Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 06:49 PM EDT

PDB ID	:	4MHI
Title	:	Crystal structure of a H5N1 influenza virus hemagglutinin from A/goose/Guangdong/1/96
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-08-29
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

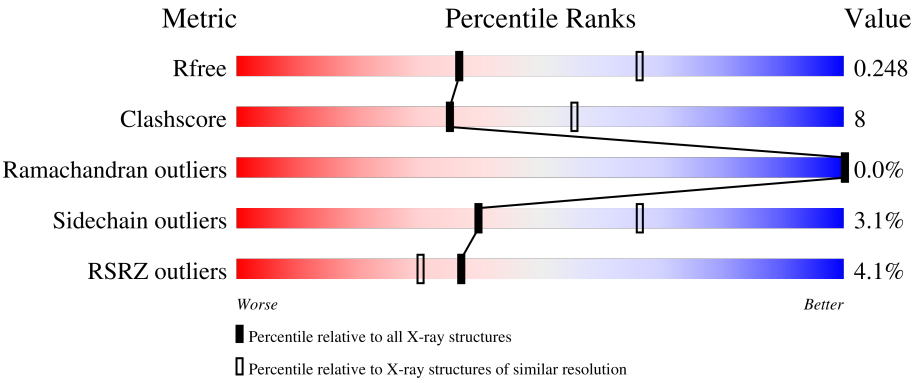
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	334	2% 77% 19%
1	C	334	7% 74% 19%
1	E	334	5% 72% 22%
1	G	334	5% 75% 20%
1	I	334	5% 78% 18%

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Mol	Chain	Length	Quality of chain
1	K	334	4% 72% 23%
1	M	334	8% 75% 20%
1	O	334	5% 76% 20%
1	Q	334	78% 17%
2	B	182	80% 15% 5%
2	D	182	77% 18% 5%
2	F	182	10% 78% 17% 5%
2	H	182	8% 77% 17% 5%
2	J	182	86% 9% 5%
2	L	182	6% 76% 18% 5%
2	N	182	3% 83% 12% 5%
2	P	182	3% 80% 15% 5%
2	R	182	82% 13% 5%
3	S	2	100%
3	T	2	100%
3	U	2	100%
3	V	2	50% 50%
3	W	2	50% 50%
3	X	2	50% 50%
3	Z	2	100%
4	Y	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36134 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	A	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	C	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	E	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	G	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	I	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	K	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	M	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	O	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	Q	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9Q0U6
A	8	ASP	-	expression tag	UNP Q9Q0U6
A	9	PRO	-	expression tag	UNP Q9Q0U6
A	10	GLY	-	expression tag	UNP Q9Q0U6
C	7	ALA	-	expression tag	UNP Q9Q0U6
C	8	ASP	-	expression tag	UNP Q9Q0U6
C	9	PRO	-	expression tag	UNP Q9Q0U6
C	10	GLY	-	expression tag	UNP Q9Q0U6
E	7	ALA	-	expression tag	UNP Q9Q0U6
E	8	ASP	-	expression tag	UNP Q9Q0U6
E	9	PRO	-	expression tag	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	expression tag	UNP Q9Q0U6
G	7	ALA	-	expression tag	UNP Q9Q0U6
G	8	ASP	-	expression tag	UNP Q9Q0U6
G	9	PRO	-	expression tag	UNP Q9Q0U6
G	10	GLY	-	expression tag	UNP Q9Q0U6
I	7	ALA	-	expression tag	UNP Q9Q0U6
I	8	ASP	-	expression tag	UNP Q9Q0U6
I	9	PRO	-	expression tag	UNP Q9Q0U6
I	10	GLY	-	expression tag	UNP Q9Q0U6
K	7	ALA	-	expression tag	UNP Q9Q0U6
K	8	ASP	-	expression tag	UNP Q9Q0U6
K	9	PRO	-	expression tag	UNP Q9Q0U6
K	10	GLY	-	expression tag	UNP Q9Q0U6
M	7	ALA	-	expression tag	UNP Q9Q0U6
M	8	ASP	-	expression tag	UNP Q9Q0U6
M	9	PRO	-	expression tag	UNP Q9Q0U6
M	10	GLY	-	expression tag	UNP Q9Q0U6
O	7	ALA	-	expression tag	UNP Q9Q0U6
O	8	ASP	-	expression tag	UNP Q9Q0U6
O	9	PRO	-	expression tag	UNP Q9Q0U6
O	10	GLY	-	expression tag	UNP Q9Q0U6
Q	7	ALA	-	expression tag	UNP Q9Q0U6
Q	8	ASP	-	expression tag	UNP Q9Q0U6
Q	9	PRO	-	expression tag	UNP Q9Q0U6
Q	10	GLY	-	expression tag	UNP Q9Q0U6

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	D	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	F	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	H	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	J	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	L	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	N	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	R	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	-	expression tag	UNP Q9Q0U6
B	177	GLY	-	expression tag	UNP Q9Q0U6
B	178	ARG	-	expression tag	UNP Q9Q0U6
B	179	LEU	-	expression tag	UNP Q9Q0U6
B	180	VAL	-	expression tag	UNP Q9Q0U6
B	181	PRO	-	expression tag	UNP Q9Q0U6
B	182	ARG	-	expression tag	UNP Q9Q0U6
D	176	SER	-	expression tag	UNP Q9Q0U6
D	177	GLY	-	expression tag	UNP Q9Q0U6
D	178	ARG	-	expression tag	UNP Q9Q0U6
D	179	LEU	-	expression tag	UNP Q9Q0U6
D	180	VAL	-	expression tag	UNP Q9Q0U6
D	181	PRO	-	expression tag	UNP Q9Q0U6
D	182	ARG	-	expression tag	UNP Q9Q0U6
F	176	SER	-	expression tag	UNP Q9Q0U6
F	177	GLY	-	expression tag	UNP Q9Q0U6
F	178	ARG	-	expression tag	UNP Q9Q0U6
F	179	LEU	-	expression tag	UNP Q9Q0U6
F	180	VAL	-	expression tag	UNP Q9Q0U6
F	181	PRO	-	expression tag	UNP Q9Q0U6
F	182	ARG	-	expression tag	UNP Q9Q0U6
H	176	SER	-	expression tag	UNP Q9Q0U6
H	177	GLY	-	expression tag	UNP Q9Q0U6
H	178	ARG	-	expression tag	UNP Q9Q0U6
H	179	LEU	-	expression tag	UNP Q9Q0U6
H	180	VAL	-	expression tag	UNP Q9Q0U6
H	181	PRO	-	expression tag	UNP Q9Q0U6
H	182	ARG	-	expression tag	UNP Q9Q0U6
J	176	SER	-	expression tag	UNP Q9Q0U6
J	177	GLY	-	expression tag	UNP Q9Q0U6
J	178	ARG	-	expression tag	UNP Q9Q0U6
J	179	LEU	-	expression tag	UNP Q9Q0U6
J	180	VAL	-	expression tag	UNP Q9Q0U6
J	181	PRO	-	expression tag	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	182	ARG	-	expression tag	UNP Q9Q0U6
L	176	SER	-	expression tag	UNP Q9Q0U6
L	177	GLY	-	expression tag	UNP Q9Q0U6
L	178	ARG	-	expression tag	UNP Q9Q0U6
L	179	LEU	-	expression tag	UNP Q9Q0U6
L	180	VAL	-	expression tag	UNP Q9Q0U6
L	181	PRO	-	expression tag	UNP Q9Q0U6
L	182	ARG	-	expression tag	UNP Q9Q0U6
N	176	SER	-	expression tag	UNP Q9Q0U6
N	177	GLY	-	expression tag	UNP Q9Q0U6
N	178	ARG	-	expression tag	UNP Q9Q0U6
N	179	LEU	-	expression tag	UNP Q9Q0U6
N	180	VAL	-	expression tag	UNP Q9Q0U6
N	181	PRO	-	expression tag	UNP Q9Q0U6
N	182	ARG	-	expression tag	UNP Q9Q0U6
P	176	SER	-	expression tag	UNP Q9Q0U6
P	177	GLY	-	expression tag	UNP Q9Q0U6
P	178	ARG	-	expression tag	UNP Q9Q0U6
P	179	LEU	-	expression tag	UNP Q9Q0U6
P	180	VAL	-	expression tag	UNP Q9Q0U6
P	181	PRO	-	expression tag	UNP Q9Q0U6
P	182	ARG	-	expression tag	UNP Q9Q0U6
R	176	SER	-	expression tag	UNP Q9Q0U6
R	177	GLY	-	expression tag	UNP Q9Q0U6
R	178	ARG	-	expression tag	UNP Q9Q0U6
R	179	LEU	-	expression tag	UNP Q9Q0U6
R	180	VAL	-	expression tag	UNP Q9Q0U6
R	181	PRO	-	expression tag	UNP Q9Q0U6
R	182	ARG	-	expression tag	UNP Q9Q0U6

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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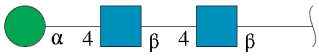
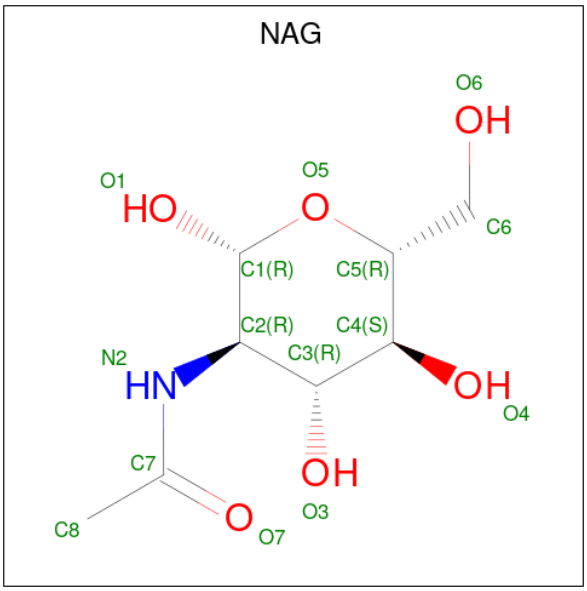
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	U	2	Total C N O 28 16 2 10	0	0	0
3	V	2	Total C N O 28 16 2 10	0	0	0
3	W	2	Total C N O 28 16 2 10	0	0	0
3	X	2	Total C N O 28 16 2 10	0	0	0
3	Z	2	Total C N O 28 16 2 10	0	0	0

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	5	Total O 5 5	0	0
6	C	6	Total O 6 6	0	0
6	D	8	Total O 8 8	0	0
6	E	6	Total O 6 6	0	0
6	F	2	Total O 2 2	0	0

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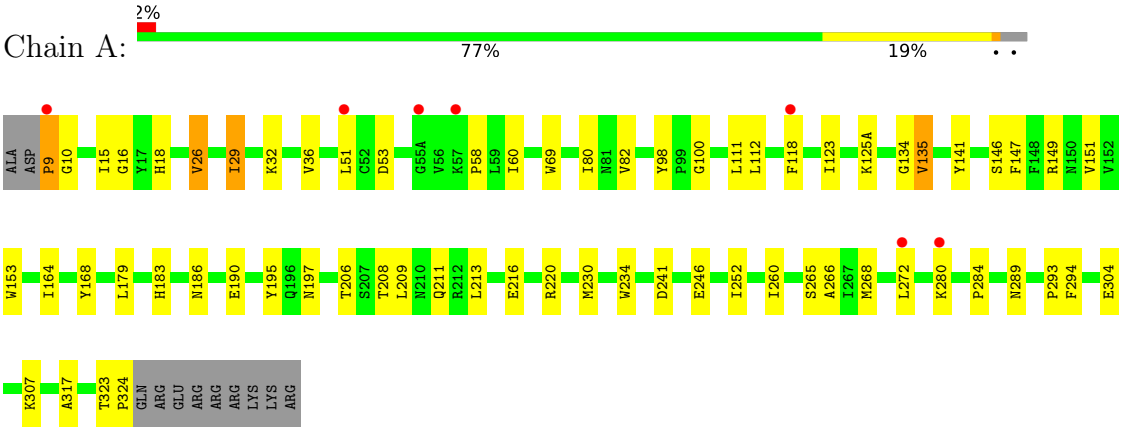
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	14	Total O 14 14	0	0
6	H	4	Total O 4 4	0	0
6	I	9	Total O 9 9	0	0
6	J	12	Total O 12 12	0	0
6	K	10	Total O 10 10	0	0
6	L	2	Total O 2 2	0	0
6	M	5	Total O 5 5	0	0
6	N	1	Total O 1 1	0	0
6	O	8	Total O 8 8	0	0
6	P	2	Total O 2 2	0	0
6	Q	8	Total O 8 8	0	0
6	R	8	Total O 8 8	0	0

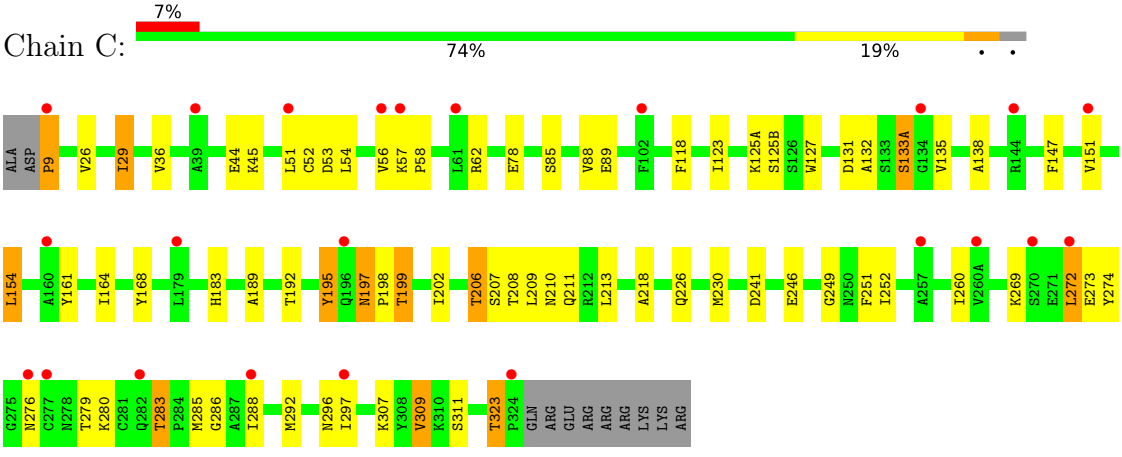
3 Residue-property plots (i)

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

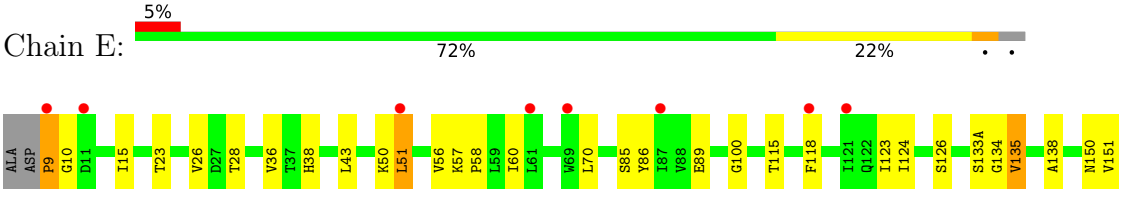
• Molecule 1: Hemagglutinin HA1 chain

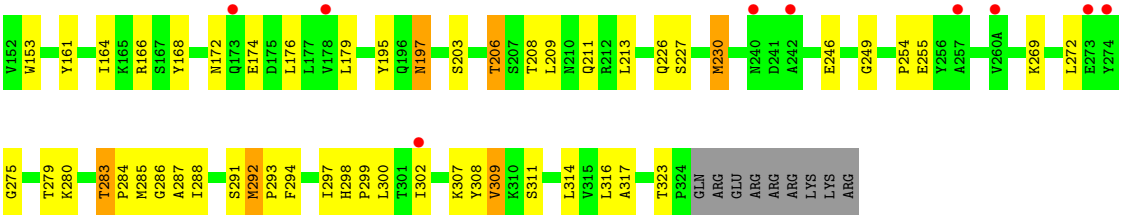


• Molecule 1: Hemagglutinin HA1 chain

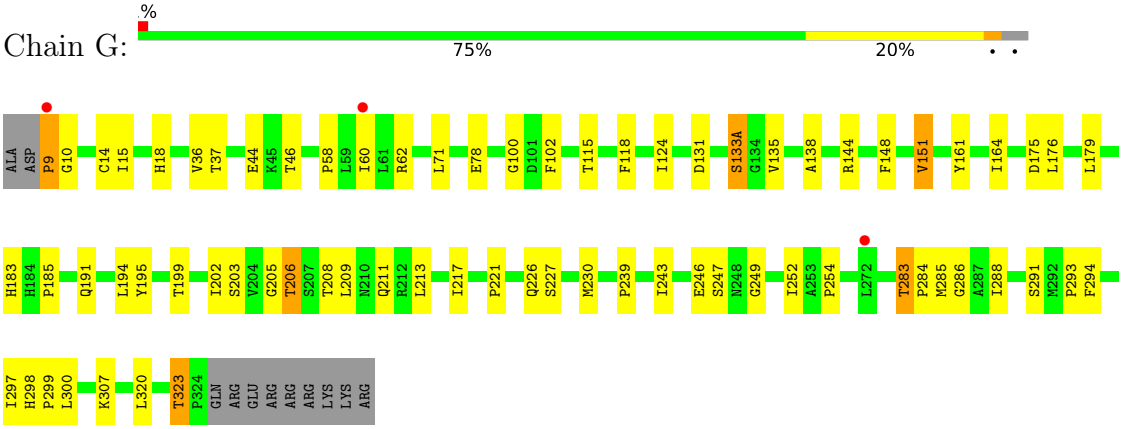


• Molecule 1: Hemagglutinin HA1 chain

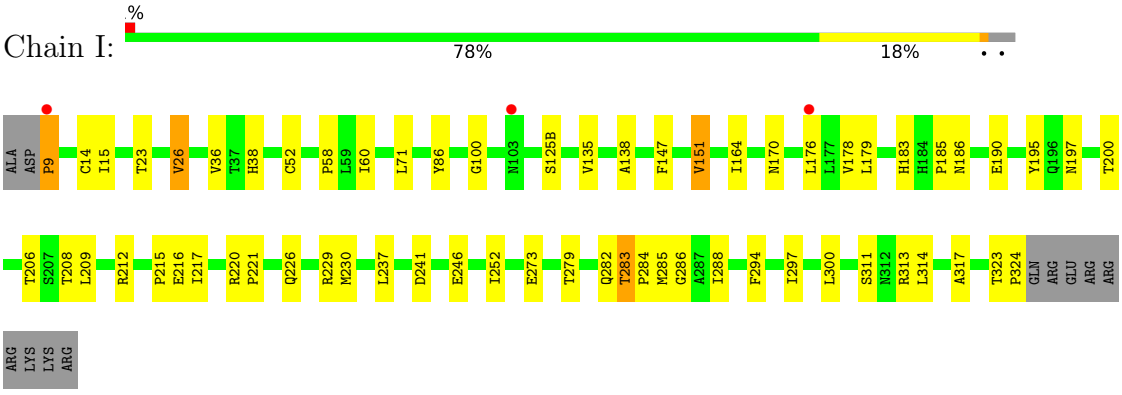




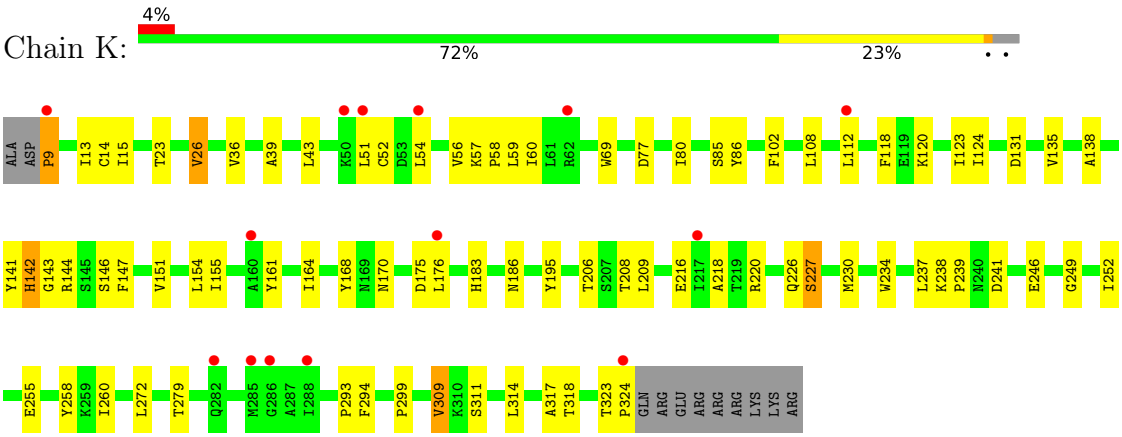
• Molecule 1: Hemagglutinin HA1 chain



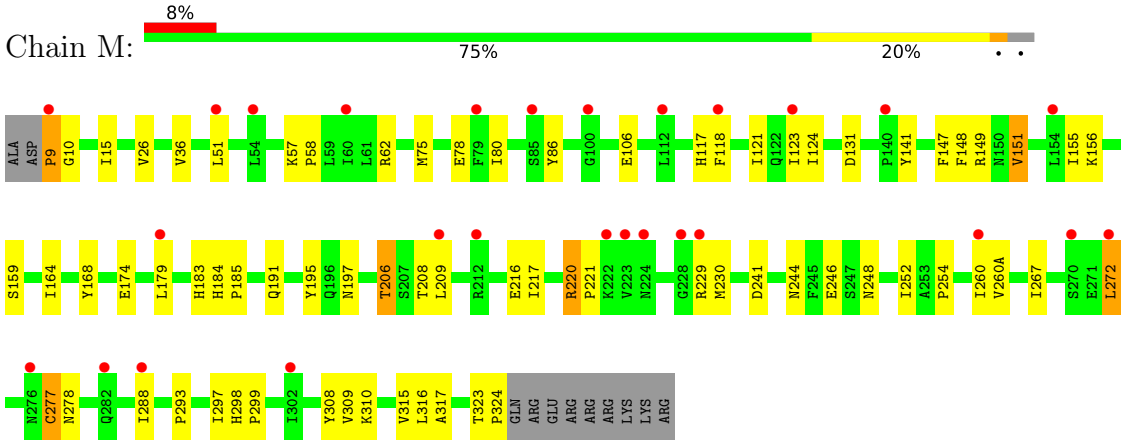
• Molecule 1: Hemagglutinin HA1 chain



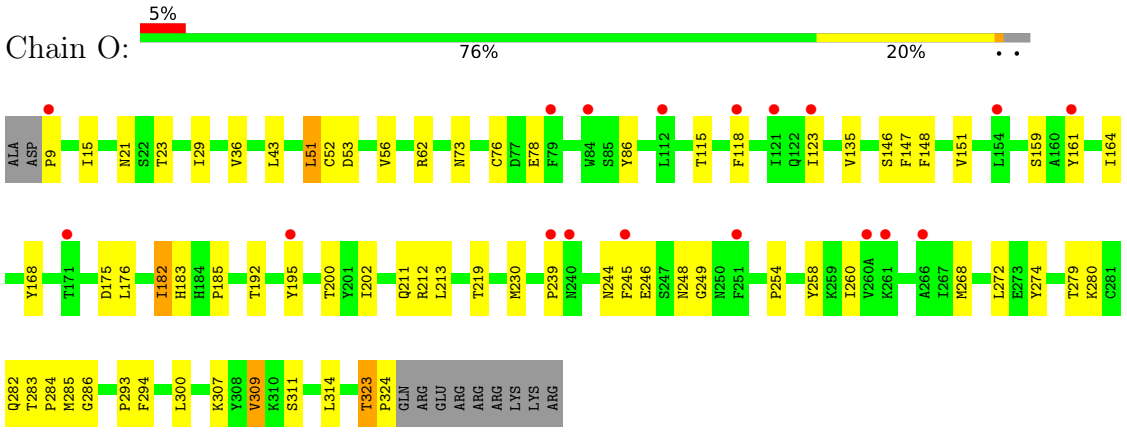
• Molecule 1: Hemagglutinin HA1 chain



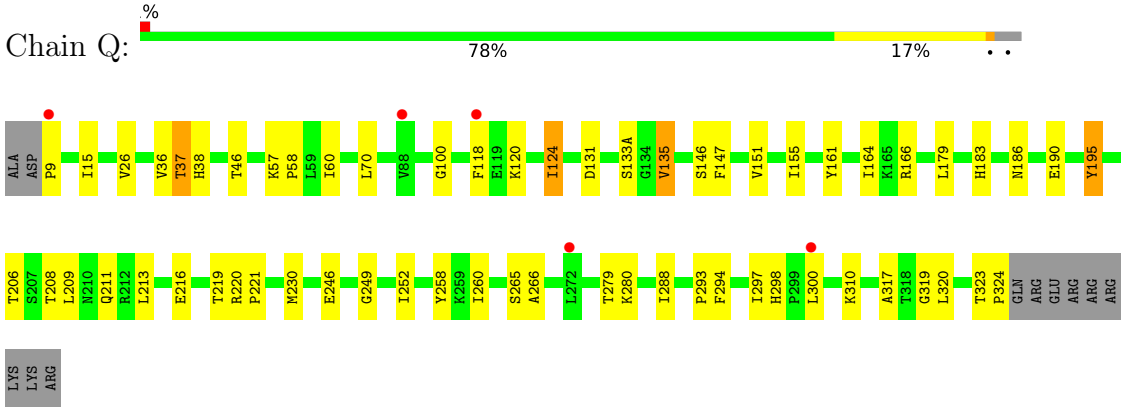
• Molecule 1: Hemagglutinin HA1 chain



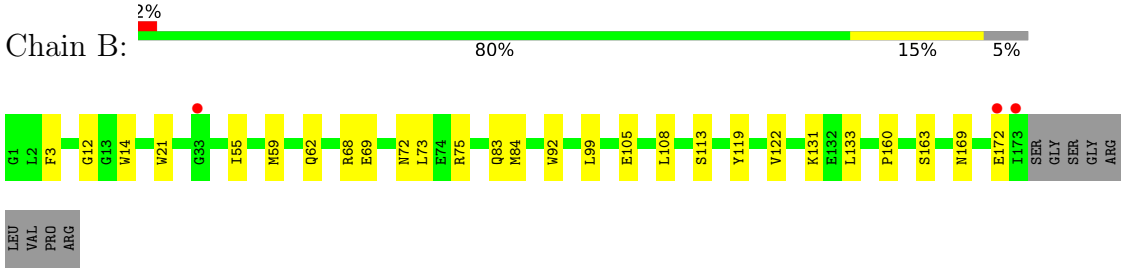
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

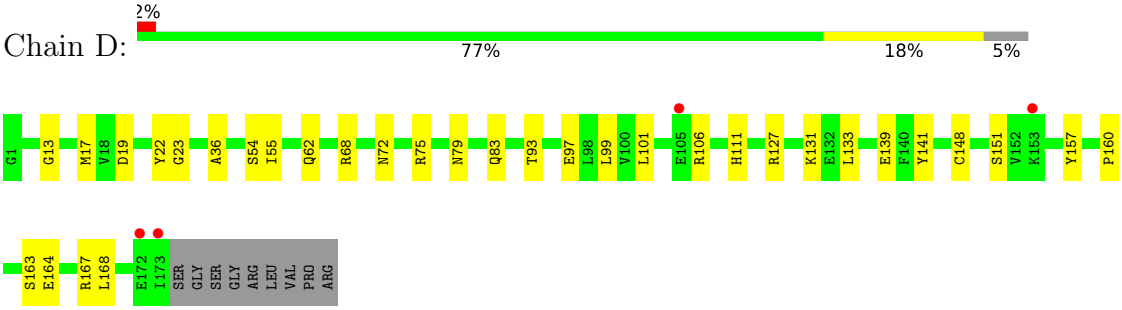


• Molecule 2: Hemagglutinin HA2 chain



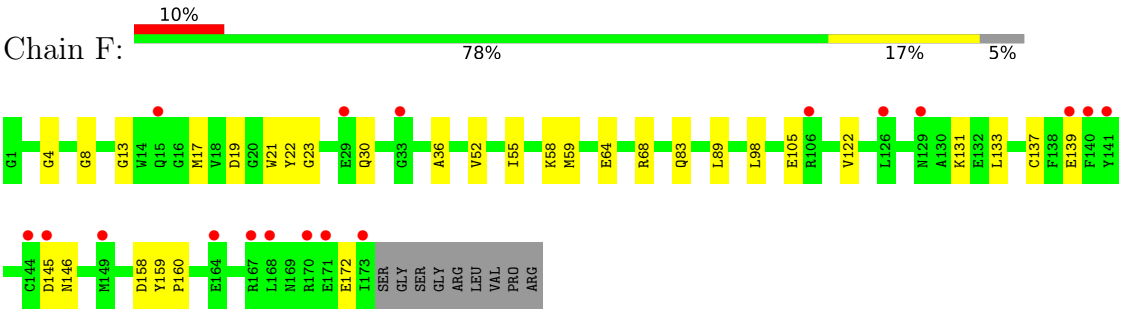
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



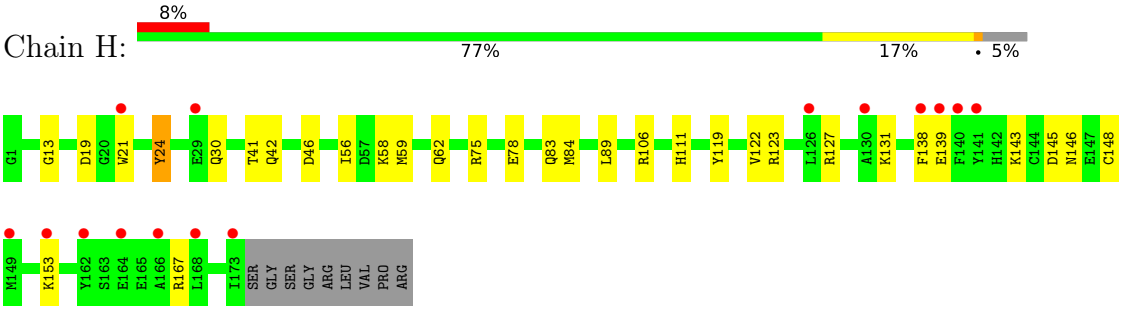
• Molecule 2: Hemagglutinin HA2 chain

Chain F:



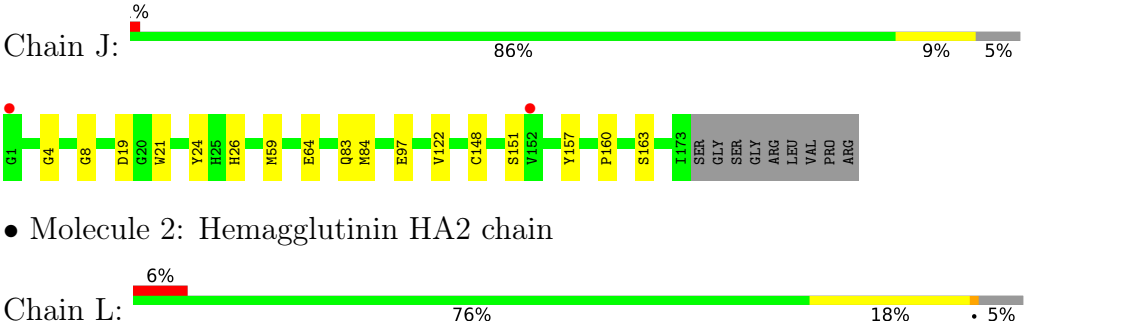
• Molecule 2: Hemagglutinin HA2 chain

Chain H:



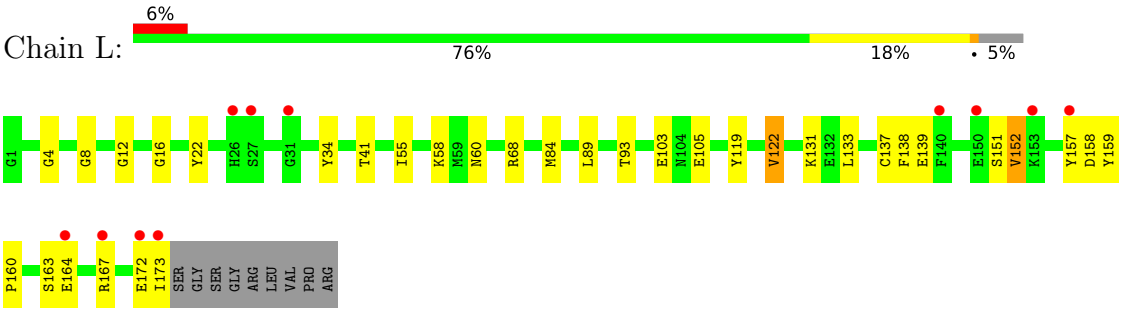
• Molecule 2: Hemagglutinin HA2 chain

Chain J:



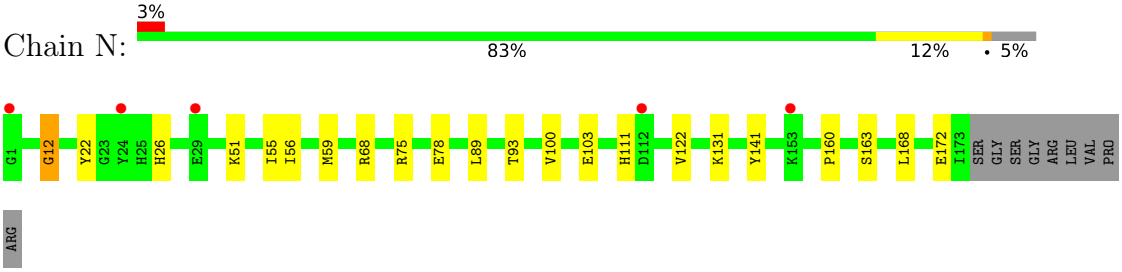
• Molecule 2: Hemagglutinin HA2 chain

Chain L:



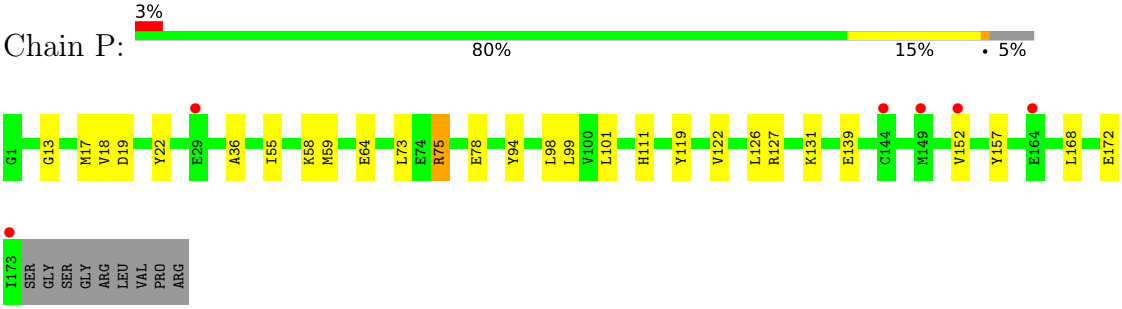
• Molecule 2: Hemagglutinin HA2 chain

Chain N:



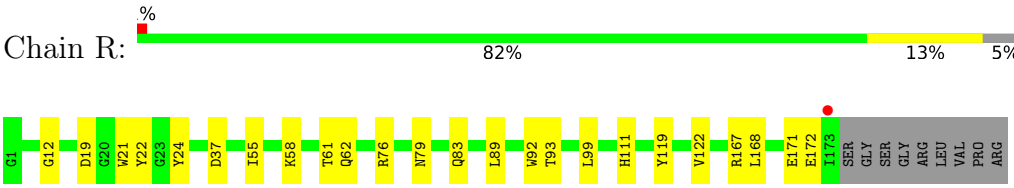
• Molecule 2: Hemagglutinin HA2 chain

Chain P:



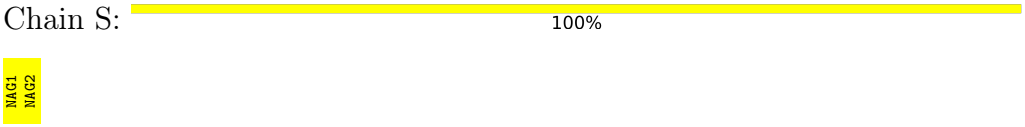
• Molecule 2: Hemagglutinin HA2 chain

Chain R:



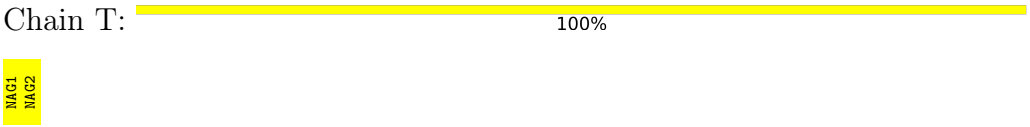
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



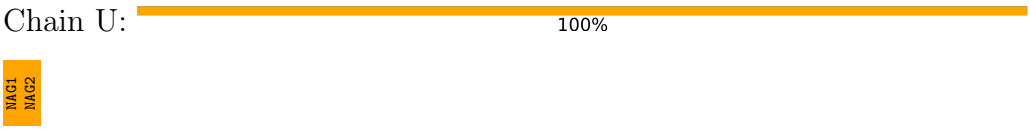
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain U:



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

Chain V:

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

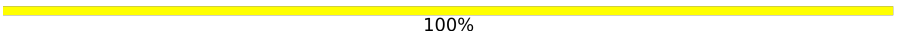
Chain W:

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

Chain X:

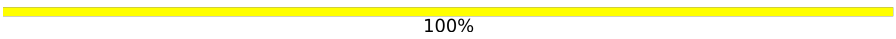
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.48Å 225.73Å 211.63Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	49.66 – 2.60 49.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.66-2.60) 95.1 (49.66-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.189 , 0.243 0.199 , 0.248	Depositor DCC
R_{free} test set	9880 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36134	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.26 % 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 2.7239e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	0/2616	0.67	1/3557 (0.0%)
1	C	0.44	0/2616	0.66	2/3557 (0.1%)
1	E	0.44	0/2616	0.65	2/3557 (0.1%)
1	G	0.46	0/2616	0.66	2/3557 (0.1%)
1	I	0.49	0/2616	0.70	1/3557 (0.0%)
1	K	0.44	0/2616	0.64	1/3557 (0.0%)
1	M	0.40	0/2616	0.62	2/3557 (0.1%)
1	O	0.42	0/2616	0.64	1/3557 (0.0%)
1	Q	0.46	0/2616	0.67	1/3557 (0.0%)
2	B	0.49	0/1430	0.65	0/1924
2	D	0.46	0/1430	0.58	0/1924
2	F	0.47	0/1430	0.60	0/1924
2	H	0.47	0/1430	0.60	0/1924
2	J	0.47	0/1430	0.61	0/1924
2	L	0.45	0/1430	0.55	0/1924
2	N	0.43	0/1430	0.59	0/1924
2	P	0.46	0/1430	0.60	0/1924
2	R	0.49	0/1430	0.62	0/1924
All	All	0.45	0/36414	0.64	13/49329 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	9	PRO	CA-N-CD	-8.94	98.98	111.50
1	C	9	PRO	CA-N-CD	-8.81	99.17	111.50
1	O	9	PRO	CA-N-CD	-8.72	99.29	111.50
1	G	9	PRO	CA-N-CD	-8.66	99.38	111.50
1	K	9	PRO	CA-N-CD	-8.51	99.59	111.50
1	A	9	PRO	CA-N-CD	-8.45	99.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	9	PRO	CA-N-CD	-8.45	99.67	111.50
1	E	9	PRO	CA-N-CD	-8.43	99.70	111.50
1	Q	9	PRO	CA-N-CD	-8.15	100.09	111.50
1	G	176	LEU	CA-CB-CG	5.97	129.03	115.30
1	E	176	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	272	LEU	CA-CB-CG	5.02	126.85	115.30
1	M	272	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2551	0	2476	45	0
1	C	2551	0	2476	55	0
1	E	2551	0	2474	54	0
1	G	2551	0	2476	54	0
1	I	2551	0	2476	49	0
1	K	2551	0	2475	58	0
1	M	2551	0	2475	60	0
1	O	2551	0	2476	48	0
1	Q	2551	0	2476	43	0
2	B	1403	0	1302	22	0
2	D	1403	0	1302	24	0
2	F	1403	0	1302	24	0
2	H	1403	0	1302	31	0
2	J	1403	0	1302	13	0
2	L	1403	0	1302	24	0
2	N	1403	0	1302	21	0
2	P	1403	0	1302	22	0
2	R	1403	0	1301	23	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	3	0
3	V	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	28	0	25	1	0
3	X	28	0	25	1	0
3	Z	28	0	25	0	0
4	Y	39	0	34	0	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	28	0	26	0	0
5	G	28	0	26	0	0
5	I	14	0	13	0	0
5	K	28	0	26	3	0
5	M	28	0	26	0	0
5	O	28	0	26	0	0
5	Q	14	0	13	0	0
6	A	7	0	0	1	0
6	B	5	0	0	0	0
6	C	6	0	0	0	0
6	D	8	0	0	0	0
6	E	6	0	0	0	0
6	F	2	0	0	0	0
6	G	14	0	0	0	0
6	H	4	0	0	0	0
6	I	9	0	0	0	0
6	J	12	0	0	0	0
6	K	10	0	0	3	0
6	L	2	0	0	0	0
6	M	5	0	0	0	0
6	N	1	0	0	0	0
6	O	8	0	0	1	0
6	P	2	0	0	0	0
6	Q	8	0	0	0	0
6	R	8	0	0	0	0
All	All	36134	0	34388	578	0

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

All (578) 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:M:9:PRO:HD2	1:M:10:GLY:H	1.17	1.07
1:E:9:PRO:HD2	1:E:10:GLY:H	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HD2	1:A:10:GLY:H	1.23	0.99
1:I:170:ASN:CG	1:I:176:LEU:HD23	1.85	0.97
1:I:170:ASN:ND2	1:I:176:LEU:HD23	1.81	0.96
1:I:206:THR:HG22	1:I:208:THR:H	1.31	0.91
1:M:9:PRO:HD2	1:M:10:GLY:N	1.86	0.90
1:K:206:THR:HG22	1:K:208:THR:H	1.38	0.89
1:E:9:PRO:HD2	1:E:10:GLY:N	1.88	0.86
1:Q:206:THR:HG22	1:Q:208:THR:H	1.40	0.84
1:A:9:PRO:HD2	1:A:10:GLY:N	1.91	0.84
2:N:131:LYS:NZ	2:P:127:ARG:HD2	1.93	0.84
1:G:323:THR:HG21	2:H:13:GLY:H	1.43	0.83
1:C:206:THR:HG22	1:C:209:LEU:H	1.44	0.83
1:M:206:THR:HG22	1:M:208:THR:H	1.44	0.82
1:O:323:THR:HG21	2:P:13:GLY:H	1.44	0.81
1:Q:206:THR:HB	1:Q:209:LEU:HB3	1.62	0.81
1:E:323:THR:HG21	2:F:13:GLY:H	1.43	0.81
1:M:323:THR:HG21	2:N:12:GLY:HA2	1.62	0.81
1:M:9:PRO:CD	1:M:10:GLY:H	1.94	0.80
1:C:56:VAL:HG23	1:C:85:SER:HB3	1.64	0.80
1:K:123:ILE:HD11	1:K:168:TYR:CE1	2.16	0.79
1:E:206:THR:HG22	1:E:209:LEU:H	1.48	0.79
1:O:283:THR:HG22	1:O:285:MET:H	1.49	0.78
1:A:206:THR:HB	1:A:209:LEU:HB3	1.66	0.78
1:M:310:LYS:H	2:N:93:THR:HG21	1.50	0.77
1:A:206:THR:HG22	1:A:208:THR:H	1.50	0.76
1:E:51:LEU:HD13	1:E:272:LEU:HD11	1.66	0.76
1:E:56:VAL:HG23	1:E:85:SER:HB3	1.66	0.76
1:A:118:PHE:HE1	1:A:260:ILE:HD13	1.49	0.75
1:K:56:VAL:HG23	1:K:85:SER:HB3	1.67	0.75
1:G:206:THR:HG22	1:G:208:THR:H	1.51	0.74
1:E:9:PRO:CD	1:E:10:GLY:H	1.98	0.74
1:M:147:PHE:HZ	1:M:230:MET:HE1	1.53	0.74
1:Q:310:LYS:H	2:R:93:THR:CG2	2.01	0.74
2:F:145:ASP:OD1	2:F:146:ASN:N	2.20	0.73
1:G:9:PRO:HD2	1:G:10:GLY:N	2.04	0.73
1:C:206:THR:HG22	1:C:208:THR:H	1.54	0.72
1:A:216:GLU:O	1:A:220:ARG:NH2	2.21	0.72
1:A:9:PRO:CD	1:A:10:GLY:H	2.02	0.72
1:Q:147:PHE:HZ	1:Q:230:MET:HE1	1.56	0.71
1:C:57:LYS:HD2	1:C:58:PRO:HD2	1.72	0.70
1:O:307:LYS:NZ	2:P:64:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:PRO:CD	1:M:10:GLY:N	2.53	0.70
1:M:123:ILE:HD11	1:M:168:TYR:CZ	2.27	0.70
1:E:206:THR:HG22	1:E:208:THR:H	1.57	0.69
1:A:307:LYS:HD3	2:B:59:MET:O	1.93	0.68
1:G:206:THR:HG22	1:G:209:LEU:H	1.58	0.68
1:G:62:ARG:NH1	1:G:78:GLU:OE1	2.27	0.68
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.73	0.68
1:O:283:THR:HB	1:O:286:GLY:O	1.93	0.68
1:Q:221:PRO:HB3	3:X:1:NAG:H81	1.76	0.68
1:A:118:PHE:CE1	1:A:260:ILE:HD13	2.28	0.68
1:G:283:THR:HG22	1:G:285:MET:H	1.57	0.68
2:D:164:GLU:OE2	2:D:167:ARG:NH2	2.21	0.67
1:Q:58:PRO:HG2	1:Q:60:ILE:HD11	1.75	0.67
1:Q:131:ASP:HB3	1:Q:155:ILE:HG13	1.74	0.67
2:N:131:LYS:HZ1	2:P:127:ARG:HD2	1.56	0.67
1:I:283:THR:HG22	1:I:285:MET:H	1.58	0.67
1:I:176:LEU:CD1	1:I:178:VAL:HG22	2.25	0.67
1:O:323:THR:HG21	2:P:13:GLY:N	2.09	0.66
2:L:164:GLU:OE2	2:L:167:ARG:NH2	2.22	0.66
1:E:9:PRO:CD	1:E:10:GLY:N	2.55	0.66
1:G:206:THR:HB	1:G:209:LEU:HB3	1.76	0.66
1:I:206:THR:HB	1:I:209:LEU:HB3	1.76	0.66
1:G:9:PRO:HD2	1:G:10:GLY:H	1.60	0.66
1:K:206:THR:HB	1:K:209:LEU:HB3	1.78	0.66
1:I:170:ASN:CG	1:I:176:LEU:CD2	2.63	0.66
1:G:115:THR:HG21	1:G:118:PHE:CE1	2.31	0.65
1:Q:186:ASN:ND2	1:Q:190:GLU:OE1	2.23	0.65
1:M:310:LYS:H	2:N:93:THR:CG2	2.10	0.65
1:Q:15:ILE:HD11	2:R:122:VAL:HG21	1.77	0.65
1:I:15:ILE:HD11	2:J:122:VAL:HG21	1.77	0.64
1:Q:310:LYS:H	2:R:93:THR:HG21	1.61	0.64
1:C:125(A):LYS:NZ	1:C:132:ALA:O	2.21	0.64
1:K:15:ILE:HD11	2:L:122:VAL:HG11	1.78	0.64
1:G:9:PRO:CD	2:H:139:GLU:OE2	2.46	0.64
1:I:230:MET:HE1	1:I:252:ILE:HG12	1.79	0.64
1:I:185:PRO:HD2	1:I:217:ILE:HD13	1.80	0.63
1:O:51:LEU:HD13	1:O:272:LEU:HD11	1.80	0.63
1:A:123:ILE:HD11	1:A:168:TYR:CZ	2.33	0.63
1:E:307:LYS:NZ	2:F:64:GLU:OE2	2.32	0.63
1:M:277:CYS:SG	1:M:278:ASN:N	2.72	0.63
1:A:9:PRO:CD	1:A:10:GLY:N	2.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:151:SER:OG	2:J:157:TYR:HA	1.99	0.62
1:K:43:LEU:HB2	1:K:314:LEU:HB2	1.81	0.62
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.81	0.62
1:O:123:ILE:HD11	1:O:168:TYR:CZ	2.33	0.62
2:H:106:ARG:HH22	2:L:105:GLU:HG2	1.65	0.62
1:M:288:ILE:HD11	1:M:297:ILE:HD11	1.82	0.62
1:C:323:THR:HG21	2:D:13:GLY:H	1.65	0.61
1:E:57:LYS:HD2	1:E:58:PRO:HD2	1.82	0.61
1:K:123:ILE:HD11	1:K:168:TYR:CZ	2.35	0.61
1:K:147:PHE:HZ	1:K:230:MET:HE1	1.66	0.61
1:I:38:HIS:HD2	2:J:21:TRP:HE1	1.48	0.61
1:M:57:LYS:HD2	1:M:58:PRO:HD2	1.83	0.60
1:A:293:PRO:HG2	1:A:294:PHE:HD1	1.66	0.60
2:D:133:LEU:HD11	2:D:139:GLU:HB2	1.82	0.60
1:I:176:LEU:CD1	1:I:178:VAL:CG2	2.79	0.60
1:K:309:VAL:HG22	2:L:93:THR:HA	1.84	0.60
1:C:53:ASP:HA	1:C:58:PRO:HD3	1.84	0.59
1:E:50:LYS:HD3	1:E:275:GLY:HA3	1.84	0.59
1:Q:323:THR:HG21	2:R:12:GLY:HA2	1.84	0.59
1:E:58:PRO:HG2	1:E:60:ILE:HD11	1.84	0.59
1:I:186:ASN:ND2	1:I:190:GLU:OE1	2.28	0.59
1:M:220:ARG:HD2	1:M:229:ARG:HG2	1.85	0.59
2:B:83:GLN:OE1	2:D:68:ARG:NH2	2.27	0.59
1:G:71:LEU:HD23	1:G:179:LEU:HD13	1.84	0.59
1:K:9:PRO:HD2	1:K:9:PRO:O	2.02	0.59
2:L:151:SER:OG	2:L:157:TYR:HA	2.03	0.59
1:E:123:ILE:HD11	1:E:168:TYR:CZ	2.38	0.59
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.37	0.58
2:L:16:GLY:HA3	2:L:34:TYR:CE2	2.37	0.58
1:Q:216:GLU:O	1:Q:220:ARG:NH2	2.35	0.58
1:A:268:MET:HG3	1:A:284:PRO:HG3	1.84	0.58
2:D:72:ASN:OD1	2:D:75:ARG:NH2	2.35	0.58
1:I:176:LEU:HD12	1:I:178:VAL:CG2	2.33	0.58
1:Q:38:HIS:HD2	2:R:21:TRP:HE1	1.49	0.58
2:J:148:CYS:O	2:J:151:SER:HB3	2.04	0.58
2:R:168:LEU:O	2:R:172:GLU:HG2	2.04	0.58
1:M:206:THR:HB	1:M:209:LEU:HB3	1.85	0.58
1:Q:37:THR:HG22	1:Q:320:LEU:H	1.69	0.58
1:C:127:TRP:CD2	1:C:154:LEU:HD21	2.39	0.58
1:Q:183:HIS:HB2	1:Q:252:ILE:HD11	1.86	0.57
2:N:131:LYS:HZ3	2:P:127:ARG:HD2	1.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:LYS:NZ	2:D:127:ARG:HH21	2.02	0.57
1:O:15:ILE:HD11	2:P:122:VAL:HG21	1.87	0.57
1:C:206:THR:HB	1:C:209:LEU:HB3	1.85	0.57
1:G:131:ASP:OD2	1:G:133(A):SER:OG	2.23	0.57
2:H:167:ARG:NH1	2:L:173:ILE:O	2.38	0.57
1:Q:310:LYS:H	2:R:93:THR:HG22	1.70	0.57
1:K:118:PHE:HE1	1:K:260:ILE:HG12	1.70	0.57
1:C:118:PHE:CE1	1:C:260:ILE:HD13	2.40	0.57
1:C:151:VAL:HG22	1:C:252:ILE:HG22	1.87	0.57
1:I:9:PRO:HD2	1:I:9:PRO:O	2.04	0.57
1:M:221:PRO:HD3	1:O:244:ASN:ND2	2.19	0.57
2:D:79:ASN:OD1	2:F:68:ARG:NH1	2.37	0.56
1:G:9:PRO:CD	1:G:10:GLY:N	2.68	0.56
1:Q:288:ILE:HD11	1:Q:297:ILE:HG13	1.86	0.56
2:D:55:ILE:HG12	2:D:99:LEU:HD21	1.87	0.56
2:H:131:LYS:HG2	2:H:139:GLU:HB3	1.86	0.56
1:Q:37:THR:CG2	1:Q:320:LEU:H	2.19	0.56
2:R:89:LEU:O	2:R:93:THR:HG23	2.06	0.56
1:C:197:ASN:N	1:C:197:ASN:OD1	2.37	0.56
1:A:15:ILE:HG13	2:B:119:TYR:HA	1.88	0.56
1:I:183:HIS:HB2	1:I:252:ILE:HD11	1.86	0.56
1:M:164:ILE:O	1:M:246:GLU:HA	2.06	0.56
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.36	0.56
1:I:283:THR:CG2	1:I:285:MET:H	2.19	0.56
1:M:117:HIS:HB3	1:M:260(A):VAL:HB	1.86	0.56
2:P:22:TYR:OH	2:P:111:HIS:ND1	2.31	0.56
1:C:131:ASP:OD2	1:C:133(A):SER:OG	2.23	0.55
1:A:293:PRO:HG2	1:A:294:PHE:CD1	2.42	0.55
2:D:83:GLN:OE1	2:F:68:ARG:NH2	2.29	0.55
1:Q:293:PRO:HG2	1:Q:294:PHE:HD1	1.70	0.55
1:C:288:ILE:HD11	1:C:297:ILE:HD11	1.88	0.55
1:E:38:HIS:HD2	2:F:21:TRP:HE1	1.54	0.55
1:M:197:ASN:ND2	1:M:248:ASN:OD1	2.39	0.55
1:C:164:ILE:O	1:C:246:GLU:HA	2.07	0.55
1:A:100:GLY:HA3	1:A:230:MET:O	2.07	0.55
2:F:131:LYS:HG2	2:F:139:GLU:HB3	1.88	0.55
2:H:42:GLN:NE2	2:H:46:ASP:OD1	2.40	0.55
2:N:68:ARG:NH1	2:R:79:ASN:OD1	2.39	0.55
1:O:15:ILE:HG13	2:P:119:TYR:HA	1.88	0.55
1:C:62:ARG:HG2	1:C:273:GLU:OE2	2.07	0.55
1:Q:100:GLY:HA3	1:Q:230:MET:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:GLN:OE1	2:H:146:ASN:N	2.39	0.54
1:I:283:THR:HB	1:I:286:GLY:O	2.07	0.54
1:M:206:THR:HG23	1:M:241:ASP:OD2	2.07	0.54
1:Q:120:LYS:HD3	1:Q:258:TYR:CE1	2.41	0.54
1:M:185:PRO:HG2	1:M:191:GLN:OE1	2.07	0.54
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.88	0.54
1:M:183:HIS:HB2	1:M:252:ILE:HD11	1.89	0.54
2:B:99:LEU:HD13	2:F:98:LEU:HD21	1.90	0.54
1:O:86:TYR:CZ	1:O:282:GLN:HG2	2.43	0.54
1:A:69:TRP:HZ3	1:A:112:LEU:HD21	1.73	0.54
1:I:221:PRO:HB3	3:W:1:NAG:H81	1.90	0.54
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.89	0.54
1:A:186:ASN:ND2	1:A:190:GLU:OE1	2.33	0.53
1:E:206:THR:HB	1:E:209:LEU:HB3	1.90	0.53
1:I:52:CYS:HB2	1:I:279:THR:HG22	1.91	0.53
5:K:2004:NAG:C8	6:K:2110:HOH:O	2.55	0.53
1:K:216:GLU:O	1:K:220:ARG:NH2	2.42	0.53
1:M:156:LYS:HE3	1:M:159:SER:HA	1.91	0.53
2:H:127:ARG:NH2	2:L:131:LYS:HE3	2.23	0.53
2:J:160:PRO:HA	2:J:163:SER:HB2	1.91	0.53
1:K:230:MET:HE1	1:K:252:ILE:HG12	1.90	0.53
1:K:138:ALA:HB2	1:K:226:GLN:HG2	1.91	0.53
1:O:135:VAL:HG22	1:O:146:SER:HA	1.90	0.53
1:A:32:LYS:NZ	2:D:54:SER:OG	2.34	0.53
1:C:118:PHE:HE1	1:C:260:ILE:HD13	1.74	0.53
1:M:230:MET:CE	1:M:252:ILE:HG12	2.39	0.53
1:O:268:MET:HE3	1:O:284:PRO:HA	1.91	0.53
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.90	0.52
1:E:316:LEU:HD13	2:F:52:VAL:HG22	1.90	0.52
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.90	0.52
1:M:293:PRO:HB3	2:N:56:ILE:HG23	1.92	0.52
1:C:51:LEU:HD13	1:C:88:VAL:HG21	1.90	0.52
1:I:176:LEU:HG	1:I:237:LEU:HB3	1.92	0.52
1:G:58:PRO:HG2	1:G:60:ILE:HD11	1.91	0.52
2:H:145:ASP:OD1	2:H:148:CYS:N	2.39	0.52
1:K:69:TRP:HZ3	1:K:112:LEU:HD21	1.75	0.52
1:A:51:LEU:HD13	1:A:272:LEU:HB2	1.90	0.52
1:C:283:THR:HG23	1:C:285:MET:H	1.75	0.52
1:G:44:GLU:OE2	1:G:46:THR:HG22	2.10	0.52
1:O:294:PHE:HZ	2:P:59:MET:HG3	1.75	0.52
1:E:123:ILE:HG23	1:E:124:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:LEU:HD12	1:I:178:VAL:HG22	1.91	0.52
1:K:123:ILE:HD11	1:K:168:TYR:CD1	2.43	0.52
1:M:123:ILE:HD11	1:M:168:TYR:CE2	2.44	0.52
1:Q:298:HIS:HE1	1:Q:300:LEU:HD12	1.73	0.52
2:B:160:PRO:HA	2:B:163:SER:HB2	1.92	0.52
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.91	0.52
1:I:100:GLY:HA3	1:I:230:MET:O	2.10	0.52
1:E:309:VAL:HG12	1:E:311:SER:H	1.75	0.52
1:K:176:LEU:HD11	1:K:237:LEU:HD23	1.91	0.52
1:K:309:VAL:HG13	1:K:311:SER:H	1.75	0.52
2:P:126:LEU:HD12	2:P:157:TYR:CE2	2.45	0.52
1:K:293:PRO:HG2	1:K:294:PHE:HD1	1.74	0.51
1:O:21:ASN:ND2	6:O:2104:HOH:O	2.39	0.51
1:C:279:THR:OG1	1:C:280:LYS:N	2.43	0.51
1:K:170:ASN:CG	1:K:176:LEU:CD2	2.79	0.51
1:E:298:HIS:HE1	1:E:300:LEU:HD12	1.75	0.51
1:K:164:ILE:O	1:K:246:GLU:HA	2.11	0.51
2:P:17:MET:HE1	2:P:36:ALA:HA	1.93	0.51
2:D:17:MET:HE1	2:D:36:ALA:HA	1.91	0.51
2:F:159:TYR:HB3	2:F:160:PRO:HD3	1.93	0.51
2:L:159:TYR:HB3	2:L:160:PRO:HD3	1.92	0.51
2:N:22:TYR:OH	2:N:111:HIS:ND1	2.35	0.51
1:G:15:ILE:HG13	2:H:119:TYR:HA	1.92	0.51
1:O:182:ILE:HD12	1:O:202:ILE:HD12	1.93	0.50
1:I:38:HIS:CD2	2:J:21:TRP:HE1	2.28	0.50
1:Q:183:HIS:ND1	1:Q:195:TYR:OH	2.36	0.50
1:G:283:THR:HB	1:G:286:GLY:O	2.11	0.50
5:K:2004:NAG:H83	6:K:2110:HOH:O	2.12	0.50
1:M:118:PHE:CE1	1:M:260:ILE:HD13	2.47	0.50
1:E:209:LEU:HD21	1:E:211:GLN:HG2	1.92	0.50
2:P:19:ASP:OD1	2:P:19:ASP:N	2.39	0.50
1:G:294:PHE:HZ	2:H:59:MET:HG3	1.77	0.50
2:P:122:VAL:HG13	2:P:152:VAL:HG21	1.94	0.50
2:D:160:PRO:HA	2:D:163:SER:HB2	1.92	0.50
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.93	0.50
1:Q:15:ILE:HG13	2:R:119:TYR:HA	1.92	0.50
1:G:9:PRO:HD3	2:H:139:GLU:OE2	2.11	0.49
1:K:26:VAL:HG11	1:K:317:ALA:HB2	1.94	0.49
2:L:152:VAL:HG12	2:L:157:TYR:HD1	1.77	0.49
1:E:26:VAL:HG11	1:E:317:ALA:HB2	1.94	0.49
1:G:9:PRO:HD2	2:H:139:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.94	0.49
1:E:28:THR:HB	2:F:105:GLU:HB2	1.94	0.49
1:M:80:ILE:HD11	1:M:149:ARG:HD2	1.93	0.49
1:C:147:PHE:HZ	1:C:230:MET:HE1	1.77	0.49
1:G:307:LYS:HD2	2:H:62:GLN:HB3	1.94	0.49
1:M:26:VAL:HG11	1:M:317:ALA:HB2	1.93	0.49
2:R:62:GLN:HG3	2:R:92:TRP:CG	2.48	0.49
1:A:323:THR:HG21	2:B:12:GLY:HA2	1.95	0.49
1:C:283:THR:HG22	1:C:286:GLY:H	1.77	0.49
2:N:75:ARG:NH1	2:N:78:GLU:OE1	2.39	0.49
2:D:131:LYS:HG2	2:D:139:GLU:HB3	1.94	0.49
1:E:164:ILE:O	1:E:246:GLU:HA	2.13	0.49
1:A:98:TYR:CD1	1:A:230:MET:HG3	2.48	0.49
1:K:120:LYS:HD3	1:K:258:TYR:CE1	2.47	0.49
1:M:151:VAL:HG22	1:M:252:ILE:HG22	1.95	0.49
1:O:182:ILE:HD11	1:O:213:LEU:HD13	1.94	0.49
2:F:17:MET:HE1	2:F:36:ALA:HA	1.95	0.49
1:I:200:THR:OG1	1:I:215:PRO:HG3	2.13	0.49
1:K:13:ILE:HG22	2:L:138:PHE:HB2	1.95	0.49
1:M:148:PHE:HB2	1:M:151:VAL:HG12	1.93	0.49
1:Q:118:PHE:HE1	1:Q:260:ILE:HG12	1.78	0.49
1:C:127:TRP:CE2	1:C:154:LEU:HD21	2.47	0.49
2:F:158:ASP:OD1	2:F:160:PRO:HD2	2.12	0.49
1:I:206:THR:HG23	1:I:241:ASP:OD2	2.12	0.49
1:O:200:THR:HA	1:O:248:ASN:HD21	1.77	0.49
1:I:147:PHE:HZ	1:I:230:MET:HE1	1.77	0.49
2:N:131:LYS:HD2	2:N:141:TYR:OH	2.13	0.49
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.96	0.48
1:C:89:GLU:OE1	1:C:269:LYS:HE2	2.13	0.48
2:D:131:LYS:HE2	2:D:141:TYR:CE1	2.47	0.48
1:E:126:SER:OG	1:E:166:ARG:NH1	2.34	0.48
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.48
1:I:216:GLU:O	1:I:220:ARG:NH2	2.46	0.48
1:K:206:THR:HG23	1:K:241:ASP:OD2	2.13	0.48
1:O:283:THR:CG2	1:O:285:MET:H	2.24	0.48
1:A:289:ASN:ND2	6:A:2105:HOH:O	2.46	0.48
1:G:9:PRO:CD	1:G:10:GLY:H	2.26	0.48
1:G:205:GLY:O	1:G:243:ILE:HA	2.12	0.48
1:M:51:LEU:HG	1:M:272:LEU:HD11	1.94	0.48
2:N:89:LEU:O	2:N:93:THR:HG23	2.12	0.48
1:O:43:LEU:HB2	1:O:314:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:CG2	1:E:285:MET:H	2.27	0.48
1:K:323:THR:HG21	2:L:12:GLY:HA2	1.95	0.48
1:M:58:PRO:HB3	1:M:86:TYR:CE1	2.48	0.48
1:C:206:THR:CG2	1:C:208:THR:H	2.26	0.48
2:D:148:CYS:O	2:D:151:SER:HB3	2.13	0.48
1:E:138:ALA:HB2	1:E:226:GLN:HG2	1.94	0.48
1:I:86:TYR:CZ	1:I:282:GLN:HG2	2.48	0.48
2:D:151:SER:OG	2:D:157:TYR:HA	2.13	0.48
2:F:172:GLU:OE1	2:F:172:GLU:N	2.46	0.48
2:J:4:GLY:O	2:J:8:GLY:HA3	2.14	0.48
1:K:15:ILE:HG13	2:L:119:TYR:HA	1.95	0.48
1:E:172:ASN:HB3	1:E:174:GLU:OE1	2.14	0.48
1:O:182:ILE:HG23	1:O:202:ILE:HD12	1.96	0.48
2:D:19:ASP:OD1	2:D:19:ASP:N	2.43	0.48
1:I:176:LEU:HD11	1:I:178:VAL:CG2	2.43	0.48
1:O:164:ILE:O	1:O:246:GLU:HA	2.14	0.48
2:P:131:LYS:HG2	2:P:139:GLU:HB3	1.95	0.48
1:G:138:ALA:HB2	1:G:226:GLN:HG2	1.96	0.48
1:M:206:THR:HG22	1:M:209:LEU:H	1.79	0.48
1:O:118:PHE:CE1	1:O:260:ILE:HD13	2.49	0.48
1:C:44:GLU:HB2	1:C:292:MET:HG3	1.96	0.47
1:E:89:GLU:OE1	1:E:269:LYS:HE2	2.14	0.47
1:M:51:LEU:HG	1:M:272:LEU:CD1	2.44	0.47
1:O:123:ILE:HD11	1:O:168:TYR:CE2	2.49	0.47
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.96	0.47
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.95	0.47
1:I:311:SER:OG	2:J:97:GLU:OE2	2.29	0.47
2:J:83:GLN:OE1	2:L:68:ARG:NH2	2.42	0.47
1:K:141:TYR:O	1:K:143:GLY:N	2.40	0.47
2:L:160:PRO:HA	2:L:163:SER:HB2	1.95	0.47
1:A:18:HIS:N	2:B:21:TRP:O	2.39	0.47
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.96	0.47
1:K:142:HIS:C	1:K:144:ARG:H	2.17	0.47
1:C:147:PHE:HZ	1:C:230:MET:CE	2.28	0.47
1:Q:58:PRO:HG2	1:Q:60:ILE:CD1	2.42	0.47
3:U:1:NAG:O3	3:U:2:NAG:H2	2.15	0.47
1:C:283:THR:CG2	1:C:285:MET:H	2.28	0.47
1:E:283:THR:HG22	1:E:286:GLY:H	1.79	0.47
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.15	0.47
1:G:320:LEU:HB3	2:H:111:HIS:CG	2.49	0.47
1:I:58:PRO:HG2	1:I:60:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:PHE:HE1	1:M:260:ILE:HD13	1.77	0.47
1:Q:135:VAL:HG22	1:Q:146:SER:HA	1.95	0.47
1:C:45:LYS:HE3	1:C:296:ASN:HD21	1.79	0.47
1:G:323:THR:HG21	2:H:13:GLY:N	2.21	0.47
1:Q:37:THR:HG23	1:Q:319:GLY:HA3	1.96	0.47
1:Q:293:PRO:HG2	1:Q:294:PHE:CD1	2.49	0.47
1:C:189:ALA:O	1:C:192:THR:HG22	2.14	0.47
1:M:316:LEU:HD23	2:N:100:VAL:HG13	1.95	0.47
2:N:168:LEU:O	2:N:172:GLU:HG2	2.14	0.47
2:B:105:GLU:HG2	2:D:106:ARG:HH22	1.80	0.47
1:G:211:GLN:NE2	1:G:213:LEU:HD11	2.29	0.47
2:H:75:ARG:NH1	2:H:78:GLU:OE1	2.46	0.47
1:A:220:ARG:NE	1:C:210:ASN:OD1	2.45	0.46
1:E:115:THR:HG21	1:E:118:PHE:CE1	2.50	0.46
1:M:217:ILE:HB	1:O:212:ARG:NH1	2.30	0.46
2:D:22:TYR:OH	2:D:111:HIS:ND1	2.36	0.46
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.97	0.46
1:G:283:THR:CG2	1:G:285:MET:H	2.24	0.46
2:N:68:ARG:NH2	2:R:83:GLN:OE1	2.44	0.46
1:Q:211:GLN:OE1	1:Q:213:LEU:HD11	2.15	0.46
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.97	0.46
1:G:299:PRO:HB3	2:H:89:LEU:HD21	1.96	0.46
1:K:118:PHE:CE1	1:K:260:ILE:HG12	2.49	0.46
1:M:174:GLU:N	1:M:174:GLU:OE1	2.48	0.46
1:Q:38:HIS:CD2	2:R:21:TRP:HE1	2.32	0.46
1:K:52:CYS:HB2	1:K:279:THR:HG22	1.97	0.46
1:M:147:PHE:HZ	1:M:230:MET:CE	2.26	0.46
2:P:55:ILE:HG23	2:P:99:LEU:HD23	1.97	0.46
1:M:62:ARG:NH1	1:M:78:GLU:OE1	2.49	0.46
1:M:184:HIS:CE1	1:M:216:GLU:H	2.34	0.46
1:E:284:PRO:HD3	1:E:300:LEU:O	2.16	0.46
1:G:284:PRO:HG2	1:G:298:HIS:CE1	2.50	0.46
2:H:127:ARG:HH21	2:L:131:LYS:HE3	1.80	0.46
1:M:131:ASP:HB3	1:M:155:ILE:HG13	1.97	0.46
1:Q:161:TYR:CZ	1:Q:249:GLY:HA2	2.50	0.46
1:A:147:PHE:HZ	1:A:230:MET:HE1	1.81	0.46
1:G:175:ASP:OD1	1:G:239:PRO:HD3	2.16	0.46
1:K:77:ASP:O	1:K:80:ILE:HG12	2.15	0.46
1:M:308:TYR:HD2	2:N:89:LEU:HD22	1.79	0.46
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.51	0.46
1:M:230:MET:HE1	1:M:252:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:135:VAL:HG22	1:K:146:SER:HA	1.98	0.46
1:K:170:ASN:CG	1:K:176:LEU:HD21	2.37	0.46
1:M:123:ILE:HG23	1:M:124:ILE:HG23	1.98	0.46
1:M:179:LEU:O	1:M:254:PRO:HB3	2.16	0.45
1:C:309:VAL:HG13	1:C:311:SER:H	1.82	0.45
1:K:131:ASP:HB3	1:K:155:ILE:HB	1.97	0.45
1:C:309:VAL:HG22	2:D:93:THR:HA	1.99	0.45
1:K:14:CYS:HA	2:L:137:CYS:HA	1.97	0.45
1:K:142:HIS:HB2	1:K:144:ARG:HG2	1.97	0.45
2:N:160:PRO:HA	2:N:163:SER:HB2	1.98	0.45
1:O:211:GLN:OE1	1:O:213:LEU:HD11	2.17	0.45
1:Q:26:VAL:HG11	1:Q:317:ALA:HB2	1.98	0.45
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.45
2:L:133:LEU:HD21	2:L:139:GLU:HB2	1.98	0.45
1:M:15:ILE:HD11	2:N:122:VAL:HG21	1.97	0.45
2:F:30:GLN:OE1	2:F:30:GLN:N	2.41	0.45
1:O:175:ASP:OD1	1:O:239:PRO:HD3	2.17	0.45
1:E:197:ASN:OD1	1:E:197:ASN:N	2.47	0.45
1:O:52:CYS:HB2	1:O:279:THR:HG22	1.97	0.45
1:A:53:ASP:HA	1:A:58:PRO:HD3	1.99	0.45
1:K:323:THR:HA	1:K:324:PRO:HD3	1.84	0.45
1:M:298:HIS:HA	1:M:299:PRO:HD3	1.77	0.45
1:O:29:ILE:HD12	2:P:101:LEU:HB3	1.98	0.45
1:A:147:PHE:CZ	1:A:230:MET:HE1	2.52	0.45
2:B:68:ARG:NH2	2:F:83:GLN:OE1	2.39	0.45
1:E:284:PRO:HG2	1:E:298:HIS:CE1	2.51	0.45
1:K:123:ILE:HD12	1:K:123:ILE:HA	1.52	0.45
2:P:98:LEU:HD21	2:R:99:LEU:HD13	1.98	0.45
2:R:167:ARG:NH1	2:R:171:GLU:OE1	2.50	0.45
1:A:141:TYR:CZ	1:A:149:ARG:NH2	2.84	0.44
1:A:323:THR:HA	1:A:324:PRO:HD3	1.77	0.44
1:C:52:CYS:HB2	1:C:279:THR:HG22	1.99	0.44
1:M:220:ARG:HD2	1:M:229:ARG:CG	2.45	0.44
1:C:230:MET:CE	1:C:252:ILE:HG12	2.48	0.44
1:K:39:ALA:HA	1:K:318:THR:HG22	1.98	0.44
2:N:55:ILE:O	2:N:59:MET:HG2	2.18	0.44
2:R:19:ASP:OD1	2:R:19:ASP:N	2.34	0.44
1:O:279:THR:OG1	1:O:280:LYS:N	2.50	0.44
2:R:58:LYS:HD3	2:R:58:LYS:HA	1.85	0.44
1:C:123:ILE:HD11	1:C:168:TYR:CE2	2.53	0.44
1:G:217:ILE:O	1:I:212:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:HIS:O	1:M:185:PRO:HD3	2.17	0.44
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.52	0.44
2:H:24:TYR:HB2	2:H:153:LYS:HE2	2.00	0.44
1:K:299:PRO:HB3	2:L:89:LEU:HD11	1.98	0.44
2:R:24:TYR:CE1	2:R:37:ASP:HB2	2.52	0.44
1:I:26:VAL:HG11	1:I:317:ALA:HB2	1.99	0.44
1:I:151:VAL:HG13	1:I:252:ILE:CG2	2.48	0.44
1:Q:323:THR:HA	1:Q:324:PRO:HD3	1.79	0.44
2:R:55:ILE:HG12	2:R:99:LEU:HD21	2.00	0.44
2:D:97:GLU:HB3	2:F:58:LYS:HE3	1.99	0.44
1:I:176:LEU:HD12	1:I:178:VAL:HG23	2.00	0.44
1:K:206:THR:HG22	1:K:209:LEU:H	1.82	0.44
1:C:51:LEU:HG	1:C:272:LEU:CD1	2.47	0.44
1:E:299:PRO:HG3	1:E:308:TYR:CE2	2.53	0.44
2:L:4:GLY:O	2:L:8:GLY:HA3	2.18	0.44
1:M:141:TYR:CZ	1:M:149:ARG:NH2	2.84	0.44
1:O:62:ARG:NH1	1:O:78:GLU:OE1	2.51	0.44
1:A:135:VAL:HG22	1:A:146:SER:HA	2.00	0.43
1:C:211:GLN:OE1	1:C:213:LEU:HD11	2.18	0.43
1:E:293:PRO:HG2	1:E:294:PHE:HD2	1.84	0.43
2:F:133:LEU:HD12	2:F:137:CYS:HB2	2.00	0.43
1:I:71:LEU:HD23	1:I:71:LEU:HA	1.80	0.43
1:C:9:PRO:HD2	1:C:9:PRO:O	2.18	0.43
1:C:202:ILE:HD11	1:C:251:PHE:HA	2.00	0.43
1:C:230:MET:HE1	1:C:252:ILE:HG12	2.00	0.43
1:G:298:HIS:HA	1:G:299:PRO:HD3	1.86	0.43
1:I:323:THR:HA	1:I:324:PRO:HD3	1.84	0.43
2:F:55:ILE:O	2:F:59:MET:HG2	2.18	0.43
1:I:284:PRO:HD3	1:I:300:LEU:O	2.18	0.43
1:A:58:PRO:HG2	1:A:60:ILE:HD11	2.00	0.43
1:C:218:ALA:HB2	1:E:203:SER:OG	2.18	0.43
1:I:294:PHE:HZ	2:J:59:MET:HG3	1.83	0.43
1:K:170:ASN:CG	1:K:176:LEU:HD23	2.38	0.43
1:O:245:PHE:CE2	1:O:254:PRO:HG2	2.54	0.43
1:G:203:SER:HB2	1:K:218:ALA:HB2	2.00	0.43
1:I:230:MET:CE	1:I:252:ILE:HG12	2.46	0.43
1:I:313:ARG:O	1:I:314:LEU:HD23	2.18	0.43
1:O:183:HIS:O	1:O:185:PRO:HD3	2.18	0.43
1:I:14:CYS:O	2:J:24:TYR:HA	2.18	0.43
2:J:19:ASP:OD1	2:J:19:ASP:N	2.51	0.43
1:K:238:LYS:HA	1:K:239:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:115:THR:HG21	1:O:118:PHE:CE1	2.53	0.43
1:Q:279:THR:OG1	1:Q:280:LYS:N	2.52	0.43
2:H:123:ARG:HB2	2:H:138:PHE:CZ	2.53	0.43
1:O:118:PHE:HE1	1:O:260:ILE:HD13	1.83	0.43
1:C:183:HIS:ND1	1:C:195:TYR:OH	2.41	0.43
1:G:124:ILE:HD12	1:G:254:PRO:HG2	2.00	0.43
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.84	0.43
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.19	0.43
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.54	0.43
1:C:62:ARG:NH1	1:C:78:GLU:OE2	2.52	0.42
1:K:175:ASP:OD1	1:K:239:PRO:HD3	2.19	0.42
1:M:106:GLU:HB3	2:R:76:ARG:HD3	2.00	0.42
1:O:309:VAL:HG12	1:O:311:SER:H	1.84	0.42
2:P:58:LYS:HD3	2:P:58:LYS:HA	1.81	0.42
2:P:94:TYR:CZ	2:P:98:LEU:HD22	2.54	0.42
1:C:307:LYS:HB3	2:D:62:GLN:NE2	2.34	0.42
1:K:9:PRO:O	1:K:9:PRO:CD	2.66	0.42
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.55	0.42
2:F:89:LEU:HD23	2:F:89:LEU:HA	1.87	0.42
1:O:148:PHE:HB2	1:O:151:VAL:HG12	2.01	0.42
1:Q:230:MET:HE1	1:Q:252:ILE:HG12	2.01	0.42
1:C:29:ILE:HD12	2:D:101:LEU:HB3	2.00	0.42
1:C:274:TYR:CZ	1:C:276:ASN:HA	2.54	0.42
1:E:15:ILE:HD11	2:F:122:VAL:HG21	2.01	0.42
1:O:314:LEU:HD23	1:O:314:LEU:HA	1.84	0.42
1:E:124:ILE:O	1:E:255:GLU:HG3	2.20	0.42
1:G:288:ILE:HD11	1:G:297:ILE:HD12	2.02	0.42
1:G:293:PRO:HB3	2:H:56:ILE:HG23	2.01	0.42
1:K:58:PRO:HB3	1:K:86:TYR:CE1	2.54	0.42
1:Q:57:LYS:HG3	1:Q:58:PRO:HD2	2.01	0.42
2:B:133:LEU:HD23	2:B:133:LEU:HA	1.77	0.42
1:C:138:ALA:HB2	1:C:226:GLN:HG2	2.01	0.42
1:G:100:GLY:HA3	1:G:230:MET:O	2.20	0.42
1:G:203:SER:OG	1:G:246:GLU:HB3	2.19	0.42
1:I:220:ARG:HD3	1:I:229:ARG:HG2	2.02	0.42
1:M:299:PRO:HG3	1:M:308:TYR:CE2	2.55	0.42
1:O:284:PRO:HD3	1:O:300:LEU:O	2.20	0.42
2:P:168:LEU:O	2:P:172:GLU:HG2	2.20	0.42
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.55	0.42
1:E:51:LEU:HA	1:E:51:LEU:HD12	1.77	0.42
1:G:284:PRO:HD3	1:G:300:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:124:ILE:HG22	1:Q:166:ARG:NH2	2.35	0.42
1:E:100:GLY:HA3	1:E:230:MET:O	2.20	0.42
1:G:37:THR:HG23	1:G:320:LEU:O	2.20	0.42
1:G:202:ILE:HG12	1:G:247:SER:OG	2.20	0.42
1:I:164:ILE:O	1:I:246:GLU:HA	2.20	0.42
1:Q:265:SER:OG	1:Q:266:ALA:N	2.53	0.42
1:A:80:ILE:HD13	1:A:80:ILE:HA	1.92	0.42
1:E:283:THR:HG23	1:E:285:MET:H	1.85	0.42
1:G:221:PRO:HB3	3:V:1:NAG:H81	2.02	0.42
1:I:283:THR:HG22	1:I:286:GLY:H	1.85	0.42
2:L:152:VAL:HG12	2:L:157:TYR:CD1	2.53	0.42
1:O:161:TYR:CZ	1:O:249:GLY:HA2	2.55	0.42
2:P:75:ARG:HH21	2:P:78:GLU:CD	2.23	0.41
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.55	0.41
1:E:292:MET:HG3	1:E:293:PRO:HD2	2.00	0.41
2:H:58:LYS:HA	2:H:58:LYS:HD2	1.83	0.41
1:Q:70:LEU:HB3	1:Q:179:LEU:HD11	2.02	0.41
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.19	0.41
1:A:16:GLY:HA3	2:B:14:TRP:CH2	2.56	0.41
2:B:169:ASN:O	2:B:172:GLU:OE1	2.37	0.41
1:C:54:LEU:O	1:C:56:VAL:HG22	2.19	0.41
1:C:198:PRO:HG2	1:C:199:THR:HG22	2.02	0.41
1:C:274:TYR:CE2	1:C:276:ASN:HA	2.55	0.41
1:E:86:TYR:HB3	1:E:302:ILE:HD13	2.01	0.41
5:K:2004:NAG:H82	6:K:2110:HOH:O	2.20	0.41
1:M:309:VAL:HB	2:N:93:THR:HG22	2.01	0.41
1:O:323:THR:HA	1:O:324:PRO:HD3	1.84	0.41
1:A:280:LYS:HE3	1:A:304:GLU:CG	2.50	0.41
2:B:73:LEU:HD23	2:B:73:LEU:HA	1.90	0.41
2:H:83:GLN:NE2	2:J:64:GLU:O	2.53	0.41
1:O:176:LEU:HD12	1:O:258:TYR:C	2.40	0.41
1:Q:310:LYS:HB2	2:R:93:THR:HG21	2.02	0.41
1:G:62:ARG:HH12	1:G:78:GLU:CD	2.23	0.41
2:H:19:ASP:OD1	2:H:19:ASP:N	2.42	0.41
1:A:164:ILE:O	1:A:246:GLU:HA	2.20	0.41
1:E:133(A):SER:O	1:E:135:VAL:N	2.53	0.41
1:G:18:HIS:N	2:H:21:TRP:O	2.49	0.41
1:I:138:ALA:HB2	1:I:226:GLN:HG2	2.03	0.41
1:M:183:HIS:HD2	1:M:230:MET:HG3	1.85	0.41
2:B:62:GLN:HG3	2:B:92:TRP:CD2	2.55	0.41
1:K:57:LYS:HG3	1:K:58:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:ILE:O	1:K:255:GLU:HG3	2.21	0.41
1:K:183:HIS:HB2	1:K:252:ILE:HD11	2.03	0.41
1:O:147:PHE:HZ	1:O:230:MET:CE	2.33	0.41
3:U:1:NAG:H4	3:U:2:NAG:H2	1.90	0.41
2:H:84:MET:HE2	2:H:84:MET:HB3	1.88	0.41
1:M:244:ASN:ND2	1:Q:221:PRO:HD3	2.36	0.41
2:N:51:LYS:HD3	2:N:103:GLU:HB3	2.03	0.41
1:C:207:SER:OG	1:C:241:ASP:OD1	2.32	0.41
1:E:279:THR:OG1	1:E:280:LYS:N	2.54	0.41
1:G:148:PHE:HB2	1:G:151:VAL:HG12	2.02	0.41
1:K:54:LEU:O	1:K:56:VAL:HG22	2.20	0.41
1:O:182:ILE:CD1	1:O:202:ILE:HD12	2.51	0.41
1:G:14:CYS:O	2:H:24:TYR:HA	2.21	0.41
1:K:58:PRO:HG2	1:K:60:ILE:HD11	2.03	0.41
1:K:108:LEU:HB2	1:K:234:TRP:CE2	2.56	0.41
2:L:158:ASP:OD1	2:L:160:PRO:HD2	2.21	0.41
1:M:221:PRO:HD3	1:O:244:ASN:HD21	1.86	0.41
1:A:211:GLN:NE2	1:A:213:LEU:HD11	2.36	0.40
2:F:19:ASP:OD1	2:F:19:ASP:N	2.42	0.40
1:G:320:LEU:HB3	2:H:111:HIS:CD2	2.56	0.40
1:I:9:PRO:O	1:I:9:PRO:CD	2.69	0.40
1:A:29:ILE:H	1:A:29:ILE:HG13	1.58	0.40
1:A:265:SER:OG	1:A:266:ALA:N	2.53	0.40
1:E:179:LEU:O	1:E:254:PRO:HB3	2.21	0.40
1:G:144:ARG:HA	1:G:144:ARG:HD2	1.89	0.40
1:K:186:ASN:OD1	1:K:227:SER:HB3	2.21	0.40
1:K:230:MET:CE	1:K:252:ILE:HG12	2.50	0.40
1:M:297:ILE:HD13	1:M:297:ILE:HG21	1.85	0.40
1:O:53:ASP:OD1	1:O:274:TYR:OH	2.25	0.40
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.90	0.40
2:H:143:LYS:O	2:H:143:LYS:HG3	2.21	0.40
2:R:22:TYR:OH	2:R:111:HIS:ND1	2.39	0.40
3:U:1:NAG:C3	3:U:2:NAG:H2	2.49	0.40
2:B:75:ARG:HD3	2:B:75:ARG:HA	1.92	0.40
2:B:84:MET:HE2	2:B:84:MET:HB3	2.00	0.40
1:E:70:LEU:O	1:E:150:ASN:ND2	2.46	0.40
1:K:51:LEU:HD13	1:K:272:LEU:HB2	2.03	0.40
2:L:55:ILE:HD11	2:L:103:GLU:HG3	2.03	0.40
2:L:58:LYS:HD2	2:L:58:LYS:HA	1.88	0.40
1:M:323:THR:HA	1:M:324:PRO:HD3	1.81	0.40
1:O:73:ASN:HB3	1:O:76:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ILE:HG23	2:B:99:LEU:HD23	2.03	0.40
2:R:62:GLN:HG3	2:R:92:TRP:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/334 (96%)	312 (97%)	9 (3%)	0	100	100
1	C	321/334 (96%)	309 (96%)	12 (4%)	0	100	100
1	E	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	G	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	I	321/334 (96%)	310 (97%)	11 (3%)	0	100	100
1	K	321/334 (96%)	311 (97%)	9 (3%)	1 (0%)	41	64
1	M	321/334 (96%)	309 (96%)	12 (4%)	0	100	100
1	O	321/334 (96%)	314 (98%)	7 (2%)	0	100	100
1	Q	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
2	B	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	D	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	F	171/182 (94%)	166 (97%)	5 (3%)	0	100	100
2	H	171/182 (94%)	168 (98%)	3 (2%)	0	100	100
2	J	171/182 (94%)	168 (98%)	3 (2%)	0	100	100
2	L	171/182 (94%)	166 (97%)	5 (3%)	0	100	100
2	N	171/182 (94%)	167 (98%)	3 (2%)	1 (1%)	25	47
2	P	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	R	171/182 (94%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4428/4644 (95%)	4301 (97%)	125 (3%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	142	HIS
2	N	12	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	287/297 (97%)	277 (96%)	10 (4%)	36 62
1	C	287/297 (97%)	273 (95%)	14 (5%)	25 48
1	E	287/297 (97%)	272 (95%)	15 (5%)	23 46
1	G	287/297 (97%)	274 (96%)	13 (4%)	27 52
1	I	287/297 (97%)	276 (96%)	11 (4%)	33 59
1	K	287/297 (97%)	277 (96%)	10 (4%)	36 62
1	M	287/297 (97%)	277 (96%)	10 (4%)	36 62
1	O	287/297 (97%)	276 (96%)	11 (4%)	33 59
1	Q	287/297 (97%)	278 (97%)	9 (3%)	40 66
2	B	148/155 (96%)	147 (99%)	1 (1%)	84 94
2	D	148/155 (96%)	147 (99%)	1 (1%)	84 94
2	F	148/155 (96%)	147 (99%)	1 (1%)	84 94
2	H	148/155 (96%)	146 (99%)	2 (1%)	67 85
2	J	148/155 (96%)	146 (99%)	2 (1%)	67 85
2	L	148/155 (96%)	141 (95%)	7 (5%)	26 50
2	N	148/155 (96%)	147 (99%)	1 (1%)	84 94
2	P	148/155 (96%)	145 (98%)	3 (2%)	55 78
2	R	148/155 (96%)	147 (99%)	1 (1%)	84 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3915/4068 (96%)	3793 (97%)	122 (3%)	40 66

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	29	ILE
1	A	36	VAL
1	A	82	VAL
1	A	111	LEU
1	A	125(A)	LYS
1	A	135	VAL
1	A	151	VAL
1	A	195	TYR
1	A	197	ASN
2	B	69	GLU
1	C	26	VAL
1	C	29	ILE
1	C	36	VAL
1	C	125(B)	SER
1	C	133(A)	SER
1	C	135	VAL
1	C	154	LEU
1	C	195	TYR
1	C	197	ASN
1	C	199	THR
1	C	206	THR
1	C	283	THR
1	C	309	VAL
1	C	323	THR
2	D	168	LEU
1	E	23	THR
1	E	36	VAL
1	E	51	LEU
1	E	135	VAL
1	E	151	VAL
1	E	195	TYR
1	E	197	ASN
1	E	206	THR
1	E	213	LEU
1	E	227	SER
1	E	230	MET

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Mol	Chain	Res	Type
1	E	283	THR
1	E	291	SER
1	E	292	MET
1	E	309	VAL
2	F	22	TYR
1	G	36	VAL
1	G	102	PHE
1	G	133(A)	SER
1	G	135	VAL
1	G	151	VAL
1	G	194	LEU
1	G	195	TYR
1	G	199	THR
1	G	206	THR
1	G	227	SER
1	G	283	THR
1	G	291	SER
1	G	323	THR
2	H	24	TYR
2	H	41	THR
1	I	23	THR
1	I	26	VAL
1	I	36	VAL
1	I	125(B)	SER
1	I	135	VAL
1	I	151	VAL
1	I	179	LEU
1	I	195	TYR
1	I	197	ASN
1	I	273	GLU
1	I	283	THR
2	J	26	HIS
2	J	84	MET
1	K	23	THR
1	K	26	VAL
1	K	36	VAL
1	K	59	LEU
1	K	102	PHE
1	K	151	VAL
1	K	154	LEU
1	K	195	TYR
1	K	227	SER

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Mol	Chain	Res	Type
1	K	309	VAL
2	L	22	TYR
2	L	41	THR
2	L	60	ASN
2	L	84	MET
2	L	122	VAL
2	L	152	VAL
2	L	172	GLU
1	M	36	VAL
1	M	75	MET
1	M	121	ILE
1	M	151	VAL
1	M	195	TYR
1	M	206	THR
1	M	220	ARG
1	M	267	ILE
1	M	277	CYS
1	M	315	VAL
2	N	26	HIS
1	O	23	THR
1	O	36	VAL
1	O	51	LEU
1	O	56	VAL
1	O	159	SER
1	O	182	ILE
1	O	192	THR
1	O	195	TYR
1	O	219	THR
1	O	309	VAL
1	O	323	THR
2	P	18	VAL
2	P	73	LEU
2	P	75	ARG
1	Q	36	VAL
1	Q	37	THR
1	Q	46	THR
1	Q	124	ILE
1	Q	133(A)	SER
1	Q	135	VAL
1	Q	151	VAL
1	Q	195	TYR
1	Q	219	THR

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Mol	Chain	Res	Type
2	R	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	C	172	ASN
1	E	38	HIS
1	E	211	GLN
2	F	129	ASN
1	G	211	GLN
1	I	38	HIS
1	M	197	ASN
1	M	211	GLN
2	N	83	GLN
2	P	26	HIS
1	Q	38	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

17 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	S	1	1,3	14,14,15	0.49	0	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	S	2	3	14,14,15	0.52	0	17,19,21	0.98	1 (5%)
3	NAG	T	1	1,3	14,14,15	0.47	0	17,19,21	1.07	1 (5%)
3	NAG	T	2	3	14,14,15	0.42	0	17,19,21	0.83	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.55	0	17,19,21	1.84	4 (23%)
3	NAG	U	2	3	14,14,15	0.52	0	17,19,21	1.38	2 (11%)
3	NAG	V	1	1,3	14,14,15	0.59	0	17,19,21	1.66	4 (23%)
3	NAG	V	2	3	14,14,15	0.54	0	17,19,21	1.00	1 (5%)
3	NAG	W	1	1,3	14,14,15	0.51	0	17,19,21	1.61	3 (17%)
3	NAG	W	2	3	14,14,15	0.54	0	17,19,21	0.70	0
3	NAG	X	1	1,3	14,14,15	0.54	0	17,19,21	1.61	3 (17%)
3	NAG	X	2	3	14,14,15	0.57	0	17,19,21	1.33	1 (5%)
4	NAG	Y	1	4,1	14,14,15	0.46	0	17,19,21	1.18	1 (5%)
4	NAG	Y	2	4	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
4	MAN	Y	3	4	11,11,12	0.52	0	15,15,17	1.66	3 (20%)
3	NAG	Z	1	2,3	14,14,15	0.62	0	17,19,21	1.58	3 (17%)
3	NAG	Z	2	3	14,14,15	0.53	0	17,19,21	1.70	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	4/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	Y	3	4	-	2/2/19/22	0/1/1/1
3	NAG	Z	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	1	NAG	C1-O5-C5	4.62	118.44	112.19
3	Z	2	NAG	C1-O5-C5	4.61	118.44	112.19
3	X	1	NAG	C1-O5-C5	4.43	118.20	112.19
3	U	2	NAG	C1-O5-C5	4.18	117.85	112.19
3	U	1	NAG	C3-C4-C5	4.06	117.48	110.24
3	Z	1	NAG	C1-O5-C5	4.06	117.69	112.19
4	Y	3	MAN	C1-O5-C5	4.03	117.65	112.19
3	W	1	NAG	C1-O5-C5	3.98	117.58	112.19
3	S	1	NAG	C1-O5-C5	3.68	117.18	112.19
3	U	1	NAG	C4-C3-C2	3.49	116.13	111.02
3	X	1	NAG	O4-C4-C3	-3.07	103.25	110.35
3	X	2	NAG	C4-C3-C2	3.07	115.52	111.02
4	Y	3	MAN	C3-C4-C5	2.97	115.53	110.24
3	Z	1	NAG	C2-N2-C7	2.93	127.08	122.90
3	Z	2	NAG	C3-C4-C5	2.91	115.42	110.24
3	V	2	NAG	C4-C3-C2	2.84	115.18	111.02
4	Y	3	MAN	O5-C5-C6	2.80	111.60	107.20
3	V	1	NAG	O4-C4-C3	-2.78	103.91	110.35
3	Z	2	NAG	O5-C5-C4	2.70	117.40	110.83
3	U	1	NAG	O4-C4-C5	-2.68	102.64	109.30
3	Z	1	NAG	C1-C2-N2	2.63	114.99	110.49
3	W	1	NAG	C2-N2-C7	-2.57	119.25	122.90
3	U	1	NAG	C1-O5-C5	2.53	115.62	112.19
3	T	1	NAG	C1-O5-C5	2.41	115.46	112.19
3	X	1	NAG	C2-N2-C7	-2.36	119.55	122.90
3	U	2	NAG	O5-C5-C6	2.32	110.84	107.20
4	Y	1	NAG	O5-C1-C2	-2.24	107.75	111.29
3	V	1	NAG	O5-C5-C6	2.20	110.66	107.20
4	Y	2	NAG	C2-N2-C7	-2.19	119.78	122.90
3	W	1	NAG	O5-C5-C6	2.16	110.60	107.20
3	T	2	NAG	C1-O5-C5	2.13	115.08	112.19
3	V	1	NAG	C1-C2-N2	2.05	114.00	110.49
3	S	2	NAG	O5-C5-C6	2.05	110.42	107.20

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	2	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
4	Y	3	MAN	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	C8-C7-N2-C2
4	Y	3	MAN	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	1	NAG	O5-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	C1-C2-N2-C7
3	W	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	S	2	NAG	O7-C7-N2-C2
3	Z	2	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C1-C2-N2-C7
3	S	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	1	NAG	3	0
3	U	2	NAG	3	0

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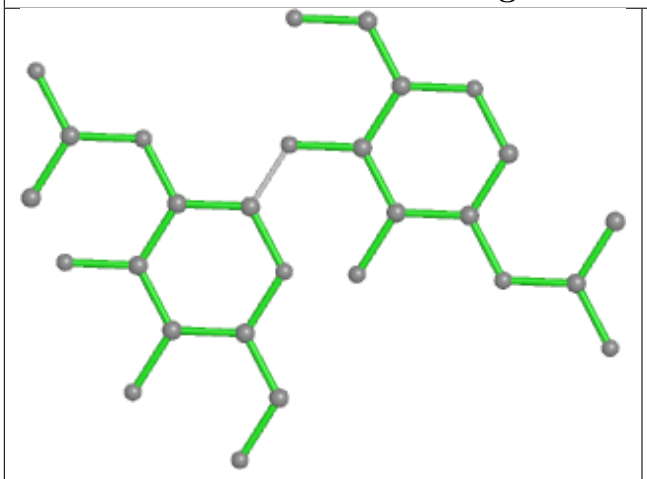
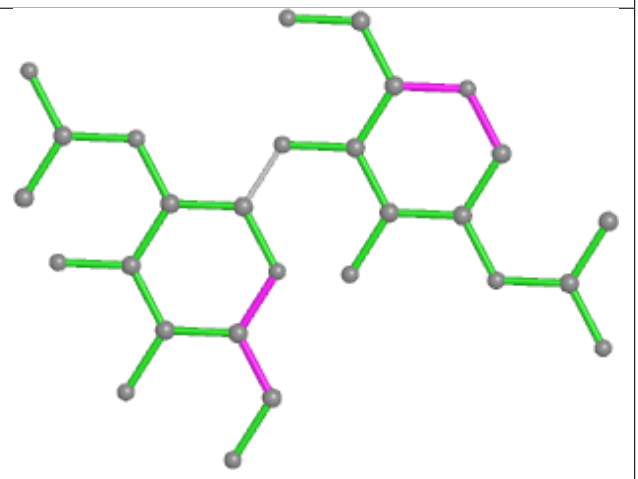
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1	NAG	1	0
3	W	1	NAG	1	0
3	V	1	NAG	1	0

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

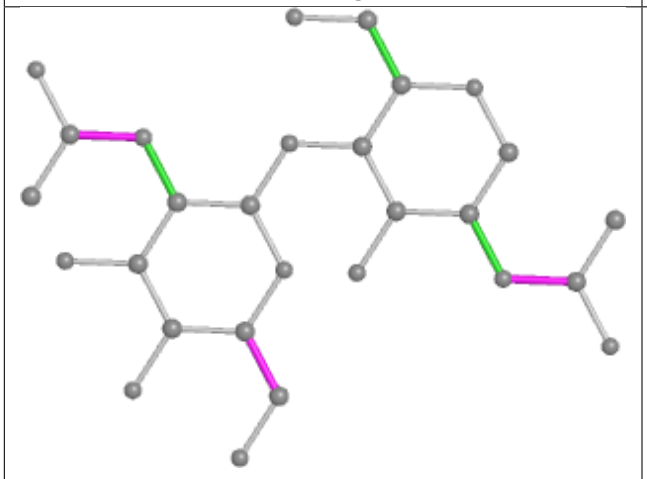
Oligosaccharide Chain S



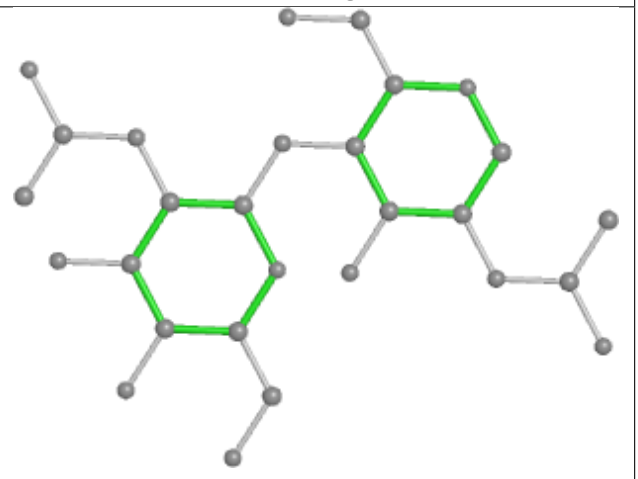
Bond lengths



Bond angles

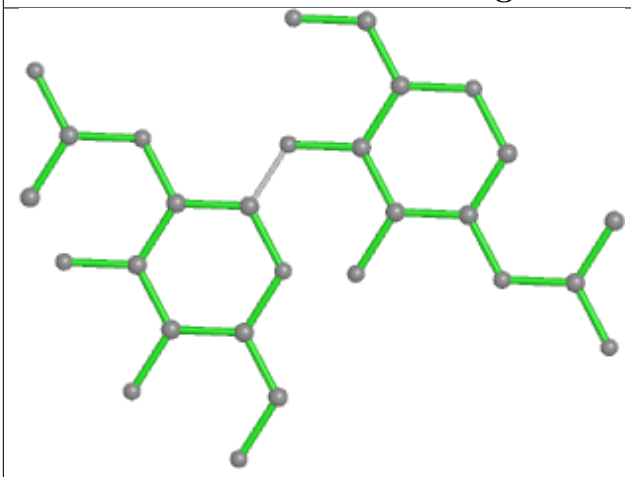


Torsions

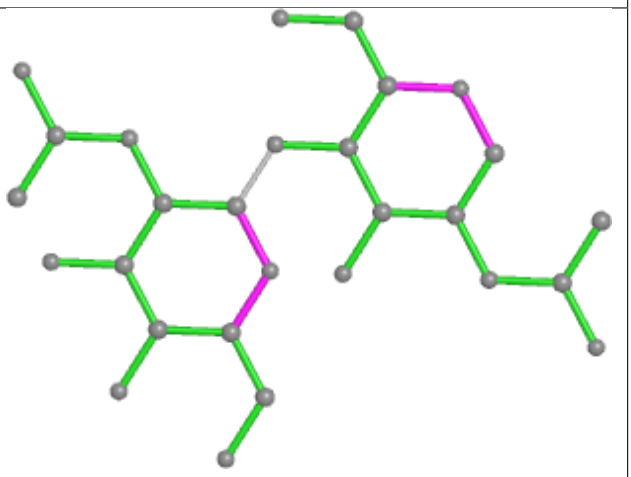


Rings

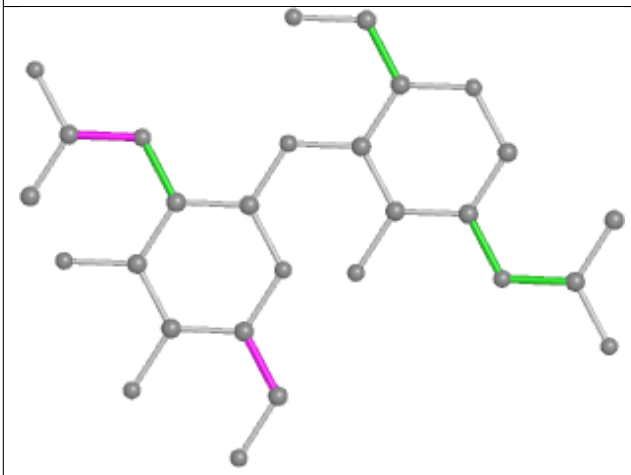
Oligosaccharide Chain T



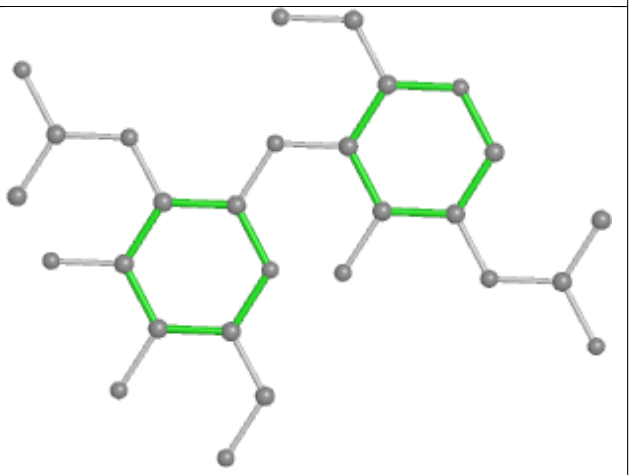
Bond lengths



Bond angles

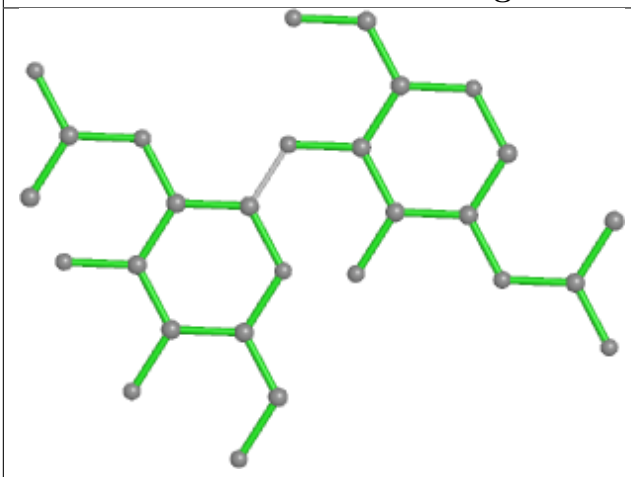


Torsions

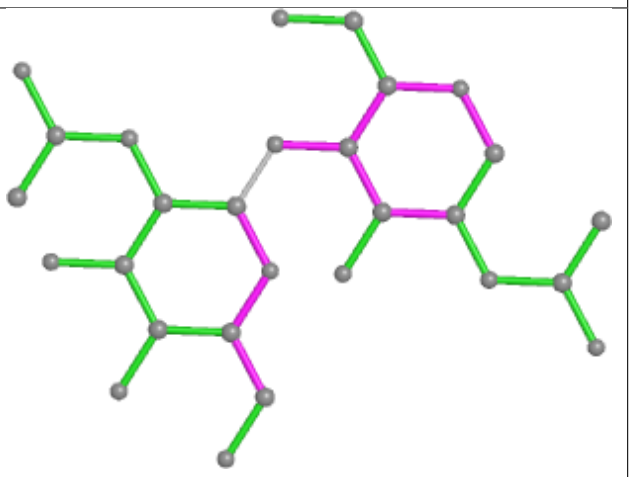


Rings

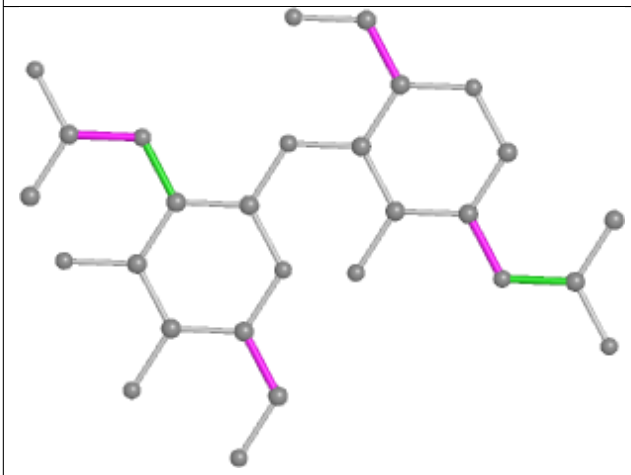
Oligosaccharide Chain U



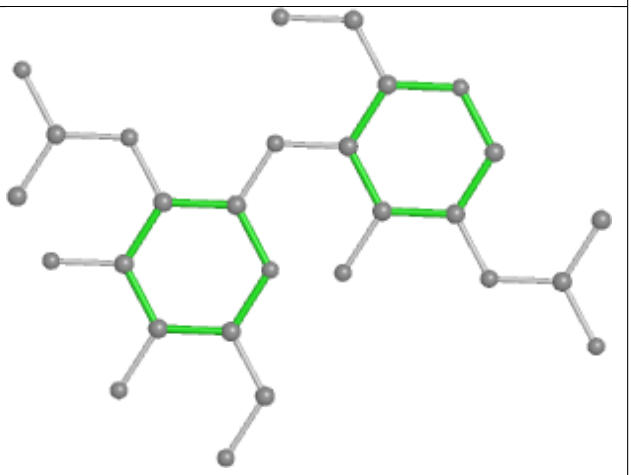
Bond lengths



Bond angles

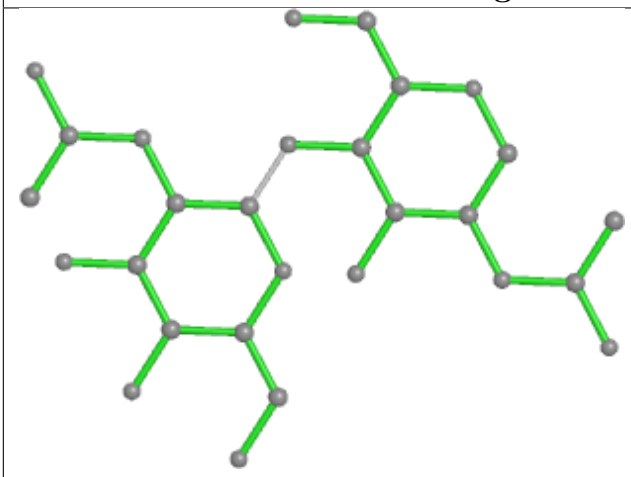


Torsions

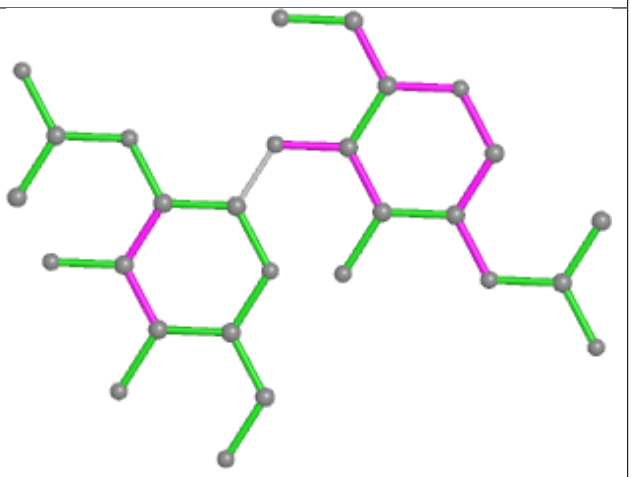


Rings

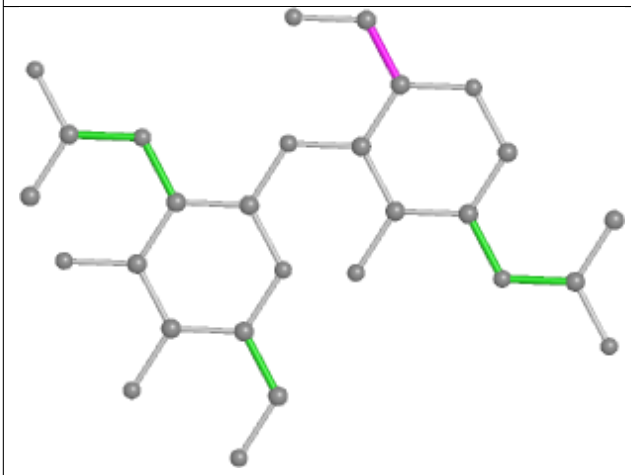
Oligosaccharide Chain V



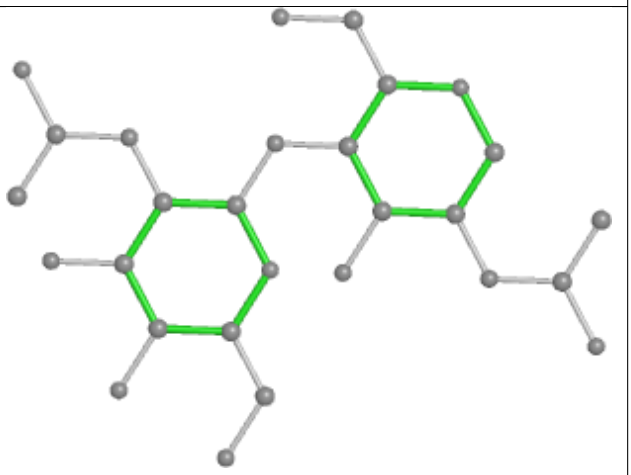
Bond lengths



Bond angles

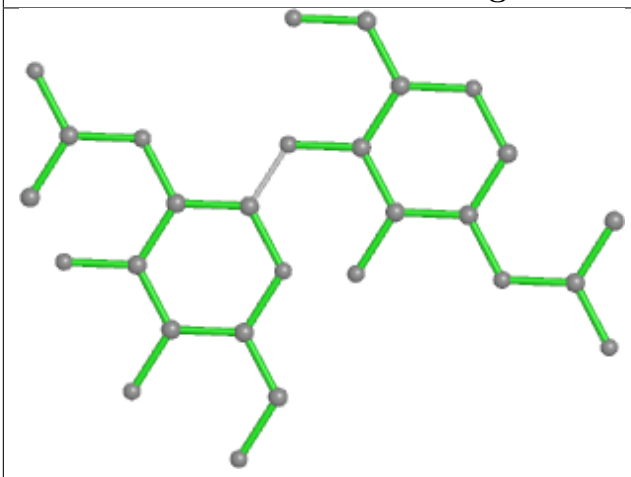


Torsions

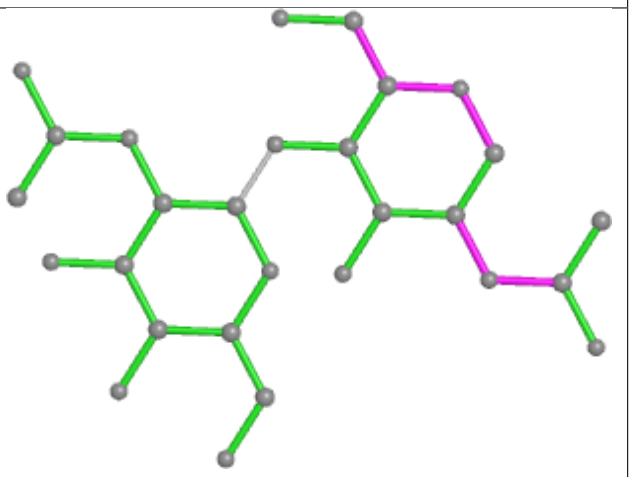


Rings

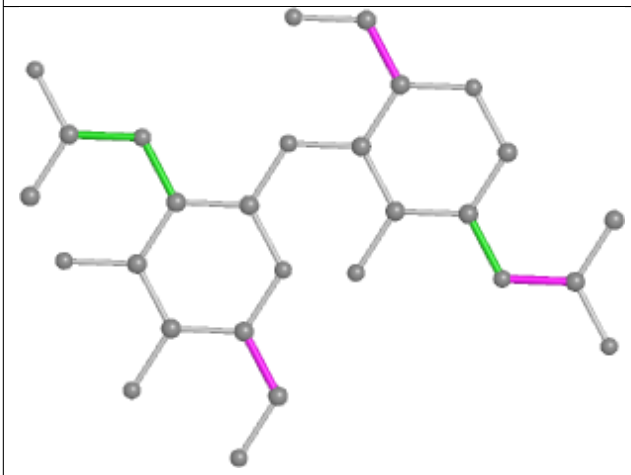
Oligosaccharide Chain W



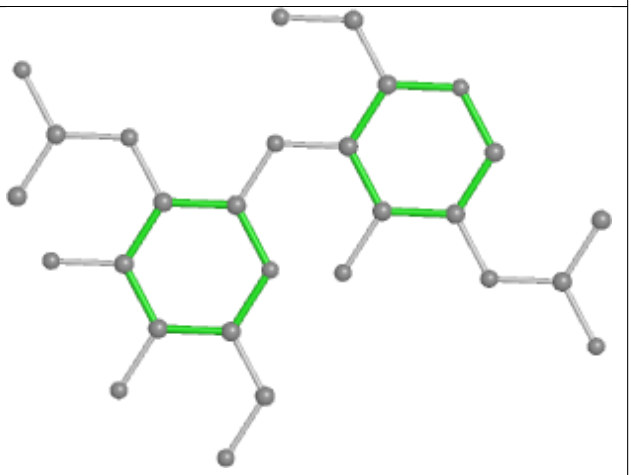
Bond lengths



Bond angles

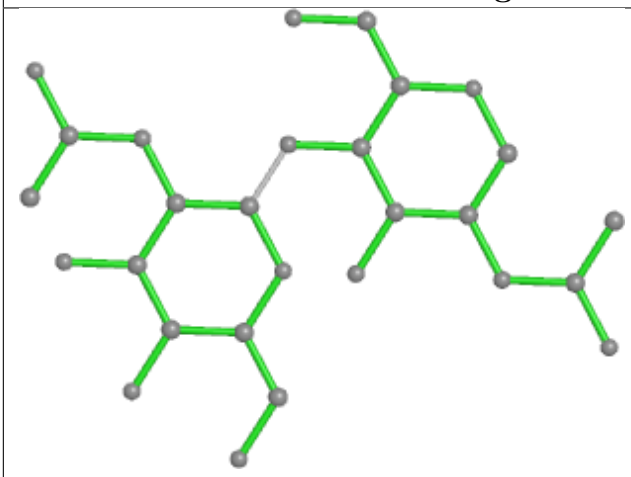


Torsions

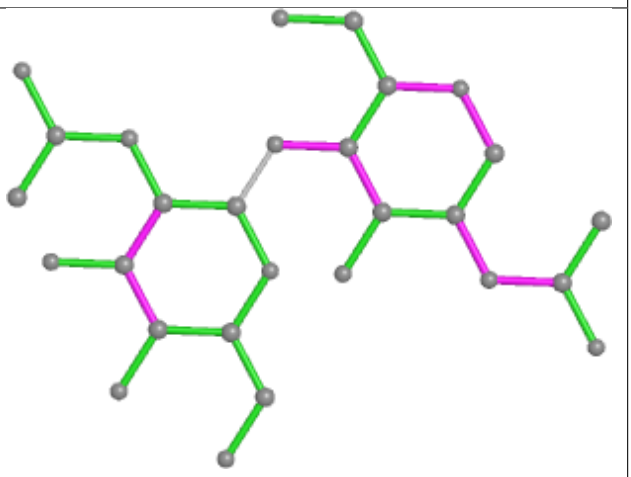


Rings

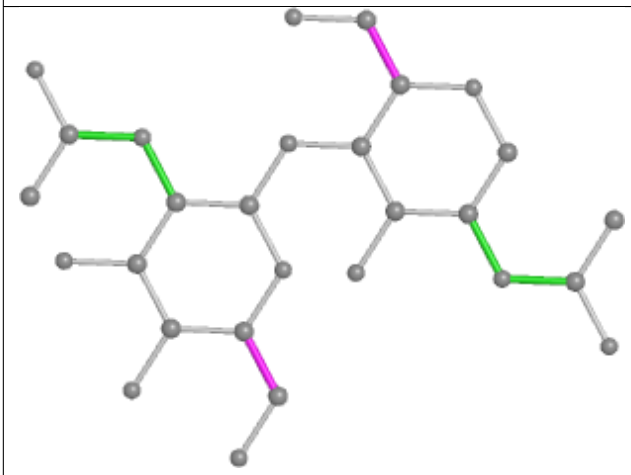
Oligosaccharide Chain X



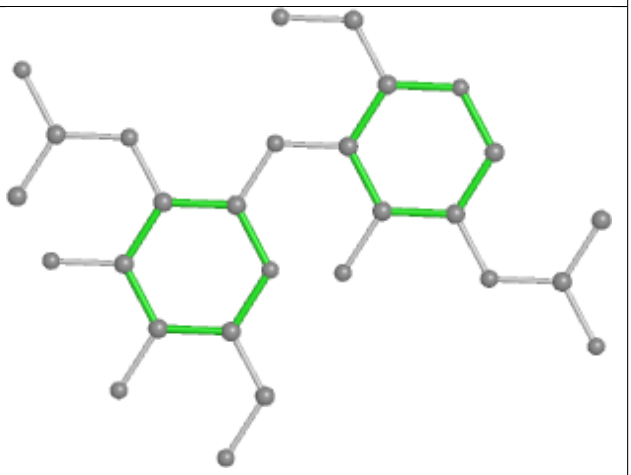
Bond lengths



Bond angles

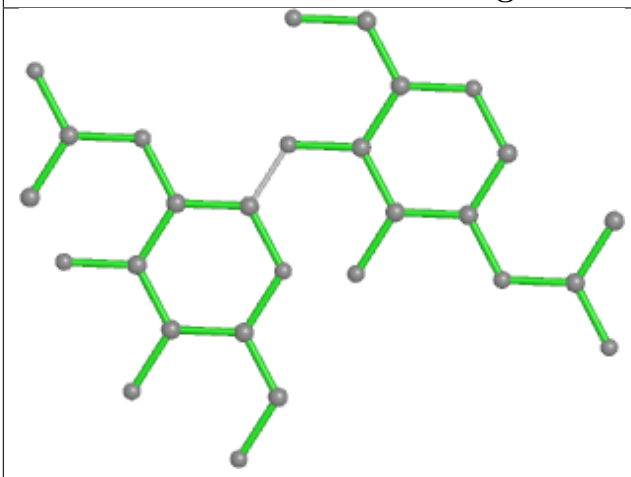


Torsions

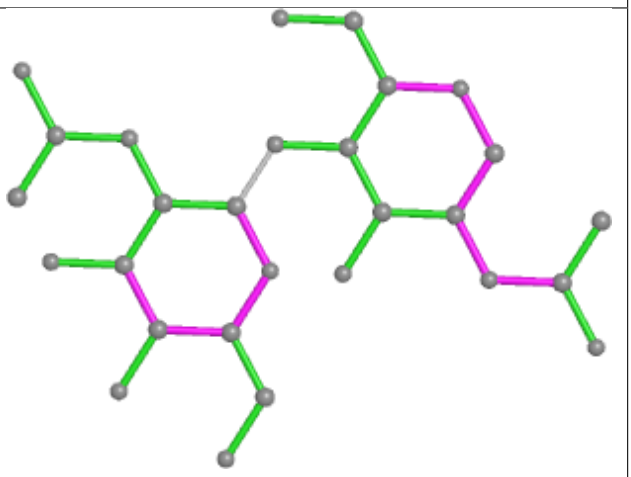


Rings

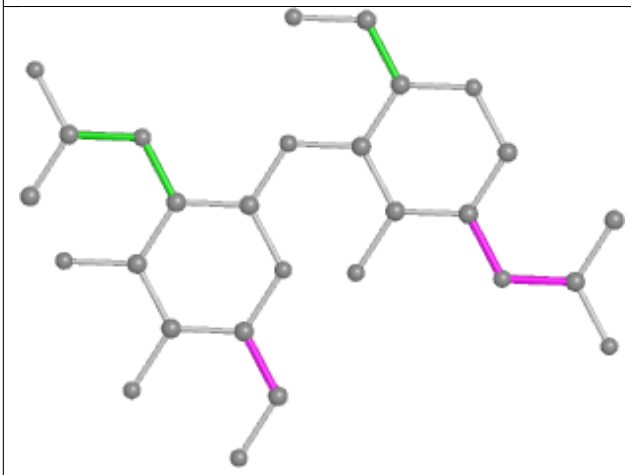
Oligosaccharide Chain Z



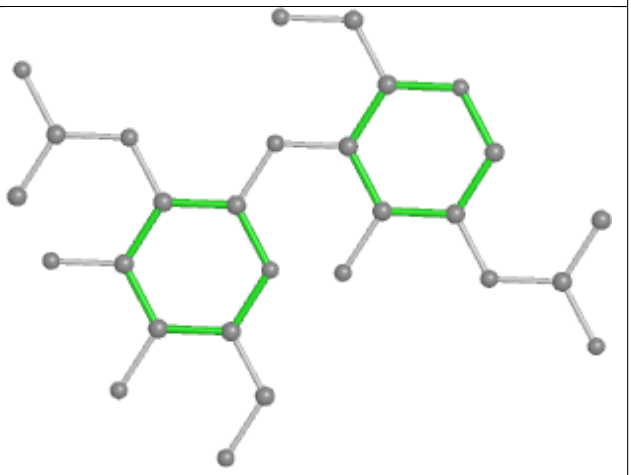
Bond lengths



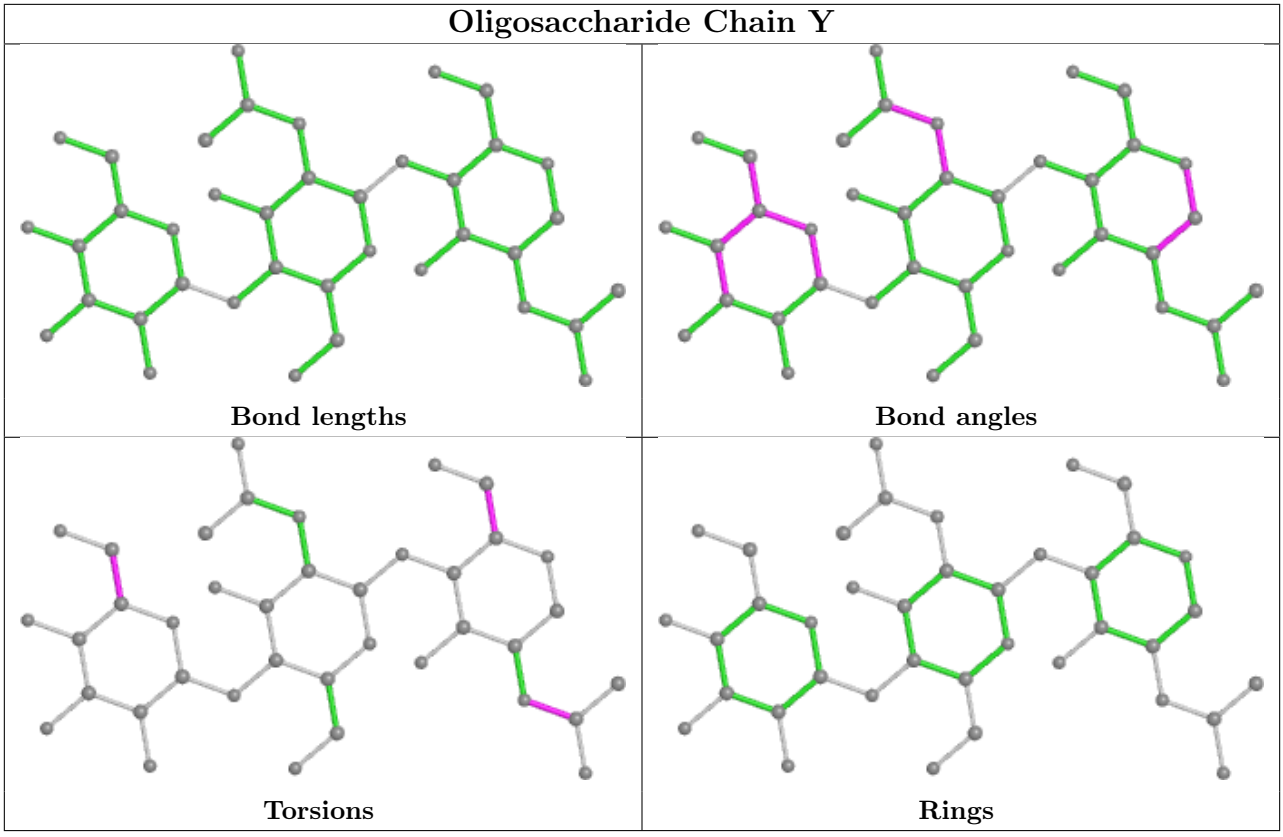
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	2004	1	14,14,15	0.40	0	17,19,21	0.77	0
5	NAG	M	2003	1	14,14,15	0.45	0	17,19,21	0.82	0
5	NAG	O	2001	1	14,14,15	0.47	0	17,19,21	1.49	2 (11%)
5	NAG	M	2004	1	14,14,15	0.52	0	17,19,21	0.81	0
5	NAG	O	2002	1	14,14,15	0.40	0	17,19,21	1.48	3 (17%)
5	NAG	G	2001	1	14,14,15	0.46	0	17,19,21	1.40	1 (5%)
5	NAG	C	2003	1	14,14,15	0.58	0	17,19,21	1.63	3 (17%)
5	NAG	G	2002	1	14,14,15	0.47	0	17,19,21	1.73	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	2001	1	14,14,15	0.48	0	17,19,21	1.10	2 (11%)
5	NAG	A	2003	1	14,14,15	0.60	0	17,19,21	1.89	6 (35%)
5	NAG	K	2003	1	14,14,15	0.61	0	17,19,21	1.64	3 (17%)
5	NAG	I	2003	1	14,14,15	0.46	0	17,19,21	1.19	1 (5%)
5	NAG	K	2004	1	14,14,15	0.43	0	17,19,21	1.24	2 (11%)
5	NAG	Q	2004	1	14,14,15	0.53	0	17,19,21	1.31	2 (11%)

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
5	NAG	E	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	M	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	O	2001	1	-	4/6/23/26	0/1/1/1
5	NAG	M	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	O	2002	1	-	0/6/23/26	0/1/1/1
5	NAG	G	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	G	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	E	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
5	NAG	K	2003	1	-	4/6/23/26	0/1/1/1
5	NAG	I	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	K	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	Q	2004	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	2002	NAG	C1-O5-C5	6.24	120.64	112.19
5	O	2001	NAG	C1-O5-C5	4.77	118.65	112.19
5	G	2001	NAG	C1-O5-C5	4.44	118.20	112.19
5	A	2003	NAG	C4-C3-C2	4.24	117.23	111.02
5	K	2003	NAG	O4-C4-C5	-4.06	99.22	109.30
5	I	2003	NAG	C1-O5-C5	3.82	117.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	2004	NAG	C1-O5-C5	3.79	117.33	112.19
5	C	2003	NAG	C3-C4-C5	3.74	116.92	110.24
5	A	2003	NAG	O5-C1-C2	-3.61	105.58	111.29
5	O	2002	NAG	C1-O5-C5	3.54	116.99	112.19
5	K	2004	NAG	C1-O5-C5	3.34	116.71	112.19
5	A	2003	NAG	C3-C4-C5	2.87	115.35	110.24
5	K	2004	NAG	C2-N2-C7	-2.69	119.07	122.90
5	C	2003	NAG	C4-C3-C2	2.67	114.93	111.02
5	C	2003	NAG	C1-O5-C5	2.66	115.80	112.19
5	E	2001	NAG	O5-C5-C6	2.59	111.26	107.20
5	E	2001	NAG	C1-O5-C5	2.49	115.56	112.19
5	O	2001	NAG	O5-C5-C6	2.38	110.93	107.20
5	A	2003	NAG	O3-C3-C2	-2.33	104.64	109.47
5	K	2003	NAG	C3-C4-C5	2.31	114.37	110.24
5	K	2003	NAG	O3-C3-C2	-2.25	104.80	109.47
5	O	2002	NAG	O5-C1-C2	-2.25	107.74	111.29
5	Q	2004	NAG	O5-C5-C6	2.24	110.72	107.20
5	O	2002	NAG	O5-C5-C6	2.21	110.67	107.20
5	A	2003	NAG	O4-C4-C5	-2.09	104.11	109.30
5	A	2003	NAG	C1-C2-N2	2.05	113.99	110.49

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2003	NAG	C8-C7-N2-C2
5	A	2003	NAG	O7-C7-N2-C2
5	E	2001	NAG	O7-C7-N2-C2
5	E	2004	NAG	C8-C7-N2-C2
5	E	2004	NAG	O7-C7-N2-C2
5	I	2003	NAG	O7-C7-N2-C2
5	M	2003	NAG	C8-C7-N2-C2
5	M	2003	NAG	O7-C7-N2-C2
5	O	2001	NAG	C8-C7-N2-C2
5	O	2001	NAG	O7-C7-N2-C2
5	E	2001	NAG	C8-C7-N2-C2
5	G	2002	NAG	O7-C7-N2-C2
5	I	2003	NAG	C8-C7-N2-C2
5	Q	2004	NAG	O5-C5-C6-O6
5	G	2002	NAG	C8-C7-N2-C2
5	K	2004	NAG	C8-C7-N2-C2
5	K	2004	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	K	2003	NAG	C4-C5-C6-O6
5	K	2003	NAG	O5-C5-C6-O6
5	K	2003	NAG	C8-C7-N2-C2
5	K	2003	NAG	O7-C7-N2-C2
5	Q	2004	NAG	C4-C5-C6-O6
5	O	2001	NAG	C4-C5-C6-O6
5	O	2001	NAG	O5-C5-C6-O6
5	G	2001	NAG	C8-C7-N2-C2
5	K	2004	NAG	C1-C2-N2-C7
5	Q	2004	NAG	C8-C7-N2-C2
5	G	2001	NAG	O7-C7-N2-C2
5	A	2003	NAG	C4-C5-C6-O6
5	Q	2004	NAG	O7-C7-N2-C2
5	K	2004	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2004	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	323/334 (96%)	0.15	7 (2%) 62 56	62, 86, 117, 157	0
1	C	323/334 (96%)	0.41	23 (7%) 16 11	69, 102, 130, 161	0
1	E	323/334 (96%)	0.26	17 (5%) 26 20	67, 94, 121, 167	0
1	G	323/334 (96%)	0.21	3 (0%) 84 82	63, 85, 112, 148	0
1	I	323/334 (96%)	0.07	3 (0%) 84 82	46, 80, 100, 138	0
1	K	323/334 (96%)	0.30	14 (4%) 35 28	52, 93, 121, 164	0
1	M	323/334 (96%)	0.50	27 (8%) 11 7	79, 112, 143, 176	0
1	O	323/334 (96%)	0.29	18 (5%) 24 19	65, 102, 130, 154	0
1	Q	323/334 (96%)	0.07	5 (1%) 73 70	61, 82, 107, 135	0
2	B	173/182 (95%)	0.26	3 (1%) 70 66	54, 83, 115, 159	0
2	D	173/182 (95%)	0.33	4 (2%) 60 54	62, 91, 124, 171	0
2	F	173/182 (95%)	0.92	18 (10%) 6 4	57, 104, 165, 216	0
2	H	173/182 (95%)	0.75	15 (8%) 10 7	62, 101, 155, 194	0
2	J	173/182 (95%)	0.19	2 (1%) 79 76	58, 84, 120, 167	0
2	L	173/182 (95%)	0.62	11 (6%) 19 14	64, 101, 153, 167	0
2	N	173/182 (95%)	0.46	5 (2%) 51 45	69, 97, 135, 155	0
2	P	173/182 (95%)	0.56	6 (3%) 44 36	63, 91, 126, 181	0
2	R	173/182 (95%)	0.20	1 (0%) 89 88	61, 79, 106, 147	0
All	All	4464/4644 (96%)	0.33	182 (4%) 37 30	46, 91, 134, 216	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	PRO	10.1
2	P	173	ILE	8.6
2	F	140	PHE	8.0

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Mol	Chain	Res	Type	RSRZ
1	E	9	PRO	7.0
2	H	173	ILE	6.8
2	F	164	GLU	6.3
2	H	140	PHE	6.1
2	L	150	GLU	6.0
2	F	149	MET	5.4
1	K	176	LEU	5.3
1	C	9	PRO	4.9
1	K	9	PRO	4.9
1	E	173	GLN	4.8
1	O	9	PRO	4.6
2	F	141	TYR	4.6
1	M	9	PRO	4.4
1	M	270	SER	4.4
1	M	100	GLY	4.3
2	H	153	LYS	4.2
1	M	228	GLY	4.2
2	F	29	GLU	4.1
2	F	168	LEU	4.1
1	I	9	PRO	4.0
2	H	149	MET	3.9
1	C	257	ALA	3.9
1	C	276	ASN	3.9
1	M	272	LEU	3.8
2	F	33	GLY	3.8
1	C	51	LEU	3.8
2	N	153	LYS	3.8
1	E	240	ASN	3.7
1	Q	118	PHE	3.7
2	H	139	GLU	3.7
1	O	251	PHE	3.6
1	A	9	PRO	3.6
1	Q	9	PRO	3.5
2	P	152	VAL	3.5
1	O	123	ILE	3.5
1	O	240	ASN	3.5
1	C	151	VAL	3.5
1	C	134	GLY	3.5
2	H	164	GLU	3.3
2	N	1	GLY	3.3
1	M	179	LEU	3.3
1	E	11	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	144	CYS	3.3
2	F	126	LEU	3.3
2	F	173	ILE	3.3
1	M	222	LYS	3.3
1	M	118	PHE	3.3
1	A	55(A)	GLY	3.2
1	C	260(A)	VAL	3.2
1	C	61	LEU	3.2
2	L	153	LYS	3.2
2	D	172	GLU	3.2
2	L	157	TYR	3.1
2	H	168	LEU	3.1
1	O	121	ILE	3.1
1	E	260(A)	VAL	3.1
1	K	51	LEU	3.1
2	L	167	ARG	3.1
1	K	160	ALA	3.1
2	H	166	ALA	3.1
2	D	173	ILE	3.0
1	C	160	ALA	3.0
1	M	212	ARG	3.0
1	E	87	ILE	3.0
2	H	138	PHE	3.0
2	B	172	GLU	3.0
2	P	149	MET	3.0
1	I	176	LEU	3.0
1	K	112	LEU	2.9
2	F	171	GLU	2.9
2	P	29	GLU	2.9
1	M	123	ILE	2.9
1	O	239	PRO	2.9
1	E	51	LEU	2.9
2	J	1	GLY	2.8
2	P	164	GLU	2.8
1	A	118	PHE	2.8
1	C	179	LEU	2.8
1	A	272	LEU	2.7
1	C	288	ILE	2.7
1	M	302	ILE	2.7
1	M	223	VAL	2.7
2	F	167	ARG	2.7
1	E	302	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	272	LEU	2.7
2	N	24	TYR	2.7
1	E	121	ILE	2.7
2	F	145	ASP	2.7
2	F	139	GLU	2.6
1	C	39	ALA	2.6
1	C	144	ARG	2.6
1	E	257	ALA	2.6
2	L	164	GLU	2.6
2	H	141	TYR	2.6
2	H	21	TRP	2.6
2	H	126	LEU	2.6
1	O	161	TYR	2.6
1	E	61	LEU	2.5
1	E	118	PHE	2.5
1	E	69	TRP	2.5
2	N	29	GLU	2.5
1	M	276	ASN	2.5
1	C	270	SER	2.5
1	I	103	ASN	2.5
2	B	33	GLY	2.5
1	K	54	LEU	2.5
1	M	51	LEU	2.5
2	F	106	ARG	2.5
1	A	51	LEU	2.4
1	C	282	GLN	2.4
1	K	324	PRO	2.4
2	B	173	ILE	2.4
2	F	129	ASN	2.4
2	H	29	GLU	2.4
2	D	153	LYS	2.4
1	O	195	TYR	2.4
1	M	79	PHE	2.4
2	L	31	GLY	2.4
2	L	140	PHE	2.4
1	M	154	LEU	2.4
2	L	27	SER	2.3
2	L	26	HIS	2.3
1	Q	300	LEU	2.3
1	K	50	LYS	2.3
1	C	272	LEU	2.3
1	C	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	102	PHE	2.3
2	J	152	VAL	2.3
2	H	130	ALA	2.3
1	O	171	THR	2.3
1	M	140	PRO	2.3
1	M	229	ARG	2.2
1	E	178	VAL	2.2
2	D	105	GLU	2.2
1	E	242	ALA	2.2
2	L	173	ILE	2.2
1	O	118	PHE	2.2
1	O	245	PHE	2.2
2	H	162	TYR	2.2
1	O	266	ALA	2.2
2	R	173	ILE	2.2
1	M	209	LEU	2.2
1	M	282	GLN	2.2
1	K	286	GLY	2.2
1	M	288	ILE	2.2
1	M	54	LEU	2.2
1	O	84	TRP	2.2
1	G	60	ILE	2.2
1	O	79	PHE	2.2
1	G	272	LEU	2.2
1	M	85	SER	2.2
1	K	217	ILE	2.1
2	F	15	GLN	2.1
2	F	170	ARG	2.1
1	E	274	TYR	2.1
1	M	60	ILE	2.1
2	L	172	GLU	2.1
2	P	144	CYS	2.1
1	C	297	ILE	2.1
1	K	288	ILE	2.1
1	A	280	LYS	2.1
1	K	285	MET	2.1
1	O	261	LYS	2.1
1	M	224	ASN	2.1
1	K	282	GLN	2.1
1	C	277	CYS	2.1
1	A	57	LYS	2.1
1	Q	88	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	260	ILE	2.0
1	K	62	ARG	2.0
2	N	112	ASP	2.0
1	C	57	LYS	2.0
1	O	260(A)	VAL	2.0
1	M	112	LEU	2.0
1	O	112	LEU	2.0
1	O	154	LEU	2.0
1	E	273	GLU	2.0
1	C	196	GLN	2.0
1	C	324	PRO	2.0

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

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

6.3 Carbohydrates (i)

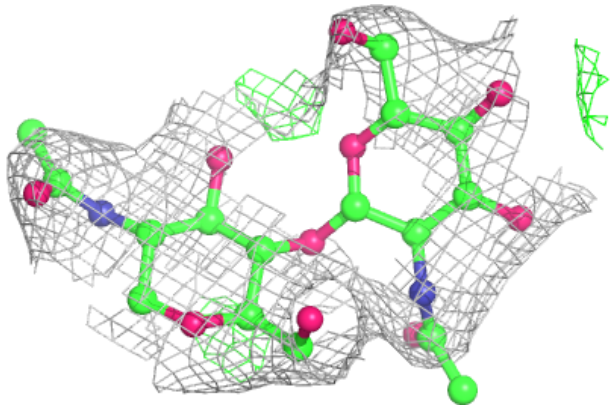
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

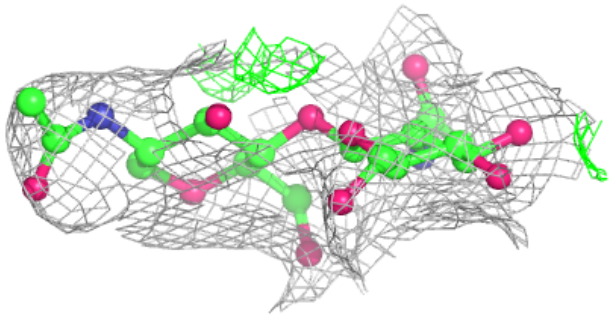
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	U	2	14/15	0.80	0.35	135,145,154,158	0
3	NAG	S	2	14/15	0.81	0.24	121,139,156,167	0
3	NAG	X	2	14/15	0.82	0.19	144,161,171,177	0
4	MAN	Y	3	11/12	0.84	0.32	143,164,169,173	0
3	NAG	U	1	14/15	0.86	0.16	92,126,137,139	0
3	NAG	T	2	14/15	0.86	0.24	109,132,145,152	0
4	NAG	Y	2	14/15	0.87	0.20	122,141,155,162	0
3	NAG	Z	1	14/15	0.88	0.31	96,115,120,135	0
3	NAG	V	2	14/15	0.89	0.20	111,122,137,152	0
3	NAG	W	2	14/15	0.90	0.17	123,135,150,165	0
3	NAG	Z	2	14/15	0.91	0.22	119,142,154,163	0
3	NAG	T	1	14/15	0.92	0.12	82,103,115,116	0
3	NAG	X	1	14/15	0.93	0.10	91,109,123,143	0
3	NAG	V	1	14/15	0.93	0.12	68,84,96,98	0
4	NAG	Y	1	14/15	0.95	0.12	86,104,121,126	0
3	NAG	S	1	14/15	0.96	0.12	85,105,126,131	0
3	NAG	W	1	14/15	0.96	0.08	74,93,106,109	0

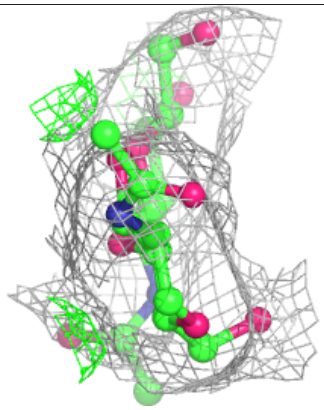
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

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

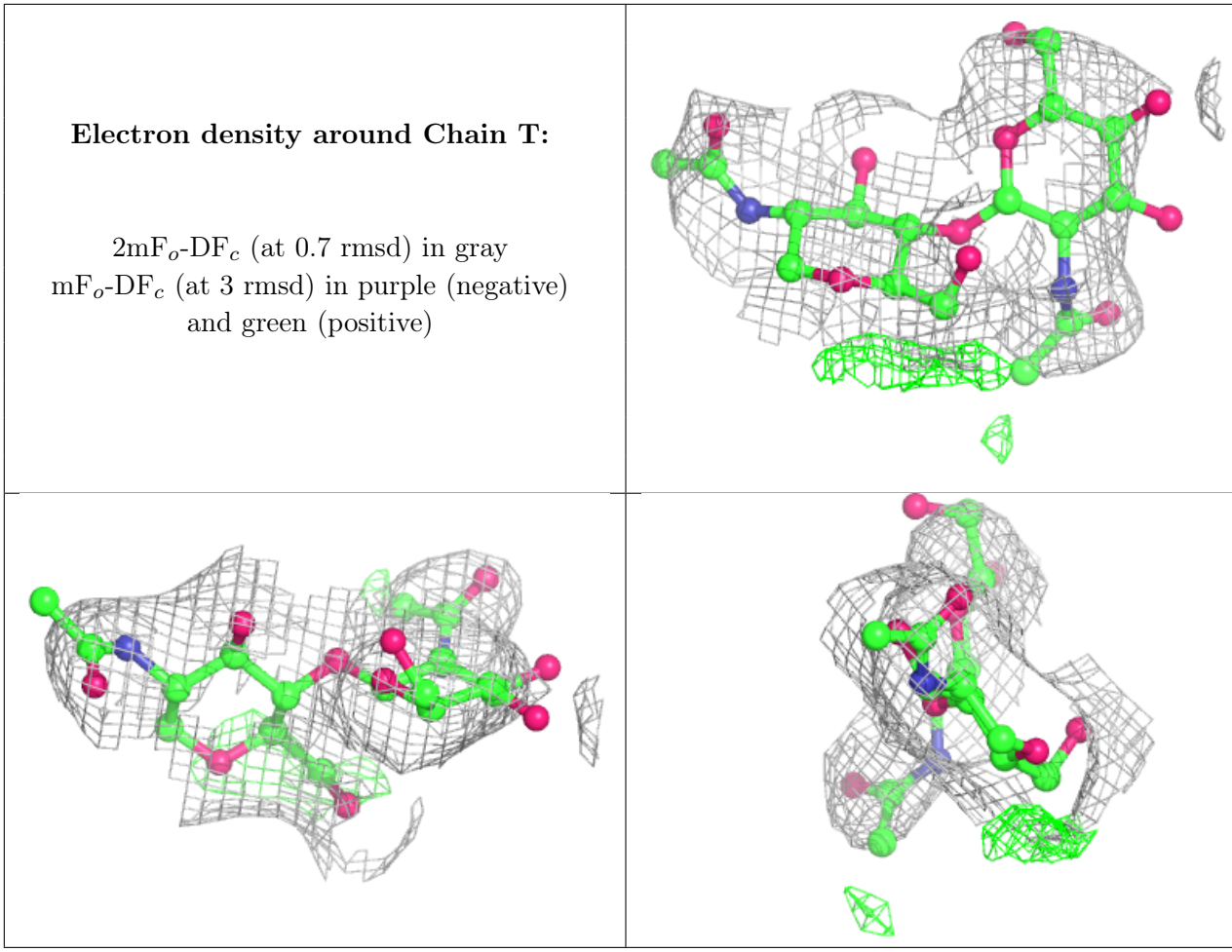






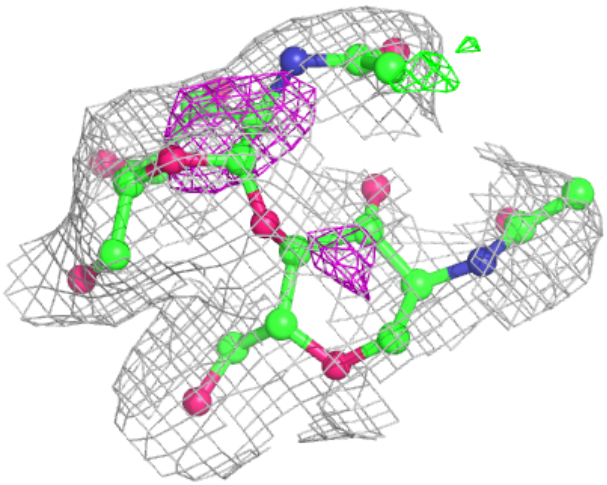
Electron density around Chain T:

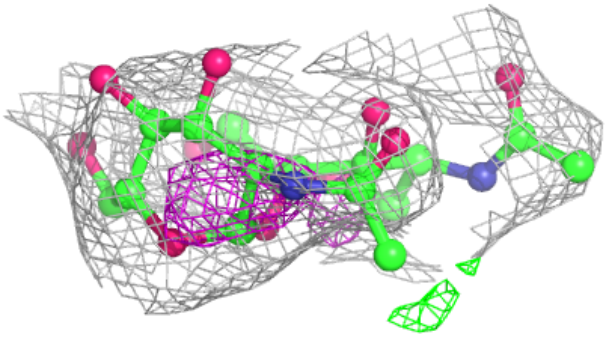
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

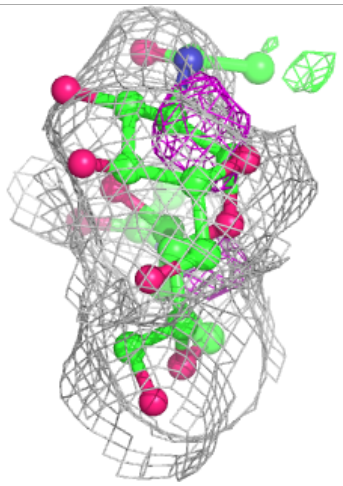


Electron density around Chain U:

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

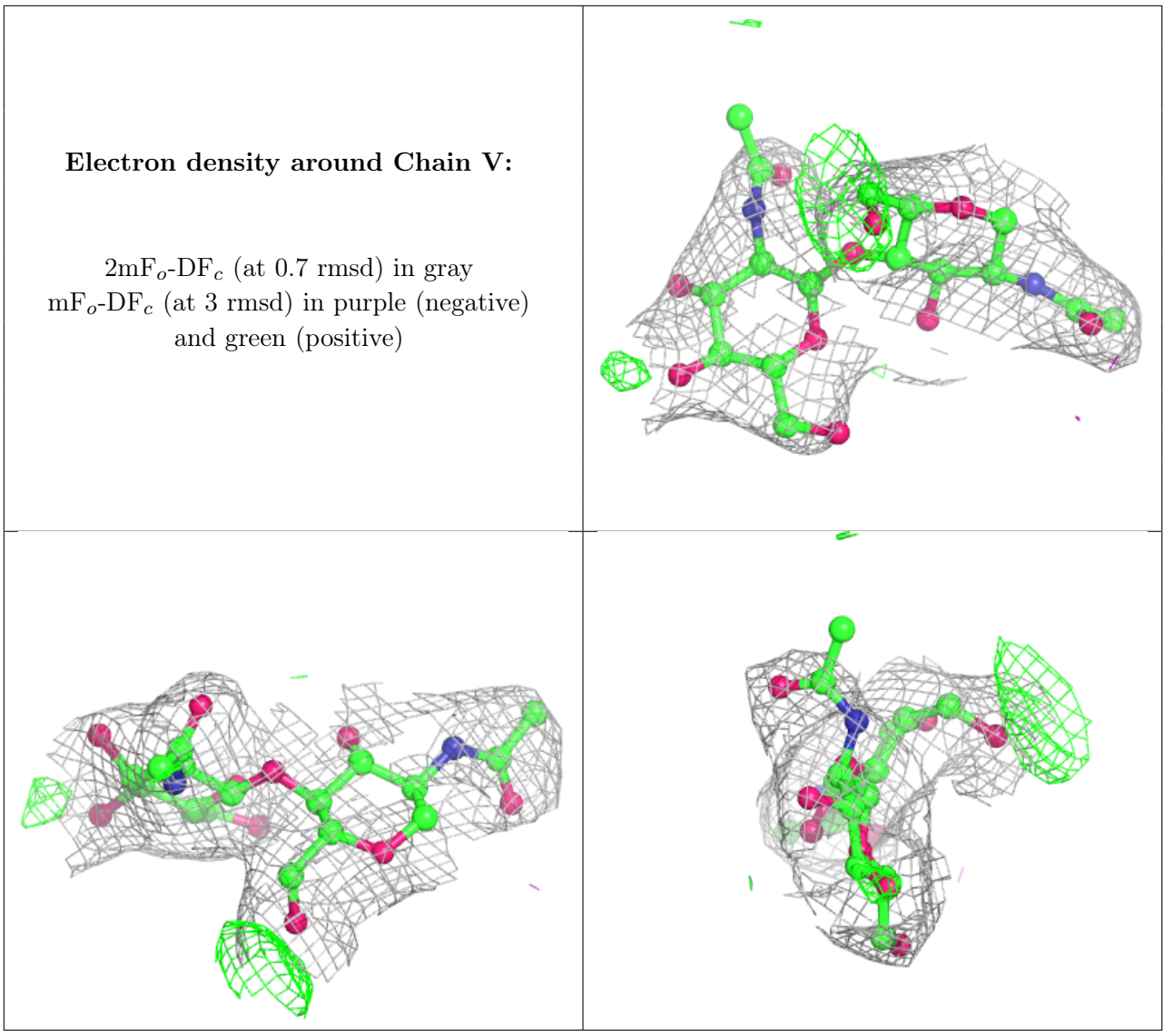






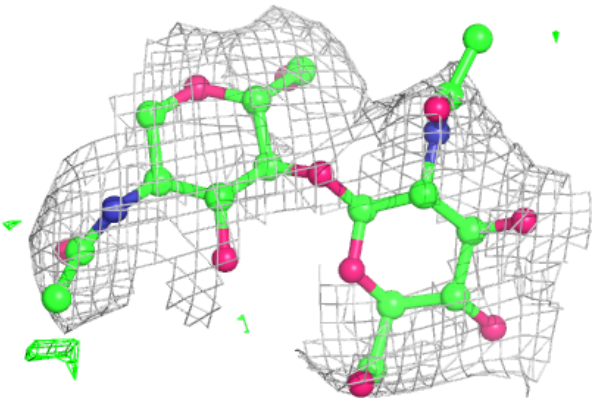
Electron density around Chain V:

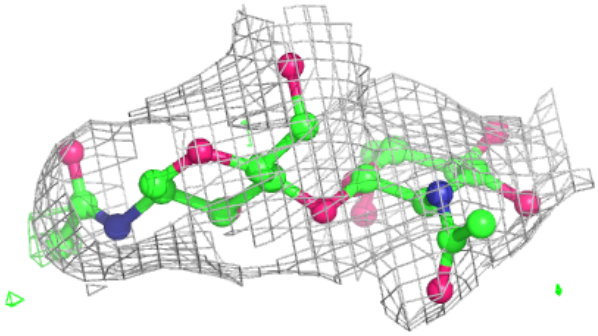
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

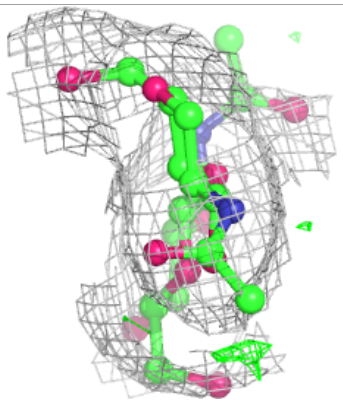


Electron density around Chain W:

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

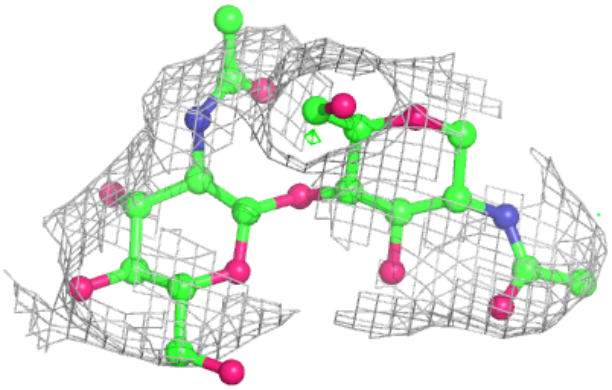


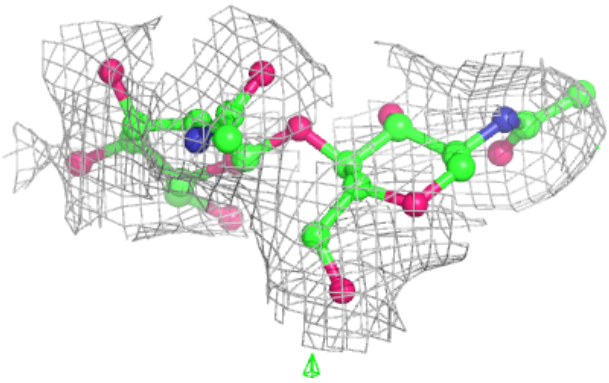


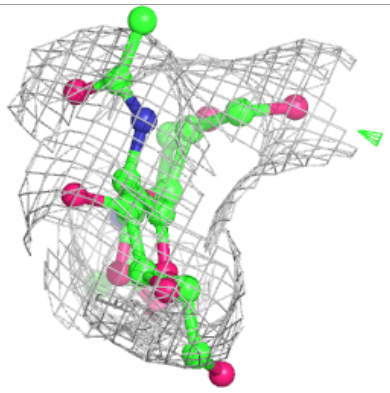


Electron density around Chain X:

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

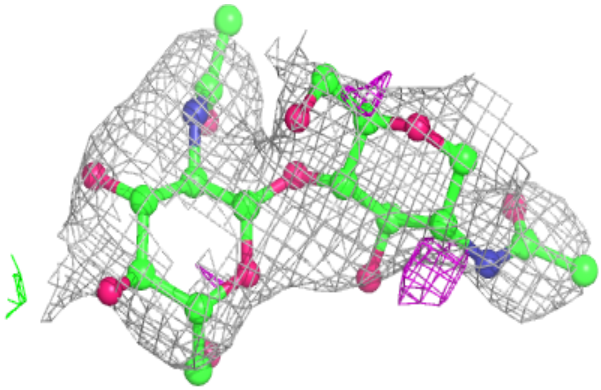


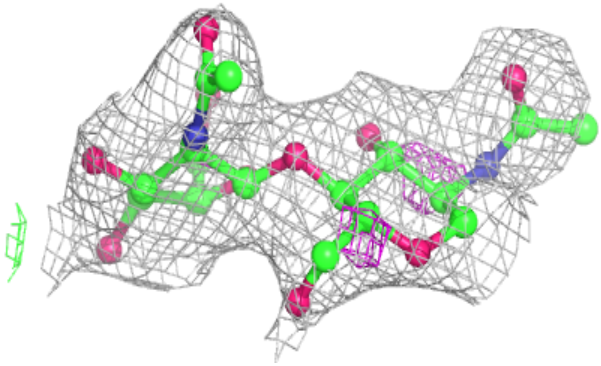


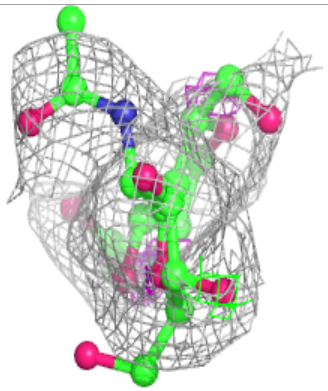


Electron density around Chain Z:

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

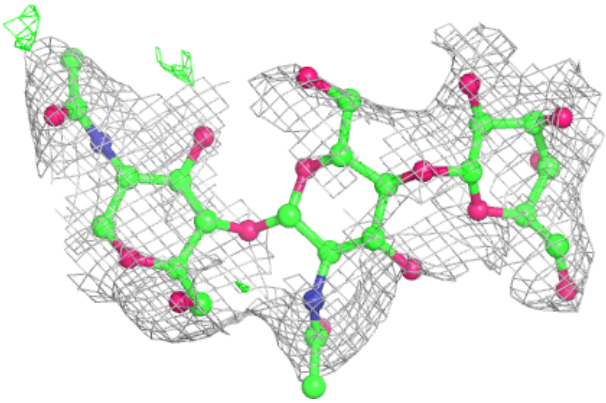


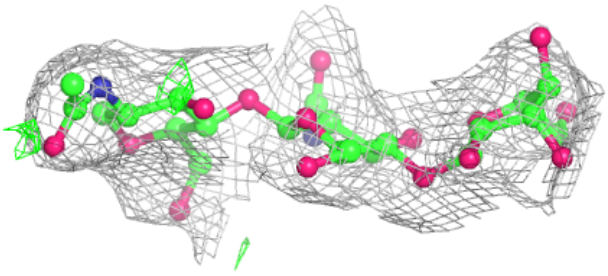


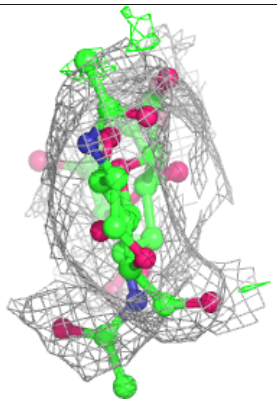


Electron density around Chain Y:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	K	2004	14/15	0.74	0.23	133,149,159,163	0
5	NAG	E	2004	14/15	0.81	0.22	119,136,150,151	0
5	NAG	K	2003	14/15	0.82	0.19	103,125,134,148	0
5	NAG	E	2001	14/15	0.84	0.30	103,118,138,158	0
5	NAG	M	2004	14/15	0.84	0.33	112,151,162,166	0
5	NAG	Q	2004	14/15	0.84	0.20	115,127,133,135	0
5	NAG	O	2001	14/15	0.86	0.18	75,105,120,122	0
5	NAG	A	2003	14/15	0.86	0.20	102,127,143,157	0
5	NAG	C	2003	14/15	0.88	0.31	115,124,136,149	0
5	NAG	M	2003	14/15	0.90	0.16	112,129,135,138	0
5	NAG	G	2001	14/15	0.91	0.15	86,106,114,116	0
5	NAG	G	2002	14/15	0.91	0.14	107,124,130,133	0
5	NAG	O	2002	14/15	0.91	0.12	92,112,118,125	0
5	NAG	I	2003	14/15	0.91	0.18	102,115,121,121	0

6.5 Other polymers (i)

There are no such residues in this entry.