



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 08:42 PM EDT

PDB ID : 3AL4  
Title : Crystal structure of the swine-origin A (H1N1)-2009 influenza A virus hemagglutinin (HA) reveals similar antigenicity to that of the 1918 pandemic virus  
Authors : Zhang, W.; Qi, J.X.; Shi, Y.; Li, Q.; Yan, J.H.; Gao, G.F.  
Deposited on : 2010-07-22  
Resolution : 2.87 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](mailto: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>.

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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 : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

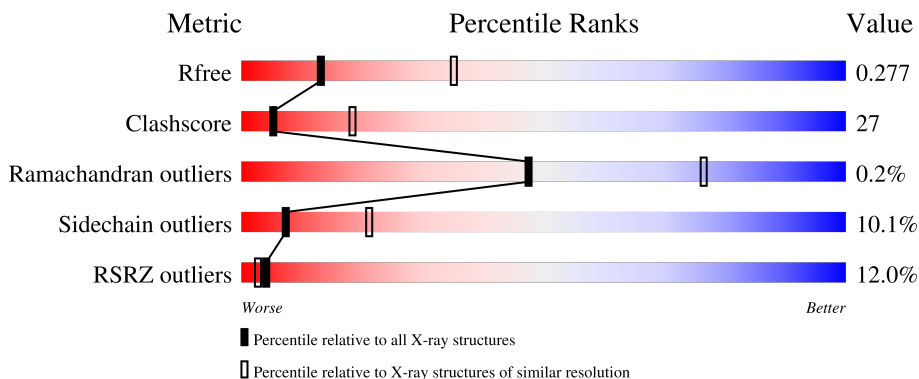
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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  $\geq 3$ , 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	333	
1	C	333	
1	E	333	
1	G	333	
1	I	333	

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Mol	Chain	Length	Quality of chain
1	K	333	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
3	M	2	
3	N	2	
3	P	2	
3	Q	2	
3	S	2	
4	O	3	
4	R	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	2	-	-	-	X
3	NAG	N	2	-	-	-	X
3	NAG	Q	2	-	-	-	X
5	NAG	A	606	-	-	-	X
5	NAG	C	601	-	-	-	X
5	NAG	C	607	-	-	-	X
5	NAG	E	601	-	-	-	X
5	NAG	E	604	-	-	-	X
5	NAG	E	605	-	-	-	X
5	NAG	F	601	-	-	-	X
5	NAG	G	602	-	-	-	X
5	NAG	G	603	-	-	-	X
5	NAG	K	603	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	NAG	K	604	-	-	-	X
5	NAG	L	601	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23626 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2505	1584	433	477	11	0	0	0
1	C	321	2509	1586	433	479	11	0	0	0
1	E	321	2509	1586	433	479	11	0	0	0
1	G	321	2505	1584	433	477	11	0	0	0
1	I	321	2509	1586	433	479	11	0	0	0
1	K	321	2511	1588	433	479	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP C3W5S1
A	2	ASP	-	expression tag	UNP C3W5S1
A	3	LEU	-	expression tag	UNP C3W5S1
A	4	GLY	-	expression tag	UNP C3W5S1
A	5	SER	-	expression tag	UNP C3W5S1
A	6	ARG	-	expression tag	UNP C3W5S1
C	1	ALA	-	expression tag	UNP C3W5S1
C	2	ASP	-	expression tag	UNP C3W5S1
C	3	LEU	-	expression tag	UNP C3W5S1
C	4	GLY	-	expression tag	UNP C3W5S1
C	5	SER	-	expression tag	UNP C3W5S1
C	6	ARG	-	expression tag	UNP C3W5S1
E	1	ALA	-	expression tag	UNP C3W5S1
E	2	ASP	-	expression tag	UNP C3W5S1
E	3	LEU	-	expression tag	UNP C3W5S1
E	4	GLY	-	expression tag	UNP C3W5S1
E	5	SER	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	ARG	-	expression tag	UNP C3W5S1
G	1	ALA	-	expression tag	UNP C3W5S1
G	2	ASP	-	expression tag	UNP C3W5S1
G	3	LEU	-	expression tag	UNP C3W5S1
G	4	GLY	-	expression tag	UNP C3W5S1
G	5	SER	-	expression tag	UNP C3W5S1
G	6	ARG	-	expression tag	UNP C3W5S1
I	1	ALA	-	expression tag	UNP C3W5S1
I	2	ASP	-	expression tag	UNP C3W5S1
I	3	LEU	-	expression tag	UNP C3W5S1
I	4	GLY	-	expression tag	UNP C3W5S1
I	5	SER	-	expression tag	UNP C3W5S1
I	6	ARG	-	expression tag	UNP C3W5S1
K	1	ALA	-	expression tag	UNP C3W5S1
K	2	ASP	-	expression tag	UNP C3W5S1
K	3	LEU	-	expression tag	UNP C3W5S1
K	4	GLY	-	expression tag	UNP C3W5S1
K	5	SER	-	expression tag	UNP C3W5S1
K	6	ARG	-	expression tag	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	162	1305	822	220	257	6	0	0	0
2	D	162	1300	818	219	257	6	0	0	0
2	F	161	1302	821	219	256	6	0	0	0
2	H	162	1305	822	220	257	6	0	0	0
2	J	162	1305	822	220	257	6	0	0	0
2	L	161	1302	821	219	256	6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP C3W5S1
B	178	LEU	-	expression tag	UNP C3W5S1
B	179	VAL	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	PRO	-	expression tag	UNP C3W5S1
B	181	ARG	-	expression tag	UNP C3W5S1
D	177	ARG	-	expression tag	UNP C3W5S1
D	178	LEU	-	expression tag	UNP C3W5S1
D	179	VAL	-	expression tag	UNP C3W5S1
D	180	PRO	-	expression tag	UNP C3W5S1
D	181	ARG	-	expression tag	UNP C3W5S1
F	177	ARG	-	expression tag	UNP C3W5S1
F	178	LEU	-	expression tag	UNP C3W5S1
F	179	VAL	-	expression tag	UNP C3W5S1
F	180	PRO	-	expression tag	UNP C3W5S1
F	181	ARG	-	expression tag	UNP C3W5S1
H	177	ARG	-	expression tag	UNP C3W5S1
H	178	LEU	-	expression tag	UNP C3W5S1
H	179	VAL	-	expression tag	UNP C3W5S1
H	180	PRO	-	expression tag	UNP C3W5S1
H	181	ARG	-	expression tag	UNP C3W5S1
J	177	ARG	-	expression tag	UNP C3W5S1
J	178	LEU	-	expression tag	UNP C3W5S1
J	179	VAL	-	expression tag	UNP C3W5S1
J	180	PRO	-	expression tag	UNP C3W5S1
J	181	ARG	-	expression tag	UNP C3W5S1
L	177	ARG	-	expression tag	UNP C3W5S1
L	178	LEU	-	expression tag	UNP C3W5S1
L	179	VAL	-	expression tag	UNP C3W5S1
L	180	PRO	-	expression tag	UNP C3W5S1
L	181	ARG	-	expression tag	UNP C3W5S1

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



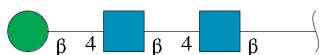
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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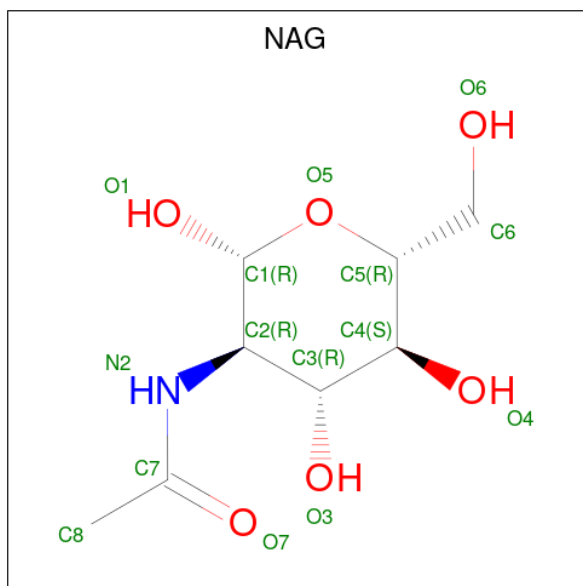
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
			Total	C	N	O			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	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	E	1	Total C N O 14 8 1 5	0	0
5	F	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	G	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	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	L	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	36	Total O 36 36	0	0
6	B	17	Total O 17 17	0	0
6	C	38	Total O 38 38	0	0
6	D	10	Total O 10 10	0	0
6	E	31	Total O 31 31	0	0

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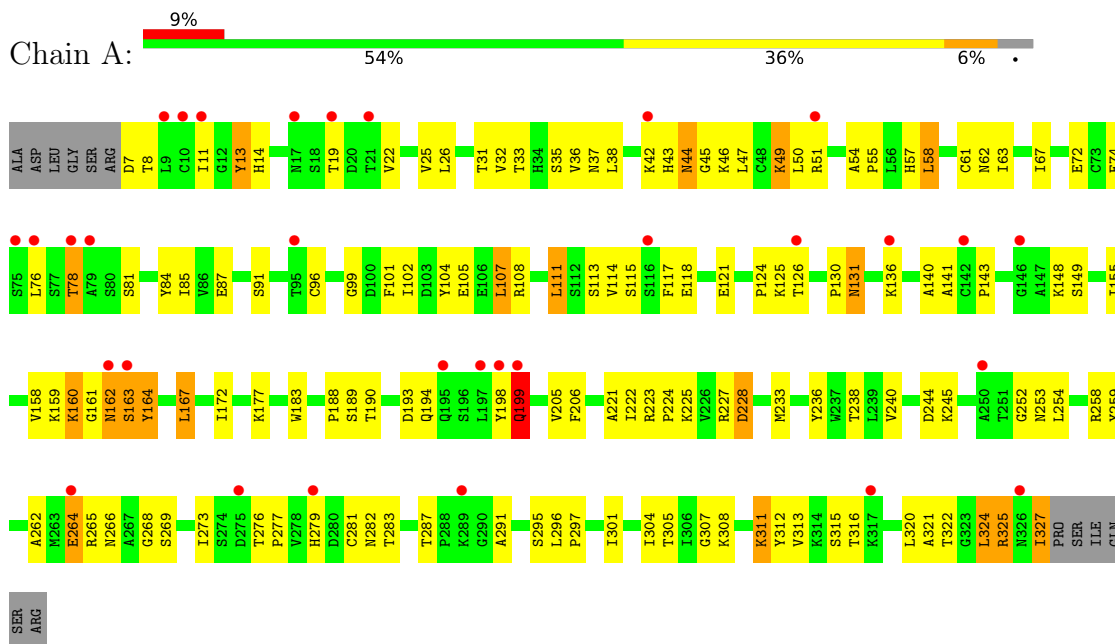
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	F	13	Total 13	O 13	0	0
6	G	45	Total 45	O 45	0	0
6	H	23	Total 23	O 23	0	0
6	I	37	Total 37	O 37	0	0
6	J	21	Total 21	O 21	0	0
6	K	35	Total 35	O 35	0	0
6	L	11	Total 11	O 11	0	0

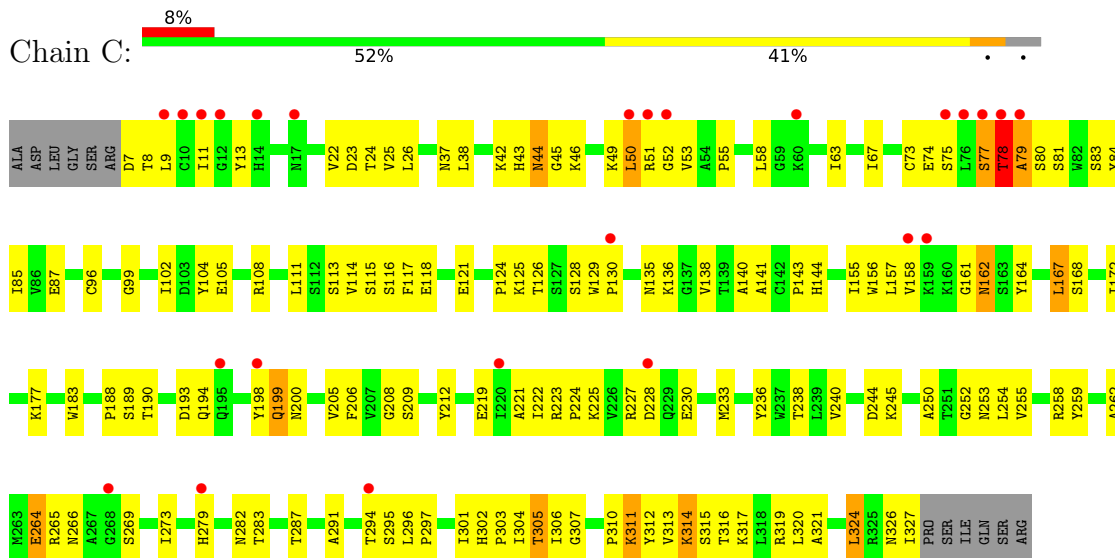
### 3 Residue-property plots

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.

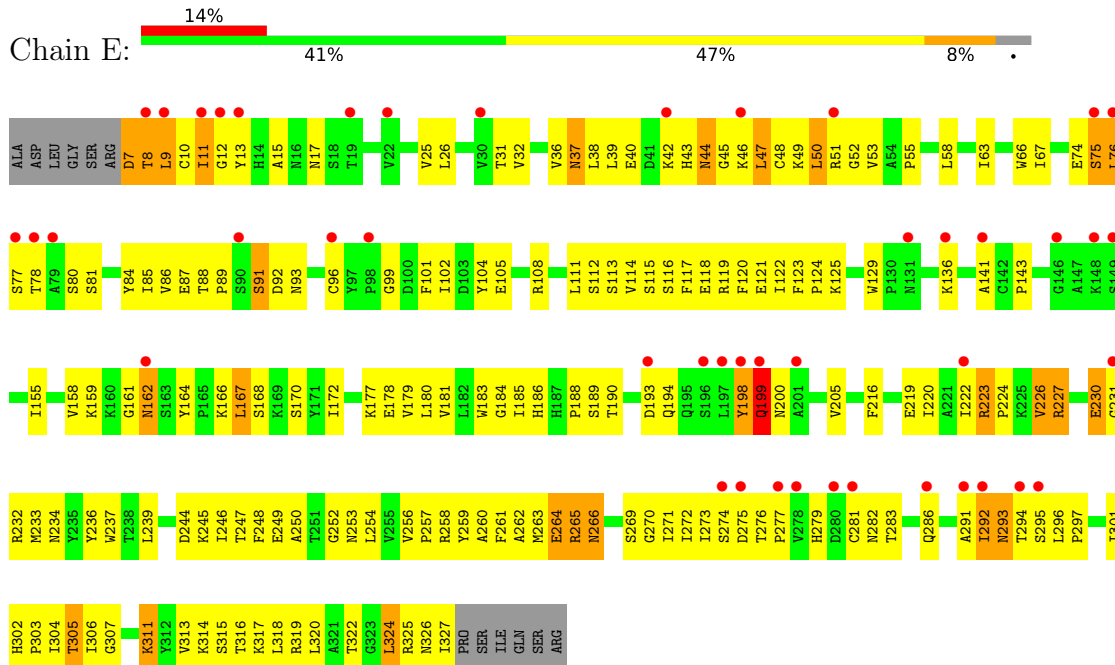
- Molecule 1: Hemagglutinin



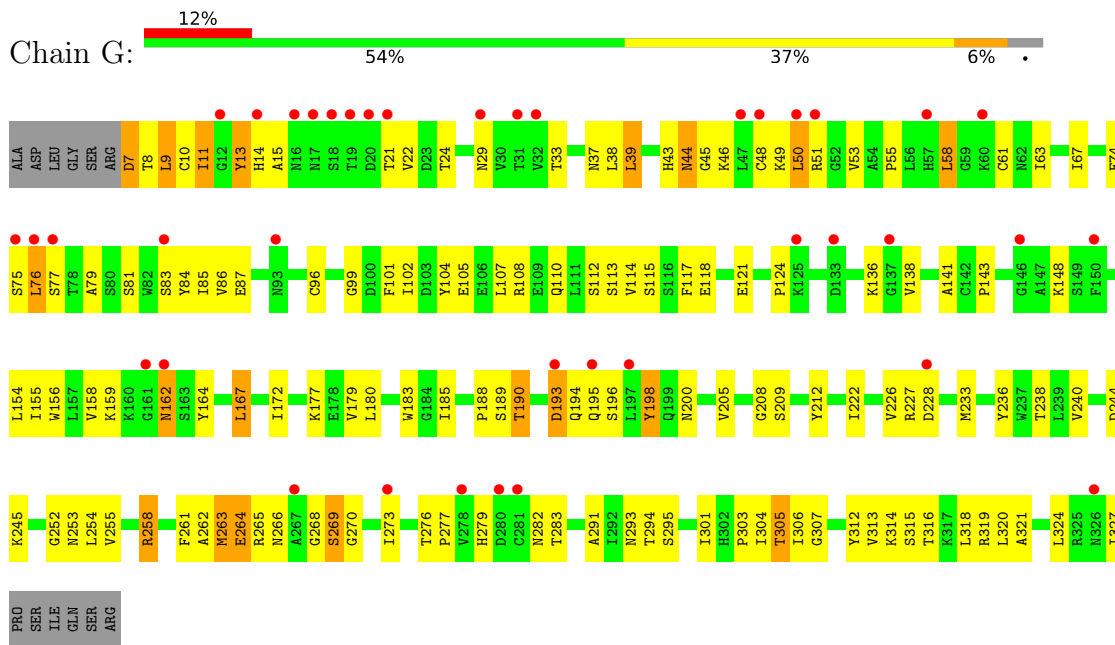
- Molecule 1: Hemagglutinin



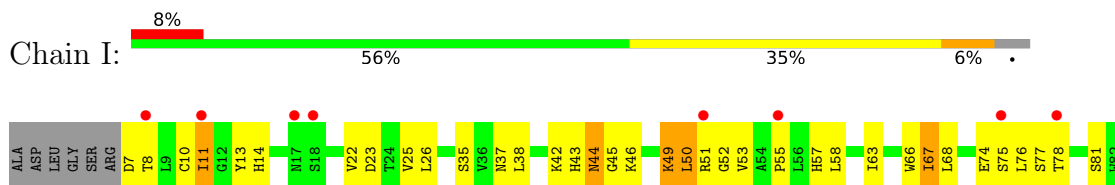
- Molecule 1: Hemagglutinin

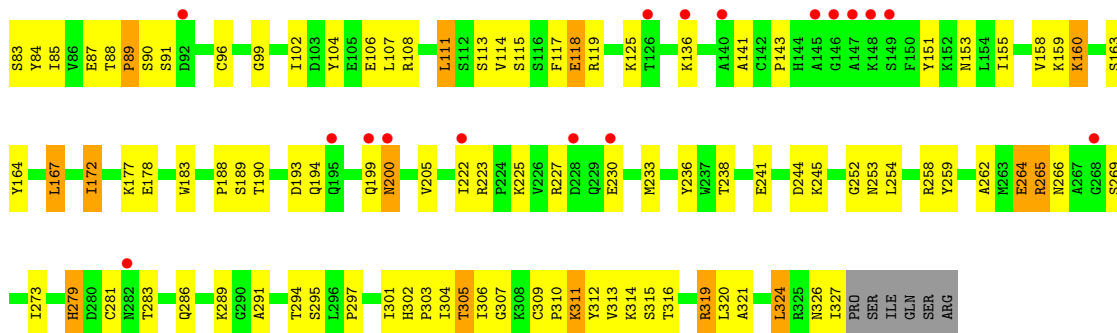


- Molecule 1: Hemagglutinin

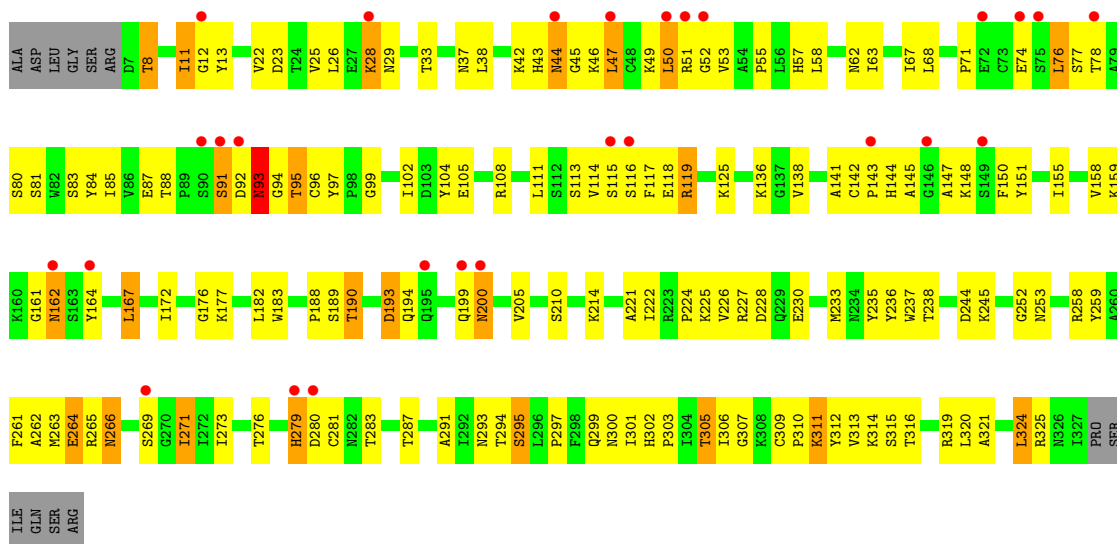


- Molecule 1: Hemagglutinin

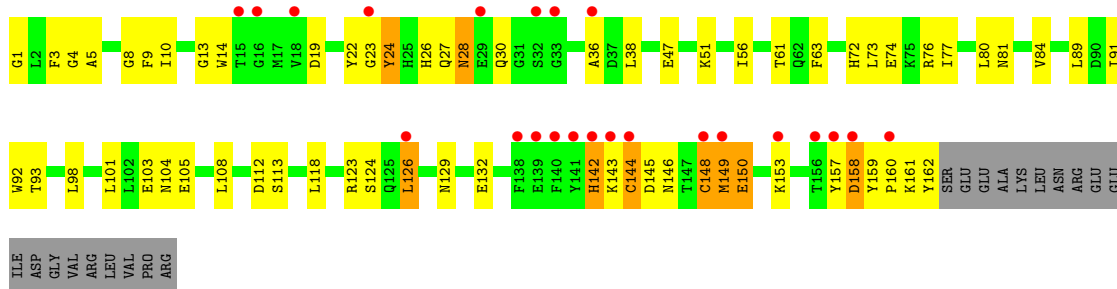




● Molecule 1: Hemagglutinin

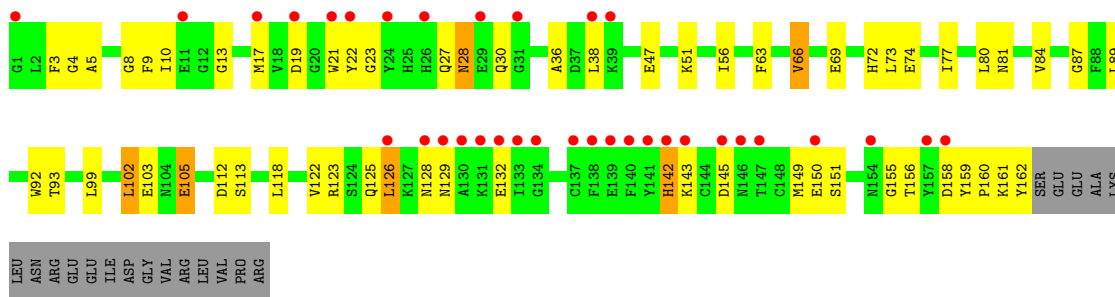


● Molecule 2: Hemagglutinin

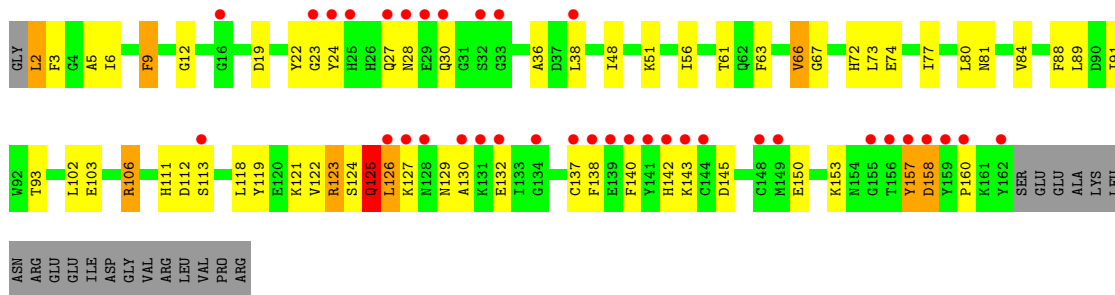


● Molecule 2: Hemagglutinin

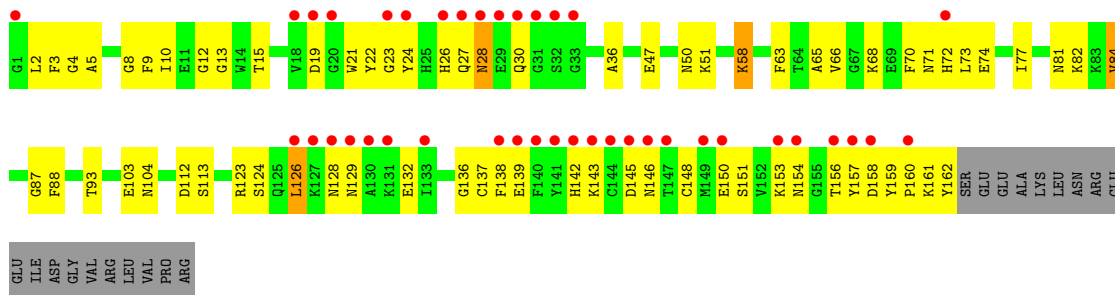




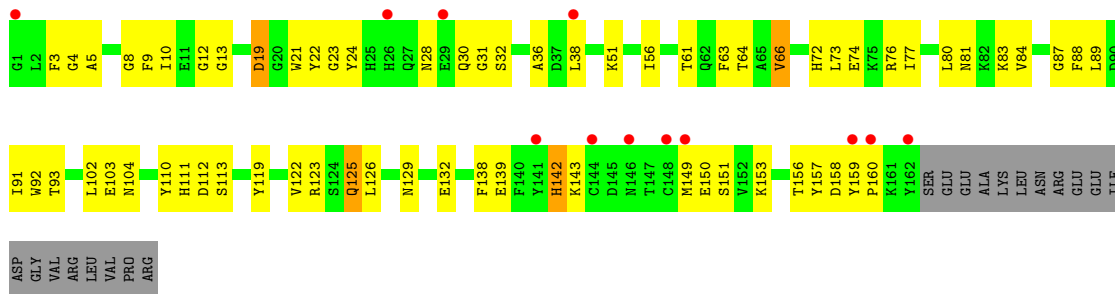
- Molecule 2: Hemagglutinin



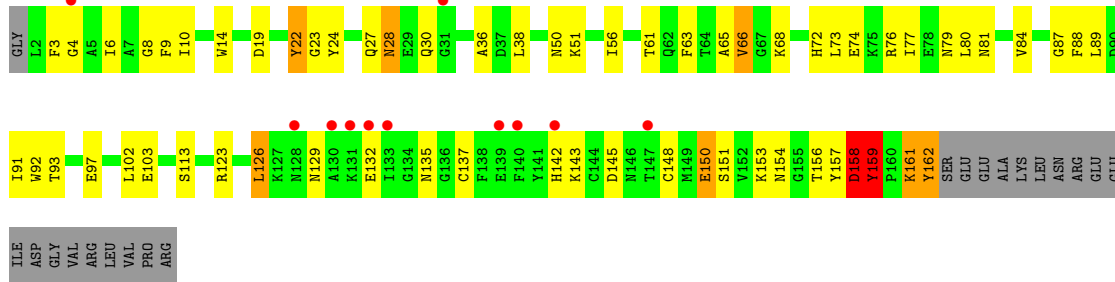
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



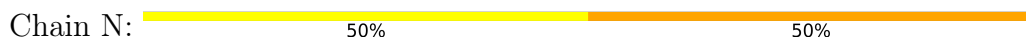
- Molecule 2: Hemagglutinin



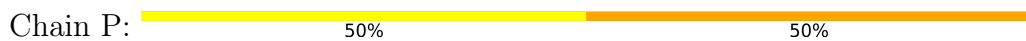
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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

Chain O:  33% 33% 33%

MAG1  
MAG2  
BMA3

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

Chain R:  33% 67%

MAG1  
MAG2  
BMA3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.02Å 115.19Å 114.98Å 62.31° 77.94° 81.05°	Depositor
Resolution (Å)	24.19 – 2.87 35.21 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.6 (24.19-2.87) 97.1 (35.21-2.87)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.85Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, $R_{free}$	0.246 , 0.270 0.254 , 0.277	Depositor DCC
$R_{free}$ test set	3295 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtrriage
Anisotropy	0.127	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/2568	0.56	5/3488 (0.1%)
1	C	0.26	0/2572	0.53	3/3493 (0.1%)
1	E	0.25	0/2572	0.62	7/3493 (0.2%)
1	G	0.26	0/2568	0.52	1/3488 (0.0%)
1	I	0.25	0/2572	0.51	3/3493 (0.1%)
1	K	0.28	0/2574	0.55	4/3497 (0.1%)
2	B	0.25	0/1333	0.43	0/1797
2	D	0.23	0/1328	0.38	0/1791
2	F	0.24	0/1330	0.45	1/1794 (0.1%)
2	H	0.25	0/1333	0.43	0/1797
2	J	0.25	0/1333	0.40	0/1797
2	L	0.28	0/1330	0.55	3/1794 (0.2%)
All	All	0.26	0/23413	0.52	27/31722 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
2	F	0	1
2	L	0	1
All	All	0	5

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	VAL	O-C-N	-14.34	99.75	122.70
1	A	199	GLN	N-CA-CB	-11.55	89.81	110.60
2	L	159	TYR	N-CA-CB	-11.34	90.19	110.60
1	E	76	LEU	N-CA-CB	-10.33	89.75	110.40
1	E	226	VAL	CA-C-N	9.25	137.55	117.20
2	L	158	ASP	CB-CA-C	-9.12	92.16	110.40
1	A	198	TYR	N-CA-C	-8.63	87.71	111.00
1	E	226	VAL	C-N-CA	8.52	143.00	121.70
1	G	269	SER	CB-CA-C	-7.88	95.12	110.10
1	I	200	ASN	N-CA-CB	7.43	123.98	110.60
1	C	79	ALA	N-CA-CB	-7.41	99.72	110.10
1	A	51	ARG	N-CA-C	-7.37	91.11	111.00
1	K	92	ASP	N-CA-C	7.32	130.77	111.00
1	E	76	LEU	N-CA-C	7.26	130.60	111.00
1	A	51	ARG	N-CA-CB	-7.26	97.53	110.60
1	I	200	ASN	N-CA-C	-7.15	91.68	111.00
1	K	93	ASN	N-CA-CB	7.12	123.41	110.60
1	E	75	SER	N-CA-C	6.77	129.28	111.00
1	K	200	ASN	N-CA-C	-6.63	93.10	111.00
1	K	200	ASN	N-CA-CB	6.49	122.29	110.60
2	L	159	TYR	N-CA-C	5.84	126.77	111.00
1	C	199	GLN	CB-CA-C	-5.71	98.99	110.40
1	I	89	PRO	N-CA-C	-5.50	97.80	112.10
1	E	78	THR	N-CA-C	-5.49	96.19	111.00
1	C	79	ALA	N-CA-C	5.28	125.25	111.00
2	F	157	TYR	N-CA-C	-5.25	96.82	111.00
1	A	199	GLN	N-CA-C	5.08	124.70	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	73	CYS	Peptide
1	C	77	SER	Peptide
1	E	226	VAL	Mainchain
2	F	125	GLN	Peptide
2	L	159	TYR	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2442	156	0
1	C	2509	0	2447	133	3
1	E	2509	0	2449	213	0
1	G	2505	0	2443	141	0
1	I	2509	0	2450	136	0
1	K	2511	0	2454	164	3
2	B	1305	0	1228	71	0
2	D	1300	0	1216	54	0
2	F	1302	0	1224	70	0
2	H	1305	0	1228	92	0
2	J	1305	0	1228	77	0
2	L	1302	0	1225	73	0
3	M	28	0	25	9	0
3	N	28	0	25	4	0
3	P	28	0	25	2	0
3	Q	28	0	25	3	0
3	S	28	0	25	5	0
4	O	39	0	34	3	0
4	R	39	0	34	3	0
5	A	28	0	26	0	0
5	C	28	0	26	3	0
5	E	42	0	39	2	0
5	F	14	0	13	0	0
5	G	42	0	39	3	0
5	K	56	0	52	9	0
5	L	14	0	13	10	0
6	A	36	0	0	19	0
6	B	17	0	0	11	0
6	C	38	0	0	15	0
6	D	10	0	0	2	0
6	E	31	0	0	10	0
6	F	13	0	0	4	0
6	G	45	0	0	25	0
6	H	23	0	0	13	0
6	I	37	0	0	21	0
6	J	21	0	0	7	0
6	K	35	0	0	15	0
6	L	11	0	0	2	0
All	All	23626	0	22435	1215	3

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 27.

All (1215) 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:E:17:ASN:HD21	5:E:601:NAG:C1	1.30	1.42
1:E:7:ASP:HA	2:F:27:GLN:O	1.37	1.21
1:E:66:TRP:HE1	1:E:77:SER:HB2	1.08	1.14
1:K:280:ASP:OD1	3:M:2:NAG:O7	1.65	1.14
1:C:282:ASN:OD1	5:C:607:NAG:O7	1.67	1.13
1:A:32:VAL:HA	6:A:338:HOH:O	1.44	1.13
1:K:52:GLY:HA3	5:K:603:NAG:H4	1.31	1.10
6:J:295:HOH:O	2:L:68:LYS:HD2	1.51	1.09
1:A:282:ASN:ND2	3:N:1:NAG:H61	1.68	1.08
1:I:66:TRP:HE3	6:I:353:HOH:O	1.37	1.07
1:G:320:LEU:HG	6:G:342:HOH:O	1.56	1.05
1:A:143:PRO:HA	6:A:341:HOH:O	1.57	1.03
1:G:327:ILE:HG12	6:G:338:HOH:O	1.56	1.02
1:G:155:ILE:HG13	1:G:258:ARG:HG3	1.41	1.02
1:A:19:THR:HB	5:L:601:NAG:H5	1.42	1.01
1:E:307:GLY:HA2	2:F:63:PHE:CE1	1.95	1.01
1:G:58:LEU:HA	1:G:76:LEU:HD11	1.41	1.00
1:E:177:LYS:HE3	1:E:264:GLU:OE2	1.62	1.00
1:E:49:LYS:O	1:E:283:THR:HG22	1.61	0.99
1:I:172:ILE:HD12	1:I:245:LYS:HB3	1.41	0.98
6:G:334:HOH:O	2:H:13:GLY:HA2	1.64	0.95
1:E:143:PRO:HD2	3:Q:1:NAG:H83	1.43	0.95
1:E:164:TYR:CZ	1:E:252:GLY:HA2	2.02	0.94
1:E:113:SER:HB2	1:E:269:SER:CB	1.96	0.94
1:E:141:ALA:O	1:E:227:ARG:NH1	2.00	0.94
1:G:269:SER:OG	1:G:270:GLY:N	1.94	0.93
1:G:9:LEU:HD22	1:G:10:CYS:H	1.33	0.92
1:A:322:THR:HG23	6:A:349:HOH:O	1.68	0.92
1:I:83:SER:HB3	6:I:338:HOH:O	1.69	0.92
1:C:282:ASN:CG	5:C:607:NAG:O7	2.09	0.91
1:E:43:HIS:HB3	1:E:301:ILE:HD13	1.52	0.91
1:C:198:TYR:O	1:C:199:GLN:HB3	1.70	0.91
2:H:123:ARG:NH1	2:J:123:ARG:HH22	1.69	0.90
1:I:160:LYS:O	1:I:160:LYS:HG3	1.72	0.90
4:R:2:NAG:H61	4:R:3:BMA:O5	1.72	0.90
1:E:183:TRP:CE2	1:E:236:TYR:HB2	2.07	0.89
1:I:8:THR:HG22	2:J:139:GLU:HA	1.54	0.89
1:E:96:CYS:O	1:E:227:ARG:HD3	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLN:O	1:C:199:GLN:HG3	1.72	0.88
2:H:158:ASP:C	2:H:160:PRO:HD3	1.94	0.88
1:E:66:TRP:NE1	1:E:77:SER:HB2	1.89	0.87
1:I:153:ASN:HA	6:I:361:HOH:O	1.75	0.87
1:K:23:ASP:OD2	5:K:602:NAG:C8	2.23	0.86
1:K:312:TYR:HD1	6:K:362:HOH:O	1.57	0.86
1:C:240:VAL:HG23	6:C:359:HOH:O	1.74	0.86
2:D:161:LYS:HB3	6:D:187:HOH:O	1.74	0.86
1:I:66:TRP:CE3	6:I:353:HOH:O	2.18	0.86
1:I:114:VAL:HG11	1:I:117:PHE:HB2	1.57	0.86
1:I:259:TYR:HD1	6:I:361:HOH:O	1.59	0.86
2:H:124:SER:HB3	6:H:188:HOH:O	1.74	0.85
1:C:114:VAL:HG11	1:C:117:PHE:HB2	1.58	0.85
1:C:313:VAL:HG12	1:C:315:SER:H	1.42	0.85
1:K:114:VAL:HG11	1:K:117:PHE:HB2	1.59	0.85
2:B:105:GLU:HB2	6:B:190:HOH:O	1.75	0.85
1:A:62:ASN:HB3	6:A:339:HOH:O	1.76	0.84
1:G:179:VAL:HG13	6:G:373:HOH:O	1.75	0.84
1:A:19:THR:CG2	5:L:601:NAG:O6	2.25	0.83
1:A:159:LYS:HD3	1:A:199:GLN:H	1.41	0.83
1:A:25:VAL:HG23	6:B:190:HOH:O	1.77	0.83
1:E:313:VAL:HG12	1:E:315:SER:H	1.44	0.82
1:K:313:VAL:HG12	1:K:315:SER:H	1.44	0.82
1:A:325:ARG:HA	6:A:338:HOH:O	1.78	0.82
1:A:160:LYS:NZ	1:A:161:GLY:HA3	1.95	0.82
1:I:313:VAL:HG12	1:I:315:SER:H	1.44	0.82
1:E:48:CYS:CB	1:E:281:CYS:SG	2.67	0.81
1:G:327:ILE:HG21	6:H:184:HOH:O	1.78	0.81
2:B:160:PRO:HD2	2:B:161:LYS:HG3	1.61	0.81
1:E:7:ASP:CA	2:F:27:GLN:O	2.26	0.81
1:A:313:VAL:HG12	1:A:315:SER:H	1.44	0.81
1:E:11:ILE:HD12	2:F:119:TYR:HA	1.63	0.81
1:G:11:ILE:HD13	1:G:11:ILE:O	1.80	0.81
1:C:143:PRO:HD2	3:P:1:NAG:H83	1.63	0.81
1:E:223:ARG:HD3	1:E:232:ARG:HG2	1.63	0.80
1:G:313:VAL:HG12	1:G:315:SER:H	1.44	0.80
2:H:47:GLU:HB3	1:K:26:LEU:HB3	1.63	0.80
1:E:172:ILE:HD12	1:E:245:LYS:HB3	1.63	0.80
2:H:123:ARG:HH22	2:L:123:ARG:HH12	1.26	0.80
1:C:168:SER:HB3	1:K:176:GLY:HA2	1.62	0.79
1:K:312:TYR:CD1	6:K:362:HOH:O	2.32	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG11	1:A:117:PHE:HB2	1.63	0.78
1:I:319:ARG:CG	1:I:319:ARG:HH11	1.96	0.78
6:I:365:HOH:O	1:K:214:LYS:HG3	1.82	0.78
2:H:12:GLY:HA2	6:H:184:HOH:O	1.82	0.78
1:E:167:LEU:HD22	1:E:250:ALA:HB3	1.63	0.78
1:E:178:GLU:OE1	1:E:265:ARG:NH1	2.17	0.78
1:E:66:TRP:HE1	1:E:77:SER:CB	1.92	0.78
1:A:19:THR:HG21	5:L:601:NAG:O6	1.84	0.77
1:E:38:LEU:HD11	1:E:320:LEU:HD22	1.65	0.77
1:G:58:LEU:HA	1:G:76:LEU:CD1	2.12	0.77
1:G:327:ILE:HG22	6:G:337:HOH:O	1.83	0.77
1:K:52:GLY:CA	5:K:603:NAG:H4	2.13	0.77
1:K:293:ASN:ND2	5:K:604:NAG:O7	2.16	0.77
1:G:86:VAL:HG23	6:G:350:HOH:O	1.83	0.77
1:A:81:SER:HB3	1:A:115:SER:O	1.84	0.77
1:A:126:THR:HA	6:A:367:HOH:O	1.84	0.77
1:G:141:ALA:O	1:G:143:PRO:HD3	1.85	0.77
1:K:183:TRP:CE3	6:K:343:HOH:O	2.36	0.77
1:A:149:SER:N	6:A:341:HOH:O	2.18	0.77
1:C:254:LEU:HD22	6:C:354:HOH:O	1.85	0.76
1:A:36:VAL:HG22	6:A:349:HOH:O	1.84	0.76
1:K:324:LEU:HD23	1:K:324:LEU:N	2.00	0.76
1:G:255:VAL:HG12	6:G:346:HOH:O	1.85	0.76
1:G:38:LEU:HD11	1:G:320:LEU:HD22	1.67	0.76
1:I:68:LEU:O	1:I:151:TYR:HB3	1.87	0.75
1:G:11:ILE:HG12	2:H:10:ILE:HD13	1.67	0.75
1:K:144:HIS:O	1:K:147:ALA:HB3	1.87	0.75
1:G:185:ILE:HD11	6:G:356:HOH:O	1.86	0.75
1:G:305:THR:H	2:H:66:VAL:HB	1.52	0.75
1:E:125:LYS:HG3	1:E:258:ARG:HH11	1.49	0.75
2:H:123:ARG:HH22	2:L:123:ARG:NH1	1.83	0.75
2:H:158:ASP:O	2:H:160:PRO:HD3	1.87	0.75
1:K:305:THR:H	2:L:66:VAL:HG13	1.50	0.75
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.69	0.74
1:E:113:SER:HB2	1:E:269:SER:HB3	1.69	0.74
1:G:177:LYS:HB2	1:G:263:MET:O	1.88	0.74
2:J:153:LYS:HB2	6:J:210:HOH:O	1.88	0.74
1:A:47:LEU:HD21	1:A:276:THR:HB	1.69	0.73
1:E:88:THR:O	1:E:91:SER:OG	2.06	0.73
1:K:102:ILE:HG13	1:K:236:TYR:CE2	2.23	0.73
1:K:311:LYS:HG2	2:L:92:TRP:CE2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:SER:HB2	1:E:269:SER:HB2	1.69	0.73
1:G:156:TRP:CE3	6:G:369:HOH:O	2.40	0.73
1:K:313:VAL:HG13	2:L:93:THR:HA	1.70	0.73
1:E:164:TYR:CE2	1:E:252:GLY:HA2	2.23	0.72
1:E:311:LYS:HE2	2:F:61:THR:HG22	1.69	0.72
1:K:266:ASN:H	1:K:266:ASN:ND2	1.87	0.72
1:E:168:SER:HA	1:E:248:PHE:O	1.89	0.72
1:K:23:ASP:OD2	5:K:602:NAG:H81	1.88	0.72
1:I:141:ALA:O	1:I:143:PRO:HD3	1.90	0.72
1:E:125:LYS:CG	1:E:258:ARG:HH11	2.03	0.72
2:H:123:ARG:HH11	2:J:123:ARG:HH22	1.35	0.72
1:E:7:ASP:O	2:F:140:PHE:HD1	1.71	0.71
1:G:141:ALA:O	1:G:227:ARG:NH1	2.22	0.71
2:H:157:TYR:CE1	6:H:186:HOH:O	2.43	0.71
1:C:199:GLN:O	1:C:199:GLN:CG	2.38	0.71
1:K:23:ASP:OD2	5:K:602:NAG:H82	1.89	0.71
1:K:182:LEU:HA	6:K:343:HOH:O	1.89	0.71
1:G:11:ILE:HD11	2:H:136:GLY:HA3	1.72	0.71
1:C:317:LYS:NZ	4:O:1:NAG:H83	2.06	0.71
1:I:258:ARG:HB3	6:I:361:HOH:O	1.91	0.70
1:I:311:LYS:HG2	2:J:92:TRP:CE2	2.26	0.70
1:E:125:LYS:HB2	1:E:258:ARG:NH1	2.05	0.70
1:G:63:ILE:HD11	1:G:85:ILE:HG21	1.72	0.70
1:C:102:ILE:HG13	1:C:236:TYR:CE2	2.26	0.70
1:E:87:GLU:O	1:E:273:ILE:HA	1.92	0.70
1:E:125:LYS:HB2	1:E:258:ARG:HH12	1.56	0.70
1:G:55:PRO:HB2	6:G:350:HOH:O	1.92	0.70
1:E:189:SER:CB	1:E:230:GLU:HB2	2.22	0.70
1:E:317:LYS:HA	6:E:356:HOH:O	1.92	0.69
1:G:188:PRO:HG2	1:G:194:GLN:NE2	2.07	0.69
1:C:8:THR:OG1	2:D:27:GLN:HB3	1.92	0.69
1:E:50:LEU:O	1:E:283:THR:O	2.11	0.69
1:E:292:ILE:HD11	1:E:301:ILE:HD12	1.74	0.69
1:C:188:PRO:HG2	1:C:194:GLN:NE2	2.08	0.69
2:B:108:LEU:N	6:B:193:HOH:O	2.20	0.69
1:G:138:VAL:HB	1:G:148:LYS:O	1.93	0.69
6:G:370:HOH:O	2:H:15:THR:HG22	1.93	0.69
1:A:258:ARG:HE	1:A:259:TYR:HE1	1.41	0.69
1:K:258:ARG:HE	1:K:259:TYR:HE1	1.41	0.69
1:K:237:TRP:HA	6:K:343:HOH:O	1.91	0.68
1:G:29:ASN:OD1	5:G:602:NAG:N2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:THR:HG22	2:H:66:VAL:HG23	1.75	0.68
2:F:118:LEU:O	2:F:122:VAL:HG13	1.94	0.68
1:I:324:LEU:HB3	2:J:111:HIS:CG	2.28	0.68
1:G:7:ASP:O	2:H:139:GLU:HA	1.92	0.68
1:C:317:LYS:HZ1	4:O:1:NAG:H83	1.59	0.68
1:G:55:PRO:HB3	1:G:84:TYR:CZ	2.27	0.68
1:K:141:ALA:O	1:K:143:PRO:HD3	1.93	0.68
1:A:107:LEU:HD22	1:A:111:LEU:HD22	1.76	0.67
1:C:63:ILE:HD11	1:C:85:ILE:HG21	1.76	0.67
1:E:188:PRO:HG2	1:E:194:GLN:NE2	2.09	0.67
1:A:31:THR:O	6:A:338:HOH:O	2.10	0.67
1:K:78:THR:HG22	1:K:78:THR:O	1.94	0.67
1:I:188:PRO:HG2	1:I:194:GLN:NE2	2.08	0.67
1:E:39:LEU:HB2	1:E:318:LEU:HB2	1.77	0.67
1:E:47:LEU:HD13	1:E:276:THR:HG21	1.76	0.67
1:K:8:THR:OG1	2:L:27:GLN:HB3	1.95	0.67
1:A:188:PRO:HG2	1:A:194:GLN:NE2	2.09	0.67
1:E:63:ILE:HD11	1:E:85:ILE:HG21	1.76	0.67
1:K:324:LEU:HD23	1:K:324:LEU:H	1.57	0.67
1:C:46:LYS:HE2	1:C:279:HIS:CE1	2.30	0.67
1:G:164:TYR:HB3	6:G:366:HOH:O	1.95	0.67
1:A:311:LYS:HG2	2:B:92:TRP:CE2	2.30	0.66
2:B:146:ASN:O	2:B:149:MET:HB2	1.95	0.66
1:G:49:LYS:O	1:G:283:THR:HG22	1.96	0.66
1:I:319:ARG:HH11	1:I:319:ARG:HG2	1.61	0.66
1:I:44:ASN:HD21	1:I:291:ALA:H	1.44	0.66
1:I:241:GLU:HG2	6:I:369:HOH:O	1.94	0.66
1:A:63:ILE:HD11	1:A:85:ILE:HG21	1.75	0.66
1:K:63:ILE:HD11	1:K:85:ILE:HG21	1.76	0.66
1:C:24:THR:HB	2:D:105:GLU:HB2	1.76	0.66
1:G:11:ILE:HG12	2:H:10:ILE:CD1	2.26	0.66
1:A:159:LYS:HE2	1:A:199:GLN:HG2	1.78	0.66
1:K:177:LYS:HE3	1:K:264:GLU:OE2	1.95	0.66
1:A:164:TYR:CE1	1:A:252:GLY:HA2	2.31	0.66
1:E:48:CYS:HB3	1:E:281:CYS:SG	2.36	0.66
1:C:188:PRO:HG2	1:C:194:GLN:HE21	1.61	0.66
1:E:183:TRP:CE2	1:E:236:TYR:CB	2.78	0.65
1:G:102:ILE:HG13	1:G:236:TYR:CE2	2.32	0.65
1:C:198:TYR:CZ	1:C:253:ASN:HA	2.31	0.65
1:G:155:ILE:CG1	1:G:258:ARG:HG3	2.22	0.65
1:I:199:GLN:O	1:I:200:ASN:OD1	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LYS:HB2	1:A:258:ARG:NH1	2.10	0.65
1:I:289:LYS:HE2	1:I:301:ILE:HG23	1.79	0.65
1:A:325:ARG:CA	6:A:338:HOH:O	2.42	0.65
1:E:258:ARG:HE	1:E:259:TYR:HE1	1.43	0.65
6:K:353:HOH:O	2:L:22:TYR:HA	1.96	0.65
1:A:160:LYS:HD3	1:A:160:LYS:O	1.95	0.65
1:E:125:LYS:HG3	1:E:155:ILE:HD11	1.79	0.65
1:C:313:VAL:HG13	2:D:93:THR:HA	1.78	0.65
1:I:102:ILE:HG13	1:I:236:TYR:CE2	2.32	0.65
2:L:135:ASN:OD1	2:L:137:CYS:N	2.30	0.65
1:E:183:TRP:NE1	1:E:236:TYR:HB2	2.12	0.64
1:A:38:LEU:HD11	1:A:320:LEU:HD22	1.79	0.64
1:G:188:PRO:HG2	1:G:194:GLN:HE21	1.63	0.64
1:K:307:GLY:HA2	2:L:63:PHE:CE1	2.33	0.64
1:C:46:LYS:HE2	1:C:279:HIS:ND1	2.13	0.64
1:I:106:GLU:OE2	6:I:341:HOH:O	2.14	0.64
1:I:188:PRO:HG2	1:I:194:GLN:HE21	1.63	0.64
1:K:188:PRO:HG2	1:K:194:GLN:NE2	2.12	0.64
1:C:311:LYS:HG2	2:D:92:TRP:CE2	2.33	0.64
1:E:188:PRO:HG2	1:E:194:GLN:HE21	1.63	0.63
1:G:313:VAL:HG13	2:H:93:THR:HA	1.80	0.63
1:K:172:ILE:HD12	1:K:245:LYS:HB3	1.80	0.63
1:K:297:PRO:HG3	2:L:56:ILE:HA	1.80	0.63
1:C:125:LYS:HB2	1:C:258:ARG:NH1	2.13	0.63
2:D:158:ASP:OD2	2:D:160:PRO:HD2	1.97	0.63
1:A:224:PRO:HG2	1:C:209:SER:HA	1.79	0.63
2:H:81:ASN:O	2:H:84:VAL:HG23	1.97	0.63
1:I:106:GLU:CD	6:I:341:HOH:O	2.35	0.63
1:I:313:VAL:HG13	2:J:93:THR:HA	1.79	0.63
1:E:108:ARG:HB3	1:E:271:ILE:CD1	2.27	0.63
2:H:159:TYR:CD2	2:H:159:TYR:O	2.52	0.63
2:D:142:HIS:CG	6:D:187:HOH:O	2.51	0.63
1:A:102:ILE:HG13	1:A:236:TYR:CE2	2.33	0.63
1:A:141:ALA:O	1:A:143:PRO:HD3	1.97	0.63
1:I:297:PRO:HG3	2:J:56:ILE:HA	1.80	0.63
1:E:87:GLU:O	1:E:274:SER:N	2.32	0.63
1:G:227:ARG:O	1:G:228:ASP:HB2	1.97	0.63
1:I:63:ILE:HD11	1:I:85:ILE:HG21	1.81	0.63
1:E:58:LEU:HD11	1:E:63:ILE:HD13	1.81	0.63
2:L:30:GLN:HE22	2:L:145:ASP:CB	2.12	0.63
1:A:313:VAL:HG13	2:B:93:THR:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:GLY:HA2	1:G:212:TYR:O	1.98	0.63
1:I:178:GLU:OE1	1:I:265:ARG:NH1	2.32	0.63
1:K:58:LEU:HD11	1:K:63:ILE:HD13	1.81	0.63
1:C:141:ALA:O	1:C:143:PRO:HD3	1.99	0.62
1:G:11:ILE:CD1	1:G:11:ILE:N	2.62	0.62
1:K:38:LEU:HD11	1:K:320:LEU:HD22	1.81	0.62
1:K:159:LYS:HZ2	1:K:199:GLN:HG3	1.64	0.62
1:A:143:PRO:HD2	3:M:1:NAG:H81	1.82	0.62
1:G:58:LEU:HB3	1:G:61:CYS:O	1.99	0.62
1:G:164:TYR:CZ	1:G:252:GLY:HA2	2.34	0.62
1:I:96:CYS:HB2	1:I:141:ALA:O	1.99	0.62
2:B:105:GLU:C	6:B:193:HOH:O	2.38	0.62
1:C:172:ILE:HD12	1:C:245:LYS:HB3	1.81	0.62
2:H:51:LYS:HB2	1:K:26:LEU:HD23	1.82	0.62
6:H:196:HOH:O	2:J:64:THR:HG22	1.98	0.62
2:J:76:ARG:HA	6:J:295:HOH:O	1.98	0.62
1:A:188:PRO:HG2	1:A:194:GLN:HE21	1.63	0.62
2:J:31:GLY:HA2	6:J:234:HOH:O	2.00	0.62
2:B:104:ASN:O	6:B:193:HOH:O	2.16	0.62
1:E:125:LYS:CG	1:E:258:ARG:NH1	2.63	0.62
1:E:141:ALA:O	1:E:143:PRO:HD3	2.00	0.62
2:H:154:ASN:OD1	2:H:154:ASN:O	2.17	0.62
1:I:259:TYR:CD1	6:I:361:HOH:O	2.41	0.62
1:K:71:PRO:HB3	1:K:144:HIS:HB2	1.81	0.62
1:G:13:TYR:HA	2:H:21:TRP:O	2.00	0.62
1:G:172:ILE:HD12	1:G:245:LYS:HB3	1.81	0.62
1:E:84:TYR:CZ	1:E:286:GLN:HG2	2.35	0.62
1:I:38:LEU:HD11	1:I:320:LEU:HD22	1.81	0.62
2:D:30:GLN:HE22	2:D:145:ASP:CB	2.13	0.61
1:E:99:GLY:HA2	6:E:340:HOH:O	1.99	0.61
1:G:183:TRP:NE1	6:G:356:HOH:O	2.31	0.61
2:H:143:LYS:HA	2:H:143:LYS:HE2	1.80	0.61
1:K:145:ALA:C	1:K:147:ALA:H	2.03	0.61
1:E:324:LEU:HB3	2:F:111:HIS:CG	2.35	0.61
1:A:307:GLY:HA2	2:B:63:PHE:CE1	2.36	0.61
2:B:30:GLN:HE22	2:B:145:ASP:CB	2.13	0.61
2:H:26:HIS:HB3	6:H:183:HOH:O	2.00	0.61
1:K:312:TYR:CD2	2:L:89:LEU:HD13	2.35	0.61
1:C:305:THR:H	2:D:66:VAL:HG13	1.65	0.61
1:K:138:VAL:HG23	1:K:148:LYS:HE3	1.83	0.61
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:TYR:CZ	1:C:252:GLY:HA2	2.36	0.60
2:F:30:GLN:HE22	2:F:145:ASP:CB	2.13	0.60
1:I:77:SER:O	1:I:78:THR:OG1	2.17	0.60
1:A:125:LYS:HB2	1:A:258:ARG:HH11	1.66	0.60
1:E:36:VAL:HG13	1:E:322:THR:HG21	1.83	0.60
2:H:51:LYS:HA	1:K:25:VAL:HG12	1.83	0.60
1:K:63:ILE:O	1:K:67:ILE:HG13	2.01	0.60
1:C:58:LEU:HD11	1:C:63:ILE:HD13	1.83	0.60
1:A:141:ALA:C	1:A:143:PRO:HD3	2.22	0.60
1:G:50:LEU:HD11	1:G:306:ILE:HG22	1.84	0.60
1:C:11:ILE:HD11	2:D:122:VAL:HG21	1.82	0.60
1:E:167:LEU:O	1:E:249:GLU:HA	2.01	0.60
2:H:2:LEU:HD11	2:J:110:TYR:HA	1.83	0.60
1:E:183:TRP:CZ2	1:E:236:TYR:HB3	2.36	0.60
1:I:141:ALA:C	1:I:143:PRO:HD3	2.22	0.60
1:C:38:LEU:HD11	1:C:320:LEU:HD22	1.82	0.60
1:I:67:ILE:HG12	6:I:353:HOH:O	2.00	0.60
1:I:125:LYS:HB2	1:I:258:ARG:NH1	2.16	0.60
1:G:8:THR:HA	2:H:138:PHE:O	2.02	0.60
1:I:258:ARG:HE	1:I:259:TYR:HE1	1.47	0.60
1:E:102:ILE:HB	6:E:357:HOH:O	2.01	0.60
1:E:314:LYS:HE2	2:F:89:LEU:HD21	1.84	0.60
1:G:180:LEU:HD12	6:G:347:HOH:O	2.01	0.60
1:I:58:LEU:HD11	1:I:63:ILE:HD13	1.83	0.60
1:I:319:ARG:CG	1:I:319:ARG:NH1	2.61	0.60
1:C:63:ILE:O	1:C:67:ILE:HG13	2.02	0.60
1:E:36:VAL:O	1:E:320:LEU:N	2.30	0.60
1:G:81:SER:HB3	1:G:115:SER:O	2.02	0.60
1:E:7:ASP:O	2:F:140:PHE:CD1	2.54	0.59
1:G:105:GLU:OE2	2:H:71:ASN:HB3	2.02	0.59
1:A:172:ILE:HD12	1:A:245:LYS:HB3	1.83	0.59
2:B:124:SER:HB3	6:B:212:HOH:O	2.01	0.59
2:B:26:HIS:HB2	2:B:149:MET:CE	2.32	0.59
1:K:49:LYS:HG3	1:K:281:CYS:O	2.03	0.59
2:L:129:ASN:ND2	2:L:161:LYS:HB2	2.17	0.59
1:A:49:LYS:O	1:A:283:THR:HG22	2.02	0.59
2:B:51:LYS:HG3	1:E:25:VAL:HG12	1.83	0.59
1:I:88:THR:C	1:I:89:PRO:O	2.39	0.59
1:K:81:SER:HB3	1:K:115:SER:O	2.02	0.59
1:K:188:PRO:HG2	1:K:194:GLN:HE21	1.67	0.59
1:A:63:ILE:O	1:A:67:ILE:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:TYR:CZ	1:I:252:GLY:HA2	2.37	0.59
1:E:47:LEU:HD13	1:E:276:THR:CG2	2.31	0.59
2:F:122:VAL:HG23	2:F:138:PHE:HE1	1.67	0.59
1:G:58:LEU:HD12	1:G:76:LEU:HD11	1.85	0.59
1:G:63:ILE:O	1:G:67:ILE:HG13	2.03	0.59
1:C:50:LEU:HD11	1:C:306:ILE:HG22	1.84	0.59
1:C:258:ARG:HE	1:C:259:TYR:HE1	1.50	0.59
1:E:170:SER:HB3	1:E:247:THR:HA	1.83	0.59
1:C:326:ASN:C	1:C:327:ILE:HG13	2.23	0.59
2:H:30:GLN:HE22	2:H:145:ASP:CB	2.16	0.59
1:A:223:ARG:HG3	1:C:206:PHE:HZ	1.67	0.58
1:C:13:TYR:HB2	1:C:324:LEU:HD11	1.85	0.58
1:I:81:SER:HB3	1:I:115:SER:O	2.03	0.58
2:L:143:LYS:HE2	2:L:143:LYS:HA	1.85	0.58
1:E:63:ILE:O	1:E:67:ILE:HG13	2.02	0.58
1:E:227:ARG:NH2	3:Q:1:NAG:O3	2.36	0.58
1:I:159:LYS:HB2	1:I:163:SER:O	2.03	0.58
2:B:101:LEU:O	6:B:190:HOH:O	2.17	0.58
2:H:123:ARG:HD2	2:H:132:GLU:OE1	2.03	0.58
1:A:160:LYS:HZ3	1:A:161:GLY:HA3	1.67	0.58
1:E:96:CYS:O	1:E:227:ARG:CD	2.50	0.58
1:G:136:LYS:HB2	1:G:158:VAL:HG21	1.85	0.58
1:C:80:SER:O	1:C:116:SER:HA	2.04	0.58
1:E:115:SER:HB2	1:E:266:ASN:OD1	2.04	0.58
1:E:292:ILE:CD1	1:E:301:ILE:HD12	2.32	0.58
2:F:122:VAL:CG2	2:F:138:PHE:HE1	2.16	0.58
2:J:123:ARG:HD2	2:J:132:GLU:OE1	2.02	0.58
2:J:123:ARG:HG3	2:J:138:PHE:HE2	1.68	0.58
2:L:150:GLU:HG2	5:L:601:NAG:H61	1.85	0.58
1:A:57:HIS:O	1:A:76:LEU:HD13	2.03	0.58
2:D:123:ARG:HD2	2:D:132:GLU:OE1	2.03	0.58
1:K:83:SER:O	1:K:269:SER:OG	2.09	0.58
1:K:125:LYS:HB2	1:K:258:ARG:NH1	2.19	0.58
2:D:123:ARG:O	2:D:126:LEU:O	2.22	0.58
1:G:44:ASN:HD21	1:G:291:ALA:H	1.50	0.58
2:H:3:PHE:CE1	2:H:113:SER:HB2	2.38	0.58
1:I:57:HIS:O	1:I:76:LEU:HD11	2.04	0.58
1:G:154:LEU:HB3	6:G:346:HOH:O	2.03	0.58
1:K:150:PHE:HB3	6:K:348:HOH:O	2.02	0.58
2:B:76:ARG:NH1	2:D:69:GLU:O	2.37	0.58
1:C:135:ASN:HB3	3:S:2:NAG:H83	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:LYS:HA	2:F:143:LYS:HE2	1.85	0.58
1:K:44:ASN:HD21	1:K:291:ALA:H	1.52	0.58
1:K:199:GLN:O	1:K:200:ASN:OD1	2.21	0.58
1:A:72:GLU:HG3	3:M:1:NAG:HN2	1.68	0.57
2:B:123:ARG:HD2	2:B:132:GLU:OE1	2.03	0.57
1:C:121:GLU:OE2	1:C:124:PRO:HA	2.02	0.57
2:D:143:LYS:HE2	2:D:143:LYS:HA	1.85	0.57
1:C:44:ASN:HD21	1:C:291:ALA:H	1.51	0.57
1:C:245:LYS:HZ3	1:K:116:SER:HB3	1.70	0.57
2:F:24:TYR:CD1	2:F:153:LYS:HE3	2.39	0.57
2:F:123:ARG:CG	2:F:124:SER:N	2.66	0.57
2:L:135:ASN:OD1	2:L:137:CYS:SG	2.62	0.57
2:D:27:GLN:O	2:D:27:GLN:HG3	2.05	0.57
1:E:189:SER:HB3	1:E:230:GLU:HB2	1.86	0.57
1:E:189:SER:HB2	1:E:230:GLU:HB2	1.85	0.57
1:I:225:LYS:HG2	1:I:230:GLU:HG3	1.86	0.57
1:I:289:LYS:HE2	1:I:301:ILE:CG2	2.34	0.57
2:L:24:TYR:CD1	2:L:153:LYS:HE3	2.40	0.57
1:E:8:THR:HG22	2:F:138:PHE:O	2.04	0.57
1:K:164:TYR:CZ	1:K:252:GLY:HA2	2.38	0.57
1:G:9:LEU:HD22	1:G:10:CYS:N	2.11	0.57
1:K:50:LEU:HD12	1:K:50:LEU:O	2.04	0.57
1:A:44:ASN:HD21	1:A:291:ALA:H	1.53	0.57
1:E:180:LEU:HA	1:E:239:LEU:HD23	1.87	0.57
2:H:123:ARG:O	2:H:126:LEU:O	2.22	0.57
2:J:24:TYR:CD1	2:J:153:LYS:HE3	2.40	0.57
1:A:55:PRO:HB3	1:A:84:TYR:CZ	2.40	0.57
2:L:150:GLU:CG	5:L:601:NAG:H61	2.35	0.57
1:A:19:THR:HG22	5:L:601:NAG:O6	2.05	0.57
2:H:159:TYR:N	2:H:160:PRO:HD3	2.18	0.57
1:I:55:PRO:HB3	1:I:84:TYR:CZ	2.39	0.57
1:I:305:THR:H	2:J:66:VAL:HG13	1.69	0.57
2:J:125:GLN:NE2	2:J:157:TYR:HB3	2.19	0.57
1:K:49:LYS:HB3	1:K:53:VAL:O	2.04	0.57
1:C:198:TYR:OH	1:C:253:ASN:HA	2.05	0.56
1:C:81:SER:HB3	1:C:115:SER:O	2.05	0.56
1:E:125:LYS:CB	1:E:258:ARG:NH1	2.68	0.56
1:G:49:LYS:HB3	1:G:53:VAL:O	2.05	0.56
1:I:118:GLU:HG2	1:I:262:ALA:HB3	1.86	0.56
1:I:259:TYR:N	6:I:361:HOH:O	2.38	0.56
5:K:604:NAG:O7	5:K:604:NAG:C1	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:30:GLN:HE22	2:L:145:ASP:HB2	1.70	0.56
1:A:159:LYS:HB2	1:A:163:SER:O	2.05	0.56
1:C:118:GLU:HG2	1:C:262:ALA:HB3	1.86	0.56
1:G:190:THR:HA	6:G:341:HOH:O	2.04	0.56
2:L:129:ASN:OD1	2:L:159:TYR:CE2	2.58	0.56
1:E:99:GLY:CA	6:E:340:HOH:O	2.52	0.56
1:G:55:PRO:HB3	1:G:84:TYR:CE1	2.41	0.56
1:K:167:LEU:HD23	1:K:167:LEU:O	2.06	0.56
1:C:55:PRO:HB3	1:C:84:TYR:CZ	2.41	0.56
2:D:125:GLN:HE22	2:D:155:GLY:HA2	1.70	0.56
1:E:81:SER:HB3	1:E:115:SER:O	2.06	0.56
1:E:223:ARG:HD3	1:E:232:ARG:CG	2.33	0.56
2:H:58:LYS:HG3	2:L:97:GLU:HB3	1.86	0.56
2:D:128:ASN:HB3	2:D:162:TYR:HE1	1.71	0.56
1:E:44:ASN:HD21	1:E:291:ALA:H	1.54	0.56
2:F:30:GLN:HE22	2:F:145:ASP:HB2	1.71	0.56
1:I:307:GLY:HA2	2:J:63:PHE:CE1	2.41	0.56
1:G:96:CYS:O	1:G:227:ARG:HD3	2.04	0.56
1:G:121:GLU:OE2	1:G:124:PRO:HA	2.06	0.56
2:H:24:TYR:CD1	2:H:153:LYS:HE3	2.40	0.56
1:I:50:LEU:HD12	1:I:50:LEU:O	2.06	0.56
1:K:145:ALA:C	1:K:147:ALA:N	2.59	0.56
1:E:216:PHE:CE2	1:E:236:TYR:CZ	2.94	0.56
2:L:154:ASN:CG	5:L:601:NAG:O7	2.45	0.56
1:E:118:GLU:O	1:E:118:GLU:HG3	2.06	0.55
1:E:219:GLU:O	1:E:223:ARG:NH2	2.32	0.55
2:L:123:ARG:O	2:L:126:LEU:O	2.23	0.55
2:D:30:GLN:HE22	2:D:145:ASP:HB2	1.70	0.55
1:A:159:LYS:HD3	1:A:199:GLN:HB2	1.88	0.55
1:E:15:ALA:HB1	1:E:327:ILE:O	2.06	0.55
1:K:55:PRO:HB3	1:K:84:TYR:CZ	2.42	0.55
2:L:51:LYS:HE3	2:L:103:GLU:OE1	2.06	0.55
1:E:55:PRO:HB3	1:E:84:TYR:CZ	2.41	0.55
1:G:118:GLU:HG2	1:G:262:ALA:HB3	1.88	0.55
2:H:68:LYS:HE3	2:L:79:ASN:HB3	1.87	0.55
1:A:327:ILE:HG21	2:B:13:GLY:H	1.72	0.55
1:E:129:TRP:CE2	1:E:256:VAL:HG21	2.42	0.55
1:E:167:LEU:O	1:E:167:LEU:HD23	2.05	0.55
1:K:324:LEU:N	1:K:324:LEU:CD2	2.68	0.55
2:H:27:GLN:O	2:H:27:GLN:HG3	2.07	0.55
1:I:125:LYS:HB2	1:I:258:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:GLY:N	2:L:14:TRP:CH2	2.75	0.55
2:F:132:GLU:HA	2:F:138:PHE:HD2	1.71	0.55
2:H:82:LYS:HE3	6:H:196:HOH:O	2.06	0.55
1:I:44:ASN:ND2	1:I:291:ALA:H	2.04	0.55
1:A:160:LYS:HZ2	1:A:161:GLY:HA3	1.70	0.55
2:H:51:LYS:HA	1:K:25:VAL:O	2.07	0.55
1:A:324:LEU:H	1:A:324:LEU:HD23	1.71	0.55
1:C:168:SER:CB	1:K:176:GLY:HA2	2.35	0.55
1:K:49:LYS:NZ	1:K:280:ASP:HA	2.21	0.55
1:K:141:ALA:O	1:K:227:ARG:NH1	2.38	0.55
3:N:1:NAG:O3	3:N:2:NAG:O5	2.22	0.55
1:E:50:LEU:O	1:E:50:LEU:HD12	2.06	0.54
2:F:67:GLY:HA2	6:F:185:HOH:O	2.08	0.54
6:I:349:HOH:O	2:L:50:ASN:ND2	2.39	0.54
2:F:123:ARG:HG2	2:F:124:SER:N	2.22	0.54
2:L:81:ASN:O	2:L:84:VAL:HG12	2.07	0.54
1:A:58:LEU:HD21	1:A:63:ILE:HD13	1.90	0.54
1:A:35:SER:HB2	1:A:320:LEU:O	2.07	0.54
1:A:49:LYS:HB3	1:A:54:ALA:HA	1.89	0.54
1:E:125:LYS:HD3	1:E:258:ARG:NH1	2.22	0.54
1:I:326:ASN:O	1:I:327:ILE:HD13	2.08	0.54
1:A:13:TYR:OH	2:B:10:ILE:O	2.23	0.54
1:A:33:THR:HG23	1:A:325:ARG:O	2.07	0.54
2:F:81:ASN:O	2:F:84:VAL:HG12	2.07	0.54
2:B:81:ASN:O	2:B:84:VAL:HG12	2.07	0.54
1:C:312:TYR:CD2	2:D:89:LEU:HD13	2.43	0.54
1:E:164:TYR:CE2	1:E:252:GLY:CA	2.89	0.54
1:G:58:LEU:HD21	1:G:63:ILE:HD13	1.89	0.54
6:K:358:HOH:O	2:L:65:ALA:HB3	2.07	0.54
2:J:83:LYS:NZ	6:J:190:HOH:O	2.30	0.54
1:A:11:ILE:HD12	2:B:24:TYR:CD2	2.43	0.54
1:C:136:LYS:HB2	1:C:158:VAL:HG21	1.89	0.54
1:E:50:LEU:HD21	1:E:306:ILE:HG22	1.90	0.54
1:E:155:ILE:HD11	1:E:258:ARG:HD2	1.88	0.54
2:H:30:GLN:HE22	2:H:145:ASP:HB2	1.73	0.54
1:I:10:CYS:O	2:J:24:TYR:HA	2.08	0.54
2:J:81:ASN:O	2:J:84:VAL:HG12	2.08	0.54
1:A:148:LYS:HA	6:A:341:HOH:O	2.07	0.54
1:A:160:LYS:HD3	1:A:160:LYS:C	2.28	0.54
1:A:160:LYS:HB3	6:A:358:HOH:O	2.08	0.54
2:B:143:LYS:HE2	2:B:143:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:TYR:CE2	1:E:252:GLY:N	2.76	0.54
1:A:58:LEU:HA	1:A:76:LEU:HD13	1.89	0.54
2:H:128:ASN:HB2	2:H:159:TYR:OH	2.09	0.54
2:J:143:LYS:HE2	2:J:143:LYS:HA	1.90	0.54
2:F:158:ASP:C	2:F:160:PRO:HD3	2.28	0.53
1:A:164:TYR:CZ	1:A:252:GLY:HA2	2.44	0.53
1:G:307:GLY:HA2	2:H:63:PHE:CE1	2.43	0.53
1:I:25:VAL:CG2	2:J:102:LEU:HD12	2.39	0.53
1:I:49:LYS:HE3	1:I:52:GLY:O	2.09	0.53
2:J:19:ASP:OD2	2:J:19:ASP:N	2.41	0.53
1:K:96:CYS:O	1:K:227:ARG:HD3	2.09	0.53
1:A:143:PRO:O	3:M:1:NAG:C8	2.56	0.53
2:F:51:LYS:HE3	2:F:103:GLU:OE1	2.08	0.53
1:I:118:GLU:CG	1:I:262:ALA:HB3	2.38	0.53
2:L:129:ASN:N	2:L:129:ASN:HD22	2.05	0.53
1:C:125:LYS:HB2	1:C:258:ARG:HH11	1.71	0.53
1:E:314:LYS:CE	2:F:89:LEU:HD21	2.38	0.53
1:K:155:ILE:HG13	1:K:258:ARG:HB2	1.90	0.53
2:B:26:HIS:HB2	2:B:149:MET:HE3	1.90	0.53
1:E:40:GLU:HB2	1:E:296:LEU:HD12	1.90	0.53
2:H:51:LYS:HB2	1:K:26:LEU:CD2	2.39	0.53
2:D:51:LYS:HE3	2:D:103:GLU:OE1	2.08	0.53
1:G:306:ILE:HA	2:H:65:ALA:HA	1.91	0.53
2:L:157:TYR:CE1	6:L:262:HOH:O	2.54	0.53
1:A:113:SER:HB2	1:A:269:SER:CB	2.39	0.53
1:I:113:SER:HB2	1:I:269:SER:CB	2.38	0.53
1:A:155:ILE:HG13	1:A:258:ARG:HB2	1.91	0.53
1:A:225:LYS:HD3	1:K:80:SER:HB3	1.89	0.53
2:B:51:LYS:HE3	2:B:103:GLU:OE1	2.09	0.53
1:C:297:PRO:HG3	2:D:56:ILE:HA	1.90	0.53
1:E:47:LEU:HD22	1:E:276:THR:HB	1.90	0.53
1:E:305:THR:H	2:F:66:VAL:HG13	1.74	0.53
1:C:136:LYS:HE3	6:C:367:HOH:O	2.07	0.53
1:C:205:VAL:HG13	6:C:354:HOH:O	2.07	0.53
1:E:13:TYR:CD2	2:F:6:ILE:HG12	2.44	0.53
2:F:72:HIS:CD2	2:F:73:LEU:HG	2.44	0.53
1:G:155:ILE:N	6:G:346:HOH:O	2.41	0.53
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.91	0.53
1:C:113:SER:HB2	1:C:269:SER:CB	2.39	0.52
6:C:357:HOH:O	2:D:13:GLY:CA	2.56	0.52
1:K:167:LEU:HD23	1:K:167:LEU:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:ND2	3:N:1:NAG:C6	2.53	0.52
1:C:78:THR:HG22	1:C:79:ALA:H	1.75	0.52
1:E:216:PHE:HE2	1:E:236:TYR:CE2	2.27	0.52
2:H:9:PHE:CD1	2:H:10:ILE:HG13	2.44	0.52
5:K:602:NAG:H82	6:K:344:HOH:O	2.10	0.52
1:E:108:ARG:O	1:E:271:ILE:HD11	2.09	0.52
1:E:167:LEU:HD23	1:E:167:LEU:C	2.29	0.52
1:G:141:ALA:C	1:G:143:PRO:HD3	2.29	0.52
1:E:136:LYS:HB2	1:E:158:VAL:HG21	1.91	0.52
1:I:23:ASP:OD2	4:R:1:NAG:O7	2.27	0.52
1:I:136:LYS:HB2	1:I:158:VAL:HG21	1.91	0.52
1:I:327:ILE:HG21	2:J:12:GLY:HA2	1.90	0.52
1:A:312:TYR:CD2	2:B:89:LEU:HD13	2.45	0.52
1:G:255:VAL:CG1	6:G:346:HOH:O	2.48	0.52
2:H:74:GLU:HA	6:I:341:HOH:O	2.09	0.52
2:H:123:ARG:HH12	2:J:123:ARG:HH12	1.58	0.52
1:I:11:ILE:HD12	2:J:119:TYR:HA	1.90	0.52
1:C:99:GLY:HA3	1:C:233:MET:O	2.09	0.52
2:D:81:ASN:O	2:D:84:VAL:HG12	2.09	0.52
1:G:205:VAL:HG11	1:G:254:LEU:HD13	1.92	0.52
2:H:123:ARG:NH1	2:J:123:ARG:NH2	2.50	0.52
2:L:135:ASN:OD1	2:L:137:CYS:CB	2.57	0.52
1:A:11:ILE:CD1	2:B:24:TYR:CD2	2.93	0.52
2:B:24:TYR:CD1	2:B:153:LYS:HE3	2.45	0.52
2:B:159:TYR:N	2:B:160:PRO:HD3	2.25	0.52
1:E:172:ILE:HA	1:E:245:LYS:HA	1.92	0.52
1:K:125:LYS:HB2	1:K:258:ARG:HH11	1.73	0.52
1:A:205:VAL:HG22	6:A:366:HOH:O	2.10	0.52
1:E:43:HIS:HB3	1:E:301:ILE:CD1	2.35	0.52
1:G:9:LEU:O	1:G:10:CYS:SG	2.68	0.52
1:G:24:THR:HG22	2:H:104:ASN:HB3	1.92	0.52
3:S:1:NAG:O3	3:S:2:NAG:O5	2.22	0.52
2:F:122:VAL:HG23	2:F:138:PHE:CE1	2.45	0.51
1:G:183:TRP:HZ3	1:G:238:THR:HG22	1.75	0.51
2:B:27:GLN:O	2:B:27:GLN:HG3	2.10	0.51
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.92	0.51
2:F:123:ARG:O	2:F:126:LEU:O	2.28	0.51
1:I:50:LEU:HB3	6:I:338:HOH:O	2.11	0.51
1:E:44:ASN:HD22	1:E:45:GLY:N	2.07	0.51
2:H:51:LYS:HE3	2:H:103:GLU:OE1	2.10	0.51
1:A:325:ARG:C	6:A:338:HOH:O	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:SER:HA	1:E:246:ILE:O	2.11	0.51
2:L:123:ARG:HD2	2:L:132:GLU:OE1	2.10	0.51
1:A:252:GLY:O	6:A:366:HOH:O	2.19	0.51
1:E:104:TYR:O	1:E:108:ARG:HG3	2.10	0.51
1:I:14:HIS:HB2	2:J:21:TRP:HA	1.93	0.51
1:A:118:GLU:HG2	1:A:262:ALA:HB3	1.92	0.51
2:B:3:PHE:HZ	2:F:2:LEU:HD13	1.75	0.51
1:E:105:GLU:HA	1:E:108:ARG:HD3	1.91	0.51
1:E:177:LYS:CE	1:E:264:GLU:OE2	2.47	0.51
1:E:293:ASN:O	1:E:293:ASN:CG	2.48	0.51
2:J:159:TYR:N	2:J:160:PRO:CD	2.74	0.51
1:A:177:LYS:HD2	1:A:262:ALA:HB1	1.93	0.51
2:B:1:GLY:N	6:B:192:HOH:O	2.42	0.51
2:B:142:HIS:O	2:B:142:HIS:CG	2.62	0.51
1:K:136:LYS:HB2	1:K:158:VAL:HG21	1.91	0.51
2:L:72:HIS:CD2	2:L:73:LEU:HG	2.46	0.51
1:A:11:ILE:HD11	2:B:118:LEU:HD23	1.91	0.51
1:A:58:LEU:HB3	1:A:61:CYS:O	2.10	0.51
1:C:141:ALA:C	1:C:143:PRO:HD3	2.31	0.51
1:C:238:THR:HG23	6:C:359:HOH:O	2.11	0.51
1:E:297:PRO:HG3	2:F:56:ILE:HA	1.93	0.51
1:G:77:SER:O	1:G:79:ALA:N	2.43	0.51
1:G:305:THR:HG22	2:H:66:VAL:CG2	2.40	0.51
1:I:57:HIS:O	1:I:76:LEU:CD1	2.58	0.51
1:K:300:ASN:HA	6:K:362:HOH:O	2.11	0.51
1:C:44:ASN:ND2	1:C:291:ALA:H	2.09	0.51
1:C:77:SER:C	1:C:78:THR:OG1	2.48	0.51
1:C:144:HIS:HA	6:C:371:HOH:O	2.10	0.51
1:E:113:SER:CB	1:E:269:SER:HB2	2.40	0.51
1:K:311:LYS:HG2	2:L:92:TRP:CD2	2.45	0.51
1:E:17:ASN:CG	5:E:601:NAG:C1	2.73	0.50
1:E:261:PHE:HD2	6:E:352:HOH:O	1.93	0.50
1:G:305:THR:O	2:H:66:VAL:N	2.44	0.50
1:I:155:ILE:HG13	1:I:258:ARG:HB2	1.91	0.50
2:J:51:LYS:HE3	2:J:103:GLU:OE1	2.09	0.50
2:J:91:ILE:HG13	6:J:185:HOH:O	2.11	0.50
2:J:129:ASN:HD22	2:J:129:ASN:N	2.09	0.50
2:D:72:HIS:CD2	2:D:73:LEU:HG	2.47	0.50
1:I:87:GLU:O	1:I:273:ILE:HA	2.11	0.50
1:I:205:VAL:HG11	1:I:254:LEU:HD13	1.94	0.50
2:J:72:HIS:CD2	2:J:73:LEU:HG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TYR:HB2	1:A:324:LEU:HD11	1.93	0.50
1:C:250:ALA:HB2	6:C:354:HOH:O	2.11	0.50
1:E:181:VAL:O	1:E:237:TRP:HA	2.10	0.50
1:G:105:GLU:CD	1:G:105:GLU:H	2.14	0.50
2:L:150:GLU:OE1	5:L:601:NAG:H61	2.12	0.50
1:E:220:ILE:N	6:E:342:HOH:O	2.44	0.50
2:F:124:SER:O	2:F:127:LYS:HE3	2.11	0.50
1:G:48:CYS:O	1:G:84:TYR:OH	2.23	0.50
1:G:76:LEU:HD22	1:G:76:LEU:O	2.11	0.50
2:H:145:ASP:CG	6:H:185:HOH:O	2.49	0.50
1:I:189:SER:HB2	1:I:222:ILE:HD13	1.94	0.50
1:A:189:SER:HB2	1:A:222:ILE:HD13	1.94	0.50
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.93	0.50
1:G:44:ASN:ND2	1:G:291:ALA:H	2.09	0.50
1:E:25:VAL:CG2	2:F:102:LEU:HD12	2.42	0.50
2:J:158:ASP:CG	2:J:160:PRO:HD2	2.32	0.50
1:K:51:ARG:O	5:K:603:NAG:H2	2.12	0.50
1:K:87:GLU:O	1:K:273:ILE:HA	2.11	0.50
2:B:123:ARG:O	2:B:126:LEU:O	2.29	0.50
1:C:155:ILE:HG13	1:C:258:ARG:HB2	1.93	0.50
2:D:145:ASP:OD2	2:D:145:ASP:N	2.45	0.50
1:C:219:GLU:O	1:C:223:ARG:NH2	2.33	0.49
1:E:166:LYS:HA	1:E:250:ALA:O	2.12	0.49
1:E:307:GLY:HA2	2:F:63:PHE:CZ	2.44	0.49
2:J:159:TYR:CG	2:J:160:PRO:HD3	2.46	0.49
1:K:113:SER:HB2	1:K:269:SER:OG	2.12	0.49
1:K:280:ASP:CG	3:M:2:NAG:O7	2.45	0.49
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.93	0.49
1:A:225:LYS:CD	1:K:80:SER:HB3	2.42	0.49
2:B:72:HIS:CD2	2:B:73:LEU:HG	2.47	0.49
1:C:307:GLY:HA2	2:D:63:PHE:CE1	2.47	0.49
2:D:129:ASN:N	2:D:129:ASN:HD22	2.10	0.49
1:E:113:SER:CB	1:E:269:SER:CB	2.83	0.49
1:G:43:HIS:HB3	1:G:301:ILE:HD13	1.94	0.49
1:I:43:HIS:HB3	1:I:301:ILE:HD13	1.94	0.49
2:J:159:TYR:CD2	2:J:160:PRO:HD3	2.47	0.49
1:A:158:VAL:HG22	6:A:343:HOH:O	2.10	0.49
1:I:51:ARG:HG3	6:I:338:HOH:O	2.11	0.49
2:L:145:ASP:OD2	2:L:145:ASP:N	2.45	0.49
1:A:50:LEU:O	1:A:283:THR:O	2.29	0.49
1:E:170:SER:CB	1:E:247:THR:HA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:VAL:HG21	1:G:321:ALA:HB2	1.94	0.49
1:A:324:LEU:HD23	1:A:324:LEU:N	2.27	0.49
6:C:357:HOH:O	2:D:13:GLY:HA2	2.13	0.49
1:E:86:VAL:HA	1:E:272:ILE:O	2.13	0.49
2:F:158:ASP:O	2:F:160:PRO:HD3	2.13	0.49
2:J:125:GLN:HE21	2:J:157:TYR:HB3	1.78	0.49
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.48	0.49
1:G:22:VAL:HG12	1:G:319:ARG:HG2	1.95	0.49
1:K:271:ILE:HG13	1:K:271:ILE:O	2.12	0.49
2:L:158:ASP:OD1	2:L:158:ASP:N	2.46	0.49
1:A:167:LEU:HD12	1:A:167:LEU:O	2.12	0.49
1:C:104:TYR:CE2	1:C:108:ARG:HD2	2.48	0.49
1:C:189:SER:HB2	1:C:222:ILE:HD13	1.95	0.49
1:I:8:THR:HG22	2:J:139:GLU:CA	2.35	0.49
1:K:44:ASN:ND2	1:K:46:LYS:H	2.10	0.49
1:K:252:GLY:C	1:K:253:ASN:HD22	2.16	0.49
1:E:189:SER:HB3	1:E:230:GLU:C	2.33	0.49
2:F:9:PHE:CD1	2:F:9:PHE:C	2.86	0.49
1:G:11:ILE:HD12	2:H:136:GLY:O	2.12	0.49
1:G:83:SER:HG	1:G:84:TYR:HD2	1.57	0.49
1:G:321:ALA:O	6:G:342:HOH:O	2.20	0.49
1:A:159:LYS:CD	1:A:199:GLN:HG2	2.43	0.49
1:A:159:LYS:CE	1:A:199:GLN:HG2	2.42	0.49
1:C:189:SER:HA	1:C:221:ALA:O	2.12	0.49
1:I:25:VAL:HG21	2:J:102:LEU:HD12	1.95	0.49
1:A:49:LYS:HG3	1:A:281:CYS:O	2.13	0.49
1:C:78:THR:CG2	1:C:79:ALA:H	2.26	0.49
1:E:80:SER:O	1:E:116:SER:HA	2.13	0.49
1:G:11:ILE:N	1:G:11:ILE:HD12	2.28	0.49
2:H:72:HIS:CD2	2:H:73:LEU:HG	2.48	0.49
1:K:159:LYS:HZ2	1:K:199:GLN:CG	2.26	0.49
2:L:135:ASN:OD1	2:L:135:ASN:C	2.52	0.49
1:A:96:CYS:O	1:A:227:ARG:HD3	2.13	0.48
1:C:9:LEU:HB2	2:D:149:MET:SD	2.53	0.48
1:E:101:PHE:HB3	1:E:104:TYR:HB2	1.94	0.48
1:I:252:GLY:C	1:I:253:ASN:HD22	2.17	0.48
1:E:183:TRP:CZ2	1:E:236:TYR:CB	2.95	0.48
1:E:184:GLY:HA2	1:E:234:ASN:O	2.13	0.48
1:K:78:THR:O	1:K:78:THR:CG2	2.61	0.48
1:K:236:TYR:O	6:K:343:HOH:O	2.20	0.48
4:R:2:NAG:C6	4:R:3:BMA:O5	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:O	1:A:162:ASN:HB2	2.13	0.48
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.94	0.48
2:J:76:ARG:CA	6:J:295:HOH:O	2.58	0.48
1:K:118:GLU:HG2	1:K:262:ALA:HB3	1.94	0.48
1:C:177:LYS:HD2	1:C:262:ALA:HB1	1.95	0.48
1:E:141:ALA:C	1:E:143:PRO:HD3	2.34	0.48
2:F:129:ASN:N	2:F:129:ASN:HD22	2.11	0.48
1:G:9:LEU:N	2:H:138:PHE:O	2.46	0.48
1:I:96:CYS:O	1:I:227:ARG:HD3	2.12	0.48
2:J:119:TYR:CE1	2:J:138:PHE:CZ	3.01	0.48
1:K:189:SER:HB2	1:K:222:ILE:HD13	1.95	0.48
1:A:205:VAL:HG11	1:A:254:LEU:HD13	1.95	0.48
1:C:43:HIS:HB3	1:C:301:ILE:HD13	1.94	0.48
1:C:121:GLU:CD	1:C:124:PRO:HA	2.34	0.48
1:C:156:TRP:CD1	6:C:346:HOH:O	2.55	0.48
1:K:8:THR:OG1	2:L:27:GLN:CB	2.60	0.48
1:A:130:PRO:HG2	1:A:131:ASN:OD1	2.13	0.48
2:B:28:ASN:OD1	2:B:146:ASN:ND2	2.46	0.48
2:B:150:GLU:O	2:B:153:LYS:N	2.47	0.48
1:E:38:LEU:HD11	1:E:320:LEU:HD13	1.94	0.48
1:E:51:ARG:O	1:E:282:ASN:OD1	2.32	0.48
1:E:224:PRO:HA	6:E:362:HOH:O	2.13	0.48
1:I:177:LYS:HD2	1:I:262:ALA:HB1	1.95	0.48
2:L:150:GLU:HG2	5:L:601:NAG:C6	2.42	0.48
1:E:44:ASN:ND2	1:E:46:LYS:H	2.11	0.48
2:F:145:ASP:OD2	2:F:145:ASP:N	2.45	0.48
2:H:74:GLU:CA	6:I:341:HOH:O	2.62	0.48
2:H:161:LYS:O	2:H:162:TYR:C	2.52	0.48
2:J:142:HIS:O	2:J:142:HIS:CG	2.66	0.48
1:A:252:GLY:C	1:A:253:ASN:HD22	2.16	0.48
1:E:185:ILE:N	1:E:234:ASN:O	2.33	0.48
1:E:216:PHE:CE2	1:E:236:TYR:CE2	3.02	0.48
1:G:252:GLY:C	1:G:253:ASN:HD22	2.17	0.48
1:K:71:PRO:CB	1:K:144:HIS:HB2	2.43	0.48
1:C:22:VAL:HG12	1:C:319:ARG:HG2	1.96	0.48
1:C:167:LEU:HD12	1:C:167:LEU:O	2.14	0.48
1:G:303:PRO:HG3	1:G:312:TYR:CE2	2.49	0.48
1:K:95:THR:HA	6:K:355:HOH:O	2.13	0.48
1:K:95:THR:OG1	1:K:97:TYR:O	2.32	0.48
1:K:44:ASN:ND2	1:K:291:ALA:H	2.11	0.48
1:C:129:TRP:N	1:C:130:PRO:HD3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ALA:O	1:C:223:ARG:NH1	2.46	0.47
1:E:167:LEU:HD22	1:E:250:ALA:CB	2.40	0.47
1:I:143:PRO:HD2	3:S:1:NAG:H83	1.94	0.47
1:K:46:LYS:HE2	1:K:279:HIS:CE1	2.48	0.47
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.49	0.47
1:E:89:PRO:HD2	1:E:275:ASP:OD2	2.14	0.47
1:I:311:LYS:HG2	2:J:92:TRP:CD2	2.48	0.47
1:I:319:ARG:NH1	1:I:319:ARG:HG3	2.29	0.47
1:K:309:CYS:O	2:L:61:THR:HG21	2.14	0.47
2:D:74:GLU:HB3	2:D:77:ILE:HD11	1.95	0.47
1:E:13:TYR:CE2	2:F:6:ILE:HA	2.49	0.47
1:E:121:GLU:HA	1:E:259:TYR:HA	1.96	0.47
1:E:189:SER:HB2	1:E:222:ILE:HD13	1.96	0.47
2:H:2:LEU:O	2:J:113:SER:OG	2.24	0.47
1:I:13:TYR:HB2	1:I:324:LEU:HD11	1.97	0.47
1:I:46:LYS:HE2	1:I:279:HIS:CE1	2.49	0.47
1:I:83:SER:CB	6:I:338:HOH:O	2.44	0.47
1:I:311:LYS:HG2	2:J:92:TRP:NE1	2.29	0.47
1:K:43:HIS:HB3	1:K:301:ILE:HD13	1.95	0.47
1:K:57:HIS:O	1:K:76:LEU:HD23	2.13	0.47
1:A:311:LYS:HG2	2:B:92:TRP:CD2	2.49	0.47
2:B:157:TYR:CD2	2:B:158:ASP:O	2.67	0.47
2:H:84:VAL:HG13	2:J:84:VAL:HG21	1.96	0.47
1:I:104:TYR:CE2	1:I:108:ARG:HD2	2.49	0.47
1:I:99:GLY:HA3	1:I:233:MET:O	2.14	0.47
1:I:294:THR:HG21	1:I:310:PRO:HG2	1.97	0.47
2:J:132:GLU:HG2	2:J:138:PHE:CE2	2.50	0.47
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.13	0.47
1:K:303:PRO:HG3	1:K:312:TYR:CZ	2.50	0.47
1:A:26:LEU:HB3	2:D:47:GLU:HB3	1.96	0.47
1:A:320:LEU:O	6:A:349:HOH:O	2.21	0.47
1:C:205:VAL:HG11	1:C:254:LEU:HD13	1.97	0.47
2:D:128:ASN:HB3	2:D:162:TYR:CE1	2.48	0.47
1:G:110:GLN:NE2	2:L:72:HIS:O	2.46	0.47
1:K:114:VAL:CG1	1:K:117:PHE:HB2	2.40	0.47
1:A:141:ALA:O	1:A:227:ARG:NH1	2.48	0.47
1:A:162:ASN:HD22	1:A:162:ASN:HA	1.55	0.47
1:A:297:PRO:HG3	2:B:56:ILE:HA	1.96	0.47
2:B:108:LEU:HB2	6:B:193:HOH:O	2.14	0.47
1:C:87:GLU:O	1:C:273:ILE:HA	2.14	0.47
1:C:294:THR:HG21	1:C:310:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:GLY:O	1:E:162:ASN:HB2	2.13	0.47
1:G:51:ARG:C	6:G:365:HOH:O	2.53	0.47
1:G:112:SER:HB2	1:G:270:GLY:HA2	1.96	0.47
1:G:167:LEU:HD12	1:G:167:LEU:O	2.14	0.47
1:G:180:LEU:N	6:G:373:HOH:O	2.48	0.47
1:G:209:SER:HA	1:K:224:PRO:HG2	1.96	0.47
1:G:244:ASP:OD2	1:G:245:LYS:N	2.48	0.47
1:G:261:PHE:N	6:G:373:HOH:O	2.28	0.47
1:G:327:ILE:C	6:G:337:HOH:O	2.53	0.47
2:H:47:GLU:CB	1:K:26:LEU:HB3	2.38	0.47
1:K:104:TYR:CE2	1:K:108:ARG:HD2	2.50	0.47
1:C:224:PRO:HG2	1:E:245:LYS:O	2.15	0.47
1:C:324:LEU:H	1:C:324:LEU:HD23	1.79	0.47
1:E:85:ILE:O	1:E:272:ILE:N	2.38	0.47
1:E:122:ILE:HB	1:E:260:ALA:CB	2.45	0.47
2:H:145:ASP:OD2	2:H:145:ASP:N	2.43	0.47
1:I:143:PRO:HD2	3:S:1:NAG:C8	2.44	0.47
1:K:102:ILE:HG13	1:K:236:TYR:CD2	2.49	0.47
1:E:123:PHE:HB2	1:E:257:PRO:O	2.15	0.47
1:G:114:VAL:HG21	1:G:117:PHE:HB2	1.97	0.47
1:I:25:VAL:HG12	2:L:51:LYS:HG3	1.96	0.47
1:I:312:TYR:CD2	2:J:89:LEU:HD13	2.50	0.47
1:K:22:VAL:HG12	1:K:319:ARG:HG2	1.96	0.47
1:A:87:GLU:O	1:A:273:ILE:HA	2.14	0.47
2:B:129:ASN:N	2:B:129:ASN:HD22	2.11	0.47
1:E:44:ASN:HD22	1:E:44:ASN:C	2.19	0.47
2:H:19:ASP:HB2	2:H:36:ALA:HB3	1.97	0.47
1:I:107:LEU:HG	1:I:111:LEU:HD22	1.97	0.47
1:K:8:THR:CB	2:L:27:GLN:HB3	2.45	0.47
1:A:99:GLY:HA3	1:A:233:MET:O	2.14	0.46
1:A:131:ASN:OD1	1:A:131:ASN:N	2.47	0.46
1:C:49:LYS:O	1:C:283:THR:HG22	2.16	0.46
2:F:106:ARG:HE	2:F:106:ARG:HB3	1.60	0.46
1:G:33:THR:HG23	1:G:324:LEU:O	2.15	0.46
1:A:44:ASN:ND2	1:A:291:ALA:H	2.12	0.46
1:A:44:ASN:O	1:A:46:LYS:HE3	2.15	0.46
1:C:44:ASN:ND2	1:C:46:LYS:H	2.13	0.46
1:C:135:ASN:HB3	3:S:2:NAG:C8	2.44	0.46
1:E:50:LEU:CD2	1:E:306:ILE:HG22	2.45	0.46
2:F:19:ASP:HB2	2:F:36:ALA:HB3	1.97	0.46
1:G:104:TYR:CE2	1:G:108:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:THR:HG21	1:K:310:PRO:HG2	1.97	0.46
1:E:25:VAL:HG21	2:F:102:LEU:HD12	1.97	0.46
1:G:226:VAL:O	1:G:227:ARG:HB2	2.15	0.46
2:J:142:HIS:O	2:J:142:HIS:CD2	2.69	0.46
1:K:99:GLY:HA3	1:K:233:MET:O	2.16	0.46
1:A:36:VAL:N	6:A:349:HOH:O	2.47	0.46
1:A:227:ARG:O	1:A:228:ASP:HB2	2.15	0.46
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.96	0.46
2:B:142:HIS:CE1	2:B:161:LYS:NZ	2.83	0.46
1:E:38:LEU:CD1	1:E:320:LEU:HB2	2.45	0.46
1:I:309:CYS:O	2:J:61:THR:HG21	2.16	0.46
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.81	0.46
1:A:72:GLU:HG3	3:M:1:NAG:N2	2.30	0.46
1:C:227:ARG:NH2	3:P:1:NAG:O3	2.49	0.46
1:K:23:ASP:OD1	1:K:28:LYS:HB3	2.16	0.46
1:G:194:GLN:O	1:G:198:TYR:O	2.33	0.46
1:I:81:SER:HA	1:I:114:VAL:HG12	1.96	0.46
1:I:183:TRP:HZ3	1:I:238:THR:HG22	1.81	0.46
1:K:42:LYS:HE3	1:K:42:LYS:HB2	1.78	0.46
1:E:172:ILE:HG13	1:E:244:ASP:O	2.16	0.46
1:G:44:ASN:HD22	1:G:45:GLY:N	2.14	0.46
1:I:302:HIS:HA	1:I:303:PRO:HD3	1.83	0.46
1:K:183:TRP:HZ3	1:K:238:THR:HG22	1.80	0.46
1:C:96:CYS:O	1:C:227:ARG:HD3	2.16	0.46
1:C:311:LYS:HA	1:C:311:LYS:HD3	1.76	0.46
1:E:125:LYS:HG3	1:E:155:ILE:CD1	2.44	0.46
1:E:155:ILE:HG13	1:E:258:ARG:HB2	1.98	0.46
2:H:13:GLY:N	6:H:184:HOH:O	2.28	0.46
2:H:88:PHE:CZ	2:L:87:GLY:HA3	2.51	0.46
1:I:167:LEU:HD12	1:I:167:LEU:O	2.15	0.46
1:I:316:THR:HG22	6:I:344:HOH:O	2.15	0.46
1:K:50:LEU:HD21	1:K:306:ILE:HG22	1.98	0.46
2:L:9:PHE:CD1	2:L:10:ILE:HG13	2.50	0.46
1:C:83:SER:HB3	6:C:334:HOH:O	2.16	0.46
1:E:11:ILE:CG2	1:E:12:GLY:N	2.79	0.46
1:E:49:LYS:HB3	1:E:53:VAL:O	2.16	0.46
1:E:108:ARG:HB3	1:E:271:ILE:HD13	1.97	0.46
1:K:244:ASP:OD2	1:K:245:LYS:N	2.49	0.46
2:L:19:ASP:HB2	2:L:36:ALA:HB3	1.98	0.46
2:L:28:ASN:C	2:L:28:ASN:HD22	2.19	0.46
1:E:93:ASN:ND2	3:Q:1:NAG:O7	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:GLU:O	1:G:273:ILE:HA	2.15	0.46
2:H:87:GLY:HA3	2:J:88:PHE:CZ	2.51	0.46
1:K:81:SER:HA	1:K:114:VAL:HG12	1.96	0.46
1:A:81:SER:HA	1:A:114:VAL:HG12	1.98	0.45
1:E:7:ASP:OD1	1:E:7:ASP:N	2.49	0.45
1:E:39:LEU:HB3	6:E:356:HOH:O	2.16	0.45
1:E:114:VAL:HG21	1:E:117:PHE:HB2	1.98	0.45
1:E:177:LYS:HB2	1:E:263:MET:O	2.16	0.45
1:G:44:ASN:ND2	1:G:46:LYS:H	2.14	0.45
1:I:44:ASN:HD22	1:I:45:GLY:N	2.14	0.45
1:K:49:LYS:HE3	3:M:2:NAG:O7	2.15	0.45
2:D:151:SER:HB2	2:D:156:THR:O	2.15	0.45
1:E:178:GLU:CD	1:E:265:ARG:NH1	2.70	0.45
1:G:105:GLU:CD	2:H:71:ASN:HD22	2.19	0.45
1:A:8:THR:OG1	2:B:27:GLN:HB3	2.17	0.45
1:A:22:VAL:HG21	1:A:321:ALA:HB2	1.99	0.45
1:A:43:HIS:HB3	1:A:301:ILE:HD13	1.97	0.45
1:A:268:GLY:O	2:B:63:PHE:HE2	2.00	0.45
2:B:123:ARG:NH2	6:B:191:HOH:O	2.49	0.45
1:C:302:HIS:HA	1:C:303:PRO:HD3	1.84	0.45
1:E:252:GLY:C	1:E:253:ASN:HD22	2.20	0.45
1:E:322:THR:O	2:F:48:ILE:HG21	2.16	0.45
2:F:119:TYR:O	2:F:122:VAL:HG22	2.16	0.45
2:F:119:TYR:CZ	2:F:138:PHE:CZ	3.04	0.45
1:I:319:ARG:HH11	1:I:319:ARG:HG3	1.80	0.45
1:K:47:LEU:HD13	1:K:276:THR:CG2	2.46	0.45
1:K:105:GLU:H	1:K:105:GLU:CD	2.20	0.45
2:L:161:LYS:O	2:L:162:TYR:C	2.54	0.45
2:B:74:GLU:HB3	2:B:77:ILE:HD11	1.97	0.45
2:D:19:ASP:HB2	2:D:36:ALA:HB3	1.97	0.45
1:E:9:LEU:HD23	1:E:9:LEU:HA	1.49	0.45
1:G:99:GLY:HA3	1:G:233:MET:O	2.15	0.45
2:B:4:GLY:O	2:B:8:GLY:HA3	2.17	0.45
1:C:81:SER:HA	1:C:114:VAL:HG12	1.99	0.45
1:I:225:LYS:CG	1:I:230:GLU:HG3	2.46	0.45
1:K:8:THR:OG1	2:L:27:GLN:O	2.34	0.45
1:K:13:TYR:HA	6:K:353:HOH:O	2.16	0.45
2:B:162:TYR:CD1	2:B:162:TYR:C	2.89	0.45
1:E:31:THR:HG22	1:E:326:ASN:HB3	1.99	0.45
1:E:179:VAL:HA	1:E:261:PHE:O	2.17	0.45
1:G:14:HIS:CD2	1:G:15:ALA:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:GLU:HB3	2:H:77:ILE:HD11	1.99	0.45
1:I:314:LYS:HB2	1:I:314:LYS:HE3	1.68	0.45
2:J:159:TYR:N	2:J:160:PRO:HD3	2.31	0.45
1:A:47:LEU:CD2	1:A:276:THR:HB	2.44	0.45
1:G:29:ASN:CG	5:G:602:NAG:N2	2.68	0.45
1:K:33:THR:HG23	1:K:325:ARG:O	2.16	0.45
1:K:47:LEU:HD22	1:K:276:THR:O	2.17	0.45
1:A:177:LYS:HE3	1:A:264:GLU:OE2	2.16	0.45
1:C:252:GLY:C	1:C:253:ASN:HD22	2.20	0.45
1:E:104:TYR:CE2	1:E:108:ARG:HD2	2.52	0.45
2:F:125:GLN:NE2	2:F:157:TYR:CG	2.85	0.45
2:H:51:LYS:HG3	1:K:25:VAL:HG12	1.99	0.45
1:I:14:HIS:N	2:J:21:TRP:O	2.49	0.45
2:J:125:GLN:HG3	2:J:125:GLN:O	2.16	0.45
1:K:314:LYS:HE3	1:K:314:LYS:HB2	1.65	0.45
1:A:104:TYR:CE2	1:A:108:ARG:HD2	2.51	0.45
1:A:143:PRO:HD2	3:M:1:NAG:C8	2.46	0.45
2:B:47:GLU:HB3	1:E:26:LEU:HB3	1.98	0.45
1:C:282:ASN:ND2	5:C:607:NAG:O7	2.50	0.45
2:F:5:ALA:HB3	2:F:112:ASP:OD2	2.16	0.45
1:G:9:LEU:HD23	1:G:9:LEU:HA	1.78	0.45
2:J:19:ASP:HB2	2:J:36:ALA:HB3	1.98	0.45
2:L:3:PHE:CE1	2:L:113:SER:HB2	2.52	0.45
1:E:324:LEU:N	1:E:324:LEU:HD23	2.32	0.45
2:F:74:GLU:HB3	2:F:77:ILE:HD11	1.99	0.45
2:F:130:ALA:N	6:F:184:HOH:O	2.50	0.45
1:I:44:ASN:ND2	1:I:46:LYS:H	2.14	0.45
1:C:105:GLU:CD	1:C:105:GLU:H	2.21	0.44
1:C:177:LYS:HE3	1:C:264:GLU:OE2	2.17	0.44
1:C:221:ALA:H	1:C:223:ARG:NH1	2.15	0.44
2:D:99:LEU:HA	2:D:102:LEU:HD23	1.99	0.44
1:E:13:TYR:CE1	2:F:6:ILE:HG23	2.52	0.44
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.52	0.44
1:E:276:THR:HA	1:E:277:PRO:HD3	1.88	0.44
1:E:325:ARG:HD3	6:E:355:HOH:O	2.17	0.44
1:K:95:THR:HG21	1:K:235:TYR:CE1	2.52	0.44
1:A:72:GLU:CG	3:M:1:NAG:HN2	2.29	0.44
1:C:42:LYS:HE3	1:C:42:LYS:HB2	1.75	0.44
1:E:198:TYR:O	1:E:200:ASN:N	2.50	0.44
2:H:51:LYS:HG3	1:K:25:VAL:CG1	2.48	0.44
2:H:68:LYS:HE3	2:L:79:ASN:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:HIS:HA	1:K:303:PRO:HD3	1.82	0.44
1:C:273:ILE:N	1:C:273:ILE:HD12	2.32	0.44
2:D:4:GLY:O	2:D:8:GLY:HA3	2.17	0.44
2:D:5:ALA:HB3	2:D:112:ASP:OD2	2.18	0.44
1:E:96:CYS:HB2	1:E:141:ALA:O	2.18	0.44
1:E:273:ILE:N	1:E:273:ILE:HD12	2.33	0.44
1:A:19:THR:HB	5:L:601:NAG:C5	2.31	0.44
2:B:145:ASP:OD2	2:B:145:ASP:N	2.50	0.44
1:C:44:ASN:HD22	1:C:45:GLY:N	2.16	0.44
1:C:324:LEU:HD23	1:C:324:LEU:N	2.33	0.44
1:I:177:LYS:HE3	1:I:264:GLU:OE2	2.17	0.44
1:A:78:THR:O	1:A:78:THR:OG1	2.35	0.44
1:A:11:ILE:HD13	2:B:24:TYR:CE2	2.53	0.44
1:A:47:LEU:N	1:A:47:LEU:HD23	2.33	0.44
1:C:245:LYS:HD2	1:K:264:GLU:OE1	2.18	0.44
2:F:119:TYR:CE1	2:F:138:PHE:CZ	3.06	0.44
1:I:63:ILE:HG23	6:I:353:HOH:O	2.17	0.44
1:K:11:ILE:O	2:L:10:ILE:HD13	2.18	0.44
1:A:136:LYS:HB2	1:A:158:VAL:HG21	1.99	0.44
2:D:159:TYR:N	2:D:160:PRO:CD	2.80	0.44
1:E:327:ILE:HG21	2:F:12:GLY:HA2	1.99	0.44
1:G:276:THR:HA	1:G:277:PRO:HD3	1.90	0.44
1:K:102:ILE:HG12	1:K:235:TYR:O	2.16	0.44
2:L:74:GLU:HB3	2:L:77:ILE:HD11	1.99	0.44
1:C:51:ARG:HB2	1:C:52:GLY:H	1.64	0.44
1:G:14:HIS:CG	1:G:15:ALA:N	2.85	0.44
2:H:129:ASN:ND2	2:H:159:TYR:CE1	2.86	0.44
2:J:87:GLY:HA3	2:L:88:PHE:CZ	2.52	0.44
1:K:28:LYS:O	1:K:29:ASN:C	2.56	0.44
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.18	0.43
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.53	0.43
2:D:87:GLY:HA3	2:F:88:PHE:CZ	2.53	0.43
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.89	0.43
1:G:74:GLU:O	1:G:75:SER:HB3	2.18	0.43
2:H:50:ASN:HD22	1:K:25:VAL:C	2.20	0.43
1:I:283:THR:HG21	1:I:286:GLN:OE1	2.18	0.43
1:K:225:LYS:NZ	1:K:230:GLU:HG3	2.33	0.43
1:A:296:LEU:HA	1:A:297:PRO:HD3	1.83	0.43
1:C:227:ARG:O	1:C:228:ASP:HB2	2.16	0.43
1:E:37:ASN:HA	1:E:319:ARG:HA	2.00	0.43
1:E:167:LEU:HD21	1:E:254:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:22:VAL:HG21	1:K:321:ALA:HB2	2.00	0.43
1:K:119:ARG:HB2	1:K:261:PHE:CE2	2.53	0.43
1:C:23:ASP:OD2	4:O:1:NAG:O7	2.35	0.43
1:C:121:GLU:CD	6:C:341:HOH:O	2.57	0.43
1:C:167:LEU:HD12	1:C:167:LEU:C	2.38	0.43
1:E:216:PHE:HE2	1:E:236:TYR:CZ	2.36	0.43
2:F:123:ARG:NH2	2:F:132:GLU:OE1	2.51	0.43
1:I:273:ILE:HD12	1:I:273:ILE:N	2.33	0.43
2:J:4:GLY:O	2:J:8:GLY:HA3	2.18	0.43
1:K:227:ARG:O	1:K:228:ASP:HB2	2.17	0.43
1:A:167:LEU:HD12	1:A:167:LEU:C	2.39	0.43
2:B:3:PHE:CE1	2:B:113:SER:HB2	2.54	0.43
1:C:22:VAL:HG21	1:C:321:ALA:HB2	2.00	0.43
1:E:266:ASN:HA	6:E:364:HOH:O	2.17	0.43
2:F:122:VAL:CG2	2:F:138:PHE:CE1	3.01	0.43
1:G:162:ASN:HD22	1:G:162:ASN:HA	1.51	0.43
1:K:62:ASN:ND2	1:K:93:ASN:O	2.51	0.43
1:A:281:CYS:HA	3:N:1:NAG:H82	2.00	0.43
1:E:104:TYR:OH	1:E:108:ARG:NH1	2.52	0.43
2:H:28:ASN:C	2:H:28:ASN:HD22	2.22	0.43
2:H:123:ARG:NH2	2:L:123:ARG:NH1	2.60	0.43
1:K:93:ASN:HB3	1:K:94:GLY:H	1.55	0.43
1:K:226:VAL:O	1:K:227:ARG:HB2	2.19	0.43
1:A:164:TYR:HD2	1:A:164:TYR:C	2.22	0.43
1:C:25:VAL:HG12	2:F:51:LYS:HG3	2.00	0.43
1:C:96:CYS:HB2	1:C:141:ALA:O	2.18	0.43
1:E:87:GLU:N	1:E:272:ILE:O	2.37	0.43
1:E:125:LYS:CD	1:E:258:ARG:NH1	2.81	0.43
1:E:302:HIS:HA	1:E:303:PRO:HD3	1.83	0.43
2:F:123:ARG:C	2:F:125:GLN:H	2.21	0.43
2:H:4:GLY:O	2:H:8:GLY:HA3	2.18	0.43
1:K:44:ASN:HD22	1:K:45:GLY:N	2.16	0.43
2:B:105:GLU:CB	6:B:190:HOH:O	2.52	0.43
1:C:161:GLY:O	1:C:162:ASN:HB2	2.19	0.43
1:E:105:GLU:CD	1:E:105:GLU:H	2.21	0.43
2:F:121:LYS:HG2	6:F:186:HOH:O	2.18	0.43
2:H:151:SER:HB2	2:H:156:THR:O	2.19	0.43
1:I:302:HIS:CE1	1:I:304:ILE:HB	2.53	0.43
2:J:159:TYR:CE1	2:J:160:PRO:HG3	2.54	0.43
1:G:9:LEU:O	2:H:137:CYS:CB	2.67	0.43
1:G:177:LYS:HE3	1:G:264:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:SER:HB2	1:G:222:ILE:HD13	2.01	0.43
1:K:49:LYS:O	1:K:283:THR:HG22	2.19	0.43
2:L:4:GLY:O	2:L:8:GLY:HA3	2.19	0.43
1:A:13:TYR:HB2	1:A:14:HIS:H	1.53	0.43
1:A:96:CYS:HB2	1:A:141:ALA:O	2.18	0.43
1:E:314:LYS:HE3	1:E:314:LYS:HB2	1.69	0.43
1:I:13:TYR:OH	2:J:10:ILE:O	2.31	0.43
1:I:88:THR:HB	1:I:89:PRO:O	2.18	0.43
2:J:91:ILE:HD13	2:L:91:ILE:HG21	1.99	0.43
1:K:162:ASN:HD22	1:K:162:ASN:HA	1.55	0.43
1:A:11:ILE:HD11	2:B:118:LEU:CD2	2.49	0.43
1:A:113:SER:HB2	1:A:269:SER:HB3	2.01	0.43
1:A:276:THR:HA	1:A:277:PRO:HD3	1.84	0.43
1:E:118:GLU:HG2	1:E:262:ALA:HB3	2.00	0.43
1:E:179:VAL:HG22	1:E:262:ALA:HA	2.00	0.43
2:F:122:VAL:O	2:F:126:LEU:HG	2.18	0.43
2:H:58:LYS:HD2	2:H:58:LYS:HA	1.51	0.43
2:J:119:TYR:CZ	2:J:138:PHE:CZ	3.06	0.43
1:K:266:ASN:ND2	1:K:266:ASN:N	2.60	0.43
1:A:91:SER:HB3	6:A:364:HOH:O	2.20	0.42
2:D:123:ARG:C	2:D:125:GLN:H	2.22	0.42
2:F:2:LEU:HD23	2:F:2:LEU:HA	1.85	0.42
1:G:44:ASN:HD22	1:G:44:ASN:C	2.22	0.42
1:G:195:GLN:HA	1:G:198:TYR:O	2.19	0.42
2:H:146:ASN:HB2	6:H:197:HOH:O	2.18	0.42
1:I:42:LYS:HB2	1:I:42:LYS:HE3	1.77	0.42
2:B:14:TRP:HZ3	2:B:23:GLY:O	2.02	0.42
1:C:162:ASN:HD22	1:C:162:ASN:HA	1.56	0.42
1:E:39:LEU:HD23	1:E:317:LYS:HA	2.00	0.42
2:H:5:ALA:HB3	2:H:112:ASP:OD2	2.19	0.42
2:J:151:SER:HB2	2:J:156:THR:O	2.18	0.42
1:C:233:MET:SD	1:C:255:VAL:HG21	2.59	0.42
2:H:66:VAL:HG22	6:H:246:HOH:O	2.18	0.42
2:H:70:PHE:HB3	2:H:74:GLU:HB2	2.01	0.42
1:I:50:LEU:HD21	1:I:306:ILE:HG22	2.01	0.42
1:I:68:LEU:HD23	1:I:68:LEU:HA	1.79	0.42
1:I:113:SER:HB2	1:I:269:SER:HB3	2.01	0.42
1:K:44:ASN:HD22	1:K:44:ASN:C	2.23	0.42
1:K:295:SER:O	2:L:56:ILE:HG23	2.19	0.42
1:A:105:GLU:CD	1:A:105:GLU:H	2.23	0.42
1:A:308:LYS:HG2	2:B:61:THR:OG1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ASP:HB2	2:B:36:ALA:CB	2.50	0.42
1:C:13:TYR:HA	2:D:21:TRP:O	2.19	0.42
1:C:141:ALA:O	1:C:227:ARG:NH1	2.53	0.42
1:E:112:SER:HB2	1:E:270:GLY:CA	2.50	0.42
1:I:22:VAL:HG21	1:I:321:ALA:HB2	2.00	0.42
1:I:88:THR:CB	1:I:89:PRO:O	2.67	0.42
1:I:114:VAL:CG1	1:I:117:PHE:HB2	2.38	0.42
1:I:311:LYS:HG2	2:J:92:TRP:CD1	2.53	0.42
1:K:210:SER:HB2	1:K:244:ASP:OD1	2.19	0.42
1:A:140:ALA:O	1:A:143:PRO:HG3	2.20	0.42
1:A:164:TYR:C	1:A:164:TYR:CD2	2.91	0.42
1:C:183:TRP:HZ3	1:C:238:THR:HG22	1.84	0.42
1:C:314:LYS:HE3	1:C:314:LYS:HB2	1.71	0.42
1:G:113:SER:HB2	1:G:269:SER:HB3	2.01	0.42
2:H:145:ASP:O	2:H:148:CYS:HB3	2.18	0.42
1:I:311:LYS:CG	2:J:92:TRP:CD1	3.02	0.42
1:K:299:GLN:CD	6:K:362:HOH:O	2.57	0.42
1:A:58:LEU:C	1:A:76:LEU:CD1	2.88	0.42
1:A:160:LYS:NZ	1:A:161:GLY:CA	2.76	0.42
1:A:304:ILE:N	1:A:304:ILE:HD12	2.35	0.42
1:C:138:VAL:HG22	6:C:352:HOH:O	2.18	0.42
2:D:28:ASN:C	2:D:28:ASN:HD22	2.21	0.42
2:F:123:ARG:C	2:F:125:GLN:N	2.70	0.42
1:G:314:LYS:HB2	1:G:314:LYS:HE3	1.66	0.42
1:I:167:LEU:HD12	1:I:167:LEU:C	2.40	0.42
1:K:177:LYS:HD2	1:K:262:ALA:HB1	1.99	0.42
1:E:51:ARG:HB2	1:E:52:GLY:H	1.70	0.42
1:E:155:ILE:CD1	1:E:258:ARG:HB2	2.50	0.42
1:E:159:LYS:HZ2	1:E:199:GLN:HG2	1.85	0.42
1:G:273:ILE:HD12	1:G:273:ILE:N	2.35	0.42
1:I:244:ASP:OD2	1:I:245:LYS:N	2.52	0.42
2:J:3:PHE:CE1	2:J:113:SER:HB2	2.54	0.42
1:C:221:ALA:H	1:C:223:ARG:HH12	1.66	0.42
2:D:105:GLU:OE2	2:F:106:ARG:NH2	2.53	0.42
1:G:121:GLU:CD	1:G:124:PRO:HA	2.40	0.42
1:G:304:ILE:HD12	1:G:304:ILE:N	2.35	0.42
1:I:11:ILE:HD11	2:J:122:VAL:HG21	2.00	0.42
1:I:223:ARG:O	1:I:230:GLU:HG2	2.19	0.42
1:A:7:ASP:OD2	2:B:28:ASN:HB2	2.20	0.42
2:B:118:LEU:HD12	2:B:118:LEU:HA	1.88	0.42
2:D:3:PHE:CE1	2:D:113:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:MET:SD	2:D:23:GLY:HA3	2.60	0.42
1:G:55:PRO:CB	6:G:350:HOH:O	2.58	0.42
1:G:155:ILE:HG13	1:G:258:ARG:CG	2.29	0.42
1:G:282:ASN:HB2	5:G:603:NAG:O7	2.19	0.42
1:I:22:VAL:HB	2:J:104:ASN:ND2	2.34	0.42
1:I:35:SER:OG	1:I:319:ARG:NH1	2.51	0.42
1:I:44:ASN:HD22	1:I:44:ASN:C	2.23	0.42
1:A:273:ILE:HD12	1:A:273:ILE:N	2.34	0.42
1:I:311:LYS:HD3	1:I:311:LYS:HA	1.79	0.42
1:K:161:GLY:O	1:K:162:ASN:HB2	2.20	0.42
1:K:311:LYS:NZ	2:L:61:THR:HG22	2.34	0.42
1:A:183:TRP:HZ3	1:A:238:THR:HG22	1.85	0.41
1:C:225:LYS:NZ	1:C:230:GLU:HG3	2.36	0.41
1:C:311:LYS:HG2	2:D:92:TRP:CD2	2.54	0.41
2:D:158:ASP:CG	2:D:160:PRO:HD2	2.40	0.41
1:E:164:TYR:CE1	1:E:252:GLY:HA2	2.54	0.41
1:G:39:LEU:HB2	1:G:318:LEU:HB2	2.00	0.41
1:I:8:THR:O	2:J:149:MET:CE	2.68	0.41
1:A:101:PHE:HB3	1:A:104:TYR:HB2	2.02	0.41
1:A:121:GLU:CD	1:A:124:PRO:HA	2.40	0.41
2:B:26:HIS:HB2	2:B:149:MET:HE2	2.00	0.41
1:C:296:LEU:HA	1:C:297:PRO:HD3	1.81	0.41
2:L:151:SER:HB2	2:L:156:THR:O	2.20	0.41
1:E:231:GLY:O	1:E:232:ARG:NH1	2.52	0.41
2:F:19:ASP:HB2	2:F:36:ALA:CB	2.50	0.41
1:G:159:LYS:HE2	1:G:196:SER:O	2.21	0.41
1:G:305:THR:CG2	6:H:194:HOH:O	2.68	0.41
2:B:142:HIS:NE2	2:B:144:CYS:SG	2.94	0.41
1:C:208:GLY:HA2	1:C:212:TYR:O	2.21	0.41
1:C:244:ASP:OD2	1:C:245:LYS:N	2.53	0.41
1:E:36:VAL:HG13	1:E:322:THR:CG2	2.48	0.41
1:E:185:ILE:O	1:E:234:ASN:N	2.51	0.41
1:G:293:ASN:OD1	1:G:293:ASN:C	2.59	0.41
1:I:63:ILE:O	1:I:67:ILE:HG13	2.20	0.41
1:K:307:GLY:HA2	2:L:63:PHE:CD1	2.55	0.41
1:A:311:LYS:NZ	2:B:61:THR:HG22	2.36	0.41
1:E:296:LEU:HA	1:E:297:PRO:HD3	1.82	0.41
1:K:25:VAL:HG21	2:L:102:LEU:HD12	2.01	0.41
2:L:19:ASP:HB2	2:L:36:ALA:CB	2.51	0.41
1:C:113:SER:HB2	1:C:269:SER:HB3	2.02	0.41
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:LEU:HG	2:D:103:GLU:N	2.32	0.41
1:E:42:LYS:HB2	1:E:42:LYS:HE3	1.77	0.41
1:G:190:THR:HG23	1:G:193:ASP:HB2	2.02	0.41
2:H:19:ASP:HB2	2:H:36:ALA:CB	2.50	0.41
2:J:74:GLU:HB3	2:J:77:ILE:HD11	2.01	0.41
1:K:8:THR:HG1	2:L:27:GLN:HB3	1.84	0.41
1:A:121:GLU:OE2	1:A:124:PRO:HA	2.20	0.41
2:D:28:ASN:C	2:D:28:ASN:ND2	2.74	0.41
1:E:244:ASP:OD2	1:E:245:LYS:N	2.52	0.41
1:E:313:VAL:HG13	2:F:93:THR:HA	2.02	0.41
1:G:118:GLU:CG	1:G:262:ALA:HB3	2.48	0.41
2:H:12:GLY:CA	6:H:184:HOH:O	2.54	0.41
1:K:25:VAL:CG2	2:L:102:LEU:HD12	2.51	0.41
2:L:28:ASN:C	2:L:28:ASN:ND2	2.74	0.41
2:B:91:ILE:HG21	2:F:91:ILE:HD13	2.03	0.41
1:C:258:ARG:NH2	6:C:341:HOH:O	2.53	0.41
2:D:19:ASP:HB2	2:D:36:ALA:CB	2.51	0.41
1:G:167:LEU:HD12	1:G:167:LEU:C	2.40	0.41
1:G:180:LEU:HB2	1:G:263:MET:HE1	2.03	0.41
1:A:244:ASP:OD2	1:A:245:LYS:N	2.53	0.41
1:C:140:ALA:O	1:C:143:PRO:HG3	2.21	0.41
1:E:11:ILE:HG23	1:E:12:GLY:N	2.36	0.41
1:E:38:LEU:HG	1:E:320:LEU:HB2	2.03	0.41
1:E:119:ARG:HB2	1:E:261:PHE:CE2	2.56	0.41
1:E:304:ILE:HD12	1:E:304:ILE:N	2.36	0.41
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.55	0.41
1:G:10:CYS:C	1:G:11:ILE:HG23	2.41	0.41
1:I:25:VAL:HG22	2:J:102:LEU:HD12	2.03	0.41
1:I:49:LYS:HB2	1:I:49:LYS:HE2	1.53	0.41
1:K:47:LEU:HD13	1:K:276:THR:HB	2.03	0.41
1:K:144:HIS:O	1:K:145:ALA:HB3	2.21	0.41
1:K:159:LYS:HD3	1:K:199:GLN:HB2	2.02	0.41
1:K:189:SER:HA	1:K:221:ALA:O	2.21	0.41
1:K:190:THR:HG23	1:K:193:ASP:HB2	2.03	0.41
1:K:311:LYS:HA	1:K:311:LYS:HD3	1.79	0.41
1:A:49:LYS:HG3	1:A:49:LYS:H	1.56	0.41
1:C:304:ILE:N	1:C:304:ILE:HD12	2.35	0.41
1:K:51:ARG:HB2	1:K:52:GLY:H	1.69	0.41
1:A:44:ASN:C	1:A:44:ASN:HD22	2.23	0.40
1:A:44:ASN:HD22	1:A:45:GLY:N	2.18	0.40
1:A:206:PHE:HZ	1:E:223:ARG:HE	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASP:OD2	2:B:148:CYS:HB3	2.21	0.40
1:C:44:ASN:HD22	1:C:44:ASN:C	2.22	0.40
1:E:121:GLU:OE2	1:E:124:PRO:HA	2.22	0.40
1:G:138:VAL:N	6:G:369:HOH:O	2.54	0.40
1:I:67:ILE:HG13	1:I:67:ILE:H	1.55	0.40
1:C:168:SER:OG	1:K:176:GLY:HA3	2.22	0.40
1:E:120:PHE:HE2	1:E:262:ALA:N	2.18	0.40
1:E:293:ASN:O	1:E:293:ASN:ND2	2.54	0.40
2:H:74:GLU:OE2	2:L:76:ARG:NH2	2.39	0.40
1:K:68:LEU:O	1:K:151:TYR:HB3	2.21	0.40
1:K:88:THR:O	1:K:91:SER:OG	2.32	0.40
1:K:299:GLN:OE1	6:K:362:HOH:O	2.21	0.40
1:A:189:SER:HA	1:A:221:ALA:O	2.22	0.40
2:F:121:LYS:HA	6:F:187:HOH:O	2.20	0.40
2:J:5:ALA:HB3	2:J:112:ASP:OD2	2.21	0.40
2:L:148:CYS:SG	6:L:262:HOH:O	2.63	0.40
1:A:44:ASN:ND2	1:A:46:LYS:H	2.19	0.40
1:E:121:GLU:CD	1:E:124:PRO:HA	2.41	0.40
1:E:186:HIS:HA	1:E:233:MET:HA	2.02	0.40
1:E:314:LYS:HB2	2:F:89:LEU:HD11	2.04	0.40
1:G:11:ILE:CD1	2:H:136:GLY:O	2.69	0.40
1:I:304:ILE:N	1:I:304:ILE:HD12	2.36	0.40
1:K:13:TYR:CE2	2:L:6:ILE:HA	2.56	0.40
2:B:24:TYR:CD1	2:B:24:TYR:N	2.89	0.40
1:C:13:TYR:C	6:C:357:HOH:O	2.60	0.40
1:G:101:PHE:HB3	1:G:104:TYR:HB2	2.04	0.40
2:H:28:ASN:C	2:H:28:ASN:ND2	2.75	0.40
1:I:327:ILE:HB	2:J:13:GLY:H	1.86	0.40
2:J:123:ARG:HG3	2:J:138:PHE:CE2	2.52	0.40

All (3) 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:C:74:GLU:OE1	1:K:144:HIS:NE2[1_455]	1.89	0.31
1:C:74:GLU:OE1	1:K:144:HIS:CD2[1_455]	2.04	0.16
1:C:74:GLU:OE2	1:K:144:HIS:ND1[1_455]	2.13	0.07

## 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	319/333 (96%)	286 (90%)	32 (10%)	1 (0%)	41	70
1	C	319/333 (96%)	296 (93%)	22 (7%)	1 (0%)	41	70
1	E	319/333 (96%)	291 (91%)	24 (8%)	4 (1%)	12	35
1	G	319/333 (96%)	299 (94%)	19 (6%)	1 (0%)	41	70
1	I	319/333 (96%)	294 (92%)	25 (8%)	0	100	100
1	K	319/333 (96%)	288 (90%)	31 (10%)	0	100	100
2	B	160/181 (88%)	143 (89%)	17 (11%)	0	100	100
2	D	160/181 (88%)	146 (91%)	14 (9%)	0	100	100
2	F	159/181 (88%)	147 (92%)	12 (8%)	0	100	100
2	H	160/181 (88%)	145 (91%)	15 (9%)	0	100	100
2	J	160/181 (88%)	148 (92%)	12 (8%)	0	100	100
2	L	159/181 (88%)	145 (91%)	14 (9%)	0	100	100
All	All	2872/3084 (93%)	2628 (92%)	237 (8%)	7 (0%)	47	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	92	ASP
1	E	199	GLN
1	A	199	GLN
1	E	75	SER
1	G	268	GLY
1	C	78	THR
1	E	227	ARG

### 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	281/292 (96%)	249 (89%)	32 (11%)	5	16
1	C	282/292 (97%)	255 (90%)	27 (10%)	8	23
1	E	282/292 (97%)	247 (88%)	35 (12%)	4	12
1	G	281/292 (96%)	252 (90%)	29 (10%)	7	20
1	I	282/292 (97%)	251 (89%)	31 (11%)	6	17
1	K	282/292 (97%)	249 (88%)	33 (12%)	5	14
2	B	139/156 (89%)	126 (91%)	13 (9%)	8	24
2	D	138/156 (88%)	128 (93%)	10 (7%)	14	37
2	F	139/156 (89%)	124 (89%)	15 (11%)	6	18
2	H	139/156 (89%)	132 (95%)	7 (5%)	24	54
2	J	139/156 (89%)	127 (91%)	12 (9%)	10	29
2	L	139/156 (89%)	127 (91%)	12 (9%)	10	29
All	All	2523/2688 (94%)	2267 (90%)	256 (10%)	7	21

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	A	37	ASN
1	A	44	ASN
1	A	49	LYS
1	A	58	LEU
1	A	74	GLU
1	A	78	THR
1	A	107	LEU
1	A	111	LEU
1	A	131	ASN
1	A	160	LYS
1	A	162	ASN
1	A	163	SER
1	A	164	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	167	LEU
1	A	190	THR
1	A	193	ASP
1	A	199	GLN
1	A	228	ASP
1	A	240	VAL
1	A	264	GLU
1	A	265	ARG
1	A	266	ASN
1	A	279	HIS
1	A	287	THR
1	A	295	SER
1	A	305	THR
1	A	311	LYS
1	A	316	THR
1	A	324	LEU
1	A	325	ARG
1	A	327	ILE
2	B	22	TYR
2	B	24	TYR
2	B	28	ASN
2	B	38	LEU
2	B	80	LEU
2	B	98	LEU
2	B	126	LEU
2	B	142	HIS
2	B	144	CYS
2	B	148	CYS
2	B	149	MET
2	B	150	GLU
2	B	158	ASP
1	C	7	ASP
1	C	26	LEU
1	C	37	ASN
1	C	44	ASN
1	C	50	LEU
1	C	53	VAL
1	C	75	SER
1	C	78	THR
1	C	111	LEU
1	C	126	THR
1	C	128	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	157	LEU
1	C	162	ASN
1	C	167	LEU
1	C	190	THR
1	C	193	ASP
1	C	200	ASN
1	C	264	GLU
1	C	265	ARG
1	C	266	ASN
1	C	287	THR
1	C	295	SER
1	C	305	THR
1	C	311	LYS
1	C	314	LYS
1	C	316	THR
1	C	324	LEU
2	D	22	TYR
2	D	28	ASN
2	D	38	LEU
2	D	66	VAL
2	D	80	LEU
2	D	102	LEU
2	D	105	GLU
2	D	126	LEU
2	D	142	HIS
2	D	150	GLU
1	E	7	ASP
1	E	8	THR
1	E	9	LEU
1	E	10	CYS
1	E	11	ILE
1	E	32	VAL
1	E	37	ASN
1	E	44	ASN
1	E	47	LEU
1	E	50	LEU
1	E	74	GLU
1	E	76	LEU
1	E	91	SER
1	E	111	LEU
1	E	162	ASN
1	E	167	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	190	THR
1	E	193	ASP
1	E	198	TYR
1	E	199	GLN
1	E	205	VAL
1	E	223	ARG
1	E	230	GLU
1	E	264	GLU
1	E	265	ARG
1	E	266	ASN
1	E	279	HIS
1	E	292	ILE
1	E	293	ASN
1	E	294	THR
1	E	295	SER
1	E	305	THR
1	E	311	LYS
1	E	316	THR
1	E	324	LEU
2	F	2	LEU
2	F	9	PHE
2	F	22	TYR
2	F	28	ASN
2	F	38	LEU
2	F	66	VAL
2	F	80	LEU
2	F	106	ARG
2	F	123	ARG
2	F	125	GLN
2	F	126	LEU
2	F	137	CYS
2	F	142	HIS
2	F	150	GLU
2	F	158	ASP
1	G	7	ASP
1	G	9	LEU
1	G	11	ILE
1	G	13	TYR
1	G	21	THR
1	G	37	ASN
1	G	39	LEU
1	G	44	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	50	LEU
1	G	58	LEU
1	G	76	LEU
1	G	107	LEU
1	G	162	ASN
1	G	167	LEU
1	G	190	THR
1	G	193	ASP
1	G	198	TYR
1	G	200	ASN
1	G	240	VAL
1	G	258	ARG
1	G	263	MET
1	G	264	GLU
1	G	265	ARG
1	G	266	ASN
1	G	279	HIS
1	G	294	THR
1	G	295	SER
1	G	305	THR
1	G	316	THR
2	H	22	TYR
2	H	28	ASN
2	H	58	LYS
2	H	84	VAL
2	H	126	LEU
2	H	142	HIS
2	H	150	GLU
1	I	7	ASP
1	I	11	ILE
1	I	26	LEU
1	I	37	ASN
1	I	44	ASN
1	I	49	LYS
1	I	50	LEU
1	I	53	VAL
1	I	67	ILE
1	I	74	GLU
1	I	75	SER
1	I	90	SER
1	I	91	SER
1	I	111	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	118	GLU
1	I	119	ARG
1	I	160	LYS
1	I	167	LEU
1	I	172	ILE
1	I	190	THR
1	I	193	ASP
1	I	264	GLU
1	I	265	ARG
1	I	266	ASN
1	I	279	HIS
1	I	281	CYS
1	I	295	SER
1	I	305	THR
1	I	311	LYS
1	I	319	ARG
1	I	324	LEU
2	J	19	ASP
2	J	22	TYR
2	J	28	ASN
2	J	30	GLN
2	J	32	SER
2	J	38	LEU
2	J	66	VAL
2	J	80	LEU
2	J	125	GLN
2	J	126	LEU
2	J	142	HIS
2	J	150	GLU
1	K	8	THR
1	K	11	ILE
1	K	28	LYS
1	K	37	ASN
1	K	44	ASN
1	K	47	LEU
1	K	50	LEU
1	K	74	GLU
1	K	76	LEU
1	K	77	SER
1	K	91	SER
1	K	93	ASN
1	K	95	THR

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Mol	Chain	Res	Type
1	K	111	LEU
1	K	119	ARG
1	K	142	CYS
1	K	162	ASN
1	K	167	LEU
1	K	190	THR
1	K	193	ASP
1	K	205	VAL
1	K	263	MET
1	K	264	GLU
1	K	265	ARG
1	K	266	ASN
1	K	271	ILE
1	K	279	HIS
1	K	287	THR
1	K	295	SER
1	K	305	THR
1	K	311	LYS
1	K	316	THR
1	K	324	LEU
2	L	22	TYR
2	L	28	ASN
2	L	38	LEU
2	L	66	VAL
2	L	80	LEU
2	L	126	LEU
2	L	142	HIS
2	L	150	GLU
2	L	158	ASP
2	L	159	TYR
2	L	161	LYS
2	L	162	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	44	ASN
1	A	132	HIS
1	A	162	ASN
1	A	194	GLN
1	A	195	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	253	ASN
1	A	266	ASN
2	B	27	GLN
2	B	28	ASN
2	B	30	GLN
2	B	125	GLN
2	B	129	ASN
2	B	142	HIS
2	B	146	ASN
1	C	37	ASN
1	C	44	ASN
1	C	132	HIS
1	C	162	ASN
1	C	194	GLN
1	C	195	GLN
1	C	199	GLN
1	C	253	ASN
1	C	266	ASN
2	D	27	GLN
2	D	28	ASN
2	D	30	GLN
2	D	125	GLN
2	D	129	ASN
2	D	146	ASN
1	E	17	ASN
1	E	37	ASN
1	E	44	ASN
1	E	132	HIS
1	E	162	ASN
1	E	194	GLN
1	E	195	GLN
1	E	253	ASN
2	F	27	GLN
2	F	28	ASN
2	F	30	GLN
2	F	95	ASN
2	F	129	ASN
2	F	146	ASN
1	G	14	HIS
1	G	37	ASN
1	G	44	ASN
1	G	132	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	162	ASN
1	G	194	GLN
1	G	195	GLN
1	G	199	GLN
1	G	253	ASN
1	G	266	ASN
1	G	279	HIS
2	H	27	GLN
2	H	28	ASN
2	H	30	GLN
2	H	125	GLN
2	H	129	ASN
2	H	146	ASN
2	H	154	ASN
1	I	37	ASN
1	I	44	ASN
1	I	132	HIS
1	I	144	HIS
1	I	194	GLN
1	I	195	GLN
1	I	253	ASN
1	I	266	ASN
1	I	279	HIS
2	J	27	GLN
2	J	28	ASN
2	J	30	GLN
2	J	95	ASN
2	J	125	GLN
2	J	129	ASN
2	J	146	ASN
1	K	37	ASN
1	K	44	ASN
1	K	93	ASN
1	K	132	HIS
1	K	162	ASN
1	K	194	GLN
1	K	195	GLN
1	K	253	ASN
1	K	266	ASN
1	K	279	HIS
2	L	27	GLN
2	L	28	ASN

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Mol	Chain	Res	Type
2	L	30	GLN
2	L	125	GLN
2	L	129	ASN
2	L	146	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

16 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	0.55	0	17,19,21	1.07	0
3	NAG	M	2	3	14,14,15	0.57	0	17,19,21	1.55	3 (17%)
3	NAG	N	1	1,3	14,14,15	0.57	0	17,19,21	0.65	0
3	NAG	N	2	3	14,14,15	0.46	0	17,19,21	1.05	1 (5%)
4	NAG	O	1	4,1	14,14,15	0.61	0	17,19,21	1.15	1 (5%)
4	NAG	O	2	4	14,14,15	0.55	0	17,19,21	1.12	1 (5%)
4	BMA	O	3	4	11,11,12	0.26	0	15,15,17	0.64	0
3	NAG	P	1	1,3	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
3	NAG	P	2	3	14,14,15	0.44	0	17,19,21	2.01	4 (23%)
3	NAG	Q	1	1,3	14,14,15	0.56	0	17,19,21	0.66	0
3	NAG	Q	2	3	14,14,15	0.58	0	17,19,21	0.81	0
4	NAG	R	1	4,1	14,14,15	0.53	0	17,19,21	1.71	3 (17%)
4	NAG	R	2	4	14,14,15	0.40	0	17,19,21	1.88	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	R	3	4	11,11,12	0.27	0	15,15,17	0.66	0
3	NAG	S	1	1,3	14,14,15	0.54	0	17,19,21	1.81	4 (23%)
3	NAG	S	2	3	14,14,15	0.61	0	17,19,21	1.13	1 (5%)

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

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

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	NAG	C1-O5-C5	6.16	120.54	112.19
4	R	2	NAG	C1-O5-C5	5.09	119.08	112.19
3	S	1	NAG	O4-C4-C3	4.96	121.81	110.35
4	R	1	NAG	C2-N2-C7	-4.92	115.90	122.90
3	M	2	NAG	C2-N2-C7	-4.29	116.80	122.90
4	R	2	NAG	C4-C3-C2	-4.13	104.97	111.02
3	P	2	NAG	C2-N2-C7	-3.35	118.13	122.90
3	S	1	NAG	C4-C3-C2	-3.26	106.23	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	NAG	C2-N2-C7	-3.15	118.42	122.90
4	R	1	NAG	C1-O5-C5	3.11	116.40	112.19
3	M	2	NAG	O5-C1-C2	-2.80	106.87	111.29
3	N	2	NAG	O5-C5-C6	2.74	111.50	107.20
3	S	2	NAG	C3-C4-C5	2.73	115.11	110.24
3	S	1	NAG	C2-N2-C7	-2.70	119.05	122.90
4	O	2	NAG	O5-C5-C6	2.68	111.41	107.20
4	R	1	NAG	C4-C3-C2	2.63	114.87	111.02
3	P	1	NAG	O5-C5-C6	2.33	110.85	107.20
3	M	2	NAG	C4-C3-C2	-2.22	107.76	111.02
3	P	2	NAG	C4-C3-C2	-2.18	107.82	111.02
4	R	2	NAG	C2-N2-C7	-2.17	119.81	122.90
3	P	2	NAG	C6-C5-C4	-2.16	107.95	113.00
4	R	2	NAG	O4-C4-C5	2.04	114.37	109.30
3	S	1	NAG	O5-C5-C6	2.03	110.39	107.20

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
4	O	3	BMA	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
4	R	3	BMA	C4-C5-C6-O6
3	P	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
4	R	3	BMA	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	N	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C3-C2-N2-C7

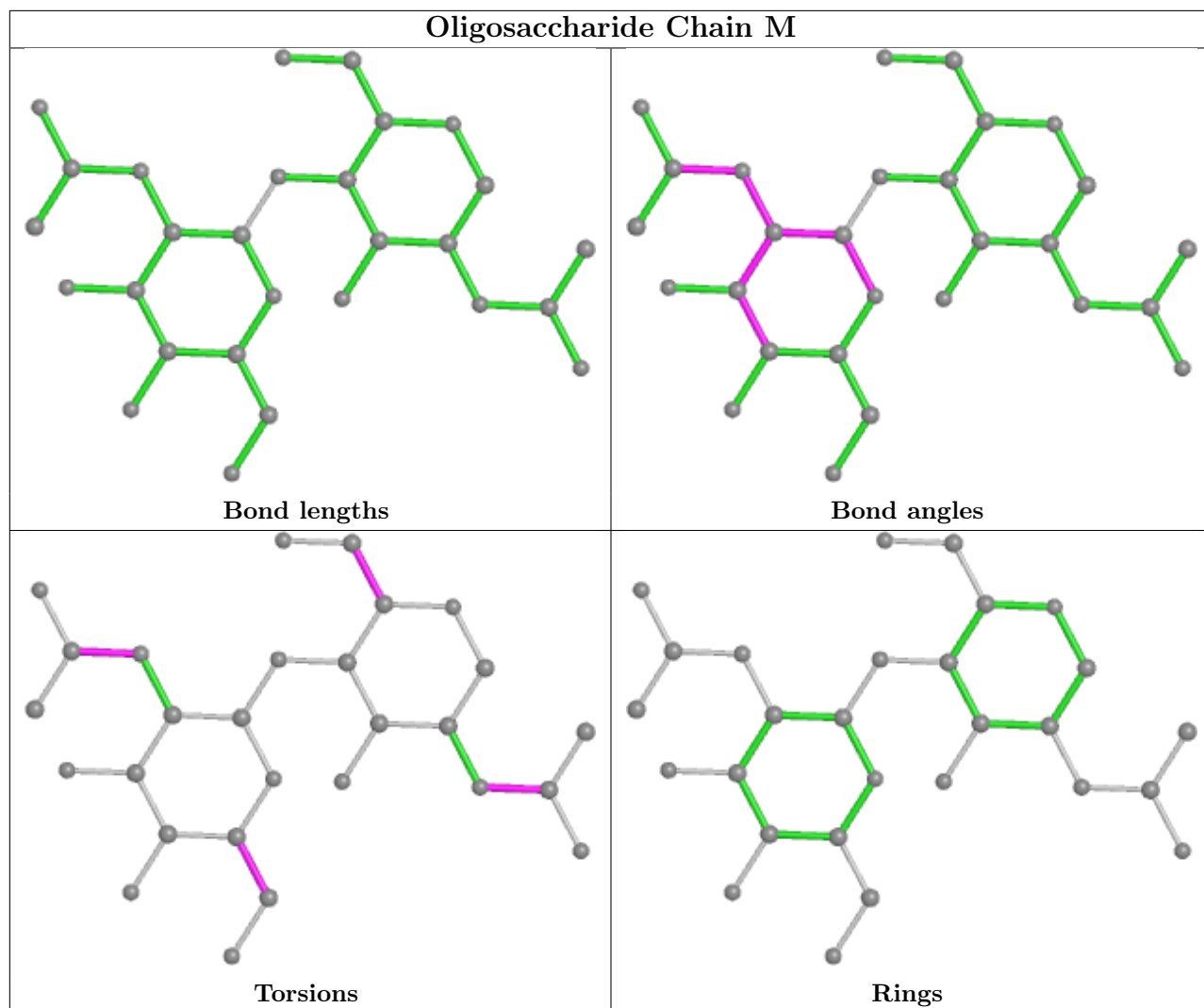
There are no ring outliers.

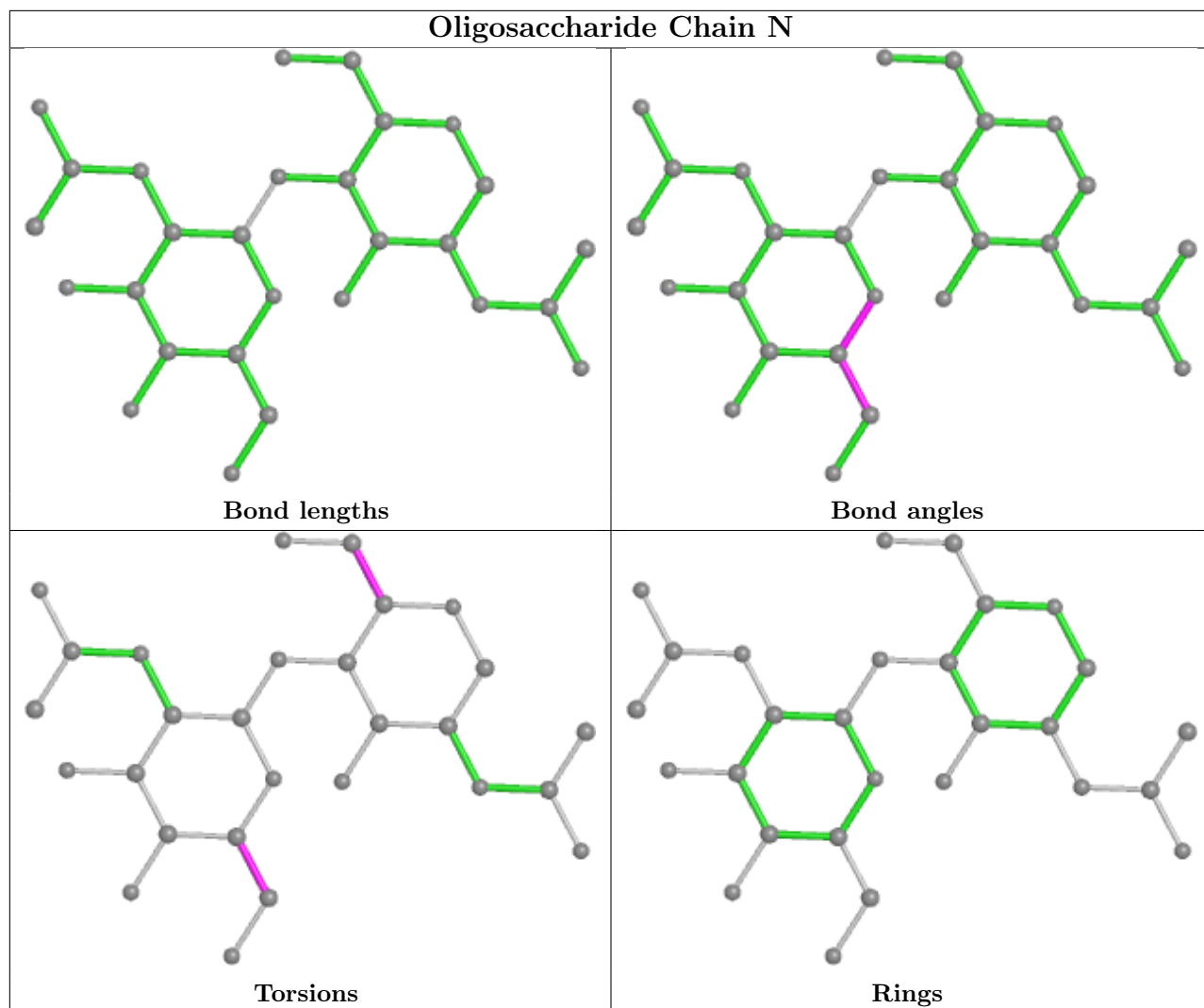
12 monomers are involved in 29 short contacts:

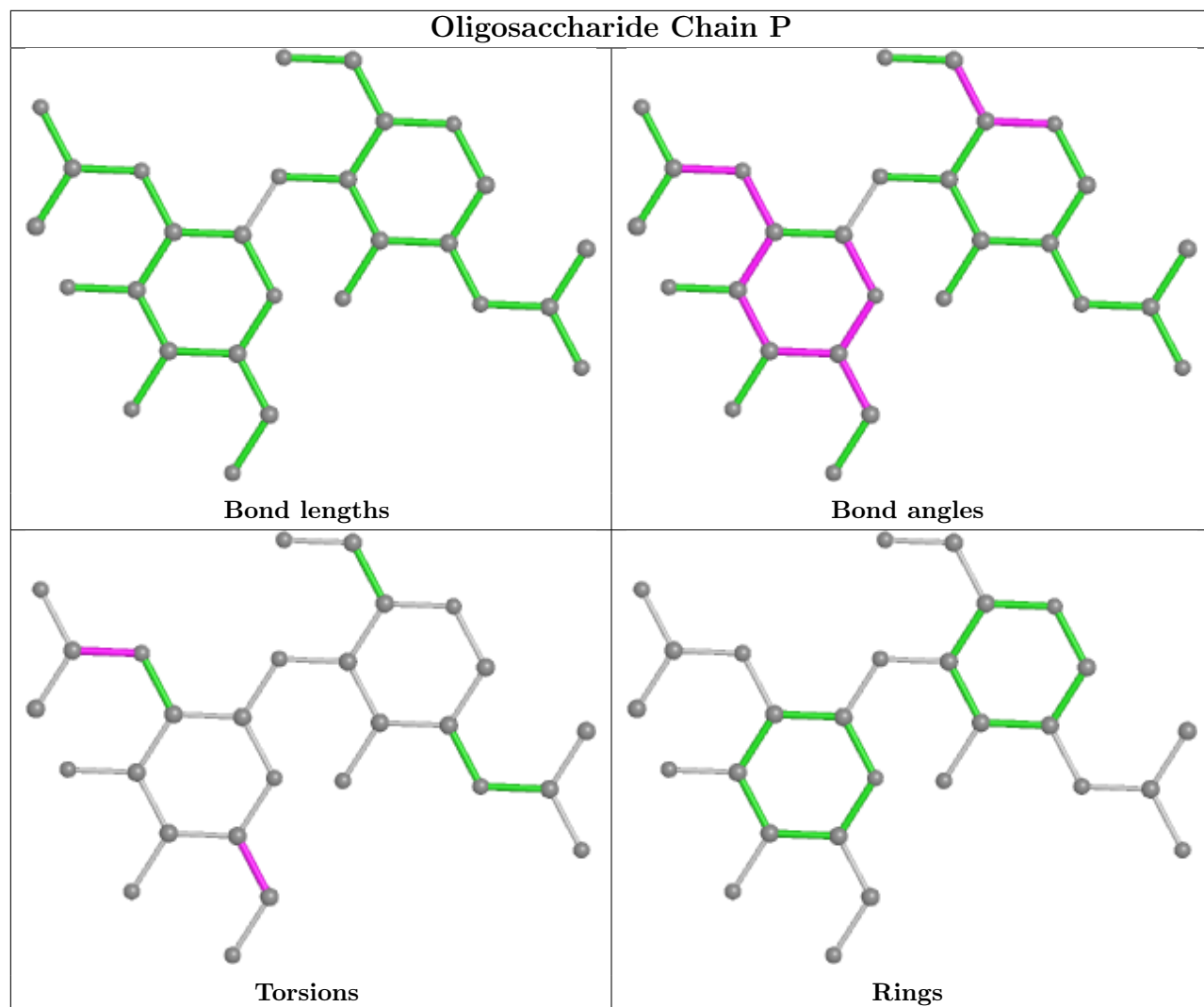
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	4	0
4	R	2	NAG	2	0
3	M	1	NAG	6	0
4	O	1	NAG	3	0
3	S	2	NAG	3	0
3	P	1	NAG	2	0
3	M	2	NAG	3	0
3	Q	1	NAG	3	0
4	R	1	NAG	1	0
4	R	3	BMA	2	0
3	S	1	NAG	3	0
3	N	2	NAG	1	0

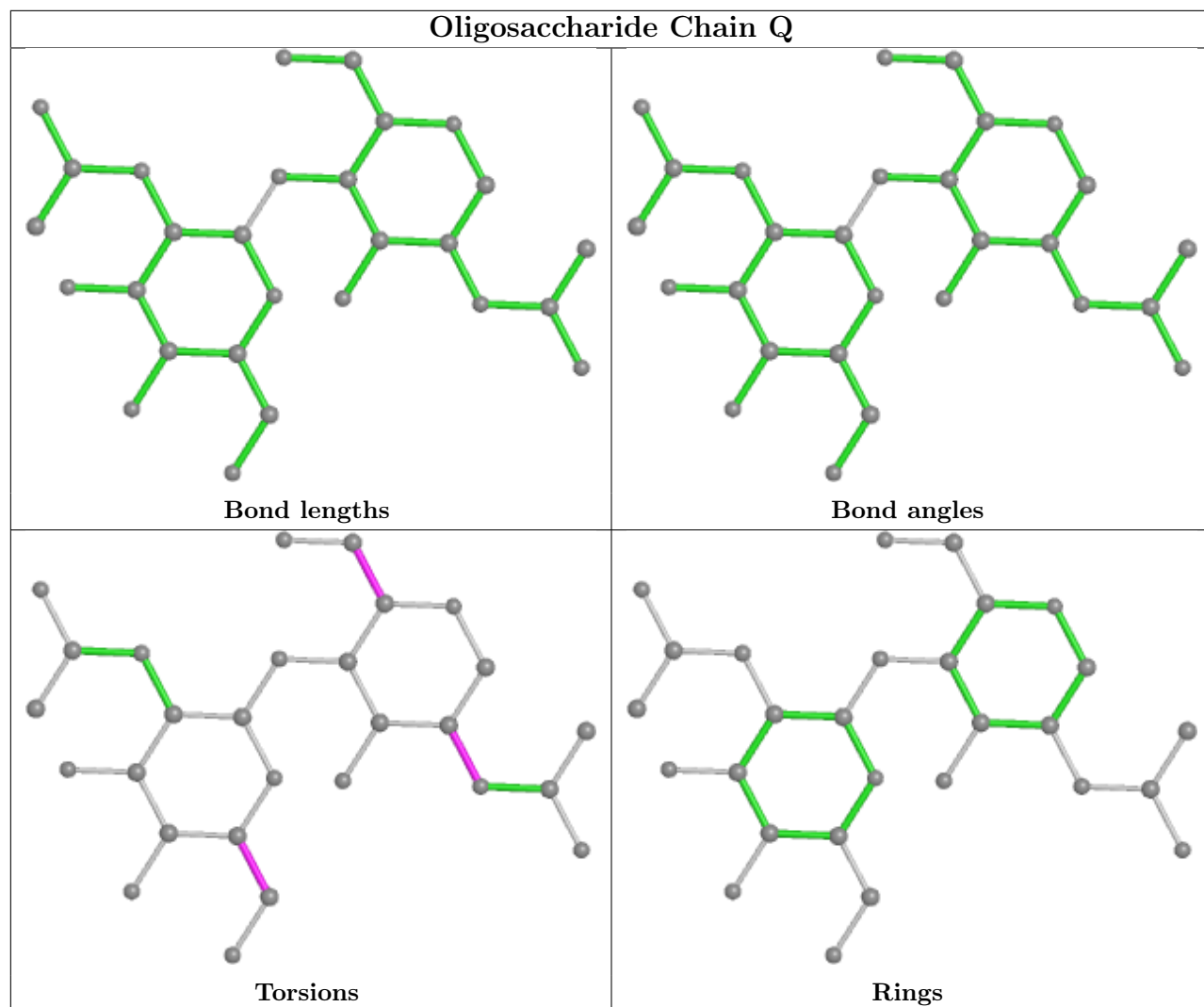
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

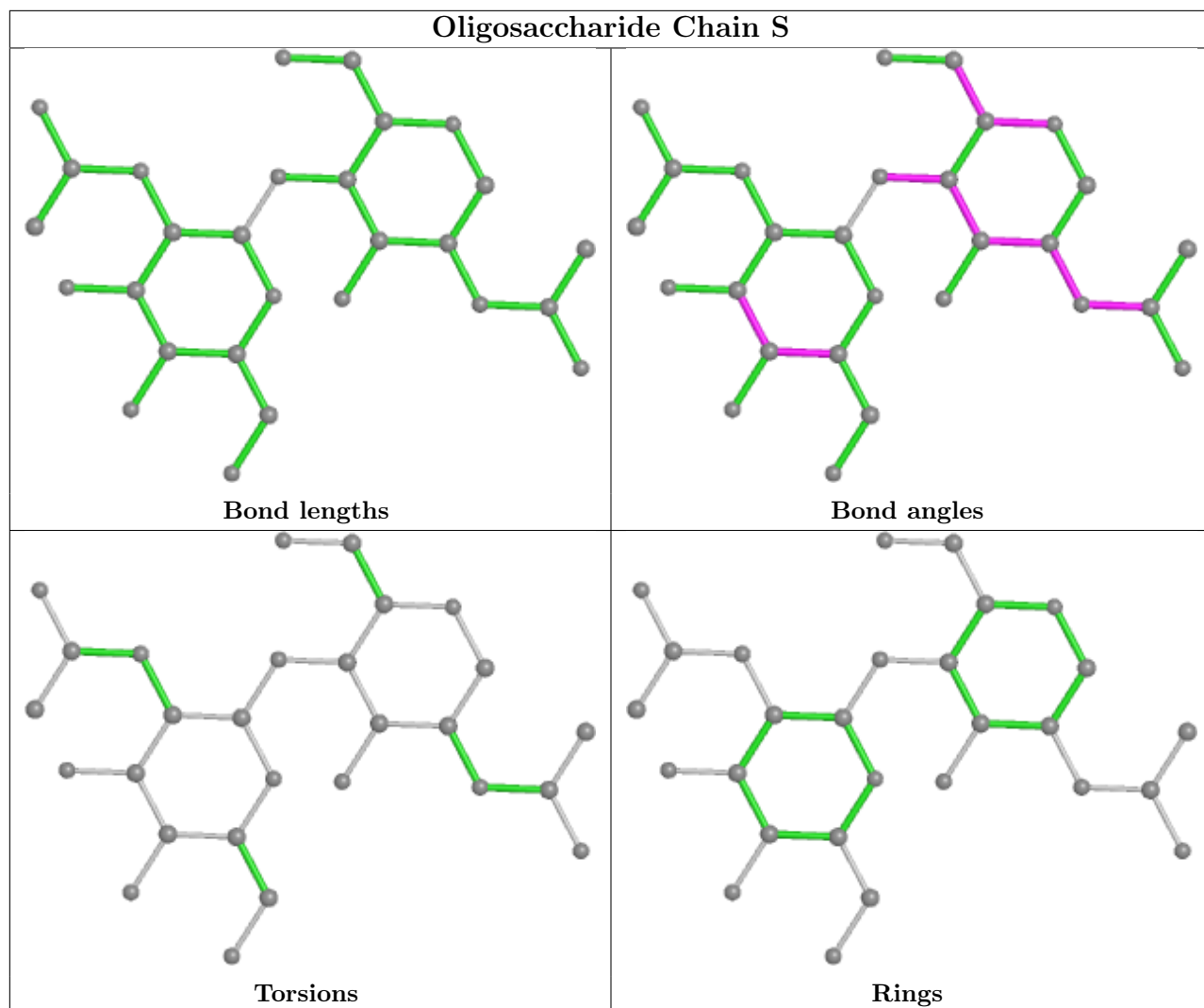


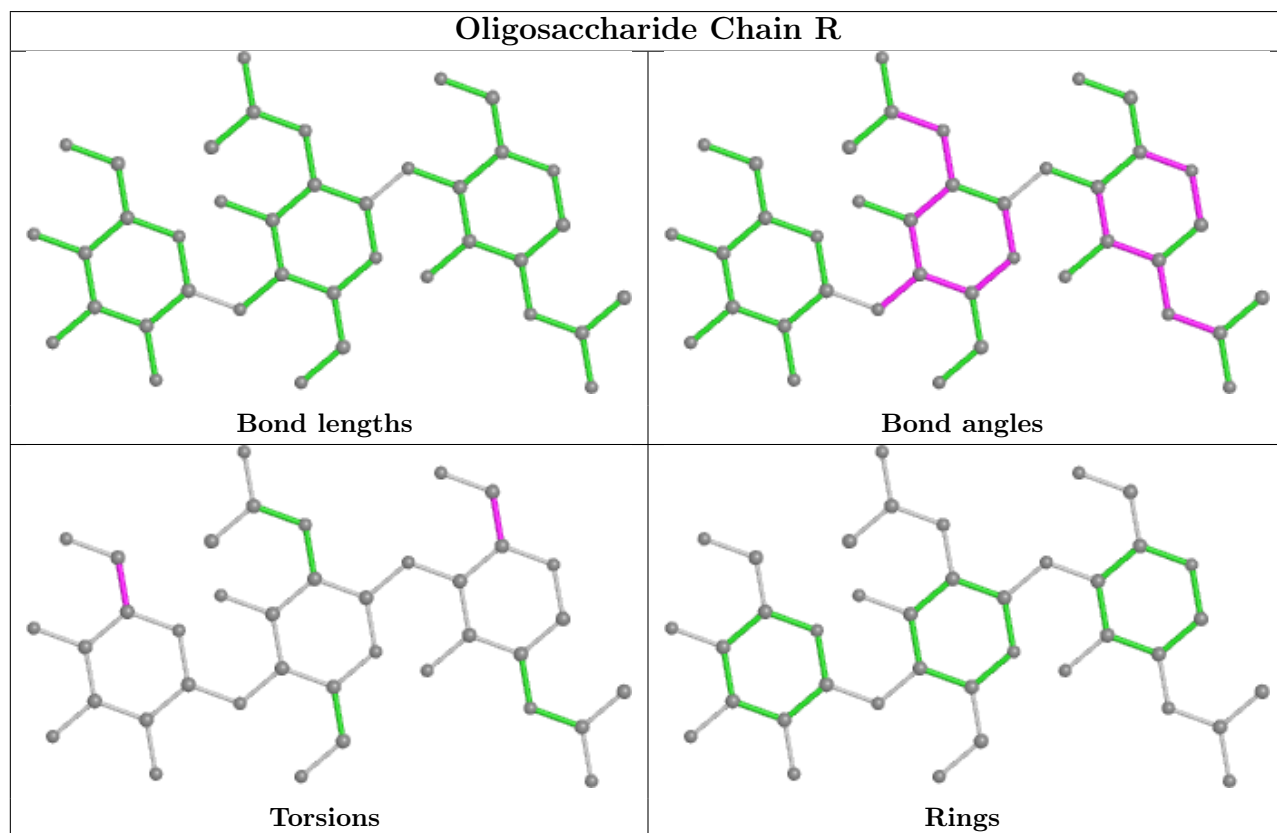
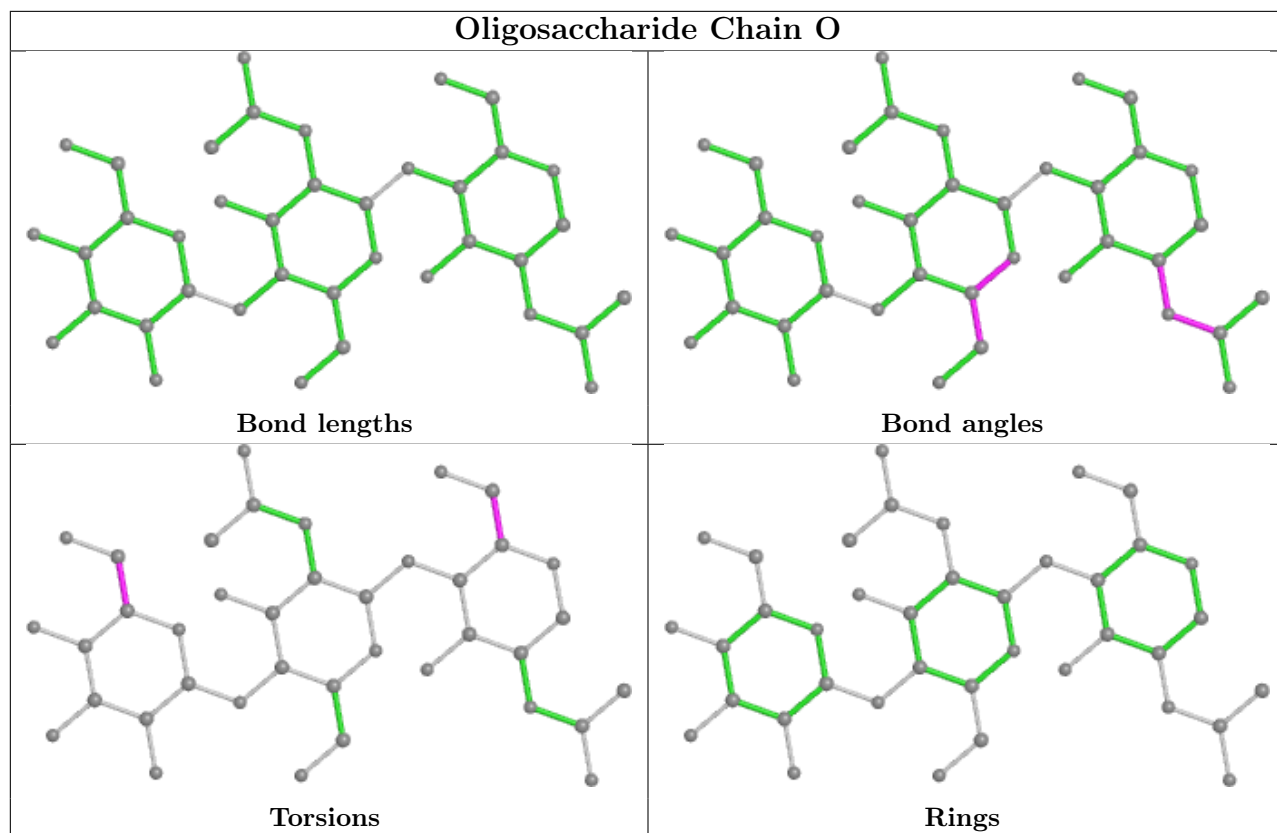












## 5.6 Ligand geometry

16 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	A	606	1	14,14,15	0.55	0	17,19,21	0.92	0
5	NAG	C	601	1	14,14,15	0.57	0	17,19,21	0.66	0
5	NAG	L	601	2	14,14,15	0.58	0	17,19,21	0.66	0
5	NAG	C	607	1	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	G	601	1	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
5	NAG	E	601	1	14,14,15	0.57	0	17,19,21	0.65	0
5	NAG	F	601	2	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	K	603	1	14,14,15	0.57	0	17,19,21	0.66	0
5	NAG	G	603	1	14,14,15	0.57	0	17,19,21	0.66	0
5	NAG	A	601	1	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	E	605	1	14,14,15	0.56	0	17,19,21	1.33	5 (29%)
5	NAG	K	601	1	14,14,15	0.46	0	17,19,21	2.46	4 (23%)
5	NAG	G	602	1	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	K	602	1	14,14,15	0.56	0	17,19,21	0.67	0
5	NAG	K	604	1	14,14,15	0.57	0	17,19,21	0.67	0
5	NAG	E	604	1	14,14,15	0.54	0	17,19,21	0.72	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
5	NAG	A	606	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	L	601	2	-	2/6/23/26	0/1/1/1
5	NAG	C	607	1	-	2/6/23/26	0/1/1/1
5	NAG	G	601	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	NAG	F	601	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	603	1	-	2/6/23/26	0/1/1/1
5	NAG	G	603	1	-	3/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	E	605	1	-	2/6/23/26	0/1/1/1
5	NAG	K	601	1	-	4/6/23/26	0/1/1/1
5	NAG	G	602	1	-	2/6/23/26	0/1/1/1
5	NAG	K	602	1	-	2/6/23/26	0/1/1/1
5	NAG	K	604	1	-	1/6/23/26	0/1/1/1
5	NAG	E	604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	601	NAG	C1-O5-C5	8.73	124.03	112.19
5	K	601	NAG	O5-C1-C2	3.11	116.20	111.29
5	E	605	NAG	O5-C1-C2	-2.68	107.05	111.29
5	E	605	NAG	C6-C5-C4	-2.43	107.32	113.00
5	G	601	NAG	O5-C5-C6	2.25	110.72	107.20
5	E	605	NAG	O5-C5-C6	2.24	110.72	107.20
5	K	601	NAG	O5-C5-C4	2.19	116.16	110.83
5	E	605	NAG	C3-C4-C5	2.14	114.06	110.24
5	K	601	NAG	C4-C3-C2	-2.07	107.98	111.02
5	E	605	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	606	NAG	C8-C7-N2-C2
5	A	606	NAG	O7-C7-N2-C2
5	K	602	NAG	C4-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6
5	K	601	NAG	C4-C5-C6-O6
5	K	601	NAG	O5-C5-C6-O6
5	G	602	NAG	O5-C5-C6-O6
5	F	601	NAG	O5-C5-C6-O6
5	K	602	NAG	O5-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	C	607	NAG	O5-C5-C6-O6
5	G	603	NAG	O5-C5-C6-O6
5	K	604	NAG	C1-C2-N2-C7
5	E	605	NAG	O5-C5-C6-O6
5	C	607	NAG	C4-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	K	601	NAG	C8-C7-N2-C2
5	K	601	NAG	O7-C7-N2-C2
5	L	601	NAG	C4-C5-C6-O6
5	G	603	NAG	C4-C5-C6-O6
5	G	602	NAG	C4-C5-C6-O6
5	K	603	NAG	O5-C5-C6-O6
5	L	601	NAG	O5-C5-C6-O6
5	E	605	NAG	C4-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	K	603	NAG	C4-C5-C6-O6
5	G	603	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	601	NAG	10	0
5	C	607	NAG	3	0
5	E	601	NAG	2	0
5	K	603	NAG	3	0
5	G	603	NAG	1	0
5	G	602	NAG	2	0
5	K	602	NAG	4	0
5	K	604	NAG	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/333 (96%)	0.56	31 (9%) 7 5	39, 70, 122, 226	0
1	C	321/333 (96%)	0.41	25 (7%) 13 10	36, 67, 116, 196	0
1	E	321/333 (96%)	0.87	45 (14%) 2 2	41, 74, 130, 215	0
1	G	321/333 (96%)	0.71	39 (12%) 4 2	46, 76, 128, 232	0
1	I	321/333 (96%)	0.54	25 (7%) 13 10	37, 70, 120, 228	0
1	K	321/333 (96%)	0.43	27 (8%) 11 8	38, 70, 121, 195	0
2	B	162/181 (89%)	0.86	23 (14%) 2 2	32, 77, 167, 209	0
2	D	162/181 (89%)	1.02	34 (20%) 1 0	34, 72, 186, 246	0
2	F	161/181 (88%)	1.02	36 (22%) 0 0	34, 74, 178, 241	0
2	H	162/181 (89%)	1.19	40 (24%) 0 0	33, 80, 174, 289	0
2	J	162/181 (89%)	0.61	12 (7%) 14 11	32, 69, 165, 200	0
2	L	161/181 (88%)	0.56	11 (6%) 17 13	36, 73, 169, 199	0
All	All	2896/3084 (93%)	0.68	348 (12%) 4 3	32, 72, 157, 289	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	159	TYR	13.4
2	F	128	ASN	9.8
2	D	139	GLU	9.4
2	H	31	GLY	8.7
2	D	140	PHE	8.4
2	H	32	SER	8.2
1	C	9	LEU	7.7
2	F	140	PHE	7.6
2	D	138	PHE	7.6
2	J	159	TYR	7.5
2	B	139	GLU	7.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	76	LEU	7.1
2	D	134	GLY	6.9
2	D	132	GLU	6.5
1	C	77	SER	6.4
2	D	142	HIS	6.3
2	B	23	GLY	6.3
2	H	158	ASP	6.2
1	E	12	GLY	6.2
1	K	12	GLY	6.2
2	D	154	ASN	6.2
2	H	140	PHE	6.2
1	A	78	THR	6.0
2	B	156	THR	6.0
1	C	78	THR	6.0
1	E	9	LEU	5.9
2	D	133	ILE	5.9
2	H	149	MET	5.9
1	C	76	LEU	5.8
2	D	129	ASN	5.8
2	D	158	ASP	5.7
2	H	154	ASN	5.4
1	C	10	CYS	5.2
1	I	78	THR	5.1
2	J	162	TYR	5.0
2	H	27	GLN	5.0
1	A	79	ALA	5.0
2	F	160	PRO	4.9
2	F	155	GLY	4.9
1	G	50	LEU	4.9
1	A	126	THR	4.8
2	D	141	TYR	4.8
2	F	131	LYS	4.7
1	I	195	GLN	4.7
1	C	75	SER	4.7
2	F	158	ASP	4.7
1	A	162	ASN	4.6
1	K	162	ASN	4.6
1	C	11	ILE	4.6
2	J	38	LEU	4.6
1	G	14	HIS	4.6
2	B	160	PRO	4.5
1	E	280	ASP	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	149	MET	4.4
2	F	143	LYS	4.4
1	G	21	THR	4.4
1	C	51	ARG	4.4
1	E	146	GLY	4.4
2	F	144	CYS	4.3
2	F	149	MET	4.3
2	B	158	ASP	4.3
1	G	146	GLY	4.3
1	E	274	SER	4.3
2	B	141	TYR	4.2
2	F	137	CYS	4.2
2	F	138	PHE	4.2
2	H	33	GLY	4.2
1	E	78	THR	4.1
2	J	29	GLU	4.1
1	E	278	VAL	4.1
2	D	31	GLY	4.1
1	I	92	ASP	4.1
2	F	141	TYR	4.1
2	H	129	ASN	4.1
1	C	195	GLN	4.0
2	B	142	HIS	4.0
1	E	149	SER	3.9
2	H	29	GLU	3.9
2	F	127	LYS	3.9
1	A	76	LEU	3.9
2	F	126	LEU	3.9
2	F	29	GLU	3.9
1	I	199	GLN	3.8
2	D	26	HIS	3.8
2	H	20	GLY	3.8
1	E	79	ALA	3.8
1	E	136	LYS	3.8
1	E	30	VAL	3.8
1	E	8	THR	3.7
1	K	199	GLN	3.7
2	H	156	THR	3.7
1	G	12	GLY	3.7
2	D	128	ASN	3.7
1	C	228	ASP	3.7
2	D	131	LYS	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	143	LYS	3.6
1	E	77	SER	3.6
2	D	145	ASP	3.6
1	I	18	SER	3.6
2	H	141	TYR	3.6
1	E	75	SER	3.6
1	G	195	GLN	3.6
1	G	326	ASN	3.6
1	E	222	ILE	3.5
1	G	60	LYS	3.5
1	A	9	LEU	3.5
1	C	159	LYS	3.5
2	H	128	ASN	3.5
1	G	280	ASP	3.5
2	D	150	GLU	3.5
1	G	32	VAL	3.4
2	D	38	LEU	3.4
2	D	126	LEU	3.4
1	K	116	SER	3.4
1	G	31	THR	3.4
2	F	132	GLU	3.4
2	H	130	ALA	3.4
1	A	17	ASN	3.4
2	D	22	TYR	3.4
1	E	148	LYS	3.4
1	A	195	GLN	3.4
1	C	12	GLY	3.4
2	F	139	GLU	3.4
2	H	150	GLU	3.4
1	K	50	LEU	3.4
2	D	146	ASN	3.4
2	F	162	TYR	3.3
1	A	19	THR	3.3
2	D	24	TYR	3.3
2	B	15	THR	3.3
1	E	13	TYR	3.3
1	I	17	ASN	3.3
1	A	11	ILE	3.3
1	I	228	ASP	3.3
1	K	149	SER	3.2
2	L	142	HIS	3.3
2	H	126	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	198	TYR	3.2
2	F	23	GLY	3.2
1	I	51	ARG	3.2
2	L	128	ASN	3.2
1	E	141	ALA	3.2
2	D	143	LYS	3.2
1	E	193	ASP	3.2
2	D	137	CYS	3.1
1	I	200	ASN	3.1
2	F	24	TYR	3.1
2	H	30	GLN	3.1
1	A	95	THR	3.1
1	K	74	GLU	3.1
2	H	131	LYS	3.1
2	F	142	HIS	3.1
1	G	77	SER	3.1
1	K	146	GLY	3.1
2	D	130	ALA	3.1
1	A	279	HIS	3.1
2	D	17	MET	3.0
1	A	142	CYS	3.0
1	G	29	ASN	3.0
1	K	75	SER	3.0
2	B	140	PHE	3.0
2	L	140	PHE	3.0
2	B	148	CYS	3.0
1	A	199	GLN	3.0
2	F	27	GLN	3.0
1	E	281	CYS	3.0
2	H	144	CYS	3.0
1	E	76	LEU	3.0
2	F	156	THR	3.0
1	A	146	GLY	2.9
2	L	131	LYS	2.9
1	K	269	SER	2.9
1	K	91	SER	2.9
1	K	52	GLY	2.9
2	H	19	ASP	2.9
2	F	30	GLN	2.9
2	H	138	PHE	2.9
1	I	146	GLY	2.9
2	F	148	CYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	132	GLU	2.9
1	G	93	ASN	2.9
1	A	250	ALA	2.9
2	L	133	ILE	2.8
2	B	126	LEU	2.8
1	E	294	THR	2.8
2	J	26	HIS	2.8
1	K	200	ASN	2.8
1	C	50	LEU	2.8
2	D	157	TYR	2.8
2	B	153	LYS	2.8
1	G	51	ARG	2.8
1	C	79	ALA	2.8
2	H	145	ASP	2.8
1	E	198	TYR	2.7
1	K	164	TYR	2.7
2	L	147	THR	2.7
2	H	147	THR	2.7
1	G	137	GLY	2.7
1	E	131	ASN	2.7
1	C	294	THR	2.7
1	I	55	PRO	2.7
2	J	160	PRO	2.7
2	F	157	TYR	2.6
1	G	19	THR	2.6
1	K	92	ASP	2.6
2	H	18	VAL	2.6
2	F	32	SER	2.6
2	H	24	TYR	2.6
1	G	228	ASP	2.6
1	A	21	THR	2.6
2	J	141	TYR	2.6
1	A	275	ASP	2.6
2	H	26	HIS	2.6
1	E	231	GLY	2.6
1	G	162	ASN	2.6
2	F	134	GLY	2.6
1	E	19	THR	2.5
1	A	116	SER	2.5
2	D	21	TRP	2.5
2	D	11	GLU	2.5
1	E	275	ASP	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	130	ALA	2.5
2	H	153	LYS	2.5
1	A	51	ARG	2.5
1	E	22	VAL	2.5
1	C	198	TYR	2.5
1	I	230	GLU	2.5
2	B	157	TYR	2.5
1	G	57	HIS	2.5
2	D	19	ASP	2.5
2	J	144	CYS	2.5
2	L	139	GLU	2.5
2	B	36	ALA	2.5
2	D	1	GLY	2.5
1	A	163	SER	2.5
2	B	18	VAL	2.5
1	K	28	LYS	2.5
1	A	75	SER	2.5
1	E	196	SER	2.5
1	I	149	SER	2.5
1	C	17	ASN	2.5
1	E	199	GLN	2.4
1	E	201	ALA	2.4
2	F	28	ASN	2.4
2	H	146	ASN	2.4
1	K	279	HIS	2.4
1	I	148	LYS	2.4
1	I	268	GLY	2.4
2	H	23	GLY	2.4
1	C	279	HIS	2.4
2	H	157	TYR	2.4
2	B	138	PHE	2.4
2	J	149	MET	2.4
1	A	42	LYS	2.4
2	B	29	GLU	2.4
2	F	38	LEU	2.4
1	I	147	ALA	2.4
2	J	148	CYS	2.4
1	I	8	THR	2.4
2	F	16	GLY	2.4
1	I	140	ALA	2.4
1	K	44	ASN	2.4
1	K	143	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	289	LYS	2.3
2	F	130	ALA	2.3
1	G	83	SER	2.3
1	G	161	GLY	2.3
1	G	281	CYS	2.3
1	E	42	LYS	2.3
1	G	20	ASP	2.3
2	H	127	LYS	2.3
1	I	145	ALA	2.3
1	I	126	THR	2.3
1	C	14	HIS	2.3
1	E	90	SER	2.3
1	E	162	ASN	2.3
1	G	278	VAL	2.3
2	H	139	GLU	2.3
1	E	291	ALA	2.3
1	E	11	ILE	2.3
1	C	60	LYS	2.3
1	K	78	THR	2.3
1	K	90	SER	2.3
2	B	32	SER	2.3
2	D	29	GLU	2.3
1	K	280	ASP	2.3
1	C	268	GLY	2.2
1	E	277	PRO	2.2
2	B	16	GLY	2.2
1	A	264	GLU	2.2
1	E	51	ARG	2.2
2	F	25	HIS	2.2
2	L	31	GLY	2.2
1	G	18	SER	2.2
1	G	193	ASP	2.2
1	C	130	PRO	2.2
1	G	48	CYS	2.2
2	B	33	GLY	2.2
2	L	4	GLY	2.2
1	E	96	CYS	2.2
2	J	146	ASN	2.2
1	G	75	SER	2.2
1	G	150	PHE	2.2
1	A	136	LYS	2.2
1	A	317	LYS	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	286	GLN	2.2
1	E	46	LYS	2.2
1	A	197	LEU	2.1
1	I	11	ILE	2.1
1	I	75	SER	2.1
2	F	33	GLY	2.1
2	J	1	GLY	2.1
1	A	326	ASN	2.1
2	H	72	HIS	2.1
2	H	142	HIS	2.1
1	C	52	GLY	2.1
2	H	1	GLY	2.1
1	G	47	LEU	2.1
1	G	273	ILE	2.1
1	E	295	SER	2.1
2	D	39	LYS	2.1
1	C	220	ILE	2.1
1	G	17	ASN	2.1
2	H	28	ASN	2.1
2	B	143	LYS	2.1
1	G	267	ALA	2.1
1	A	10	CYS	2.1
1	G	16	ASN	2.1
2	B	144	CYS	2.1
1	E	197	LEU	2.1
1	E	292	ILE	2.1
1	K	51	ARG	2.1
2	H	160	PRO	2.1
1	G	197	LEU	2.1
1	K	115	SER	2.1
1	C	158	VAL	2.1
1	K	47	LEU	2.1
2	H	133	ILE	2.1
1	I	222	ILE	2.0
2	D	147	THR	2.0
1	G	125	LYS	2.0
1	I	136	LYS	2.0
1	K	195	GLN	2.0
1	I	282	ASN	2.0
1	G	133	ASP	2.0
1	E	98	PRO	2.0
1	K	72	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	113	SER	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](#)

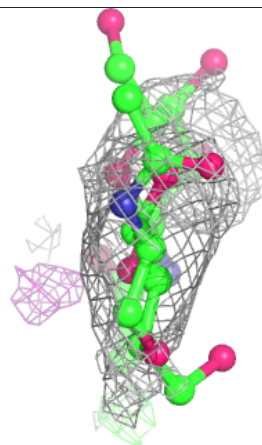
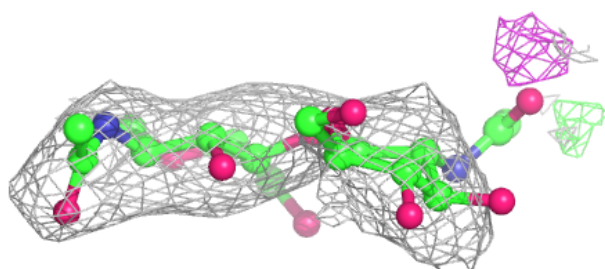
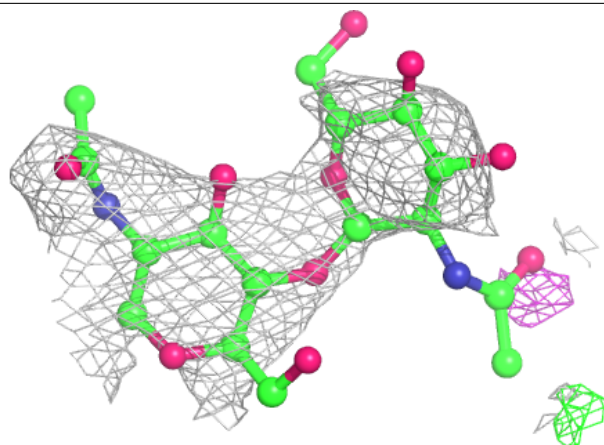
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	R	3	11/12	0.46	0.30	108,135,142,143	0
3	NAG	N	2	14/15	0.61	0.40	124,134,147,148	0
3	NAG	M	2	14/15	0.67	0.55	120,148,155,174	0
3	NAG	Q	2	14/15	0.73	0.52	119,139,166,193	0
4	BMA	O	3	11/12	0.77	0.27	89,112,124,151	0
3	NAG	P	2	14/15	0.77	0.33	91,106,136,144	0
3	NAG	S	2	14/15	0.78	0.30	128,134,141,147	0
3	NAG	N	1	14/15	0.79	0.34	68,108,117,126	0
3	NAG	Q	1	14/15	0.79	0.27	108,129,134,135	0
3	NAG	S	1	14/15	0.80	0.27	94,114,139,150	0
4	NAG	R	1	14/15	0.81	0.21	72,82,95,97	0
4	NAG	O	2	14/15	0.82	0.28	55,84,111,120	0
3	NAG	M	1	14/15	0.87	0.40	82,113,129,130	0
3	NAG	P	1	14/15	0.89	0.19	70,86,98,99	0
4	NAG	O	1	14/15	0.89	0.14	61,76,95,102	0
4	NAG	R	2	14/15	0.91	0.33	92,117,138,145	0

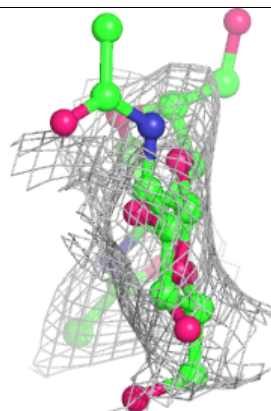
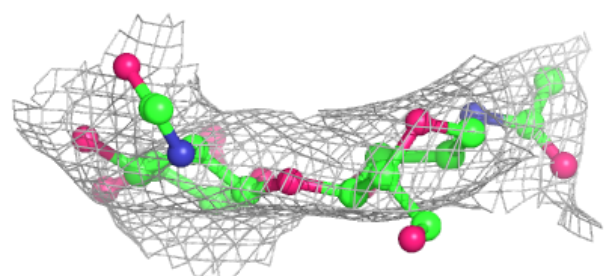
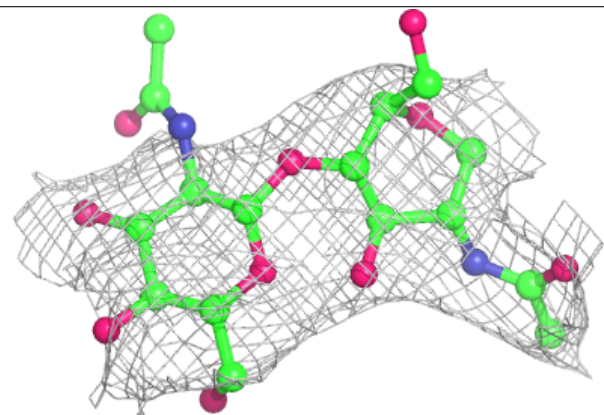
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

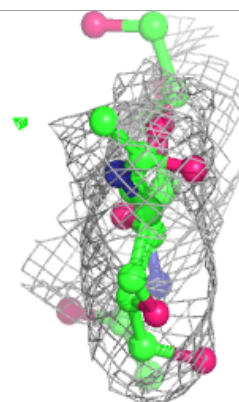
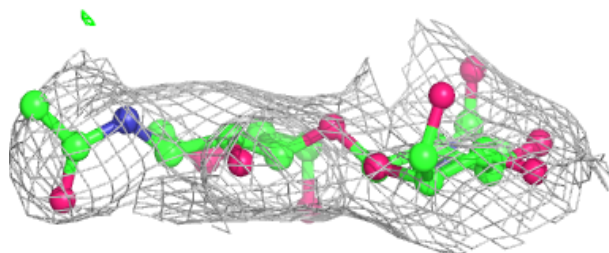
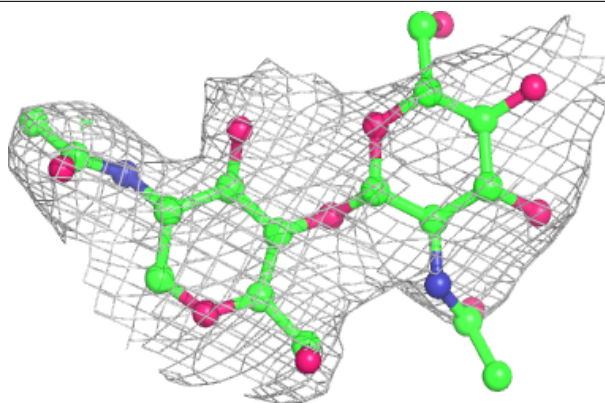
**Electron density around Chain N:**

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

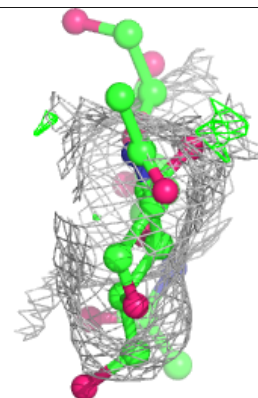
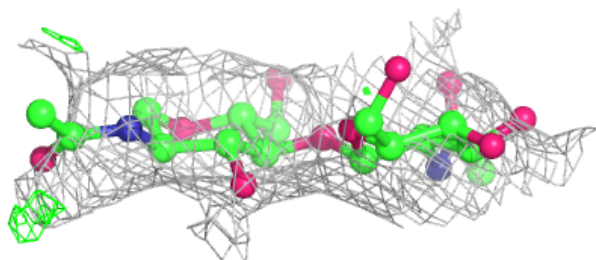
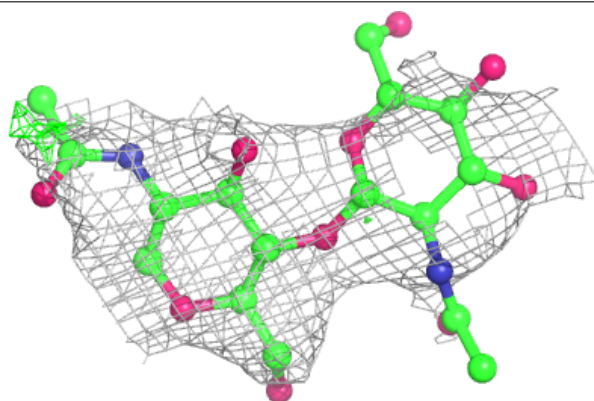


**Electron density around Chain P:**

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

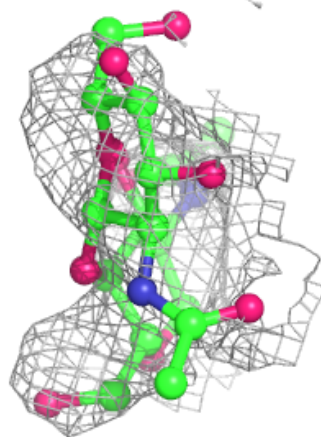
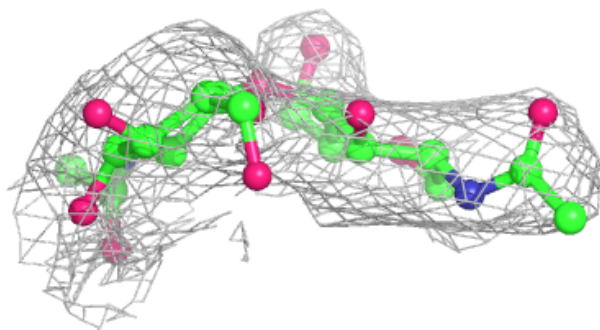
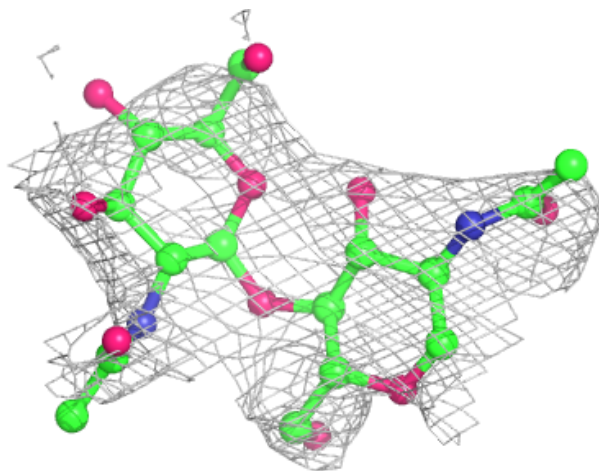
**Electron density around Chain Q:**

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



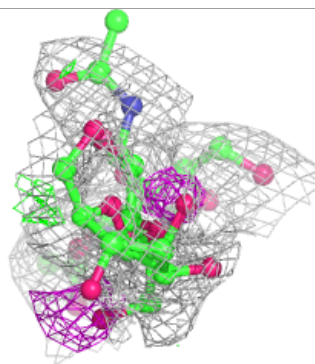
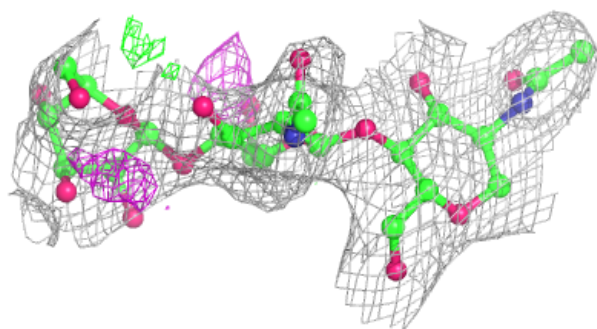
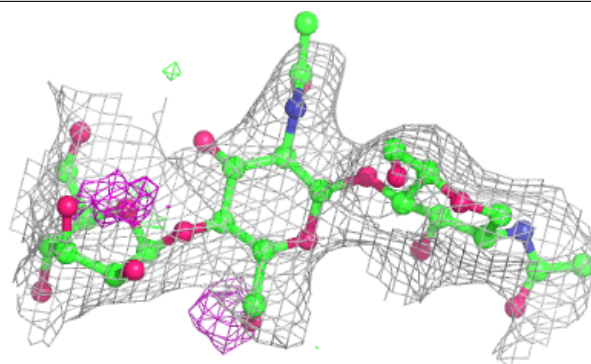
**Electron density around Chain S:**

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

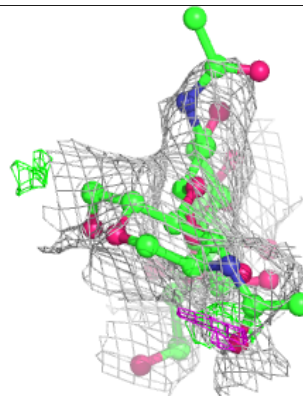
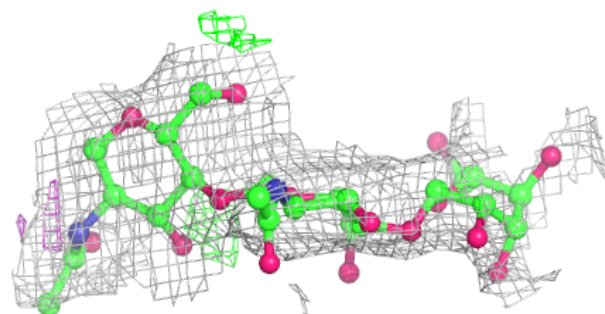
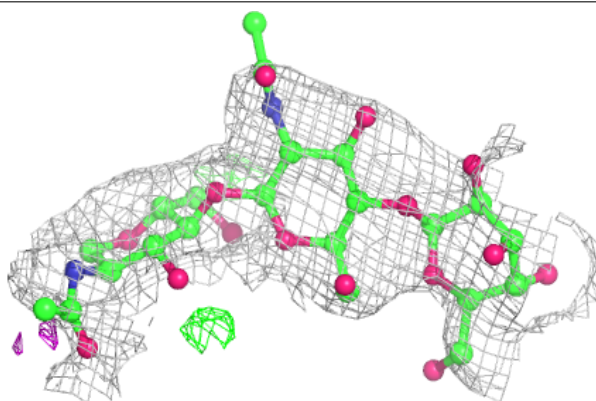


**Electron density around Chain O:**

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

**Electron density around Chain R:**

$2mF_o-DF_c$  (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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	L	601	14/15	0.31	0.54	132,161,178,187	0
5	NAG	E	601	14/15	0.48	0.53	117,156,185,194	0
5	NAG	A	606	14/15	0.51	0.51	103,126,141,143	0
5	NAG	E	605	14/15	0.54	0.59	134,171,193,199	0
5	NAG	K	601	14/15	0.56	0.36	88,113,140,142	0
5	NAG	F	601	14/15	0.58	0.44	154,173,188,194	0
5	NAG	K	602	14/15	0.63	0.34	68,115,138,139	0
5	NAG	A	601	14/15	0.64	0.34	53,78,94,104	0
5	NAG	C	601	14/15	0.66	0.50	157,180,192,198	0
5	NAG	C	607	14/15	0.66	0.42	95,116,142,146	0
5	NAG	G	602	14/15	0.67	0.49	171,186,198,202	0
5	NAG	G	601	14/15	0.69	0.33	141,158,176,181	0
5	NAG	K	603	14/15	0.72	0.51	84,126,147,153	0
5	NAG	K	604	14/15	0.72	0.50	108,133,146,153	0
5	NAG	E	604	14/15	0.72	0.53	26,28,30,30	0
5	NAG	G	603	14/15	0.75	0.41	139,163,185,199	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.