ALA:HB2	1:A:229:TYR:CD1	2.34	0.61
1:A:100:GLU:HG2	2:J:76:ARG:NE	2.15	0.61
6:W:2:NAG:O3	6:W:3:BMA:H61	1.99	0.61
2:H:145:ASN:ND2	2:H:147:GLU:OE1	2.34	0.61
1:K:212:GLU:O	1:K:216:ARG:NH2	2.33	0.61
1:G:64:ASN:HD21	3:V:1:NAG:H83	1.66	0.61
1:A:203:SER:HB2	1:I:219:VAL:HG11	1.81	0.61
1:G:7:TYR:CZ	2:H:6:ILE:HG23	2.36	0.61
1:G:207:ARG:NH2	9:G:503:HOH:O	2.34	0.60
2:L:37:ASP:OD1	2:L:38:GLN:N	2.35	0.60
2:J:18:VAL:HG12	2:J:19:ASP:H	1.64	0.60
2:J:130:ALA:HB2	2:J:140:PHE:CD1	2.36	0.60
1:E:116:ILE:HD13	1:E:253:ALA:HB2	1.83	0.60
2:L:70:PHE:CD2	2:L:78:GLU:HA	2.37	0.60
1:A:87:ASN:ND2	4:P:1:NAG:O7	2.35	0.60
1:C:179:HIS:ND1	1:C:191:TYR:OH	2.30	0.60
2:D:80:LEU:HD13	2:J:81:ASN:OD1	2.02	0.60
1:I:18:THR:OG1	2:J:105:GLU:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ASP:O	1:E:190:LEU:HB2	2.02	0.60
1:I:212:GLU:O	1:I:216:ARG:NH2	2.35	0.60
1:K:281:PRO:HG2	1:K:295:HIS:CE1	2.36	0.60
2:B:76:ARG:HG2	1:C:103:GLU:HG3	1.83	0.60
1:G:181:PRO:HG2	1:G:187:GLN:HB2	1.84	0.60
1:A:230:TRP:HZ3	1:A:232:LEU:HD12	1.66	0.59
1:G:170:LYS:NZ	1:G:257:SER:OG	2.18	0.59
1:E:26:VAL:HG21	1:E:314:VAL:HG11	1.83	0.59
1:K:212:GLU:HB3	1:E:208:LYS:HD3	1.85	0.59
1:K:95:PHE:HB3	1:K:98:TYR:HB2	1.85	0.59
2:L:51:LYS:HG2	1:G:19:VAL:HG22	1.84	0.59
1:I:49:PRO:HD2	1:I:271:MET:HE1	1.85	0.59
1:I:180:HIS:ND1	1:I:211:PRO:HA	2.18	0.59
1:I:145:LYS:NZ	9:I:501:HOH:O	2.36	0.59
1:I:292:GLN:OE1	1:I:294:VAL:N	2.36	0.58
1:G:65:PRO:O	1:G:68:GLU:HG3	2.02	0.58
2:F:125:GLN:HE22	2:F:155:GLY:HA3	1.68	0.58
1:K:64:ASN:HB3	1:K:67:CYS:SG	2.44	0.58
2:L:131:LYS:NZ	2:L:141:TYR:HB3	2.18	0.58
1:I:180:HIS:CE1	1:I:211:PRO:HA	2.39	0.58
1:A:128:VAL:HG12	1:A:150:LEU:HD22	1.86	0.57
1:E:16:VAL:HG21	1:E:314:VAL:HG12	1.85	0.57
2:F:154:ASN:OD1	2:F:155:GLY:N	2.36	0.57
1:K:261:GLY:O	2:L:64:THR:HG21	2.04	0.57
1:C:10:ASN:O	1:C:319:ASN:ND2	2.30	0.57
1:E:122:SER:O	1:E:162:LYS:HE2	2.04	0.57
2:F:81:ASN:C	2:F:81:ASN:HD22	2.10	0.57
1:I:27:THR:HG22	1:I:317:LEU:O	2.04	0.57
2:J:37:ASP:OD1	2:J:38:GLN:N	2.37	0.57
1:K:119:LYS:NZ	9:K:504:HOH:O	2.37	0.57
1:K:311:LEU:HD21	2:L:97:GLU:HG2	1.85	0.57
1:A:170:LYS:HE3	1:A:257:SER:OG	2.04	0.57
1:A:56:SER:HB3	1:A:85:PRO:HB2	1.85	0.57
2:J:141:TYR:OH	2:J:161:LYS:HG3	2.05	0.57
2:L:50:ASN:HB3	1:G:20:LEU:HA	1.86	0.57
1:A:15:THR:CG2	1:A:23:ASN:HA	2.35	0.57
1:A:186:ASP:O	1:A:190:LEU:HB2	2.05	0.57
1:C:196:ALA:HB1	1:C:211:PRO:HG2	1.87	0.57
1:G:50:LEU:HD11	1:G:60:TRP:CZ2	2.39	0.57
1:I:261:GLY:O	2:J:64:THR:HG21	2.05	0.56
1:A:27:THR:HG22	1:A:317:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:CYS:SG	1:A:303:PRO:HD2	2.45	0.56
1:E:300:GLY:O	2:F:63:PHE:HA	2.04	0.56
2:H:129:ASN:HA	2:H:141:TYR:CE2	2.40	0.56
2:H:154:ASN:OD1	2:H:155:GLY:N	2.36	0.56
1:I:127:THR:OG1	1:I:152:GLY:O	2.22	0.56
1:A:117:PHE:CD1	1:A:162:LYS:HG2	2.41	0.56
1:A:157:TYR:CZ	1:A:245:GLY:HA2	2.40	0.56
1:C:82:LYS:HG3	9:C:512:HOH:O	2.05	0.56
1:K:127:THR:HG23	1:K:153:LYS:HB2	1.87	0.56
2:B:51:LYS:HG2	1:I:19:VAL:O	2.06	0.56
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.41	0.56
2:J:125:GLN:HE22	2:J:155:GLY:HA3	1.69	0.56
1:K:31:ASN:O	1:K:31:ASN:ND2	2.38	0.56
1:K:198:VAL:HB	1:K:209:PHE:HB2	1.88	0.56
1:C:18:THR:HG22	1:C:21:GLU:O	2.05	0.56
2:D:37:ASP:OD1	2:D:38:GLN:N	2.38	0.56
1:G:27:THR:HG22	1:G:317:LEU:O	2.05	0.56
1:C:96:ALA:HB2	1:C:229:TYR:CD1	2.40	0.55
2:B:98:LEU:HD21	2:D:99:LEU:HD13	1.89	0.55
1:K:201:VAL:HG11	1:G:216:ARG:HB3	1.89	0.55
2:L:145:ASN:ND2	2:L:147:GLU:OE1	2.39	0.55
1:A:114:PHE:CE2	1:A:116:ILE:HG23	2.41	0.55
1:G:302:CYS:O	2:H:62:GLN:N	2.39	0.55
2:J:130:ALA:HB2	2:J:140:PHE:HD1	1.70	0.55
1:K:23:ASN:CG	7:K:401:NAG:H83	2.32	0.55
1:K:90:CYS:O	1:K:220:ARG:HD3	2.07	0.55
2:B:37:ASP:OD1	2:B:38:GLN:N	2.39	0.55
1:C:28:HIS:CE1	2:D:21:TRP:HE1	2.25	0.55
1:G:18:THR:OG1	2:H:105:GLU:HG2	2.06	0.55
2:H:28:ASN:HD21	2:H:145:ASN:C	2.14	0.55
1:I:170:LYS:N	1:I:235:PRO:HG3	2.21	0.55
1:C:233:LEU:HG	1:C:237:ASP:HB3	1.88	0.55
1:G:161:SER:HA	1:G:241:PHE:O	2.06	0.55
2:D:28:ASN:ND2	2:D:146:ASP:OD1	2.35	0.55
2:B:27:GLN:HA	2:B:32:SER:HB2	1.89	0.55
1:C:34:GLU:HG2	1:C:289:LEU:HD12	1.89	0.55
1:C:291:PHE:CE2	2:D:96:ALA:HB2	2.42	0.55
2:H:119:TYR:CE1	2:H:136:GLY:HA2	2.41	0.55
1:E:54:ASN:OD1	1:E:82:LYS:NZ	2.28	0.55
1:E:62:LEU:HD21	1:E:228:TYR:CD1	2.42	0.55
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:HB2	1:I:219:VAL:CG1	2.37	0.54
1:E:260:PHE:HD1	1:E:260:PHE:H	1.54	0.54
2:H:28:ASN:ND2	2:H:146:ASP:OD1	2.27	0.54
2:L:148:CYS:HA	2:L:151:SER:HB3	1.89	0.54
1:C:27:THR:HG22	1:C:317:LEU:O	2.06	0.54
1:E:16:VAL:HG21	1:E:314:VAL:CG1	2.37	0.54
1:E:6:GLY:HA3	2:F:14:TRP:CZ2	2.42	0.54
2:D:141:TYR:HE2	2:D:162:TYR:H	1.54	0.54
1:E:64:ASN:ND2	1:E:87:ASN:HB3	2.18	0.54
1:G:172:VAL:HA	1:G:254:PHE:O	2.07	0.54
1:C:16:VAL:HG22	1:C:312:ARG:HB3	1.89	0.54
1:I:16:VAL:HG21	1:I:314:VAL:HG12	1.90	0.54
1:I:292:GLN:NE2	1:I:295:HIS:O	2.32	0.54
1:A:99:GLU:H	1:A:99:GLU:CD	2.16	0.54
2:D:127:LYS:HD3	2:D:159:TYR:OH	2.08	0.54
1:K:87:ASN:HA	4:N:1:NAG:H83	1.90	0.54
1:K:115:GLU:CD	1:K:118:PRO:HA	2.33	0.54
1:C:302:CYS:SG	1:C:303:PRO:HD2	2.48	0.54
1:G:297:VAL:HG13	2:H:66:VAL:HG12	1.90	0.54
1:A:233:LEU:HD13	1:A:239:ILE:HB	1.90	0.53
2:B:132:GLU:HG3	2:B:138:PHE:HE1	1.73	0.53
1:G:64:ASN:HD21	3:V:1:NAG:C8	2.21	0.53
1:E:133:ALA:O	1:E:136:SER:OG	2.21	0.53
1:I:304:LYS:HE2	2:J:92:TRP:CD1	2.43	0.53
1:A:109:SER:HB3	1:A:259:GLY:HA3	1.90	0.53
2:B:51:LYS:HG2	1:I:19:VAL:HG22	1.90	0.53
1:E:287:SER:HB2	1:E:303:PRO:HD3	1.90	0.53
1:G:16:VAL:HG22	1:G:312:ARG:HB3	1.90	0.53
1:I:296:PRO:HG3	1:I:305:TYR:CE2	2.44	0.53
1:A:91:TYR:CD1	1:A:92:PRO:HD2	2.44	0.53
1:A:115:GLU:OE2	1:A:251:ARG:NE	2.33	0.53
1:G:116:ILE:HG22	1:G:117:PHE:CG	2.44	0.53
1:E:176:TRP:NE1	1:E:200:VAL:HG21	2.23	0.53
1:A:100:GLU:HG3	2:J:76:ARG:HH21	1.72	0.53
2:B:76:ARG:HG3	1:C:103:GLU:HG3	1.90	0.53
1:E:197:TYR:CE1	1:E:244:ASN:HB2	2.44	0.53
1:E:234:GLU:N	9:E:502:HOH:O	2.27	0.53
1:K:18:THR:HB	2:L:105:GLU:HG2	1.91	0.52
1:A:307:ARG:CZ	2:B:89:ILE:HG21	2.39	0.52
1:C:157:TYR:CE1	1:C:245:GLY:HA2	2.45	0.52
2:D:60:ASN:O	2:D:61:THR:HG23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:O	2:D:10:ILE:HD13	2.09	0.52
2:B:94:TYR:HD1	2:B:95:ASN:HD22	1.56	0.52
1:E:92:PRO:HB2	1:E:225:ARG:HD3	1.91	0.52
1:E:202:SER:OG	1:E:203:SER:N	2.43	0.52
1:E:184:ILE:HD12	1:E:184:ILE:H	1.75	0.52
1:E:104:GLN:NE2	9:E:503:HOH:O	2.30	0.52
1:E:263:GLY:HA3	2:F:66:VAL:HG11	1.92	0.52
1:A:127:THR:HG23	1:A:153:LYS:HB2	1.91	0.52
2:B:59:MET:HE3	2:B:59:MET:HA	1.92	0.52
1:C:62:LEU:HD21	1:C:228:TYR:CD1	2.45	0.52
2:D:3:PHE:HB2	2:D:112:ASP:CG	2.35	0.52
1:E:292:GLN:HG2	1:E:303:PRO:HG2	1.91	0.52
4:P:5:NAG:O7	4:P:5:NAG:O3	2.23	0.52
2:L:20:GLY:HA2	2:L:41:THR:HG21	1.92	0.52
1:A:100:GLU:O	1:A:104:GLN:HG2	2.09	0.52
1:E:116:ILE:HD11	1:E:250:PRO:HB2	1.92	0.52
1:G:26:VAL:HG21	1:G:314:VAL:HG11	1.92	0.52
1:I:112:GLU:HG3	9:I:544:HOH:O	2.10	0.52
1:C:96:ALA:HB3	1:C:229:TYR:HA	1.92	0.51
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.46	0.51
1:G:310:LYS:HG2	1:G:312:ARG:NH1	2.25	0.51
2:F:28:ASN:HD21	2:F:145:ASN:HA	1.75	0.51
1:I:64:ASN:HD21	5:X:1:NAG:C8	2.23	0.51
1:I:87:ASN:HA	5:X:1:NAG:H83	1.92	0.51
1:I:214:ALA:O	1:I:216:ARG:NH1	2.43	0.51
1:K:216:ARG:O	1:K:223:GLU:HG3	2.09	0.51
1:G:292:GLN:HG2	1:G:303:PRO:HG2	1.93	0.51
2:J:119:TYR:HE1	2:J:136:GLY:HA2	1.75	0.51
1:E:16:VAL:HG22	1:E:312:ARG:HG2	1.92	0.51
2:B:71:ASN:ND2	2:B:74:GLU:HG3	2.26	0.51
2:F:26:HIS:HB2	2:F:149:MET:SD	2.50	0.51
1:A:38:ASN:HB3	1:A:284:ALA:N	2.25	0.51
1:C:112:GLU:HB3	1:C:255:ALA:HB3	1.93	0.51
1:E:57:VAL:HG23	1:E:81:GLU:OE2	2.11	0.51
1:E:292:GLN:HB3	1:E:303:PRO:HG2	1.91	0.51
1:A:128:VAL:HB	1:A:148:LEU:HD21	1.93	0.51
2:B:74:GLU:OE1	2:J:76:ARG:NH1	2.43	0.51
2:F:28:ASN:ND2	2:F:144:CYS:O	2.43	0.51
2:H:154:ASN:CG	2:H:155:GLY:H	2.18	0.51
1:I:135:CYS:O	1:I:142:SER:HB3	2.11	0.51
1:A:63:GLY:O	1:A:145:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:TYR:CE2	2:D:6:ILE:HA	2.45	0.51
1:G:58:ALA:HB2	1:G:98:TYR:CE2	2.46	0.51
2:H:129:ASN:HA	2:H:141:TYR:HE2	1.76	0.51
2:L:125:GLN:NE2	2:L:152:VAL:O	2.44	0.51
1:C:96:ALA:O	1:C:230:TRP:NE1	2.40	0.51
1:I:302:CYS:SG	1:I:303:PRO:HD2	2.51	0.51
1:K:58:ALA:HB2	1:K:98:TYR:CE1	2.46	0.51
1:K:276:ALA:HB2	1:K:284:ALA:HB1	1.92	0.51
1:E:215:LYS:HG3	1:G:240:ILE:HD13	1.92	0.51
1:I:28:HIS:CE1	2:J:21:TRP:HE1	2.29	0.51
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.93	0.51
1:K:33:LEU:HD12	1:K:311:LEU:HD12	1.93	0.50
2:B:3:PHE:CZ	2:B:113:SER:HB2	2.46	0.50
1:I:213:ILE:HD12	9:I:539:HOH:O	2.10	0.50
1:A:205:TYR:OH	1:A:207:ARG:HD3	2.11	0.50
1:A:4:CYS:O	2:B:24:TYR:HA	2.11	0.50
1:G:300:GLY:O	2:H:63:PHE:HA	2.11	0.50
1:K:87:ASN:ND2	4:N:1:NAG:H83	2.13	0.50
1:K:99:GLU:H	1:K:99:GLU:CD	2.20	0.50
1:C:157:TYR:CZ	1:C:245:GLY:HA2	2.46	0.50
1:C:298:THR:O	2:D:64:THR:HA	2.11	0.50
1:G:49:PRO:HB3	1:G:78:TYR:CZ	2.45	0.50
1:I:99:GLU:CD	2:J:71:ASN:HB2	2.37	0.50
2:J:121:LYS:O	2:J:125:GLN:HG3	2.11	0.50
1:K:276:ALA:CB	1:K:284:ALA:HB1	2.42	0.50
2:F:76:ARG:CG	1:G:103:GLU:HG3	2.39	0.50
1:K:58:ALA:O	1:K:62:LEU:HB2	2.11	0.50
3:M:1:NAG:H4	3:M:2:NAG:H61	1.92	0.50
1:E:299:ILE:HA	2:F:64:THR:CG2	2.40	0.50
1:K:205:TYR:C	1:K:205:TYR:CD1	2.89	0.50
1:C:292:GLN:OE1	1:C:294:VAL:HG22	2.12	0.50
2:J:141:TYR:HB2	2:J:164:GLU:HG3	1.92	0.50
1:C:71:ILE:HD13	1:C:145:LYS:HD3	1.93	0.49
1:G:41:LEU:N	1:G:270:PRO:O	2.31	0.49
1:G:112:GLU:OE2	1:G:168:LYS:NZ	2.45	0.49
1:E:116:ILE:CD1	1:E:250:PRO:HB2	2.42	0.49
2:F:9:PHE:CD1	2:F:10:ILE:HG13	2.47	0.49
2:L:9:PHE:CD1	2:L:10:ILE:HG13	2.47	0.49
1:A:219:VAL:HG11	1:C:203:SER:HB3	1.93	0.49
1:A:286:ASN:OD1	7:A:413:NAG:H4	2.12	0.49
7:A:414:NAG:H3	9:A:533:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:THR:OG1	2:F:105:GLU:HG2	2.12	0.49
1:E:91:TYR:HB3	1:E:228:TYR:OH	2.11	0.49
1:E:98:TYR:HE2	1:E:102:ARG:HD2	1.77	0.49
1:A:16:VAL:HG22	2:B:104:ASN:ND2	2.28	0.49
1:G:95:PHE:HE1	1:G:230:TRP:CD1	2.30	0.49
1:K:41:LEU:HD13	1:K:80:VAL:HG21	1.94	0.49
2:L:76:ARG:CG	1:E:103:GLU:HG3	2.39	0.49
1:G:4:CYS:O	2:H:24:TYR:HA	2.12	0.49
1:A:123:TRP:CZ3	1:A:162:LYS:HD3	2.47	0.49
1:A:181:PRO:HG2	1:A:213:ILE:HG12	1.94	0.49
2:H:28:ASN:HD21	2:H:145:ASN:HA	1.78	0.49
1:I:201:VAL:HG12	1:I:202:SER:O	2.13	0.49
2:D:76:ARG:CG	1:I:103:GLU:HG3	2.41	0.49
2:L:73:LEU:HD13	1:E:97:ASP:OD1	2.13	0.49
1:C:123:TRP:CZ3	1:C:160:LEU:HD21	2.45	0.48
1:C:216:ARG:HA	1:I:240:ILE:HD12	1.94	0.48
1:G:196:ALA:HA	1:G:244:ASN:HB3	1.95	0.48
1:I:16:VAL:HG22	1:I:312:ARG:CG	2.43	0.48
2:H:30:GLN:OE1	2:H:145:ASN:HB2	2.13	0.48
2:H:122:VAL:HA	2:H:125:GLN:HB2	1.95	0.48
1:C:7:TYR:CD2	2:D:6:ILE:HG22	2.48	0.48
1:C:123:TRP:CZ3	1:C:160:LEU:HD11	2.49	0.48
1:I:49:PRO:HB3	1:I:78:TYR:CZ	2.48	0.48
5:U:4:MAN:H61	5:U:4:MAN:O2	2.14	0.48
1:C:19:VAL:CG2	2:J:51:LYS:HG2	2.41	0.48
1:E:64:ASN:OD1	1:E:65:PRO:HD2	2.13	0.48
1:A:72:SER:OG	9:A:501:HOH:O	2.20	0.48
1:C:38:ASN:HB3	1:C:284:ALA:HB3	1.95	0.48
1:E:234:GLU:OE1	1:E:235:PRO:HD2	2.13	0.48
5:T:1:NAG:H62	5:T:2:NAG:O7	2.14	0.48
1:A:171:GLU:OE1	1:A:258:ARG:NH1	2.46	0.48
1:I:16:VAL:HG21	1:I:314:VAL:CG1	2.44	0.48
1:I:57:VAL:HG21	1:I:264:ILE:HD13	1.94	0.48
1:A:71:ILE:CD1	1:A:145:LYS:HD3	2.43	0.48
2:B:18:VAL:O	2:B:19:ASP:OD1	2.31	0.48
1:I:79:ILE:HB	1:I:264:ILE:HG12	1.95	0.48
1:I:115:GLU:OE2	1:I:118:PRO:HA	2.13	0.48
1:A:188:ARG:HH21	1:A:194:GLU:CD	2.22	0.48
1:C:292:GLN:HG2	1:C:303:PRO:HG2	1.94	0.48
1:G:116:ILE:HG13	1:G:253:ALA:HB3	1.96	0.48
1:G:291:PHE:CE1	2:H:96:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:ASP:C	2:H:160:PRO:HD2	2.38	0.48
2:B:80:LEU:HD13	2:D:81:ASN:OD1	2.12	0.47
1:C:74:GLU:OE2	1:C:113:ARG:HB3	2.13	0.47
1:E:224:GLY:O	1:E:225:ARG:NH1	2.46	0.47
1:K:285:ILE:HD11	1:K:294:VAL:CG2	2.44	0.47
1:A:64:ASN:OD1	1:A:65:PRO:HD2	2.14	0.47
1:K:7:TYR:HE1	1:K:320:ILE:HD13	1.79	0.47
2:L:145:ASN:OD1	2:L:145:ASN:N	2.42	0.47
1:A:30:VAL:O	1:A:312:ARG:O	2.32	0.47
2:H:120:GLU:C	2:H:122:VAL:H	2.21	0.47
1:K:197:TYR:CE1	1:K:244:ASN:HB2	2.49	0.47
2:L:69:GLU:HA	9:L:202:HOH:O	2.15	0.47
1:A:46:GLY:N	1:A:275:ASP:OD1	2.47	0.47
1:K:215:LYS:HE3	1:E:240:ILE:HG21	1.95	0.47
2:B:125:GLN:NE2	2:B:154:ASN:O	2.42	0.47
1:E:212:GLU:HB3	1:G:208:LYS:HD3	1.95	0.47
1:G:292:GLN:HB3	1:G:303:PRO:HG2	1.96	0.47
1:I:91:TYR:CD1	1:I:92:PRO:HD2	2.49	0.47
1:I:320:ILE:O	2:J:13:GLY:N	2.38	0.47
2:D:126:LEU:HD23	2:D:157:TYR:CE2	2.49	0.47
1:E:41:LEU:N	1:E:270:PRO:O	2.34	0.47
2:F:21:TRP:H	2:F:41:THR:HG23	1.80	0.47
1:I:276:ALA:HB1	1:I:284:ALA:HB1	1.97	0.47
1:K:180:HIS:ND1	1:K:211:PRO:HA	2.30	0.47
2:D:120:GLU:C	2:D:122:VAL:H	2.22	0.47
1:E:4:CYS:O	2:F:24:TYR:HA	2.14	0.47
1:E:10:ASN:O	1:E:319:ASN:ND2	2.47	0.47
1:E:46:GLY:N	1:E:275:ASP:OD1	2.41	0.47
1:E:289:LEU:O	1:E:303:PRO:HB3	2.15	0.47
2:F:98:LEU:HD21	2:H:99:LEU:HD13	1.96	0.47
2:F:120:GLU:C	2:F:122:VAL:H	2.22	0.47
2:F:131:LYS:HG3	2:F:141:TYR:CE1	2.50	0.47
1:G:19:VAL:HB	2:H:101:LEU:HD23	1.96	0.47
1:G:281:PRO:HG2	1:G:295:HIS:CE1	2.48	0.47
1:I:55:CYS:HA	1:I:87:ASN:O	2.14	0.47
1:I:302:CYS:SG	1:I:303:PRO:CD	3.03	0.47
2:J:60:ASN:O	2:J:61:THR:OG1	2.31	0.47
2:B:120:GLU:C	2:B:122:VAL:H	2.22	0.47
1:G:16:VAL:HG22	1:G:312:ARG:CB	2.44	0.47
1:G:115:GLU:OE2	1:G:118:PRO:HA	2.15	0.47
1:K:15:THR:CG2	1:K:23:ASN:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLY:HA2	2:D:10:ILE:HG21	1.97	0.47
2:D:148:CYS:O	2:D:151:SER:HB3	2.15	0.47
1:I:64:ASN:HB3	1:I:67:CYS:SG	2.55	0.47
1:I:81:GLU:O	1:I:266:ASN:HA	2.15	0.47
1:C:7:TYR:CE2	2:D:6:ILE:HG22	2.50	0.46
1:G:63:GLY:O	1:G:144:TYR:HA	2.15	0.46
1:G:157:TYR:CE1	1:G:245:GLY:HA2	2.50	0.46
1:A:26:VAL:HG21	1:A:314:VAL:CG1	2.40	0.46
1:A:180:HIS:CE1	1:A:211:PRO:HA	2.50	0.46
1:C:216:ARG:O	1:C:223:GLU:HG3	2.15	0.46
2:D:82:LYS:HE2	2:D:86:ASP:OD2	2.15	0.46
2:H:55:VAL:HG13	2:H:99:LEU:HD21	1.98	0.46
2:L:120:GLU:C	2:L:122:VAL:N	2.73	0.46
2:B:160:PRO:O	9:B:201:HOH:O	2.20	0.46
2:D:20:GLY:HA2	2:D:41:THR:HG21	1.97	0.46
2:F:154:ASN:CG	2:F:155:GLY:H	2.20	0.46
1:G:46:GLY:N	1:G:275:ASP:OD1	2.48	0.46
1:G:313:MET:HA	2:H:104:ASN:OD1	2.16	0.46
4:N:3:BMA:H3	4:N:4:MAN:H3	1.98	0.46
1:K:7:TYR:CE1	1:K:320:ILE:HD13	2.50	0.46
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.96	0.46
2:J:18:VAL:HG12	2:J:19:ASP:N	2.30	0.46
3:S:3:BMA:H61	3:S:6:MAN:H2	1.73	0.46
1:A:19:VAL:HG12	2:B:105:GLU:CG	2.45	0.46
1:A:31:ASN:O	1:A:33:LEU:N	2.48	0.46
1:A:116:ILE:CD1	1:A:253:ALA:HB2	2.44	0.46
1:A:159:ASN:ND2	7:A:414:NAG:H83	2.31	0.46
1:C:314:VAL:N	2:D:104:ASN:OD1	2.48	0.46
1:E:7:TYR:CE2	2:F:6:ILE:HG22	2.50	0.46
1:G:170:LYS:HZ2	1:G:257:SER:HG	1.52	0.46
1:G:300:GLY:H	2:H:64:THR:HG23	1.80	0.46
1:K:215:LYS:O	1:K:215:LYS:HG3	2.15	0.46
1:A:18:THR:HG23	1:A:20:LEU:H	1.80	0.46
1:A:36:SER:HB3	9:A:550:HOH:O	2.15	0.46
1:A:184:ILE:HD12	1:A:184:ILE:H	1.80	0.46
1:C:92:PRO:HB2	1:C:225:ARG:HD3	1.97	0.46
1:C:171:GLU:H	1:C:171:GLU:HG2	1.36	0.46
1:C:232:LEU:HD12	9:C:548:HOH:O	2.15	0.46
1:G:101:LEU:HB2	1:G:230:TRP:CZ2	2.51	0.46
1:I:95:PHE:HB3	1:I:98:TYR:HB2	1.98	0.46
1:C:238:THR:HG21	9:C:531:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ALA:O	1:G:62:LEU:HB2	2.15	0.46
2:H:51:LYS:NZ	2:H:103:GLU:HB3	2.31	0.46
2:H:116:LYS:O	2:H:120:GLU:HG2	2.16	0.46
1:A:64:ASN:HB3	1:A:67:CYS:SG	2.55	0.46
1:A:96:ALA:HB2	1:A:229:TYR:HD1	1.77	0.46
2:D:126:LEU:HD23	2:D:157:TYR:HE2	1.81	0.46
1:I:93:GLY:HA3	1:I:226:ILE:O	2.15	0.46
1:I:311:LEU:HD21	2:J:97:GLU:HG2	1.98	0.46
1:E:19:VAL:HG22	2:H:51:LYS:HG2	1.97	0.46
1:E:299:ILE:HA	2:F:64:THR:HA	1.98	0.46
2:J:20:GLY:HA2	2:J:41:THR:HG21	1.98	0.46
2:J:122:VAL:O	2:J:126:LEU:N	2.40	0.46
1:K:170:LYS:HD2	1:K:257:SER:OG	2.17	0.45
2:L:157:TYR:C	2:L:159:TYR:N	2.74	0.45
1:A:28:HIS:CD2	2:B:21:TRP:HE1	2.35	0.45
1:G:203:SER:OG	1:G:237:ASP:OD1	2.33	0.45
1:A:16:VAL:CG2	1:A:314:VAL:HG13	2.40	0.45
1:A:317:LEU:HB3	2:B:111:HIS:ND1	2.31	0.45
1:G:64:ASN:HB3	1:G:67:CYS:SG	2.56	0.45
2:B:3:PHE:HB2	2:B:112:ASP:CG	2.42	0.45
1:C:220:ARG:NH2	5:R:1:NAG:O3	2.42	0.45
1:E:38:ASN:HB3	1:E:284:ALA:N	2.31	0.45
1:G:160:LEU:O	1:G:242:GLU:HA	2.15	0.45
1:I:64:ASN:O	1:I:66:GLU:N	2.50	0.45
2:J:129:ASN:HA	2:J:141:TYR:CE2	2.51	0.45
9:K:508:HOH:O	1:E:201:VAL:HB	2.15	0.45
1:I:26:VAL:HG21	1:I:314:VAL:HG11	1.98	0.45
1:I:74:GLU:OE2	1:I:113:ARG:HB3	2.17	0.45
1:I:177:GLY:CA	1:I:248:ILE:HB	2.46	0.45
3:M:3:BMA:H3	3:M:4:MAN:H5	1.98	0.45
1:K:151:THR:HG22	1:K:152:GLY:N	2.32	0.45
2:L:94:TYR:CZ	2:L:98:LEU:HD22	2.52	0.45
1:C:198:VAL:HG22	1:C:243:ALA:HB1	1.98	0.45
1:C:215:LYS:HG2	1:I:242:GLU:OE2	2.17	0.45
1:E:115:GLU:HG2	1:E:118:PRO:HA	1.98	0.45
1:G:16:VAL:HG21	1:G:314:VAL:HG12	1.99	0.45
1:K:42:CYS:HB3	1:K:274:CYS:O	2.17	0.45
1:A:209:PHE:CE2	1:A:229:TYR:CD2	3.04	0.45
1:C:16:VAL:HG21	1:C:314:VAL:HG12	1.97	0.45
1:C:173:LEU:HB2	1:C:256:LEU:HD21	1.98	0.45
1:G:19:VAL:CG1	2:H:105:GLU:HG3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:LEU:HD12	2:J:105:GLU:HG3	1.99	0.45
1:I:116:ILE:HG13	1:I:164:TYR:CD1	2.52	0.45
1:K:140:LYS:HG2	5:O:2:NAG:H62	1.98	0.45
2:L:132:GLU:HG3	2:L:138:PHE:HE1	1.82	0.45
1:E:215:LYS:HG2	1:G:242:GLU:OE2	2.17	0.45
1:G:92:PRO:HB3	1:G:219:VAL:HG13	1.98	0.45
1:G:310:LYS:CB	1:G:312:ARG:HD3	2.29	0.45
1:I:198:VAL:O	1:I:209:PHE:HD1	2.00	0.45
1:K:16:VAL:HG22	1:K:312:ARG:HB3	1.99	0.45
2:L:129:ASN:HA	2:L:141:TYR:CE2	2.52	0.45
1:C:18:THR:OG1	2:D:105:GLU:HG2	2.16	0.45
1:C:123:TRP:CE3	1:C:160:LEU:HD11	2.52	0.45
2:B:51:LYS:NZ	2:B:107:THR:HG23	2.32	0.45
1:K:186:ASP:O	1:K:190:LEU:HB2	2.17	0.44
2:L:131:LYS:HZ2	2:L:141:TYR:HB3	1.81	0.44
1:K:292:GLN:HG3	1:K:305:TYR:HA	1.98	0.44
1:G:88:GLY:O	1:G:90:CYS:N	2.50	0.44
1:E:123:TRP:CD2	1:E:150:LEU:HD11	2.53	0.44
2:F:70:PHE:HZ	2:F:81:ASN:OD1	2.00	0.44
1:G:216:ARG:O	1:G:223:GLU:HG3	2.17	0.44
2:H:28:ASN:HD21	2:H:145:ASN:CA	2.30	0.44
3:M:3:BMA:H62	3:M:6:MAN:H2	1.77	0.44
1:K:81:GLU:O	1:K:266:ASN:HA	2.18	0.44
1:K:262:SER:OG	1:K:263:GLY:N	2.50	0.44
2:L:80:LEU:HD12	2:L:80:LEU:O	2.17	0.44
1:A:8:HIS:ND1	2:B:17:MET:O	2.50	0.44
1:A:215:LYS:HG2	1:A:223:GLU:OE2	2.17	0.44
1:G:290:PRO:HG2	1:G:291:PHE:CD2	2.53	0.44
2:H:51:LYS:HZ2	2:H:103:GLU:HB3	1.82	0.44
2:L:159:TYR:N	2:L:160:PRO:HD2	2.33	0.44
1:C:127:THR:N	1:C:153:LYS:HB2	2.33	0.44
1:C:281:PRO:HG2	1:C:295:HIS:CE1	2.51	0.44
1:E:34:GLU:HG2	1:E:289:LEU:HD12	2.00	0.44
1:E:216:ARG:HB3	1:G:201:VAL:HG11	1.98	0.44
1:G:183:ASN:HB2	1:G:186:ASP:H	1.83	0.44
1:G:310:LYS:HD3	1:G:312:ARG:HD3	1.99	0.44
1:I:239:ILE:HG12	1:I:241:PHE:CE1	2.53	0.44
1:K:50:LEU:HD12	1:K:76:TRP:CE3	2.53	0.44
1:K:301:GLU:HG2	2:L:63:PHE:CE1	2.53	0.44
1:I:19:VAL:HG12	2:J:105:GLU:HG3	1.99	0.44
2:J:131:LYS:NZ	2:J:141:TYR:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLY:C	1:C:248:ILE:HB	2.42	0.44
1:E:49:PRO:HG3	1:E:78:TYR:CZ	2.53	0.44
1:I:92:PRO:HB3	1:I:219:VAL:CG2	2.47	0.44
1:E:5:ILE:HG13	2:F:119:TYR:HA	1.99	0.44
1:E:198:VAL:HB	1:E:209:PHE:HB2	1.99	0.44
1:G:31:ASN:C	1:G:31:ASN:HD22	2.25	0.44
2:H:87:GLY:O	2:H:91:VAL:HG23	2.18	0.44
1:I:127:THR:HG23	1:I:153:LYS:HB2	2.00	0.44
1:I:297:VAL:HG13	2:J:66:VAL:HG12	1.99	0.44
1:A:285:ILE:HD11	1:A:294:VAL:HG21	1.99	0.44
1:E:98:TYR:CE2	1:E:102:ARG:HD2	2.53	0.44
2:H:70:PHE:CE1	2:H:78:GLU:HA	2.53	0.44
1:I:226:ILE:HD13	1:I:226:ILE:HG21	1.82	0.44
2:B:3:PHE:CE1	2:B:113:SER:HB2	2.53	0.43
2:D:141:TYR:HB2	2:D:164:GLU:HG3	1.99	0.43
1:E:129:THR:HG23	1:E:129:THR:O	2.18	0.43
1:G:15:THR:HB	1:G:312:ARG:HH21	1.82	0.43
1:G:26:VAL:HG21	1:G:314:VAL:CG1	2.48	0.43
1:G:116:ILE:HG22	1:G:117:PHE:CD2	2.53	0.43
1:I:320:ILE:HG21	2:J:11:GLU:O	2.18	0.43
2:L:116:LYS:O	2:L:120:GLU:HG2	2.18	0.43
1:A:31:ASN:C	1:A:33:LEU:H	2.26	0.43
2:B:26:HIS:HD2	2:B:26:HIS:O	2.01	0.43
1:C:147:LEU:HD22	1:C:176:TRP:HA	2.00	0.43
1:C:201:VAL:HA	1:C:205:TYR:O	2.18	0.43
1:G:19:VAL:HG12	2:H:105:GLU:HG3	2.00	0.43
1:G:298:THR:O	2:H:64:THR:HA	2.18	0.43
1:I:88:GLY:O	1:I:90:CYS:N	2.49	0.43
1:K:181:PRO:HG2	1:K:187:GLN:HB2	1.99	0.43
2:L:131:LYS:HZ3	2:L:141:TYR:HB3	1.82	0.43
1:A:104:GLN:OE1	1:A:258:ARG:NH2	2.51	0.43
1:I:41:LEU:HD11	1:I:80:VAL:HG11	1.99	0.43
1:A:129:THR:OG1	1:A:130:GLY:N	2.50	0.43
1:A:203:SER:HA	1:I:225:ARG:HH21	1.84	0.43
1:C:186:ASP:O	1:C:190:LEU:HB2	2.18	0.43
1:G:51:GLN:HE21	1:G:51:GLN:HB2	1.48	0.43
2:B:74:GLU:CD	2:J:76:ARG:HH12	2.25	0.43
1:I:30:VAL:O	1:I:312:ARG:O	2.37	0.43
1:K:3:ILE:HD12	2:L:26:HIS:HB3	2.00	0.43
2:B:72:LYS:HA	2:B:72:LYS:HD3	1.81	0.43
2:B:79:ASN:ND2	1:C:103:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:TYR:HD2	2:H:58:LYS:O	2.01	0.43
2:F:159:TYR:O	2:F:160:PRO:C	2.60	0.43
1:K:176:TRP:CE2	1:K:200:VAL:HG21	2.53	0.43
1:K:292:GLN:HB3	1:K:303:PRO:CG	2.46	0.43
2:L:103:GLU:OE1	2:H:102:LEU:HD11	2.19	0.43
1:A:136:SER:OG	3:M:6:MAN:H4	2.18	0.43
1:C:199:SER:N	1:C:242:GLU:O	2.38	0.43
2:D:2:LEU:HD23	2:D:3:PHE:CE1	2.53	0.43
1:I:151:THR:OG1	1:I:152:GLY:N	2.51	0.43
1:K:120:GLU:HB2	9:K:556:HOH:O	2.18	0.43
2:L:132:GLU:HG3	2:L:138:PHE:CE1	2.53	0.43
2:B:62:GLN:O	2:B:63:PHE:CD2	2.72	0.43
1:C:220:ARG:NH2	5:R:1:NAG:H82	2.34	0.43
1:G:256:LEU:HD23	1:G:258:ARG:NH2	2.33	0.43
1:K:112:GLU:HB3	1:K:255:ALA:HB3	2.00	0.43
1:K:305:TYR:CD1	1:K:305:TYR:C	2.95	0.43
1:A:289:LEU:O	1:A:303:PRO:HB3	2.18	0.43
1:I:101:LEU:HA	1:I:101:LEU:HD12	1.69	0.43
1:I:125:ASN:OD1	7:I:409:NAG:H83	2.19	0.43
2:J:70:PHE:CD1	2:J:78:GLU:HA	2.54	0.43
1:A:49:PRO:HD2	1:A:271:MET:HE1	2.01	0.43
1:A:90:CYS:HB3	4:P:1:NAG:H81	2.01	0.43
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.54	0.43
1:K:171:GLU:OE2	1:K:232:LEU:HD22	2.19	0.42
1:C:313:MET:HA	2:D:104:ASN:OD1	2.19	0.42
2:D:71:ASN:CB	2:D:74:GLU:HG3	2.45	0.42
1:G:69:LEU:HD12	1:G:69:LEU:H	1.84	0.42
1:I:287:SER:OG	1:I:288:SER:N	2.50	0.42
1:E:38:ASN:HB3	1:E:284:ALA:H	1.84	0.42
1:I:317:LEU:HD12	1:I:318:ARG:O	2.19	0.42
1:K:320:ILE:HB	2:L:13:GLY:H	1.83	0.42
2:L:47:GLY:CA	1:G:20:LEU:HB2	2.49	0.42
2:L:141:TYR:OH	2:L:161:LYS:HG3	2.20	0.42
1:A:15:THR:HG23	1:A:23:ASN:HA	2.01	0.42
1:E:68:GLU:CD	1:E:137:HIS:HE2	2.27	0.42
1:E:201:VAL:HG13	1:E:206:SER:HB2	2.02	0.42
1:I:58:ALA:O	1:I:62:LEU:HB2	2.19	0.42
1:K:16:VAL:HG22	1:K:312:ARG:CB	2.50	0.42
2:F:20:GLY:CA	2:F:41:THR:HG21	2.48	0.42
1:G:119:LYS:HD2	1:G:251:ARG:CZ	2.49	0.42
2:H:60:ASN:OD1	2:H:60:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:LEU:HD12	1:I:311:LEU:HD12	2.02	0.42
1:C:292:GLN:HB3	1:C:303:PRO:HG2	2.02	0.42
2:D:51:LYS:HE3	2:D:51:LYS:HB3	1.89	0.42
1:E:264:ILE:HD13	1:E:264:ILE:HG21	1.81	0.42
1:G:285:ILE:HD11	1:G:294:VAL:CG2	2.50	0.42
2:J:23:GLY:HA2	2:J:37:ASP:H	1.84	0.42
1:A:38:ASN:HB3	1:A:284:ALA:H	1.84	0.42
1:A:86:GLU:HB3	4:P:1:NAG:H62	2.02	0.42
1:A:114:PHE:CE2	1:A:168:LYS:HE3	2.55	0.42
1:A:203:SER:HA	1:I:225:ARG:NH2	2.34	0.42
2:B:119:TYR:CD1	2:B:136:GLY:HA2	2.54	0.42
1:C:127:THR:OG1	1:C:152:GLY:O	2.38	0.42
1:K:19:VAL:HA	2:L:101:LEU:HD21	2.01	0.42
1:E:62:LEU:HD13	1:E:95:PHE:HE2	1.84	0.42
1:E:92:PRO:HB3	1:E:219:VAL:HG13	2.02	0.42
1:E:176:TRP:HB3	1:E:250:PRO:HG3	2.01	0.42
1:G:23:ASN:OD1	7:G:402:NAG:O6	2.33	0.42
1:G:92:PRO:HB2	1:G:225:ARG:HD3	2.01	0.42
1:A:60:TRP:CZ3	1:A:105:LEU:HD13	2.54	0.42
9:E:533:HOH:O	2:F:69:GLU:HG3	2.19	0.42
1:G:18:THR:OG1	1:G:19:VAL:N	2.53	0.42
1:G:66:GLU:CD	1:G:137:HIS:HD1	2.28	0.42
1:G:241:PHE:CZ	1:G:250:PRO:HG2	2.54	0.42
1:C:62:LEU:HB3	1:C:144:TYR:CD2	2.55	0.42
2:D:26:HIS:HB2	2:D:149:MET:SD	2.60	0.42
2:F:120:GLU:OE1	2:F:121:LYS:N	2.53	0.42
1:G:10:ASN:O	1:G:319:ASN:ND2	2.50	0.42
1:G:15:THR:CG2	1:G:23:ASN:HA	2.50	0.42
2:J:154:ASN:OD1	2:J:155:GLY:N	2.43	0.42
1:A:18:THR:OG1	1:A:19:VAL:N	2.53	0.42
1:C:261:GLY:HA2	2:D:64:THR:HG21	2.02	0.42
1:G:115:GLU:CD	1:G:118:PRO:HA	2.44	0.42
2:J:145:ASN:OD1	2:J:145:ASN:N	2.43	0.42
1:A:19:VAL:O	2:D:51:LYS:HG2	2.19	0.41
1:E:285:ILE:HD11	1:E:294:VAL:CG2	2.50	0.41
2:H:159:TYR:N	2:H:160:PRO:HD2	2.35	0.41
1:K:178:VAL:O	1:K:226:ILE:HA	2.20	0.41
1:K:209:PHE:CD1	1:K:209:PHE:N	2.88	0.41
1:A:63:GLY:O	1:A:144:TYR:HA	2.19	0.41
1:A:82:LYS:HG3	9:A:561:HOH:O	2.19	0.41
2:D:70:PHE:CD1	2:D:70:PHE:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PRO:O	1:E:122:SER:HB2	2.20	0.41
1:E:217:PRO:HG2	1:G:203:SER:HA	2.02	0.41
2:F:71:ASN:CG	2:F:74:GLU:HG3	2.45	0.41
1:I:209:PHE:HE2	1:I:229:TYR:CE1	2.38	0.41
1:K:5:ILE:HG13	2:L:24:TYR:CD2	2.55	0.41
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.83	0.41
1:E:115:GLU:CD	1:E:118:PRO:HA	2.44	0.41
1:A:87:ASN:HD22	1:A:87:ASN:HA	1.67	0.41
1:A:207:ARG:HG2	1:A:209:PHE:CZ	2.55	0.41
1:C:217:PRO:HG2	1:I:203:SER:HA	2.02	0.41
1:E:198:VAL:HG22	1:E:243:ALA:HB1	2.03	0.41
1:G:90:CYS:CB	3:V:1:NAG:H81	2.47	0.41
1:K:30:VAL:O	1:K:312:ARG:O	2.38	0.41
1:K:31:ASN:O	1:K:33:LEU:N	2.54	0.41
1:K:87:ASN:HD22	4:N:1:NAG:C8	2.15	0.41
1:C:26:VAL:HG21	1:C:314:VAL:HG11	2.03	0.41
1:C:51:GLN:HE21	1:C:53:GLY:H	1.69	0.41
1:C:103:GLU:HG2	9:D:202:HOH:O	2.20	0.41
1:C:127:THR:HG23	1:C:153:LYS:HB2	2.03	0.41
1:E:117:PHE:HB2	1:E:250:PRO:O	2.20	0.41
1:E:196:ALA:HB1	1:E:246:ASN:OD1	2.21	0.41
2:B:80:LEU:O	2:B:84:VAL:HG23	2.20	0.41
1:E:64:ASN:O	1:E:65:PRO:C	2.63	0.41
2:F:62:GLN:O	2:F:63:PHE:CD2	2.74	0.41
1:G:266:ASN:O	1:G:281:PRO:HB3	2.20	0.41
1:A:33:LEU:HD12	1:A:311:LEU:HD12	2.02	0.41
1:A:287:SER:OG	1:A:288:SER:N	2.53	0.41
7:A:402:NAG:H3	7:A:402:NAG:H83	2.02	0.41
2:B:70:PHE:CD1	2:B:70:PHE:N	2.88	0.41
1:C:96:ALA:HB2	1:C:229:TYR:HD1	1.81	0.41
1:E:75:SER:O	1:E:76:TRP:HB3	2.20	0.41
1:G:105:LEU:HA	1:G:105:LEU:HD23	1.78	0.41
1:I:64:ASN:O	1:I:65:PRO:C	2.62	0.41
2:L:99:LEU:HD13	2:H:98:LEU:HD21	2.02	0.41
1:A:38:ASN:HD22	1:A:284:ALA:H	1.69	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.88	0.41
1:A:176:TRP:CZ3	1:A:230:TRP:HA	2.55	0.41
1:C:58:ALA:O	1:C:62:LEU:HB2	2.21	0.41
1:E:5:ILE:O	2:F:10:ILE:HD13	2.21	0.41
1:E:155:GLY:HA2	1:E:192:HIS:CE1	2.56	0.41
1:G:126:HIS:HE1	1:G:157:TYR:CD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:PRO:HB3	1:I:78:TYR:CE2	2.56	0.41
1:K:122:SER:HA	1:K:162:LYS:NZ	2.35	0.41
2:L:101:LEU:HD13	2:F:58:LYS:HE2	2.02	0.41
1:A:39:GLY:H	1:A:283:GLY:HA3	1.86	0.41
1:A:62:LEU:HD13	1:A:95:PHE:HE2	1.86	0.41
1:A:115:GLU:HA	1:A:252:TYR:HA	2.03	0.41
1:A:285:ILE:HD11	1:A:294:VAL:CG2	2.51	0.41
1:A:292:GLN:HG2	1:A:303:PRO:HG2	2.02	0.41
1:C:200:VAL:HG22	1:C:241:PHE:CD1	2.56	0.41
2:D:87:GLY:O	2:D:91:VAL:HG23	2.20	0.41
9:D:209:HOH:O	2:J:65:ALA:HB1	2.20	0.41
1:E:41:LEU:HD23	1:E:41:LEU:HA	1.87	0.41
1:E:50:LEU:HD11	1:E:60:TRP:CZ2	2.56	0.41
1:G:9:ALA:HA	1:G:319:ASN:OD1	2.21	0.41
1:G:31:ASN:C	1:G:31:ASN:ND2	2.79	0.41
1:G:310:LYS:HB3	1:G:312:ARG:CD	2.29	0.41
2:H:9:PHE:CD1	2:H:10:ILE:HG13	2.55	0.41
1:I:134:SER:HG	1:I:222:GLN:HG2	1.84	0.41
2:J:59:MET:HE3	2:J:59:MET:HA	2.03	0.41
1:A:292:GLN:HB3	1:A:303:PRO:HG2	2.03	0.41
2:B:23:GLY:HA2	2:B:37:ASP:H	1.86	0.41
2:F:148:CYS:O	2:F:151:SER:HB3	2.21	0.41
1:G:62:LEU:O	1:G:144:TYR:HB3	2.21	0.41
1:I:57:VAL:HG21	1:I:264:ILE:CD1	2.51	0.41
1:K:62:LEU:HD12	1:K:175:LEU:HD22	2.03	0.40
1:K:97:ASP:O	1:K:98:TYR:C	2.63	0.40
1:K:285:ILE:HD11	1:K:294:VAL:HG22	2.02	0.40
1:K:317:LEU:HD12	1:K:318:ARG:O	2.20	0.40
1:A:10:ASN:ND2	1:A:28:HIS:CE1	2.89	0.40
1:A:38:ASN:ND2	1:A:42:CYS:SG	2.94	0.40
1:C:173:LEU:CB	1:C:256:LEU:HD21	2.50	0.40
2:D:110:PHE:HB2	9:D:205:HOH:O	2.20	0.40
1:E:41:LEU:HD13	1:E:80:VAL:HG21	2.03	0.40
1:E:181:PRO:HG2	1:E:187:GLN:HB2	2.02	0.40
1:G:233:LEU:HD13	1:G:239:ILE:HB	2.03	0.40
2:J:154:ASN:CG	2:J:155:GLY:H	2.26	0.40
1:K:218:LYS:HA	1:K:222:GLN:O	2.21	0.40
2:L:10:ILE:HG12	2:L:136:GLY:HA3	2.03	0.40
1:A:57:VAL:HG23	1:A:81:GLU:OE2	2.21	0.40
2:B:23:GLY:CA	2:B:37:ASP:H	2.35	0.40
2:B:106:ARG:NH1	2:J:106:ARG:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:ASN:OD1	2:D:155:GLY:N	2.46	0.40
1:G:99:GLU:O	1:G:102:ARG:HB2	2.22	0.40
1:I:160:LEU:O	1:I:242:GLU:HA	2.21	0.40
1:K:122:SER:HA	1:K:162:LYS:HZ1	1.85	0.40
1:A:43:LEU:HD23	1:A:46:GLY:O	2.21	0.40
1:A:205:TYR:CD1	1:A:205:TYR:C	3.00	0.40
1:C:216:ARG:HB3	1:C:217:PRO:HD2	2.04	0.40
2:F:141:TYR:CG	2:F:164:GLU:HG3	2.57	0.40
1:I:90:CYS:HB3	5:X:1:NAG:H81	2.02	0.40
3:M:6:MAN:HO3	3:M:6:MAN:HO6	1.68	0.40
1:K:4:CYS:O	2:L:24:TYR:HA	2.21	0.40
1:K:5:ILE:HG13	2:L:24:TYR:HD2	1.86	0.40
1:K:51:GLN:HG2	9:K:536:HOH:O	2.21	0.40
7:C:409:NAG:H83	9:C:544:HOH:O	2.22	0.40
2:D:79:ASN:ND2	1:I:103:GLU:OE1	2.55	0.40
1:A:175:LEU:O	1:A:250:PRO:HB3	2.21	0.40
1:E:277:LYS:HD3	1:E:287:SER:HB3	2.03	0.40
1:E:299:ILE:CA	2:F:64:THR:HG22	2.47	0.40
2:F:125:GLN:NE2	2:F:155:GLY:HA3	2.33	0.40
1:I:112:GLU:CB	1:I:255:ALA:HB3	2.44	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:GLU:OE2	1:I:68:GLU:OE2[3_555]	2.09	0.11

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	319/330 (97%)	291 (91%)	24 (8%)	4 (1%)	9 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	319/330 (97%)	290 (91%)	28 (9%)	1 (0%)	36	66
1	E	319/330 (97%)	291 (91%)	27 (8%)	1 (0%)	36	66
1	G	318/330 (96%)	289 (91%)	27 (8%)	2 (1%)	21	53
1	I	318/330 (96%)	288 (91%)	27 (8%)	3 (1%)	14	44
1	K	319/330 (97%)	290 (91%)	25 (8%)	4 (1%)	9	37
2	B	163/183 (89%)	143 (88%)	18 (11%)	2 (1%)	10	38
2	D	163/183 (89%)	146 (90%)	17 (10%)	0	100	100
2	F	163/183 (89%)	145 (89%)	16 (10%)	2 (1%)	10	38
2	H	163/183 (89%)	149 (91%)	14 (9%)	0	100	100
2	J	163/183 (89%)	146 (90%)	17 (10%)	0	100	100
2	L	163/183 (89%)	147 (90%)	16 (10%)	0	100	100
All	All	2890/3078 (94%)	2615 (90%)	256 (9%)	19 (1%)	18	50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	32	LEU
1	A	32	LEU
2	B	62	GLN
2	B	63	PHE
2	F	62	GLN
2	F	63	PHE
1	K	261	GLY
1	E	196	ALA
1	I	261	GLY
1	A	261	GLY
1	K	90	CYS
1	A	196	ALA
1	G	196	ALA
1	G	261	GLY
1	I	276	ALA
1	K	196	ALA
1	A	276	ALA
1	C	90	CYS
1	I	32	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/288 (98%)	281 (100%)	0	100	100
1	C	281/288 (98%)	281 (100%)	0	100	100
1	E	281/288 (98%)	281 (100%)	0	100	100
1	G	280/288 (97%)	280 (100%)	0	100	100
1	I	280/288 (97%)	280 (100%)	0	100	100
1	K	281/288 (98%)	281 (100%)	0	100	100
2	B	141/157 (90%)	141 (100%)	0	100	100
2	D	141/157 (90%)	141 (100%)	0	100	100
2	F	141/157 (90%)	141 (100%)	0	100	100
2	H	141/157 (90%)	141 (100%)	0	100	100
2	J	141/157 (90%)	141 (100%)	0	100	100
2	L	141/157 (90%)	141 (100%)	0	100	100
All	All	2530/2670 (95%)	2530 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	64	ASN
1	K	138	ASN
1	K	154	ASN
2	L	25	HIS
2	L	28	ASN
2	L	53	ASN
2	L	60	ASN
2	L	95	ASN
2	L	129	ASN
1	A	28	HIS
1	A	31	ASN

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Mol	Chain	Res	Type
1	A	38	ASN
1	A	279	GLN
2	B	28	ASN
2	B	53	ASN
2	B	95	ASN
2	B	129	ASN
1	C	28	HIS
1	C	31	ASN
1	C	51	GLN
1	C	94	HIS
1	C	167	ASN
1	C	266	ASN
2	D	26	HIS
2	D	79	ASN
2	D	128	ASN
1	E	28	HIS
1	E	126	HIS
1	E	204	HIS
1	E	227	ASN
2	F	26	HIS
2	F	117	ASN
2	F	125	GLN
1	G	8	HIS
1	G	28	HIS
1	G	31	ASN
1	G	51	GLN
1	G	64	ASN
1	G	126	HIS
1	G	244	ASN
1	G	266	ASN
2	H	26	HIS
2	H	27	GLN
2	H	30	GLN
2	H	79	ASN
2	H	95	ASN
2	H	142	HIS
1	I	31	ASN
1	I	204	HIS
1	I	244	ASN
2	J	25	HIS
2	J	53	ASN
2	J	125	GLN

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Mol	Chain	Res	Type
2	J	128	ASN
2	J	142	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

55 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	M	1	1,3	14,14,15	0.40	0	17,19,21	2.45	3 (17%)
3	NAG	M	2	3	14,14,15	1.20	1 (7%)	17,19,21	1.60	2 (11%)
3	BMA	M	3	3	11,11,12	2.14	4 (36%)	15,15,17	1.36	3 (20%)
3	MAN	M	4	3	11,11,12	2.51	3 (27%)	15,15,17	1.69	2 (13%)
3	NAG	M	5	3	14,14,15	0.90	1 (7%)	17,19,21	0.71	1 (5%)
3	MAN	M	6	3	11,11,12	1.83	3 (27%)	15,15,17	1.55	3 (20%)
4	NAG	N	1	4,1	14,14,15	0.21	0	17,19,21	0.93	1 (5%)
4	NAG	N	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.59	1 (5%)
4	BMA	N	3	4	11,11,12	1.72	3 (27%)	15,15,17	1.36	1 (6%)
4	MAN	N	4	4	11,11,12	2.19	4 (36%)	15,15,17	2.37	5 (33%)
4	NAG	N	5	4	14,14,15	0.77	0	17,19,21	0.88	1 (5%)
5	NAG	O	1	1,5	14,14,15	0.45	0	17,19,21	0.96	0
5	NAG	O	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.68	3 (17%)
5	BMA	O	3	5	11,11,12	2.12	3 (27%)	15,15,17	2.12	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	O	4	5	11,11,12	1.99	4 (36%)	15,15,17	1.77	3 (20%)
4	NAG	P	1	4,1	14,14,15	0.93	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	P	2	4	14,14,15	0.31	0	17,19,21	0.94	1 (5%)
4	BMA	P	3	4	11,11,12	2.59	3 (27%)	15,15,17	1.82	2 (13%)
4	MAN	P	4	4	11,11,12	3.93	7 (63%)	15,15,17	2.62	6 (40%)
4	NAG	P	5	4	14,14,15	0.97	1 (7%)	17,19,21	1.42	3 (17%)
5	NAG	Q	1	1,5	14,14,15	0.25	0	17,19,21	0.81	0
5	NAG	Q	2	5	14,14,15	0.36	0	17,19,21	1.25	0
5	BMA	Q	3	5	11,11,12	2.32	4 (36%)	15,15,17	2.01	5 (33%)
5	MAN	Q	4	5	11,11,12	1.81	4 (36%)	15,15,17	1.25	2 (13%)
5	NAG	R	1	1,5	14,14,15	0.94	2 (14%)	17,19,21	0.92	1 (5%)
5	NAG	R	2	5	14,14,15	0.91	2 (14%)	17,19,21	1.10	1 (5%)
5	BMA	R	3	5	11,11,12	1.90	2 (18%)	15,15,17	1.97	5 (33%)
5	MAN	R	4	5	11,11,12	2.30	4 (36%)	15,15,17	1.23	1 (6%)
3	NAG	S	1	1,3	14,14,15	0.52	0	17,19,21	2.39	2 (11%)
3	NAG	S	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.44	3 (17%)
3	BMA	S	3	3	11,11,12	3.44	7 (63%)	15,15,17	1.78	4 (26%)
3	MAN	S	4	3	11,11,12	2.98	6 (54%)	15,15,17	2.88	5 (33%)
3	NAG	S	5	3	14,14,15	2.69	2 (14%)	17,19,21	3.12	3 (17%)
3	MAN	S	6	3	11,11,12	2.81	6 (54%)	15,15,17	1.68	3 (20%)
5	NAG	T	1	1,5	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
5	NAG	T	2	5	14,14,15	0.67	1 (7%)	17,19,21	1.65	2 (11%)
5	BMA	T	3	5	11,11,12	2.30	3 (27%)	15,15,17	2.40	4 (26%)
5	MAN	T	4	5	11,11,12	2.24	3 (27%)	15,15,17	1.30	3 (20%)
5	NAG	U	1	1,5	14,14,15	1.09	2 (14%)	17,19,21	1.54	2 (11%)
5	NAG	U	2	5	14,14,15	0.74	0	17,19,21	1.29	2 (11%)
5	BMA	U	3	5	11,11,12	2.23	5 (45%)	15,15,17	1.59	3 (20%)
5	MAN	U	4	5	11,11,12	2.33	5 (45%)	15,15,17	2.16	4 (26%)
3	NAG	V	1	1,3	14,14,15	0.37	0	17,19,21	1.13	2 (11%)
3	NAG	V	2	3	14,14,15	0.50	0	17,19,21	1.06	2 (11%)
3	BMA	V	3	3	11,11,12	1.71	1 (9%)	15,15,17	1.35	2 (13%)
3	MAN	V	4	3	11,11,12	3.41	5 (45%)	15,15,17	2.43	7 (46%)
3	NAG	V	5	3	14,14,15	1.91	2 (14%)	17,19,21	1.54	1 (5%)
3	MAN	V	6	3	11,11,12	1.90	3 (27%)	15,15,17	1.16	1 (6%)
6	NAG	W	1	1,6	14,14,15	0.70	1 (7%)	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	W	2	6	14,14,15	0.34	0	17,19,21	0.70	0
6	BMA	W	3	6	11,11,12	2.06	3 (27%)	15,15,17	1.82	4 (26%)
5	NAG	X	1	1,5	14,14,15	1.12	1 (7%)	17,19,21	1.04	2 (11%)
5	NAG	X	2	5	14,14,15	0.32	0	17,19,21	0.88	0
5	BMA	X	3	5	11,11,12	2.16	4 (36%)	15,15,17	1.64	3 (20%)
5	MAN	X	4	5	11,11,12	1.53	2 (18%)	15,15,17	1.31	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	1/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
3	MAN	S	4	3	-	1/2/19/22	0/1/1/1
3	NAG	S	5	3	-	1/6/23/26	0/1/1/1
3	MAN	S	6	3	-	2/2/19/22	1/1/1/1
5	NAG	T	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	4/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	MAN	T	4	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
5	MAN	U	4	5	-	1/2/19/22	1/1/1/1
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	1/6/23/26	0/1/1/1
3	BMA	V	3	3	-	2/2/19/22	0/1/1/1
3	MAN	V	4	3	-	2/2/19/22	0/1/1/1
3	NAG	V	5	3	-	2/6/23/26	0/1/1/1
3	MAN	V	6	3	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	BMA	W	3	6	-	1/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	BMA	X	3	5	-	1/2/19/22	1/1/1/1
5	MAN	X	4	5	-	1/2/19/22	1/1/1/1

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	5	NAG	O5-C1	9.31	1.59	1.43
4	P	4	MAN	C2-C3	7.75	1.64	1.52
4	P	4	MAN	O2-C2	6.85	1.57	1.43
3	S	3	BMA	C4-C5	6.60	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	4	MAN	O2-C2	6.41	1.56	1.43
3	V	4	MAN	O5-C5	6.04	1.55	1.43
3	S	4	MAN	O5-C5	5.96	1.55	1.43
5	T	4	MAN	C2-C3	5.78	1.61	1.52
4	P	3	BMA	C2-C3	-5.77	1.43	1.52
3	M	4	MAN	C1-C2	5.72	1.65	1.52
3	V	5	NAG	O5-C1	5.46	1.52	1.43
5	X	3	BMA	C2-C3	5.29	1.60	1.52
5	U	4	MAN	O5-C5	4.92	1.53	1.43
3	S	6	MAN	C1-C2	4.90	1.63	1.52
4	P	4	MAN	C4-C3	4.84	1.64	1.52
3	S	3	BMA	O5-C5	4.83	1.52	1.43
3	M	4	MAN	C2-C3	4.82	1.59	1.52
5	R	4	MAN	O5-C5	4.81	1.52	1.43
3	V	4	MAN	O5-C1	4.81	1.51	1.43
5	U	3	BMA	C4-C5	4.71	1.63	1.53
3	S	4	MAN	C1-C2	4.68	1.63	1.52
3	V	5	NAG	C1-C2	4.57	1.58	1.52
5	Q	3	BMA	O5-C1	4.57	1.51	1.43
6	W	3	BMA	C2-C3	4.52	1.59	1.52
4	N	4	MAN	O5-C5	4.48	1.52	1.43
3	S	4	MAN	O5-C1	4.43	1.51	1.43
5	O	3	BMA	C4-C3	4.39	1.63	1.52
5	R	3	BMA	C4-C5	4.36	1.62	1.53
3	S	3	BMA	O3-C3	4.35	1.53	1.43
3	M	2	NAG	O5-C1	4.29	1.50	1.43
4	P	3	BMA	C4-C5	4.28	1.62	1.53
5	T	3	BMA	C4-C5	4.24	1.62	1.53
3	M	3	BMA	C4-C3	4.23	1.63	1.52
5	O	3	BMA	C4-C5	4.12	1.61	1.53
5	R	4	MAN	C4-C5	4.03	1.61	1.53
5	T	3	BMA	C4-C3	4.02	1.62	1.52
3	S	6	MAN	O5-C5	3.97	1.51	1.43
5	Q	4	MAN	C1-C2	3.87	1.61	1.52
5	T	3	BMA	C1-C2	3.85	1.61	1.52
5	R	3	BMA	C4-C3	3.84	1.62	1.52
3	V	4	MAN	C4-C5	3.80	1.61	1.53
5	O	4	MAN	C4-C5	3.71	1.60	1.53
3	S	3	BMA	C4-C3	3.70	1.61	1.52
5	X	1	NAG	O5-C1	-3.70	1.37	1.43
3	S	5	NAG	C1-C2	3.65	1.57	1.52
5	U	4	MAN	O5-C1	3.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	3	BMA	C2-C3	3.60	1.58	1.52
3	M	6	MAN	O5-C5	3.57	1.50	1.43
3	S	3	BMA	C2-C3	-3.55	1.47	1.52
3	V	6	MAN	C4-C3	3.55	1.61	1.52
5	O	4	MAN	O5-C5	3.47	1.50	1.43
6	W	3	BMA	O5-C5	3.44	1.50	1.43
3	S	6	MAN	O2-C2	3.33	1.50	1.43
4	P	4	MAN	O5-C1	3.33	1.49	1.43
3	V	3	BMA	C4-C3	3.29	1.60	1.52
4	P	1	NAG	O5-C1	-3.28	1.38	1.43
3	M	3	BMA	O3-C3	3.28	1.51	1.43
3	S	6	MAN	C6-C5	3.27	1.62	1.51
5	Q	3	BMA	C1-C2	3.27	1.60	1.52
4	N	4	MAN	O5-C1	3.15	1.49	1.43
4	P	4	MAN	C1-C2	3.15	1.59	1.52
5	X	4	MAN	C1-C2	3.15	1.59	1.52
4	P	5	NAG	O5-C1	3.15	1.49	1.43
5	T	4	MAN	C1-C2	3.15	1.59	1.52
4	P	3	BMA	C4-C3	3.12	1.60	1.52
4	N	4	MAN	C1-C2	3.10	1.59	1.52
5	U	1	NAG	O5-C1	-3.09	1.38	1.43
3	S	6	MAN	C2-C3	3.08	1.57	1.52
3	S	3	BMA	O5-C1	3.06	1.48	1.43
4	P	4	MAN	O5-C5	3.05	1.49	1.43
3	M	6	MAN	C1-C2	3.03	1.59	1.52
4	N	3	BMA	O5-C1	2.97	1.48	1.43
4	N	3	BMA	O5-C5	2.93	1.49	1.43
5	X	3	BMA	C1-C2	2.92	1.59	1.52
3	V	6	MAN	O5-C5	2.86	1.49	1.43
3	S	2	NAG	O5-C1	-2.85	1.38	1.43
5	O	4	MAN	C1-C2	2.83	1.59	1.52
5	U	3	BMA	O5-C5	2.83	1.48	1.43
5	U	4	MAN	C6-C5	2.77	1.61	1.51
4	N	4	MAN	O2-C2	2.70	1.49	1.43
5	O	3	BMA	C1-C2	2.68	1.58	1.52
5	O	2	NAG	O5-C1	-2.67	1.39	1.43
5	U	3	BMA	O4-C4	2.66	1.49	1.43
3	V	6	MAN	O5-C1	2.60	1.48	1.43
5	T	4	MAN	C4-C3	2.60	1.59	1.52
4	N	2	NAG	O5-C1	2.57	1.48	1.43
5	R	4	MAN	C4-C3	2.53	1.58	1.52
3	M	3	BMA	O5-C5	2.52	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	6	MAN	O5-C1	2.49	1.47	1.43
3	S	4	MAN	C4-C5	2.48	1.58	1.53
5	R	4	MAN	O5-C1	2.45	1.47	1.43
3	M	5	NAG	C1-C2	2.42	1.55	1.52
5	U	3	BMA	C2-C3	2.40	1.56	1.52
5	X	3	BMA	O3-C3	2.39	1.48	1.43
3	S	4	MAN	O2-C2	2.39	1.48	1.43
3	M	4	MAN	O2-C2	2.36	1.48	1.43
5	U	1	NAG	C1-C2	-2.34	1.49	1.52
5	R	1	NAG	O5-C1	-2.31	1.39	1.43
5	Q	4	MAN	C2-C3	2.30	1.56	1.52
3	S	3	BMA	O2-C2	2.30	1.48	1.43
3	M	3	BMA	O5-C1	2.29	1.47	1.43
6	W	3	BMA	C6-C5	2.28	1.59	1.51
5	R	2	NAG	O5-C1	-2.26	1.39	1.43
5	X	4	MAN	O5-C5	2.26	1.47	1.43
5	R	2	NAG	C1-C2	-2.23	1.49	1.52
4	N	3	BMA	C4-C3	2.22	1.58	1.52
6	W	1	NAG	O5-C1	2.21	1.47	1.43
5	U	4	MAN	C4-C3	2.20	1.58	1.52
3	S	6	MAN	C4-C3	2.15	1.57	1.52
5	T	2	NAG	O5-C1	-2.13	1.40	1.43
5	O	4	MAN	C2-C3	2.11	1.55	1.52
5	U	4	MAN	O2-C2	2.10	1.47	1.43
3	V	4	MAN	C2-C3	2.10	1.55	1.52
5	Q	3	BMA	C6-C5	2.07	1.58	1.51
5	Q	4	MAN	O3-C3	2.06	1.48	1.43
5	R	1	NAG	C1-C2	-2.05	1.49	1.52
5	X	3	BMA	O5-C5	2.03	1.47	1.43
4	P	4	MAN	C6-C5	2.03	1.58	1.51
5	U	3	BMA	C1-C2	2.02	1.57	1.52
3	S	4	MAN	C6-C5	2.01	1.58	1.51
5	Q	4	MAN	O2-C2	2.00	1.47	1.43

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	5	NAG	C1-O5-C5	11.12	127.09	112.19
3	M	1	NAG	C1-O5-C5	8.34	123.37	112.19
3	S	1	NAG	C1-O5-C5	8.28	123.29	112.19
3	S	4	MAN	C1-O5-C5	8.19	123.16	112.19
3	V	4	MAN	C1-O5-C5	6.42	120.79	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	4	MAN	C1-O5-C5	6.38	120.73	112.19
5	T	3	BMA	C1-O5-C5	-6.19	103.89	112.19
4	N	4	MAN	C1-O5-C5	6.03	120.27	112.19
3	V	5	NAG	C1-O5-C5	5.95	120.17	112.19
4	N	2	NAG	C1-O5-C5	5.90	120.10	112.19
5	O	3	BMA	C1-O5-C5	-5.82	104.39	112.19
5	U	4	MAN	C1-O5-C5	5.58	119.66	112.19
3	S	4	MAN	O2-C2-C3	-5.36	99.06	110.15
5	R	3	BMA	C1-C2-C3	-4.84	102.60	109.64
3	S	5	NAG	C2-N2-C7	4.81	129.34	122.90
5	T	2	NAG	C1-O5-C5	4.64	118.40	112.19
4	P	3	BMA	C3-C4-C5	4.57	118.52	110.23
5	X	3	BMA	C1-O5-C5	4.52	118.25	112.19
3	M	2	NAG	C1-O5-C5	4.52	118.25	112.19
5	U	1	NAG	C1-O5-C5	4.52	118.24	112.19
4	P	4	MAN	C2-C3-C4	4.52	118.80	110.86
5	O	2	NAG	C3-C4-C5	4.48	118.35	110.23
3	S	1	NAG	O4-C4-C3	-4.39	100.03	110.38
5	O	4	MAN	C1-O5-C5	4.34	118.00	112.19
3	S	3	BMA	C2-C3-C4	-4.34	103.23	110.86
5	Q	3	BMA	C1-O5-C5	4.33	117.99	112.19
4	N	3	BMA	C1-O5-C5	4.31	117.96	112.19
3	M	6	MAN	C1-O5-C5	4.29	117.94	112.19
3	S	6	MAN	C1-O5-C5	4.25	117.89	112.19
5	T	3	BMA	C3-C4-C5	4.22	117.88	110.23
4	P	5	NAG	C1-O5-C5	4.21	117.83	112.19
6	W	3	BMA	C1-O5-C5	4.15	117.75	112.19
5	U	4	MAN	O5-C5-C6	4.13	115.71	107.66
3	M	2	NAG	O4-C4-C5	3.94	119.04	109.32
3	V	4	MAN	O2-C2-C1	3.86	118.06	109.22
3	M	4	MAN	C1-O5-C5	3.72	117.18	112.19
3	M	4	MAN	C1-C2-C3	3.68	115.00	109.64
5	R	3	BMA	C3-C4-C5	3.66	116.88	110.23
4	P	3	BMA	C1-O5-C5	3.66	117.10	112.19
3	V	3	BMA	C3-C4-C5	3.64	116.83	110.23
5	Q	3	BMA	O5-C5-C6	3.63	114.73	107.66
5	T	3	BMA	C1-C2-C3	-3.58	104.43	109.64
4	N	4	MAN	O2-C2-C3	-3.52	102.87	110.15
5	O	3	BMA	O3-C3-C4	3.47	118.55	110.38
5	O	2	NAG	C1-O5-C5	-3.40	107.62	112.19
5	Q	3	BMA	C2-C3-C4	3.26	116.59	110.86
5	R	4	MAN	C1-C2-C3	-3.26	104.90	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C3-C4-C5	3.22	116.06	110.23
5	X	4	MAN	O2-C2-C1	3.14	116.40	109.22
4	N	4	MAN	C2-C3-C4	-3.11	105.39	110.86
4	P	4	MAN	C3-C4-C5	3.09	115.83	110.23
5	U	2	NAG	C3-C4-C5	3.09	115.83	110.23
5	U	3	BMA	O5-C1-C2	-3.08	103.44	110.79
3	M	1	NAG	O5-C5-C6	-3.06	101.72	107.66
3	M	3	BMA	O5-C1-C2	-3.05	103.52	110.79
5	O	2	NAG	C4-C3-C2	3.04	115.47	111.02
3	S	4	MAN	O3-C3-C4	-3.04	103.22	110.38
6	W	3	BMA	C1-C2-C3	3.03	114.06	109.64
4	N	4	MAN	C1-C2-C3	-3.02	105.25	109.64
3	S	2	NAG	C1-O5-C5	-3.00	108.16	112.19
3	S	2	NAG	C3-C4-C5	2.98	115.64	110.23
4	N	4	MAN	O3-C3-C2	2.95	116.07	110.05
4	P	4	MAN	O2-C2-C1	2.90	115.87	109.22
3	S	6	MAN	O5-C5-C6	2.90	113.30	107.66
3	V	1	NAG	O4-C4-C3	-2.90	103.55	110.38
4	P	4	MAN	C1-C2-C3	2.89	113.86	109.64
5	T	2	NAG	C3-C4-C5	2.88	115.45	110.23
6	W	3	BMA	C2-C3-C4	2.87	115.91	110.86
5	U	3	BMA	O3-C3-C2	2.79	115.74	110.05
3	M	6	MAN	O2-C2-C1	2.77	115.57	109.22
5	R	1	NAG	O4-C4-C3	-2.76	103.88	110.38
5	Q	4	MAN	C1-O5-C5	2.73	115.85	112.19
6	W	3	BMA	O5-C5-C6	2.71	112.94	107.66
5	X	3	BMA	O3-C3-C2	2.68	115.52	110.05
3	S	3	BMA	O3-C3-C4	2.67	116.68	110.38
5	R	2	NAG	C3-C4-C5	2.67	115.07	110.23
4	P	4	MAN	O2-C2-C3	2.67	115.67	110.15
3	V	4	MAN	C2-C3-C4	-2.66	106.19	110.86
5	O	3	BMA	C6-C5-C4	2.64	119.51	113.02
4	P	5	NAG	C3-C4-C5	2.64	115.02	110.23
3	V	6	MAN	C1-O5-C5	2.64	115.73	112.19
5	U	2	NAG	C1-O5-C5	2.63	115.71	112.19
5	U	3	BMA	C1-C2-C3	-2.56	105.92	109.64
4	P	2	NAG	O4-C4-C3	-2.53	104.41	110.38
3	V	4	MAN	O3-C3-C2	2.53	115.21	110.05
5	X	1	NAG	O4-C4-C5	-2.48	103.23	109.32
4	N	5	NAG	C3-C4-C5	2.47	114.71	110.23
5	O	4	MAN	C1-C2-C3	2.45	113.22	109.64
3	M	1	NAG	O4-C4-C3	-2.45	104.60	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2	NAG	C2-N2-C7	2.44	126.17	122.90
5	R	3	BMA	O6-C6-C5	-2.42	103.08	111.33
3	S	3	BMA	C3-C4-C5	2.42	114.62	110.23
3	S	5	NAG	C1-C2-N2	-2.38	106.68	110.43
5	T	1	NAG	C1-O5-C5	2.38	115.37	112.19
3	S	3	BMA	C1-C2-C3	-2.36	106.21	109.64
3	V	3	BMA	O5-C5-C6	2.35	112.24	107.66
5	U	4	MAN	O2-C2-C1	2.35	114.59	109.22
5	T	4	MAN	C2-C3-C4	2.33	114.96	110.86
4	N	1	NAG	C1-O5-C5	2.32	115.30	112.19
5	X	4	MAN	C1-O5-C5	2.32	115.30	112.19
3	S	4	MAN	O5-C5-C6	2.32	112.17	107.66
5	X	1	NAG	C1-O5-C5	-2.30	109.10	112.19
5	T	4	MAN	O5-C1-C2	-2.28	105.36	110.79
3	V	4	MAN	O5-C5-C6	2.26	112.06	107.66
5	Q	3	BMA	C3-C4-C5	2.26	114.33	110.23
5	Q	4	MAN	O2-C2-C1	2.25	114.39	109.22
4	P	5	NAG	C1-C2-N2	2.24	113.97	110.43
5	X	3	BMA	C1-C2-C3	2.23	112.89	109.64
3	M	3	BMA	O5-C5-C6	2.23	112.01	107.66
5	R	3	BMA	C1-O5-C5	2.21	115.15	112.19
3	S	2	NAG	O4-C4-C5	-2.20	103.89	109.32
3	S	6	MAN	O2-C2-C1	2.19	114.23	109.22
3	M	3	BMA	C1-C2-C3	-2.18	106.47	109.64
3	V	4	MAN	O5-C5-C4	2.18	116.12	110.83
5	Q	3	BMA	C1-C2-C3	2.16	112.79	109.64
5	T	3	BMA	O5-C5-C6	2.12	111.79	107.66
5	O	4	MAN	O2-C2-C1	2.10	114.04	109.22
3	S	4	MAN	C3-C4-C5	2.10	114.04	110.23
3	V	4	MAN	O2-C2-C3	2.09	114.48	110.15
5	R	3	BMA	O5-C5-C6	-2.05	103.67	107.66
3	V	2	NAG	C3-C4-C5	2.04	113.93	110.23
3	V	1	NAG	C1-O5-C5	2.04	114.92	112.19
4	P	1	NAG	O4-C4-C3	-2.04	105.58	110.38
3	M	6	MAN	C1-C2-C3	-2.02	106.70	109.64
3	M	5	NAG	C2-N2-C7	2.02	125.61	122.90
5	U	4	MAN	C2-C3-C4	2.02	114.41	110.86
5	T	4	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	2	NAG	C1-C2-N2-C7
3	S	5	NAG	C3-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	P	1	NAG	C3-C2-N2-C7
4	P	2	NAG	O5-C5-C6-O6
3	M	5	NAG	C4-C5-C6-O6
5	Q	4	MAN	C4-C5-C6-O6
3	V	4	MAN	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
5	Q	4	MAN	O5-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
3	M	5	NAG	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
4	N	4	MAN	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
3	V	5	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
3	V	5	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
4	P	5	NAG	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
6	W	1	NAG	C4-C5-C6-O6
4	N	5	NAG	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
3	V	4	MAN	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
4	N	5	NAG	C4-C5-C6-O6
4	P	4	MAN	C4-C5-C6-O6
4	P	5	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-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	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
3	M	3	BMA	O5-C5-C6-O6
5	X	4	MAN	O5-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
3	S	6	MAN	C4-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
3	V	3	BMA	C4-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	O	4	MAN	O5-C5-C6-O6
3	S	4	MAN	O5-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	M	5	NAG	C3-C2-N2-C7
3	V	2	NAG	C3-C2-N2-C7
5	R	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	V	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C1-C2-N2-C7
5	T	2	NAG	C1-C2-N2-C7
3	M	3	BMA	C4-C5-C6-O6
3	S	6	MAN	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C3-C2-N2-C7
4	N	5	NAG	C3-C2-N2-C7
4	P	5	NAG	C3-C2-N2-C7
5	O	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
4	N	1	NAG	C4-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C1-C2-N2-C7
4	P	5	NAG	C1-C2-N2-C7
5	O	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
3	V	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	U	4	MAN	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
4	P	3	BMA	C4-C5-C6-O6

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	3	BMA	C1-C2-C3-C4-C5-O5
3	S	6	MAN	C1-C2-C3-C4-C5-O5
5	U	4	MAN	C1-C2-C3-C4-C5-O5
5	X	4	MAN	C1-C2-C3-C4-C5-O5
5	Q	4	MAN	C1-C2-C3-C4-C5-O5
4	N	3	BMA	C1-C2-C3-C4-C5-O5

23 monomers are involved in 34 short contacts:

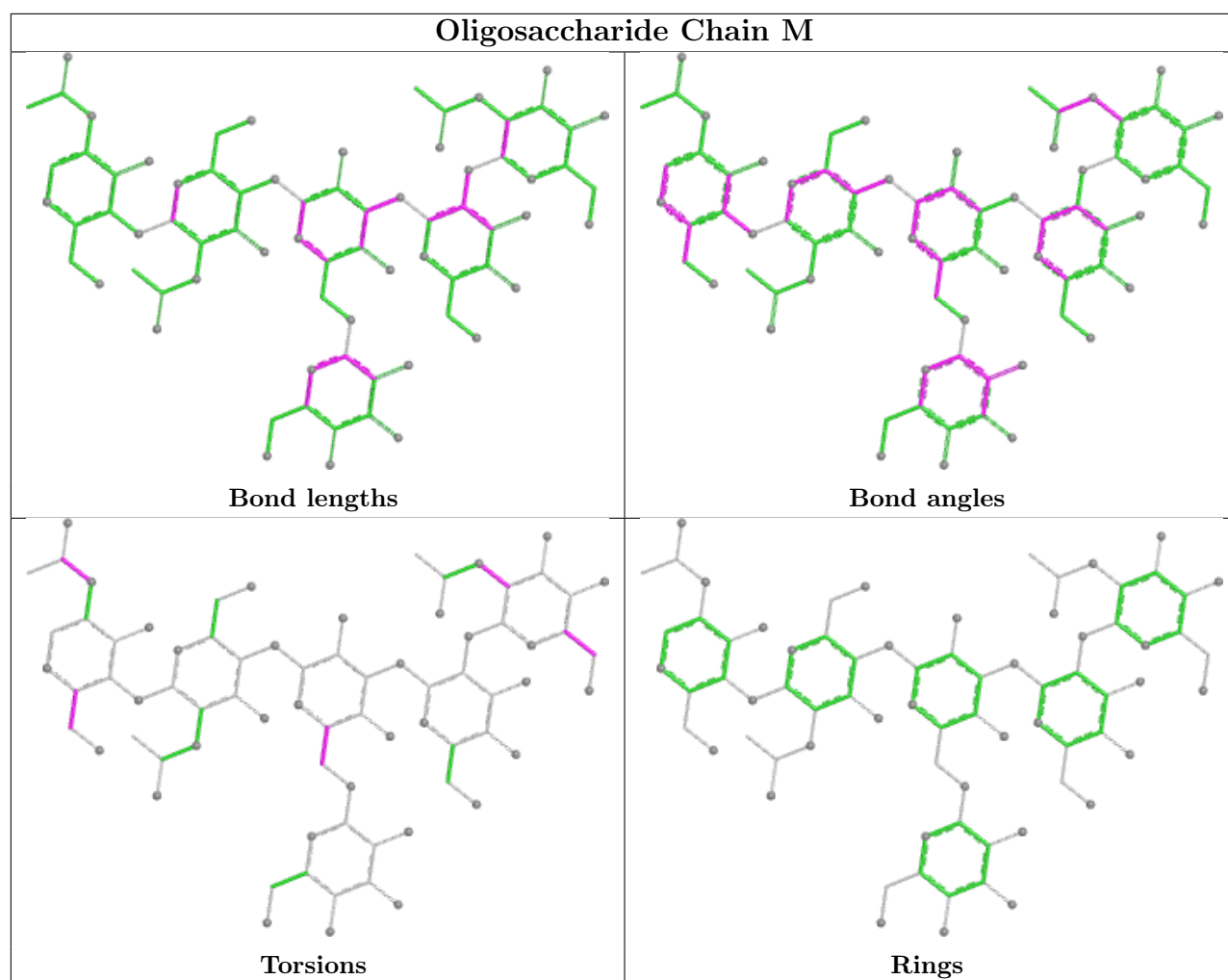
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	6	MAN	3	0
3	M	2	NAG	1	0

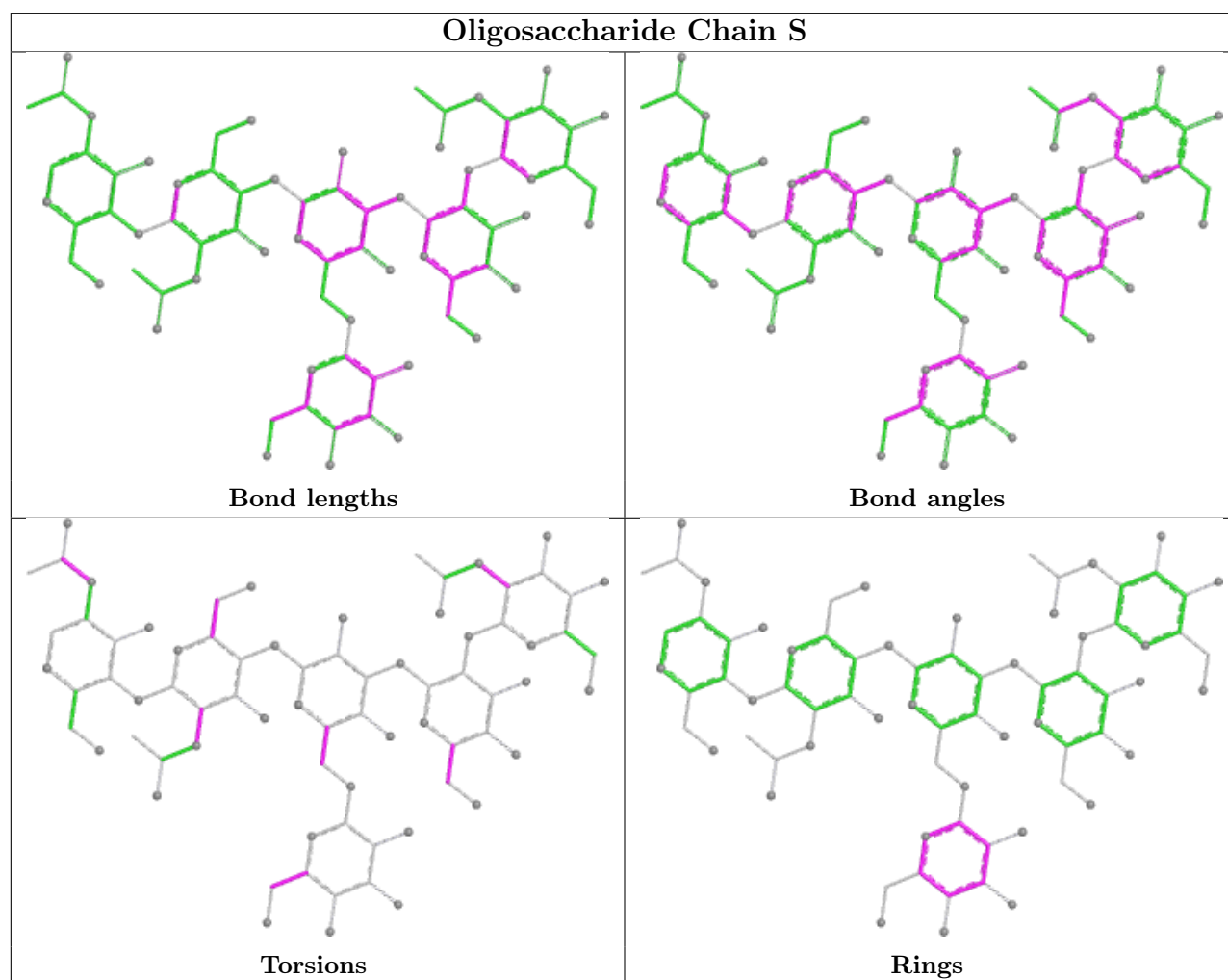
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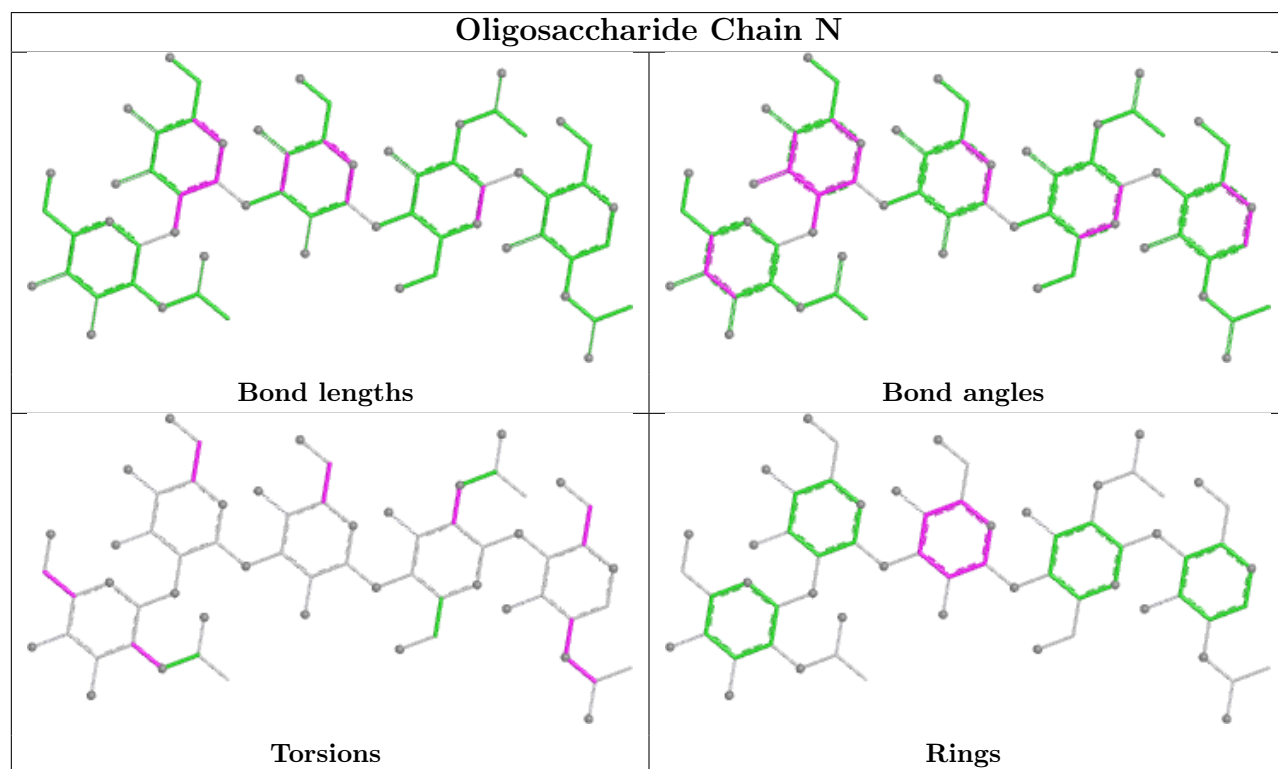
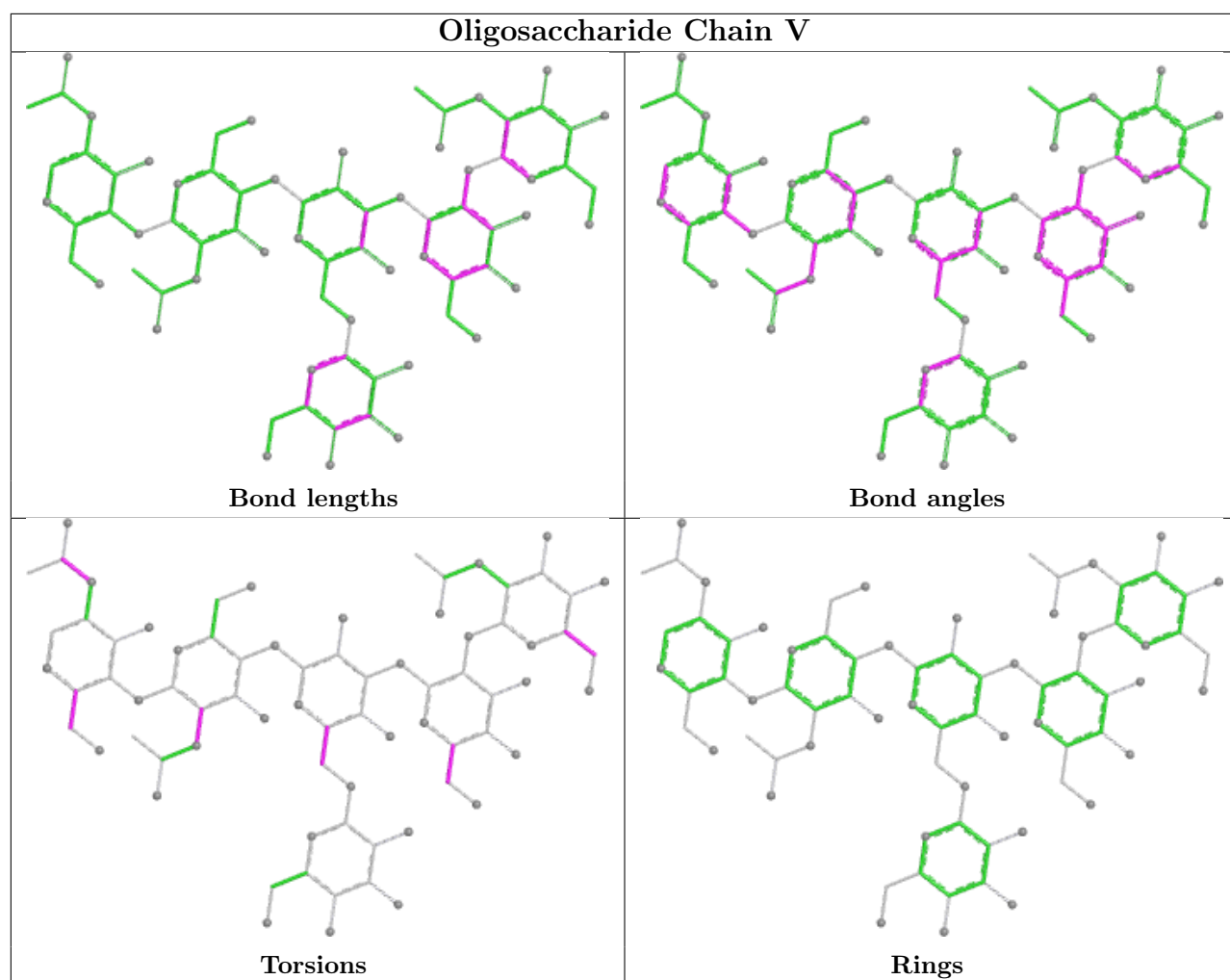
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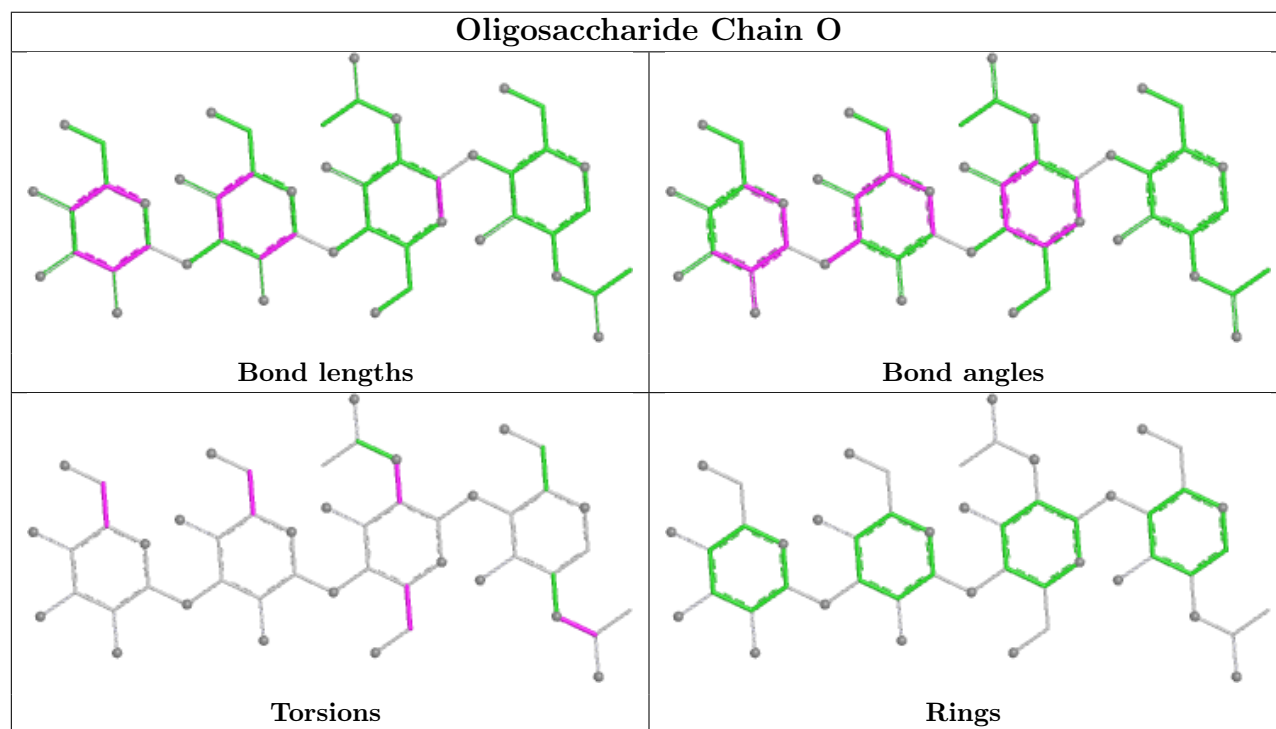
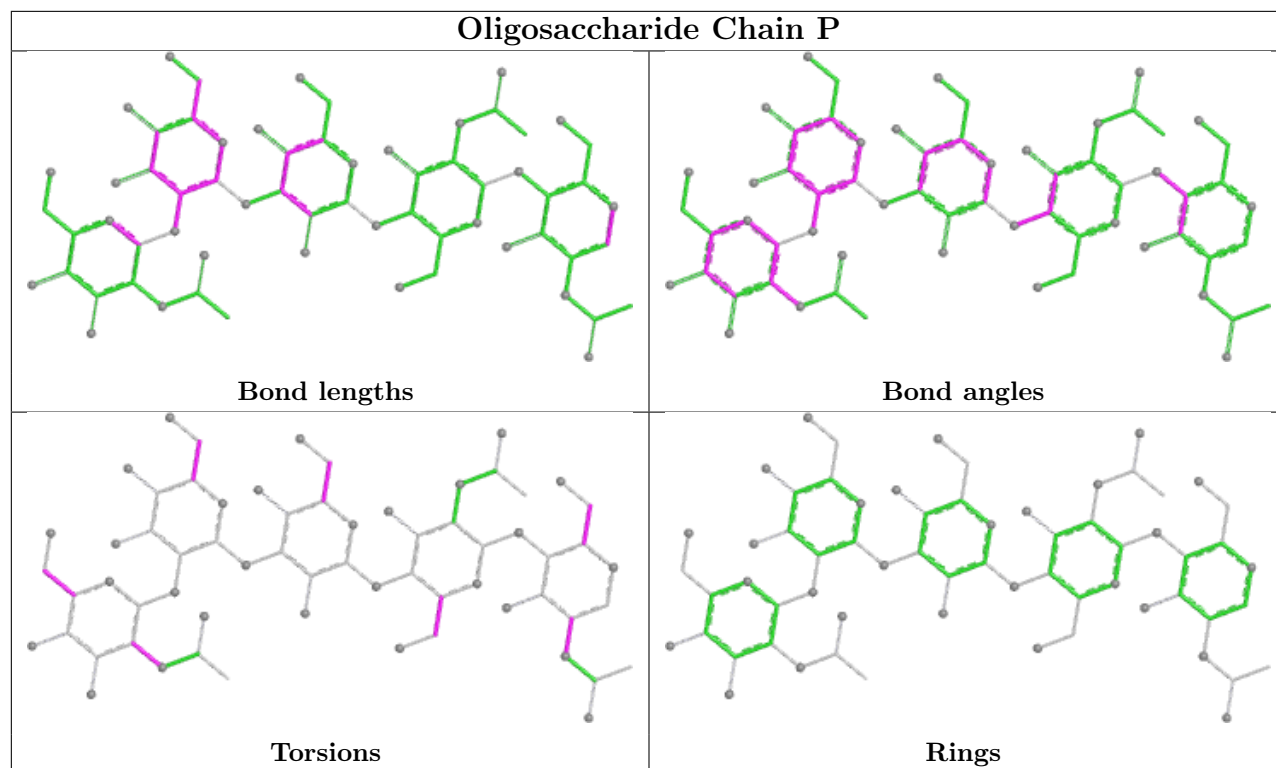
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	NAG	5	0
5	X	1	NAG	4	0
5	O	2	NAG	1	0
5	U	4	MAN	1	0
4	P	5	NAG	1	0
5	R	1	NAG	3	0
3	M	1	NAG	1	0
3	V	1	NAG	5	0
3	S	3	BMA	1	0
3	S	6	MAN	1	0
3	M	3	BMA	2	0
3	M	4	MAN	1	0
6	W	3	BMA	1	0
4	N	3	BMA	1	0
5	R	2	NAG	1	0
5	T	2	NAG	1	0
4	P	1	NAG	3	0
5	T	1	NAG	2	0
4	N	4	MAN	1	0
6	W	2	NAG	1	0
3	S	5	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.

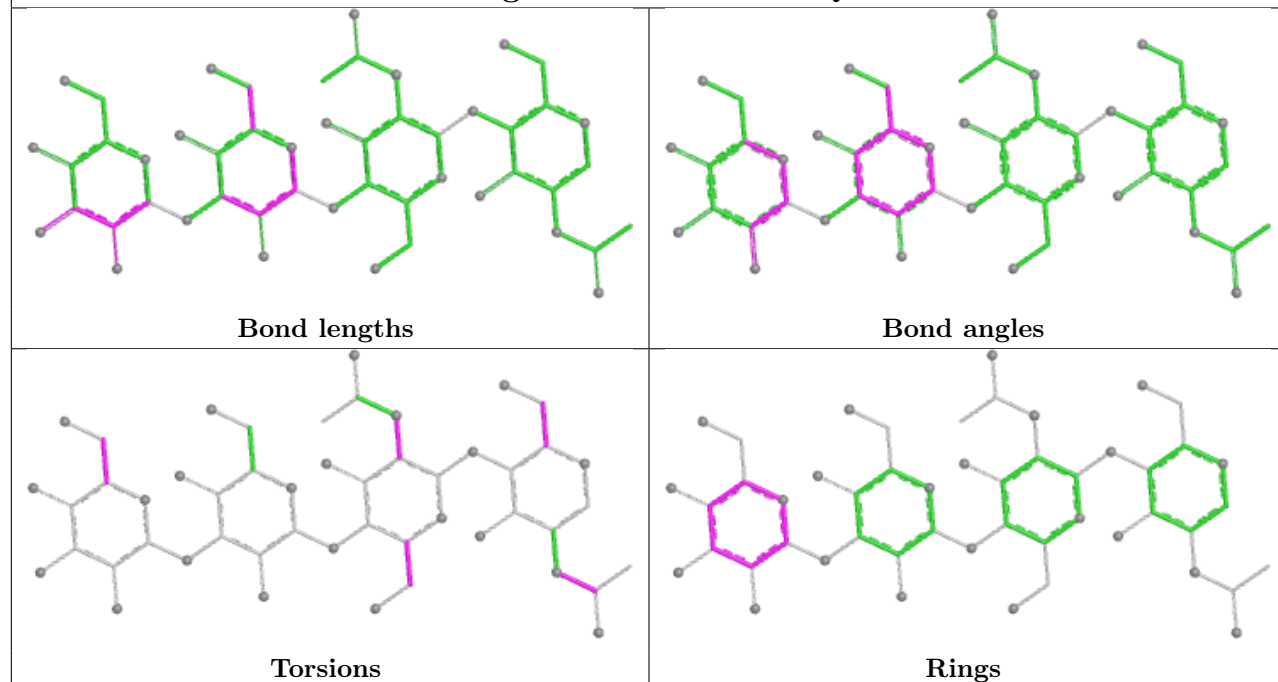




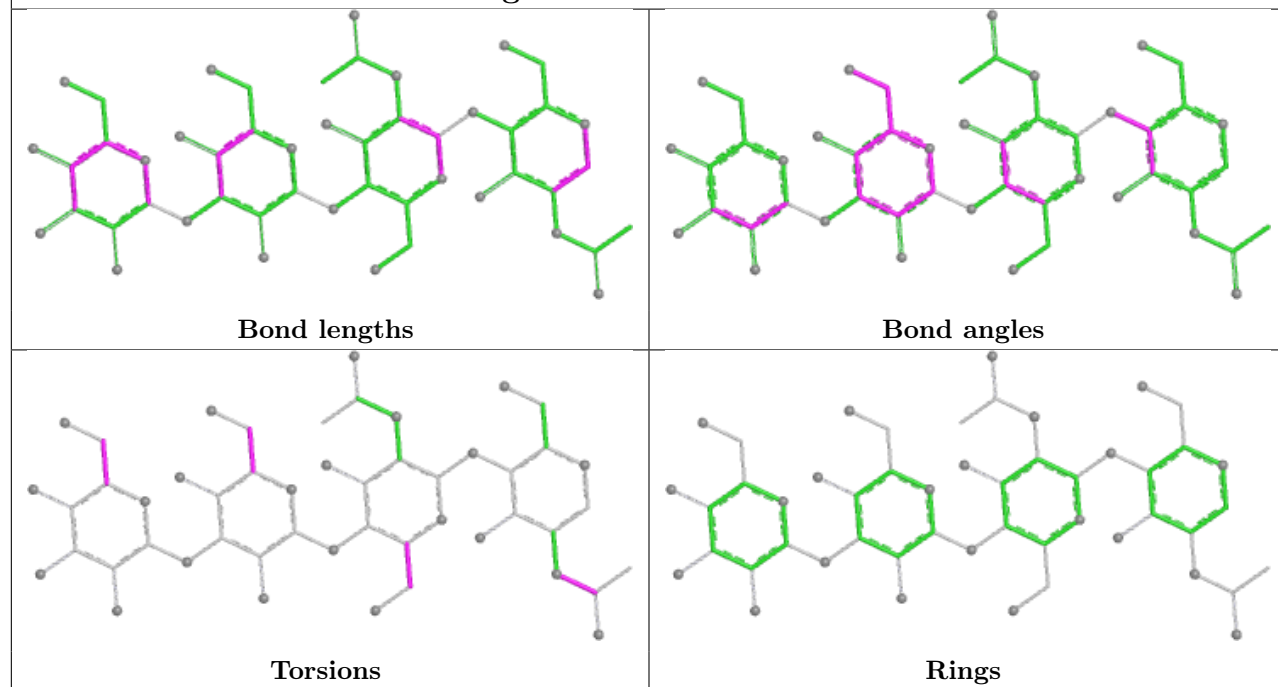




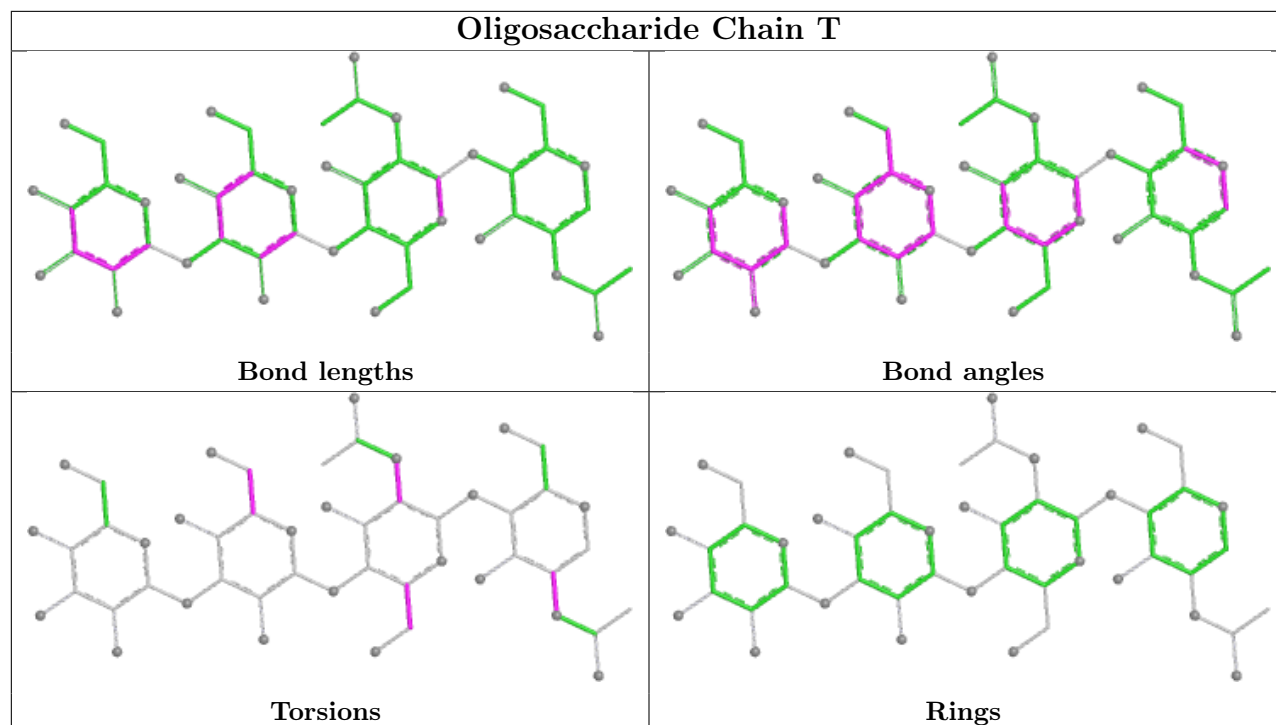
Oligosaccharide Chain Q



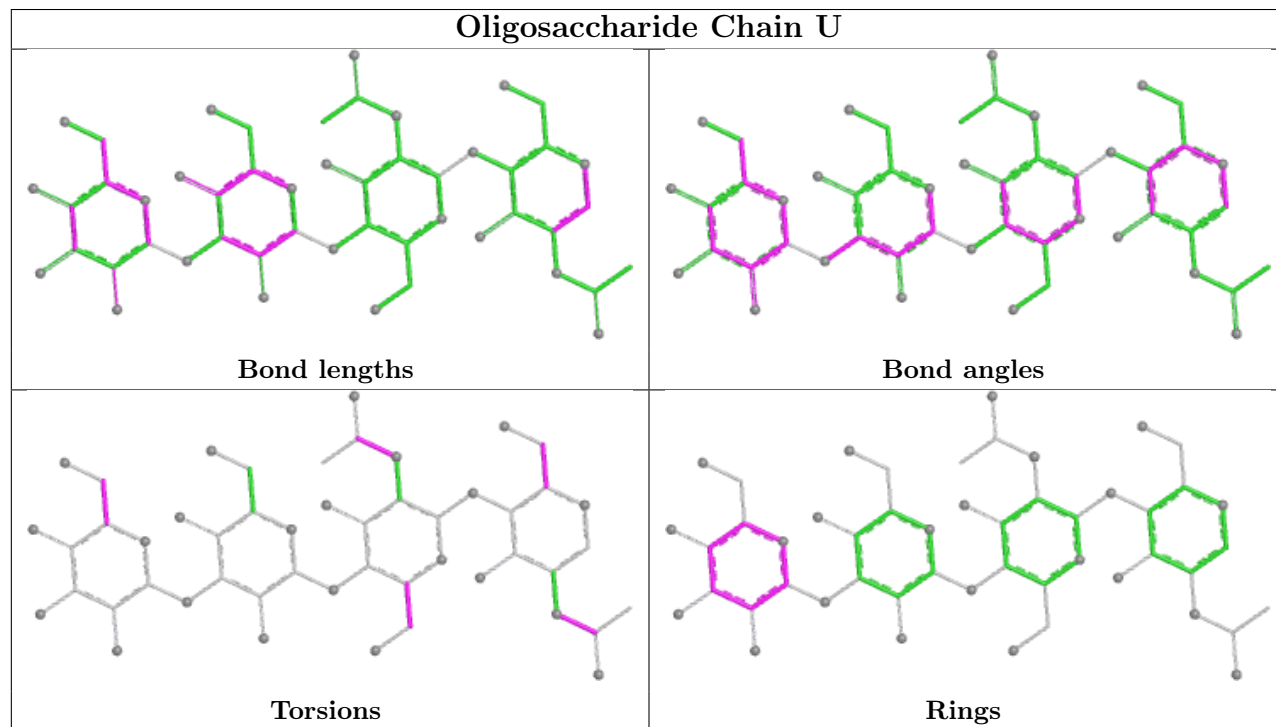
Oligosaccharide Chain R

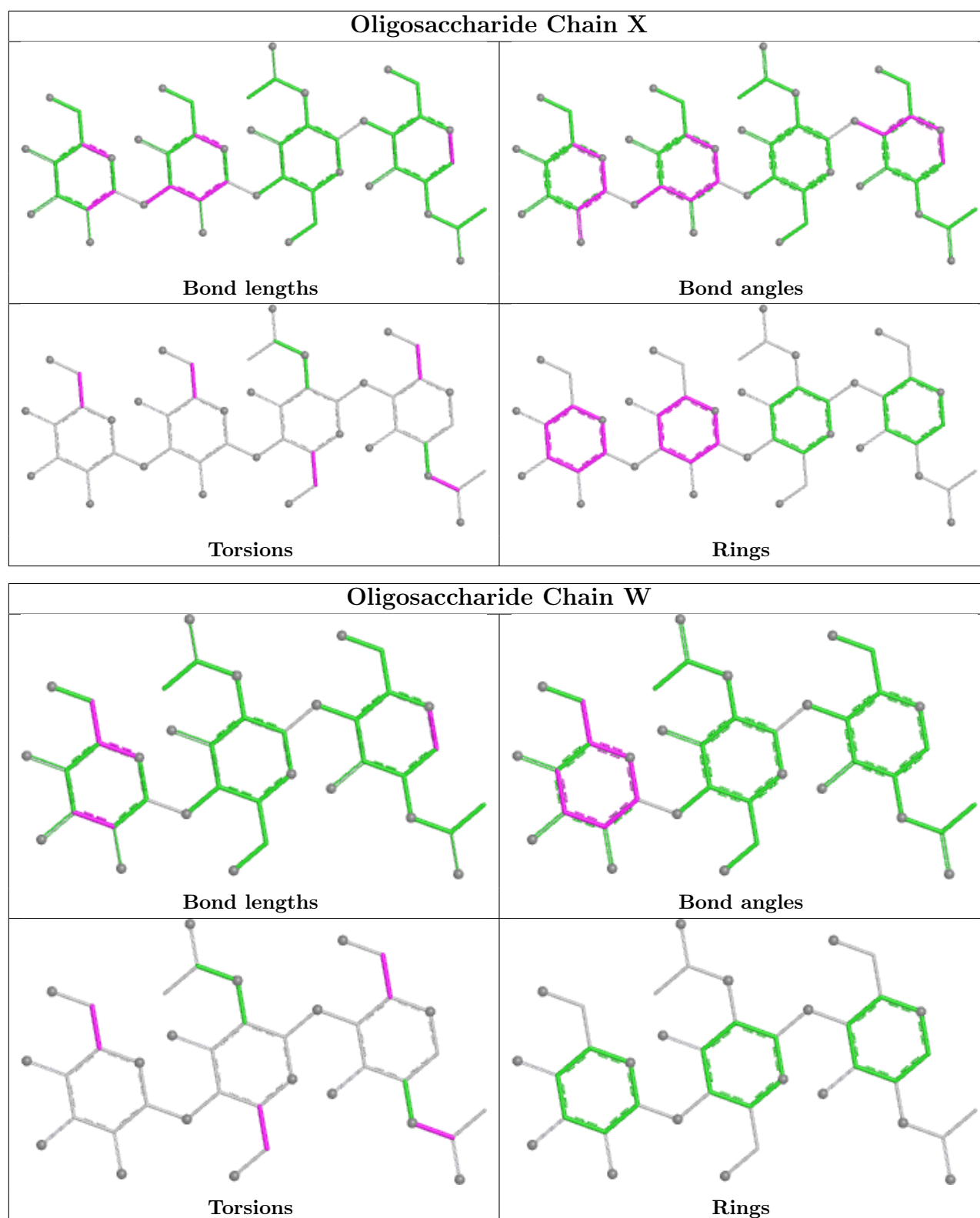


Oligosaccharide Chain T



Oligosaccharide Chain U





5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	$\# Z > 2$
7	NAG	I	410	1	14,14,15	0.22	0	17,19,21	0.87	0
7	NAG	A	412	1	14,14,15	1.80	2 (14%)	17,19,21	1.43	1 (5%)
7	NAG	I	401	1	14,14,15	0.52	0	17,19,21	0.49	0
7	NAG	I	409	1	14,14,15	0.47	0	17,19,21	1.20	1 (5%)
7	NAG	G	413	1	14,14,15	2.08	2 (14%)	17,19,21	2.74	1 (5%)
7	NAG	G	401	1	14,14,15	1.52	1 (7%)	17,19,21	1.89	1 (5%)
7	NAG	K	414	1	14,14,15	1.08	2 (14%)	17,19,21	1.53	1 (5%)
7	NAG	A	401	1	14,14,15	0.84	1 (7%)	17,19,21	1.32	1 (5%)
7	NAG	C	409	1	14,14,15	0.63	0	17,19,21	0.66	0
7	NAG	E	414	1	14,14,15	1.97	2 (14%)	17,19,21	1.94	1 (5%)
7	NAG	E	413	1	14,14,15	0.61	1 (7%)	17,19,21	0.88	1 (5%)
7	NAG	G	402	1	14,14,15	0.96	2 (14%)	17,19,21	1.75	1 (5%)
7	NAG	K	413	1	14,14,15	0.42	0	17,19,21	0.68	0
7	NAG	E	412	1	14,14,15	1.23	1 (7%)	17,19,21	1.05	2 (11%)
7	NAG	K	401	1	14,14,15	0.70	0	17,19,21	0.66	0
7	NAG	A	413	1	14,14,15	1.78	2 (14%)	17,19,21	1.27	1 (5%)
7	NAG	E	401	1	14,14,15	1.07	1 (7%)	17,19,21	0.74	0
7	NAG	A	402	1	14,14,15	0.76	1 (7%)	17,19,21	2.39	3 (17%)
7	NAG	A	414	1	14,14,15	0.83	1 (7%)	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	410	1	-	4/6/23/26	0/1/1/1
7	NAG	A	412	1	-	4/6/23/26	0/1/1/1
7	NAG	I	401	1	-	3/6/23/26	0/1/1/1
7	NAG	I	409	1	-	4/6/23/26	0/1/1/1
7	NAG	G	413	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	401	1	-	3/6/23/26	0/1/1/1
7	NAG	K	414	1	-	2/6/23/26	0/1/1/1
7	NAG	A	401	1	-	3/6/23/26	0/1/1/1
7	NAG	C	409	1	-	3/6/23/26	0/1/1/1
7	NAG	E	414	1	-	3/6/23/26	0/1/1/1
7	NAG	E	413	1	-	2/6/23/26	0/1/1/1
7	NAG	G	402	1	-	4/6/23/26	0/1/1/1
7	NAG	K	413	1	-	4/6/23/26	0/1/1/1
7	NAG	E	412	1	-	3/6/23/26	0/1/1/1
7	NAG	K	401	1	-	4/6/23/26	0/1/1/1
7	NAG	A	413	1	-	4/6/23/26	0/1/1/1
7	NAG	E	401	1	-	4/6/23/26	0/1/1/1
7	NAG	A	402	1	-	4/6/23/26	0/1/1/1
7	NAG	A	414	1	-	4/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	413	NAG	O5-C1	7.08	1.55	1.43
7	E	414	NAG	O5-C1	6.24	1.54	1.43
7	G	401	NAG	O5-C1	5.42	1.52	1.43
7	A	412	NAG	O5-C1	5.36	1.52	1.43
7	A	413	NAG	C1-C2	5.11	1.59	1.52
7	E	412	NAG	C1-C2	4.03	1.57	1.52
7	A	413	NAG	O5-C1	4.01	1.50	1.43
7	A	412	NAG	C1-C2	3.99	1.57	1.52
7	E	401	NAG	O5-C1	-3.87	1.37	1.43
7	E	414	NAG	C1-C2	3.81	1.57	1.52
7	G	413	NAG	C1-C2	3.17	1.56	1.52
7	K	414	NAG	O5-C1	3.14	1.49	1.43
7	G	402	NAG	O5-C1	2.68	1.48	1.43
7	A	401	NAG	O5-C1	2.66	1.48	1.43
7	A	402	NAG	O5-C1	2.51	1.47	1.43
7	K	414	NAG	C1-C2	2.49	1.55	1.52
7	A	414	NAG	C1-C2	2.38	1.55	1.52
7	G	402	NAG	C1-C2	2.18	1.55	1.52
7	E	413	NAG	O5-C1	2.04	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	413	NAG	C1-O5-C5	11.18	127.17	112.19
7	E	414	NAG	C1-O5-C5	7.63	122.42	112.19
7	A	402	NAG	C1-O5-C5	7.38	122.07	112.19
7	G	401	NAG	C1-O5-C5	7.06	121.64	112.19
7	G	402	NAG	C1-O5-C5	6.64	121.09	112.19
7	K	414	NAG	C1-O5-C5	6.21	120.50	112.19
7	A	412	NAG	C1-O5-C5	4.92	118.79	112.19
7	A	401	NAG	C1-O5-C5	4.91	118.77	112.19
7	A	402	NAG	C2-N2-C7	4.75	129.27	122.90
7	A	413	NAG	C1-O5-C5	4.59	118.34	112.19
7	E	413	NAG	C1-O5-C5	2.93	116.11	112.19
7	E	412	NAG	C1-O5-C5	-2.91	108.29	112.19
7	A	402	NAG	C1-C2-N2	2.86	114.94	110.43
7	I	409	NAG	C1-O5-C5	2.61	115.68	112.19
7	E	412	NAG	C4-C3-C2	2.21	114.25	111.02

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	414	NAG	C1-C2-N2-C7
7	E	401	NAG	O5-C5-C6-O6
7	I	410	NAG	O5-C5-C6-O6
7	A	414	NAG	O5-C5-C6-O6
7	E	413	NAG	O5-C5-C6-O6
7	I	410	NAG	C4-C5-C6-O6
7	E	413	NAG	C4-C5-C6-O6
7	E	401	NAG	C4-C5-C6-O6
7	A	414	NAG	C4-C5-C6-O6
7	A	412	NAG	O5-C5-C6-O6
7	A	412	NAG	C4-C5-C6-O6
7	G	402	NAG	O5-C5-C6-O6
7	I	409	NAG	O5-C5-C6-O6
7	K	413	NAG	O5-C5-C6-O6
7	I	409	NAG	C4-C5-C6-O6
7	K	401	NAG	C8-C7-N2-C2
7	K	401	NAG	O7-C7-N2-C2
7	K	413	NAG	C8-C7-N2-C2
7	K	413	NAG	O7-C7-N2-C2
7	K	414	NAG	C8-C7-N2-C2
7	K	414	NAG	O7-C7-N2-C2
7	A	401	NAG	C8-C7-N2-C2
7	A	401	NAG	O7-C7-N2-C2

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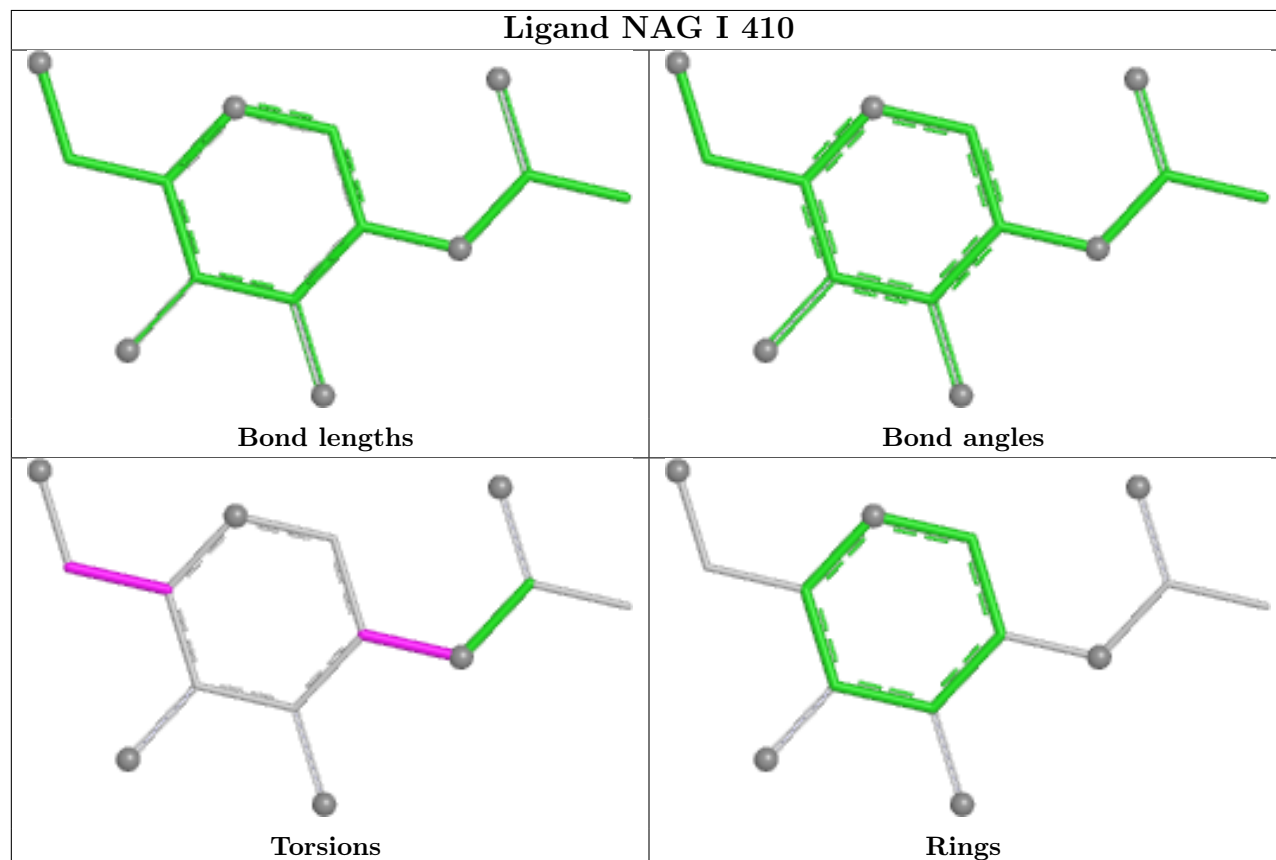
Mol	Chain	Res	Type	Atoms
7	A	402	NAG	C8-C7-N2-C2
7	A	402	NAG	O7-C7-N2-C2
7	A	413	NAG	C8-C7-N2-C2
7	A	413	NAG	O7-C7-N2-C2
7	A	414	NAG	C8-C7-N2-C2
7	A	414	NAG	O7-C7-N2-C2
7	C	409	NAG	C8-C7-N2-C2
7	C	409	NAG	O7-C7-N2-C2
7	E	401	NAG	C8-C7-N2-C2
7	E	401	NAG	O7-C7-N2-C2
7	E	412	NAG	C8-C7-N2-C2
7	E	412	NAG	O7-C7-N2-C2
7	G	401	NAG	C8-C7-N2-C2
7	G	401	NAG	O7-C7-N2-C2
7	G	413	NAG	C8-C7-N2-C2
7	G	413	NAG	O7-C7-N2-C2
7	I	401	NAG	C8-C7-N2-C2
7	I	401	NAG	O7-C7-N2-C2
7	I	409	NAG	C8-C7-N2-C2
7	I	409	NAG	O7-C7-N2-C2
7	G	401	NAG	O5-C5-C6-O6
7	E	412	NAG	O5-C5-C6-O6
7	C	409	NAG	O5-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	A	412	NAG	C3-C2-N2-C7
7	A	413	NAG	C4-C5-C6-O6
7	K	413	NAG	C4-C5-C6-O6
7	K	401	NAG	C4-C5-C6-O6
7	A	413	NAG	O5-C5-C6-O6
7	A	412	NAG	C1-C2-N2-C7
7	K	401	NAG	O5-C5-C6-O6
7	A	402	NAG	C3-C2-N2-C7
7	G	402	NAG	C3-C2-N2-C7
7	I	410	NAG	C3-C2-N2-C7
7	G	402	NAG	C4-C5-C6-O6
7	A	402	NAG	C1-C2-N2-C7
7	G	402	NAG	C1-C2-N2-C7
7	I	410	NAG	C1-C2-N2-C7
7	I	401	NAG	O5-C5-C6-O6
7	E	414	NAG	C4-C5-C6-O6
7	E	414	NAG	O5-C5-C6-O6

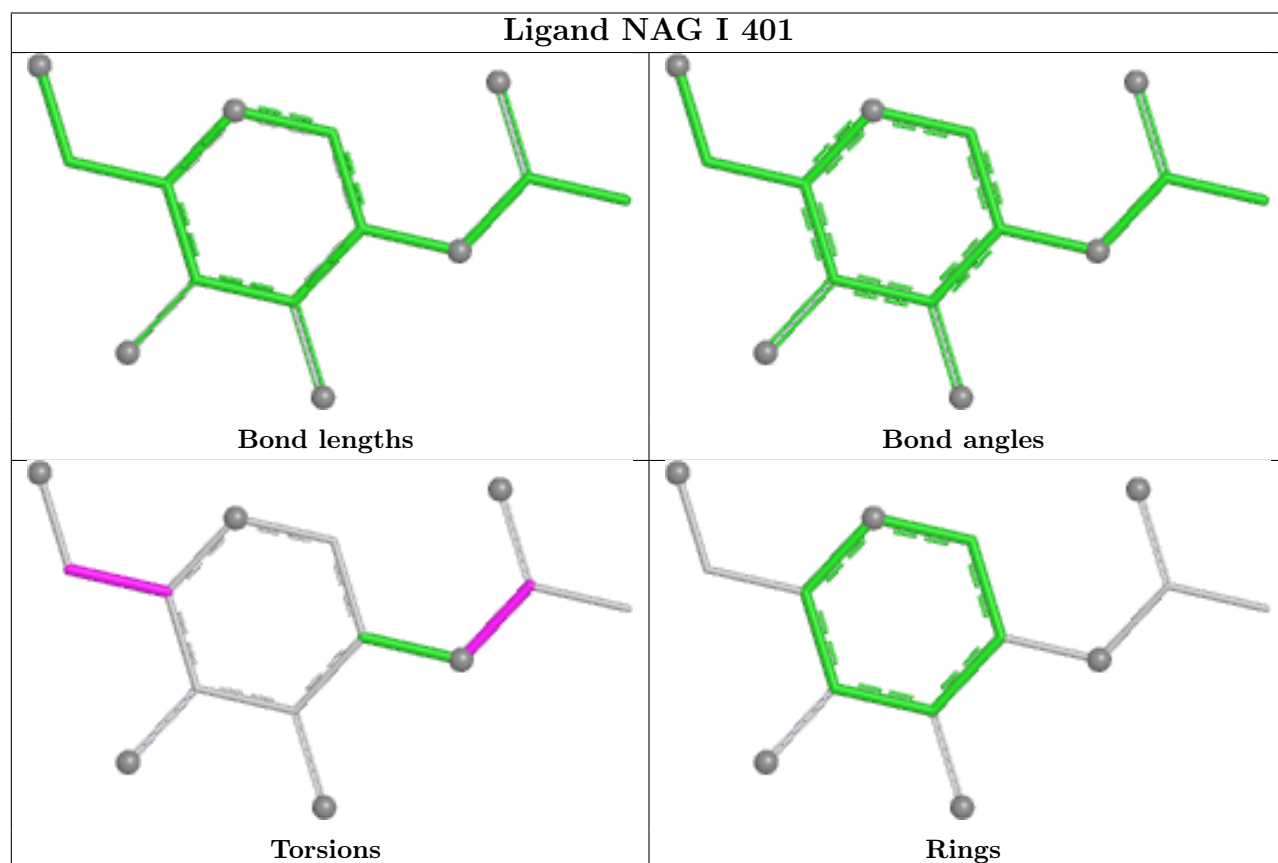
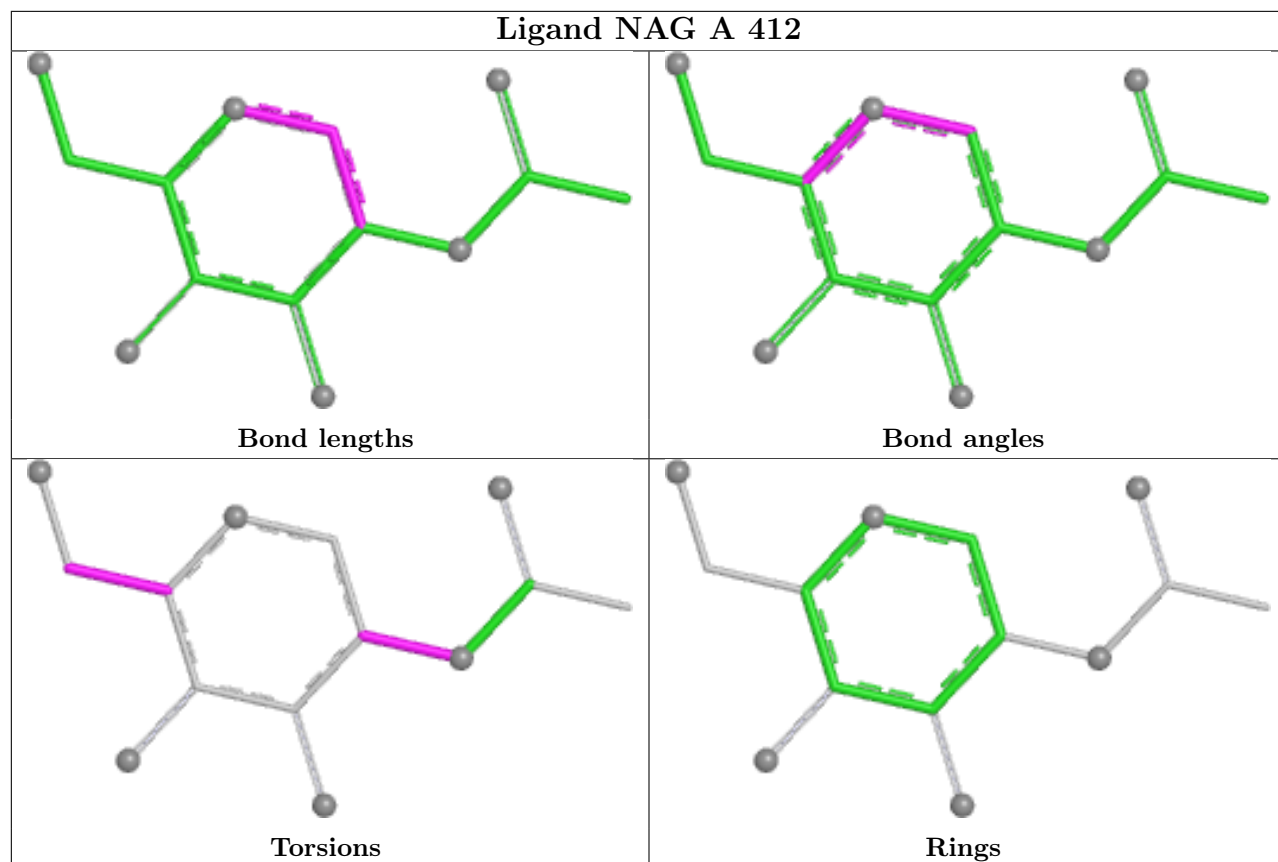
There are no ring outliers.

7 monomers are involved in 8 short contacts:

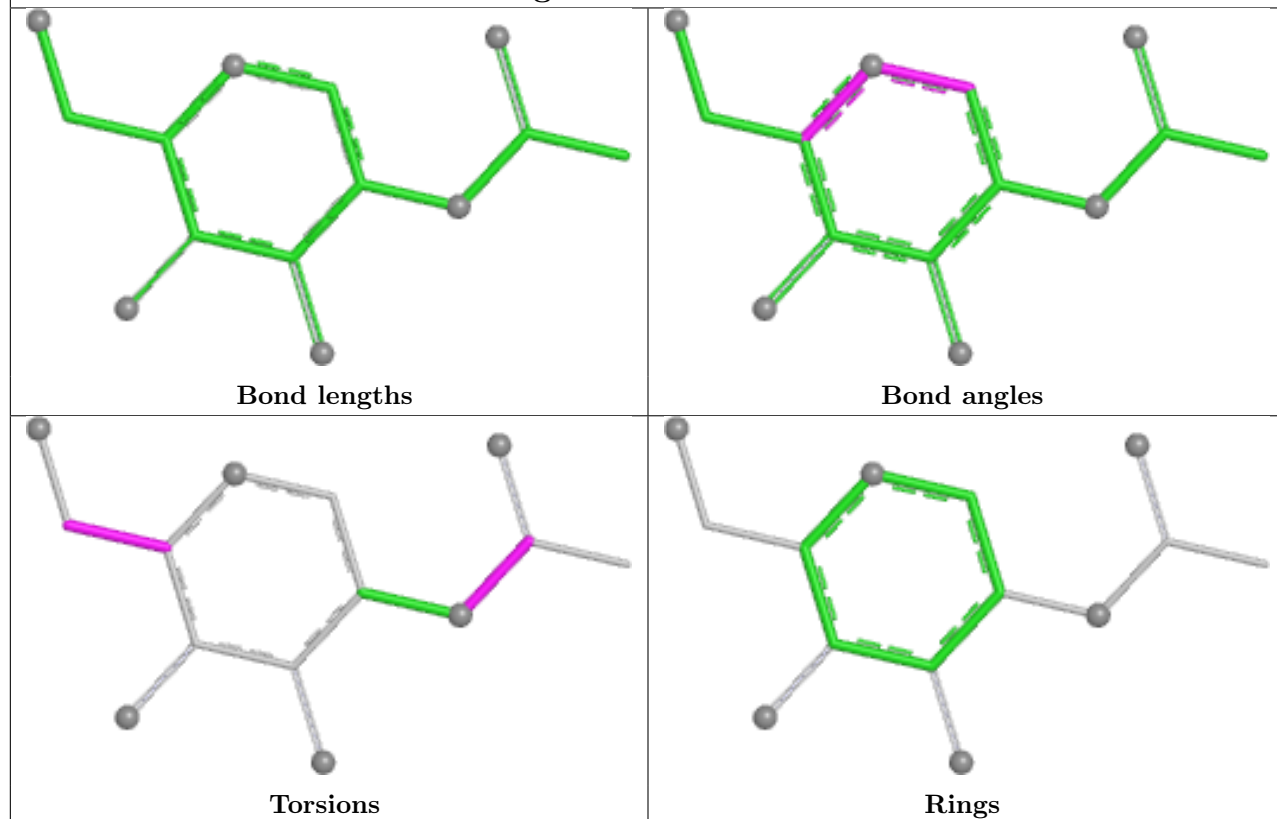
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	409	NAG	1	0
7	C	409	NAG	1	0
7	G	402	NAG	1	0
7	K	401	NAG	1	0
7	A	413	NAG	1	0
7	A	402	NAG	1	0
7	A	414	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

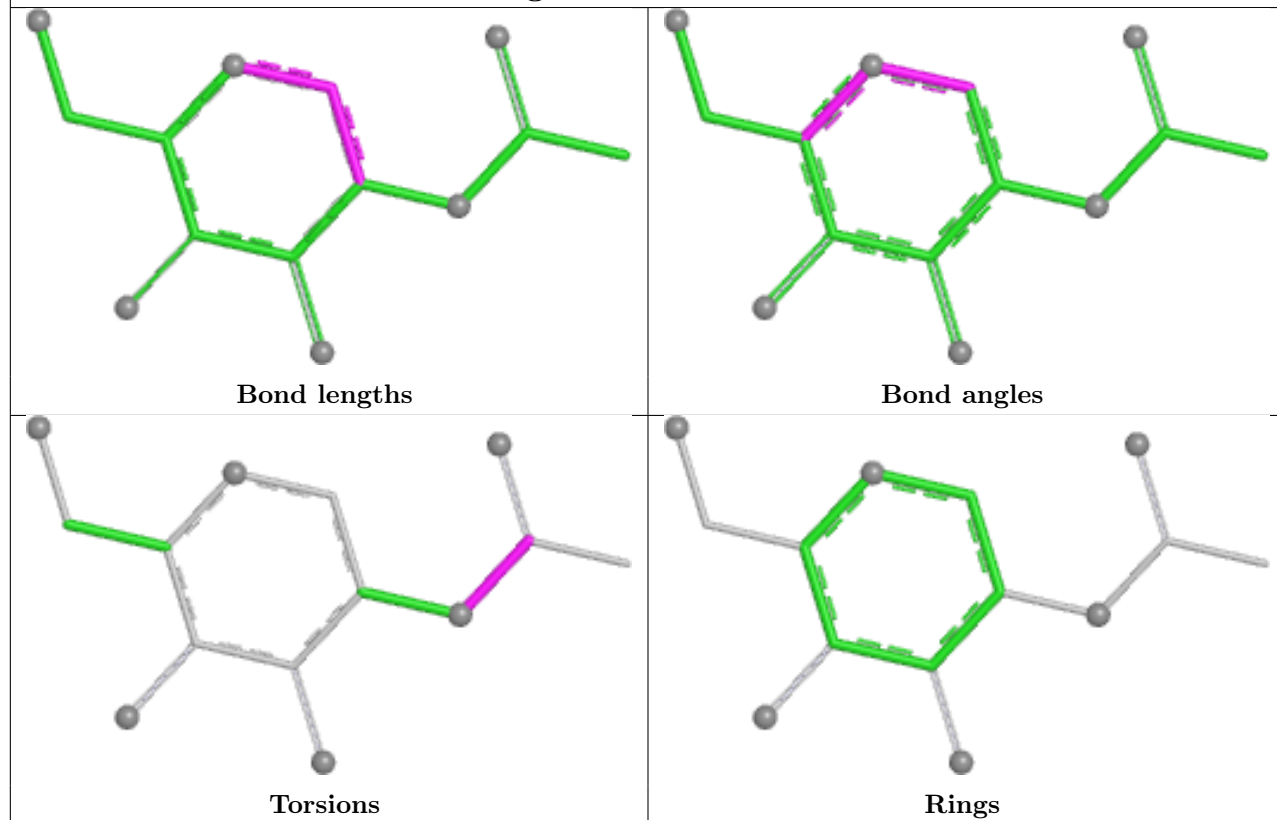


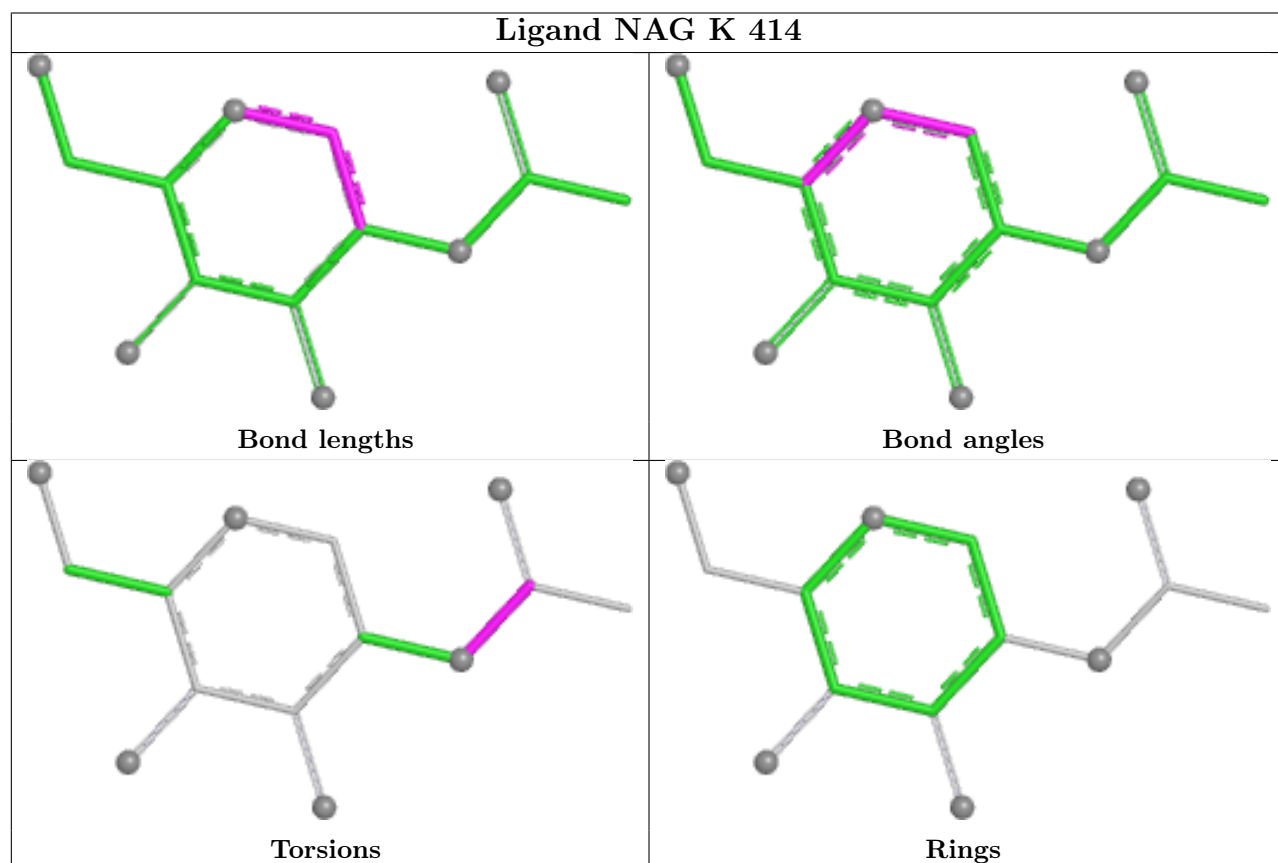
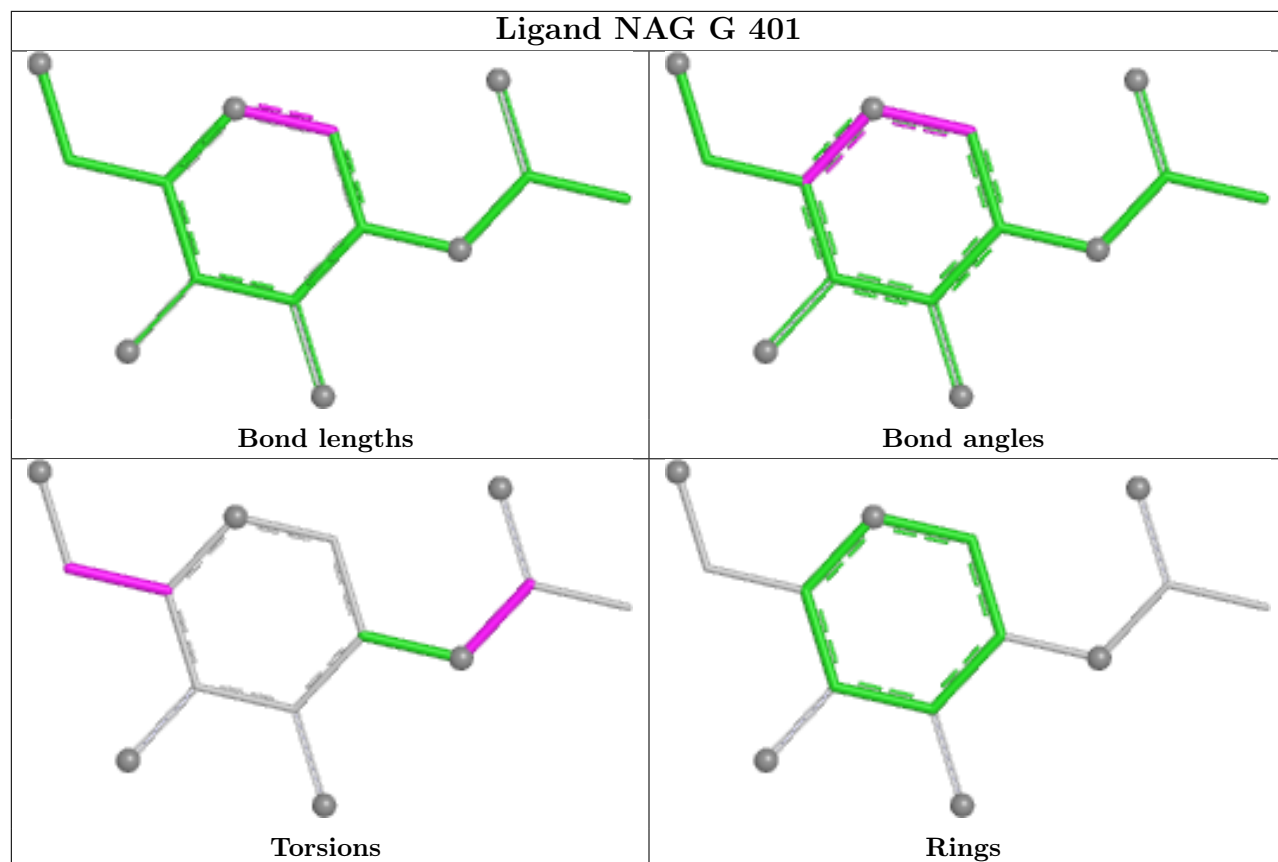


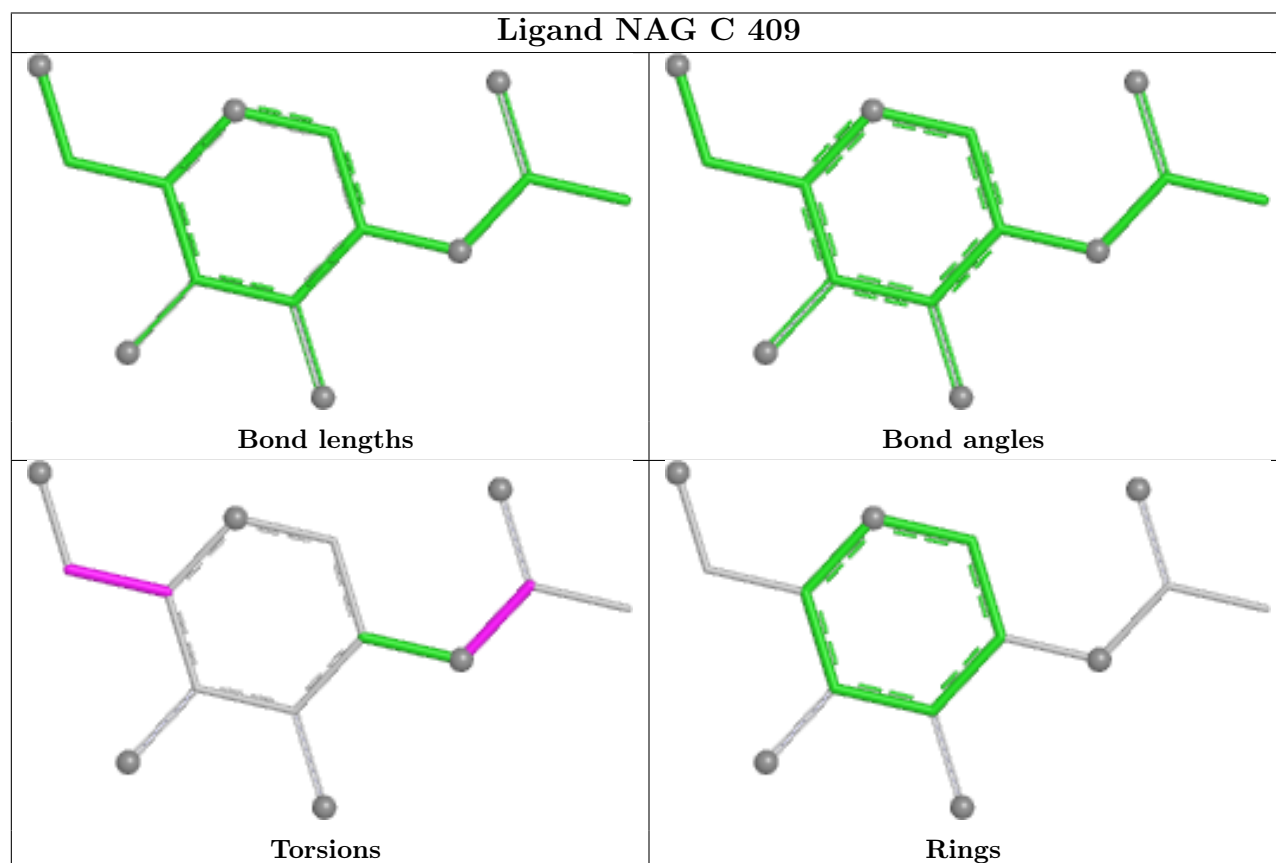
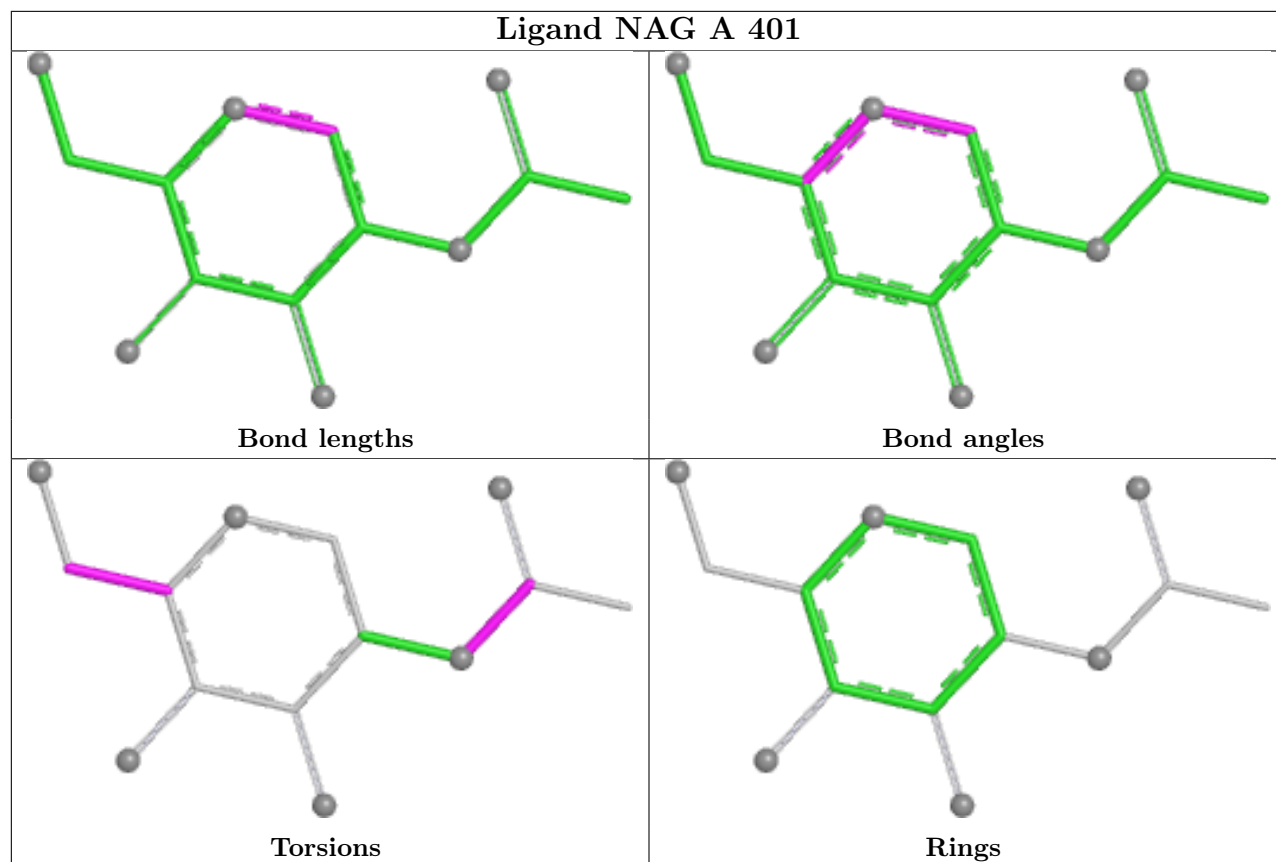
Ligand NAG I 409

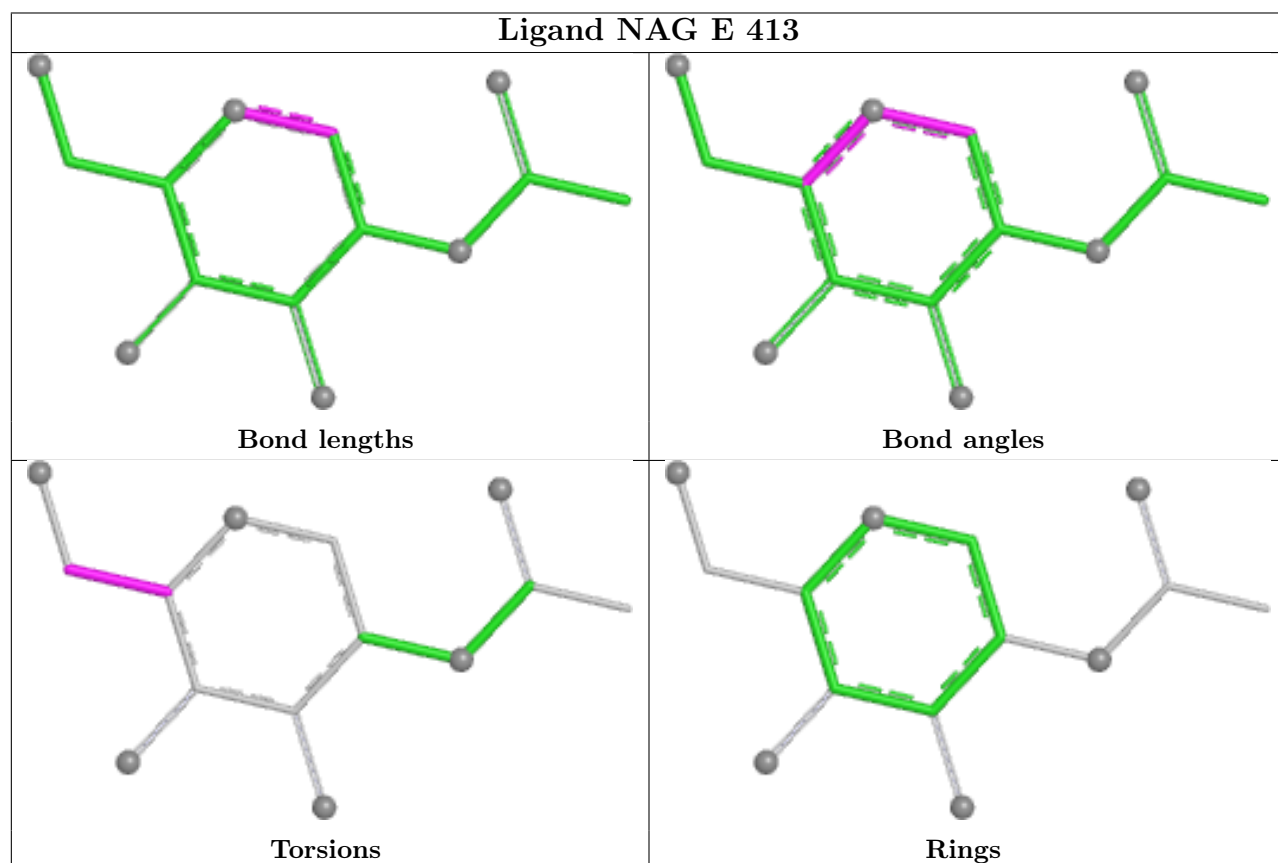
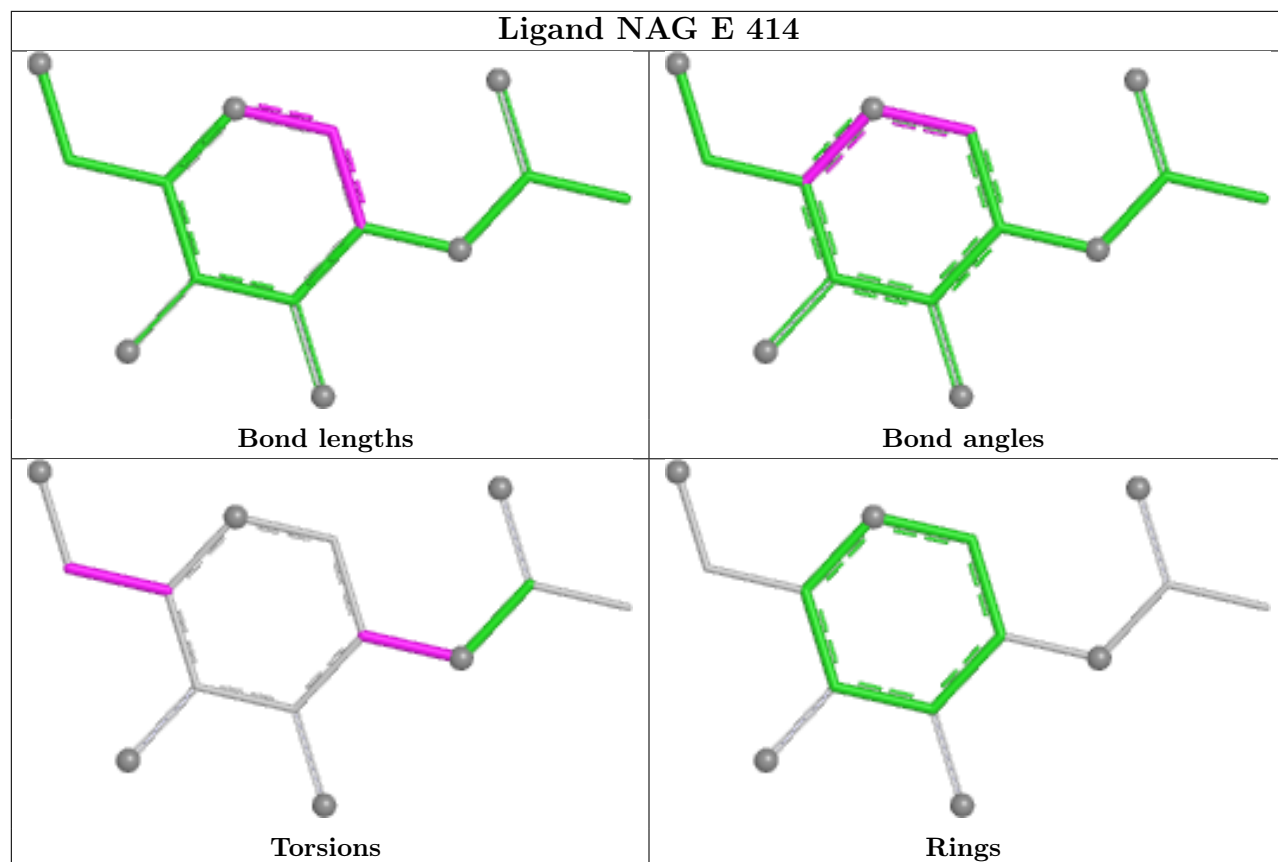


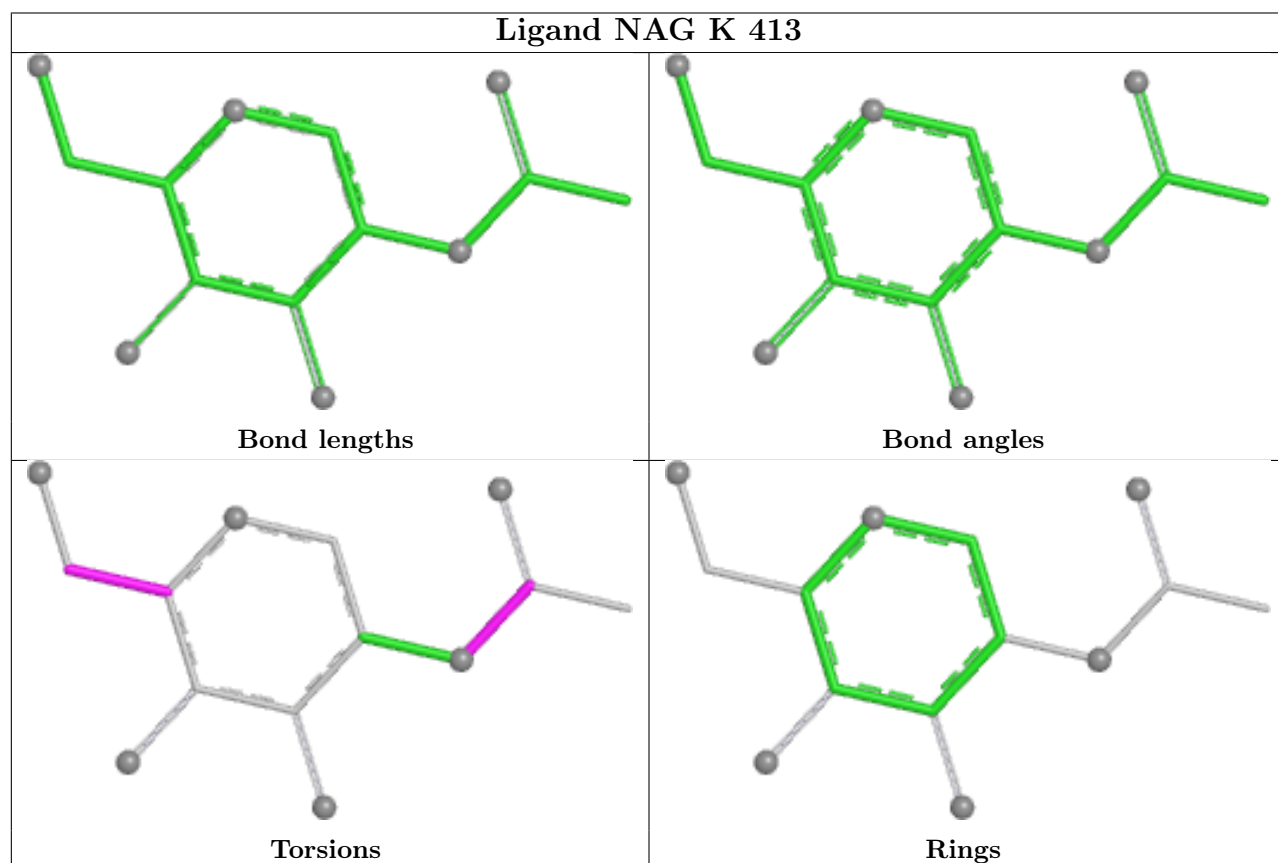
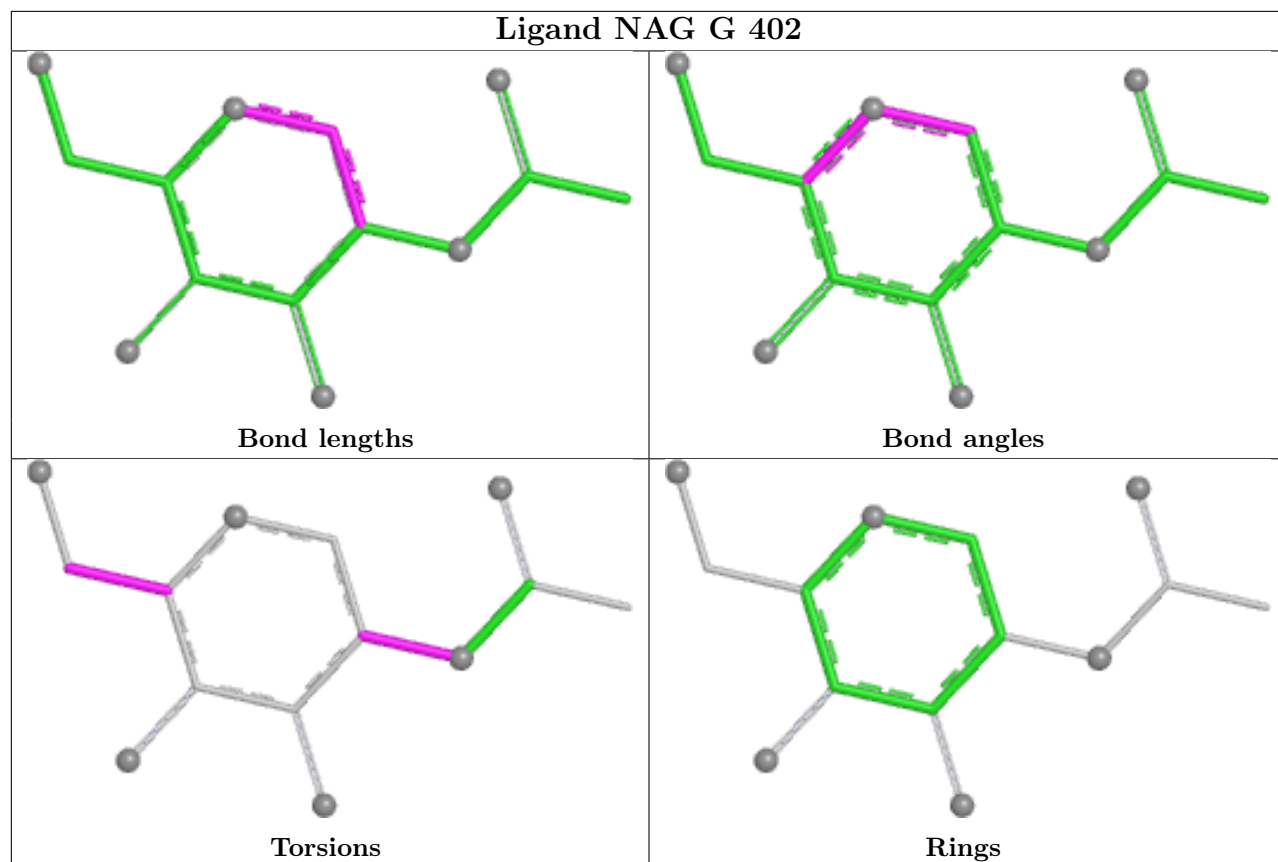
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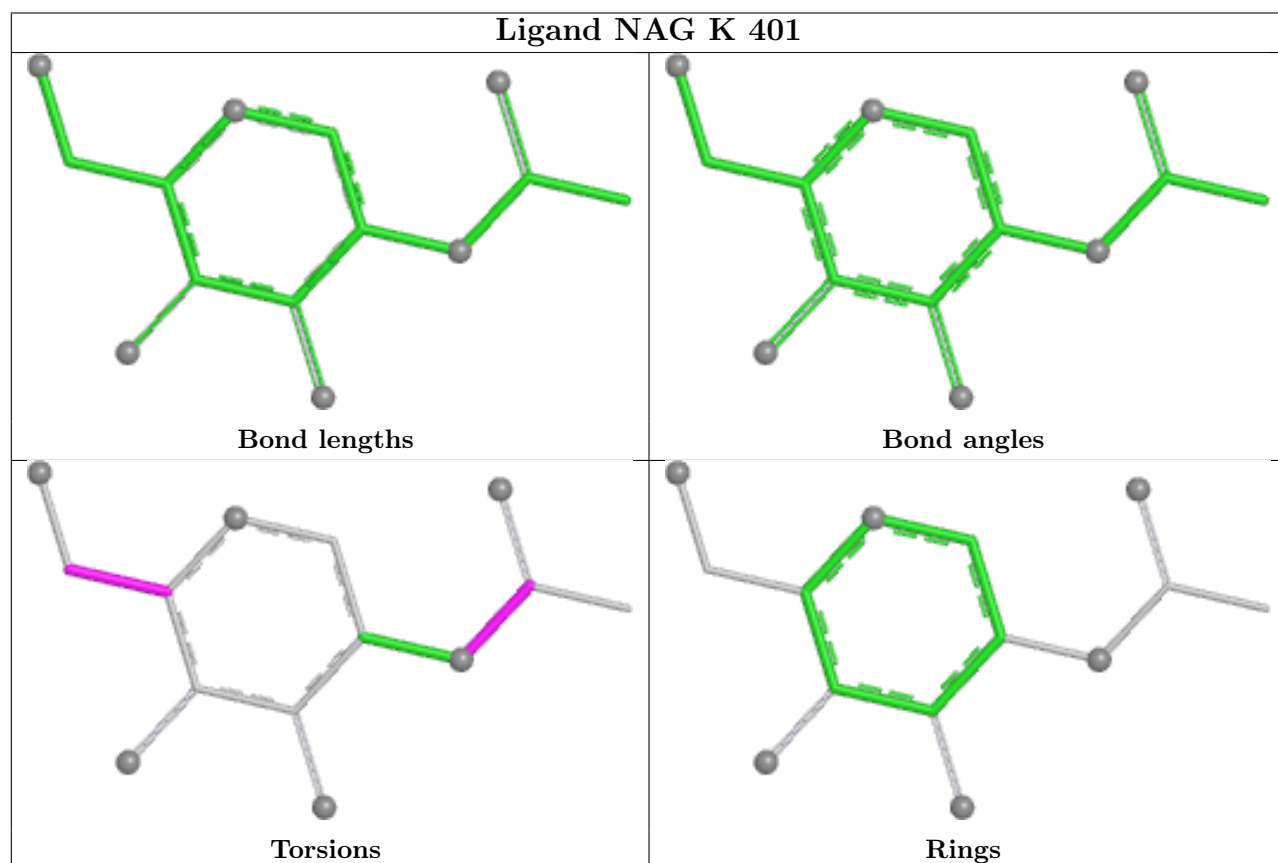
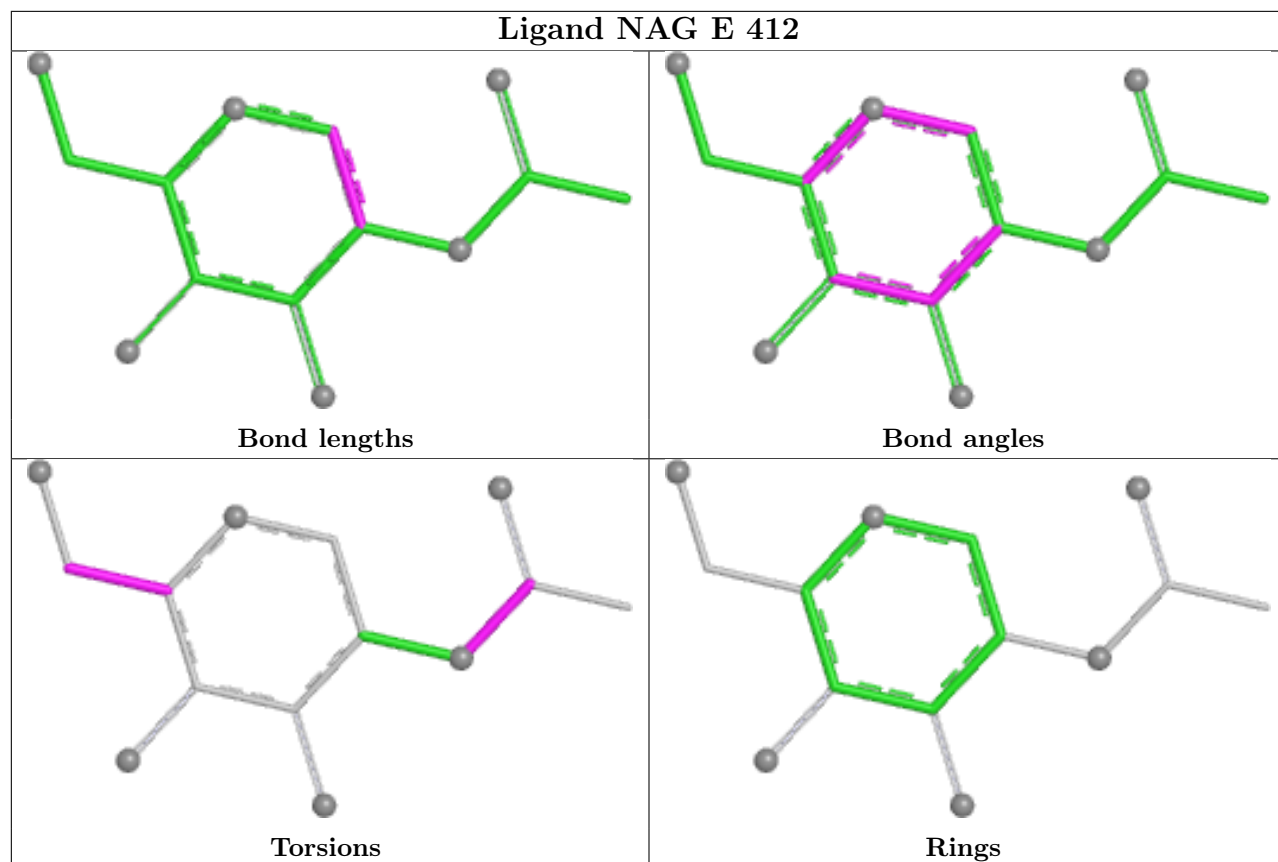


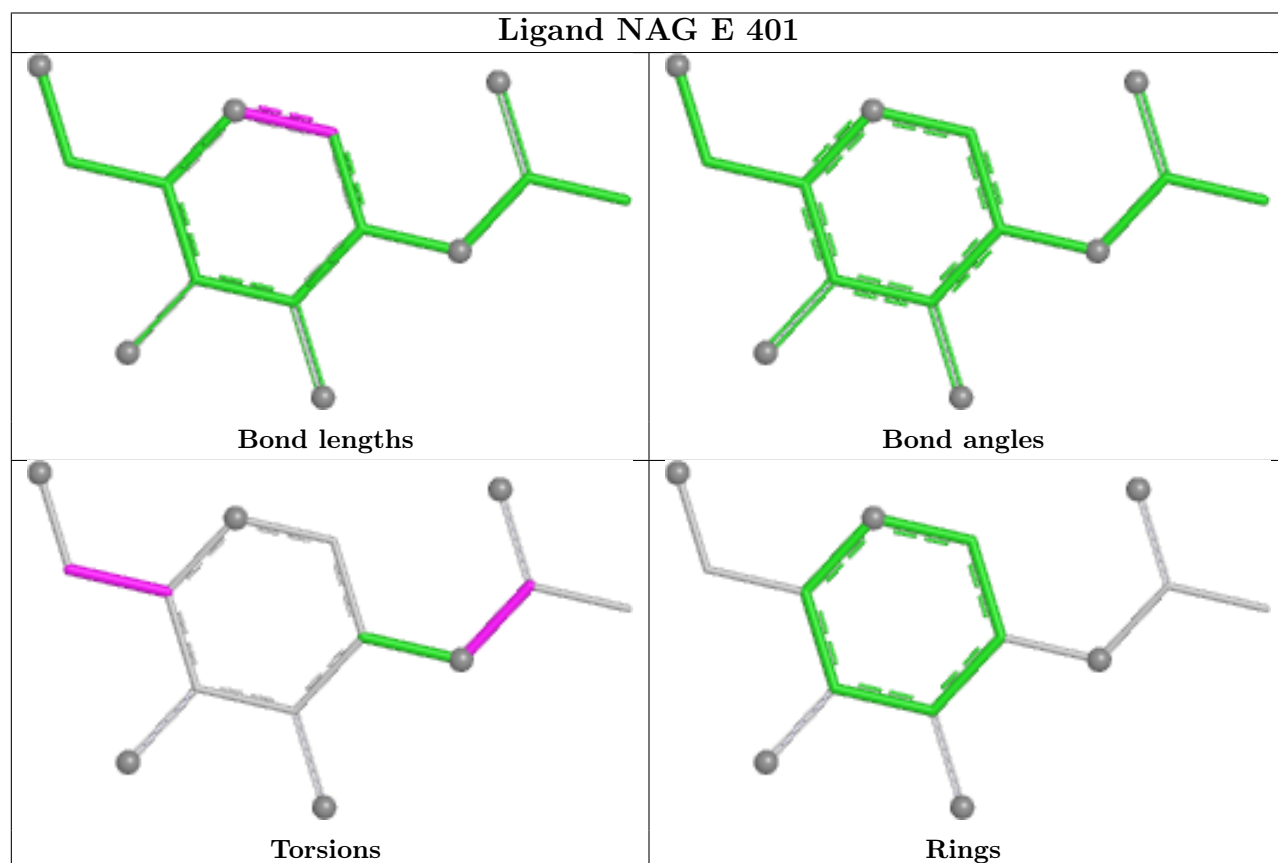
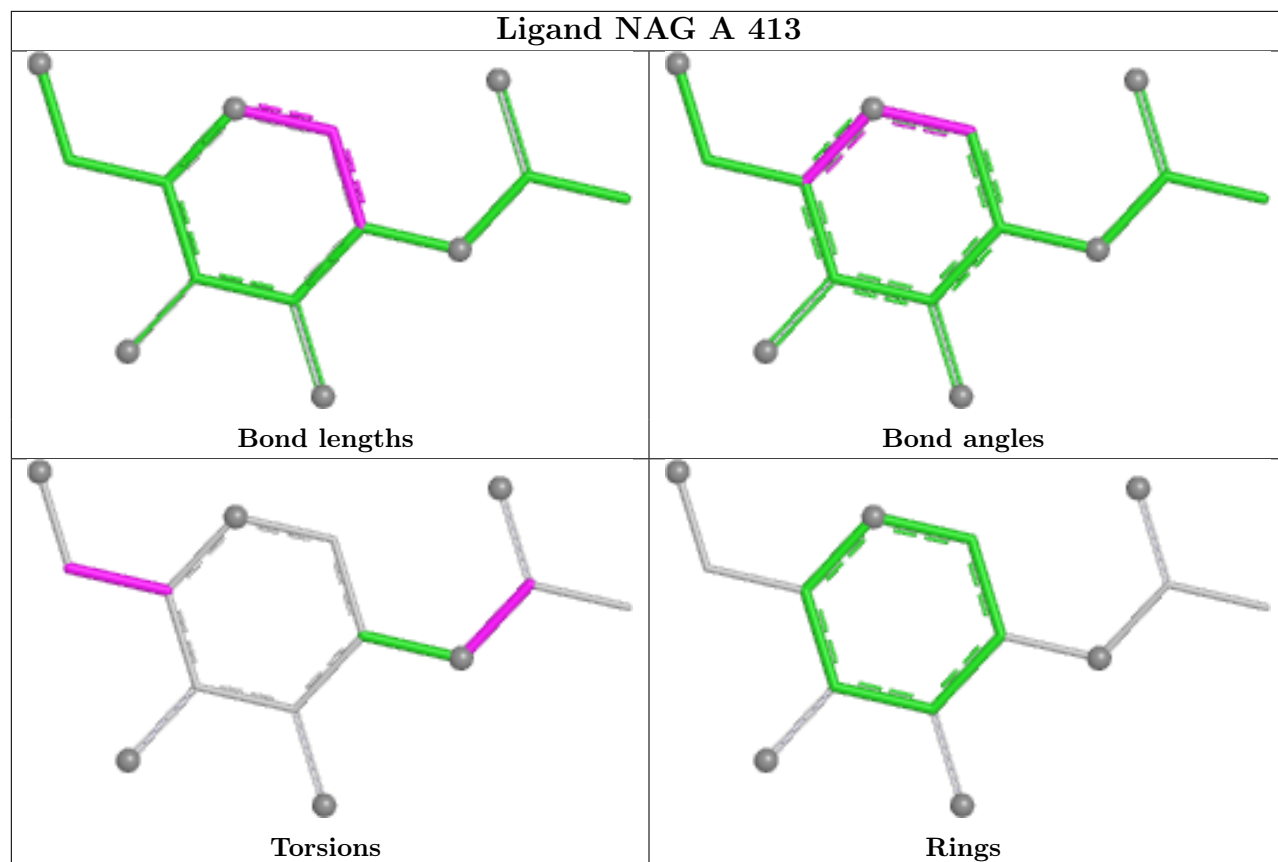


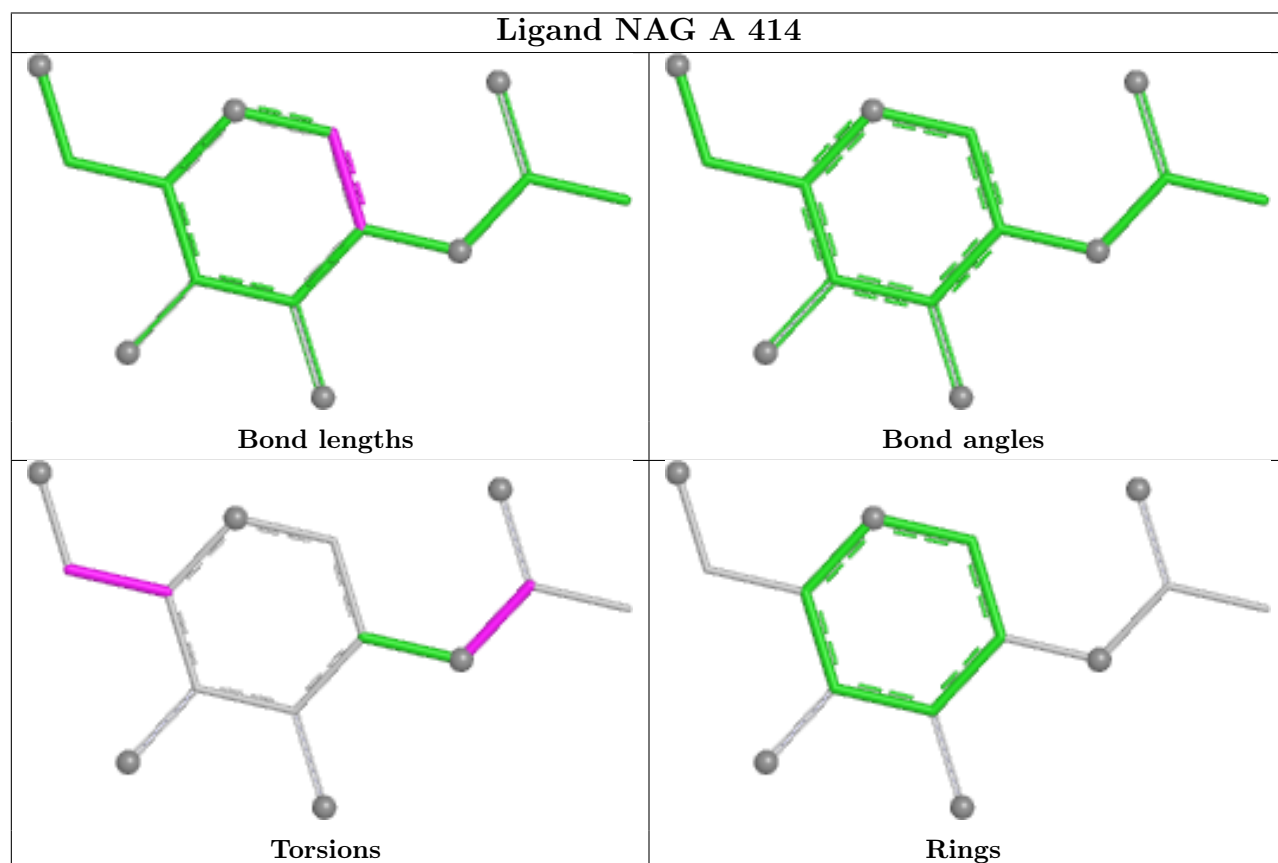
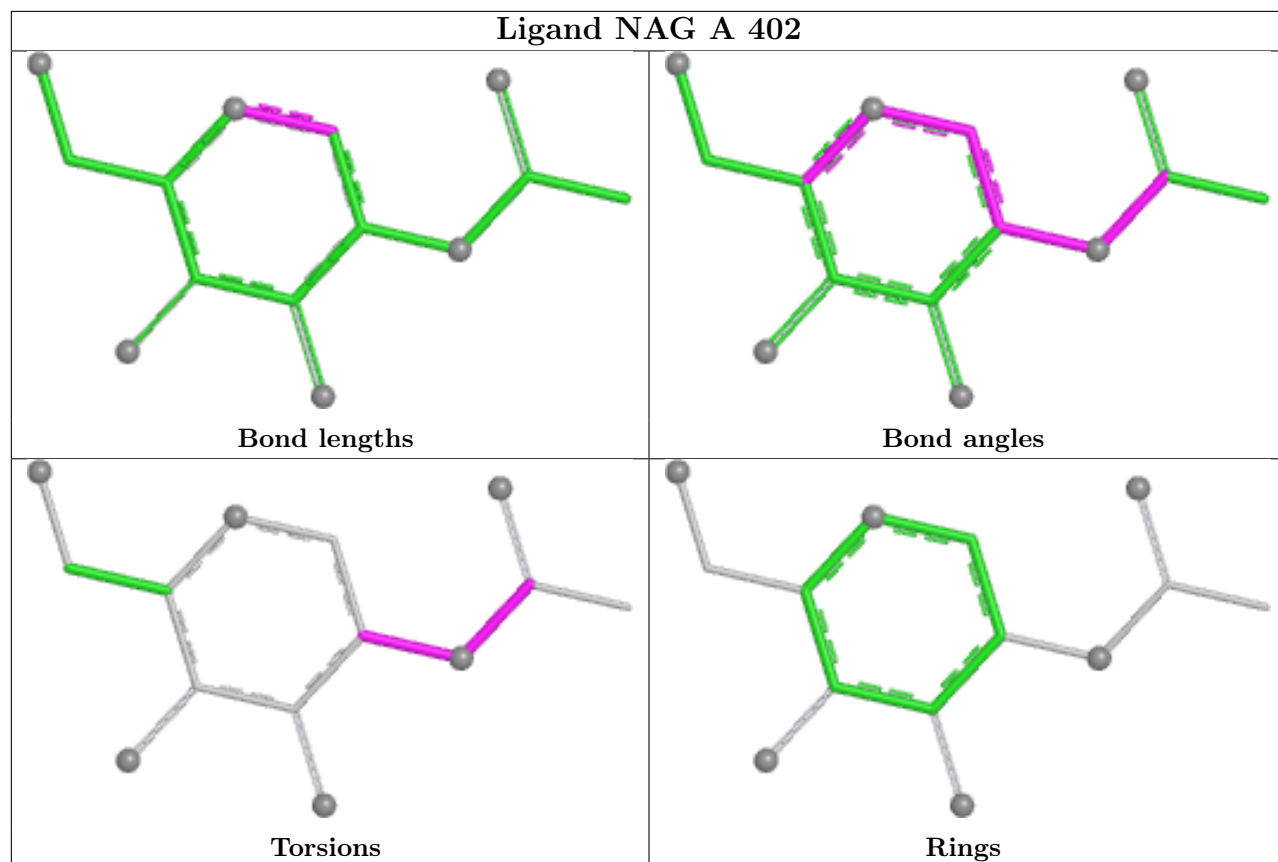












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	321/330 (97%)	0.65	27 (8%) 17 12	20, 54, 117, 244	0
1	C	321/330 (97%)	0.66	30 (9%) 14 10	26, 54, 108, 183	0
1	E	321/330 (97%)	0.59	15 (4%) 36 23	19, 57, 93, 133	0
1	G	320/330 (96%)	0.50	9 (2%) 55 36	28, 56, 92, 143	0
1	I	320/330 (96%)	0.69	23 (7%) 21 14	25, 58, 122, 170	0
1	K	321/330 (97%)	0.57	20 (6%) 26 17	26, 54, 103, 176	0
2	B	165/183 (90%)	1.43	43 (26%) 1 2	37, 117, 172, 201	0
2	D	165/183 (90%)	1.61	53 (32%) 1 1	35, 121, 195, 238	0
2	F	165/183 (90%)	1.35	43 (26%) 1 2	31, 94, 154, 206	0
2	H	165/183 (90%)	1.14	34 (20%) 2 2	31, 82, 131, 177	0
2	J	165/183 (90%)	1.68	58 (35%) 1 1	34, 112, 180, 205	0
2	L	165/183 (90%)	1.02	24 (14%) 6 5	34, 95, 153, 186	0
All	All	2914/3078 (94%)	0.87	379 (13%) 7 6	19, 65, 150, 244	0

All (379) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	GLY	9.0
2	J	163	SER	8.6
2	D	4	GLY	6.7
2	J	118	LEU	6.3
2	J	114	ASN	5.6
1	A	3	ILE	5.5
2	J	138	PHE	5.5
2	D	22	TYR	5.3
2	F	21	TRP	5.3
2	D	116	LYS	5.2
2	D	6	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	117	ASN	5.0
1	C	213	ILE	4.9
2	J	122	VAL	4.7
2	D	126	LEU	4.7
1	I	260	PHE	4.7
1	A	323	ILE	4.5
1	A	4	CYS	4.5
2	B	124	SER	4.4
1	C	3	ILE	4.4
2	F	159	TYR	4.4
1	K	5	ILE	4.4
2	F	50	ASN	4.3
2	H	156	THR	4.3
2	B	116	LYS	4.3
2	J	119	TYR	4.2
2	J	40	SER	4.1
2	D	115	VAL	4.1
2	D	118	LEU	4.1
1	K	323	ILE	4.1
1	A	5	ILE	4.1
2	B	44	ALA	4.1
2	J	159	TYR	4.1
2	J	116	LYS	4.1
2	F	163	SER	4.1
2	J	6	ILE	4.0
2	F	116	LYS	4.0
2	D	114	ASN	4.0
2	H	128	ASN	4.0
2	J	126	LEU	4.0
2	F	160	PRO	3.9
1	G	263	GLY	3.9
2	B	138	PHE	3.9
2	J	110	PHE	3.9
2	F	133	ILE	3.9
2	D	5	ALA	3.9
1	K	129	THR	3.9
2	B	15	THR	3.9
2	D	35	ALA	3.9
2	F	162	TYR	3.8
2	D	156	THR	3.8
2	F	134	GLY	3.8
2	L	138	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	132	GLU	3.8
2	L	121	LYS	3.7
1	A	138	ASN	3.7
2	F	129	ASN	3.7
2	B	143	LYS	3.7
2	H	61	THR	3.7
2	H	131	LYS	3.7
1	I	3	ILE	3.7
2	B	2	LEU	3.7
2	B	126	LEU	3.7
2	F	131	LYS	3.6
1	C	323	ILE	3.6
2	D	36	ALA	3.6
2	J	22	TYR	3.6
2	B	139	GLU	3.6
2	B	134	GLY	3.5
2	J	160	PRO	3.5
2	B	133	ILE	3.5
2	D	105	GLU	3.5
2	D	119	TYR	3.5
2	H	141	TYR	3.5
2	B	35	ALA	3.5
1	K	183	ASN	3.5
1	I	6	GLY	3.5
2	L	133	ILE	3.5
2	J	134	GLY	3.4
1	I	317	LEU	3.4
2	D	152	VAL	3.4
2	D	19	ASP	3.4
2	F	3	PHE	3.4
2	B	141	TYR	3.4
2	L	1	GLY	3.4
2	H	140	PHE	3.4
2	J	121	LYS	3.4
2	B	128	ASN	3.3
2	J	140	PHE	3.3
2	B	131	LYS	3.3
1	E	5	ILE	3.3
2	J	117	ASN	3.3
2	F	147	GLU	3.3
1	C	313	MET	3.3
1	I	17	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	143	LYS	3.3
1	G	231	THR	3.3
2	J	123	LYS	3.3
2	D	64	THR	3.2
2	L	159	TYR	3.2
2	D	2	LEU	3.2
2	F	124	SER	3.2
2	H	102	LEU	3.2
2	J	156	THR	3.2
2	F	132	GLU	3.2
2	D	39	LYS	3.2
2	F	22	TYR	3.2
2	F	102	LEU	3.2
1	K	4	CYS	3.2
2	J	59	MET	3.2
1	I	263	GLY	3.2
2	J	20	GLY	3.2
1	C	23	ASN	3.2
1	A	20	LEU	3.2
1	E	4	CYS	3.2
2	B	158	ASP	3.1
1	E	6	GLY	3.1
2	D	134	GLY	3.1
2	D	102	LEU	3.1
1	I	20	LEU	3.1
1	E	129	THR	3.1
2	F	23	GLY	3.1
1	C	288	SER	3.1
2	D	106	ARG	3.1
1	E	323	ILE	3.1
1	I	8	HIS	3.0
1	I	318	ARG	3.0
2	F	4	GLY	3.0
2	H	162	TYR	3.0
1	C	261	GLY	3.0
2	L	134	GLY	3.0
2	J	115	VAL	3.0
1	A	273	GLU	3.0
1	A	313	MET	3.0
2	D	24	TYR	3.0
2	D	34	TYR	3.0
2	B	3	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	18	VAL	3.0
1	K	84	ASN	3.0
2	J	158	ASP	2.9
1	I	5	ILE	2.9
2	L	6	ILE	2.9
1	C	32	LEU	2.9
2	H	143	LYS	2.9
2	J	58	LYS	2.9
2	B	119	TYR	2.9
2	J	157	TYR	2.9
2	F	63	PHE	2.9
2	B	19	ASP	2.9
1	E	138	ASN	2.9
1	G	23	ASN	2.9
2	J	136	GLY	2.9
2	B	127	LYS	2.9
2	D	127	LYS	2.9
2	H	2	LEU	2.9
2	L	3	PHE	2.9
2	L	25	HIS	2.8
2	D	7	ALA	2.8
1	K	6	GLY	2.8
2	D	131	LYS	2.8
2	B	159	TYR	2.8
1	E	287	SER	2.8
1	G	321	PRO	2.8
2	F	64	THR	2.8
2	J	109	ASP	2.8
1	C	314	VAL	2.8
2	D	21	TRP	2.8
1	K	195	ASN	2.8
2	L	124	SER	2.8
2	B	163	SER	2.8
2	J	19	ASP	2.8
2	B	129	ASN	2.8
2	J	128	ASN	2.8
1	C	4	CYS	2.8
2	B	152	VAL	2.8
2	F	121	LYS	2.8
2	J	152	VAL	2.8
1	E	273	GLU	2.8
1	C	316	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	7	TYR	2.8
2	F	141	TYR	2.8
1	I	262	SER	2.8
1	E	120	GLU	2.8
2	D	157	TYR	2.7
2	H	159	TYR	2.7
1	K	30	VAL	2.7
1	I	51	GLN	2.7
2	J	1	GLY	2.7
2	F	19	ASP	2.7
1	I	31	ASN	2.7
2	F	157	TYR	2.7
2	L	163	SER	2.7
2	J	149	MET	2.7
2	H	130	ALA	2.7
2	H	157	TYR	2.7
1	I	314	VAL	2.7
2	F	142	HIS	2.7
1	I	313	MET	2.7
1	A	318	ARG	2.7
2	L	127	LYS	2.7
2	F	130	ALA	2.7
2	J	127	LYS	2.6
2	F	137	CYS	2.6
2	B	118	LEU	2.6
2	D	18	VAL	2.6
2	J	141	TYR	2.6
2	B	38	GLN	2.6
2	D	11	GLU	2.6
2	B	21	TRP	2.6
2	L	162	TYR	2.6
2	H	3	PHE	2.6
2	F	158	ASP	2.6
2	J	139	GLU	2.6
2	B	122	VAL	2.6
1	I	231	THR	2.6
1	A	310	LYS	2.6
2	L	140	PHE	2.6
2	D	9	PHE	2.6
2	J	25	HIS	2.6
2	H	19	ASP	2.6
1	C	20	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	101	LEU	2.6
2	F	150	GLU	2.6
1	K	196	ALA	2.6
1	I	22	LYS	2.6
2	B	157	TYR	2.5
2	D	38	GLN	2.5
2	H	134	GLY	2.5
1	A	183	ASN	2.5
2	J	143	LYS	2.5
1	I	289	LEU	2.5
2	J	2	LEU	2.5
2	L	154	ASN	2.5
1	C	299	ILE	2.5
2	J	61	THR	2.5
1	A	7	TYR	2.5
1	G	8	HIS	2.5
2	F	24	TYR	2.5
2	H	22	TYR	2.5
1	K	178	VAL	2.5
1	C	244	ASN	2.5
2	H	129	ASN	2.5
1	G	20	LEU	2.5
2	D	23	GLY	2.5
2	L	27	GLN	2.5
1	I	72	SER	2.5
2	H	160	PRO	2.5
2	F	16	GLY	2.5
2	H	16	GLY	2.5
1	A	268	ASN	2.4
2	J	153	LYS	2.4
1	A	18	THR	2.4
2	B	160	PRO	2.4
2	J	35	ALA	2.4
2	D	133	ILE	2.4
2	B	120	GLU	2.4
2	B	132	GLU	2.4
2	D	132	GLU	2.4
1	E	310	LYS	2.4
2	H	138	PHE	2.4
2	D	98	LEU	2.4
2	F	123	LYS	2.4
2	D	110	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	121	SER	2.4
1	A	315	THR	2.4
2	D	43	ASN	2.4
2	B	56	ILE	2.4
2	D	10	ILE	2.4
2	F	127	LYS	2.4
1	I	121	SER	2.4
2	F	128	ASN	2.4
2	L	157	TYR	2.4
2	H	165	GLU	2.4
1	E	315	THR	2.3
2	H	35	ALA	2.3
1	A	143	PHE	2.3
2	L	108	LEU	2.3
2	F	38	GLN	2.3
2	J	9	PHE	2.3
1	G	73	LYS	2.3
2	H	121	LYS	2.3
1	C	188	ARG	2.3
1	E	278	CYS	2.3
2	J	133	ILE	2.3
1	C	246	ASN	2.3
2	B	140	PHE	2.3
2	F	161	LYS	2.3
2	D	32	SER	2.3
2	H	135	ASN	2.3
2	D	3	PHE	2.3
1	C	187	GLN	2.3
2	H	29	GLU	2.3
1	A	320	ILE	2.3
2	L	22	TYR	2.3
1	A	291	PHE	2.3
1	K	3	ILE	2.2
2	D	160	PRO	2.2
1	A	276	ALA	2.2
2	F	35	ALA	2.2
1	A	22	LYS	2.2
1	C	310	LYS	2.2
2	L	117	ASN	2.2
2	J	62	GLN	2.2
2	D	29	GLU	2.2
2	J	120	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	20	LEU	2.2
1	K	186	ASP	2.2
1	C	317	LEU	2.2
1	A	277	LYS	2.2
1	A	304	LYS	2.2
1	A	157	TYR	2.2
2	H	24	TYR	2.2
2	D	16	GLY	2.2
2	D	37	ASP	2.2
2	J	37	ASP	2.2
1	K	89	THR	2.2
1	I	28	HIS	2.2
2	H	142	HIS	2.2
1	A	144	TYR	2.2
1	C	311	LEU	2.2
2	L	7	ALA	2.2
2	B	135	ASN	2.2
1	C	19	VAL	2.1
2	J	162	TYR	2.1
2	J	17	MET	2.1
2	H	31	GLY	2.1
2	D	95	ASN	2.1
2	F	66	VAL	2.1
1	K	210	THR	2.1
2	L	156	THR	2.1
2	B	156	THR	2.1
2	D	128	ASN	2.1
1	C	17	ASP	2.1
2	H	152	VAL	2.1
2	H	118	LEU	2.1
1	G	9	ALA	2.1
2	D	130	ALA	2.1
2	L	8	GLY	2.1
2	J	8	GLY	2.1
1	E	29	SER	2.1
1	G	75	SER	2.1
2	J	53	ASN	2.1
1	K	219	VAL	2.1
2	J	137	CYS	2.1
2	H	119	TYR	2.1
2	J	34	TYR	2.1
2	D	155	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	PRO	2.1
1	C	273	GLU	2.1
1	K	82	LYS	2.1
1	C	7	TYR	2.1
2	B	20	GLY	2.1
2	B	31	GLY	2.1
2	D	20	GLY	2.1
2	D	30	GLN	2.1
2	F	1	GLY	2.1
2	F	125	GLN	2.1
2	J	164	GLU	2.1
1	E	30	VAL	2.0
2	J	131	LYS	2.0
2	F	149	MET	2.0
1	C	210	THR	2.0
1	I	27	THR	2.0
1	A	111	PHE	2.0
1	E	88	GLY	2.0
2	B	9	PHE	2.0
1	K	317	LEU	2.0
1	K	29	SER	2.0
1	C	320	ILE	2.0
2	H	124	SER	2.0
2	L	149	MET	2.0
2	B	25	HIS	2.0
2	B	59	MET	2.0
1	C	315	THR	2.0
2	J	24	TYR	2.0
1	C	6	GLY	2.0
2	B	27	GLN	2.0
2	J	132	GLU	2.0
1	C	5	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	N	5	14/15	0.48	0.17	73,91,104,110	0
4	MAN	N	4	11/12	0.56	0.16	82,115,129,130	0
3	MAN	V	4	11/12	0.58	0.18	78,108,117,120	0
5	BMA	O	3	11/12	0.58	0.16	85,115,121,131	0
5	BMA	X	3	11/12	0.61	0.19	101,108,114,116	0
3	MAN	S	4	11/12	0.62	0.16	75,91,111,113	0
3	NAG	V	5	14/15	0.63	0.18	87,108,116,123	0
3	NAG	M	5	14/15	0.65	0.17	76,102,119,119	0
3	BMA	V	3	11/12	0.65	0.14	91,99,104,114	0
3	MAN	M	4	11/12	0.69	0.12	59,104,113,116	0
5	MAN	T	4	11/12	0.69	0.15	87,109,122,125	0
3	MAN	V	6	11/12	0.69	0.15	56,76,83,86	0
5	MAN	R	4	11/12	0.70	0.12	74,98,103,107	0
3	NAG	S	5	14/15	0.71	0.14	58,94,100,100	0
5	NAG	U	1	14/15	0.73	0.17	61,71,92,93	0
5	MAN	O	4	11/12	0.73	0.17	85,94,108,121	0
3	NAG	M	2	14/15	0.74	0.15	83,94,106,108	0
5	NAG	U	2	14/15	0.74	0.19	73,94,99,100	0
4	BMA	N	3	11/12	0.74	0.14	64,92,108,124	0
4	MAN	P	4	11/12	0.76	0.12	72,91,95,108	0
5	BMA	Q	3	11/12	0.77	0.12	78,91,103,104	0
4	BMA	P	3	11/12	0.77	0.10	70,88,95,96	0
3	BMA	S	3	11/12	0.78	0.14	60,82,98,107	0
5	NAG	O	2	14/15	0.78	0.13	60,84,97,104	0
6	BMA	W	3	11/12	0.78	0.12	79,86,95,97	0
3	NAG	S	2	14/15	0.79	0.13	61,83,87,93	0
3	BMA	M	3	11/12	0.80	0.14	75,82,103,119	0
5	NAG	Q	2	14/15	0.80	0.13	73,83,91,98	0
4	NAG	P	5	14/15	0.80	0.11	55,72,77,83	0
5	NAG	R	2	14/15	0.81	0.14	57,74,95,102	0
6	NAG	W	2	14/15	0.81	0.13	53,92,106,115	0
5	BMA	U	3	11/12	0.81	0.12	59,68,74,78	0
5	BMA	T	3	11/12	0.82	0.09	70,80,86,89	0
5	NAG	Q	1	14/15	0.82	0.12	36,50,56,71	0
3	NAG	V	2	14/15	0.83	0.13	46,65,70,71	0
5	MAN	X	4	11/12	0.83	0.10	56,67,76,78	0
5	BMA	R	3	11/12	0.84	0.09	67,73,78,81	0
5	NAG	X	2	14/15	0.84	0.12	68,80,92,98	0
3	MAN	M	6	11/12	0.84	0.13	47,69,82,83	0
3	NAG	S	1	14/15	0.85	0.11	33,62,74,79	0
4	NAG	N	2	14/15	0.86	0.12	47,61,75,88	0

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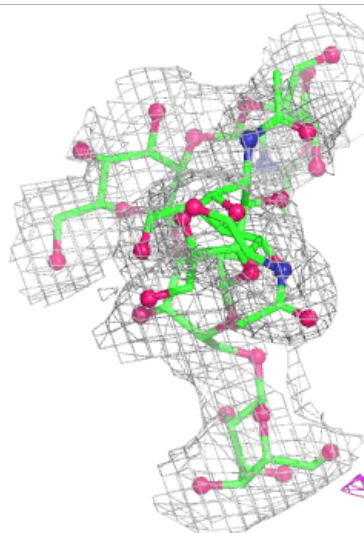
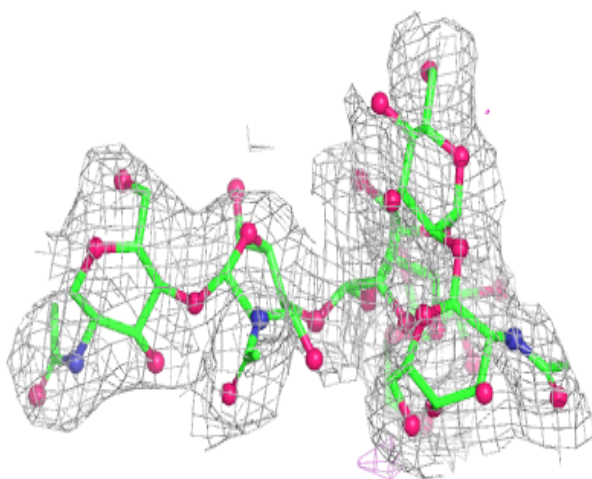
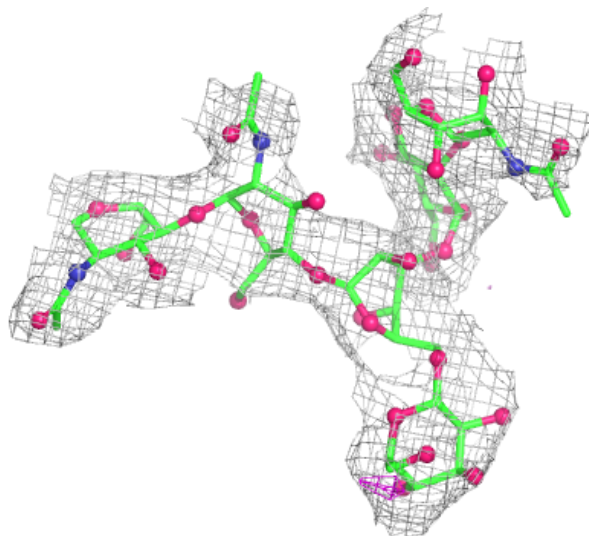
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	S	6	11/12	0.86	0.10	35,45,52,52	0
5	MAN	U	4	11/12	0.86	0.12	39,59,70,73	0
5	NAG	T	2	14/15	0.86	0.14	52,66,72,82	0
5	MAN	Q	4	11/12	0.88	0.14	67,80,105,112	0
3	NAG	M	1	14/15	0.88	0.12	51,54,59,59	0
6	NAG	W	1	14/15	0.89	0.09	53,56,60,65	0
4	NAG	P	2	14/15	0.89	0.12	44,52,68,69	0
5	NAG	O	1	14/15	0.89	0.10	31,52,63,73	0
5	NAG	R	1	14/15	0.90	0.11	37,40,44,46	0
4	NAG	P	1	14/15	0.91	0.12	34,45,58,67	0
5	NAG	T	1	14/15	0.91	0.12	34,49,57,63	0
3	NAG	V	1	14/15	0.91	0.12	32,37,40,42	0
4	NAG	N	1	14/15	0.94	0.12	32,34,36,46	0
5	NAG	X	1	14/15	0.94	0.09	32,39,55,58	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.

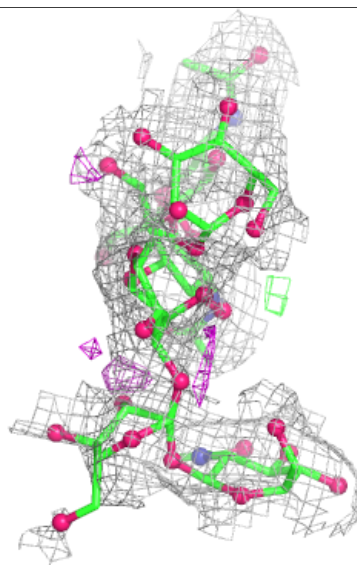
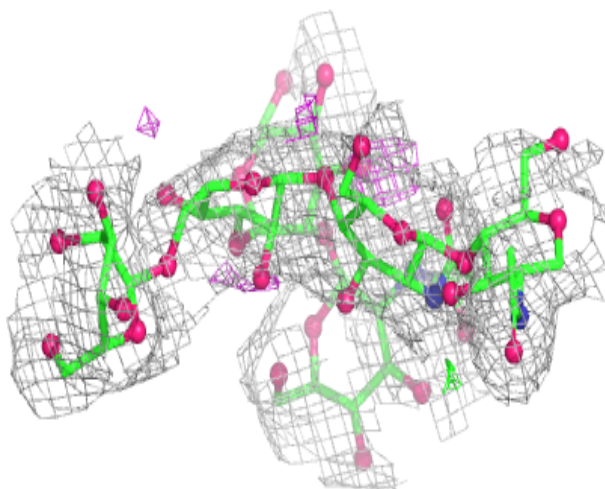
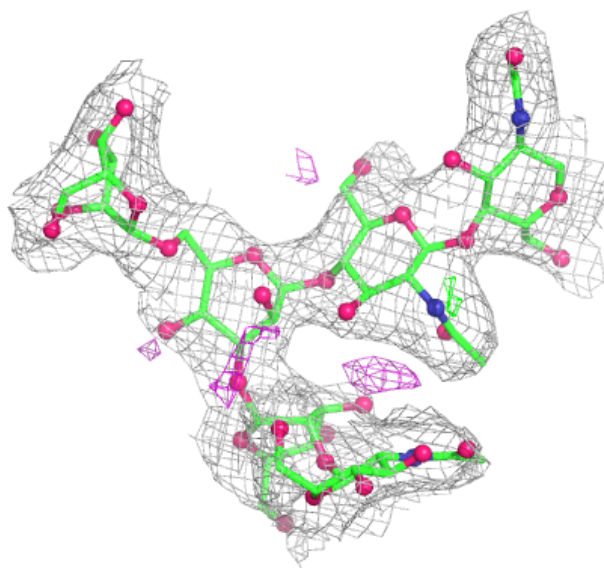
Electron density around Chain M:

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



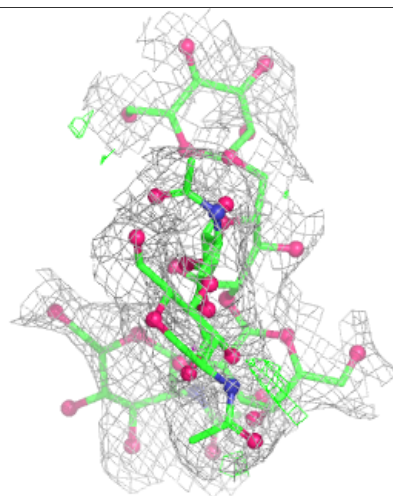
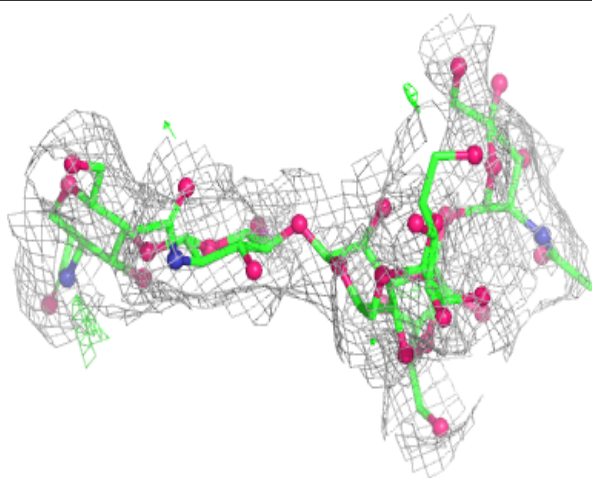
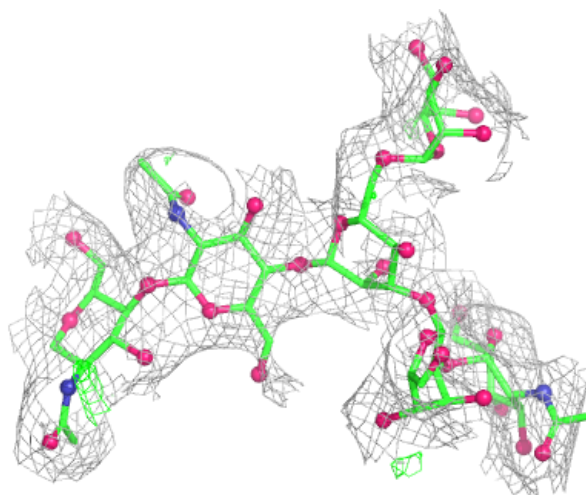
Electron density around Chain S:

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



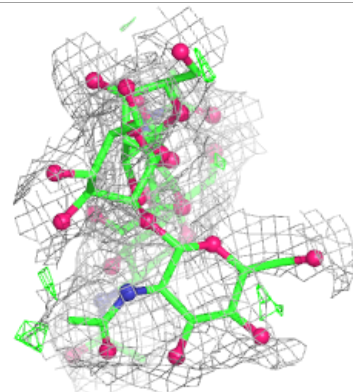
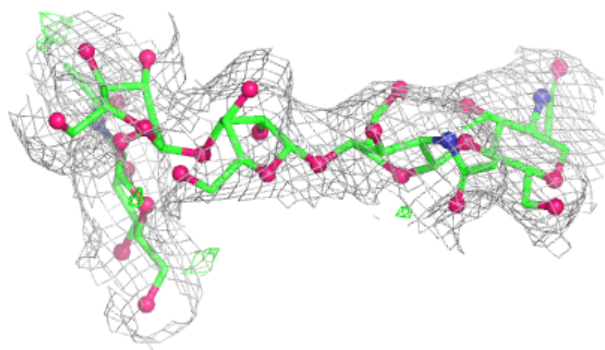
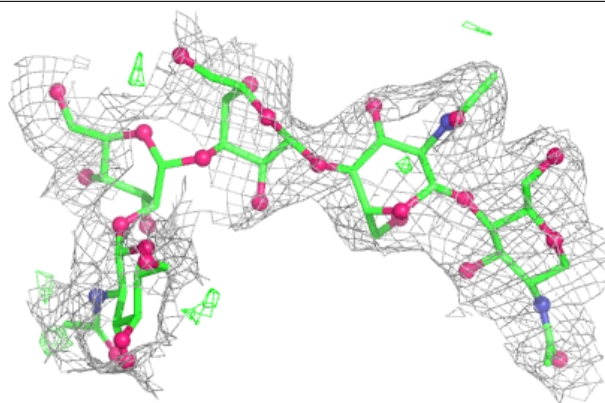
Electron density around Chain V:

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



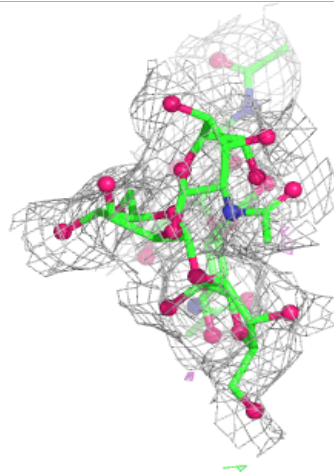
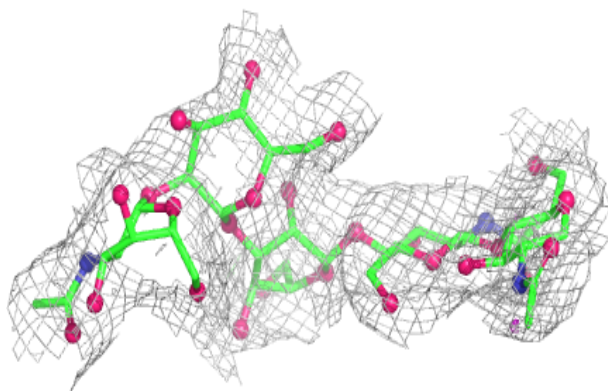
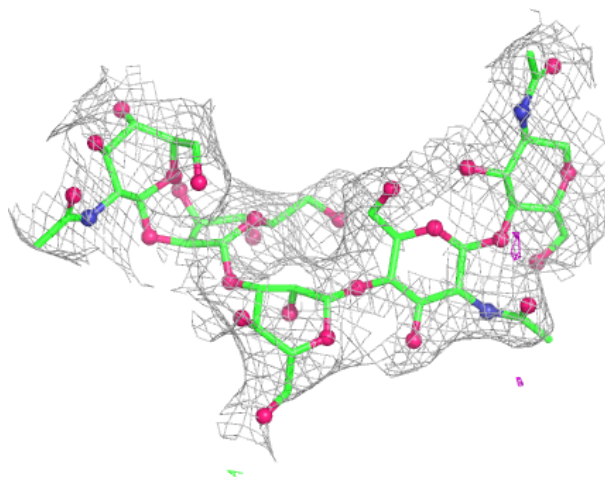
Electron density around Chain N:

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



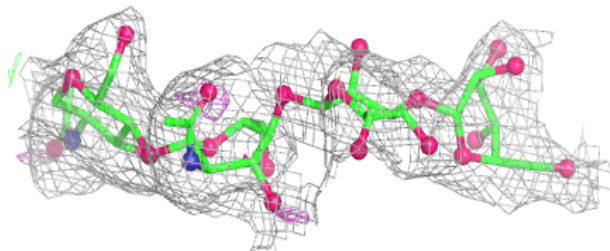
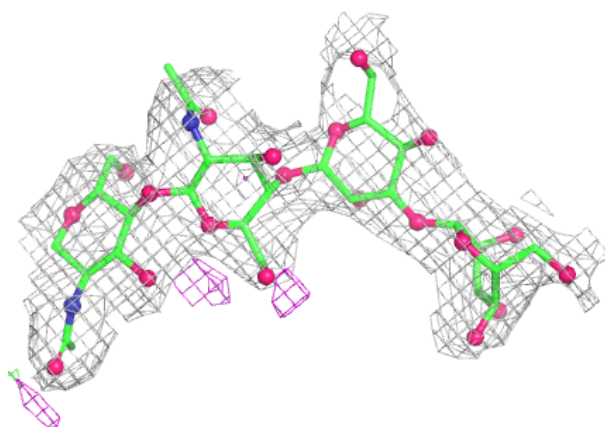
Electron density around Chain P:

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

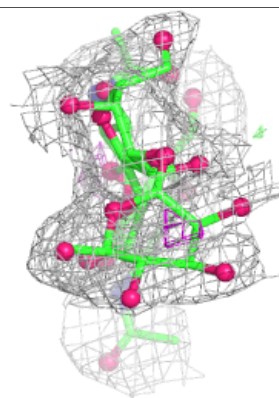
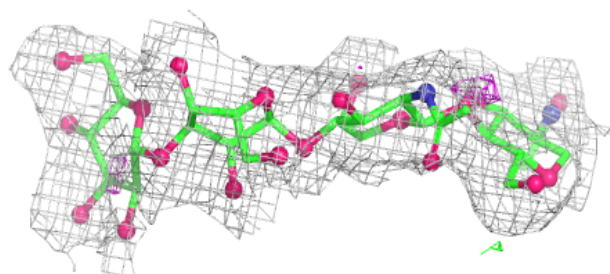
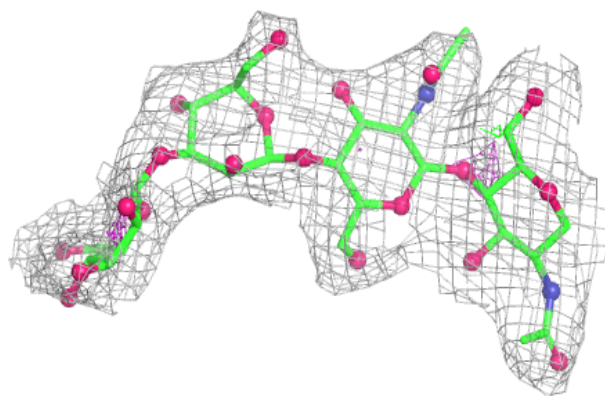


Electron density around Chain O:

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

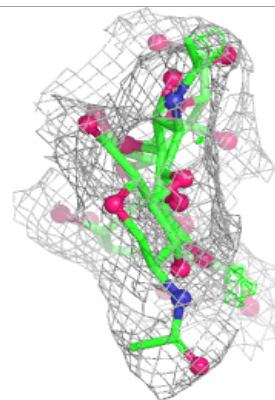
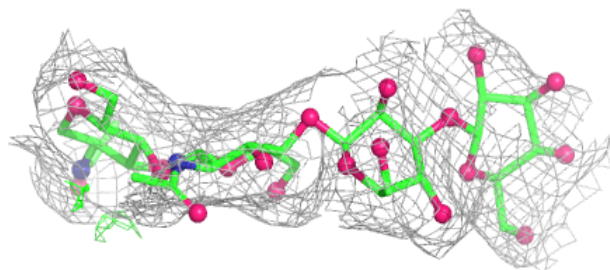
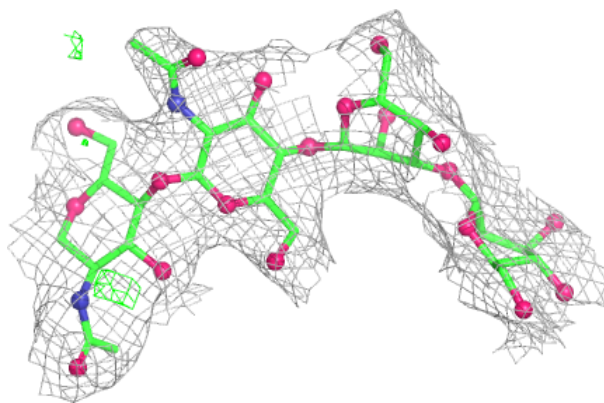
**Electron density around Chain Q:**

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

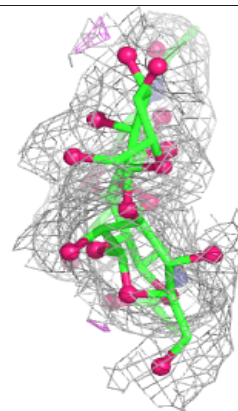
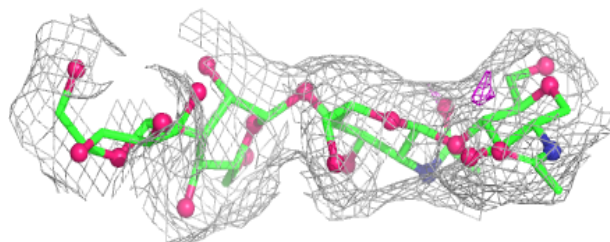
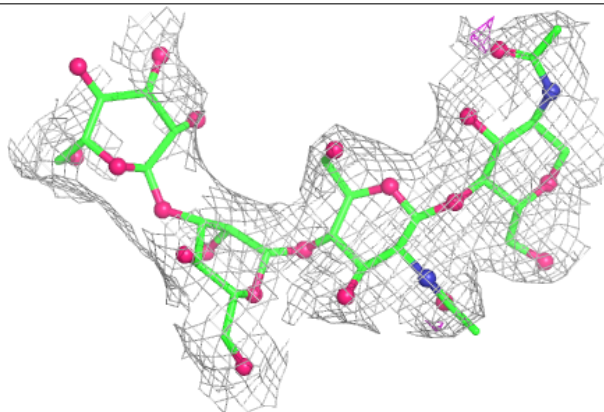


Electron density around Chain R:

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

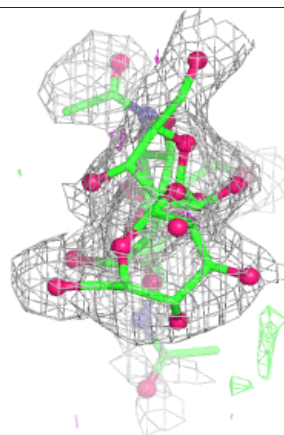
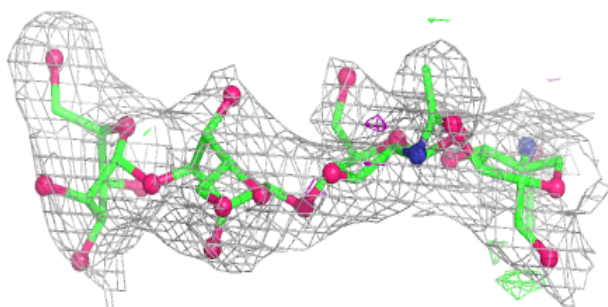
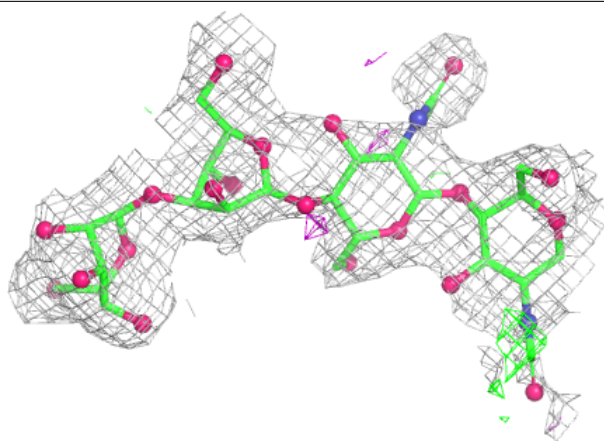
**Electron density around Chain T:**

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

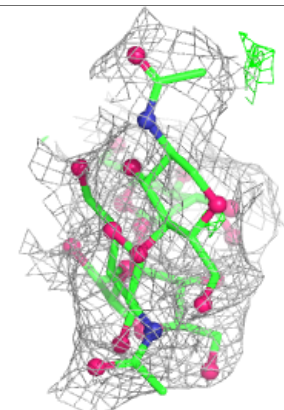
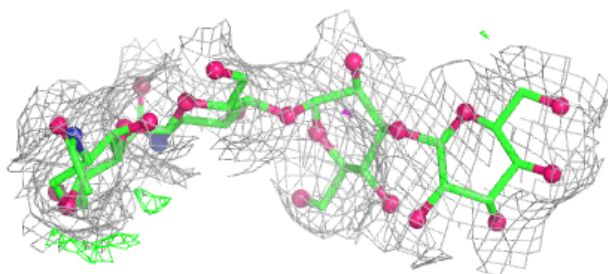
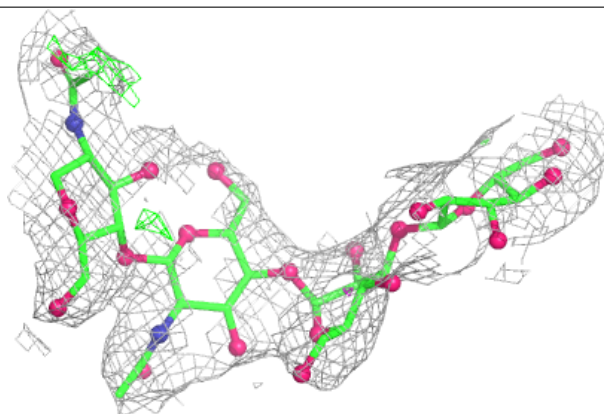


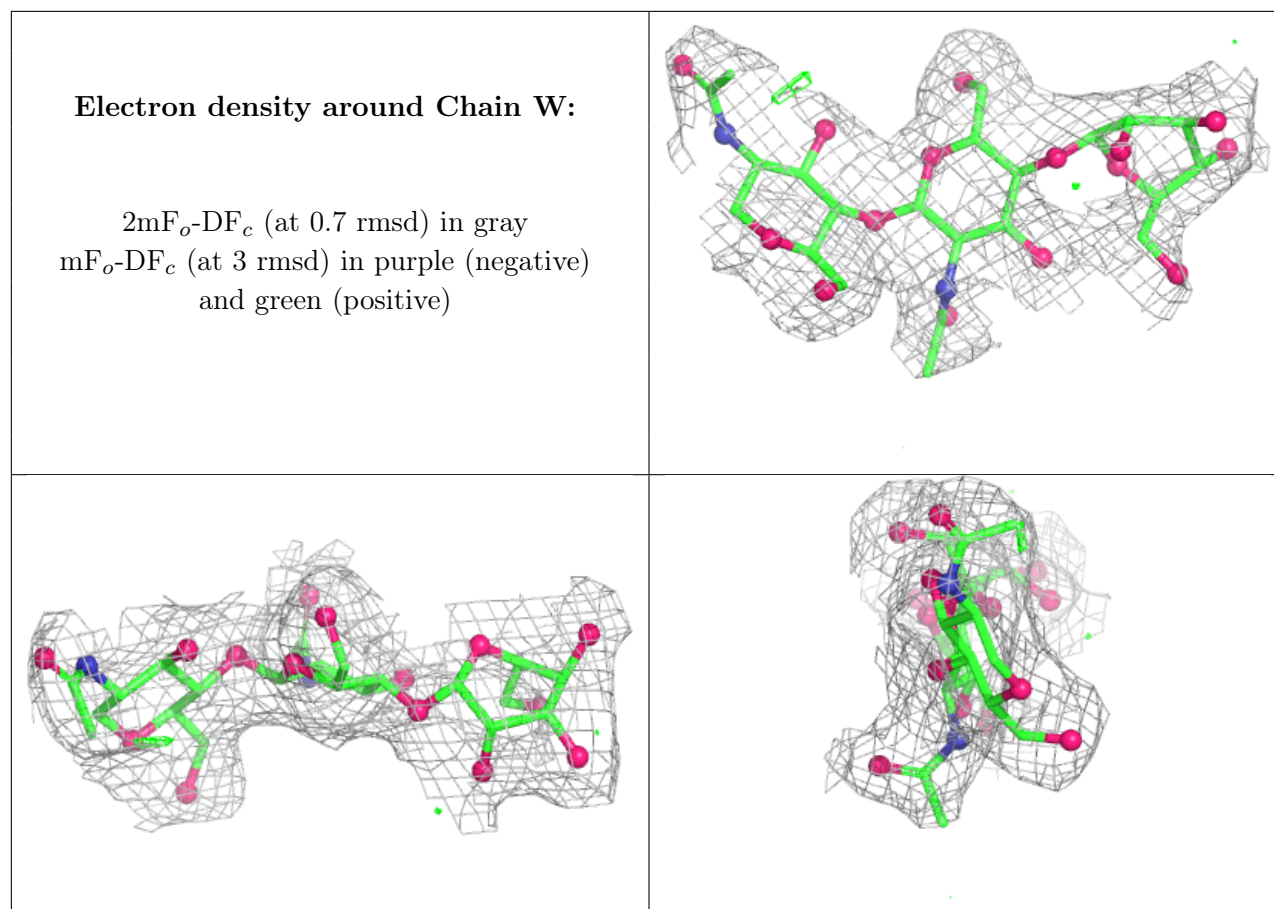
Electron density around Chain U:

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

**Electron density around Chain X:**

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





6.4 Ligands ⓘ

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

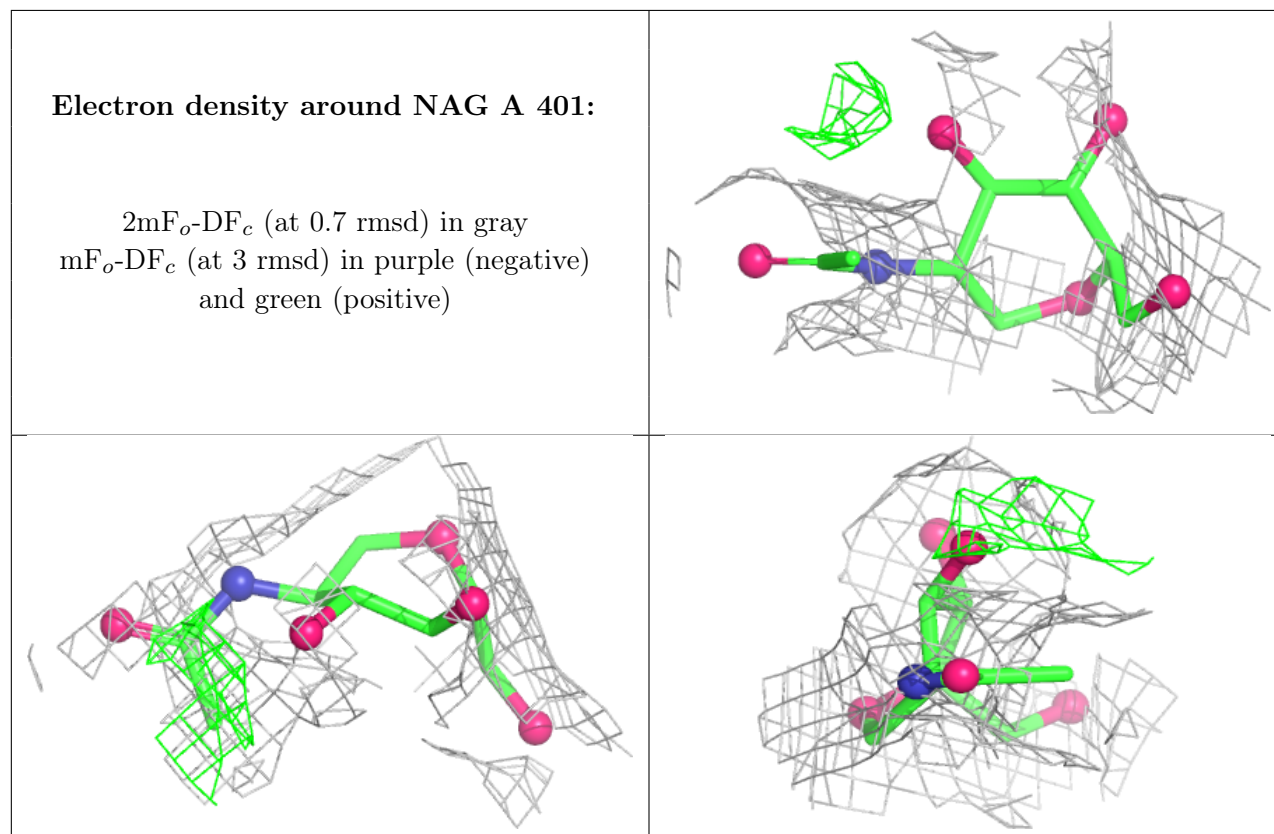
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	401	14/15	0.34	0.17	108,129,155,157	0
7	NAG	K	401	14/15	0.44	0.18	102,134,139,140	0
7	NAG	I	401	14/15	0.44	0.15	118,132,146,152	0
7	NAG	K	413	14/15	0.46	0.17	79,112,140,143	0
7	NAG	I	410	14/15	0.48	0.14	100,131,137,147	0
7	NAG	E	414	14/15	0.53	0.16	103,124,132,137	0
7	NAG	E	412	14/15	0.56	0.15	98,123,129,130	0
7	NAG	A	402	14/15	0.61	0.16	118,155,164,170	0
7	NAG	E	413	14/15	0.62	0.15	75,88,96,98	0
7	NAG	C	409	14/15	0.64	0.15	84,91,98,101	0
7	NAG	E	401	14/15	0.65	0.15	66,91,109,110	0
7	NAG	I	409	14/15	0.65	0.16	75,90,97,99	0
7	NAG	G	402	14/15	0.65	0.16	82,107,120,120	0

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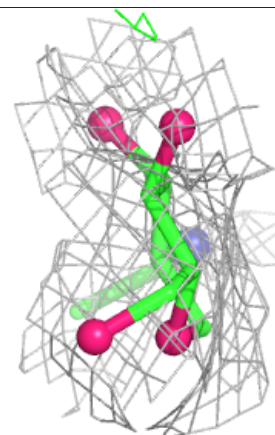
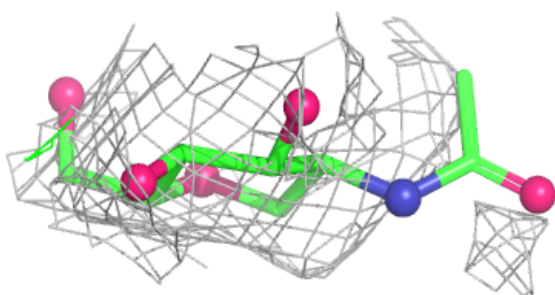
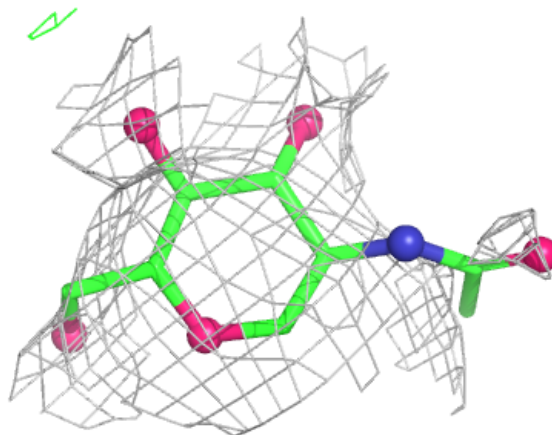
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	412	14/15	0.66	0.14	60,112,127,129	0
7	NAG	A	413	14/15	0.67	0.14	80,93,100,101	0
7	NAG	K	414	14/15	0.72	0.14	103,115,122,122	0
7	NAG	G	401	14/15	0.73	0.14	71,80,91,92	0
7	NAG	A	414	14/15	0.74	0.13	62,80,86,88	0
7	NAG	G	413	14/15	0.79	0.11	57,80,96,97	0
8	ZN	K	415	1/1	0.99	0.04	47,47,47,47	0
8	ZN	G	414	1/1	0.99	0.03	40,40,40,40	0
8	ZN	I	411	1/1	0.99	0.05	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

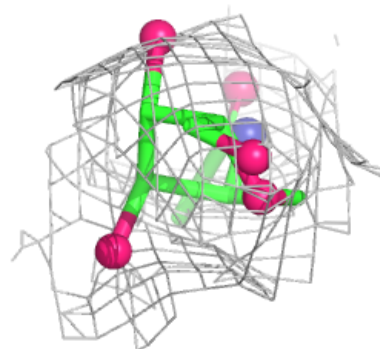
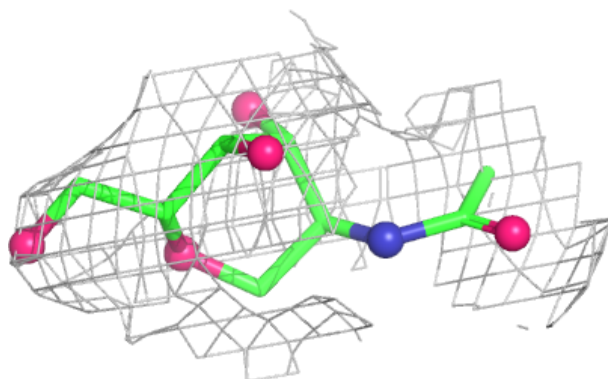
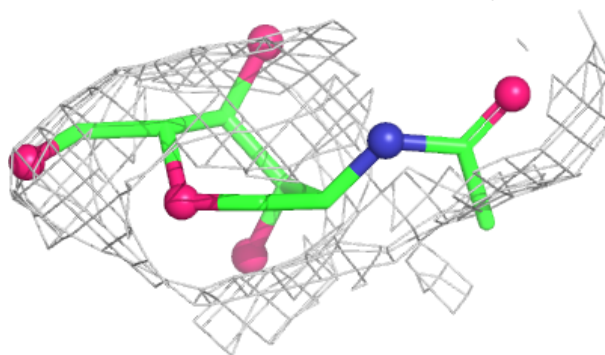


Electron density around NAG K 401:

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

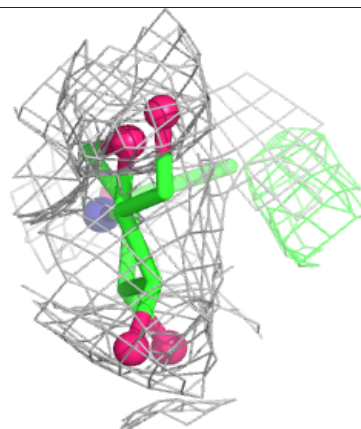
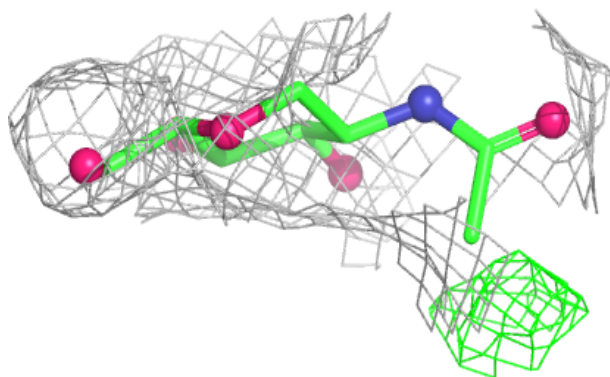
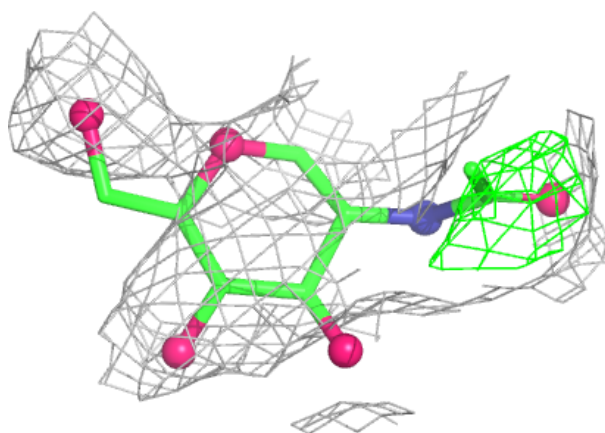
**Electron density around NAG I 401:**

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

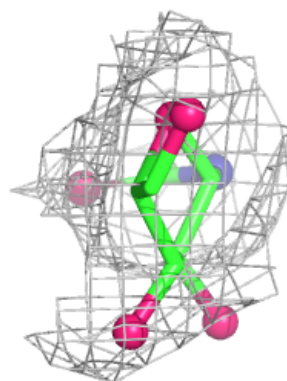
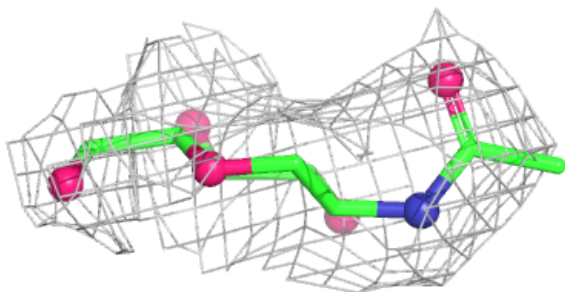
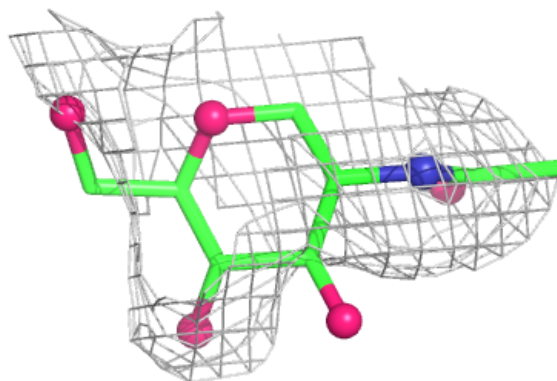


Electron density around NAG K 413:

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

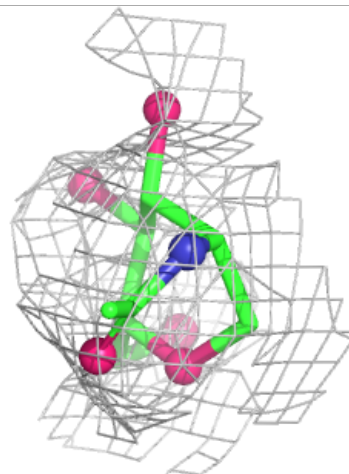
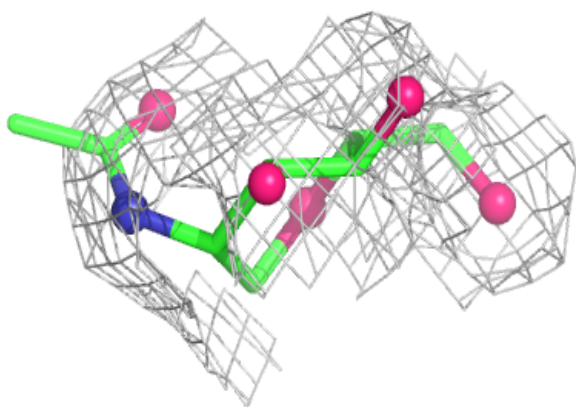
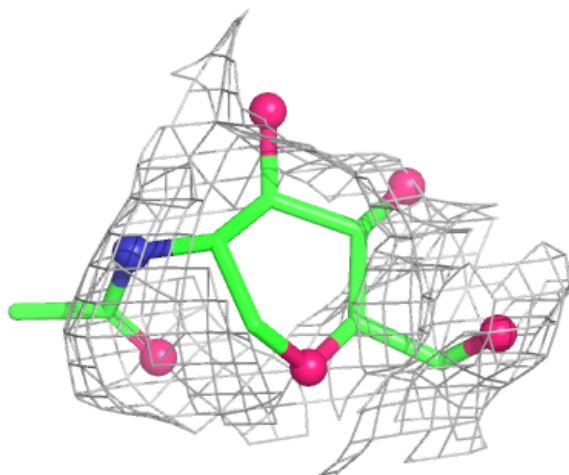
**Electron density around NAG I 410:**

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



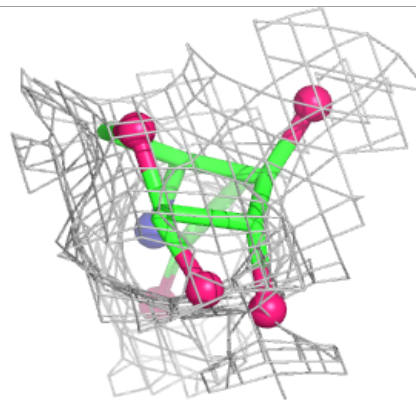
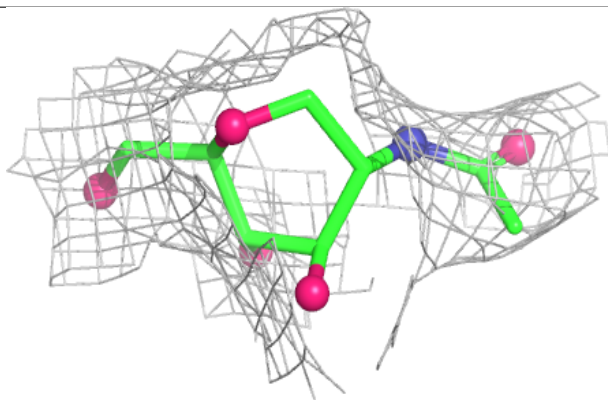
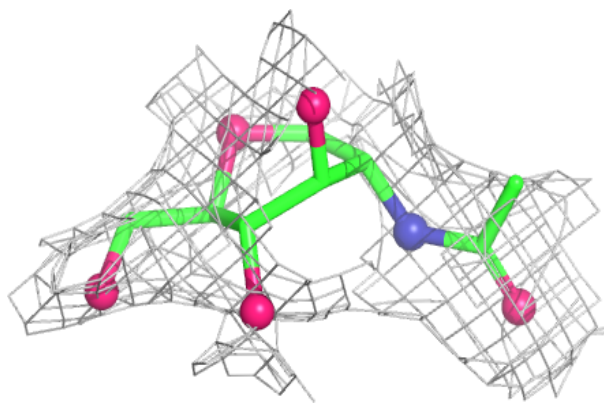
Electron density around NAG E 414:

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

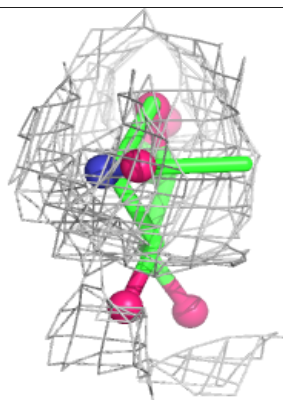
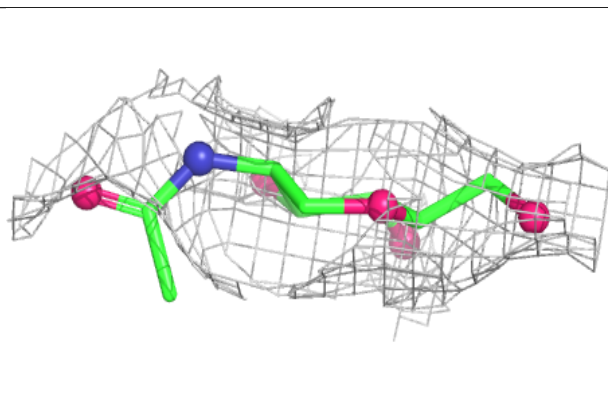
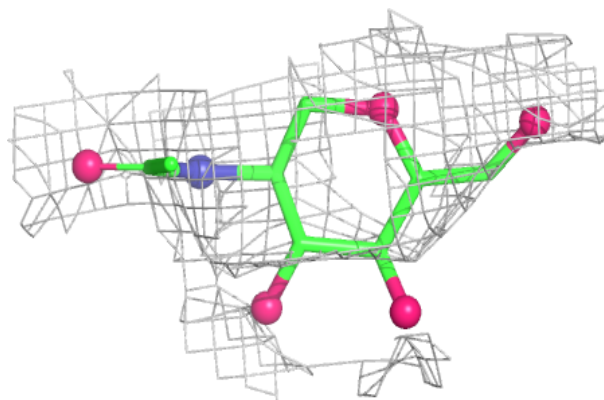


Electron density around NAG E 412:

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

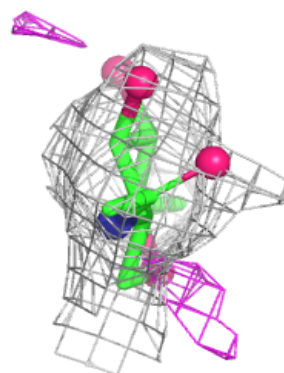
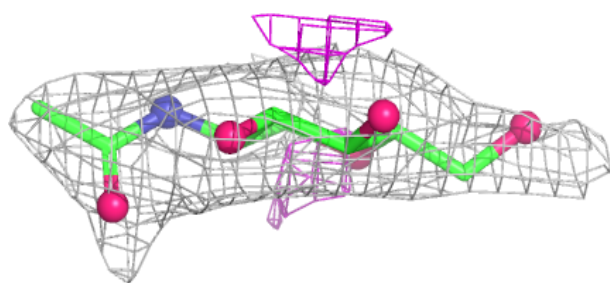
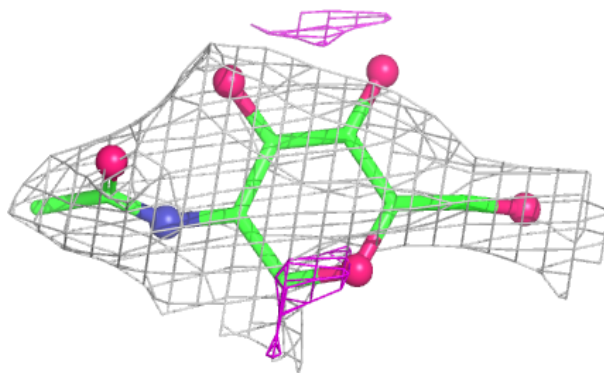
**Electron density around NAG A 402:**

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

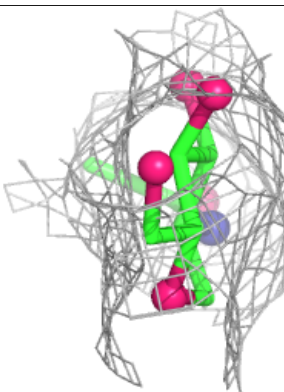
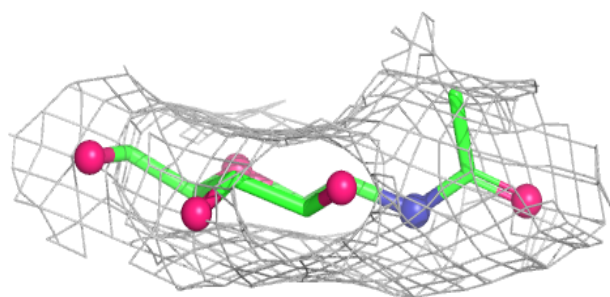
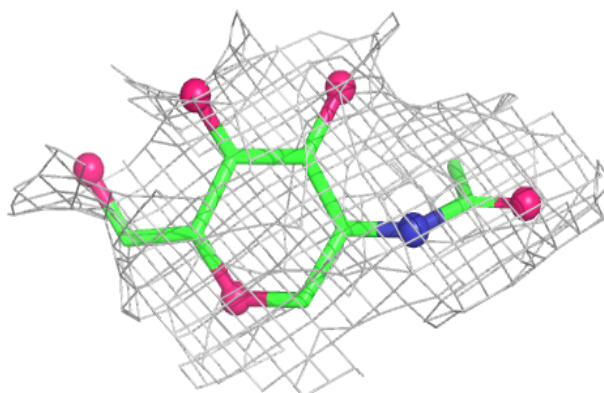


Electron density around NAG E 413:

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

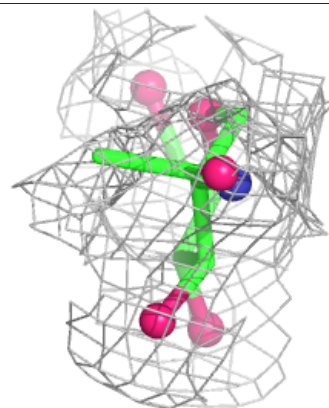
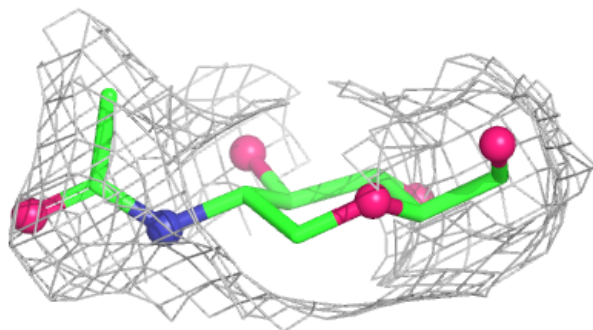
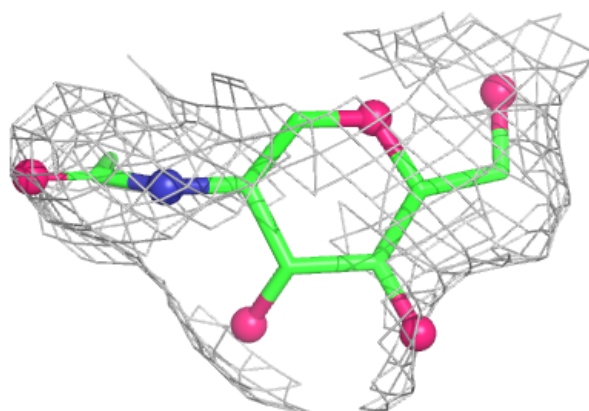
**Electron density around NAG C 409:**

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

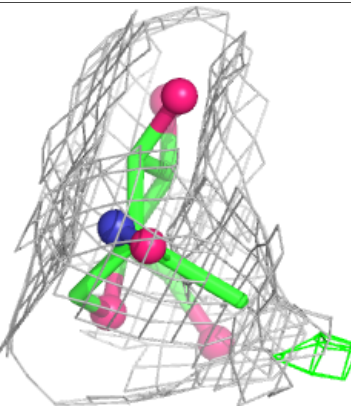
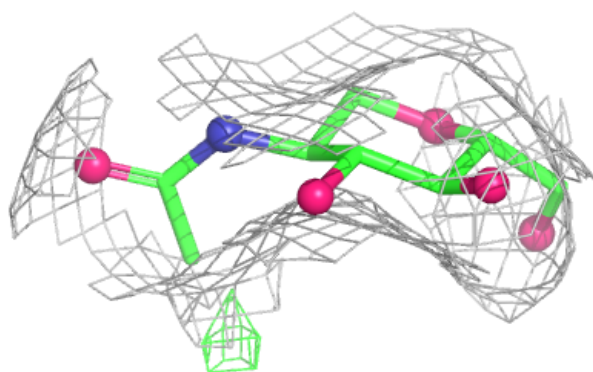
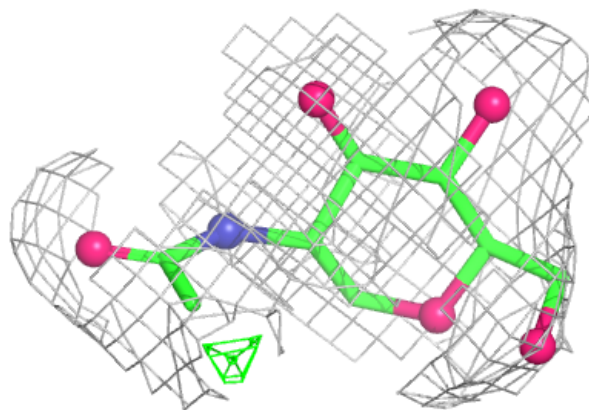


Electron density around NAG E 401:

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

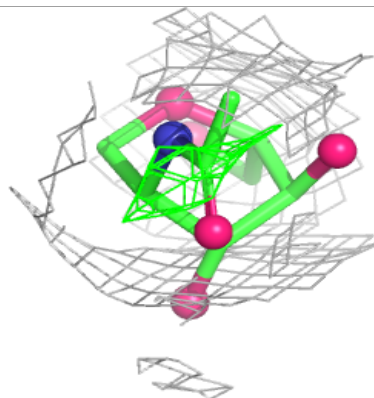
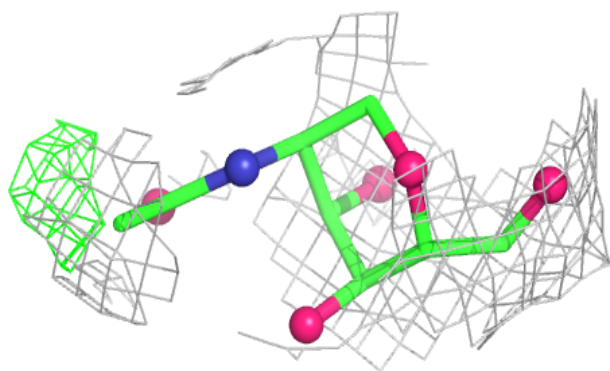
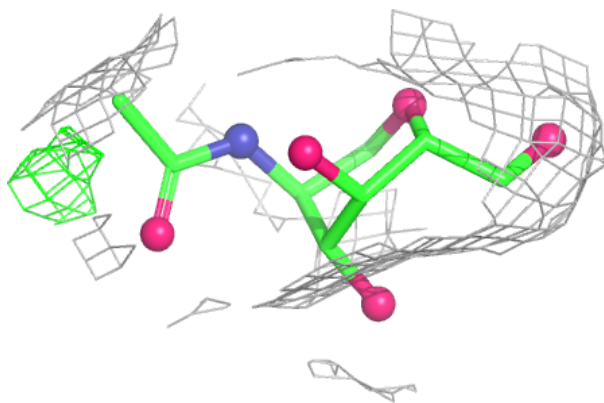
**Electron density around NAG I 409:**

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

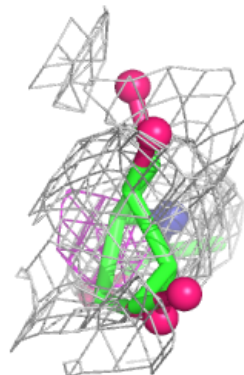
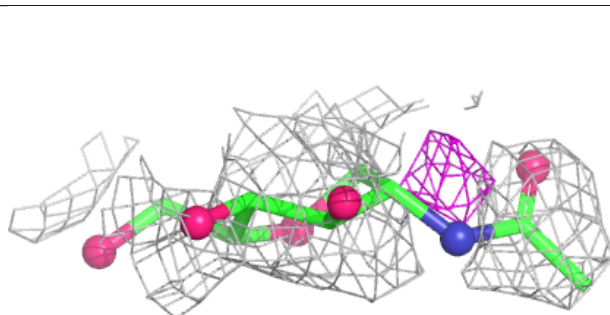
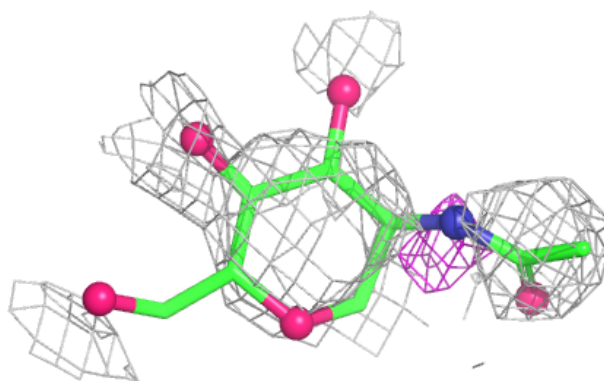


Electron density around NAG G 402:

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

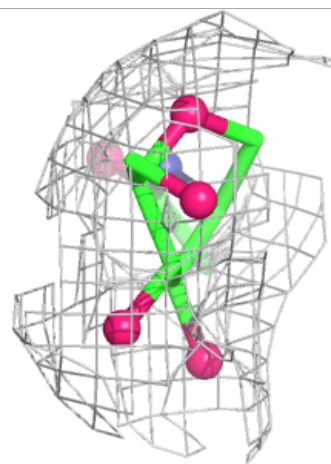
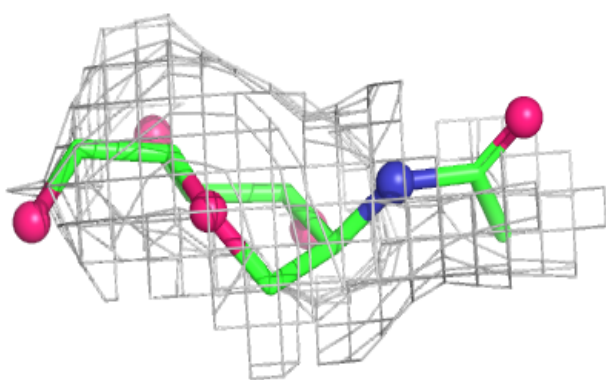
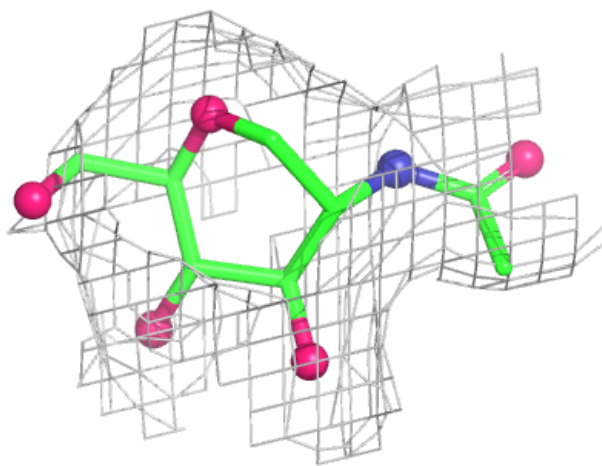
**Electron density around NAG A 412:**

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



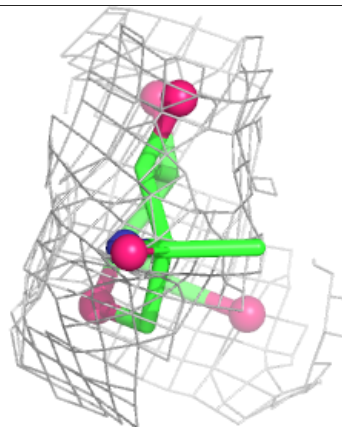
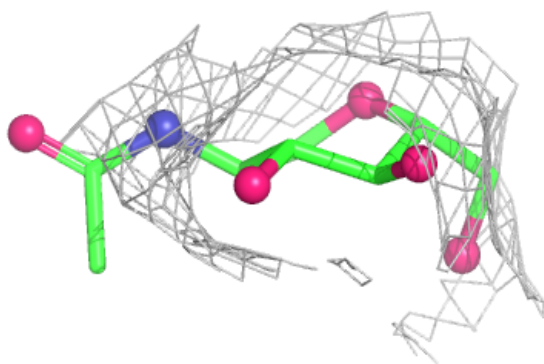
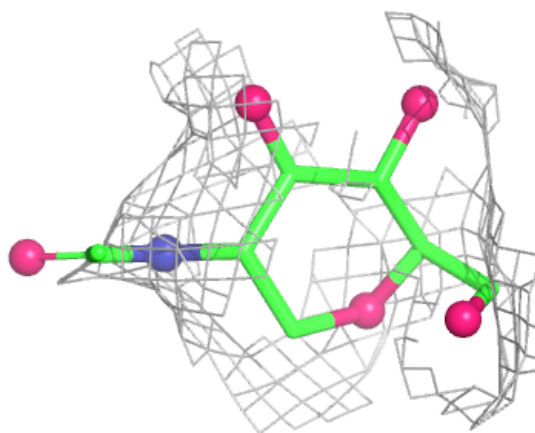
Electron density around NAG A 413:

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

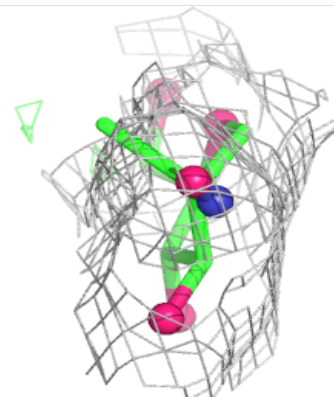
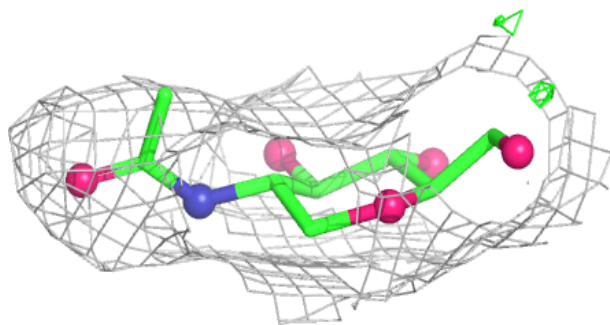
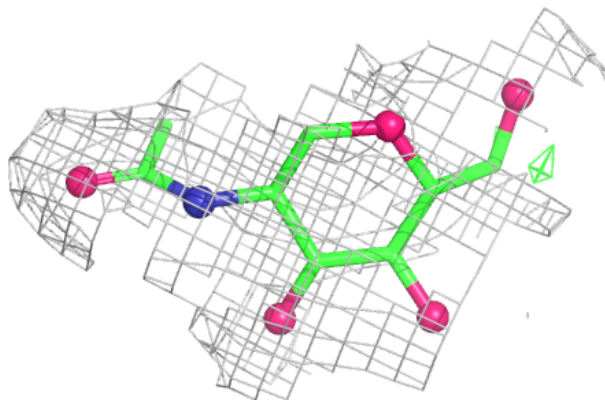


Electron density around NAG K 414:

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

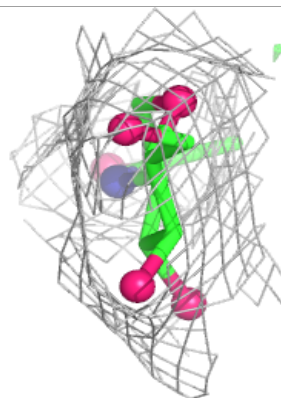
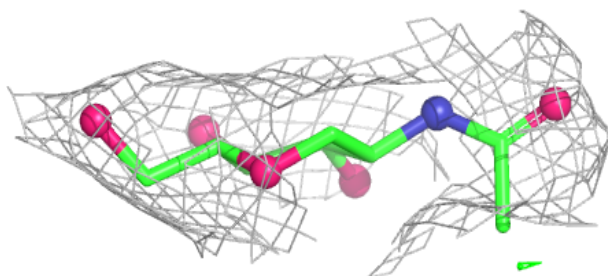
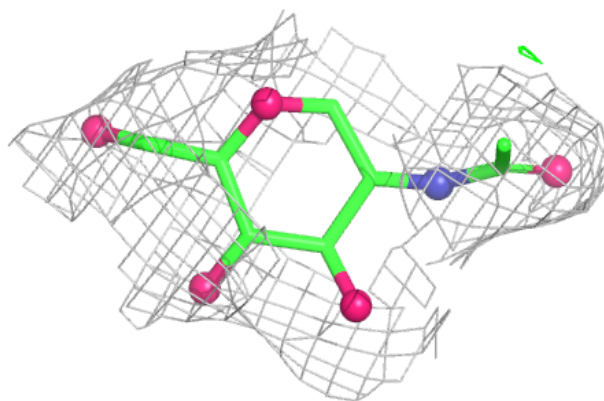
**Electron density around NAG G 401:**

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

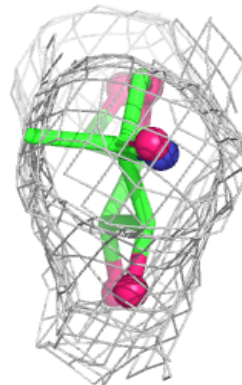
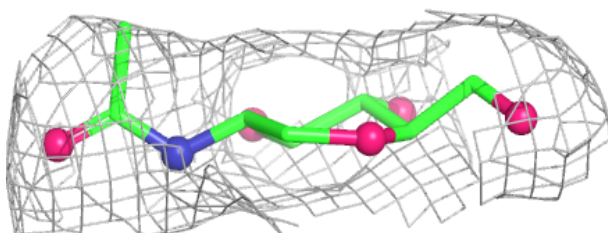
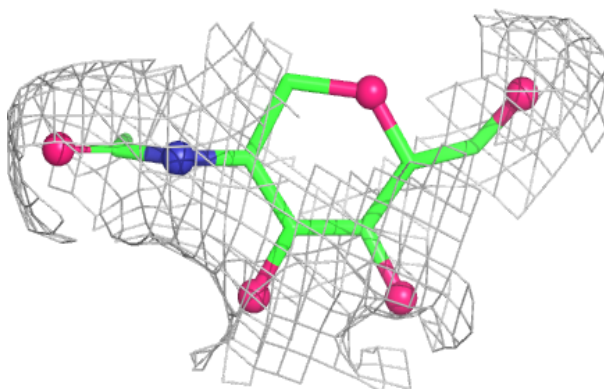


Electron density around NAG A 414:

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

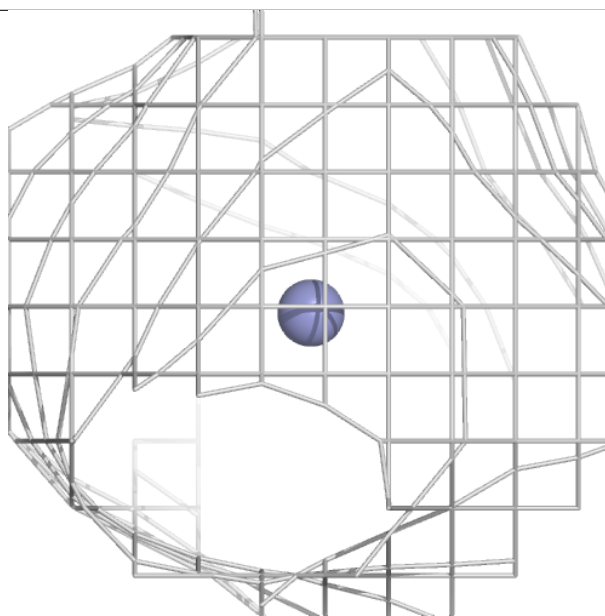
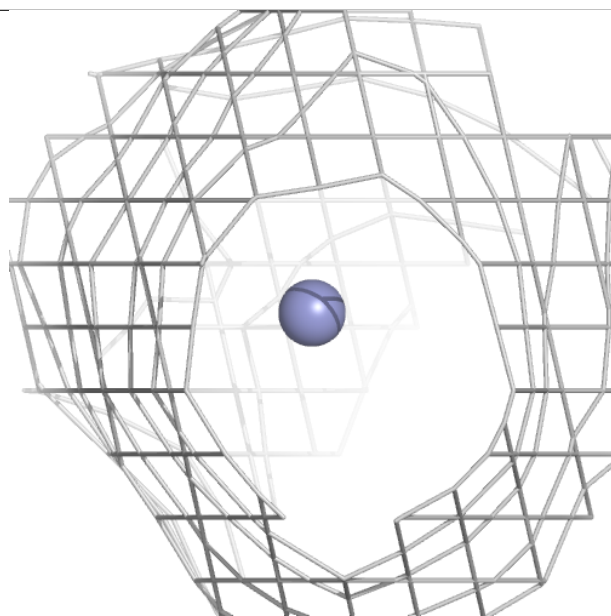
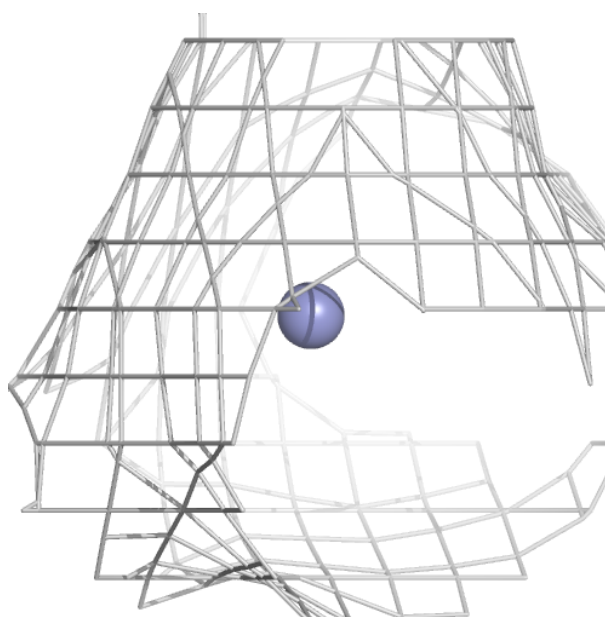
**Electron density around NAG G 413:**

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



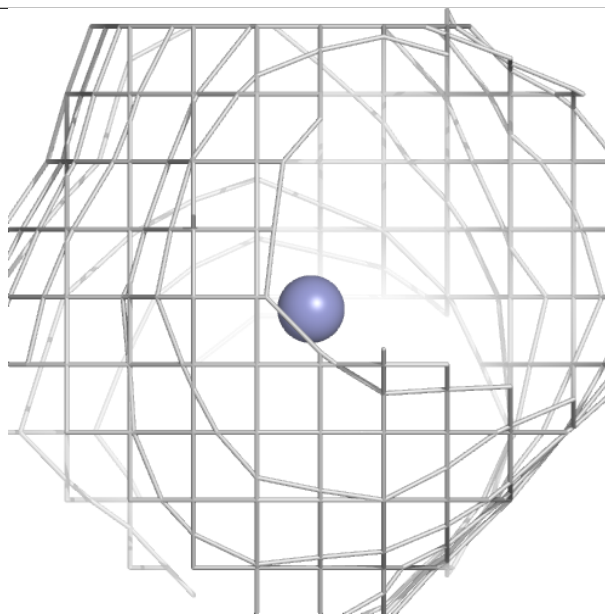
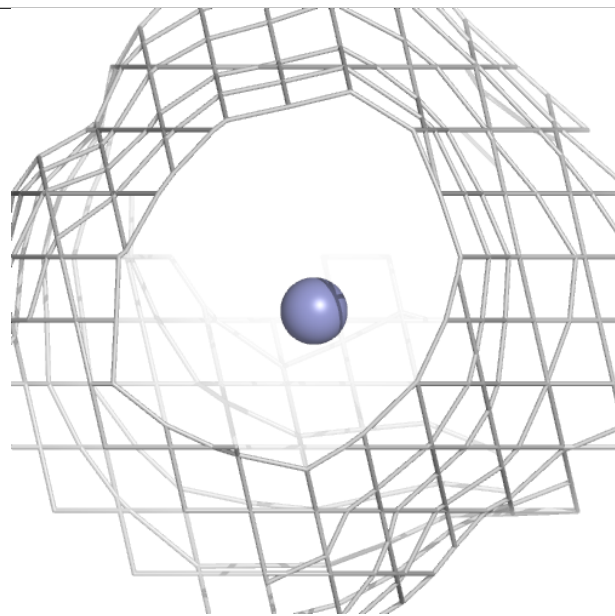
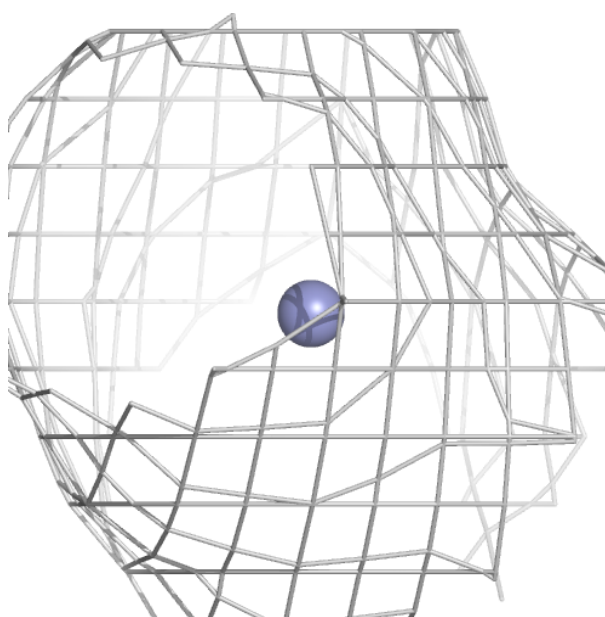
Electron density around ZN K 415:

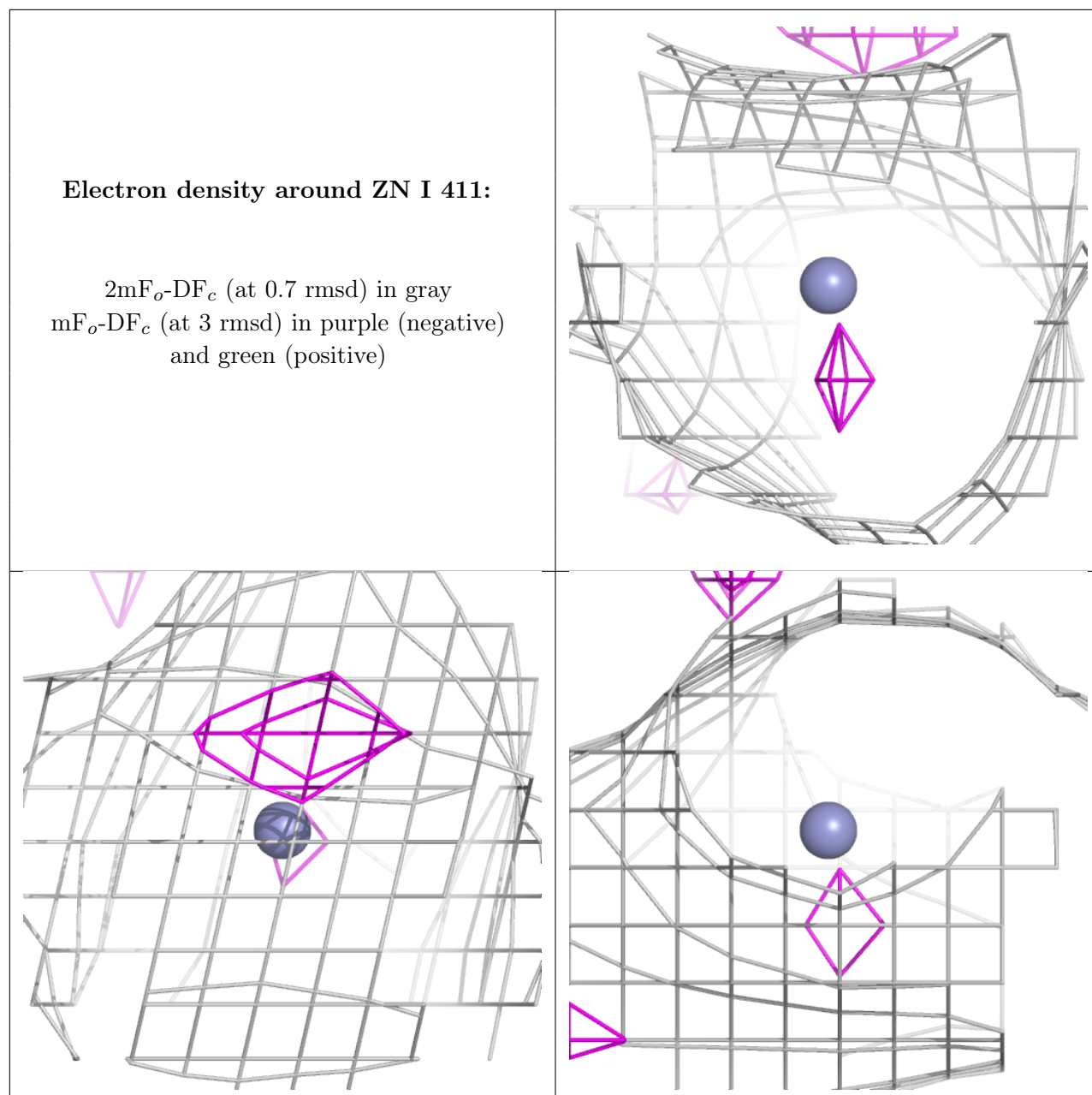
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN G 414:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.