



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:22 AM BST

PDB ID : 2FK0  
Title : Crystal Structure of a H5N1 influenza virus hemagglutinin.  
Authors : Stevens, J.; Wilson, I.A.  
Deposited on : 2006-01-03  
Resolution : 2.95 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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

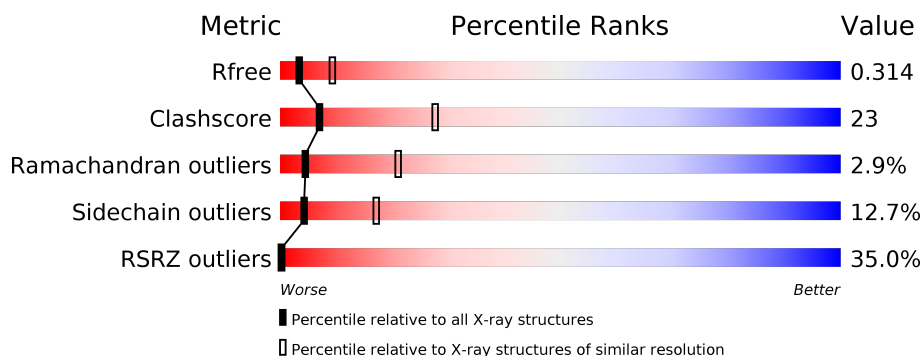
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on 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	334	<div> <div>15%</div> <div>61%</div> <div>29%</div> <div>6%</div> <div>• •</div> </div>
1	C	334	<div> <div>13%</div> <div>60%</div> <div>31%</div> <div>• • •</div> </div>
1	E	334	<div> <div>14%</div> <div>56%</div> <div>34%</div> <div>6%</div> <div>• •</div> </div>
1	G	334	<div> <div>13%</div> <div>58%</div> <div>32%</div> <div>6%</div> <div>• •</div> </div>
1	I	334	<div> <div>15%</div> <div>57%</div> <div>32%</div> <div>7%</div> <div>• •</div> </div>
1	K	334	<div> <div>18%</div> <div>57%</div> <div>33%</div> <div>5%</div> <div>• •</div> </div>


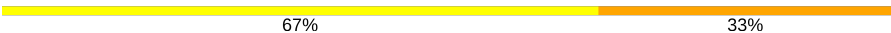
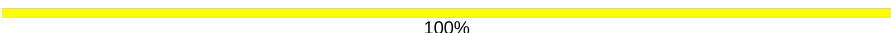
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Mol	Chain	Length	Quality of chain
1	M	334	
1	O	334	
1	Q	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	
3	S	2	
3	U	2	
3	V	2	
3	W	2	
3	Y	2	
3	a	2	
3	b	2	
3	c	2	
3	d	2	
3	e	2	
3	f	2	
3	g	2	
3	h	2	

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Mol	Chain	Length	Quality of chain
4	T	3	
4	X	3	
4	Z	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	S	1	-	-	-	X
3	NAG	S	2	-	-	-	X
3	NAG	U	1	-	-	-	X
3	NAG	U	2	-	-	-	X
3	NAG	V	1	X	-	-	-
3	NAG	V	2	-	-	-	X
3	NAG	W	2	-	-	-	X
3	NAG	Y	2	-	-	-	X
3	NAG	a	1	-	-	-	X
3	NAG	a	2	-	-	-	X
3	NAG	b	1	X	-	-	-
3	NAG	b	2	-	-	-	X
3	NAG	c	1	-	-	-	X
3	NAG	c	2	-	-	-	X
3	NAG	d	1	X	-	-	-
3	NAG	d	2	-	-	-	X
3	NAG	e	1	-	-	-	X
3	NAG	e	2	-	-	-	X
3	NAG	f	1	X	-	-	X
3	NAG	g	1	-	-	-	X
3	NAG	g	2	-	-	-	X
3	NAG	h	1	X	-	-	X
3	NAG	h	2	-	-	-	X
4	NAG	T	1	X	-	-	-
4	NAG	T	2	-	-	-	X
4	BMA	T	3	-	-	-	X
4	NAG	X	1	X	-	-	-
4	BMA	X	3	-	-	-	X
4	BMA	Z	3	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36202 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
1	A	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	C	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	E	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	G	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	I	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	K	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	M	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	O	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	Q	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	cloning artifact	GB 50296053
A	8	ASP	-	cloning artifact	GB 50296053
A	9	PRO	-	cloning artifact	GB 50296053
A	10	GLY	-	cloning artifact	GB 50296053
C	7	ALA	-	cloning artifact	GB 50296053
C	8	ASP	-	cloning artifact	GB 50296053
C	9	PRO	-	cloning artifact	GB 50296053
C	10	GLY	-	cloning artifact	GB 50296053
E	7	ALA	-	cloning artifact	GB 50296053
E	8	ASP	-	cloning artifact	GB 50296053
E	9	PRO	-	cloning artifact	GB 50296053

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	cloning artifact	GB 50296053
G	7	ALA	-	cloning artifact	GB 50296053
G	8	ASP	-	cloning artifact	GB 50296053
G	9	PRO	-	cloning artifact	GB 50296053
G	10	GLY	-	cloning artifact	GB 50296053
I	7	ALA	-	cloning artifact	GB 50296053
I	8	ASP	-	cloning artifact	GB 50296053
I	9	PRO	-	cloning artifact	GB 50296053
I	10	GLY	-	cloning artifact	GB 50296053
K	7	ALA	-	cloning artifact	GB 50296053
K	8	ASP	-	cloning artifact	GB 50296053
K	9	PRO	-	cloning artifact	GB 50296053
K	10	GLY	-	cloning artifact	GB 50296053
M	7	ALA	-	cloning artifact	GB 50296053
M	8	ASP	-	cloning artifact	GB 50296053
M	9	PRO	-	cloning artifact	GB 50296053
M	10	GLY	-	cloning artifact	GB 50296053
O	7	ALA	-	cloning artifact	GB 50296053
O	8	ASP	-	cloning artifact	GB 50296053
O	9	PRO	-	cloning artifact	GB 50296053
O	10	GLY	-	cloning artifact	GB 50296053
Q	7	ALA	-	cloning artifact	GB 50296053
Q	8	ASP	-	cloning artifact	GB 50296053
Q	9	PRO	-	cloning artifact	GB 50296053
Q	10	GLY	-	cloning artifact	GB 50296053

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	H	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	J	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	L	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	N	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	R	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	cloning artifact	GB 58618438
B	176	GLY	-	cloning artifact	GB 58618438
B	177	ARG	-	cloning artifact	GB 58618438
B	178	LEU	-	cloning artifact	GB 58618438
B	179	VAL	-	cloning artifact	GB 58618438
B	180	PRO	-	cloning artifact	GB 58618438
B	181	ARG	-	cloning artifact	GB 58618438
D	175	SER	-	cloning artifact	GB 58618438
D	176	GLY	-	cloning artifact	GB 58618438
D	177	ARG	-	cloning artifact	GB 58618438
D	178	LEU	-	cloning artifact	GB 58618438
D	179	VAL	-	cloning artifact	GB 58618438
D	180	PRO	-	cloning artifact	GB 58618438
D	181	ARG	-	cloning artifact	GB 58618438
F	175	SER	-	cloning artifact	GB 58618438
F	176	GLY	-	cloning artifact	GB 58618438
F	177	ARG	-	cloning artifact	GB 58618438
F	178	LEU	-	cloning artifact	GB 58618438
F	179	VAL	-	cloning artifact	GB 58618438
F	180	PRO	-	cloning artifact	GB 58618438
F	181	ARG	-	cloning artifact	GB 58618438
H	175	SER	-	cloning artifact	GB 58618438
H	176	GLY	-	cloning artifact	GB 58618438
H	177	ARG	-	cloning artifact	GB 58618438
H	178	LEU	-	cloning artifact	GB 58618438
H	179	VAL	-	cloning artifact	GB 58618438
H	180	PRO	-	cloning artifact	GB 58618438
H	181	ARG	-	cloning artifact	GB 58618438
J	175	SER	-	cloning artifact	GB 58618438
J	176	GLY	-	cloning artifact	GB 58618438
J	177	ARG	-	cloning artifact	GB 58618438
J	178	LEU	-	cloning artifact	GB 58618438
J	179	VAL	-	cloning artifact	GB 58618438
J	180	PRO	-	cloning artifact	GB 58618438

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Chain	Residue	Modelled	Actual	Comment	Reference
J	181	ARG	-	cloning artifact	GB 58618438
L	175	SER	-	cloning artifact	GB 58618438
L	176	GLY	-	cloning artifact	GB 58618438
L	177	ARG	-	cloning artifact	GB 58618438
L	178	LEU	-	cloning artifact	GB 58618438
L	179	VAL	-	cloning artifact	GB 58618438
L	180	PRO	-	cloning artifact	GB 58618438
L	181	ARG	-	cloning artifact	GB 58618438
N	175	SER	-	cloning artifact	GB 58618438
N	176	GLY	-	cloning artifact	GB 58618438
N	177	ARG	-	cloning artifact	GB 58618438
N	178	LEU	-	cloning artifact	GB 58618438
N	179	VAL	-	cloning artifact	GB 58618438
N	180	PRO	-	cloning artifact	GB 58618438
N	181	ARG	-	cloning artifact	GB 58618438
P	175	SER	-	cloning artifact	GB 58618438
P	176	GLY	-	cloning artifact	GB 58618438
P	177	ARG	-	cloning artifact	GB 58618438
P	178	LEU	-	cloning artifact	GB 58618438
P	179	VAL	-	cloning artifact	GB 58618438
P	180	PRO	-	cloning artifact	GB 58618438
P	181	ARG	-	cloning artifact	GB 58618438
R	175	SER	-	cloning artifact	GB 58618438
R	176	GLY	-	cloning artifact	GB 58618438
R	177	ARG	-	cloning artifact	GB 58618438
R	178	LEU	-	cloning artifact	GB 58618438
R	179	VAL	-	cloning artifact	GB 58618438
R	180	PRO	-	cloning artifact	GB 58618438
R	181	ARG	-	cloning artifact	GB 58618438

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	g	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	h	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.

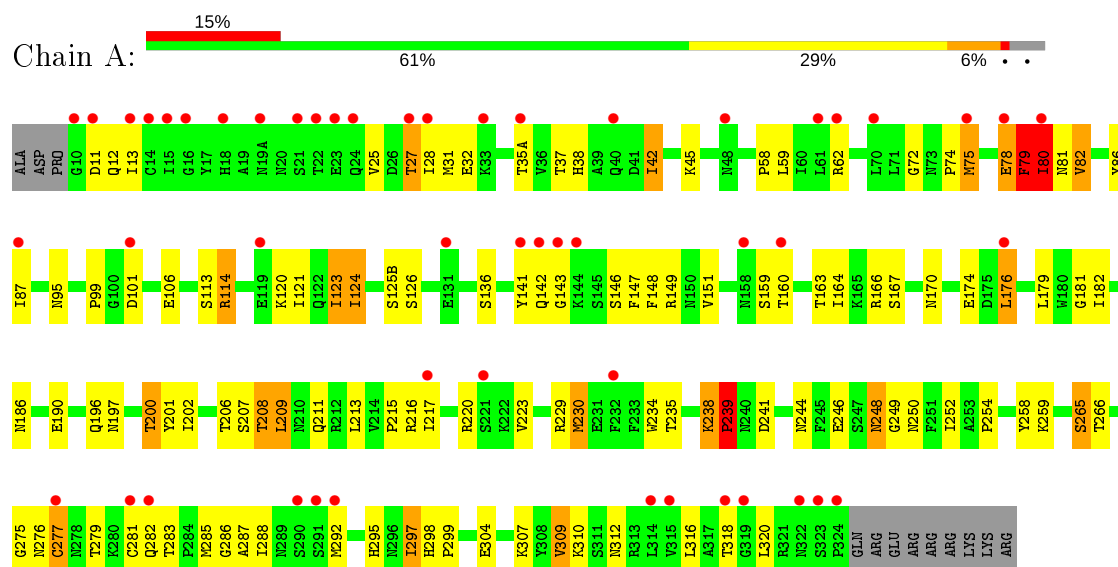


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			

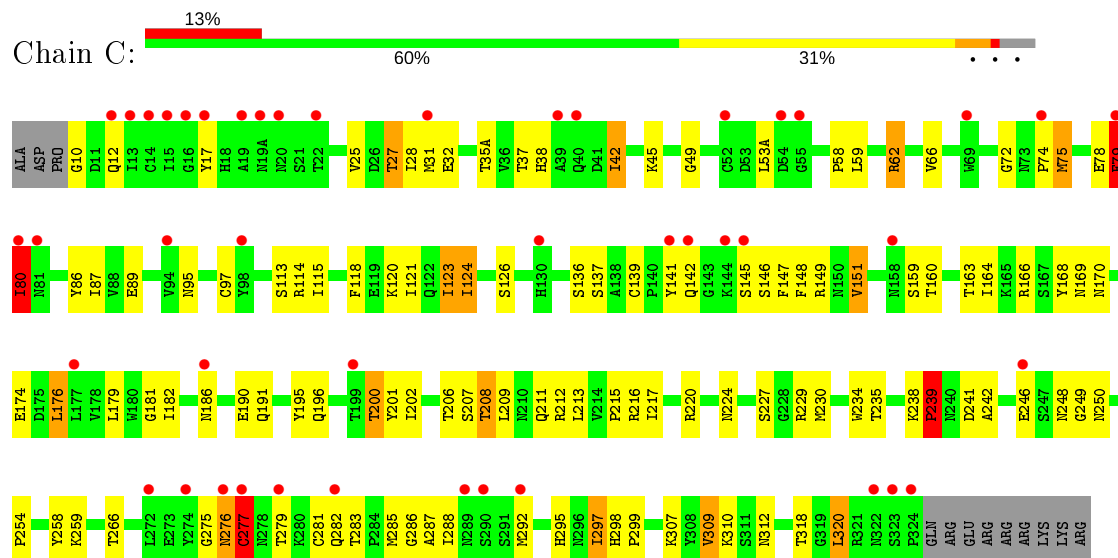
### 3 Residue-property plots [i](#)

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

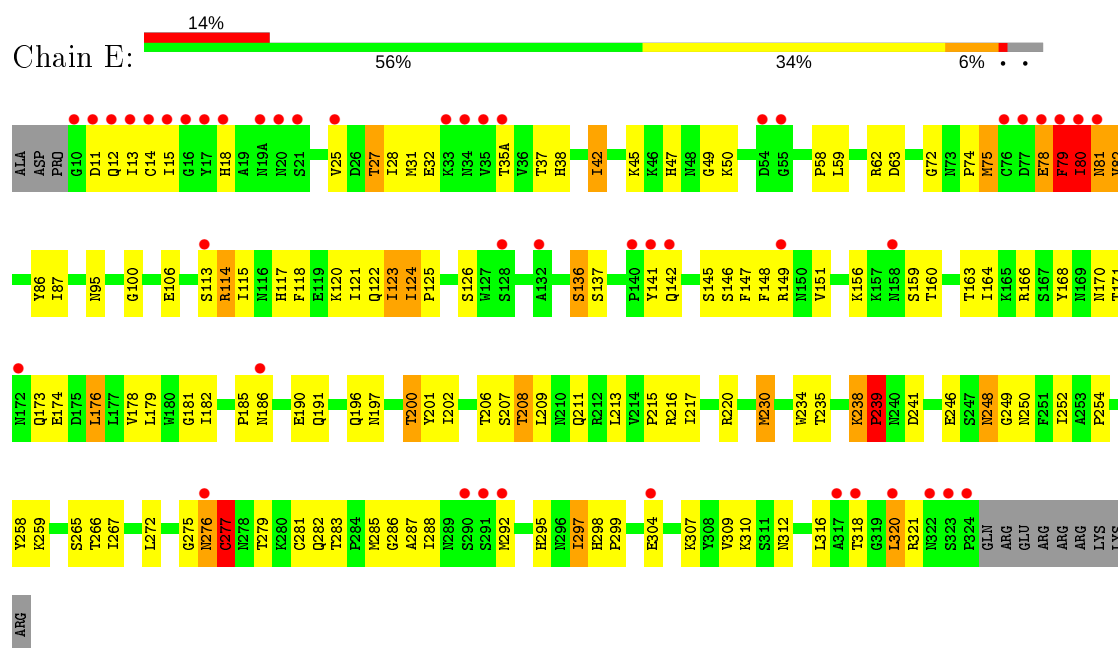
- Molecule 1: hemagglutinin



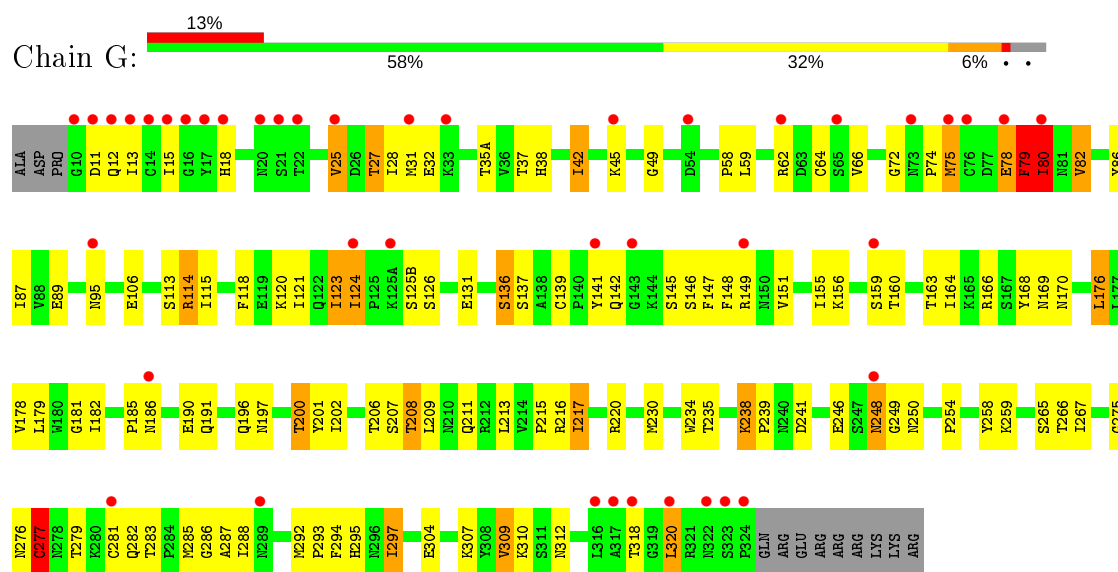
- Molecule 1: hemagglutinin



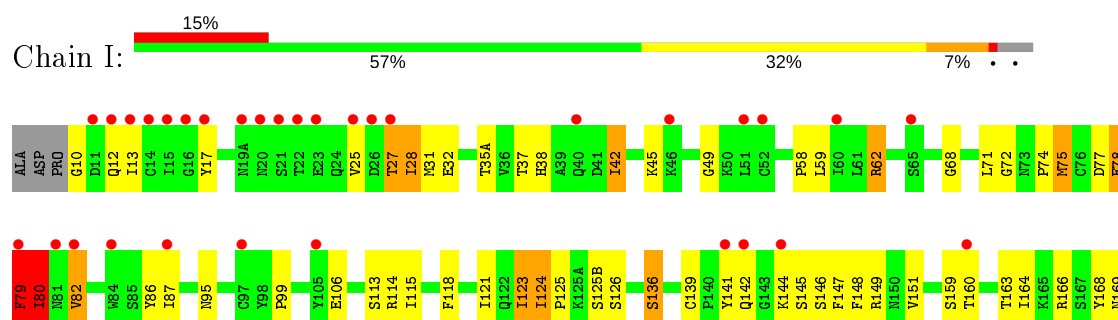
- Molecule 1: hemagglutinin

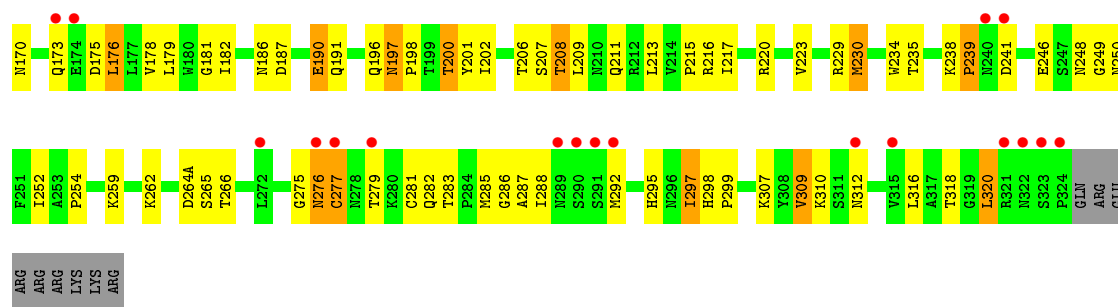


• Molecule 1: hemagglutinin

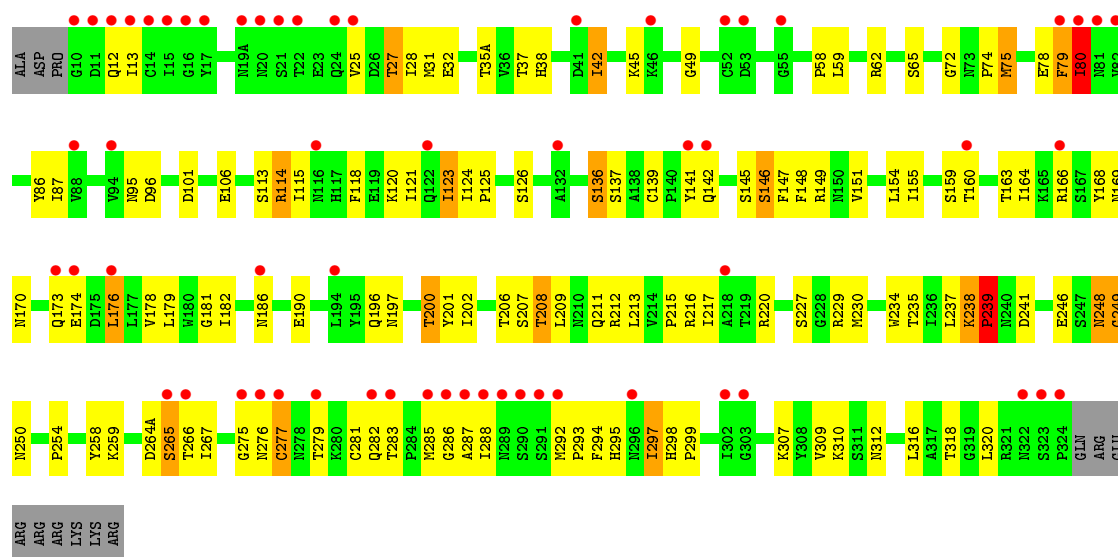


• Molecule 1: hemagglutinin

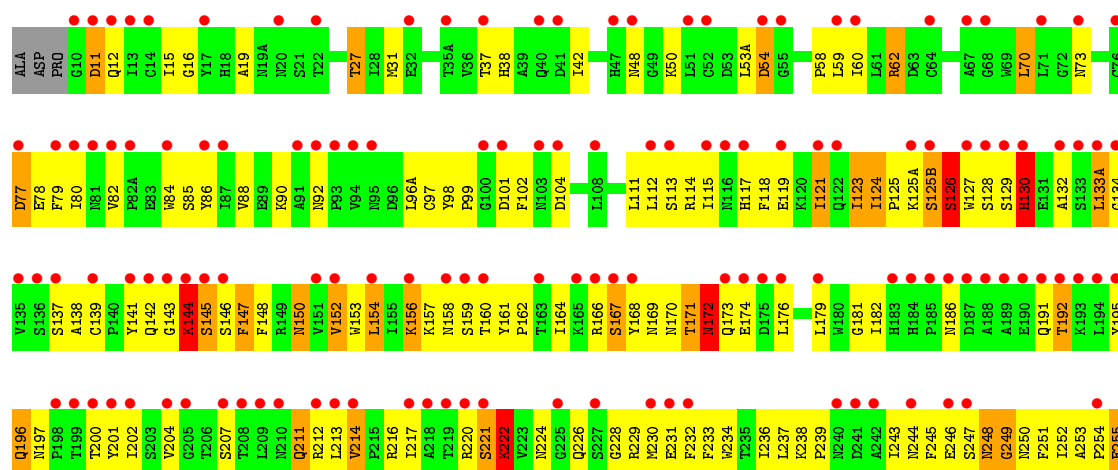
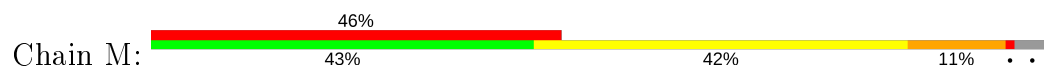


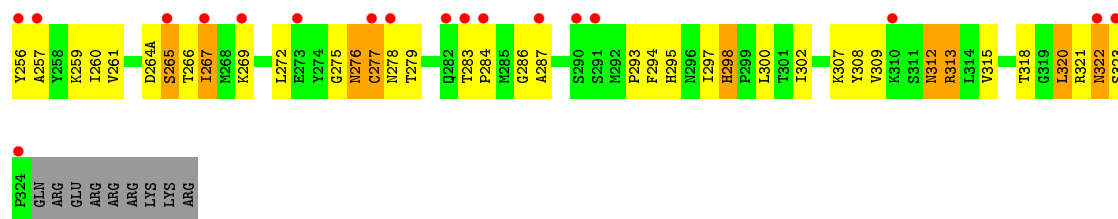


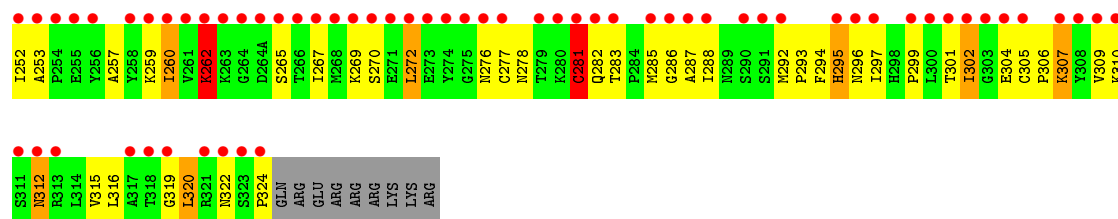
• Molecule 1: hemagglutinin



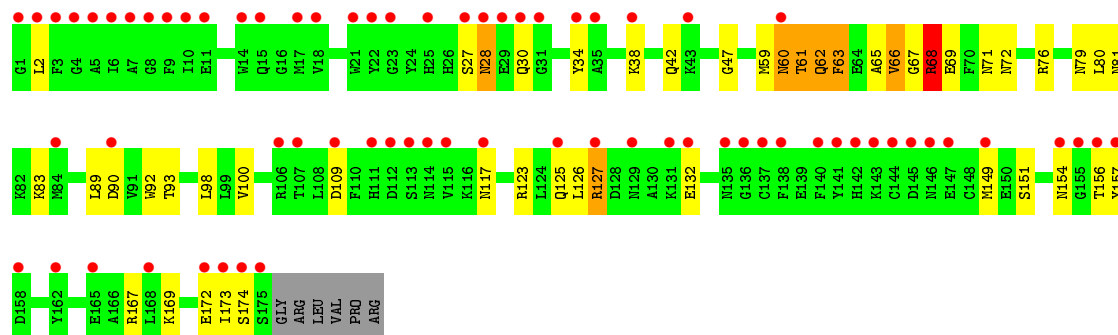
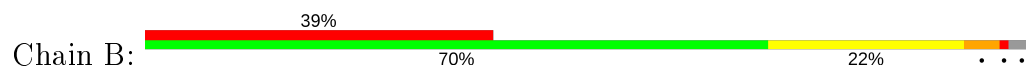
• Molecule 1: hemagglutinin



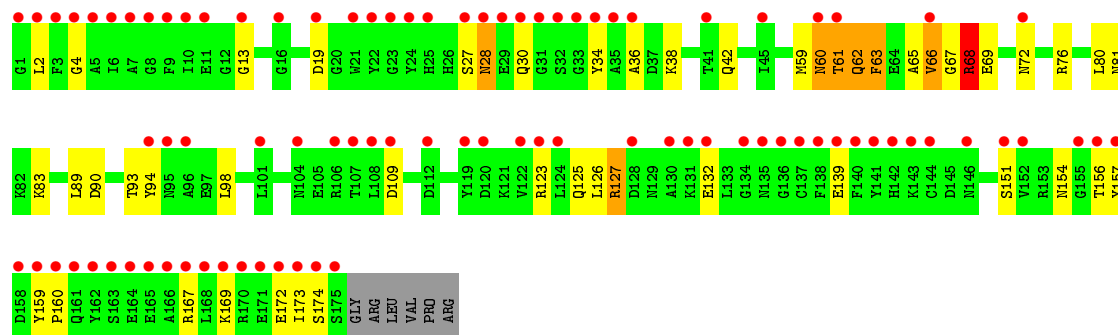




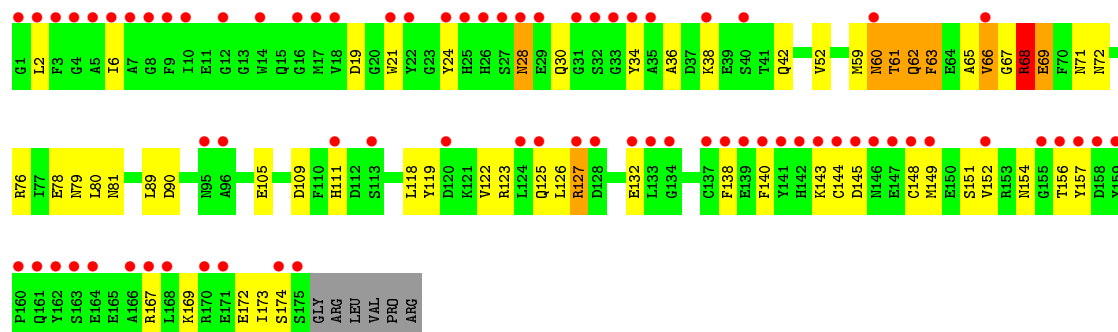
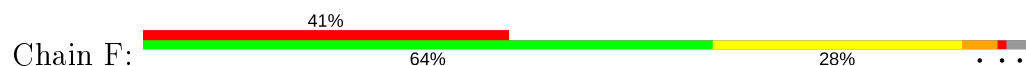
• Molecule 2: hemagglutinin



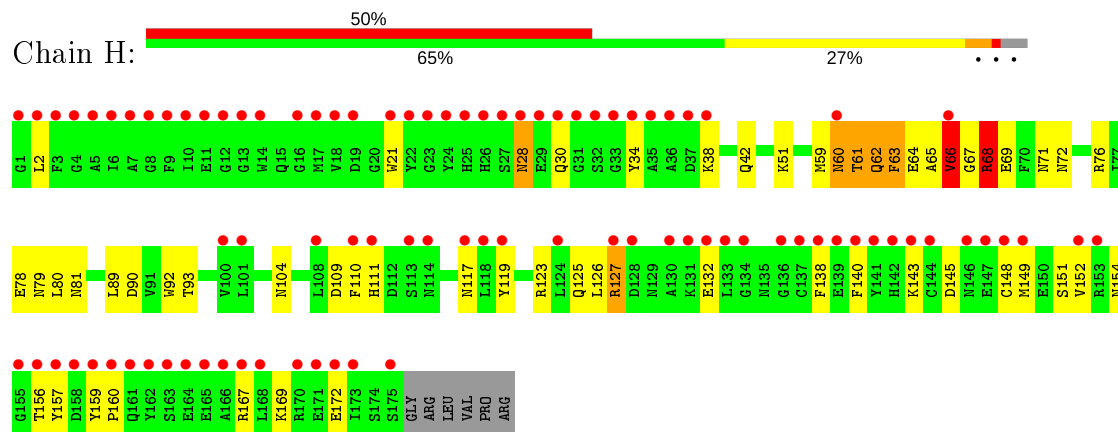
• Molecule 2: hemagglutinin



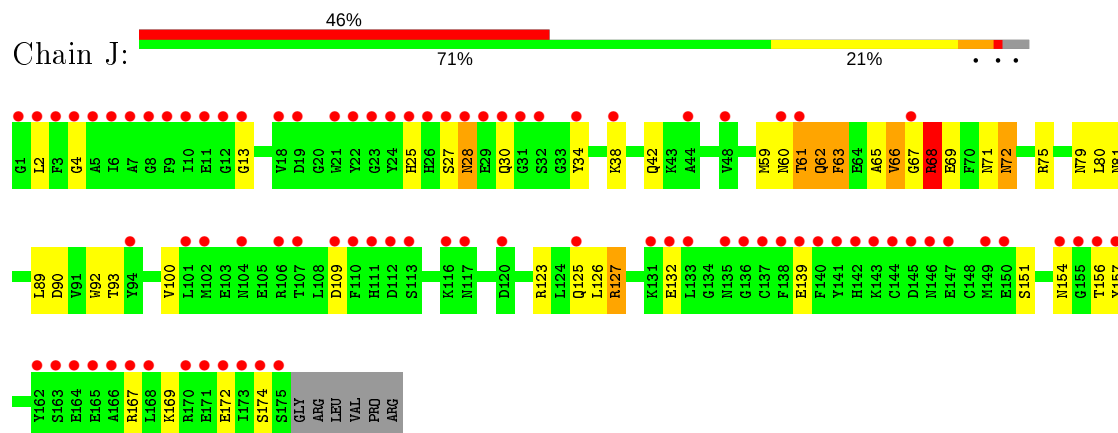
• Molecule 2: hemagglutinin



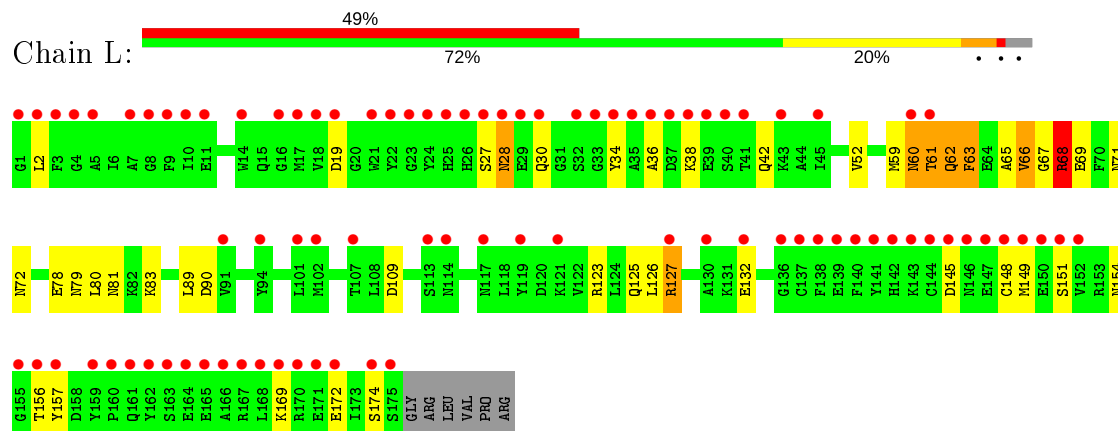
- Molecule 2: hemagglutinin



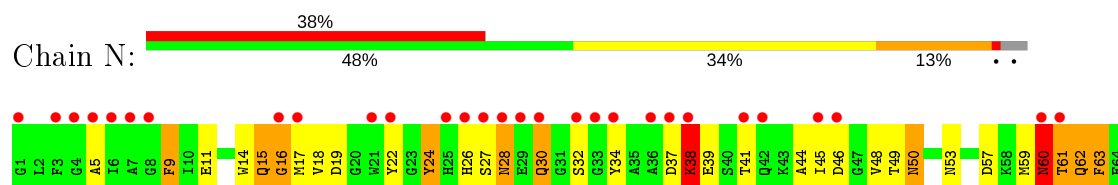
- Molecule 2: hemagglutinin

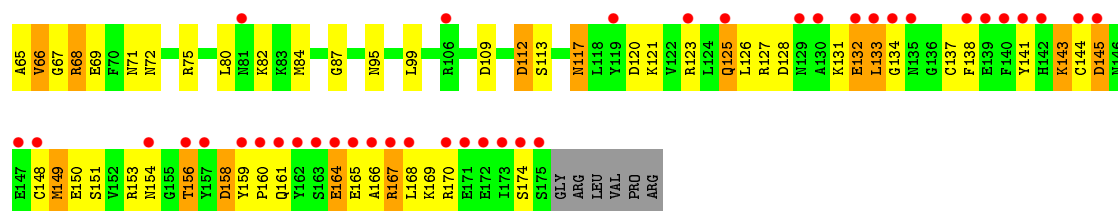


- Molecule 2: hemagglutinin

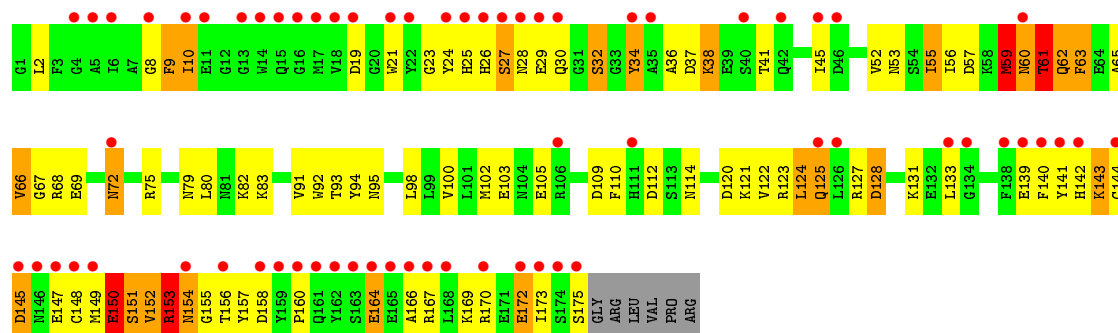
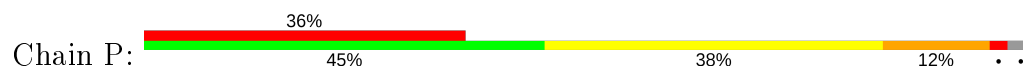


- Molecule 2: hemagglutinin

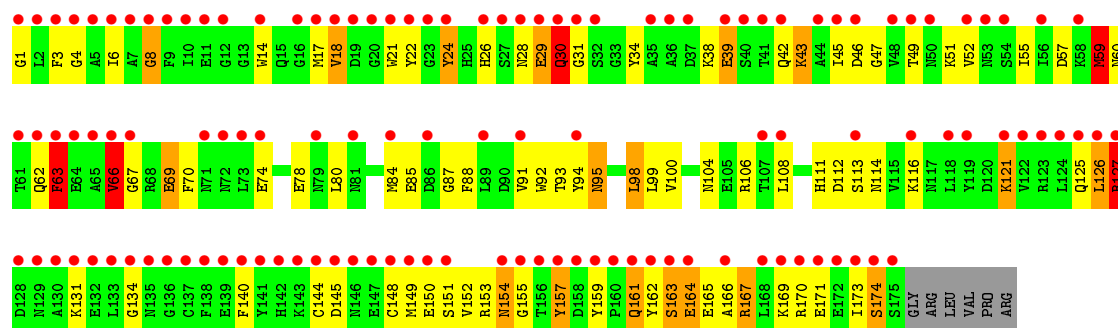




• Molecule 2: hemagglutinin



• 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

Chain V:  100%

NAG1  
NAG2

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

Chain W:  100%

NAG1  
NAG2

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

Chain Y:  100%

NAG1  
NAG2

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

Chain a:  100%

NAG1  
NAG2

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

Chain b:  100%

NAG1  
NAG2

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

Chain c:  100%

NAG1  
NAG2

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

Chain d:  100%

MAG1  
MAG2


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

Chain e:  100%MAG1  
MAG2


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

Chain f:  100%MAG1  
MAG2

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

Chain g:  100%MAG1  
MAG2


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

Chain h:  100%MAG1  
MAG2

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

Chain T:  33% 67%MAG1  
MAG2  
BXI3

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

Chain X:  67% 33%MAG1  
MAG2  
BXI3

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

Chain Z:

100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.94Å 197.94Å 134.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	171.50 – 2.95 49.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (171.50-2.95) 98.9 (49.49-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.268 , 0.319 0.266 , 0.314	Depositor DCC
$R_{free}$ test set	1233 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 98.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.008 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	36202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.76	0/2615	0.83	3/3551 (0.1%)
1	C	0.84	3/2615 (0.1%)	0.87	2/3551 (0.1%)
1	E	0.84	1/2615 (0.0%)	0.87	4/3551 (0.1%)
1	G	0.84	3/2615 (0.1%)	0.85	3/3551 (0.1%)
1	I	0.80	2/2615 (0.1%)	0.85	4/3551 (0.1%)
1	K	0.79	1/2615 (0.0%)	0.83	2/3551 (0.1%)
1	M	1.12	21/2615 (0.8%)	0.87	5/3551 (0.1%)
1	O	1.49	22/2615 (0.8%)	0.91	9/3551 (0.3%)
1	Q	0.65	2/2615 (0.1%)	0.70	0/3551
2	B	0.67	0/1443	0.70	3/1939 (0.2%)
2	D	0.68	0/1443	0.71	3/1939 (0.2%)
2	F	0.70	3/1443 (0.2%)	0.71	3/1939 (0.2%)
2	H	0.67	1/1443 (0.1%)	0.70	3/1939 (0.2%)
2	J	0.64	0/1443	0.68	2/1939 (0.1%)
2	L	0.67	1/1443 (0.1%)	0.67	2/1939 (0.1%)
2	N	1.29	7/1443 (0.5%)	0.86	5/1939 (0.3%)
2	P	1.38	13/1443 (0.9%)	0.88	5/1939 (0.3%)
2	R	0.74	5/1443 (0.3%)	0.69	0/1939
All	All	0.91	85/36522 (0.2%)	0.81	58/49410 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
1	G	0	2
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	3
1	M	0	1
1	O	0	3
1	Q	0	1
2	B	0	3
2	D	0	3
2	F	0	3
2	H	0	3
2	J	0	2
2	L	0	3
2	N	0	2
2	P	0	2
All	All	0	38

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	125(B)	SER	CB-OG	34.55	1.87	1.42
2	N	38	LYS	CE-NZ	31.98	2.29	1.49
2	P	143	LYS	CE-NZ	27.78	2.18	1.49
1	O	157	LYS	CD-CE	22.51	2.07	1.51
1	O	130	HIS	CE1-NE2	20.34	1.79	1.32
1	O	125(A)	LYS	CE-NZ	18.91	1.96	1.49
1	M	130	HIS	CE1-NE2	18.73	1.75	1.32
2	P	38	LYS	CE-NZ	17.21	1.92	1.49
2	P	145	ASP	CG-OD1	16.80	1.64	1.25
1	O	157	LYS	CE-NZ	16.52	1.90	1.49
2	N	38	LYS	CD-CE	15.33	1.89	1.51
1	O	219	THR	CB-OG1	15.01	1.73	1.43
1	M	130	HIS	CG-ND1	14.75	1.71	1.38
1	M	247	SER	CB-OG	14.60	1.61	1.42
1	M	166	ARG	C-O	14.56	1.51	1.23
2	N	165	GLU	CD-OE2	14.41	1.41	1.25
1	O	160	THR	CB-OG1	14.28	1.71	1.43
1	O	159	SER	CB-OG	14.14	1.60	1.42
2	P	143	LYS	CD-CE	14.06	1.86	1.51
1	Q	130	HIS	CE1-NE2	13.35	1.63	1.32
1	O	125(A)	LYS	CD-CE	13.06	1.83	1.51
1	O	130	HIS	CG-ND1	12.82	1.67	1.38
1	M	159	SER	CB-OG	12.05	1.57	1.42
1	O	128	SER	CB-OG	11.90	1.57	1.42
2	R	150	GLU	CD-OE1	11.71	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	158	ASN	CG-OD1	11.48	1.49	1.24
2	N	38	LYS	CG-CD	11.47	1.91	1.52
1	M	158	ASN	CG-ND2	11.43	1.61	1.32
1	M	126	SER	CB-OG	11.06	1.56	1.42
2	P	145	ASP	CG-OD2	10.45	1.49	1.25
1	O	157	LYS	CG-CD	10.41	1.87	1.52
1	O	156	LYS	CE-NZ	10.31	1.74	1.49
2	P	175	SER	C-O	9.61	1.41	1.23
2	N	11	GLU	CG-CD	9.14	1.65	1.51
1	O	119	GLU	CD-OE2	8.90	1.35	1.25
2	P	125	GLN	CD-NE2	8.60	1.54	1.32
1	Q	130	HIS	CG-ND1	8.52	1.57	1.38
2	P	125	GLN	CG-CD	8.52	1.70	1.51
2	N	165	GLU	CD-OE1	8.35	1.34	1.25
1	M	137	SER	CB-OG	8.21	1.52	1.42
2	R	116	LYS	CD-CE	8.07	1.71	1.51
2	P	150	GLU	CD-OE1	7.94	1.34	1.25
2	R	39	GLU	CD-OE2	7.92	1.34	1.25
1	K	139	CYS	CB-SG	-7.75	1.69	1.82
1	M	166	ARG	CZ-NH1	7.71	1.43	1.33
1	O	165	LYS	CD-CE	7.71	1.70	1.51
2	R	39	GLU	CD-OE1	7.45	1.33	1.25
1	C	139	CYS	CB-SG	-7.40	1.69	1.82
1	M	154	LEU	CG-CD1	7.34	1.78	1.51
1	M	172	ASN	CG-OD1	7.33	1.40	1.24
1	E	277	CYS	CB-SG	-7.20	1.70	1.82
1	G	139	CYS	CB-SG	-7.14	1.70	1.82
1	M	172	ASN	CG-ND2	6.69	1.49	1.32
1	I	139	CYS	CB-SG	-6.67	1.71	1.82
1	M	222	LYS	CE-NZ	6.61	1.65	1.49
1	O	216	ARG	CZ-NH1	6.38	1.41	1.33
1	G	277	CYS	CB-SG	-6.33	1.71	1.82
2	L	78	GLU	CG-CD	6.29	1.61	1.51
2	P	125	GLN	CB-CG	6.21	1.69	1.52
2	P	150	GLU	CG-CD	6.20	1.61	1.51
1	G	64	CYS	CB-SG	-6.14	1.71	1.82
1	O	10	GLY	N-CA	6.13	1.55	1.46
2	N	11	GLU	CB-CG	6.10	1.63	1.52
2	P	125	GLN	CD-OE1	6.04	1.37	1.24
1	C	277	CYS	CB-SG	-6.03	1.72	1.82
2	R	150	GLU	CB-CG	5.99	1.63	1.52
1	M	73	ASN	CG-OD1	5.96	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	38	LYS	CD-CE	5.94	1.66	1.51
1	O	158	ASN	CG-OD1	5.93	1.37	1.24
2	H	78	GLU	CG-CD	5.78	1.60	1.51
1	M	152	VAL	C-O	5.76	1.34	1.23
1	M	166	ARG	CZ-NH2	5.68	1.40	1.33
1	M	128	SER	CB-OG	5.59	1.49	1.42
2	F	68	ARG	N-CA	5.58	1.57	1.46
1	M	166	ARG	C-N	5.54	1.46	1.34
1	O	160	THR	CB-CG2	5.41	1.70	1.52
1	M	186	ASN	CG-ND2	5.40	1.46	1.32
1	O	193	LYS	CE-NZ	5.38	1.62	1.49
1	O	210	ASN	C-O	5.32	1.33	1.23
1	C	151	VAL	CB-CG2	-5.30	1.41	1.52
2	F	69	GLU	CD-OE2	5.22	1.31	1.25
2	F	78	GLU	CG-CD	5.21	1.59	1.51
1	I	190	GLU	CG-CD	5.17	1.59	1.51
1	M	167	SER	CB-OG	5.16	1.49	1.42
1	O	219	THR	CB-CG2	5.08	1.69	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	38	LYS	CD-CE-NZ	-14.03	79.42	111.70
1	M	166	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	O	125(A)	LYS	CD-CE-NZ	-11.74	84.70	111.70
1	M	154	LEU	CB-CG-CD2	11.21	130.05	111.00
2	P	143	LYS	CD-CE-NZ	-10.31	87.98	111.70
2	P	145	ASP	CB-CG-OD1	-9.66	109.61	118.30
1	M	154	LEU	CB-CG-CD1	-8.27	96.94	111.00
1	O	157	LYS	CG-CD-CE	-8.05	87.74	111.90
1	A	176	LEU	CA-CB-CG	7.27	132.02	115.30
1	O	157	LYS	CD-CE-NZ	-7.16	95.24	111.70
2	F	76	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	K	176	LEU	CA-CB-CG	6.98	131.34	115.30
1	O	157	LYS	CB-CG-CD	-6.81	93.90	111.60
1	I	176	LEU	CA-CB-CG	6.79	130.92	115.30
2	N	38	LYS	CG-CD-CE	-6.72	91.74	111.90
2	D	68	ARG	N-CA-C	6.57	128.74	111.00
2	P	38	LYS	CD-CE-NZ	-6.48	96.80	111.70
1	G	176	LEU	CA-CB-CG	6.46	130.17	115.30
2	P	143	LYS	CG-CD-CE	-6.41	92.67	111.90
2	B	68	ARG	N-CA-C	6.38	128.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	68	ARG	N-CA-C	6.30	128.01	111.00
2	H	76	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	L	68	ARG	N-CA-C	6.15	127.61	111.00
1	K	80	ILE	N-CA-C	-6.13	94.44	111.00
1	E	176	LEU	CA-CB-CG	6.09	129.30	115.30
2	J	68	ARG	N-CA-C	6.00	127.21	111.00
1	C	176	LEU	CA-CB-CG	6.00	129.11	115.30
1	O	160	THR	CA-CB-CG2	-6.00	104.01	112.40
2	J	66	VAL	N-CA-C	5.99	127.17	111.00
1	E	63	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	O	125(B)	SER	CA-CB-OG	-5.93	95.20	111.20
2	F	68	ARG	N-CA-C	5.92	126.98	111.00
1	E	176	LEU	CB-CG-CD2	-5.89	100.98	111.00
2	D	66	VAL	N-CA-C	5.68	126.34	111.00
1	I	80	ILE	N-CA-C	-5.67	95.70	111.00
1	G	80	ILE	N-CA-C	-5.62	95.83	111.00
2	B	76	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	80	ILE	N-CA-C	-5.57	95.97	111.00
1	I	62	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	I	175	ASP	CB-CG-OD1	5.46	123.21	118.30
1	M	166	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	80	ILE	N-CA-C	-5.44	96.31	111.00
1	E	80	ILE	N-CA-C	-5.38	96.48	111.00
2	B	66	VAL	N-CA-C	5.37	125.50	111.00
2	F	66	VAL	N-CA-C	5.37	125.50	111.00
1	O	277	CYS	CA-CB-SG	5.32	123.58	114.00
2	H	66	VAL	N-CA-C	5.26	125.21	111.00
1	O	166	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	D	76	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	N	38	LYS	CB-CG-CD	-5.17	98.14	111.60
1	A	209	LEU	CB-CG-CD2	-5.17	102.22	111.00
1	O	216	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	P	59	MET	CA-CB-CG	-5.13	104.58	113.30
2	L	66	VAL	N-CA-C	5.13	124.85	111.00
2	N	165	GLU	OE1-CD-OE2	5.12	129.45	123.30
2	N	66	VAL	N-CA-C	5.10	124.77	111.00
1	M	154	LEU	CD1-CG-CD2	5.08	125.74	110.50
1	G	176	LEU	CB-CG-CD2	-5.06	102.41	111.00

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ASN	Peptide
1	A	276	ASN	Peptide
2	B	60	ASN	Peptide
2	B	61	THR	Peptide
2	B	68	ARG	Peptide
1	C	249	GLY	Peptide
1	C	276	ASN	Peptide
2	D	60	ASN	Peptide
2	D	61	THR	Peptide
2	D	68	ARG	Peptide
1	E	248	ASN	Peptide
1	E	276	ASN	Peptide
2	F	60	ASN	Peptide
2	F	61	THR	Peptide
2	F	68	ARG	Peptide
1	G	248	ASN	Peptide
1	G	276	ASN	Peptide
2	H	60	ASN	Peptide
2	H	61	THR	Peptide
2	H	68	ARG	Peptide
1	I	276	ASN	Peptide
2	J	61	THR	Peptide
2	J	68	ARG	Peptide
1	K	248	ASN	Peptide
1	K	249	GLY	Peptide
1	K	276	ASN	Peptide
2	L	60	ASN	Peptide
2	L	61	THR	Peptide
2	L	68	ARG	Peptide
1	M	130	HIS	Sidechain
2	N	61	THR	Peptide
2	N	68	ARG	Peptide
1	O	225	GLY	Peptide
1	O	276	ASN	Peptide
1	O	313	ARG	Peptide
2	P	60	ASN	Peptide
2	P	61	THR	Peptide
1	Q	240	ASN	Peptide

## 5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2496	118	2
1	C	2553	0	2496	118	3
1	E	2553	0	2496	169	0
1	G	2553	0	2496	131	3
1	I	2553	0	2496	139	0
1	K	2553	0	2496	117	2
1	M	2553	0	2496	166	0
1	O	2553	0	2496	190	0
1	Q	2553	0	2498	132	0
2	B	1416	0	1320	48	0
2	D	1416	0	1320	46	0
2	F	1416	0	1320	72	0
2	H	1416	0	1320	60	0
2	J	1416	0	1320	42	0
2	L	1416	0	1320	39	0
2	N	1416	0	1320	75	0
2	P	1416	0	1320	82	0
2	R	1416	0	1320	77	0
3	S	28	0	25	1	0
3	U	28	0	25	1	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	Y	28	0	25	2	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
4	T	39	0	34	3	0
4	X	39	0	34	3	0
4	Z	39	0	34	0	0
All	All	36202	0	34773	1618	5

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 23.

All (1618) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:LEU:CD1	1:M:154:LEU:CG	1.79	1.60
1:M:130:HIS:CG	1:M:130:HIS:ND1	1.71	1.54
1:M:130:HIS:NE2	1:M:130:HIS:CE1	1.75	1.53
1:O:125(A):LYS:CE	1:O:125(A):LYS:CD	1.83	1.52
2:P:143:LYS:CE	2:P:143:LYS:CD	1.86	1.51
2:N:38:LYS:CD	2:N:38:LYS:CE	1.89	1.49
2:N:38:LYS:CD	2:N:38:LYS:CG	1.91	1.48
1:O:157:LYS:CG	1:O:157:LYS:CD	1.87	1.48
1:O:156:LYS:NZ	1:O:156:LYS:CE	1.74	1.45
1:O:160:THR:CB	1:O:160:THR:OG1	1.71	1.37
1:O:219:THR:OG1	1:O:219:THR:CB	1.73	1.34
1:O:157:LYS:NZ	1:O:157:LYS:CE	1.90	1.34
2:P:145:ASP:CG	2:P:145:ASP:OD1	1.64	1.34
1:G:141:TYR:HE2	1:G:142:GLN:NE2	1.28	1.31
2:P:38:LYS:CE	2:P:38:LYS:NZ	1.92	1.31
1:I:141:TYR:HE2	1:I:142:GLN:NE2	1.29	1.31
1:O:157:LYS:CD	1:O:157:LYS:CE	2.07	1.31
1:E:141:TYR:HE2	1:E:142:GLN:NE2	1.26	1.30
1:O:130:HIS:NE2	1:O:130:HIS:CE1	1.79	1.30
1:O:125(A):LYS:CE	1:O:125(A):LYS:NZ	1.96	1.29
1:C:141:TYR:HE2	1:C:142:GLN:NE2	1.27	1.27
1:A:141:TYR:HE2	1:A:142:GLN:NE2	1.31	1.26
1:E:78:GLU:OE2	1:I:142:GLN:OE1	1.56	1.23
1:O:125(B):SER:OG	1:O:125(B):SER:CB	1.87	1.22
1:K:141:TYR:HE2	1:K:142:GLN:NE2	1.41	1.16
1:Q:206:THR:HG22	1:Q:207:SER:H	1.04	1.14
1:G:75:MET:HB2	1:G:95:ASN:ND2	1.66	1.10
1:E:200:THR:HG21	1:E:250:ASN:OD1	1.51	1.10
1:K:200:THR:HG21	1:K:250:ASN:OD1	1.52	1.10
1:E:75:MET:HB2	1:E:95:ASN:ND2	1.67	1.09
1:G:200:THR:HG21	1:G:250:ASN:OD1	1.49	1.09
1:E:182:ILE:HD12	1:E:202:ILE:HD13	1.34	1.08
1:I:200:THR:HG21	1:I:250:ASN:OD1	1.51	1.07
1:A:75:MET:HB2	1:A:95:ASN:ND2	1.69	1.07
2:P:143:LYS:CE	2:P:143:LYS:NZ	2.18	1.07
1:A:75:MET:HB2	1:A:95:ASN:HD22	1.21	1.04
1:K:182:ILE:HD12	1:K:202:ILE:HD13	1.38	1.04
1:M:130:HIS:CG	1:M:130:HIS:CE1	2.40	1.04
1:A:200:THR:HG21	1:A:250:ASN:OD1	1.55	1.04
1:C:75:MET:HB2	1:C:95:ASN:ND2	1.73	1.04
1:I:75:MET:HB2	1:I:95:ASN:ND2	1.73	1.04
1:G:182:ILE:HD11	1:G:213:LEU:HD12	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:MET:HB2	1:G:95:ASN:HD22	1.24	1.02
1:E:75:MET:HB2	1:E:95:ASN:HD22	1.23	1.01
1:G:79:PHE:C	1:G:79:PHE:HD1	1.65	1.00
1:C:200:THR:HG21	1:C:250:ASN:OD1	1.61	0.99
2:B:59:MET:O	2:B:61:THR:N	1.94	0.99
1:E:13:ILE:CD1	2:F:152:VAL:HG11	1.93	0.98
1:K:75:MET:HB2	1:K:95:ASN:ND2	1.79	0.98
2:P:59:MET:O	2:P:61:THR:N	1.95	0.98
2:R:165:GLU:O	2:R:169:LYS:HB3	1.64	0.98
1:Q:282:GLN:O	1:Q:301:THR:HB	1.64	0.98
1:A:79:PHE:HD1	1:A:79:PHE:C	1.68	0.97
1:C:283:THR:HB	1:C:286:GLY:O	1.64	0.97
2:F:59:MET:O	2:F:61:THR:N	1.97	0.97
1:I:283:THR:HB	1:I:286:GLY:O	1.64	0.97
1:C:75:MET:HB2	1:C:95:ASN:HD22	1.29	0.97
1:E:283:THR:HB	1:E:286:GLY:O	1.65	0.97
2:N:150:GLU:O	2:N:154:ASN:HB2	1.64	0.96
1:O:283:THR:HG22	1:O:285:MET:H	1.30	0.96
1:G:182:ILE:HD12	1:G:202:ILE:HD13	1.46	0.96
1:E:182:ILE:HD11	1:E:213:LEU:HD12	1.47	0.96
2:N:38:LYS:NZ	2:N:38:LYS:CE	2.29	0.95
1:I:182:ILE:HD11	1:I:213:LEU:HD12	1.46	0.95
1:I:79:PHE:C	1:I:79:PHE:HD1	1.70	0.95
1:A:182:ILE:HD12	1:A:202:ILE:HD13	1.49	0.95
1:E:11:ASP:OD2	2:F:143:LYS:HA	1.66	0.95
1:E:79:PHE:HD1	1:E:79:PHE:C	1.68	0.94
1:O:28:ILE:HD11	2:P:102:MET:HG3	1.47	0.94
1:C:182:ILE:HD12	1:C:202:ILE:HD13	1.44	0.94
1:I:182:ILE:HD12	1:I:202:ILE:HD13	1.47	0.94
1:I:75:MET:HB2	1:I:95:ASN:HD22	1.32	0.94
1:O:141:TYR:HB2	1:O:146:SER:HB3	1.46	0.94
1:O:251:PHE:CE1	1:O:253:ALA:HA	2.03	0.93
1:E:272:LEU:HD21	1:M:171:THR:HG21	1.51	0.93
1:G:283:THR:HB	1:G:286:GLY:O	1.69	0.93
1:M:27:THR:HG22	1:M:31:MET:H	1.31	0.93
1:G:275:GLY:O	1:G:277:CYS:HB3	1.69	0.92
1:K:275:GLY:O	1:K:277:CYS:HB3	1.69	0.92
2:J:59:MET:O	2:J:61:THR:N	2.02	0.92
1:Q:206:THR:CG2	1:Q:207:SER:H	1.83	0.92
1:C:182:ILE:HD11	1:C:213:LEU:HD12	1.52	0.92
2:R:30:GLN:HA	2:R:30:GLN:HE21	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:GLY:O	1:E:277:CYS:HB3	1.70	0.91
2:R:127:ARG:HB2	2:R:127:ARG:HH11	1.36	0.91
1:A:283:THR:HB	1:A:286:GLY:O	1.70	0.91
1:G:283:THR:HG22	1:G:285:MET:H	1.35	0.90
1:K:79:PHE:HD1	1:K:79:PHE:C	1.74	0.90
2:L:59:MET:O	2:L:61:THR:N	2.04	0.90
1:M:50:LYS:HD3	1:M:275:GLY:HA3	1.50	0.90
1:K:182:ILE:HD11	1:K:213:LEU:HD12	1.53	0.90
2:H:59:MET:O	2:H:61:THR:N	2.05	0.90
1:A:182:ILE:HD11	1:A:213:LEU:HD12	1.53	0.90
2:N:145:ASP:O	2:N:148:CYS:HB3	1.72	0.90
2:P:145:ASP:OD1	2:P:148:CYS:HB2	1.71	0.90
1:Q:206:THR:HG22	1:Q:207:SER:N	1.85	0.90
1:M:275:GLY:O	1:M:277:CYS:HB3	1.71	0.89
1:I:79:PHE:O	1:I:80:ILE:HD13	1.72	0.89
2:P:151:SER:HB2	2:P:157:TYR:HA	1.55	0.89
1:C:275:GLY:O	1:C:277:CYS:HB3	1.71	0.89
1:C:79:PHE:C	1:C:79:PHE:HD1	1.76	0.89
1:E:13:ILE:HD12	2:F:152:VAL:HG11	1.53	0.89
1:A:275:GLY:O	1:A:277:CYS:HB3	1.73	0.89
1:M:201:TYR:H	1:M:248:ASN:HB2	1.38	0.88
1:Q:16:GLY:HA3	2:R:14:TRP:HD1	1.39	0.87
1:O:157:LYS:CB	1:O:157:LYS:CD	2.53	0.87
1:K:79:PHE:CD1	1:K:79:PHE:C	2.46	0.87
1:E:79:PHE:C	1:E:79:PHE:CD1	2.42	0.86
1:A:159:SER:O	1:A:196:GLN:HG3	1.74	0.86
1:I:283:THR:HG22	1:I:285:MET:H	1.40	0.86
2:H:63:PHE:N	2:H:63:PHE:HD1	1.73	0.86
2:D:59:MET:O	2:D:61:THR:N	2.09	0.85
1:M:200:THR:HA	1:M:248:ASN:HB3	1.57	0.85
1:K:283:THR:HB	1:K:286:GLY:O	1.75	0.84
1:O:135:VAL:HG22	1:O:146:SER:HA	1.58	0.84
1:A:79:PHE:C	1:A:79:PHE:CD1	2.42	0.84
1:C:124:ILE:HD11	1:C:254:PRO:O	1.77	0.84
1:I:275:GLY:O	1:I:277:CYS:HB3	1.76	0.84
1:C:79:PHE:CD1	1:C:79:PHE:C	2.49	0.84
1:E:283:THR:HG22	1:E:285:MET:H	1.43	0.84
1:I:79:PHE:C	1:I:79:PHE:CD1	2.44	0.84
1:M:114:ARG:HB2	1:M:265:SER:HB3	1.59	0.84
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.59	0.83
2:L:63:PHE:HD1	2:L:63:PHE:N	1.73	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:143:LYS:CE	2:P:143:LYS:CG	2.55	0.83
2:P:63:PHE:HD1	2:P:63:PHE:N	1.77	0.83
1:A:283:THR:HG22	1:A:285:MET:H	1.44	0.83
1:M:130:HIS:CE1	1:M:130:HIS:CD2	2.66	0.83
1:G:79:PHE:CD1	1:G:79:PHE:C	2.39	0.83
1:M:38:HIS:HB2	1:M:318:THR:HB	1.61	0.83
1:K:283:THR:HG22	1:K:285:MET:H	1.44	0.82
1:K:75:MET:HB2	1:K:95:ASN:HD22	1.42	0.82
1:M:154:LEU:CB	1:M:154:LEU:CD1	2.56	0.82
1:E:27:THR:HG22	1:E:31:MET:H	1.43	0.82
1:E:272:LEU:CD2	1:M:171:THR:HG21	2.10	0.82
1:G:288:ILE:HD11	1:G:297:ILE:HG13	1.60	0.82
2:N:144:CYS:SG	2:N:149:MET:HG3	2.20	0.81
1:E:126:SER:HB2	1:E:166:ARG:HH22	1.45	0.81
1:E:79:PHE:CG	1:I:144:LYS:HE3	2.16	0.81
1:Q:44:GLU:HB2	1:Q:294:PHE:O	1.81	0.81
2:H:63:PHE:CD1	2:H:63:PHE:N	2.45	0.80
1:C:79:PHE:O	1:C:80:ILE:HD13	1.82	0.80
2:J:63:PHE:N	2:J:63:PHE:HD1	1.78	0.80
2:H:61:THR:OG1	1:I:310:LYS:HD3	1.82	0.80
1:O:53(A):LEU:HD11	1:O:302:ILE:HG22	1.62	0.80
1:I:27:THR:HG22	1:I:31:MET:H	1.47	0.80
1:K:79:PHE:O	1:K:80:ILE:HD13	1.81	0.80
1:M:267:ILE:HD12	1:M:267:ILE:H	1.45	0.80
2:D:63:PHE:N	2:D:63:PHE:HD1	1.78	0.80
2:L:63:PHE:N	2:L:63:PHE:CD1	2.44	0.80
2:N:143:LYS:H	2:N:143:LYS:HD3	1.44	0.79
1:K:288:ILE:HD11	1:K:297:ILE:HG13	1.64	0.79
1:C:27:THR:HG22	1:C:31:MET:H	1.46	0.79
1:Q:225:GLY:O	1:Q:226:GLN:HB2	1.83	0.79
2:F:63:PHE:HD1	2:F:63:PHE:N	1.80	0.79
1:K:126:SER:HB2	1:K:166:ARG:HH22	1.48	0.79
1:K:27:THR:HG22	1:K:31:MET:H	1.44	0.79
1:E:87:ILE:HD12	1:E:113:SER:HA	1.64	0.79
1:M:266:THR:HG21	2:N:67:GLY:H	1.47	0.78
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.64	0.78
2:R:95:ASN:O	2:R:99:LEU:HB2	1.84	0.78
1:A:288:ILE:HD11	1:A:297:ILE:HG13	1.66	0.78
1:Q:260:ILE:HG23	1:Q:262:LYS:HB3	1.64	0.78
1:C:283:THR:HG22	1:C:285:MET:H	1.49	0.78
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:SER:OG	1:M:266:THR:N	2.15	0.78
2:B:167:ARG:HD3	2:D:174:SER:HA	1.66	0.77
1:E:18:HIS:HB2	2:F:21:TRP:HA	1.65	0.77
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.66	0.77
1:K:179:LEU:HD23	1:K:234:TRP:HB3	1.65	0.77
2:P:63:PHE:N	2:P:63:PHE:CD1	2.48	0.77
1:A:121:ILE:HG22	1:A:123:ILE:HD13	1.64	0.77
1:C:288:ILE:HD11	1:C:297:ILE:HG13	1.66	0.77
1:G:27:THR:HG22	1:G:31:MET:H	1.48	0.77
1:K:141:TYR:CE2	1:K:142:GLN:NE2	2.29	0.77
1:O:238:LYS:HG3	1:O:239:PRO:HD2	1.65	0.77
1:G:79:PHE:O	1:G:79:PHE:CD1	2.39	0.76
2:D:63:PHE:N	2:D:63:PHE:CD1	2.50	0.76
1:I:79:PHE:CD1	1:I:79:PHE:O	2.39	0.76
1:E:11:ASP:HB2	2:F:140:PHE:HD1	1.51	0.76
1:I:59:LEU:HD11	1:I:80:ILE:HG23	1.67	0.76
2:N:132:GLU:O	2:N:134:GLY:N	2.18	0.76
2:D:167:ARG:HD3	2:F:174:SER:HA	1.67	0.76
1:O:307:LYS:HD2	2:P:92:TRP:CE2	2.21	0.76
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.67	0.75
1:A:282:GLN:HE21	1:A:283:THR:H	1.32	0.75
1:E:282:GLN:HE21	1:E:283:THR:H	1.34	0.75
1:M:283:THR:HG22	1:M:284:PRO:HD2	1.67	0.75
1:O:300:LEU:HD21	2:P:68:ARG:HH21	1.51	0.75
2:F:63:PHE:N	2:F:63:PHE:CD1	2.52	0.75
1:E:11:ASP:O	2:F:140:PHE:N	2.16	0.75
2:R:4:GLY:HA2	2:R:8:GLY:HA3	1.68	0.75
1:E:47:HIS:HE1	1:M:171:THR:O	1.69	0.75
1:O:293:PRO:HG2	1:O:294:PHE:CD1	2.22	0.75
1:K:13:ILE:HD11	2:L:149:MET:HG2	1.68	0.74
1:C:59:LEU:HD11	1:C:80:ILE:HG23	1.69	0.74
1:Q:16:GLY:HA3	2:R:14:TRP:CD1	2.20	0.74
1:C:124:ILE:CG1	1:C:254:PRO:O	2.35	0.74
1:G:206:THR:HG22	1:G:207:SER:N	2.02	0.74
1:M:201:TYR:H	1:M:248:ASN:CB	2.00	0.74
1:I:146:SER:OG	1:I:147:PHE:N	2.19	0.74
1:K:80:ILE:O	1:K:80:ILE:HG22	1.88	0.74
1:A:206:THR:HB	1:A:209:LEU:H	1.52	0.74
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.67	0.74
1:G:124:ILE:HD11	1:G:254:PRO:O	1.88	0.74
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:63:PHE:CD1	2:J:63:PHE:N	2.50	0.74
1:M:204:VAL:HA	1:M:244:ASN:O	1.88	0.73
1:A:79:PHE:O	1:A:79:PHE:CD1	2.42	0.73
1:O:206:THR:HB	1:O:208:THR:H	1.53	0.73
1:G:206:THR:HG22	1:G:208:THR:H	1.54	0.73
1:I:266:THR:HG21	2:J:67:GLY:H	1.53	0.73
2:B:63:PHE:N	2:B:63:PHE:HD1	1.87	0.73
2:P:164:GLU:HA	2:P:167:ARG:HB2	1.69	0.73
2:P:37:ASP:O	2:P:41:THR:OG1	2.07	0.73
1:I:179:LEU:HD23	1:I:234:TRP:HB3	1.70	0.73
1:C:182:ILE:HD13	1:C:182:ILE:N	2.02	0.73
4:T:2:NAG:HN2	4:T:2:NAG:H5	1.54	0.73
1:A:126:SER:HB2	1:A:166:ARG:HH22	1.54	0.73
3:S:1:NAG:H62	3:S:2:NAG:H2	1.70	0.73
1:C:124:ILE:CD1	1:C:254:PRO:O	2.37	0.72
1:E:11:ASP:CB	2:F:140:PHE:HD1	2.02	0.72
1:E:79:PHE:O	1:E:79:PHE:CD1	2.42	0.72
1:I:124:ILE:HD11	1:I:254:PRO:O	1.89	0.72
1:O:219:THR:HG22	1:O:220:ARG:H	1.54	0.72
2:P:25:HIS:HA	2:P:34:TYR:HB3	1.71	0.72
1:E:272:LEU:HD21	1:M:171:THR:CG2	2.20	0.72
2:R:30:GLN:HA	2:R:30:GLN:NE2	2.04	0.72
1:M:211:GLN:NE2	1:M:213:LEU:HD21	2.05	0.72
1:Q:104:ASP:HB2	1:Q:234:TRP:HE1	1.55	0.72
1:G:279:THR:HG21	1:G:287:ALA:HB1	1.72	0.72
1:C:279:THR:HG21	1:C:287:ALA:HB1	1.72	0.72
1:G:79:PHE:O	1:G:80:ILE:HD13	1.90	0.72
1:M:37:THR:HB	1:M:320:LEU:H	1.54	0.72
1:E:121:ILE:HG22	1:E:123:ILE:HD13	1.72	0.71
1:E:59:LEU:HD11	1:E:80:ILE:HG23	1.70	0.71
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.72	0.71
1:A:27:THR:HG22	1:A:31:MET:H	1.55	0.71
1:O:134:GLY:HA2	1:O:155:ILE:HD13	1.72	0.71
1:C:307:LYS:NZ	2:D:62:GLN:HB3	2.06	0.71
1:C:141:TYR:CE2	1:C:142:GLN:NE2	2.18	0.71
1:O:27:THR:HG22	1:O:31:MET:H	1.55	0.71
1:C:159:SER:O	1:C:196:GLN:HG3	1.91	0.71
1:O:200:THR:HG21	1:O:250:ASN:HB2	1.73	0.71
1:Q:56:VAL:O	1:Q:85:SER:OG	2.09	0.71
1:G:159:SER:O	1:G:196:GLN:HG3	1.91	0.71
1:O:27:THR:HB	1:O:32:GLU:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:MET:CB	1:E:95:ASN:ND2	2.52	0.70
1:I:159:SER:O	1:I:196:GLN:HG3	1.90	0.70
1:K:124:ILE:HD11	1:K:254:PRO:O	1.90	0.70
1:M:123:ILE:HG23	1:M:124:ILE:HG12	1.72	0.70
1:C:80:ILE:HG22	1:C:80:ILE:O	1.90	0.70
1:O:62:ARG:HD2	1:O:63:ASP:HB2	1.74	0.70
1:E:11:ASP:HB2	2:F:140:PHE:CD1	2.26	0.70
1:G:59:LEU:HD11	1:G:80:ILE:HG23	1.71	0.70
1:O:125(A):LYS:CE	1:O:125(A):LYS:CG	2.70	0.70
1:Q:87:ILE:HD11	1:Q:267:ILE:HA	1.73	0.70
1:M:200:THR:HA	1:M:248:ASN:CB	2.21	0.70
1:K:307:LYS:NZ	2:L:62:GLN:HB3	2.06	0.70
1:A:206:THR:HG22	1:A:208:THR:H	1.56	0.70
1:A:72:GLY:O	1:A:148:PHE:HA	1.92	0.70
1:C:126:SER:HB2	1:C:166:ARG:HH22	1.56	0.70
1:C:181:GLY:C	1:C:182:ILE:HD13	2.11	0.70
1:I:182:ILE:HD13	1:I:182:ILE:N	2.07	0.70
1:E:206:THR:HG22	1:E:207:SER:N	2.07	0.70
1:G:11:ASP:OD2	2:H:143:LYS:HA	1.92	0.70
1:C:206:THR:HG22	1:C:207:SER:N	2.06	0.70
1:O:223:VAL:O	1:O:224:ASN:HB2	1.91	0.70
1:E:206:THR:HB	1:E:209:LEU:H	1.57	0.70
1:K:159:SER:O	1:K:196:GLN:HG3	1.92	0.70
1:A:59:LEU:HD11	1:A:80:ILE:HG23	1.72	0.69
2:N:37:ASP:O	2:N:39:GLU:N	2.24	0.69
1:Q:181:GLY:O	1:Q:182:ILE:HD13	1.92	0.69
1:G:121:ILE:HG22	1:G:123:ILE:HD13	1.72	0.69
2:H:65:ALA:C	2:H:66:VAL:HG13	2.11	0.69
2:N:38:LYS:CD	2:N:38:LYS:CB	2.69	0.69
2:P:59:MET:C	2:P:61:THR:H	1.95	0.69
2:B:63:PHE:CD1	2:B:63:PHE:N	2.59	0.69
1:O:125(A):LYS:CD	1:O:125(A):LYS:NZ	2.56	0.69
1:Q:16:GLY:CA	2:R:14:TRP:HD1	2.04	0.69
1:G:206:THR:CG2	1:G:207:SER:N	2.55	0.69
1:M:202:ILE:HB	1:M:213:LEU:HD12	1.74	0.69
1:C:141:TYR:CD2	1:C:142:GLN:HG3	2.28	0.69
1:M:243:ILE:HG12	1:M:245:PHE:CE1	2.27	0.69
1:E:146:SER:OG	1:E:147:PHE:N	2.26	0.69
2:F:65:ALA:C	2:F:66:VAL:HG13	2.13	0.69
1:E:124:ILE:HD11	1:E:254:PRO:O	1.92	0.69
1:M:279:THR:HG21	1:M:287:ALA:HB1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:HD12	1:C:113:SER:HA	1.75	0.69
1:I:124:ILE:CG1	1:I:254:PRO:O	2.40	0.69
1:I:282:GLN:HE21	1:I:283:THR:H	1.40	0.69
2:N:117:ASN:O	2:N:121:LYS:HG2	1.93	0.69
1:M:114:ARG:HH11	1:M:265:SER:HB2	1.59	0.68
1:A:206:THR:HG22	1:A:207:SER:N	2.08	0.68
1:A:206:THR:HG22	1:A:208:THR:N	2.09	0.68
1:I:206:THR:HG22	1:I:207:SER:N	2.08	0.68
1:C:206:THR:CG2	1:C:207:SER:N	2.56	0.68
1:I:38:HIS:HB2	1:I:318:THR:HB	1.75	0.68
1:G:206:THR:HB	1:G:209:LEU:H	1.57	0.68
1:O:295:HIS:HD2	1:O:297:ILE:H	1.39	0.68
1:I:121:ILE:HG22	1:I:123:ILE:HD13	1.75	0.68
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.73	0.68
1:E:18:HIS:N	2:F:21:TRP:O	2.25	0.68
1:I:126:SER:HB2	1:I:166:ARG:HH22	1.59	0.68
1:Q:172:ASN:ND2	1:Q:259:LYS:HE2	2.09	0.68
1:G:72:GLY:O	1:G:148:PHE:HA	1.94	0.67
1:I:72:GLY:O	1:I:148:PHE:HA	1.94	0.67
2:P:59:MET:HE1	2:P:62:GLN:HG3	1.75	0.67
1:A:124:ILE:HD13	1:A:254:PRO:HG2	1.76	0.67
1:A:75:MET:CB	1:A:95:ASN:ND2	2.54	0.67
1:A:181:GLY:C	1:A:182:ILE:HD13	2.14	0.67
1:A:229:ARG:HH21	1:E:207:SER:HA	1.59	0.67
1:E:307:LYS:NZ	2:F:62:GLN:HB3	2.08	0.67
1:G:13:ILE:CD1	2:H:152:VAL:HG11	2.24	0.67
1:C:79:PHE:O	1:C:79:PHE:CD1	2.48	0.67
1:E:124:ILE:HD13	1:E:254:PRO:HG2	1.75	0.67
1:M:202:ILE:HA	1:M:246:GLU:O	1.94	0.67
1:O:182:ILE:HG23	1:O:215:PRO:HB3	1.77	0.67
1:K:124:ILE:HD13	1:K:254:PRO:HG2	1.76	0.67
1:A:124:ILE:HD11	1:A:254:PRO:O	1.95	0.67
1:A:124:ILE:CG1	1:A:254:PRO:O	2.42	0.67
1:C:206:THR:HG22	1:C:208:THR:H	1.59	0.67
1:G:126:SER:HB2	1:G:166:ARG:HH22	1.60	0.67
1:K:59:LEU:HD11	1:K:80:ILE:HG23	1.76	0.67
1:O:211:GLN:NE2	1:O:213:LEU:HD11	2.09	0.67
1:E:126:SER:CB	1:E:166:ARG:HH22	2.06	0.66
1:I:27:THR:HG22	1:I:32:GLU:H	1.60	0.66
1:K:121:ILE:HG22	1:K:123:ILE:HD13	1.75	0.66
1:K:206:THR:HG22	1:K:207:SER:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:120:ASP:OD1	2:N:123:ARG:NH1	2.28	0.66
1:Q:14:CYS:O	2:R:24:TYR:HB3	1.95	0.66
1:I:181:GLY:C	1:I:182:ILE:HD13	2.15	0.66
1:K:282:GLN:HE21	1:K:283:THR:H	1.41	0.66
1:M:172:ASN:H	1:M:172:ASN:HD22	1.43	0.66
1:E:72:GLY:O	1:E:148:PHE:HA	1.95	0.66
1:I:206:THR:CG2	1:I:207:SER:N	2.58	0.66
1:E:206:THR:CG2	1:E:207:SER:N	2.59	0.66
1:G:266:THR:HG21	2:H:67:GLY:H	1.60	0.66
1:K:206:THR:CG2	1:K:207:SER:N	2.58	0.66
2:N:38:LYS:CE	2:N:38:LYS:CG	2.73	0.66
2:P:27:SER:HA	2:P:32:SER:HB2	1.76	0.66
2:N:59:MET:O	2:N:61:THR:N	2.29	0.66
1:C:282:GLN:HE21	1:C:283:THR:H	1.42	0.66
1:C:72:GLY:O	1:C:148:PHE:HA	1.96	0.66
1:I:206:THR:HB	1:I:209:LEU:H	1.61	0.66
2:P:63:PHE:HD1	2:P:63:PHE:H	1.43	0.66
1:K:146:SER:OG	1:K:147:PHE:N	2.27	0.66
1:K:279:THR:HG21	1:K:287:ALA:HB1	1.78	0.66
2:B:90:ASP:OD1	2:F:63:PHE:HE1	1.79	0.65
1:G:282:GLN:HE21	1:G:283:THR:H	1.42	0.65
1:K:206:THR:HG22	1:K:208:THR:N	2.11	0.65
2:N:166:ALA:HA	2:N:169:LYS:HB3	1.78	0.65
1:O:157:LYS:CG	1:O:157:LYS:CE	2.74	0.65
2:P:80:LEU:HD12	2:P:83:LYS:HE3	1.78	0.65
1:A:141:TYR:CE2	1:A:142:GLN:NE2	2.22	0.65
1:O:58:PRO:HB3	1:O:86:TYR:CE2	2.30	0.65
1:I:206:THR:HG22	1:I:208:THR:H	1.61	0.65
1:C:38:HIS:HB2	1:C:318:THR:HB	1.77	0.65
1:O:27:THR:HG23	2:P:105:GLU:HB2	1.79	0.65
4:T:2:NAG:N2	4:T:2:NAG:H5	2.08	0.65
1:G:206:THR:HG22	1:G:208:THR:N	2.10	0.65
1:G:75:MET:CB	1:G:95:ASN:ND2	2.55	0.65
2:R:166:ALA:HB1	2:R:170:ARG:HD3	1.78	0.65
1:E:79:PHE:O	1:E:80:ILE:HD13	1.96	0.65
1:K:186:ASN:HB3	1:K:190:GLU:OE2	1.97	0.65
1:O:123:ILE:N	1:O:255:GLU:O	2.27	0.65
1:A:27:THR:HG22	1:A:32:GLU:H	1.61	0.65
1:C:27:THR:HG22	1:C:32:GLU:H	1.62	0.65
1:I:206:THR:HG22	1:I:208:THR:N	2.12	0.65
1:M:277:CYS:SG	1:M:278:ASN:N	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:133:LEU:HB2	2:N:137:CYS:O	1.97	0.65
2:P:128:ASP:HB3	2:P:170:ARG:HH12	1.62	0.65
1:E:126:SER:HB3	1:I:79:PHE:CZ	2.32	0.65
1:O:38:HIS:HD2	1:O:319:GLY:HA3	1.62	0.65
1:C:141:TYR:CE2	1:C:142:GLN:HG3	2.32	0.64
1:Q:200:THR:HG23	1:Q:249:GLY:H	1.62	0.64
1:A:275:GLY:O	1:A:277:CYS:CB	2.45	0.64
1:E:50:LYS:HZ2	1:M:121:ILE:HG23	1.60	0.64
2:B:174:SER:HA	2:F:167:ARG:HD3	1.77	0.64
1:K:79:PHE:CD1	1:K:79:PHE:O	2.50	0.64
1:O:177:LEU:HD23	1:O:258:TYR:HD1	1.62	0.64
1:A:79:PHE:O	1:A:80:ILE:HD13	1.97	0.64
2:N:57:ASP:O	2:N:60:ASN:HB2	1.98	0.64
2:H:66:VAL:HG21	2:J:79:ASN:HD21	1.63	0.64
1:I:80:ILE:HG22	1:I:80:ILE:O	1.96	0.64
1:M:221:SER:O	1:M:229:ARG:NH2	2.29	0.64
1:A:12:GLN:HB2	2:B:27:SER:OG	1.98	0.64
2:N:63:PHE:CD1	2:N:63:PHE:N	2.62	0.64
2:P:133:LEU:HD21	2:P:139:GLU:HB2	1.78	0.64
1:A:206:THR:CG2	1:A:207:SER:N	2.61	0.64
2:N:151:SER:HB2	2:N:156:THR:O	1.98	0.64
1:Q:320:LEU:HD12	2:R:6:ILE:HG21	1.80	0.64
1:A:266:THR:HG21	2:B:67:GLY:H	1.62	0.64
2:H:68:ARG:HG3	2:H:68:ARG:O	1.96	0.64
1:Q:53(A):LEU:O	1:Q:278:ASN:HA	1.98	0.64
1:O:57:LYS:H	1:O:57:LYS:CD	2.11	0.64
1:Q:22:THR:CG2	1:Q:324:PRO:HD3	2.27	0.64
1:K:38:HIS:HB2	1:K:318:THR:HB	1.80	0.64
2:P:59:MET:CE	2:P:62:GLN:HG3	2.28	0.64
1:O:172:ASN:N	1:O:172:ASN:ND2	2.47	0.63
1:G:38:HIS:HB2	1:G:318:THR:HB	1.80	0.63
1:C:206:THR:HB	1:C:209:LEU:H	1.63	0.63
1:I:79:PHE:O	1:I:80:ILE:CD1	2.46	0.63
1:K:181:GLY:C	1:K:182:ILE:HD13	2.17	0.63
1:Q:104:ASP:CB	1:Q:234:TRP:HE1	2.11	0.63
1:E:171:THR:HB	1:I:121:ILE:HD13	1.81	0.63
1:K:182:ILE:N	1:K:182:ILE:HD13	2.12	0.63
1:E:47:HIS:CE1	1:M:171:THR:O	2.51	0.63
1:E:266:THR:HG21	2:F:67:GLY:H	1.64	0.63
1:G:206:THR:HG23	1:G:241:ASP:OD2	1.99	0.63
1:M:172:ASN:N	1:M:172:ASN:HD22	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:TYR:CD2	1:K:142:GLN:HG3	2.32	0.63
1:O:38:HIS:HB2	1:O:318:THR:HB	1.81	0.63
1:C:206:THR:HG22	1:C:208:THR:N	2.14	0.62
1:M:228:GLY:O	1:M:229:ARG:NH1	2.32	0.62
1:E:38:HIS:HB2	1:E:318:THR:HB	1.81	0.62
1:O:102:PHE:HB3	1:O:105:TYR:HB2	1.81	0.62
1:O:214:VAL:O	1:O:216:ARG:HD3	2.00	0.62
1:Q:11:ASP:HB2	2:R:140:PHE:HD1	1.65	0.62
1:I:182:ILE:HD11	1:I:213:LEU:CD1	2.28	0.62
1:K:126:SER:CB	1:K:166:ARG:HH22	2.11	0.62
1:K:201:TYR:CE2	1:K:248:ASN:HB2	2.34	0.62
1:M:114:ARG:NH1	1:M:265:SER:HB2	2.14	0.62
1:O:146:SER:OG	1:O:147:PHE:N	2.32	0.62
1:M:170:ASN:ND2	1:M:239:PRO:HA	2.14	0.62
2:B:62:GLN:N	2:B:62:GLN:CD	2.51	0.62
2:H:63:PHE:HE1	2:J:90:ASP:OD1	1.81	0.62
1:I:27:THR:CG2	1:I:31:MET:H	2.12	0.62
1:O:313:ARG:HB3	1:O:315:VAL:HG23	1.81	0.62
1:Q:90:LYS:HD3	1:Q:270:SER:O	2.00	0.62
1:Q:63:ASP:HB3	1:Q:95:ASN:HD21	1.65	0.62
1:I:141:TYR:CD2	1:I:142:GLN:HG3	2.35	0.61
1:K:27:THR:HG22	1:K:32:GLU:H	1.64	0.61
2:N:63:PHE:HD1	2:N:63:PHE:H	1.48	0.61
1:Q:316:LEU:HD13	2:R:100:VAL:HG22	1.82	0.61
1:C:124:ILE:HG12	1:C:254:PRO:O	2.00	0.61
1:E:206:THR:HG22	1:E:208:THR:N	2.14	0.61
1:K:141:TYR:CE2	1:K:142:GLN:HG3	2.35	0.61
1:C:27:THR:CG2	1:C:31:MET:H	2.11	0.61
1:M:313:ARG:HD2	1:M:315:VAL:HG21	1.82	0.61
2:R:95:ASN:O	2:R:99:LEU:N	2.31	0.61
1:A:182:ILE:HD13	1:A:182:ILE:N	2.16	0.61
1:G:87:ILE:HD12	1:G:113:SER:HA	1.83	0.61
1:M:182:ILE:CD1	1:M:202:ILE:HD13	2.30	0.61
1:M:167:SER:HB2	1:M:243:ILE:O	2.00	0.61
1:G:170:ASN:O	1:G:239:PRO:O	2.18	0.61
2:N:63:PHE:HD1	2:N:63:PHE:N	1.99	0.61
1:K:206:THR:HG22	1:K:208:THR:H	1.66	0.61
1:A:38:HIS:HB2	1:A:318:THR:HB	1.83	0.61
1:E:15:ILE:HD13	2:F:119:TYR:HA	1.82	0.61
1:G:283:THR:HG22	1:G:285:MET:N	2.14	0.61
1:A:282:GLN:NE2	1:A:283:THR:H	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:CG2	1:C:207:SER:H	2.14	0.61
1:E:179:LEU:CD2	1:E:234:TRP:HB3	2.30	0.61
1:G:80:ILE:HG22	1:G:80:ILE:O	2.01	0.61
1:E:117:HIS:CD2	1:I:125(B):SER:HB3	2.35	0.61
1:Q:127:TRP:CE3	1:Q:127:TRP:HA	2.35	0.61
1:G:11:ASP:HB2	2:H:140:PHE:HD1	1.66	0.61
1:M:171:THR:H	1:M:172:ASN:HD22	1.49	0.61
1:O:172:ASN:HD22	1:O:172:ASN:H	1.49	0.61
2:R:145:ASP:O	2:R:148:CYS:HB3	2.00	0.61
1:E:27:THR:CG2	1:E:31:MET:H	2.12	0.60
2:N:164:GLU:HA	2:N:167:ARG:HB2	1.83	0.60
1:O:127:TRP:CZ3	1:O:154:LEU:HD11	2.36	0.60
1:E:320:LEU:HB3	2:F:111:HIS:CD2	2.34	0.60
1:G:179:LEU:CD2	1:G:234:TRP:HB3	2.31	0.60
2:J:167:ARG:HD3	2:L:174:SER:HA	1.83	0.60
1:C:79:PHE:O	1:C:80:ILE:CD1	2.49	0.60
1:M:123:ILE:HD13	1:M:257:ALA:HB3	1.83	0.60
1:Q:53:ASP:HB2	1:Q:276:ASN:ND2	2.16	0.60
1:E:141:TYR:CE2	1:E:142:GLN:NE2	2.18	0.60
1:G:124:ILE:CG1	1:G:254:PRO:O	2.49	0.60
1:K:72:GLY:O	1:K:148:PHE:HA	2.02	0.60
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.83	0.60
1:M:283:THR:HG22	1:M:284:PRO:CD	2.31	0.60
1:E:282:GLN:NE2	1:E:283:THR:H	1.98	0.60
1:G:79:PHE:O	1:G:79:PHE:HD1	1.79	0.60
1:K:182:ILE:HD11	1:K:213:LEU:CD1	2.30	0.60
2:P:65:ALA:C	2:P:66:VAL:HG13	2.22	0.60
1:A:230:MET:SD	1:A:252:ILE:HD11	2.42	0.60
1:G:181:GLY:C	1:G:182:ILE:HD13	2.22	0.60
1:I:124:ILE:CD1	1:I:254:PRO:O	2.49	0.60
2:N:37:ASP:C	2:N:39:GLU:H	2.04	0.60
1:O:172:ASN:N	1:O:172:ASN:HD22	1.99	0.60
1:O:177:LEU:HD23	1:O:258:TYR:CD1	2.36	0.60
1:C:275:GLY:O	1:C:277:CYS:CB	2.48	0.60
1:A:310:LYS:HD3	2:F:61:THR:OG1	2.01	0.60
1:G:121:ILE:HG13	1:G:259:LYS:HE3	1.84	0.60
1:G:141:TYR:CD2	1:G:142:GLN:HG3	2.36	0.60
1:G:124:ILE:CD1	1:G:254:PRO:O	2.50	0.60
1:O:283:THR:HB	1:O:286:GLY:O	2.02	0.60
1:E:206:THR:HG22	1:E:208:THR:H	1.67	0.60
2:P:59:MET:C	2:P:61:THR:N	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:262:LYS:HG3	1:Q:262:LYS:O	2.02	0.60
1:G:59:LEU:HD11	1:G:80:ILE:CG2	2.32	0.60
1:M:152:VAL:HG23	1:M:255:GLU:HG3	1.82	0.60
2:D:81:ASN:HD22	2:F:80:LEU:HD13	1.66	0.59
2:R:164:GLU:HA	2:R:167:ARG:HD2	1.83	0.59
1:E:141:TYR:CD2	1:E:142:GLN:HG3	2.37	0.59
1:E:179:LEU:HD23	1:E:234:TRP:CB	2.32	0.59
1:G:307:LYS:NZ	2:H:62:GLN:HB3	2.17	0.59
1:M:15:ILE:HD12	1:M:15:ILE:H	1.68	0.59
1:M:172:ASN:N	1:M:172:ASN:ND2	2.49	0.59
1:G:27:THR:HG22	1:G:32:GLU:H	1.66	0.59
1:O:218:ALA:HB3	1:O:220:ARG:HH21	1.66	0.59
1:E:159:SER:O	1:E:196:GLN:HG3	2.02	0.59
1:G:13:ILE:HD12	2:H:152:VAL:HG11	1.84	0.59
1:Q:80:ILE:C	1:Q:82:VAL:H	2.06	0.59
1:A:124:ILE:CD1	1:A:254:PRO:HG2	2.31	0.59
1:Q:260:ILE:HG22	1:Q:260:ILE:O	2.02	0.59
1:E:182:ILE:HD11	1:E:213:LEU:CD1	2.26	0.59
1:M:123:ILE:HG22	1:M:255:GLU:C	2.23	0.59
1:O:222:LYS:HD2	1:O:222:LYS:N	2.18	0.59
2:D:61:THR:OG1	1:E:310:LYS:HD3	2.02	0.59
1:K:206:THR:HB	1:K:209:LEU:H	1.66	0.59
1:M:313:ARG:HD2	1:M:315:VAL:CG2	2.33	0.59
1:O:184:HIS:HB2	1:O:220:ARG:HH12	1.67	0.59
1:O:222:LYS:HA	1:O:226:GLN:O	2.03	0.59
1:O:295:HIS:HD2	1:O:297:ILE:N	2.00	0.59
2:P:120:ASP:OD1	2:P:123:ARG:NH1	2.36	0.59
2:N:159:TYR:N	2:N:160:PRO:HD2	2.18	0.59
1:M:101:ASP:HB3	1:M:231:GLU:HG3	1.84	0.59
2:R:93:THR:HG22	2:R:93:THR:O	2.03	0.59
1:I:124:ILE:HD13	1:I:254:PRO:HG2	1.84	0.59
1:Q:320:LEU:HA	2:R:108:LEU:HD23	1.85	0.59
2:D:62:GLN:N	2:D:62:GLN:CD	2.53	0.58
1:O:124:ILE:HD11	1:O:254:PRO:HG2	1.84	0.58
2:P:9:PHE:HD1	2:P:10:ILE:HG13	1.67	0.58
2:B:61:THR:OG1	1:C:310:LYS:HD3	2.04	0.58
1:M:161:TYR:CZ	1:M:249:GLY:HA2	2.39	0.58
1:Q:53:ASP:HB2	1:Q:276:ASN:HD22	1.68	0.58
2:D:63:PHE:HE1	2:F:90:ASP:OD1	1.87	0.58
1:G:310:LYS:HD3	2:L:61:THR:OG1	2.02	0.58
1:M:27:THR:HG22	1:M:31:MET:N	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:ILE:HD11	2:P:122:VAL:HG21	1.84	0.58
1:Q:282:GLN:H	1:Q:302:ILE:HG22	1.67	0.58
1:E:18:HIS:CB	2:F:21:TRP:HA	2.33	0.58
1:G:275:GLY:O	1:G:277:CYS:CB	2.49	0.58
1:I:179:LEU:CD2	1:I:234:TRP:HB3	2.32	0.58
1:C:266:THR:HG21	2:D:67:GLY:H	1.68	0.58
2:B:2:LEU:HB2	2:B:109:ASP:OD2	2.04	0.58
1:K:206:THR:HG23	1:K:241:ASP:OD2	2.04	0.58
1:M:27:THR:CG2	1:M:31:MET:H	2.11	0.58
1:A:126:SER:CB	1:A:166:ARG:HH22	2.16	0.58
2:D:59:MET:O	2:D:61:THR:O	2.22	0.58
1:A:87:ILE:HD12	1:A:113:SER:HA	1.85	0.58
2:P:24:TYR:CE1	2:P:153:ARG:HB3	2.39	0.58
1:Q:296:ASN:HB3	1:Q:309:VAL:O	2.03	0.58
2:F:62:GLN:N	2:F:62:GLN:CD	2.58	0.58
1:K:74:PRO:HB3	1:K:141:TYR:HD1	1.69	0.58
1:M:169:ASN:HB3	1:M:171:THR:HG23	1.86	0.58
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.65	0.58
2:P:150:GLU:HA	2:P:153:ARG:CZ	2.33	0.58
1:Q:200:THR:HG21	1:Q:250:ASN:HB2	1.85	0.58
1:E:13:ILE:HD13	2:F:152:VAL:HG11	1.80	0.57
1:K:124:ILE:CG1	1:K:254:PRO:O	2.52	0.57
1:C:124:ILE:HD13	1:C:254:PRO:HG2	1.86	0.57
1:E:81:ASN:HB2	1:I:144:LYS:NZ	2.19	0.57
2:L:2:LEU:HB2	2:L:109:ASP:OD2	2.04	0.57
1:G:11:ASP:O	2:H:140:PHE:N	2.30	0.57
1:M:114:ARG:HH11	1:M:265:SER:CB	2.17	0.57
1:M:293:PRO:HG2	1:M:294:PHE:CD1	2.39	0.57
1:A:141:TYR:CD2	1:A:142:GLN:HG3	2.39	0.57
1:G:75:MET:HB2	1:G:95:ASN:HD21	1.64	0.57
1:O:178:VAL:O	1:O:234:TRP:HA	2.04	0.57
2:P:128:ASP:CB	2:P:170:ARG:HH12	2.16	0.57
1:Q:74:PRO:HG3	1:Q:139:CYS:HB3	1.86	0.57
2:R:87:GLY:O	2:R:91:VAL:HG23	2.04	0.57
1:E:74:PRO:HB3	1:E:141:TYR:HD1	1.68	0.57
1:E:206:THR:CG2	1:E:207:SER:H	2.18	0.57
1:K:266:THR:HG21	2:L:67:GLY:H	1.69	0.57
1:M:125:PRO:HB2	1:M:126:SER:OG	2.05	0.57
1:Q:11:ASP:H	2:R:140:PHE:HB2	1.69	0.57
1:A:27:THR:CG2	1:A:31:MET:H	2.16	0.57
1:C:146:SER:OG	1:C:147:PHE:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:TYR:HE1	1:C:246:GLU:HG2	1.69	0.57
1:E:141:TYR:CE2	1:E:142:GLN:HG3	2.40	0.57
1:O:141:TYR:HB2	1:O:146:SER:CB	2.27	0.57
1:K:316:LEU:HD23	2:L:52:VAL:HG22	1.86	0.57
1:G:206:THR:CG2	1:G:207:SER:H	2.17	0.57
1:G:42:ILE:O	1:G:292:MET:HB3	2.05	0.57
1:O:124:ILE:HG21	1:O:166:ARG:HE	1.70	0.57
1:G:179:LEU:HD23	1:G:234:TRP:CB	2.33	0.57
1:K:27:THR:CG2	1:K:31:MET:H	2.13	0.57
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.05	0.57
1:E:59:LEU:HD11	1:E:80:ILE:CG2	2.35	0.57
1:M:320:LEU:H	1:M:320:LEU:HD23	1.69	0.57
2:P:38:LYS:CD	2:P:38:LYS:NZ	2.68	0.57
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.87	0.57
1:C:126:SER:CB	1:C:166:ARG:HH22	2.18	0.56
1:M:90:LYS:O	1:M:269:LYS:HD3	2.04	0.56
1:O:87:ILE:HD11	1:O:112:LEU:O	2.04	0.56
2:D:2:LEU:HB2	2:D:109:ASP:OD2	2.05	0.56
2:B:68:ARG:HG3	2:B:68:ARG:O	2.05	0.56
2:J:2:LEU:HB2	2:J:109:ASP:OD2	2.05	0.56
2:L:59:MET:O	2:L:61:THR:O	2.22	0.56
1:M:144:LYS:HD2	1:M:145:SER:OG	2.05	0.56
2:N:109:ASP:HA	2:N:112:ASP:HB2	1.87	0.56
2:P:79:ASN:ND2	2:P:83:LYS:HE2	2.20	0.56
2:L:151:SER:HA	2:L:154:ASN:HB2	1.88	0.56
1:M:59:LEU:HD11	1:M:80:ILE:HG21	1.86	0.56
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.45	0.56
1:A:186:ASN:HB3	1:A:190:GLU:OE2	2.06	0.56
2:F:59:MET:C	2:F:61:THR:N	2.59	0.56
2:H:151:SER:HA	2:H:154:ASN:HB2	1.88	0.56
2:N:38:LYS:CD	2:N:38:LYS:NZ	2.69	0.56
1:O:87:ILE:HD12	1:O:113:SER:HA	1.86	0.56
1:O:266:THR:HG21	2:P:67:GLY:H	1.70	0.56
1:Q:13:ILE:HD13	2:R:152:VAL:HG11	1.87	0.56
2:R:63:PHE:N	2:R:63:PHE:CD1	2.73	0.56
1:C:186:ASN:HB3	1:C:190:GLU:OE2	2.06	0.56
1:O:151:VAL:HG23	1:O:254:PRO:HA	1.88	0.56
1:E:121:ILE:HG13	1:E:259:LYS:HE3	1.86	0.56
1:G:182:ILE:HD11	1:G:213:LEU:CD1	2.27	0.56
1:I:282:GLN:NE2	1:I:283:THR:H	2.02	0.56
1:M:266:THR:CG2	1:M:302:ILE:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:291:SER:HB2	1:O:292:MET:CE	2.35	0.56
1:Q:251:PHE:CE2	1:Q:253:ALA:HB2	2.40	0.56
1:A:124:ILE:CD1	1:A:254:PRO:O	2.54	0.56
1:E:27:THR:HG22	1:E:32:GLU:H	1.71	0.56
1:I:121:ILE:HG13	1:I:259:LYS:HE3	1.87	0.56
1:K:282:GLN:NE2	1:K:283:THR:H	2.04	0.56
1:G:141:TYR:CE2	1:G:142:GLN:HG3	2.41	0.56
1:I:126:SER:CB	1:I:166:ARG:HH22	2.18	0.56
1:I:141:TYR:CE2	1:I:142:GLN:NE2	2.21	0.56
1:I:75:MET:HB2	1:I:95:ASN:HD21	1.68	0.56
1:K:75:MET:HB2	1:K:95:ASN:HD21	1.68	0.56
2:B:79:ASN:HD21	2:F:66:VAL:HG21	1.70	0.56
1:K:307:LYS:HG3	2:L:59:MET:SD	2.46	0.56
1:O:307:LYS:HD2	2:P:92:TRP:CZ2	2.41	0.56
1:Q:155:ILE:HG12	1:Q:194:LEU:HD22	1.88	0.56
1:C:170:ASN:O	1:C:239:PRO:O	2.24	0.55
1:E:14:CYS:O	2:F:24:TYR:HA	2.06	0.55
1:G:207:SER:HA	1:I:229:ARG:HH21	1.72	0.55
2:H:59:MET:O	2:H:61:THR:O	2.23	0.55
1:K:275:GLY:O	1:K:277:CYS:CB	2.50	0.55
1:M:212:ARG:O	1:M:213:LEU:HD23	2.06	0.55
1:O:204:VAL:HG12	1:O:205:GLY:N	2.21	0.55
1:C:295:HIS:HD2	1:C:297:ILE:H	1.52	0.55
2:D:65:ALA:C	2:D:66:VAL:HG13	2.26	0.55
1:E:124:ILE:CD1	1:E:254:PRO:HG2	2.36	0.55
1:E:79:PHE:HD1	1:E:79:PHE:O	1.81	0.55
1:E:80:ILE:HG22	1:E:80:ILE:O	2.06	0.55
1:G:282:GLN:NE2	1:G:283:THR:H	2.04	0.55
1:I:141:TYR:CE2	1:I:142:GLN:HG3	2.41	0.55
1:I:206:THR:HG23	1:I:241:ASP:OD2	2.07	0.55
2:L:59:MET:O	2:L:61:THR:C	2.45	0.55
1:Q:98:TYR:CD2	1:Q:230:MET:HB2	2.41	0.55
1:A:80:ILE:C	1:A:82:VAL:H	2.10	0.55
1:C:121:ILE:HG22	1:C:123:ILE:HD13	1.86	0.55
1:G:27:THR:CG2	1:G:31:MET:H	2.16	0.55
2:J:66:VAL:HG21	2:L:79:ASN:HD21	1.71	0.55
1:E:272:LEU:HD21	1:M:171:THR:CB	2.37	0.55
1:M:19:ALA:HB1	1:M:322:ASN:ND2	2.21	0.55
1:G:120:LYS:HG3	1:G:258:TYR:CE2	2.42	0.55
1:I:206:THR:CG2	1:I:207:SER:H	2.18	0.55
1:K:124:ILE:CD1	1:K:254:PRO:HG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ILE:HG13	1:C:259:LYS:HE3	1.88	0.55
1:G:106:GLU:OE2	2:H:71:ASN:HB3	2.07	0.55
1:G:126:SER:CB	1:G:166:ARG:HH22	2.19	0.55
2:H:80:LEU:HD13	2:L:81:ASN:HD22	1.71	0.55
1:Q:293:PRO:HB2	1:Q:294:PHE:CD1	2.42	0.55
2:B:59:MET:C	2:B:61:THR:H	2.10	0.55
1:K:295:HIS:HD2	1:K:297:ILE:H	1.53	0.55
1:O:141:TYR:CB	1:O:146:SER:HB3	2.31	0.55
2:P:23:GLY:HA2	2:P:36:ALA:HA	1.89	0.55
1:Q:127:TRP:HE3	1:Q:127:TRP:HA	1.72	0.55
2:R:127:ARG:NH1	2:R:159:TYR:OH	2.40	0.55
2:B:80:LEU:HD13	2:F:81:ASN:HD22	1.71	0.55
1:M:283:THR:CG2	1:M:298:HIS:HB3	2.37	0.55
1:A:11:ASP:OD1	2:B:28:ASN:HA	2.07	0.55
1:E:124:ILE:CG1	1:E:254:PRO:O	2.55	0.55
2:F:68:ARG:O	2:F:68:ARG:HG3	2.06	0.55
1:G:79:PHE:O	1:G:80:ILE:CD1	2.55	0.55
1:A:141:TYR:CE2	1:A:142:GLN:HG3	2.42	0.54
1:E:15:ILE:HG23	2:F:118:LEU:HD23	1.90	0.54
1:I:74:PRO:HB3	1:I:141:TYR:HD1	1.71	0.54
1:O:125(B):SER:OG	1:O:125(B):SER:CA	2.53	0.54
2:R:14:TRP:HB3	2:R:34:TYR:HE2	1.72	0.54
2:R:94:TYR:O	2:R:98:LEU:HB2	2.07	0.54
1:G:141:TYR:CE2	1:G:142:GLN:NE2	2.20	0.54
1:G:123:ILE:HD11	1:G:168:TYR:CZ	2.42	0.54
1:G:320:LEU:HB3	2:H:111:HIS:CD2	2.43	0.54
1:O:71:LEU:H	1:O:71:LEU:HD23	1.72	0.54
1:I:216:ARG:O	1:I:220:ARG:NH2	2.41	0.54
1:I:27:THR:HG22	1:I:32:GLU:N	2.22	0.54
1:I:79:PHE:HD1	1:I:79:PHE:O	1.84	0.54
2:J:59:MET:O	2:J:61:THR:O	2.25	0.54
1:I:106:GLU:OE2	2:J:71:ASN:HB3	2.08	0.54
2:N:159:TYR:OH	2:N:167:ARG:NH2	2.40	0.54
1:K:179:LEU:CD2	1:K:234:TRP:HB3	2.35	0.54
1:O:206:THR:HG22	1:O:241:ASP:OD2	2.07	0.54
1:Q:55:GLY:HA2	4:X:3:BMA:H62	1.88	0.54
1:C:27:THR:HG22	1:C:32:GLU:N	2.23	0.54
1:O:211:GLN:HE22	1:O:213:LEU:HD11	1.72	0.54
2:P:9:PHE:CD1	2:P:10:ILE:HG13	2.42	0.54
2:R:52:VAL:HA	2:R:55:ILE:HD12	1.89	0.54
1:O:135:VAL:CG2	1:O:146:SER:HA	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:25:VAL:HG13	1:Q:26:ASP:N	2.23	0.54
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.07	0.54
1:E:307:LYS:HZ3	2:F:62:GLN:HB3	1.70	0.54
1:K:124:ILE:CD1	1:K:254:PRO:O	2.55	0.54
1:Q:109:LYS:HE3	1:Q:267:ILE:HG12	1.90	0.54
2:R:165:GLU:O	2:R:169:LYS:CB	2.49	0.54
1:A:124:ILE:HG12	1:A:254:PRO:O	2.07	0.54
2:N:141:TYR:HB3	2:N:169:LYS:HG2	1.88	0.54
1:G:80:ILE:C	1:G:82:VAL:H	2.12	0.54
1:M:320:LEU:N	1:M:320:LEU:HD23	2.22	0.54
1:O:125(B):SER:OG	1:O:125(B):SER:N	2.40	0.54
1:O:209:LEU:HD12	1:O:211:GLN:HB3	1.90	0.54
1:O:238:LYS:HG3	1:O:239:PRO:CD	2.36	0.54
2:P:29:GLU:CD	2:P:29:GLU:H	2.11	0.54
2:B:151:SER:HA	2:B:154:ASN:HB2	1.90	0.54
1:E:42:ILE:O	1:E:292:MET:HB3	2.07	0.54
1:G:124:ILE:HD13	1:G:254:PRO:HG2	1.89	0.54
1:M:267:ILE:HD12	1:M:267:ILE:N	2.20	0.54
1:Q:121:ILE:HD11	1:Q:259:LYS:HE3	1.90	0.54
2:B:59:MET:O	2:B:61:THR:C	2.46	0.53
1:C:307:LYS:HZ1	2:D:62:GLN:HB3	1.71	0.53
1:E:124:ILE:CD1	1:E:254:PRO:O	2.56	0.53
2:F:151:SER:HA	2:F:154:ASN:HB2	1.89	0.53
1:I:78:GLU:O	1:I:80:ILE:N	2.40	0.53
2:J:62:GLN:N	2:J:62:GLN:CD	2.61	0.53
1:M:295:HIS:CE1	1:M:308:TYR:HB2	2.43	0.53
1:M:37:THR:HB	1:M:320:LEU:N	2.21	0.53
1:E:206:THR:HB	1:E:209:LEU:HB3	1.90	0.53
2:J:61:THR:OG1	1:K:310:LYS:HD3	2.07	0.53
2:P:52:VAL:O	2:P:55:ILE:HG22	2.08	0.53
1:Q:320:LEU:HD12	2:R:6:ILE:CG2	2.38	0.53
1:C:59:LEU:HD11	1:C:80:ILE:CG2	2.36	0.53
2:F:2:LEU:HB2	2:F:109:ASP:OD2	2.07	0.53
1:M:141:TYR:HB3	1:M:146:SER:HB2	1.90	0.53
1:M:220:ARG:O	1:M:222:LYS:NZ	2.32	0.53
1:O:53(A):LEU:HD11	1:O:302:ILE:CG2	2.35	0.53
1:Q:90:LYS:O	1:Q:92:ASN:N	2.42	0.53
2:R:100:VAL:O	2:R:104:ASN:HB2	2.09	0.53
1:A:106:GLU:OE2	2:B:71:ASN:HB3	2.08	0.53
1:C:282:GLN:NE2	1:C:283:THR:H	2.06	0.53
1:G:182:ILE:N	1:G:182:ILE:HD13	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:LEU:HD11	1:I:80:ILE:CG2	2.36	0.53
1:A:146:SER:OG	1:A:147:PHE:N	2.41	0.53
1:A:42:ILE:O	1:A:292:MET:HB3	2.08	0.53
2:D:151:SER:HA	2:D:154:ASN:HB2	1.90	0.53
1:E:164:ILE:O	1:E:246:GLU:HA	2.07	0.53
1:E:79:PHE:O	1:E:80:ILE:CD1	2.56	0.53
1:G:181:GLY:O	1:G:182:ILE:HD13	2.08	0.53
1:I:309:VAL:HG22	2:J:93:THR:HA	1.91	0.53
2:P:153:ARG:O	2:P:155:GLY:N	2.41	0.53
1:A:121:ILE:HG13	1:A:259:LYS:HE3	1.89	0.53
1:C:75:MET:CB	1:C:95:ASN:ND2	2.61	0.53
1:G:279:THR:HB	1:G:281:CYS:H	1.74	0.53
2:H:117:ASN:HD21	2:J:4:GLY:N	2.05	0.53
1:G:18:HIS:HB2	2:H:21:TRP:HA	1.91	0.53
1:M:191:GLN:HE21	1:M:195:TYR:HB2	1.74	0.53
1:M:152:VAL:CG2	1:M:255:GLU:HG3	2.39	0.53
1:O:18:HIS:HB2	2:P:21:TRP:HA	1.90	0.53
1:Q:190:GLU:HA	1:Q:193:LYS:HB2	1.90	0.53
1:G:124:ILE:O	1:G:124:ILE:CG1	2.56	0.53
1:M:312:ASN:ND2	1:M:312:ASN:N	2.57	0.53
1:Q:260:ILE:CG2	1:Q:260:ILE:O	2.57	0.53
1:Q:78:GLU:O	1:Q:78:GLU:HG2	2.09	0.53
1:G:146:SER:OG	1:G:147:PHE:N	2.41	0.53
1:K:206:THR:CG2	1:K:207:SER:H	2.21	0.53
1:A:59:LEU:HD11	1:A:80:ILE:CG2	2.37	0.53
2:B:59:MET:C	2:B:61:THR:N	2.60	0.53
2:H:65:ALA:C	2:H:66:VAL:CG1	2.76	0.53
1:K:283:THR:HG22	1:K:285:MET:N	2.18	0.53
1:Q:22:THR:HG21	1:Q:324:PRO:HD3	1.89	0.53
1:A:279:THR:HB	1:A:281:CYS:H	1.73	0.53
1:C:201:TYR:CE2	1:C:248:ASN:HB2	2.44	0.53
1:C:74:PRO:HB3	1:C:141:TYR:HD1	1.73	0.53
2:J:151:SER:HA	2:J:154:ASN:HB2	1.91	0.53
2:H:79:ASN:HD21	2:L:66:VAL:HG21	1.74	0.53
1:M:156:LYS:O	1:M:156:LYS:HD2	2.09	0.53
1:M:182:ILE:HD11	1:M:202:ILE:HD13	1.90	0.53
1:O:200:THR:HG21	1:O:250:ASN:CB	2.39	0.53
1:O:309:VAL:HG22	2:P:93:THR:HA	1.91	0.53
2:J:59:MET:C	2:J:61:THR:N	2.63	0.52
1:O:57:LYS:HD2	1:O:57:LYS:H	1.73	0.52
2:R:144:CYS:SG	2:R:149:MET:HG3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:63:PHE:N	2:R:63:PHE:HD1	2.07	0.52
1:A:206:THR:CG2	1:A:207:SER:H	2.22	0.52
1:E:216:ARG:O	1:E:220:ARG:NH2	2.42	0.52
1:M:156:LYS:HB3	1:M:161:TYR:HB2	1.90	0.52
1:O:157:LYS:CD	1:O:157:LYS:HB3	2.37	0.52
1:Q:16:GLY:CA	2:R:14:TRP:CD1	2.88	0.52
2:B:47:GLY:O	1:C:31:MET:HG2	2.09	0.52
2:L:68:ARG:HG3	2:L:68:ARG:O	2.08	0.52
2:F:59:MET:O	2:F:61:THR:C	2.48	0.52
1:I:279:THR:HB	1:I:281:CYS:H	1.73	0.52
1:O:151:VAL:HG22	1:O:252:ILE:HG22	1.90	0.52
2:D:59:MET:O	2:D:61:THR:C	2.48	0.52
1:E:13:ILE:HD11	2:F:149:MET:HG2	1.91	0.52
1:I:42:ILE:O	1:I:292:MET:HB3	2.10	0.52
2:N:68:ARG:O	2:N:68:ARG:HG3	2.09	0.52
1:O:74:PRO:HG2	1:O:139:CYS:HB3	1.92	0.52
1:Q:44:GLU:OE1	1:Q:292:MET:HB2	2.09	0.52
2:B:59:MET:O	2:B:61:THR:O	2.26	0.52
1:E:11:ASP:OD2	2:F:143:LYS:CA	2.48	0.52
2:H:51:LYS:HA	1:I:28:ILE:O	2.09	0.52
2:J:59:MET:C	2:J:61:THR:H	2.13	0.52
1:K:58:PRO:HB3	1:K:86:TYR:CZ	2.44	0.52
2:B:65:ALA:C	2:B:66:VAL:HG13	2.30	0.52
1:I:298:HIS:ND1	1:I:299:PRO:HD2	2.25	0.52
1:C:80:ILE:CG2	1:C:80:ILE:O	2.58	0.52
1:G:13:ILE:HD11	2:H:149:MET:HG2	1.91	0.52
2:J:81:ASN:HD22	2:L:80:LEU:HD13	1.75	0.52
1:C:10:GLY:HA3	2:D:139:GLU:OE2	2.09	0.52
2:D:66:VAL:HG21	2:F:79:ASN:HD21	1.74	0.52
1:K:201:TYR:HE1	1:K:246:GLU:HG2	1.75	0.52
1:M:297:ILE:O	1:M:298:HIS:HB2	2.10	0.52
1:A:170:ASN:O	1:A:239:PRO:O	2.28	0.52
1:E:122:GLN:OE1	1:I:77:ASP:HB2	2.09	0.52
1:G:74:PRO:HB3	1:G:141:TYR:HD1	1.75	0.52
1:O:228:GLY:O	1:O:229:ARG:NH1	2.42	0.52
1:O:220:ARG:HG2	1:O:229:ARG:NH2	2.25	0.52
2:H:2:LEU:HB2	2:H:109:ASP:OD2	2.10	0.51
1:I:170:ASN:O	1:I:239:PRO:O	2.28	0.51
1:K:115:ILE:HG21	1:K:118:PHE:HB2	1.92	0.51
1:M:176:LEU:HD23	1:M:237:LEU:HD23	1.91	0.51
2:P:149:MET:HA	2:P:152:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:PHE:HE1	2:D:90:ASP:OD1	1.93	0.51
1:E:279:THR:CG2	1:E:287:ALA:HB1	2.38	0.51
1:I:283:THR:HG22	1:I:285:MET:N	2.18	0.51
1:K:42:ILE:O	1:K:292:MET:HB3	2.10	0.51
2:N:24:TYR:CE1	2:N:153:ARG:HG2	2.45	0.51
1:O:123:ILE:HG23	1:O:124:ILE:HG12	1.91	0.51
1:Q:22:THR:HG22	1:Q:324:PRO:HD3	1.90	0.51
2:R:42:GLN:HA	2:R:45:ILE:HD12	1.92	0.51
1:C:42:ILE:O	1:C:292:MET:HB3	2.10	0.51
1:M:295:HIS:HD2	1:M:297:ILE:HG12	1.75	0.51
1:M:321:ARG:HH11	1:M:321:ARG:HB3	1.75	0.51
1:A:200:THR:HG22	1:A:215:PRO:CD	2.40	0.51
1:I:164:ILE:O	1:I:246:GLU:HA	2.10	0.51
1:I:72:GLY:HA3	1:I:149:ARG:HB2	1.91	0.51
1:K:179:LEU:HD23	1:K:234:TRP:CB	2.36	0.51
2:P:82:LYS:O	2:P:83:LYS:C	2.49	0.51
1:Q:123:ILE:HG12	1:Q:257:ALA:HB3	1.92	0.51
1:A:164:ILE:O	1:A:246:GLU:HA	2.11	0.51
1:A:27:THR:HG22	1:A:32:GLU:N	2.24	0.51
1:C:279:THR:HB	1:C:281:CYS:H	1.75	0.51
1:M:200:THR:HG21	1:M:250:ASN:HB2	1.93	0.51
1:O:200:THR:HG21	1:O:250:ASN:OD1	2.10	0.51
1:Q:91:ALA:HA	1:Q:269:LYS:HD2	1.93	0.51
1:E:122:GLN:HE22	1:I:77:ASP:CB	2.24	0.51
1:E:279:THR:HB	1:E:281:CYS:H	1.75	0.51
1:E:80:ILE:C	1:E:82:VAL:H	2.13	0.51
1:I:10:GLY:HA3	2:J:139:GLU:OE2	2.10	0.51
2:L:59:MET:C	2:L:61:THR:N	2.64	0.51
1:M:192:THR:HG23	1:M:196:GLN:HA	1.92	0.51
1:M:70:LEU:HD13	1:M:179:LEU:HD11	1.92	0.51
1:G:72:GLY:HA3	1:G:149:ARG:HB2	1.92	0.51
2:H:68:ARG:HH11	2:H:68:ARG:HB2	1.76	0.51
1:M:156:LYS:HG2	1:M:196:GLN:HG2	1.93	0.51
2:N:27:SER:HA	2:N:32:SER:HB3	1.92	0.51
1:Q:182:ILE:HD11	1:Q:202:ILE:HG21	1.93	0.51
1:Q:225:GLY:O	1:Q:226:GLN:CB	2.57	0.51
2:F:59:MET:C	2:F:61:THR:H	2.14	0.51
2:J:68:ARG:HG3	2:J:68:ARG:O	2.10	0.51
1:K:80:ILE:O	1:K:80:ILE:CG2	2.58	0.51
1:O:52:CYS:HA	1:O:277:CYS:HB3	1.93	0.51
2:F:65:ALA:C	2:F:66:VAL:CG1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:ILE:HG12	1:I:254:PRO:O	2.09	0.51
1:E:81:ASN:H	1:I:144:LYS:HZ2	1.57	0.51
1:Q:182:ILE:HD11	1:Q:202:ILE:HG12	1.92	0.51
2:H:59:MET:C	2:H:61:THR:N	2.64	0.51
1:M:16:GLY:HA3	2:N:14:TRP:NE1	2.26	0.51
1:A:238:LYS:HG3	1:A:239:PRO:HD2	1.92	0.50
1:C:238:LYS:HG3	1:C:239:PRO:HD2	1.93	0.50
1:E:124:ILE:CG1	1:E:124:ILE:O	2.58	0.50
1:G:295:HIS:HD2	1:G:297:ILE:H	1.58	0.50
1:I:49:GLY:HA2	1:I:285:MET:O	2.11	0.50
1:K:87:ILE:HD12	1:K:113:SER:HA	1.92	0.50
1:M:182:ILE:HD12	1:M:202:ILE:HD13	1.93	0.50
1:M:283:THR:CG2	1:M:284:PRO:HD2	2.40	0.50
3:U:1:NAG:C7	3:U:1:NAG:O3	2.60	0.50
1:A:79:PHE:O	1:A:80:ILE:CD1	2.59	0.50
1:C:216:ARG:O	1:C:220:ARG:NH2	2.44	0.50
1:E:238:LYS:HG3	1:E:239:PRO:HD2	1.93	0.50
2:F:59:MET:O	2:F:61:THR:O	2.29	0.50
1:K:238:LYS:HG3	1:K:239:PRO:HD2	1.93	0.50
2:L:65:ALA:C	2:L:66:VAL:HG13	2.32	0.50
2:N:158:ASP:OD1	2:N:161:GLN:HG3	2.11	0.50
1:O:156:LYS:NZ	1:O:156:LYS:CD	2.69	0.50
1:O:291:SER:HB2	1:O:292:MET:HE3	1.93	0.50
2:P:150:GLU:HA	2:P:153:ARG:NH1	2.26	0.50
2:R:47:GLY:O	2:R:51:LYS:HB3	2.11	0.50
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.46	0.50
1:C:276:ASN:O	1:C:277:CYS:HB2	2.11	0.50
1:E:283:THR:HG22	1:E:285:MET:N	2.19	0.50
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.46	0.50
1:G:124:ILE:HG12	1:G:254:PRO:O	2.11	0.50
1:E:11:ASP:H	2:F:140:PHE:HB2	1.76	0.50
1:E:298:HIS:ND1	1:E:299:PRO:HD2	2.26	0.50
2:F:125:GLN:HG2	2:F:157:TYR:HB3	1.94	0.50
1:G:45:LYS:HE2	1:G:312:ASN:O	2.12	0.50
1:I:179:LEU:HD23	1:I:234:TRP:CB	2.38	0.50
1:O:291:SER:CB	1:O:292:MET:HE2	2.42	0.50
1:O:74:PRO:HB3	1:O:141:TYR:HA	1.94	0.50
1:Q:92:ASN:O	1:Q:92:ASN:ND2	2.45	0.50
1:G:216:ARG:HG2	1:K:212:ARG:HB2	1.92	0.50
2:H:59:MET:O	2:H:61:THR:C	2.49	0.50
1:I:282:GLN:HG3	1:I:283:THR:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:MET:O	2:J:61:THR:C	2.50	0.50
1:O:226:GLN:HE22	1:O:228:GLY:H	1.59	0.50
1:O:292:MET:HB3	1:O:293:PRO:CD	2.41	0.50
2:P:34:TYR:N	2:P:34:TYR:CD1	2.79	0.50
1:A:283:THR:HG22	1:A:285:MET:N	2.19	0.50
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.47	0.50
1:E:27:THR:HG22	1:E:31:MET:N	2.19	0.50
2:J:65:ALA:C	2:J:66:VAL:HG13	2.32	0.50
1:O:232:PHE:N	1:O:232:PHE:CD1	2.78	0.50
1:O:320:LEU:HD23	1:O:320:LEU:N	2.27	0.50
2:D:68:ARG:HG3	2:D:68:ARG:O	2.11	0.50
2:J:63:PHE:HE1	2:L:90:ASP:OD1	1.94	0.50
2:N:166:ALA:C	2:N:168:LEU:H	2.13	0.50
1:O:23:GLU:O	1:O:35(A):THR:HA	2.12	0.50
1:A:179:LEU:CD2	1:A:234:TRP:HB3	2.40	0.50
1:E:114:ARG:HH11	1:E:265:SER:HB3	1.77	0.50
2:J:38:LYS:O	2:J:42:GLN:HB2	2.12	0.50
1:K:216:ARG:O	1:K:220:ARG:NH2	2.45	0.50
1:O:189:ALA:O	1:O:193:LYS:N	2.36	0.50
1:C:283:THR:HG22	1:C:285:MET:N	2.22	0.50
1:I:201:TYR:HE1	1:I:246:GLU:HG2	1.76	0.50
1:I:279:THR:CG2	1:I:287:ALA:HB1	2.38	0.50
1:M:179:LEU:O	1:M:254:PRO:HB3	2.12	0.50
2:N:68:ARG:HA	2:N:69:GLU:OE1	2.11	0.50
1:O:195:TYR:CZ	1:O:250:ASN:HA	2.47	0.50
1:O:295:HIS:CD2	1:O:297:ILE:H	2.26	0.50
1:O:52:CYS:SG	1:O:287:ALA:HB2	2.52	0.50
1:O:68:GLY:O	1:O:71:LEU:O	2.29	0.50
2:R:171:GLU:HA	2:R:174:SER:HB3	1.93	0.50
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.48	0.49
1:E:182:ILE:CD1	1:E:202:ILE:HD13	2.24	0.49
2:J:125:GLN:HG2	2:J:157:TYR:HB3	1.94	0.49
1:K:164:ILE:O	1:K:246:GLU:HA	2.12	0.49
1:K:79:PHE:O	1:K:80:ILE:CD1	2.54	0.49
2:R:30:GLN:CA	2:R:30:GLN:HE21	2.17	0.49
1:O:37:THR:OG1	1:O:320:LEU:N	2.45	0.49
2:P:65:ALA:C	2:P:66:VAL:CG1	2.80	0.49
1:A:201:TYR:HE1	1:A:246:GLU:HG2	1.77	0.49
1:E:72:GLY:HA3	1:E:149:ARG:HB2	1.94	0.49
1:E:206:THR:HG23	1:E:241:ASP:OD2	2.13	0.49
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:295:HIS:CD2	1:M:297:ILE:H	2.29	0.49
1:A:307:LYS:HD2	2:B:92:TRP:CE2	2.47	0.49
1:Q:267:ILE:H	1:Q:267:ILE:HD12	1.78	0.49
3:Y:1:NAG:H62	3:Y:2:NAG:HN2	1.78	0.49
1:C:75:MET:HB2	1:C:95:ASN:HD21	1.71	0.49
1:E:45:LYS:HE2	1:E:312:ASN:O	2.12	0.49
1:E:321:ARG:HD2	2:F:6:ILE:HD12	1.94	0.49
1:M:212:ARG:C	1:M:213:LEU:HD23	2.32	0.49
1:O:120:LYS:HE3	1:O:258:TYR:HE2	1.77	0.49
1:O:157:LYS:O	1:O:159:SER:N	2.46	0.49
2:P:150:GLU:O	2:P:154:ASN:HB2	2.12	0.49
1:Q:234:TRP:HZ3	1:Q:236:ILE:HG13	1.78	0.49
1:I:307:LYS:NZ	2:J:62:GLN:HB3	2.28	0.49
1:Q:37:THR:HB	1:Q:319:GLY:HA3	1.95	0.49
1:Q:98:TYR:HD2	1:Q:230:MET:HB2	1.77	0.49
2:R:38:LYS:O	2:R:42:GLN:HG2	2.12	0.49
1:C:307:LYS:HZ3	2:D:62:GLN:HB3	1.76	0.49
2:D:59:MET:C	2:D:61:THR:N	2.66	0.49
1:E:170:ASN:O	1:E:239:PRO:O	2.31	0.49
2:H:68:ARG:NH1	2:H:68:ARG:HB2	2.28	0.49
1:I:27:THR:HG22	1:I:31:MET:N	2.22	0.49
1:M:139:CYS:O	1:M:146:SER:O	2.31	0.49
1:O:94:VAL:HG12	1:O:95:ASN:OD1	2.12	0.49
1:A:201:TYR:CE2	1:A:248:ASN:HB2	2.47	0.49
1:E:201:TYR:CE2	1:E:248:ASN:HB2	2.48	0.49
1:E:200:THR:HG22	1:E:215:PRO:CD	2.42	0.49
1:E:295:HIS:HD2	1:E:297:ILE:H	1.60	0.49
2:H:38:LYS:O	2:H:42:GLN:HB2	2.13	0.49
1:K:121:ILE:HG13	1:K:259:LYS:HE3	1.93	0.49
2:P:19:ASP:HB2	2:P:36:ALA:HB2	1.95	0.49
1:Q:316:LEU:HD12	2:R:104:ASN:OD1	2.13	0.49
1:A:74:PRO:HB3	1:A:141:TYR:HD1	1.77	0.49
1:C:179:LEU:HD23	1:C:234:TRP:CB	2.39	0.49
1:E:238:LYS:O	1:E:239:PRO:C	2.50	0.49
1:G:58:PRO:HB3	1:G:86:TYR:CZ	2.48	0.49
1:K:45:LYS:HE2	1:K:312:ASN:O	2.12	0.49
1:K:307:LYS:HZ1	2:L:62:GLN:HB3	1.77	0.49
1:O:279:THR:OG1	1:O:287:ALA:HB1	2.12	0.49
1:Q:223:VAL:C	1:Q:225:GLY:H	2.15	0.49
1:Q:222:LYS:HG2	1:Q:227:SER:HB2	1.95	0.49
1:A:143:GLY:HA3	1:Q:285:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:53:ASP:HA	1:Q:58:PRO:HD3	1.95	0.49
1:G:238:LYS:HG3	1:G:239:PRO:HD2	1.94	0.49
1:I:201:TYR:CE2	1:I:248:ASN:HB2	2.48	0.49
1:I:45:LYS:HE2	1:I:312:ASN:O	2.13	0.49
1:O:140:PRO:O	1:O:141:TYR:C	2.51	0.49
1:Q:200:THR:HG21	1:Q:250:ASN:N	2.27	0.49
2:B:117:ASN:HD21	2:D:4:GLY:N	2.11	0.48
1:E:79:PHE:O	1:E:80:ILE:CG1	2.61	0.48
1:E:304:GLU:HG2	2:F:63:PHE:HA	1.95	0.48
1:K:298:HIS:ND1	1:K:299:PRO:HD2	2.28	0.48
1:O:123:ILE:HD12	1:O:123:ILE:HA	1.68	0.48
2:P:94:TYR:O	2:P:95:ASN:C	2.50	0.48
1:Q:27:THR:CG2	1:Q:28:ILE:N	2.76	0.48
1:Q:82:VAL:O	1:Q:83:GLU:N	2.33	0.48
1:A:27:THR:HG22	1:A:31:MET:N	2.26	0.48
1:E:122:GLN:OE1	1:E:125:PRO:HB3	2.13	0.48
1:E:275:GLY:O	1:E:277:CYS:CB	2.52	0.48
1:Q:109:LYS:NZ	1:Q:267:ILE:HG21	2.28	0.48
1:A:13:ILE:HD11	2:B:149:MET:HG2	1.95	0.48
2:J:28:ASN:HD22	2:J:28:ASN:H	1.62	0.48
1:M:202:ILE:H	1:M:213:LEU:HB2	1.78	0.48
1:E:75:MET:CB	1:E:95:ASN:HD21	2.24	0.48
2:H:90:ASP:OD1	2:L:63:PHE:HE1	1.95	0.48
1:I:12:GLN:HB2	2:J:27:SER:OG	2.12	0.48
2:L:63:PHE:HD1	2:L:63:PHE:H	1.57	0.48
1:O:164:ILE:O	1:O:246:GLU:HA	2.14	0.48
1:Q:116:ASN:O	1:Q:117:HIS:HB2	2.12	0.48
1:Q:168:TYR:O	1:Q:242:ALA:HA	2.13	0.48
1:Q:200:THR:HA	1:Q:248:ASN:HB3	1.95	0.48
1:A:120:LYS:HG3	1:A:258:TYR:CE2	2.48	0.48
1:C:179:LEU:CD2	1:C:234:TRP:HB3	2.40	0.48
2:D:28:ASN:HD22	2:D:28:ASN:H	1.61	0.48
1:G:87:ILE:HB	1:G:267:ILE:HG13	1.96	0.48
1:I:206:THR:HB	1:I:209:LEU:HB3	1.95	0.48
1:O:169:ASN:HB3	1:O:171:THR:HG23	1.96	0.48
1:G:279:THR:CG2	1:G:287:ALA:HB1	2.42	0.48
1:I:238:LYS:HG3	1:I:239:PRO:HD2	1.96	0.48
1:E:126:SER:CB	1:I:79:PHE:CZ	2.77	0.48
1:M:230:MET:HG2	1:M:232:PHE:CZ	2.49	0.48
2:N:150:GLU:O	2:N:154:ASN:CB	2.51	0.48
2:N:46:ASP:O	2:N:50:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:GLU:HA	1:O:23:GLU:OE2	2.14	0.48
1:A:45:LYS:HE2	1:A:312:ASN:O	2.13	0.48
2:D:63:PHE:HD1	2:D:63:PHE:H	1.60	0.48
2:P:153:ARG:O	2:P:154:ASN:C	2.52	0.48
2:R:14:TRP:HB3	2:R:34:TYR:CE2	2.49	0.48
1:A:143:GLY:O	1:Q:272:LEU:HG	2.14	0.48
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.28	0.48
1:I:58:PRO:HB3	1:I:86:TYR:CZ	2.48	0.48
1:K:124:ILE:CG1	1:K:124:ILE:O	2.62	0.48
1:Q:220:ARG:NH1	1:Q:228:GLY:HA2	2.28	0.48
1:Q:53(A):LEU:HG	1:Q:282:GLN:HB2	1.96	0.48
1:I:123:ILE:HD11	1:I:168:TYR:CZ	2.48	0.48
2:H:81:ASN:HD22	2:J:80:LEU:HD13	1.79	0.48
2:L:62:GLN:N	2:L:62:GLN:CD	2.68	0.48
2:P:150:GLU:C	2:P:154:ASN:HB2	2.34	0.48
2:R:166:ALA:O	2:R:170:ARG:HB2	2.13	0.48
1:A:304:GLU:HG2	2:B:63:PHE:HA	1.95	0.47
2:N:123:ARG:HG3	2:N:138:PHE:HZ	1.78	0.47
2:N:71:ASN:C	2:N:71:ASN:OD1	2.52	0.47
2:P:72:ASN:HB2	2:P:75:ARG:HD2	1.95	0.47
1:A:80:ILE:HG22	1:A:80:ILE:O	2.14	0.47
2:B:28:ASN:H	2:B:28:ASN:HD22	1.62	0.47
2:B:68:ARG:HH11	2:B:68:ARG:HB2	1.78	0.47
1:G:136:SER:O	1:G:145:SER:HB2	2.13	0.47
1:O:206:THR:HB	1:O:208:THR:N	2.24	0.47
1:C:309:VAL:HG22	2:D:93:THR:HA	1.96	0.47
2:B:90:ASP:OD1	2:F:63:PHE:CE1	2.62	0.47
2:H:62:GLN:N	2:H:62:GLN:CD	2.67	0.47
1:K:170:ASN:O	1:K:239:PRO:O	2.32	0.47
1:O:143:GLY:O	1:O:144:LYS:C	2.51	0.47
2:P:2:LEU:HB2	2:P:109:ASP:OD2	2.14	0.47
2:P:9:PHE:HD1	2:P:10:ILE:N	2.12	0.47
1:Q:11:ASP:HB2	2:R:140:PHE:CD1	2.48	0.47
1:Q:247:SER:OG	1:Q:251:PHE:HB2	2.13	0.47
1:Q:75:MET:HE1	1:Q:140:PRO:HD2	1.95	0.47
1:A:307:LYS:HZ1	2:B:62:GLN:HB3	1.80	0.47
1:M:60:ILE:HG23	1:M:88:VAL:HB	1.97	0.47
1:O:201:TYR:CE2	1:O:248:ASN:ND2	2.82	0.47
1:O:316:LEU:HD13	2:P:100:VAL:HG22	1.97	0.47
1:Q:292:MET:HB3	1:Q:293:PRO:HD2	1.96	0.47
2:R:169:LYS:HG3	2:R:169:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:24:TYR:CE2	2:R:153:ARG:HG2	2.50	0.47
1:E:181:GLY:C	1:E:182:ILE:HD13	2.35	0.47
2:H:125:GLN:HG2	2:H:157:TYR:HB3	1.96	0.47
1:I:42:ILE:HA	1:I:42:ILE:HD13	1.68	0.47
1:K:27:THR:HG22	1:K:31:MET:N	2.21	0.47
1:M:307:LYS:HA	1:M:307:LYS:HD3	1.56	0.47
1:O:226:GLN:NE2	1:O:228:GLY:H	2.11	0.47
1:A:174:GLU:N	1:A:174:GLU:OE2	2.45	0.47
2:B:125:GLN:HG2	2:B:157:TYR:HB3	1.95	0.47
1:C:62:ARG:H	1:C:62:ARG:HD3	1.80	0.47
1:G:114:ARG:HH11	1:G:265:SER:HB3	1.79	0.47
1:K:307:LYS:HZ3	2:L:62:GLN:HB3	1.76	0.47
2:P:149:MET:HA	2:P:152:VAL:HG23	1.97	0.47
1:Q:82:VAL:C	1:Q:83:GLU:H	2.17	0.47
1:C:12:GLN:HB2	2:D:27:SER:OG	2.15	0.47
1:I:307:LYS:HD2	2:J:92:TRP:CE2	2.49	0.47
1:K:27:THR:HG22	1:K:32:GLU:N	2.29	0.47
2:B:68:ARG:NH1	2:B:68:ARG:HB2	2.30	0.47
2:D:123:ARG:HD2	2:D:132:GLU:OE1	2.15	0.47
2:B:81:ASN:HD22	2:D:80:LEU:HD13	1.79	0.47
1:E:49:GLY:HA2	1:E:285:MET:O	2.15	0.47
1:I:316:LEU:HD13	2:J:100:VAL:HG22	1.95	0.47
1:K:123:ILE:HD12	1:K:123:ILE:HA	1.41	0.47
1:M:154:LEU:HD12	1:M:251:PHE:HB3	1.97	0.47
1:O:124:ILE:HD12	1:O:127:TRP:HZ2	1.80	0.47
1:O:64:CYS:SG	1:O:95:ASN:HB2	2.54	0.47
2:R:169:LYS:O	2:R:169:LYS:CG	2.62	0.47
2:R:28:ASN:HB3	2:R:31:GLY:CA	2.45	0.47
1:A:181:GLY:O	1:A:182:ILE:HD13	2.13	0.47
2:B:38:LYS:O	2:B:42:GLN:HB2	2.14	0.47
1:C:45:LYS:HE2	1:C:312:ASN:O	2.14	0.47
1:E:123:ILE:HD11	1:E:168:TYR:CZ	2.49	0.47
1:K:72:GLY:HA3	1:K:149:ARG:H	1.79	0.47
1:K:279:THR:HB	1:K:281:CYS:H	1.80	0.47
1:A:59:LEU:CD1	1:A:80:ILE:HG23	2.42	0.47
2:L:59:MET:C	2:L:61:THR:H	2.19	0.47
1:O:220:ARG:HH11	1:O:229:ARG:HG2	1.79	0.47
1:Q:312:ASN:OD1	1:Q:312:ASN:N	2.47	0.47
1:C:72:GLY:HA3	1:C:149:ARG:HB2	1.97	0.47
1:O:47:HIS:HB3	1:O:297:ILE:CD1	2.45	0.47
2:P:41:THR:O	2:P:45:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:18:HIS:CE1	2:R:18:VAL:HA	2.50	0.47
1:A:216:ARG:O	1:A:220:ARG:NH2	2.48	0.46
1:E:137:SER:HA	1:E:145:SER:HB2	1.97	0.46
2:L:28:ASN:H	2:L:28:ASN:HD22	1.63	0.46
1:M:172:ASN:OD1	1:M:259:LYS:HD3	2.15	0.46
1:M:236:ILE:H	1:M:236:ILE:HD12	1.80	0.46
1:O:134:GLY:CA	1:O:155:ILE:HD13	2.45	0.46
1:O:36:VAL:HG12	1:O:38:HIS:H	1.78	0.46
3:Y:1:NAG:H62	3:Y:2:NAG:N2	2.30	0.46
1:A:230:MET:SD	1:A:252:ILE:CD1	3.02	0.46
1:C:123:ILE:HA	1:C:123:ILE:HD12	1.32	0.46
1:C:181:GLY:O	1:C:182:ILE:HD13	2.15	0.46
1:C:279:THR:CG2	1:C:287:ALA:HB1	2.41	0.46
1:E:27:THR:HG22	1:E:32:GLU:N	2.30	0.46
1:M:200:THR:HA	1:M:248:ASN:CG	2.36	0.46
2:N:30:GLN:HE22	2:N:145:ASP:HB2	1.80	0.46
1:O:124:ILE:HD12	1:O:127:TRP:CZ2	2.51	0.46
1:O:279:THR:HG21	1:O:287:ALA:HB1	1.97	0.46
1:O:27:THR:HG22	1:O:28:ILE:N	2.31	0.46
1:O:60:ILE:CD1	1:O:274:TYR:HB2	2.45	0.46
2:P:169:LYS:HA	2:P:172:GLU:HB2	1.97	0.46
1:Q:262:LYS:O	1:Q:262:LYS:CG	2.63	0.46
1:C:27:THR:HG22	1:C:31:MET:N	2.23	0.46
2:D:63:PHE:CE1	2:F:90:ASP:OD1	2.67	0.46
1:E:182:ILE:N	1:E:182:ILE:HD13	2.30	0.46
2:H:65:ALA:O	2:H:66:VAL:CG1	2.64	0.46
2:B:83:LYS:HD3	2:F:66:VAL:HG22	1.96	0.46
2:F:65:ALA:O	2:F:66:VAL:CG1	2.64	0.46
2:H:28:ASN:H	2:H:28:ASN:HD22	1.63	0.46
1:I:86:TYR:HA	1:I:113:SER:O	2.15	0.46
1:M:117:HIS:HB3	1:M:261:VAL:HG23	1.98	0.46
1:C:307:LYS:HG2	2:D:59:MET:HE3	1.97	0.46
1:G:12:GLN:HA	2:H:138:PHE:O	2.16	0.46
1:M:96(A):LEU:HB3	1:M:98:TYR:O	2.15	0.46
1:O:129:SER:HA	1:O:157:LYS:HD2	1.97	0.46
1:O:219:THR:HG22	1:O:220:ARG:N	2.27	0.46
1:O:71:LEU:N	1:O:71:LEU:HD23	2.31	0.46
1:G:66:VAL:HG23	1:G:89:GLU:OE2	2.16	0.46
1:I:75:MET:CB	1:I:95:ASN:ND2	2.63	0.46
1:K:123:ILE:HD11	1:K:168:TYR:CZ	2.51	0.46
1:O:149:ARG:HB3	1:O:149:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:141:TYR:O	2:P:169:LYS:HG2	2.15	0.46
2:P:91:VAL:HG12	2:P:92:TRP:N	2.30	0.46
2:D:62:GLN:CD	2:D:62:GLN:H	2.17	0.46
1:E:295:HIS:CD2	1:E:297:ILE:H	2.33	0.46
1:G:200:THR:HG22	1:G:215:PRO:CD	2.46	0.46
1:I:124:ILE:CD1	1:I:254:PRO:HG2	2.44	0.46
2:H:63:PHE:CE1	2:J:90:ASP:OD1	2.66	0.46
1:K:206:THR:HB	1:K:209:LEU:HB3	1.97	0.46
1:K:295:HIS:CD2	1:K:297:ILE:H	2.32	0.46
2:N:59:MET:O	2:N:61:THR:C	2.54	0.46
2:R:151:SER:HA	2:R:154:ASN:HB2	1.98	0.46
1:A:249:GLY:O	1:A:250:ASN:OD1	2.34	0.46
1:E:124:ILE:HG12	1:E:254:PRO:O	2.16	0.46
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.98	0.46
2:F:68:ARG:HH11	2:F:68:ARG:HB2	1.81	0.46
1:G:309:VAL:HG22	2:H:93:THR:HA	1.98	0.46
2:H:59:MET:C	2:H:61:THR:H	2.19	0.46
1:I:136:SER:O	1:I:145:SER:HB2	2.15	0.46
1:I:17:TYR:CD1	2:J:13:GLY:HA3	2.51	0.46
2:N:59:MET:CE	2:N:62:GLN:HG3	2.44	0.46
1:E:186:ASN:HB3	1:E:190:GLU:OE2	2.16	0.46
1:K:136:SER:O	1:K:145:SER:HB2	2.16	0.46
1:M:125(A):LYS:O	1:M:125(B):SER:C	2.53	0.46
2:N:49:THR:HG22	2:N:53:ASN:HD21	1.80	0.46
2:R:111:HIS:HA	2:R:114:ASN:ND2	2.31	0.46
1:G:11:ASP:HB2	2:H:140:PHE:CD1	2.48	0.46
1:G:123:ILE:HA	1:G:123:ILE:HD12	1.36	0.46
1:I:178:VAL:O	1:I:234:TRP:HA	2.15	0.46
1:M:275:GLY:O	1:M:276:ASN:C	2.53	0.46
1:O:251:PHE:CZ	1:O:253:ALA:HA	2.51	0.46
1:O:37:THR:HG1	1:O:320:LEU:H	1.63	0.46
1:Q:39:ALA:O	1:Q:40:GLN:HB2	2.16	0.46
1:A:279:THR:CG2	1:A:287:ALA:HB1	2.43	0.45
1:K:87:ILE:HB	1:K:267:ILE:HG13	1.98	0.45
1:M:230:MET:SD	1:M:252:ILE:CD1	3.04	0.45
2:P:110:PHE:O	2:P:114:ASN:OD1	2.34	0.45
2:P:140:PHE:C	2:P:142:HIS:H	2.20	0.45
2:P:53:ASN:O	2:P:57:ASP:N	2.46	0.45
1:Q:50:LYS:O	1:Q:286:GLY:HA2	2.17	0.45
1:Q:51:LEU:HD11	1:Q:88:VAL:HG21	1.98	0.45
1:A:179:LEU:HD23	1:A:234:TRP:CB	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ARG:HB2	1:E:216:ARG:HG2	1.97	0.45
1:I:87:ILE:HD12	1:I:113:SER:HA	1.98	0.45
1:K:79:PHE:HD1	1:K:80:ILE:N	2.14	0.45
2:L:125:GLN:HG2	2:L:157:TYR:HB3	1.97	0.45
1:O:220:ARG:HB3	1:O:227:SER:HB2	1.98	0.45
1:A:79:PHE:HD1	1:A:79:PHE:O	1.84	0.45
2:H:51:LYS:HG3	1:I:28:ILE:HG23	1.97	0.45
1:O:42:ILE:O	1:O:293:PRO:HD2	2.16	0.45
1:Q:281:CYS:SG	1:Q:288:ILE:HD12	2.55	0.45
1:A:316:LEU:HD13	2:B:100:VAL:HG22	1.98	0.45
2:B:62:GLN:H	2:B:62:GLN:CD	2.18	0.45
1:C:49:GLY:HA2	1:C:285:MET:O	2.17	0.45
1:I:80:ILE:C	1:I:82:VAL:H	2.20	0.45
1:I:80:ILE:CG2	1:I:80:ILE:O	2.63	0.45
1:M:124:ILE:O	1:M:125:PRO:C	2.54	0.45
1:M:222:LYS:HA	1:M:226:GLN:O	2.17	0.45
1:M:58:PRO:HB3	1:M:86:TYR:CE2	2.52	0.45
1:A:72:GLY:HA3	1:A:149:ARG:HB2	1.98	0.45
1:E:125:PRO:HG3	1:I:79:PHE:HA	1.12	0.45
1:G:201:TYR:CE2	1:G:248:ASN:HB2	2.51	0.45
1:M:62:ARG:NH2	1:M:77:ASP:OD1	2.49	0.45
1:O:234:TRP:O	1:O:235:THR:CB	2.64	0.45
1:Q:13:ILE:HD11	2:R:149:MET:HG2	1.98	0.45
1:A:114:ARG:HH11	1:A:265:SER:HB3	1.82	0.45
1:C:78:GLU:O	1:C:80:ILE:N	2.49	0.45
1:G:137:SER:HA	1:G:145:SER:HB2	1.99	0.45
1:G:216:ARG:O	1:G:220:ARG:NH2	2.49	0.45
1:O:190:GLU:C	1:O:192:THR:H	2.20	0.45
1:K:59:LEU:HD11	1:K:80:ILE:CG2	2.44	0.45
1:M:15:ILE:HD12	1:M:15:ILE:N	2.31	0.45
2:N:166:ALA:C	2:N:168:LEU:N	2.70	0.45
2:N:26:HIS:O	2:N:32:SER:HB2	2.16	0.45
2:N:65:ALA:C	2:N:66:VAL:CG1	2.85	0.45
1:O:161:TYR:OH	1:O:164:ILE:HD11	2.16	0.45
1:M:134:GLY:O	1:M:153:TRP:HB3	2.17	0.45
2:N:159:TYR:HB3	2:N:160:PRO:CD	2.46	0.45
2:N:59:MET:HB3	2:N:59:MET:HE2	1.78	0.45
1:O:185:PRO:O	1:O:217:ILE:HG23	2.17	0.45
1:O:251:PHE:HE1	1:O:253:ALA:HA	1.75	0.45
1:Q:320:LEU:HA	2:R:108:LEU:CD2	2.46	0.45
1:A:75:MET:HB2	1:A:95:ASN:HD21	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:GLU:O	1:E:80:ILE:N	2.49	0.45
1:K:137:SER:HA	1:K:145:SER:HB2	1.98	0.45
1:M:283:THR:HG23	1:M:298:HIS:HB3	1.97	0.45
1:O:49:GLY:HA2	1:O:285:MET:O	2.17	0.45
1:Q:301:THR:OG1	1:Q:305:CYS:SG	2.61	0.45
2:D:59:MET:C	2:D:61:THR:H	2.20	0.45
1:E:201:TYR:HE1	1:E:246:GLU:HG2	1.82	0.45
1:E:282:GLN:HG3	1:E:283:THR:N	2.32	0.45
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.99	0.45
1:O:200:THR:CG2	1:O:250:ASN:HB2	2.45	0.45
1:O:42:ILE:HD13	1:O:42:ILE:HA	1.48	0.45
1:Q:206:THR:CG2	1:Q:207:SER:N	2.54	0.45
2:F:38:LYS:O	2:F:42:GLN:HB2	2.17	0.44
1:K:227:SER:HA	1:K:229:ARG:HH12	1.82	0.44
1:K:279:THR:CG2	1:K:287:ALA:HB1	2.45	0.44
1:M:129:SER:HA	1:M:157:LYS:HD3	2.00	0.44
1:M:202:ILE:HD12	1:M:202:ILE:N	2.32	0.44
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.18	0.44
1:Q:223:VAL:C	1:Q:225:GLY:N	2.70	0.44
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.52	0.44
1:E:316:LEU:HD23	2:F:52:VAL:HG22	1.99	0.44
1:G:186:ASN:HB3	1:G:190:GLU:OE2	2.17	0.44
1:G:27:THR:HG22	1:G:32:GLU:N	2.30	0.44
2:L:38:LYS:O	2:L:42:GLN:HB2	2.18	0.44
4:T:1:NAG:H61	4:T:2:NAG:C1	2.48	0.44
1:G:307:LYS:HZ1	2:H:62:GLN:HB3	1.83	0.44
1:I:206:THR:HB	1:I:209:LEU:CB	2.47	0.44
2:J:123:ARG:HD2	2:J:132:GLU:OE1	2.18	0.44
1:M:85:SER:O	1:M:114:ARG:NH1	2.51	0.44
1:Q:139:CYS:SG	1:Q:147:PHE:HA	2.57	0.44
1:Q:48:ASN:OD1	1:Q:287:ALA:N	2.50	0.44
2:R:95:ASN:O	2:R:99:LEU:CB	2.60	0.44
1:C:59:LEU:CD1	1:C:80:ILE:HG23	2.44	0.44
1:E:124:ILE:HA	1:E:125:PRO:HD2	1.68	0.44
1:G:27:THR:HG22	1:G:31:MET:N	2.25	0.44
2:J:72:ASN:HB2	2:J:75:ARG:HD2	1.99	0.44
1:M:283:THR:HB	1:M:286:GLY:H	1.81	0.44
1:O:70:LEU:HD23	1:O:70:LEU:HA	1.68	0.44
1:Q:201:TYR:CD2	1:Q:248:ASN:HB2	2.53	0.44
1:A:307:LYS:NZ	2:B:62:GLN:HB3	2.32	0.44
1:G:206:THR:HB	1:G:209:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:THR:CB	1:I:121:ILE:HD13	2.47	0.44
1:I:124:ILE:CG1	1:I:124:ILE:O	2.65	0.44
1:I:186:ASN:HB3	1:I:190:GLU:OE2	2.17	0.44
1:I:230:MET:SD	1:I:252:ILE:HD11	2.57	0.44
2:N:59:MET:CE	2:N:62:GLN:CG	2.95	0.44
1:O:25:VAL:CG1	1:O:26:ASP:N	2.80	0.44
1:A:78:GLU:O	1:A:80:ILE:N	2.50	0.44
2:B:66:VAL:HG22	2:D:83:LYS:HD3	2.00	0.44
1:C:182:ILE:HD11	1:C:213:LEU:CD1	2.35	0.44
2:D:38:LYS:O	2:D:42:GLN:HB2	2.18	0.44
1:K:307:LYS:HG2	2:L:59:MET:HE1	1.99	0.44
1:M:104:ASP:HB2	1:M:234:TRP:HE1	1.83	0.44
1:M:144:LYS:HE3	1:M:144:LYS:HB3	1.80	0.44
1:O:160:THR:HG1	1:O:160:THR:CB	2.15	0.44
1:O:185:PRO:HG2	1:O:217:ILE:HG23	1.99	0.44
1:C:174:GLU:OE2	1:C:174:GLU:N	2.51	0.44
1:K:200:THR:HG22	1:K:215:PRO:CD	2.48	0.44
1:M:152:VAL:N	1:M:253:ALA:O	2.38	0.44
1:Q:182:ILE:CD1	1:Q:202:ILE:HG12	2.48	0.44
2:R:57:ASP:O	2:R:59:MET:N	2.47	0.44
1:A:124:ILE:CG1	1:A:124:ILE:O	2.65	0.44
1:A:123:ILE:HG22	1:A:124:ILE:HG23	1.99	0.44
1:A:159:SER:O	1:A:196:GLN:CG	2.58	0.44
2:F:123:ARG:HD2	2:F:132:GLU:OE1	2.17	0.44
2:F:19:ASP:HB3	2:F:36:ALA:HB3	2.00	0.44
1:E:307:LYS:HZ1	2:F:62:GLN:HB3	1.79	0.44
1:G:11:ASP:CB	2:H:140:PHE:HD1	2.28	0.44
1:M:11:ASP:N	1:M:11:ASP:OD2	2.51	0.44
1:M:37:THR:HG22	1:M:38:HIS:CD2	2.52	0.44
1:O:52:CYS:CA	1:O:277:CYS:HB3	2.45	0.44
1:Q:295:HIS:HD2	1:Q:297:ILE:HG12	1.82	0.44
2:R:148:CYS:O	2:R:151:SER:OG	2.35	0.44
1:C:17:TYR:CD1	2:D:13:GLY:HA3	2.53	0.44
1:E:79:PHE:O	1:E:80:ILE:HG12	2.18	0.44
1:G:79:PHE:O	1:G:80:ILE:CG1	2.66	0.44
1:M:245:PHE:CD1	1:M:245:PHE:N	2.85	0.44
1:M:97:CYS:HB2	1:M:138:ALA:O	2.18	0.44
1:O:112:LEU:HA	1:O:112:LEU:HD23	1.67	0.44
1:Q:104:ASP:HB2	1:Q:234:TRP:NE1	2.27	0.44
1:C:124:ILE:CD1	1:C:254:PRO:HG2	2.47	0.43
2:F:145:ASP:O	2:F:148:CYS:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:154:LEU:O	1:K:155:ILE:HD12	2.17	0.43
1:M:134:GLY:CA	1:M:153:TRP:HB3	2.48	0.43
1:Q:283:THR:HB	1:Q:286:GLY:O	2.18	0.43
2:R:45:ILE:HG13	2:R:45:ILE:H	1.63	0.43
1:C:120:LYS:HG3	1:C:258:TYR:CE2	2.52	0.43
1:G:293:PRO:HG2	1:G:294:PHE:CE1	2.53	0.43
1:I:121:ILE:HA	1:I:121:ILE:HD13	1.89	0.43
2:N:5:ALA:HA	2:N:9:PHE:CD1	2.53	0.43
1:O:307:LYS:HZ1	2:P:62:GLN:HB3	1.83	0.43
1:O:302:ILE:HA	2:P:65:ALA:O	2.18	0.43
1:Q:20:ASN:N	1:Q:20:ASN:OD1	2.38	0.43
2:R:52:VAL:O	2:R:55:ILE:HB	2.18	0.43
1:A:295:HIS:HD2	1:A:297:ILE:H	1.66	0.43
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.33	0.43
1:A:79:PHE:O	1:A:80:ILE:CG1	2.66	0.43
1:C:115:ILE:HG21	1:C:118:PHE:HB2	2.01	0.43
1:C:53(A):LEU:HD23	1:C:53(A):LEU:HA	1.63	0.43
1:C:97:CYS:O	1:C:224:ASN:ND2	2.50	0.43
1:G:307:LYS:HZ3	2:H:62:GLN:HB3	1.83	0.43
1:I:320:LEU:N	1:I:320:LEU:HD23	2.33	0.43
1:K:114:ARG:HH11	1:K:265:SER:HB3	1.83	0.43
1:O:149:ARG:HH11	1:O:149:ARG:CG	2.32	0.43
1:O:182:ILE:CG2	1:O:215:PRO:HB3	2.48	0.43
1:O:285:MET:CE	1:O:285:MET:HA	2.49	0.43
2:P:145:ASP:OD1	2:P:148:CYS:CB	2.54	0.43
1:E:120:LYS:HG3	1:E:258:TYR:CE2	2.54	0.43
1:I:59:LEU:CD1	1:I:80:ILE:HG23	2.44	0.43
1:M:84:TRP:NE1	1:M:112:LEU:O	2.50	0.43
2:P:144:CYS:SG	2:P:149:MET:HG2	2.58	0.43
1:Q:86:TYR:HA	1:Q:265:SER:CB	2.49	0.43
2:R:28:ASN:HB3	2:R:31:GLY:HA3	2.00	0.43
1:C:206:THR:HB	1:C:209:LEU:HB3	2.00	0.43
1:E:230:MET:SD	1:E:252:ILE:HD11	2.58	0.43
1:I:200:THR:HG22	1:I:215:PRO:CD	2.48	0.43
1:Q:142:GLN:HG3	1:Q:142:GLN:O	2.19	0.43
1:Q:200:THR:HG23	1:Q:249:GLY:N	2.29	0.43
1:Q:295:HIS:CD2	1:Q:297:ILE:H	2.37	0.43
2:R:151:SER:O	2:R:154:ASN:HB2	2.18	0.43
1:Q:55:GLY:C	4:X:3:BMA:O4	2.57	0.43
2:F:28:ASN:HD22	2:F:28:ASN:H	1.67	0.43
2:N:30:GLN:NE2	2:N:145:ASP:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:143:LYS:NZ	2:P:143:LYS:CD	2.82	0.43
1:Q:141:TYR:CG	1:Q:142:GLN:N	2.85	0.43
1:O:230:MET:HB3	1:O:232:PHE:CE1	2.53	0.43
2:R:127:ARG:H	2:R:127:ARG:HD3	1.84	0.43
1:G:124:ILE:CD1	1:G:254:PRO:HG2	2.47	0.43
1:G:25:VAL:HG13	2:H:104:ASN:ND2	2.33	0.43
1:M:230:MET:SD	1:M:252:ILE:HD11	2.58	0.43
2:R:18:VAL:O	2:R:18:VAL:HG12	2.18	0.43
2:R:88:PHE:O	2:R:92:TRP:HD1	2.01	0.43
1:C:297:ILE:H	1:C:297:ILE:HG12	1.70	0.43
1:G:201:TYR:HE1	1:G:246:GLU:HG2	1.83	0.43
2:H:167:ARG:HD3	2:J:174:SER:HA	2.01	0.43
1:K:65:SER:OG	1:K:96:ASP:HA	2.19	0.43
1:M:279:THR:CG2	1:M:287:ALA:HB1	2.44	0.43
2:N:141:TYR:CD1	2:N:166:ALA:HB1	2.53	0.43
1:Q:305:CYS:O	1:Q:307:LYS:N	2.51	0.43
1:E:115:ILE:HG21	1:E:118:PHE:HB2	2.01	0.43
1:E:174:GLU:N	1:E:174:GLU:OE2	2.47	0.43
1:G:307:LYS:HD2	2:H:92:TRP:CE2	2.53	0.43
1:M:118:PHE:CE1	1:M:260:ILE:HD11	2.54	0.43
1:M:141:TYR:O	1:M:143:GLY:N	2.52	0.43
1:M:147:PHE:CG	1:M:148:PHE:N	2.86	0.43
1:M:202:ILE:HG12	1:M:251:PHE:HD1	1.84	0.43
1:M:181:GLY:HA3	1:M:252:ILE:HB	2.01	0.43
2:N:131:LYS:C	2:N:133:LEU:H	2.21	0.43
1:O:260:ILE:HG23	1:O:261:VAL:N	2.34	0.43
2:P:140:PHE:HB3	2:P:142:HIS:O	2.18	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.19	0.42
2:N:44:ALA:O	2:N:45:ILE:C	2.57	0.42
1:O:231:GLU:O	1:O:233:PHE:CE1	2.72	0.42
1:O:291:SER:HB2	1:O:292:MET:HE2	2.00	0.42
1:O:266:THR:HG22	1:O:302:ILE:HD11	2.01	0.42
2:R:70:PHE:HB2	2:R:78:GLU:HB2	2.01	0.42
2:R:84:MET:HE1	2:R:85:GLU:HG3	2.01	0.42
2:R:99:LEU:HD12	2:R:99:LEU:HA	1.86	0.42
1:C:200:THR:HG23	1:C:201:TYR:N	2.34	0.42
2:D:125:GLN:HG2	2:D:157:TYR:HB3	2.00	0.42
1:G:207:SER:HA	1:I:229:ARG:NH2	2.34	0.42
1:M:19:ALA:HB1	1:M:322:ASN:HD21	1.84	0.42
1:O:220:ARG:HD2	1:O:229:ARG:HG2	2.01	0.42
1:O:52:CYS:HB3	1:O:277:CYS:HB3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:26:HIS:CE1	2:P:32:SER:HA	2.54	0.42
1:O:42:ILE:HD12	2:P:56:ILE:HD11	2.01	0.42
1:Q:55:GLY:HA2	1:Q:278:ASN:HD21	1.84	0.42
1:A:123:ILE:CG2	1:A:124:ILE:HG23	2.49	0.42
1:C:206:THR:HG23	1:C:207:SER:H	1.84	0.42
1:G:178:VAL:O	1:G:234:TRP:HA	2.18	0.42
1:M:168:TYR:O	1:M:243:ILE:HG22	2.18	0.42
1:O:220:ARG:HH11	1:O:229:ARG:CG	2.33	0.42
1:Q:122:GLN:HE21	1:Q:125:PRO:HA	1.84	0.42
2:R:155:GLY:C	2:R:157:TYR:H	2.22	0.42
1:C:137:SER:HA	1:C:145:SER:HB2	2.01	0.42
2:H:123:ARG:HD2	2:H:132:GLU:OE1	2.20	0.42
1:M:12:GLN:HB2	2:N:27:SER:OG	2.19	0.42
2:N:37:ASP:C	2:N:39:GLU:N	2.70	0.42
2:N:84:MET:O	2:N:87:GLY:N	2.53	0.42
1:O:173:GLN:HB2	1:O:173:GLN:HE21	1.55	0.42
1:C:195:TYR:CE1	1:C:250:ASN:ND2	2.87	0.42
2:D:19:ASP:HB3	2:D:36:ALA:HB3	2.02	0.42
1:E:106:GLU:OE2	2:F:71:ASN:HB3	2.20	0.42
1:E:12:GLN:HG2	2:F:138:PHE:O	2.19	0.42
1:E:136:SER:O	1:E:145:SER:HB2	2.20	0.42
1:I:276:ASN:O	1:I:277:CYS:HB2	2.19	0.42
1:I:13:ILE:HA	2:J:25:HIS:O	2.20	0.42
1:K:106:GLU:OE2	2:L:71:ASN:HB3	2.19	0.42
1:M:114:ARG:HD2	1:M:264(A):ASP:O	2.20	0.42
1:M:118:PHE:HE1	1:M:260:ILE:HD11	1.84	0.42
1:O:186:ASN:HB2	1:O:227:SER:O	2.19	0.42
2:B:173:ILE:O	2:F:167:ARG:NH1	2.53	0.42
1:K:59:LEU:CD1	1:K:80:ILE:HG23	2.46	0.42
1:O:38:HIS:HB2	1:O:319:GLY:H	1.84	0.42
1:Q:293:PRO:HB2	1:Q:294:PHE:HD1	1.84	0.42
1:E:171:THR:HB	1:I:121:ILE:CD1	2.48	0.42
1:A:229:ARG:NH2	1:E:207:SER:HA	2.29	0.42
1:E:178:VAL:O	1:E:234:TRP:HA	2.19	0.42
1:I:115:ILE:HG21	1:I:118:PHE:HB2	2.01	0.42
1:K:124:ILE:HA	1:K:125:PRO:HD2	1.87	0.42
1:M:123:ILE:HG23	1:M:124:ILE:N	2.35	0.42
1:M:77:ASP:HB2	1:M:79:PHE:H	1.82	0.42
2:N:28:ASN:HD22	2:N:28:ASN:H	1.67	0.42
1:O:146:SER:HG	1:O:147:PHE:H	1.64	0.42
1:O:32:GLU:HB3	1:O:35:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:61:LEU:HB3	1:O:64:CYS:O	2.18	0.42
1:A:206:THR:HB	1:A:209:LEU:N	2.28	0.42
2:B:167:ARG:NH1	2:D:173:ILE:O	2.52	0.42
2:B:59:MET:HG3	2:D:94:TYR:CD1	2.55	0.42
1:C:79:PHE:O	1:C:80:ILE:CG1	2.68	0.42
2:F:68:ARG:NH1	2:F:68:ARG:HB2	2.35	0.42
1:G:115:ILE:HG21	1:G:118:PHE:HB2	2.01	0.42
1:G:15:ILE:HD13	2:H:119:TYR:HA	2.02	0.42
1:G:304:GLU:HG2	2:H:63:PHE:HA	2.01	0.42
1:K:174:GLU:N	1:K:174:GLU:OE2	2.52	0.42
2:L:123:ARG:HD2	2:L:132:GLU:OE1	2.19	0.42
1:M:115:ILE:HG21	1:M:118:PHE:HB2	2.02	0.42
1:M:170:ASN:OD1	1:M:171:THR:N	2.53	0.42
2:N:17:MET:HG3	2:N:34:TYR:HB3	2.02	0.42
2:N:38:LYS:NZ	2:N:38:LYS:HD2	2.34	0.42
1:Q:295:HIS:CD2	1:Q:297:ILE:HG12	2.55	0.42
1:A:297:ILE:H	1:A:297:ILE:HG12	1.71	0.42
1:C:227:SER:HA	1:C:229:ARG:HH12	1.85	0.42
1:E:11:ASP:OD2	2:F:144:CYS:N	2.52	0.42
1:E:156:LYS:HD2	1:E:196:GLN:HG2	2.02	0.42
1:G:159:SER:C	1:G:196:GLN:HG3	2.40	0.42
1:G:49:GLY:HA2	1:G:285:MET:O	2.20	0.42
1:I:181:GLY:O	1:I:182:ILE:HD13	2.20	0.42
1:O:108:LEU:HD22	1:O:234:TRP:CD1	2.55	0.42
1:Q:60:ILE:HA	1:Q:88:VAL:HB	2.01	0.42
1:A:75:MET:CB	1:A:95:ASN:HD21	2.30	0.42
1:E:87:ILE:HB	1:E:267:ILE:HG13	2.01	0.42
1:G:295:HIS:CD2	1:G:297:ILE:H	2.36	0.42
1:G:72:GLY:HA3	1:G:149:ARG:H	1.84	0.42
1:K:206:THR:HG23	1:K:207:SER:H	1.84	0.42
1:M:141:TYR:CB	1:M:146:SER:HB2	2.49	0.42
1:M:294:PHE:HA	1:M:307:LYS:O	2.20	0.42
2:N:128:ASP:O	2:N:170:ARG:NH1	2.53	0.42
2:N:95:ASN:O	2:N:99:LEU:HB2	2.20	0.42
1:O:292:MET:HB3	1:O:293:PRO:HD2	2.01	0.42
1:Q:184:HIS:HA	1:Q:185:PRO:HD3	1.63	0.42
1:Q:220:ARG:HD2	1:Q:227:SER:O	2.20	0.42
2:R:121:LYS:O	2:R:125:GLN:HB2	2.20	0.42
1:A:238:LYS:O	1:A:239:PRO:C	2.57	0.41
1:G:18:HIS:N	2:H:21:TRP:O	2.48	0.41
1:K:178:VAL:O	1:K:234:TRP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:ASN:ND2	1:Q:238:LYS:O	2.52	0.41
2:D:167:ARG:NH1	2:F:173:ILE:O	2.53	0.41
1:E:123:ILE:HD12	1:E:123:ILE:HA	1.46	0.41
1:K:120:LYS:HG3	1:K:258:TYR:CE2	2.54	0.41
1:K:201:TYR:CE1	1:K:246:GLU:HG2	2.54	0.41
1:O:190:GLU:OE2	1:O:190:GLU:HA	2.20	0.41
2:P:155:GLY:O	2:P:157:TYR:N	2.49	0.41
1:Q:251:PHE:HE2	1:Q:253:ALA:HB2	1.83	0.41
1:A:309:VAL:HG22	2:B:93:THR:HA	2.01	0.41
1:I:124:ILE:HA	1:I:125:PRO:HD2	1.82	0.41
2:H:117:ASN:ND2	2:J:4:GLY:CA	2.84	0.41
1:M:125(A):LYS:HG3	1:M:132:ALA:HB1	2.02	0.41
1:M:161:TYR:CE2	1:M:249:GLY:HA2	2.55	0.41
2:N:143:LYS:N	2:N:143:LYS:HD3	2.22	0.41
1:E:185:PRO:HG3	1:E:191:GLN:HG2	2.02	0.41
2:L:145:ASP:O	2:L:148:CYS:HB3	2.20	0.41
2:P:59:MET:HB3	2:P:59:MET:HE2	1.97	0.41
1:Q:75:MET:HG2	1:Q:75:MET:H	1.51	0.41
2:R:1:GLY:HA3	2:R:8:GLY:H	1.85	0.41
2:D:81:ASN:HD22	2:F:80:LEU:CD1	2.30	0.41
1:I:68:GLY:O	1:I:71:LEU:O	2.39	0.41
1:K:49:GLY:HA2	1:K:285:MET:O	2.20	0.41
1:M:144:LYS:HG2	1:M:145:SER:N	2.36	0.41
1:M:161:TYR:HB2	1:M:196:GLN:HG3	2.02	0.41
2:N:117:ASN:HA	2:N:117:ASN:HD22	1.65	0.41
2:N:143:LYS:CD	2:N:143:LYS:H	2.21	0.41
1:O:42:ILE:CD1	2:P:56:ILE:HD11	2.51	0.41
1:Q:278:ASN:HD21	4:X:3:BMA:H62	1.86	0.41
1:A:206:THR:HB	1:A:209:LEU:HB3	2.02	0.41
1:A:99:PRO:HB3	1:A:223:VAL:CG1	2.51	0.41
1:C:201:TYR:CE1	1:C:246:GLU:HG2	2.52	0.41
1:G:266:THR:HB	2:H:66:VAL:HB	2.02	0.41
1:K:238:LYS:O	1:K:239:PRO:C	2.58	0.41
1:K:86:TYR:HA	1:K:113:SER:O	2.21	0.41
1:M:266:THR:HG23	1:M:302:ILE:HD11	2.01	0.41
1:Q:147:PHE:CG	1:Q:148:PHE:N	2.89	0.41
2:R:24:TYR:N	2:R:24:TYR:CD1	2.89	0.41
2:R:43:LYS:HA	2:R:46:ASP:HB2	2.02	0.41
1:A:86:TYR:HA	1:A:113:SER:O	2.20	0.41
1:C:66:VAL:HG23	1:C:89:GLU:OE2	2.21	0.41
2:F:59:MET:O	2:F:61:THR:CA	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:99:PRO:HD2	1:M:226:GLN:HG3	2.02	0.41
2:N:132:GLU:C	2:N:134:GLY:H	2.23	0.41
1:O:152:VAL:N	1:O:253:ALA:O	2.54	0.41
2:R:26:HIS:CD2	2:R:153:ARG:HH22	2.39	0.41
1:E:11:ASP:HB2	2:F:140:PHE:HB2	2.02	0.41
1:E:276:ASN:O	1:E:277:CYS:HB2	2.20	0.41
1:I:262:LYS:NZ	1:I:264(A):ASP:OD1	2.39	0.41
1:K:72:GLY:HA3	1:K:149:ARG:HB2	2.02	0.41
2:J:66:VAL:HG22	2:L:83:LYS:HD3	2.03	0.41
1:M:48:ASN:HD21	1:M:287:ALA:HB3	1.85	0.41
2:N:72:ASN:HA	2:N:75:ARG:HG3	2.02	0.41
2:N:80:LEU:HD12	2:N:80:LEU:HA	1.92	0.41
1:C:141:TYR:CE2	1:C:142:GLN:CG	3.03	0.41
1:G:185:PRO:HG3	1:G:191:GLN:HG2	2.03	0.41
2:H:63:PHE:H	2:H:63:PHE:HD1	1.59	0.41
1:I:187:ASP:C	1:I:187:ASP:OD2	2.60	0.41
1:I:197:ASN:HA	1:I:198:PRO:HD3	1.96	0.41
1:K:293:PRO:HG2	1:K:294:PHE:CE1	2.56	0.41
1:M:119:GLU:O	1:M:259:LYS:N	2.53	0.41
1:M:293:PRO:HG2	1:M:294:PHE:CE1	2.56	0.41
1:M:295:HIS:CD2	1:M:297:ILE:HG12	2.56	0.41
2:N:125:GLN:HE21	2:N:125:GLN:HB2	1.71	0.41
2:N:59:MET:O	2:N:61:THR:O	2.38	0.41
1:O:86:TYR:HA	1:O:113:SER:O	2.21	0.41
1:O:147:PHE:O	1:O:148:PHE:C	2.59	0.41
1:O:184:HIS:HA	1:O:185:PRO:HD2	1.88	0.41
1:O:251:PHE:CD1	1:O:251:PHE:C	2.94	0.41
1:O:117:HIS:H	1:O:261:VAL:HB	1.86	0.41
1:O:266:THR:HG23	1:O:267:ILE:N	2.36	0.41
1:O:70:LEU:O	1:O:258:TYR:OH	2.37	0.41
2:P:21:TRP:HB2	2:P:41:THR:HG23	2.02	0.41
1:C:320:LEU:HD23	1:C:320:LEU:N	2.36	0.41
1:C:86:TYR:HA	1:C:113:SER:O	2.20	0.41
1:E:206:THR:HB	1:E:209:LEU:CB	2.50	0.41
1:G:185:PRO:HG2	1:G:217:ILE:HG13	2.02	0.41
1:I:275:GLY:O	1:I:277:CYS:CB	2.58	0.41
1:I:295:HIS:HD2	1:I:297:ILE:H	1.68	0.41
1:I:297:ILE:HG12	1:I:297:ILE:H	1.64	0.41
2:H:110:PHE:CD1	2:J:2:LEU:HD21	2.56	0.41
1:M:176:LEU:O	1:M:237:LEU:N	2.54	0.41
1:M:232:PHE:C	1:M:233:PHE:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:127:TRP:HZ3	1:O:164:ILE:HD13	1.86	0.41
1:Q:80:ILE:C	1:Q:82:VAL:N	2.74	0.41
2:R:66:VAL:HB	2:R:67:GLY:H	1.62	0.41
1:A:167:SER:CB	1:A:244:ASN:OD1	2.69	0.41
1:E:100:GLY:HA3	1:E:230:MET:O	2.21	0.41
1:G:75:MET:CB	1:G:95:ASN:HD21	2.28	0.41
1:E:149:ARG:NH1	1:I:142:GLN:OE1	2.54	0.41
1:I:72:GLY:HA3	1:I:149:ARG:H	1.86	0.41
1:M:130:HIS:NE2	1:M:162:PRO:HD2	2.35	0.41
2:N:15:GLN:HA	2:N:15:GLN:HE21	1.86	0.41
2:N:28:ASN:HB2	2:N:144:CYS:O	2.20	0.41
2:P:98:LEU:HA	2:P:98:LEU:HD23	1.77	0.41
1:Q:161:TYR:CD2	1:Q:161:TYR:C	2.95	0.41
2:R:29:GLU:O	2:R:30:GLN:CB	2.69	0.41
2:D:159:TYR:N	2:D:160:PRO:HD2	2.37	0.40
2:D:98:LEU:HA	2:D:98:LEU:HD23	1.84	0.40
1:E:266:THR:HB	2:F:66:VAL:HB	2.03	0.40
1:E:27:THR:HG23	2:F:105:GLU:HB2	2.04	0.40
1:E:81:ASN:HB2	1:I:144:LYS:HZ3	1.85	0.40
2:F:65:ALA:O	2:F:66:VAL:HG13	2.21	0.40
1:G:131:GLU:HB2	1:G:155:ILE:O	2.19	0.40
1:G:59:LEU:CD1	1:G:80:ILE:HG23	2.45	0.40
1:O:155:ILE:CG2	1:O:156:LYS:N	2.84	0.40
2:R:63:PHE:H	2:R:63:PHE:HD1	1.68	0.40
1:A:282:GLN:HG3	1:A:283:THR:N	2.37	0.40
1:C:241:ASP:CG	1:C:242:ALA:H	2.25	0.40
1:E:59:LEU:CD1	1:E:80:ILE:HG23	2.45	0.40
2:H:145:ASP:O	2:H:148:CYS:HB3	2.21	0.40
1:I:206:THR:HG23	1:I:207:SER:H	1.86	0.40
2:L:19:ASP:HB3	2:L:36:ALA:HB3	2.03	0.40
1:O:27:THR:HG23	2:P:105:GLU:CB	2.50	0.40
2:P:120:ASP:O	2:P:124:LEU:HD12	2.22	0.40
2:P:141:TYR:HB2	2:P:166:ALA:HB1	2.02	0.40
1:K:249:GLY:O	1:K:250:ASN:OD1	2.39	0.40
2:L:145:ASP:H	2:L:148:CYS:HB3	1.86	0.40
1:M:150:ASN:HA	1:M:256:TYR:HD1	1.86	0.40
1:O:295:HIS:HB3	1:O:306:PRO:HG2	2.04	0.40
2:R:126:LEU:O	2:R:126:LEU:HD12	2.21	0.40
2:R:127:ARG:HB2	2:R:127:ARG:NH1	2.18	0.40
2:B:62:GLN:NE2	2:B:62:GLN:H	2.19	0.40
2:D:65:ALA:C	2:D:66:VAL:CG1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:TYR:N	2:H:160:PRO:HD2	2.36	0.40
1:I:99:PRO:HB3	1:I:223:VAL:CG1	2.52	0.40
1:I:307:LYS:HD2	2:J:92:TRP:CZ2	2.57	0.40
1:K:237:LEU:CD1	1:K:241:ASP:HB3	2.52	0.40
1:K:12:GLN:HB2	2:L:27:SER:OG	2.22	0.40
1:M:126:SER:O	1:M:127:TRP:CD1	2.75	0.40
1:E:272:LEU:HD23	1:M:171:THR:HG21	1.98	0.40
1:M:62:ARG:H	1:M:62:ARG:HH11	1.69	0.40
2:N:16:GLY:HA3	2:N:34:TYR:CZ	2.56	0.40
1:O:182:ILE:HD13	1:O:182:ILE:HA	1.93	0.40
2:B:123:ARG:HD2	2:B:132:GLU:OE1	2.22	0.40
2:B:98:LEU:HD23	2:B:98:LEU:HA	1.91	0.40
1:C:200:THR:HG22	1:C:215:PRO:CD	2.51	0.40
1:M:284:PRO:HD3	1:M:300:LEU:O	2.22	0.40
2:N:65:ALA:C	2:N:66:VAL:HG13	2.41	0.40
1:Q:109:LYS:HZ1	2:R:69:GLU:HG2	1.87	0.40
1:Q:58:PRO:HG2	1:Q:60:ILE:HD11	2.03	0.40
2:R:162:TYR:O	2:R:163:SER:HB3	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE2	1:K:142:GLN:OE1[3_455]	1.69	0.51
1:C:142:GLN:OE1	1:G:78:GLU:OE2[2_555]	1.87	0.33
1:C:79:PHE:CE2	1:G:125(B):SER:C[2_555]	1.94	0.26
1:C:142:GLN:OE1	1:G:149:ARG:NH1[2_555]	2.17	0.03
1:A:125(B):SER:C	1:K:79:PHE:CE2[3_455]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/334 (96%)	289 (90%)	25 (8%)	6 (2%)	8	32
1	C	320/334 (96%)	290 (91%)	26 (8%)	4 (1%)	12	41
1	E	320/334 (96%)	289 (90%)	25 (8%)	6 (2%)	8	32
1	G	320/334 (96%)	285 (89%)	31 (10%)	4 (1%)	12	41
1	I	320/334 (96%)	285 (89%)	29 (9%)	6 (2%)	8	32
1	K	320/334 (96%)	287 (90%)	28 (9%)	5 (2%)	9	36
1	M	320/334 (96%)	255 (80%)	52 (16%)	13 (4%)	3	13
1	O	320/334 (96%)	248 (78%)	57 (18%)	15 (5%)	2	11
1	Q	320/334 (96%)	237 (74%)	63 (20%)	20 (6%)	1	6
2	B	173/181 (96%)	161 (93%)	10 (6%)	2 (1%)	13	43
2	D	173/181 (96%)	164 (95%)	7 (4%)	2 (1%)	13	43
2	F	173/181 (96%)	162 (94%)	9 (5%)	2 (1%)	13	43
2	H	173/181 (96%)	162 (94%)	8 (5%)	3 (2%)	9	34
2	J	173/181 (96%)	163 (94%)	8 (5%)	2 (1%)	13	43
2	L	173/181 (96%)	164 (95%)	7 (4%)	2 (1%)	13	43
2	N	173/181 (96%)	132 (76%)	35 (20%)	6 (4%)	3	17
2	P	173/181 (96%)	126 (73%)	37 (21%)	10 (6%)	1	7
2	R	173/181 (96%)	124 (72%)	29 (17%)	20 (12%)	0	1
All	All	4437/4635 (96%)	3823 (86%)	486 (11%)	128 (3%)	4	21

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
2	B	127	ARG
2	D	60	ASN
2	D	127	ARG
1	E	80	ILE
2	F	60	ASN
2	F	127	ARG
1	G	80	ILE
2	H	60	ASN
2	H	127	ARG
2	J	60	ASN
2	J	127	ARG
1	K	80	ILE
2	L	60	ASN

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Mol	Chain	Res	Type
2	L	127	ARG
1	M	133(A)	LEU
1	M	142	GLN
1	M	145	SER
2	N	38	LYS
2	N	60	ASN
2	N	133	LEU
1	O	158	ASN
2	P	60	ASN
2	P	151	SER
2	P	153	ARG
2	P	154	ASN
1	Q	91	ALA
1	Q	226	GLN
1	Q	307	LYS
2	R	63	PHE
2	R	74	GLU
2	R	163	SER
1	A	79	PHE
1	A	80	ILE
1	C	79	PHE
1	C	80	ILE
1	E	79	PHE
1	G	79	PHE
1	I	79	PHE
1	M	113	SER
1	M	147	PHE
1	M	150	ASN
1	O	134	GLY
1	O	144	LYS
1	O	235	THR
1	O	239	PRO
2	P	152	VAL
1	Q	71	LEU
1	Q	96(A)	LEU
1	Q	142	GLN
1	Q	158	ASN
1	Q	249	GLY
1	Q	281	CYS
2	R	8	GLY
2	R	30	GLN
2	R	39	GLU

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Mol	Chain	Res	Type
2	R	59	MET
2	R	154	ASN
2	R	157	TYR
1	C	277	CYS
1	E	277	CYS
1	G	277	CYS
1	M	144	LYS
1	M	249	GLY
1	M	276	ASN
2	N	167	ARG
1	O	96	ASP
1	O	133(A)	LEU
2	P	150	GLU
1	Q	81	ASN
1	Q	82(A)	PRO
1	Q	83	GLU
1	Q	299	PRO
1	Q	306	PRO
2	R	60	ASN
2	R	161	GLN
2	R	174	SER
1	A	277	CYS
1	I	80	ILE
1	I	277	CYS
1	K	277	CYS
1	M	214	VAL
1	O	62	ARG
1	O	141	TYR
1	Q	45	LYS
1	Q	80	ILE
1	E	81	ASN
1	I	265	SER
1	K	146	SER
1	K	265	SER
1	M	54	ASP
2	N	132	GLU
1	O	99	PRO
1	O	106	GLU
1	O	224	ASN
1	O	236	ILE
1	O	289	ASN
1	Q	21	SER

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Mol	Chain	Res	Type
1	Q	117	HIS
1	Q	262	LYS
2	R	29	GLU
1	A	81	ASN
1	A	239	PRO
1	A	265	SER
1	C	239	PRO
1	I	239	PRO
2	P	156	THR
2	R	17	MET
2	R	49	THR
2	R	66	VAL
2	R	127	ARG
2	R	134	GLY
1	E	239	PRO
2	P	8	GLY
1	K	239	PRO
2	N	16	GLY
1	Q	25	VAL
1	E	249	GLY
1	M	298	HIS
2	P	66	VAL
1	G	249	GLY
2	H	66	VAL
1	M	123	ILE
1	O	93	PRO
2	R	18	VAL
2	R	173	ILE
1	I	249	GLY
2	P	160	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	289/300 (96%)	257 (89%)	32 (11%)	6 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	289/300 (96%)	260 (90%)	29 (10%)	7	26
1	E	289/300 (96%)	257 (89%)	32 (11%)	6	22
1	G	289/300 (96%)	258 (89%)	31 (11%)	6	23
1	I	289/300 (96%)	256 (89%)	33 (11%)	5	21
1	K	289/300 (96%)	255 (88%)	34 (12%)	5	20
1	M	289/300 (96%)	239 (83%)	50 (17%)	2	8
1	O	289/300 (96%)	246 (85%)	43 (15%)	3	12
1	Q	289/300 (96%)	238 (82%)	51 (18%)	2	8
2	B	149/155 (96%)	135 (91%)	14 (9%)	8	29
2	D	149/155 (96%)	135 (91%)	14 (9%)	8	29
2	F	149/155 (96%)	135 (91%)	14 (9%)	8	29
2	H	149/155 (96%)	134 (90%)	15 (10%)	7	26
2	J	149/155 (96%)	135 (91%)	14 (9%)	8	29
2	L	149/155 (96%)	135 (91%)	14 (9%)	8	29
2	N	149/155 (96%)	121 (81%)	28 (19%)	1	7
2	P	149/155 (96%)	121 (81%)	28 (19%)	1	7
2	R	149/155 (96%)	125 (84%)	24 (16%)	2	10
All	All	3942/4095 (96%)	3442 (87%)	500 (13%)	4	17

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	27	THR
1	A	28	ILE
1	A	35(A)	THR
1	A	37	THR
1	A	42	ILE
1	A	62	ARG
1	A	75	MET
1	A	78	GLU
1	A	79	PHE
1	A	82	VAL
1	A	101	ASP
1	A	114	ARG
1	A	123	ILE

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Mol	Chain	Res	Type
1	A	124	ILE
1	A	136	SER
1	A	151	VAL
1	A	160	THR
1	A	163	THR
1	A	176	LEU
1	A	197	ASN
1	A	200	THR
1	A	208	THR
1	A	211	GLN
1	A	217	ILE
1	A	230	MET
1	A	235	THR
1	A	238	LYS
1	A	239	PRO
1	A	297	ILE
1	A	309	VAL
1	A	320	LEU
2	B	28	ASN
2	B	30	GLN
2	B	34	TYR
2	B	62	GLN
2	B	63	PHE
2	B	68	ARG
2	B	69	GLU
2	B	72	ASN
2	B	89	LEU
2	B	126	LEU
2	B	127	ARG
2	B	156	THR
2	B	169	LYS
2	B	172	GLU
1	C	25	VAL
1	C	27	THR
1	C	28	ILE
1	C	35(A)	THR
1	C	37	THR
1	C	42	ILE
1	C	62	ARG
1	C	75	MET
1	C	79	PHE
1	C	114	ARG

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Mol	Chain	Res	Type
1	C	123	ILE
1	C	124	ILE
1	C	136	SER
1	C	151	VAL
1	C	160	THR
1	C	163	THR
1	C	169	ASN
1	C	176	LEU
1	C	191	GLN
1	C	200	THR
1	C	208	THR
1	C	211	GLN
1	C	217	ILE
1	C	230	MET
1	C	235	THR
1	C	239	PRO
1	C	297	ILE
1	C	309	VAL
1	C	320	LEU
2	D	28	ASN
2	D	30	GLN
2	D	34	TYR
2	D	62	GLN
2	D	63	PHE
2	D	68	ARG
2	D	69	GLU
2	D	72	ASN
2	D	89	LEU
2	D	126	LEU
2	D	127	ARG
2	D	156	THR
2	D	169	LYS
2	D	172	GLU
1	E	25	VAL
1	E	27	THR
1	E	28	ILE
1	E	35(A)	THR
1	E	37	THR
1	E	42	ILE
1	E	62	ARG
1	E	75	MET
1	E	78	GLU

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Mol	Chain	Res	Type
1	E	79	PHE
1	E	82	VAL
1	E	114	ARG
1	E	123	ILE
1	E	124	ILE
1	E	136	SER
1	E	151	VAL
1	E	160	THR
1	E	163	THR
1	E	173	GLN
1	E	176	LEU
1	E	197	ASN
1	E	200	THR
1	E	208	THR
1	E	211	GLN
1	E	217	ILE
1	E	230	MET
1	E	235	THR
1	E	238	LYS
1	E	239	PRO
1	E	297	ILE
1	E	309	VAL
1	E	320	LEU
2	F	28	ASN
2	F	30	GLN
2	F	34	TYR
2	F	62	GLN
2	F	63	PHE
2	F	68	ARG
2	F	69	GLU
2	F	72	ASN
2	F	89	LEU
2	F	126	LEU
2	F	127	ARG
2	F	156	THR
2	F	169	LYS
2	F	172	GLU
1	G	25	VAL
1	G	27	THR
1	G	28	ILE
1	G	35(A)	THR
1	G	37	THR

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Mol	Chain	Res	Type
1	G	42	ILE
1	G	62	ARG
1	G	75	MET
1	G	78	GLU
1	G	79	PHE
1	G	82	VAL
1	G	114	ARG
1	G	123	ILE
1	G	124	ILE
1	G	136	SER
1	G	151	VAL
1	G	160	THR
1	G	163	THR
1	G	169	ASN
1	G	176	LEU
1	G	197	ASN
1	G	200	THR
1	G	208	THR
1	G	211	GLN
1	G	217	ILE
1	G	230	MET
1	G	235	THR
1	G	238	LYS
1	G	297	ILE
1	G	309	VAL
1	G	320	LEU
2	H	28	ASN
2	H	30	GLN
2	H	34	TYR
2	H	62	GLN
2	H	63	PHE
2	H	64	GLU
2	H	68	ARG
2	H	69	GLU
2	H	72	ASN
2	H	89	LEU
2	H	126	LEU
2	H	127	ARG
2	H	156	THR
2	H	169	LYS
2	H	172	GLU
1	I	25	VAL

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Mol	Chain	Res	Type
1	I	27	THR
1	I	28	ILE
1	I	35(A)	THR
1	I	37	THR
1	I	42	ILE
1	I	62	ARG
1	I	75	MET
1	I	78	GLU
1	I	79	PHE
1	I	80	ILE
1	I	82	VAL
1	I	114	ARG
1	I	123	ILE
1	I	124	ILE
1	I	136	SER
1	I	151	VAL
1	I	160	THR
1	I	163	THR
1	I	169	ASN
1	I	173	GLN
1	I	176	LEU
1	I	191	GLN
1	I	197	ASN
1	I	200	THR
1	I	208	THR
1	I	211	GLN
1	I	217	ILE
1	I	230	MET
1	I	235	THR
1	I	297	ILE
1	I	309	VAL
1	I	320	LEU
2	J	28	ASN
2	J	30	GLN
2	J	34	TYR
2	J	62	GLN
2	J	63	PHE
2	J	68	ARG
2	J	69	GLU
2	J	72	ASN
2	J	89	LEU
2	J	126	LEU

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Mol	Chain	Res	Type
2	J	127	ARG
2	J	156	THR
2	J	169	LYS
2	J	172	GLU
1	K	25	VAL
1	K	27	THR
1	K	28	ILE
1	K	35(A)	THR
1	K	37	THR
1	K	42	ILE
1	K	62	ARG
1	K	75	MET
1	K	78	GLU
1	K	79	PHE
1	K	80	ILE
1	K	101	ASP
1	K	114	ARG
1	K	123	ILE
1	K	136	SER
1	K	151	VAL
1	K	160	THR
1	K	163	THR
1	K	169	ASN
1	K	173	GLN
1	K	176	LEU
1	K	197	ASN
1	K	200	THR
1	K	208	THR
1	K	211	GLN
1	K	217	ILE
1	K	230	MET
1	K	235	THR
1	K	238	LYS
1	K	239	PRO
1	K	264(A)	ASP
1	K	297	ILE
1	K	309	VAL
1	K	320	LEU
2	L	28	ASN
2	L	30	GLN
2	L	34	TYR
2	L	62	GLN

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Mol	Chain	Res	Type
2	L	63	PHE
2	L	68	ARG
2	L	69	GLU
2	L	72	ASN
2	L	89	LEU
2	L	126	LEU
2	L	127	ARG
2	L	156	THR
2	L	169	LYS
2	L	172	GLU
1	M	11	ASP
1	M	27	THR
1	M	42	ILE
1	M	53(A)	LEU
1	M	54	ASP
1	M	62	ARG
1	M	70	LEU
1	M	77	ASP
1	M	78	GLU
1	M	82	VAL
1	M	92	ASN
1	M	102	PHE
1	M	111	LEU
1	M	121	ILE
1	M	124	ILE
1	M	125(B)	SER
1	M	126	SER
1	M	133(A)	LEU
1	M	144	LYS
1	M	156	LYS
1	M	160	THR
1	M	164	ILE
1	M	171	THR
1	M	172	ASN
1	M	173	GLN
1	M	174	GLU
1	M	192	THR
1	M	196	GLN
1	M	197	ASN
1	M	207	SER
1	M	211	GLN
1	M	214	VAL

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Mol	Chain	Res	Type
1	M	216	ARG
1	M	217	ILE
1	M	221	SER
1	M	222	LYS
1	M	224	ASN
1	M	238	LYS
1	M	248	ASN
1	M	255	GLU
1	M	265	SER
1	M	267	ILE
1	M	272	LEU
1	M	277	CYS
1	M	309	VAL
1	M	312	ASN
1	M	313	ARG
1	M	320	LEU
1	M	322	ASN
1	M	323	SER
2	N	9	PHE
2	N	15	GLN
2	N	18	VAL
2	N	19	ASP
2	N	22	TYR
2	N	24	TYR
2	N	28	ASN
2	N	30	GLN
2	N	41	THR
2	N	48	VAL
2	N	50	ASN
2	N	60	ASN
2	N	62	GLN
2	N	63	PHE
2	N	82	LYS
2	N	112	ASP
2	N	113	SER
2	N	117	ASN
2	N	125	GLN
2	N	126	LEU
2	N	127	ARG
2	N	143	LYS
2	N	145	ASP
2	N	149	MET

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Mol	Chain	Res	Type
2	N	156	THR
2	N	158	ASP
2	N	164	GLU
2	N	174	SER
1	O	22	THR
1	O	42	ILE
1	O	57	LYS
1	O	62	ARG
1	O	63	ASP
1	O	71	LEU
1	O	77	ASP
1	O	80	ILE
1	O	82	VAL
1	O	96(A)	LEU
1	O	102	PHE
1	O	111	LEU
1	O	114	ARG
1	O	121	ILE
1	O	123	ILE
1	O	125(B)	SER
1	O	130	HIS
1	O	149	ARG
1	O	152	VAL
1	O	160	THR
1	O	163	THR
1	O	171	THR
1	O	172	ASN
1	O	173	GLN
1	O	187	ASP
1	O	191	GLN
1	O	197	ASN
1	O	199	THR
1	O	206	THR
1	O	209	LEU
1	O	214	VAL
1	O	216	ARG
1	O	230	MET
1	O	248	ASN
1	O	251	PHE
1	O	260	ILE
1	O	266	THR
1	O	273	GLU

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Mol	Chain	Res	Type
1	O	277	CYS
1	O	285	MET
1	O	309	VAL
1	O	320	LEU
1	O	322	ASN
2	P	9	PHE
2	P	10	ILE
2	P	27	SER
2	P	28	ASN
2	P	30	GLN
2	P	32	SER
2	P	34	TYR
2	P	55	ILE
2	P	59	MET
2	P	61	THR
2	P	62	GLN
2	P	63	PHE
2	P	69	GLU
2	P	72	ASN
2	P	103	GLU
2	P	112	ASP
2	P	121	LYS
2	P	124	LEU
2	P	125	GLN
2	P	127	ARG
2	P	128	ASP
2	P	131	LYS
2	P	147	GLU
2	P	153	ARG
2	P	158	ASP
2	P	164	GLU
2	P	172	GLU
2	P	173	ILE
1	Q	11	ASP
1	Q	17	TYR
1	Q	20	ASN
1	Q	23	GLU
1	Q	25	VAL
1	Q	44	GLU
1	Q	46	LYS
1	Q	48	ASN
1	Q	51	LEU

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Mol	Chain	Res	Type
1	Q	52	CYS
1	Q	57	LYS
1	Q	61	LEU
1	Q	62	ARG
1	Q	75	MET
1	Q	85	SER
1	Q	95	ASN
1	Q	102	PHE
1	Q	115	ILE
1	Q	118	PHE
1	Q	124	ILE
1	Q	125(B)	SER
1	Q	127	TRP
1	Q	133(A)	LEU
1	Q	135	VAL
1	Q	151	VAL
1	Q	161	TYR
1	Q	169	ASN
1	Q	170	ASN
1	Q	175	ASP
1	Q	176	LEU
1	Q	186	ASN
1	Q	191	GLN
1	Q	195	TYR
1	Q	199	THR
1	Q	211	GLN
1	Q	223	VAL
1	Q	236	ILE
1	Q	238	LYS
1	Q	260	ILE
1	Q	262	LYS
1	Q	272	LEU
1	Q	277	CYS
1	Q	281	CYS
1	Q	295	HIS
1	Q	302	ILE
1	Q	304	GLU
1	Q	310	LYS
1	Q	312	ASN
1	Q	315	VAL
1	Q	320	LEU
1	Q	322	ASN

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Mol	Chain	Res	Type
2	R	3	PHE
2	R	21	TRP
2	R	22	TYR
2	R	24	TYR
2	R	30	GLN
2	R	43	LYS
2	R	59	MET
2	R	62	GLN
2	R	63	PHE
2	R	66	VAL
2	R	69	GLU
2	R	80	LEU
2	R	95	ASN
2	R	98	LEU
2	R	106	ARG
2	R	112	ASP
2	R	113	SER
2	R	121	LYS
2	R	126	LEU
2	R	127	ARG
2	R	131	LYS
2	R	161	GLN
2	R	164	GLU
2	R	167	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
2	B	79	ASN
2	B	81	ASN
2	B	117	ASN
1	C	38	HIS
1	C	295	HIS
1	C	322	ASN
2	D	15	GLN
2	D	79	ASN
2	D	81	ASN
2	D	117	ASN
1	E	47	HIS
1	E	295	HIS
2	F	79	ASN

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Mol	Chain	Res	Type
2	F	81	ASN
2	F	117	ASN
1	G	295	HIS
1	G	322	ASN
2	H	79	ASN
2	H	81	ASN
2	H	117	ASN
1	I	38	HIS
1	I	322	ASN
2	J	15	GLN
2	J	79	ASN
2	J	81	ASN
2	J	117	ASN
1	K	226	GLN
1	K	295	HIS
1	K	322	ASN
2	L	79	ASN
2	L	81	ASN
1	M	110	HIS
1	M	117	HIS
1	M	172	ASN
1	M	191	GLN
1	M	226	GLN
1	M	250	ASN
1	M	295	HIS
1	M	312	ASN
2	N	15	GLN
2	N	26	HIS
2	N	30	GLN
2	N	53	ASN
2	N	117	ASN
2	N	125	GLN
2	N	135	ASN
1	O	38	HIS
1	O	117	HIS
1	O	172	ASN
1	O	173	GLN
1	O	211	GLN
1	O	224	ASN
1	O	226	GLN
1	O	248	ASN
1	O	282	GLN

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Mol	Chain	Res	Type
1	O	322	ASN
2	P	53	ASN
2	P	79	ASN
2	P	117	ASN
2	P	129	ASN
1	Q	24	GLN
1	Q	92	ASN
1	Q	95	ASN
1	Q	116	ASN
1	Q	122	GLN
1	Q	170	ASN
1	Q	276	ASN
1	Q	278	ASN
2	R	15	GLN
2	R	26	HIS
2	R	28	ASN
2	R	30	GLN
2	R	42	GLN
2	R	81	ASN
2	R	114	ASN
2	R	135	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

35 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	S	1	1,3	14,14,15	0.64	0	17,19,21	1.47	3 (17%)
3	NAG	S	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.07	2 (11%)
4	NAG	T	1	1,4	14,14,15	0.72	0	17,19,21	1.77	3 (17%)
4	NAG	T	2	4	14,14,15	0.76	0	17,19,21	1.85	5 (29%)
4	BMA	T	3	4	11,11,12	0.69	0	15,15,17	1.43	2 (13%)
3	NAG	U	1	1,3	14,14,15	0.69	0	17,19,21	2.74	7 (41%)
3	NAG	U	2	3	14,14,15	0.63	0	17,19,21	1.64	3 (17%)
3	NAG	V	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	2.34	6 (35%)
3	NAG	V	2	3	14,14,15	0.60	0	17,19,21	1.77	4 (23%)
3	NAG	W	1	1,3	14,14,15	0.58	0	17,19,21	1.83	5 (29%)
3	NAG	W	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.76	3 (17%)
4	NAG	X	1	1,4	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
4	NAG	X	2	4	14,14,15	0.59	0	17,19,21	1.38	3 (17%)
4	BMA	X	3	4	11,11,12	0.86	0	15,15,17	2.57	4 (26%)
3	NAG	Y	1	1,3	14,14,15	0.66	0	17,19,21	1.25	1 (5%)
3	NAG	Y	2	3	14,14,15	1.00	1 (7%)	17,19,21	1.51	2 (11%)
4	NAG	Z	1	1,4	14,14,15	0.79	0	17,19,21	2.44	5 (29%)
4	NAG	Z	2	4	14,14,15	0.75	0	17,19,21	1.49	3 (17%)
4	BMA	Z	3	4	11,11,12	0.56	0	15,15,17	2.49	2 (13%)
3	NAG	a	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	2.88	8 (47%)
3	NAG	a	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.63	4 (23%)
3	NAG	b	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	1.57	5 (29%)
3	NAG	b	2	3	14,14,15	0.66	0	17,19,21	1.57	4 (23%)
3	NAG	c	1	1,3	14,14,15	0.77	0	17,19,21	2.24	5 (29%)
3	NAG	c	2	3	14,14,15	1.03	1 (7%)	17,19,21	2.74	6 (35%)
3	NAG	d	1	1,3	14,14,15	0.71	0	17,19,21	1.83	4 (23%)
3	NAG	d	2	3	14,14,15	0.53	0	17,19,21	1.35	2 (11%)
3	NAG	e	1	1,3	14,14,15	0.82	0	17,19,21	1.69	4 (23%)
3	NAG	e	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.17	1 (5%)
3	NAG	f	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	1.89	4 (23%)
3	NAG	f	2	3	14,14,15	0.88	0	17,19,21	2.04	5 (29%)
3	NAG	g	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	2.03	6 (35%)
3	NAG	g	2	3	14,14,15	1.21	1 (7%)	17,19,21	1.90	4 (23%)
3	NAG	h	1	1,3	14,14,15	0.73	0	17,19,21	2.63	7 (41%)
3	NAG	h	2	3	14,14,15	0.89	1 (7%)	17,19,21	1.36	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	S	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
4	NAG	T	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	T	2	4	-	4/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	NAG	V	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	W	2	3	-	4/6/23/26	0/1/1/1
4	NAG	X	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	1/2/19/22	0/1/1/1
3	NAG	Y	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	5/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	c	2	3	-	1/6/23/26	0/1/1/1
3	NAG	d	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	4/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	3/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	g	2	3	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	h	1	1,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	5/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	NAG	C1-C2	3.66	1.57	1.52
3	S	2	NAG	C1-C2	2.81	1.56	1.52
3	e	2	NAG	C1-C2	2.73	1.56	1.52
3	Y	2	NAG	C1-C2	2.73	1.56	1.52
3	g	1	NAG	C1-C2	2.72	1.56	1.52
3	c	2	NAG	C1-C2	2.59	1.56	1.52
3	f	1	NAG	C1-C2	2.51	1.56	1.52
3	W	2	NAG	C1-C2	2.47	1.56	1.52
3	h	2	NAG	C1-C2	2.26	1.55	1.52
3	a	1	NAG	C1-C2	2.25	1.55	1.52
3	V	1	NAG	O5-C1	-2.21	1.40	1.43
3	b	1	NAG	C1-C2	2.15	1.55	1.52
3	a	2	NAG	C1-C2	2.08	1.55	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	3	BMA	C1-O5-C5	8.68	123.95	112.19
3	U	1	NAG	C1-O5-C5	8.51	123.73	112.19
3	a	1	NAG	C1-O5-C5	8.22	123.33	112.19
4	X	3	BMA	C1-C2-C3	6.55	117.71	109.67
4	Z	1	NAG	O5-C1-C2	-6.39	101.19	111.29
3	c	2	NAG	C1-O5-C5	6.25	120.66	112.19
3	h	1	NAG	C4-C3-C2	-5.77	102.56	111.02
3	V	1	NAG	C1-O5-C5	-5.75	104.40	112.19
3	h	1	NAG	C1-O5-C5	5.33	119.42	112.19
4	T	1	NAG	O5-C1-C2	-5.16	103.15	111.29
3	c	2	NAG	O5-C5-C6	5.16	115.29	107.20
3	c	1	NAG	C1-O5-C5	5.11	119.12	112.19
4	X	3	BMA	C1-O5-C5	5.02	119.00	112.19
3	f	1	NAG	O5-C1-C2	-4.91	103.54	111.29
3	V	2	NAG	C2-N2-C7	-4.74	116.16	122.90
4	Z	1	NAG	C1-O5-C5	4.72	118.59	112.19
3	h	1	NAG	O5-C1-C2	-4.65	103.95	111.29
3	W	2	NAG	C2-N2-C7	4.59	129.44	122.90
3	f	2	NAG	C2-N2-C7	4.57	129.41	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1	NAG	O5-C1-C2	4.55	118.48	111.29
3	g	2	NAG	C1-O5-C5	4.55	118.36	112.19
4	T	2	NAG	C1-O5-C5	-4.47	106.13	112.19
3	U	2	NAG	C3-C4-C5	4.43	118.15	110.24
3	V	1	NAG	C2-N2-C7	-4.33	116.73	122.90
3	c	2	NAG	C3-C4-C5	4.27	117.85	110.24
3	f	2	NAG	C4-C3-C2	4.22	117.20	111.02
3	d	1	NAG	C2-N2-C7	4.14	128.81	122.90
3	W	1	NAG	C2-N2-C7	-4.11	117.06	122.90
3	c	1	NAG	C4-C3-C2	4.04	116.93	111.02
3	c	1	NAG	O5-C5-C6	3.98	113.45	107.20
3	g	1	NAG	C3-C4-C5	-3.98	103.15	110.24
3	W	2	NAG	C4-C3-C2	3.96	116.82	111.02
3	c	2	NAG	C4-C3-C2	3.93	116.78	111.02
4	T	3	BMA	C1-O5-C5	3.93	117.51	112.19
3	a	2	NAG	C1-O5-C5	3.89	117.46	112.19
3	W	1	NAG	C1-O5-C5	3.84	117.40	112.19
4	X	3	BMA	O5-C1-C2	3.84	116.70	110.77
4	X	1	NAG	O5-C1-C2	-3.78	105.32	111.29
4	Z	2	NAG	C4-C3-C2	3.77	116.54	111.02
3	U	1	NAG	C4-C3-C2	-3.72	105.57	111.02
3	h	2	NAG	C4-C3-C2	3.69	116.42	111.02
3	e	1	NAG	C2-N2-C7	3.63	128.07	122.90
3	d	2	NAG	C1-O5-C5	3.53	116.97	112.19
3	a	1	NAG	C4-C3-C2	-3.49	105.91	111.02
4	X	2	NAG	C4-C3-C2	3.48	116.12	111.02
3	c	1	NAG	C3-C4-C5	3.42	116.33	110.24
3	h	1	NAG	C2-N2-C7	-3.40	118.06	122.90
3	V	2	NAG	C1-O5-C5	3.36	116.75	112.19
3	c	2	NAG	C2-N2-C7	3.34	127.67	122.90
3	c	2	NAG	O5-C1-C2	3.31	116.52	111.29
3	g	2	NAG	O5-C1-C2	3.29	116.49	111.29
3	S	1	NAG	C4-C3-C2	-3.25	106.26	111.02
3	g	1	NAG	C4-C3-C2	-3.22	106.30	111.02
3	V	1	NAG	C8-C7-N2	3.17	121.47	116.10
3	d	1	NAG	C1-O5-C5	3.14	116.45	112.19
3	g	2	NAG	C2-N2-C7	3.13	127.36	122.90
4	T	2	NAG	O5-C5-C6	3.10	112.07	107.20
3	b	2	NAG	O5-C5-C4	-3.08	103.33	110.83
3	f	2	NAG	C3-C4-C5	3.07	115.72	110.24
3	f	2	NAG	C1-O5-C5	-3.07	108.03	112.19
3	W	1	NAG	O5-C5-C6	3.05	111.98	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	1	NAG	C2-N2-C7	3.03	127.22	122.90
3	f	1	NAG	C3-C4-C5	-2.99	104.91	110.24
3	U	2	NAG	O5-C1-C2	-2.97	106.60	111.29
4	Z	2	NAG	C2-N2-C7	-2.95	118.70	122.90
4	T	1	NAG	C1-O5-C5	-2.92	108.23	112.19
3	b	1	NAG	O5-C1-C2	-2.90	106.70	111.29
3	h	1	NAG	O4-C4-C5	2.90	116.50	109.30
3	e	1	NAG	C4-C3-C2	2.90	115.27	111.02
3	Y	2	NAG	O5-C5-C6	2.89	111.74	107.20
3	g	1	NAG	C1-C2-N2	2.89	115.43	110.49
3	e	1	NAG	C1-O5-C5	2.89	116.11	112.19
3	Y	2	NAG	C2-N2-C7	2.88	127.01	122.90
3	f	1	NAG	O5-C5-C6	2.85	111.68	107.20
4	X	1	NAG	C1-O5-C5	2.81	116.00	112.19
3	S	2	NAG	O5-C1-C2	2.81	115.72	111.29
3	a	1	NAG	O4-C4-C3	2.81	116.83	110.35
3	Y	1	NAG	C1-O5-C5	2.77	115.94	112.19
3	a	1	NAG	O5-C5-C6	2.77	111.54	107.20
3	S	1	NAG	C1-O5-C5	2.76	115.94	112.19
3	V	1	NAG	O5-C5-C4	-2.75	104.13	110.83
3	b	2	NAG	C1-C2-N2	-2.72	105.84	110.49
3	b	2	NAG	C3-C4-C5	-2.72	105.39	110.24
3	a	2	NAG	C4-C3-C2	2.71	114.98	111.02
3	d	1	NAG	C1-C2-N2	-2.70	105.88	110.49
3	W	2	NAG	O5-C5-C6	2.63	111.33	107.20
3	b	1	NAG	C3-C4-C5	2.63	114.94	110.24
3	g	1	NAG	C1-O5-C5	2.63	115.76	112.19
3	U	1	NAG	O5-C5-C6	2.59	111.27	107.20
3	g	1	NAG	O4-C4-C5	2.58	115.71	109.30
4	Z	1	NAG	O5-C5-C6	-2.56	103.19	107.20
4	T	2	NAG	O3-C3-C2	-2.54	104.20	109.47
4	Z	2	NAG	C1-C2-N2	-2.54	106.15	110.49
3	V	1	NAG	O5-C5-C6	2.53	111.18	107.20
3	U	1	NAG	O3-C3-C2	2.53	114.71	109.47
4	T	2	NAG	O5-C5-C4	-2.48	104.80	110.83
4	Z	1	NAG	C2-N2-C7	-2.47	119.38	122.90
4	X	2	NAG	C3-C4-C5	2.45	114.62	110.24
3	U	1	NAG	O4-C4-C5	2.45	115.38	109.30
3	b	2	NAG	O5-C5-C6	2.43	111.02	107.20
3	c	1	NAG	O4-C4-C5	-2.43	103.26	109.30
3	a	2	NAG	C3-C4-C5	2.43	114.57	110.24
4	Z	3	BMA	O5-C5-C4	2.42	116.72	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	2	NAG	O5-C5-C6	2.41	110.98	107.20
3	a	2	NAG	O5-C1-C2	2.40	115.08	111.29
3	U	1	NAG	C3-C4-C5	-2.36	106.03	110.24
4	T	3	BMA	O5-C1-C2	2.30	114.33	110.77
4	X	3	BMA	C2-C3-C4	2.30	114.87	110.89
3	V	2	NAG	O5-C1-C2	2.29	114.91	111.29
3	W	1	NAG	C3-C4-C5	-2.29	106.15	110.24
3	d	2	NAG	O4-C4-C5	2.27	114.95	109.30
3	f	1	NAG	C1-C2-N2	2.26	114.35	110.49
3	V	1	NAG	O5-C1-C2	-2.25	107.73	111.29
3	d	1	NAG	O5-C1-C2	-2.24	107.75	111.29
3	S	2	NAG	O5-C5-C6	2.24	110.72	107.20
4	Z	1	NAG	C1-C2-N2	-2.23	106.67	110.49
3	U	2	NAG	C4-C3-C2	2.22	114.27	111.02
4	X	2	NAG	C1-O5-C5	2.21	115.19	112.19
3	e	2	NAG	C4-C3-C2	2.21	114.25	111.02
3	S	1	NAG	C2-N2-C7	2.17	125.99	122.90
3	W	1	NAG	O5-C1-C2	-2.17	107.87	111.29
3	a	1	NAG	C1-C2-N2	2.15	114.16	110.49
3	h	1	NAG	C1-C2-N2	2.11	114.10	110.49
3	V	2	NAG	C3-C4-C5	2.10	113.99	110.24
3	b	1	NAG	C1-C2-N2	2.10	114.07	110.49
4	T	1	NAG	O4-C4-C5	2.08	114.47	109.30
3	a	1	NAG	C3-C4-C5	-2.08	106.53	110.24
3	e	1	NAG	C6-C5-C4	2.08	117.87	113.00
3	b	1	NAG	O7-C7-C8	-2.05	118.25	122.06
3	f	2	NAG	C8-C7-N2	2.03	119.53	116.10
3	a	1	NAG	O3-C3-C4	2.02	115.02	110.35
4	T	2	NAG	O5-C1-C2	2.01	114.46	111.29
3	h	1	NAG	O5-C5-C4	2.01	115.71	110.83
3	U	1	NAG	C1-C2-N2	2.01	113.92	110.49
3	g	1	NAG	O5-C5-C6	2.00	110.34	107.20

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	f	1	NAG	C1
3	h	1	NAG	C1
3	b	1	NAG	C1
4	X	1	NAG	C1
3	V	1	NAG	C1
3	d	1	NAG	C1

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Mol	Chain	Res	Type	Atom
4	T	1	NAG	C1

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	f	1	NAG	C8-C7-N2-C2
3	f	1	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	c	1	NAG	C3-C2-N2-C7
3	c	1	NAG	C8-C7-N2-C2
3	c	1	NAG	O7-C7-N2-C2
3	h	1	NAG	C8-C7-N2-C2
3	h	1	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C3-C2-N2-C7
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	g	1	NAG	C8-C7-N2-C2
3	g	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	Y	2	NAG	C3-C2-N2-C7
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	h	2	NAG	C3-C2-N2-C7
3	h	2	NAG	C8-C7-N2-C2
3	h	2	NAG	O7-C7-N2-C2
3	e	1	NAG	C3-C2-N2-C7
3	e	1	NAG	C8-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
3	e	2	NAG	C8-C7-N2-C2
3	e	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	g	2	NAG	C8-C7-N2-C2
3	g	2	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	f	2	NAG	C3-C2-N2-C7
3	f	2	NAG	C8-C7-N2-C2
3	f	2	NAG	O7-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	O7-C7-N2-C2
3	e	1	NAG	C4-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O7-C7-N2-C2
3	d	2	NAG	O5-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
3	d	2	NAG	C8-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
3	c	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C1-C2-N2-C7
3	V	2	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6

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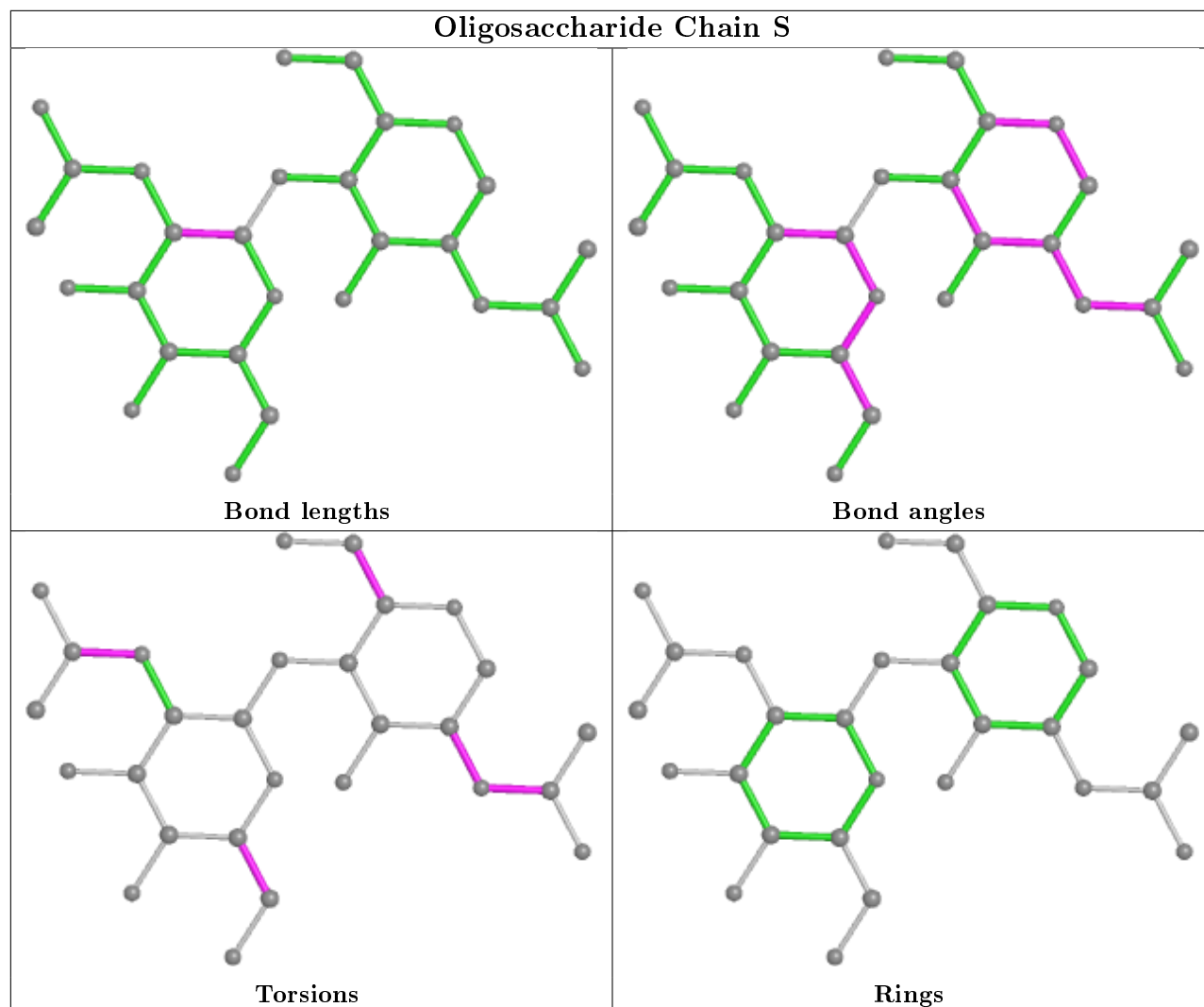
Mol	Chain	Res	Type	Atoms
3	d	2	NAG	O7-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
3	b	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	C1-C2-N2-C7
3	g	2	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	d	1	NAG	O7-C7-N2-C2
3	d	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C3-C2-N2-C7
4	Z	2	NAG	C8-C7-N2-C2
3	h	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	T	1	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	C3-C2-N2-C7
3	h	2	NAG	C4-C5-C6-O6

There are no ring outliers.

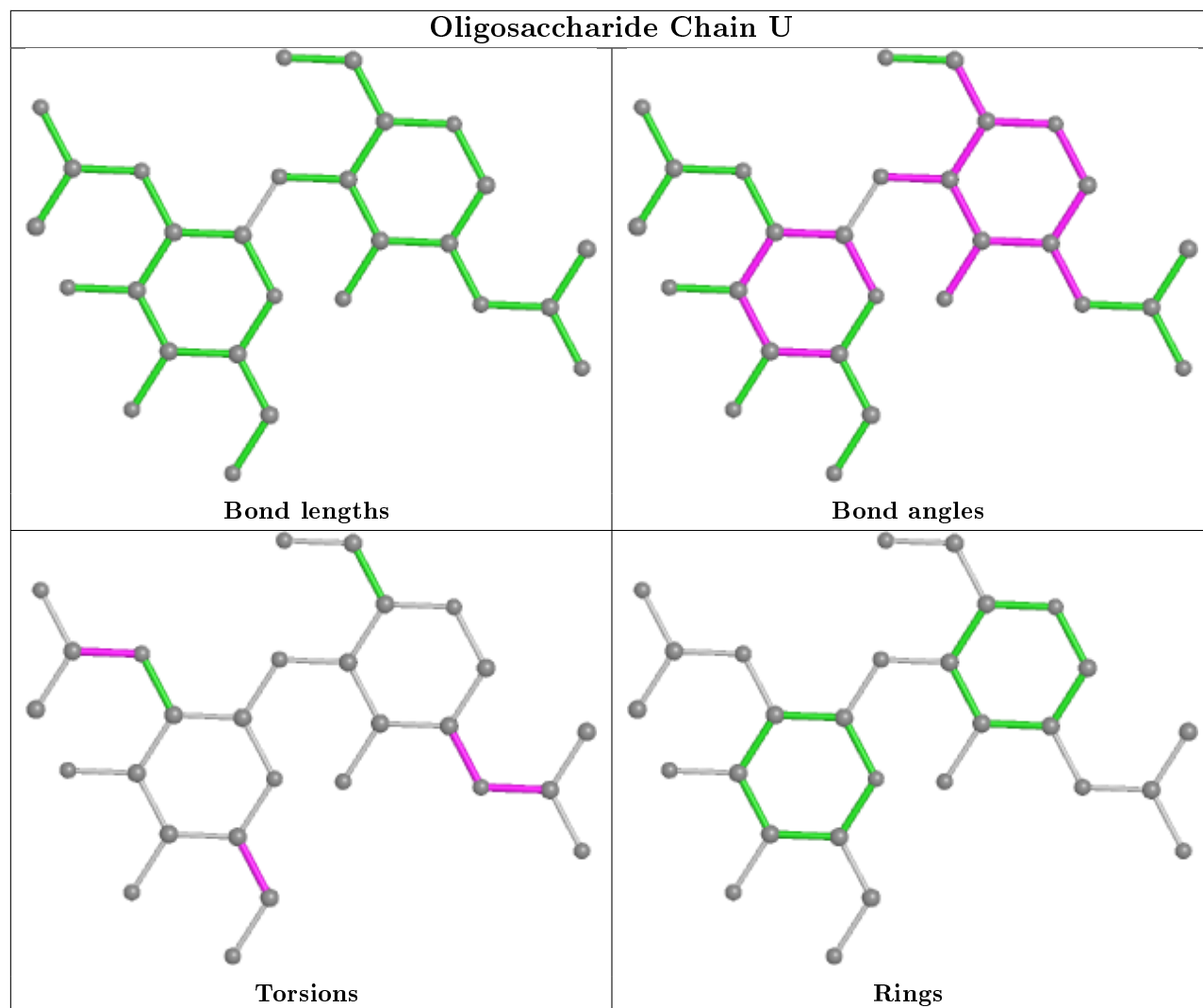
8 monomers are involved in 10 short contacts:

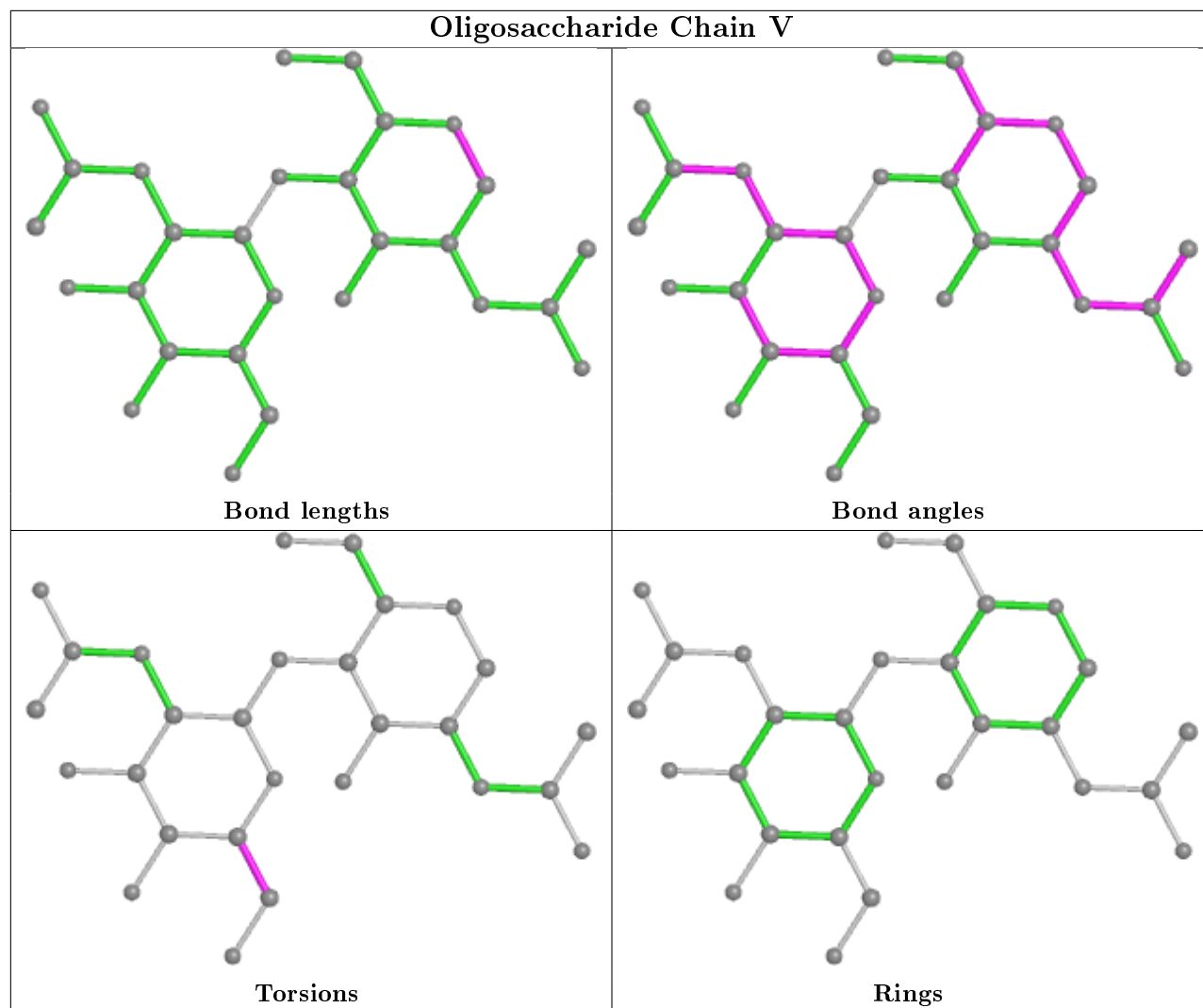
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	2	NAG	1	0
3	Y	1	NAG	2	0
3	S	1	NAG	1	0
3	Y	2	NAG	2	0
4	T	2	NAG	3	0
4	X	3	BMA	3	0
3	U	1	NAG	1	0
4	T	1	NAG	1	0

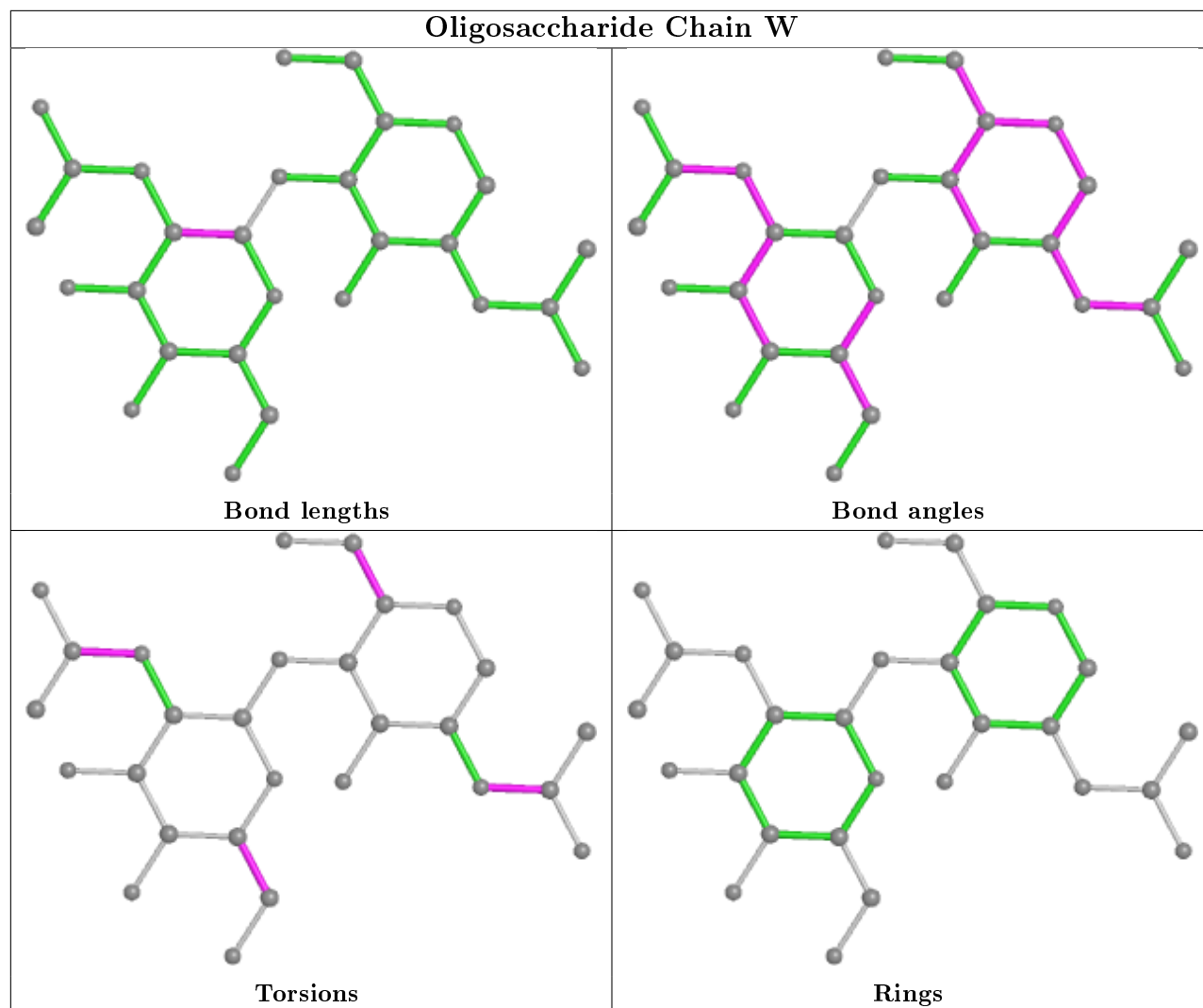
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

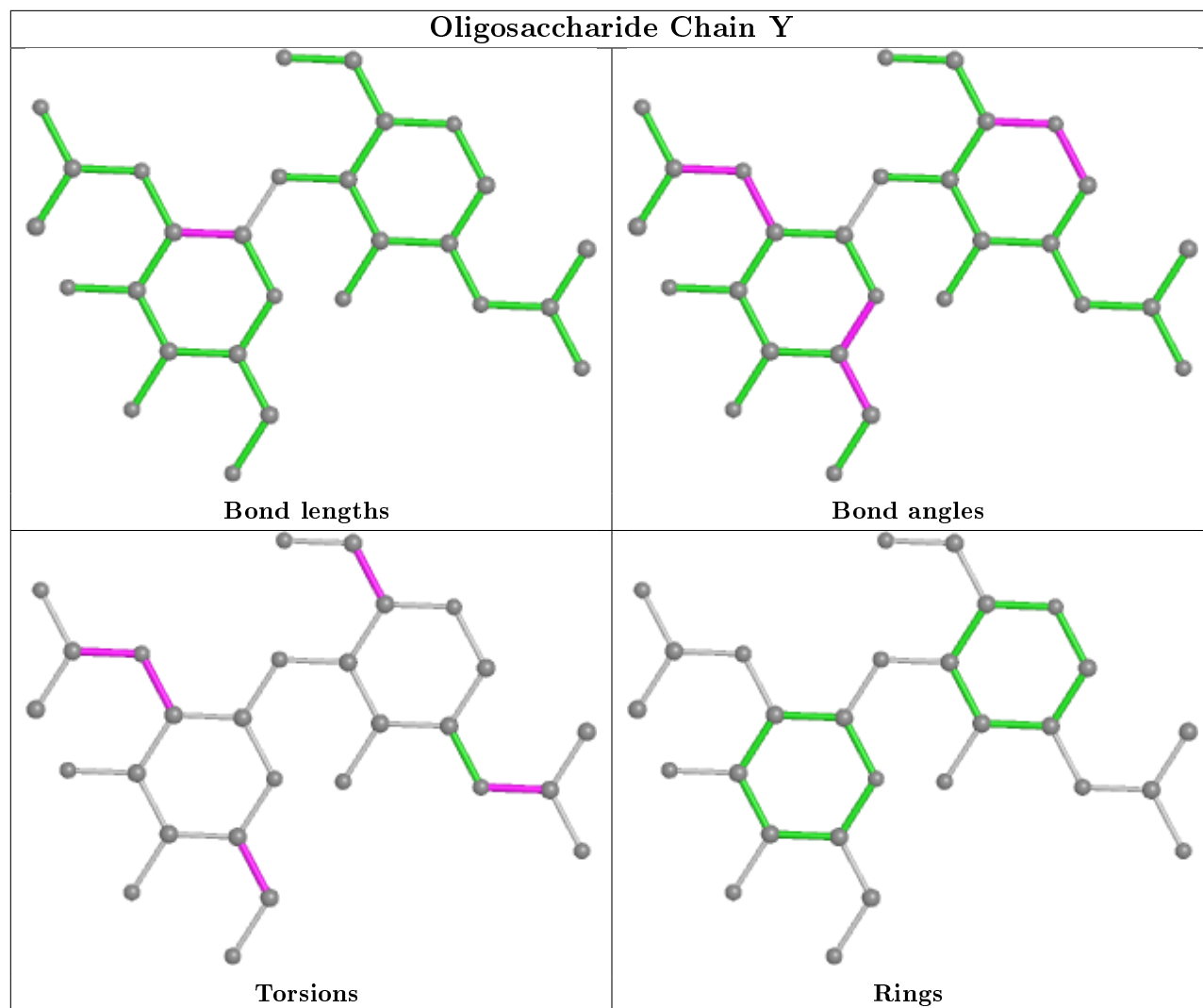


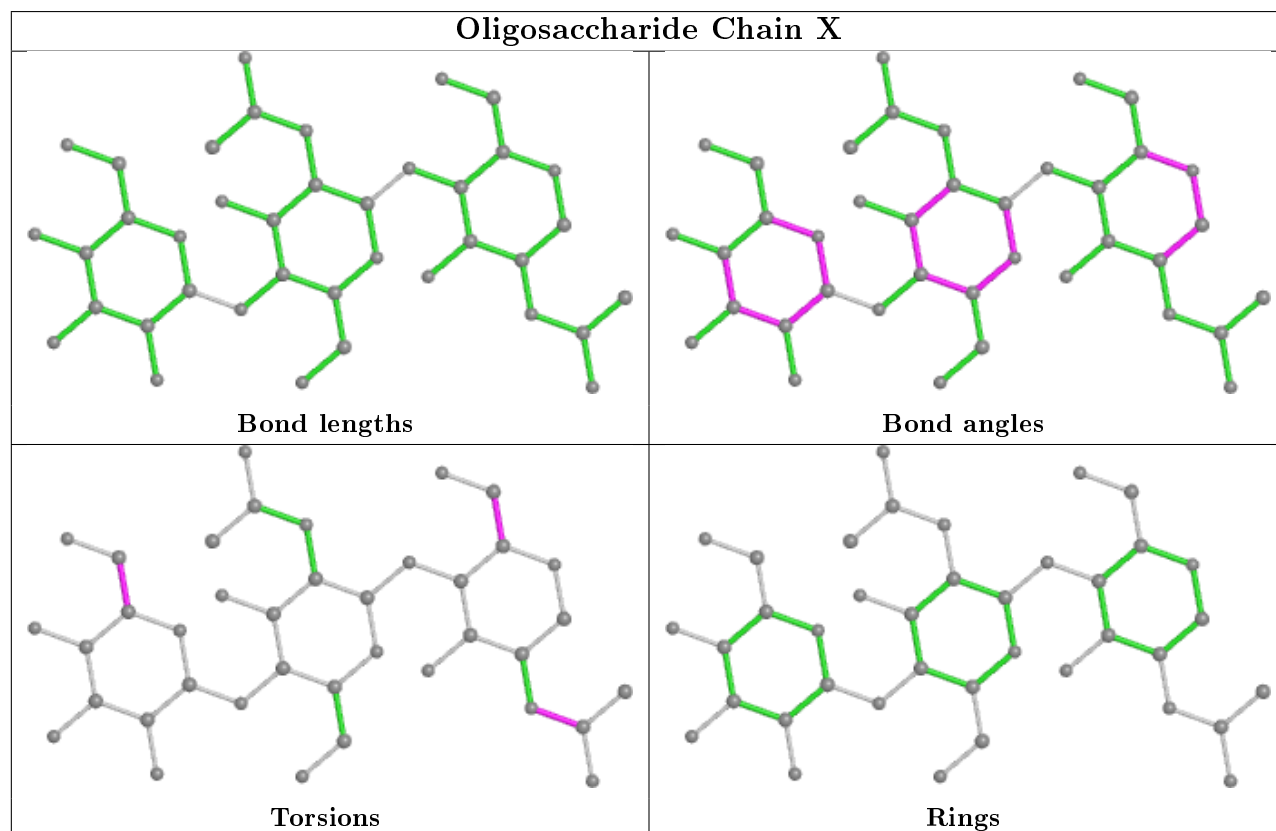
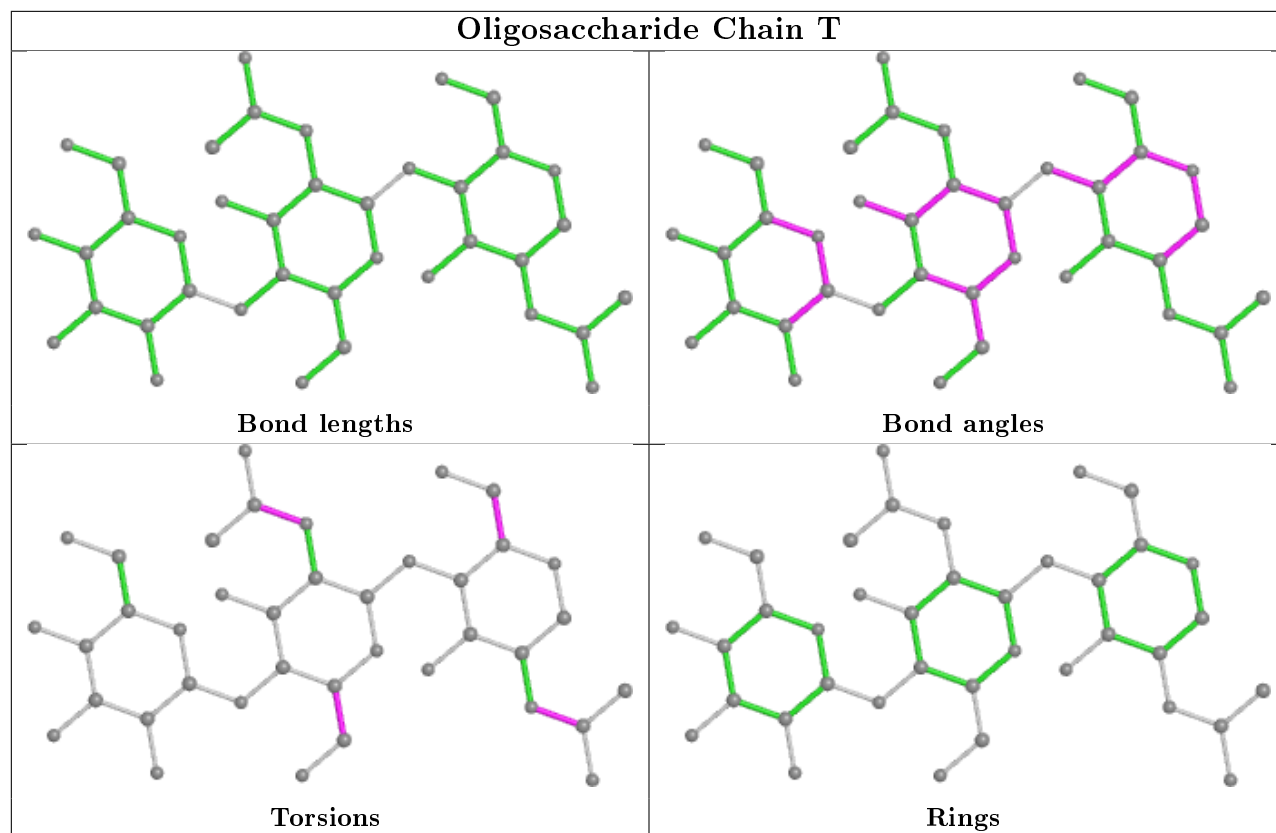


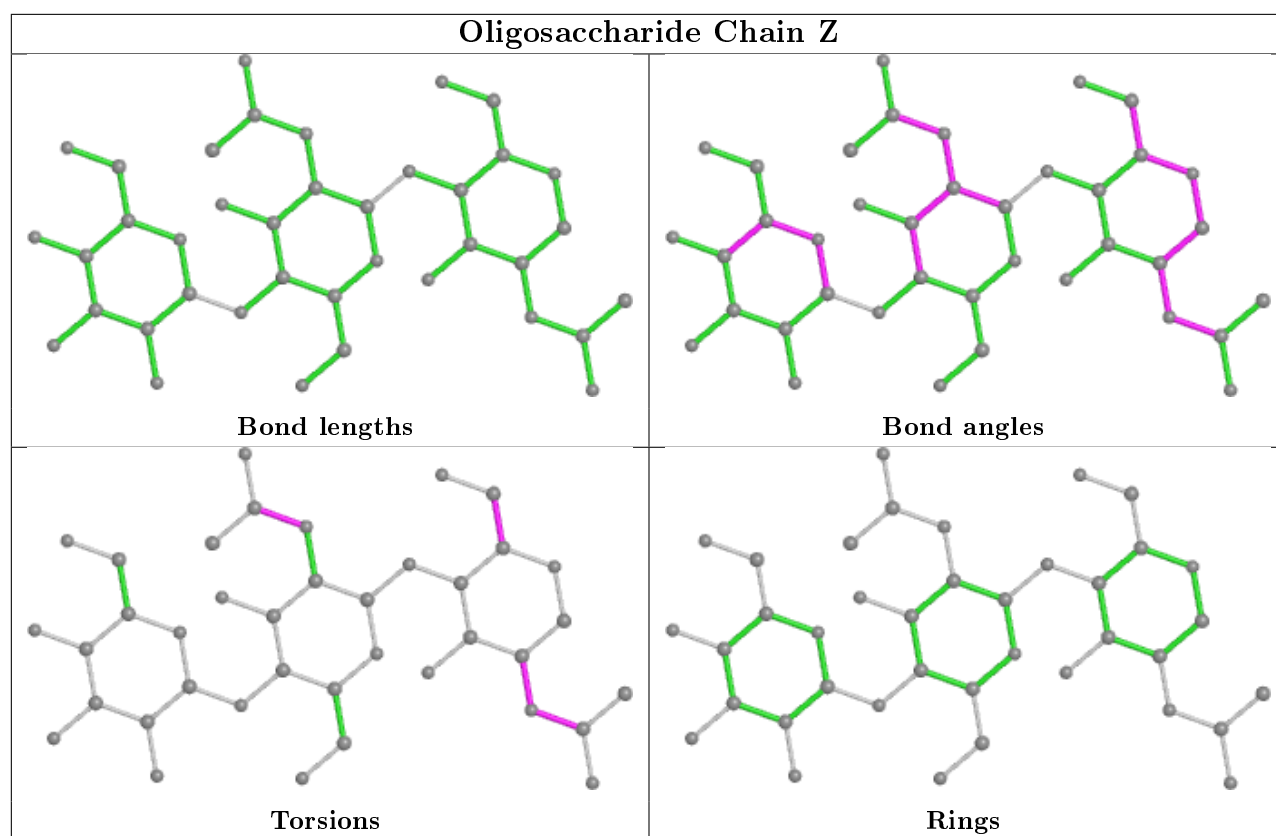












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	322/334 (96%)	1.28	51 (15%) 2 1	70, 71, 72, 73	0
1	C	322/334 (96%)	1.19	45 (13%) 2 1	70, 71, 72, 73	0
1	E	322/334 (96%)	1.35	46 (14%) 2 1	70, 71, 72, 73	0
1	G	322/334 (96%)	1.30	42 (13%) 3 2	70, 71, 72, 73	0
1	I	322/334 (96%)	1.28	50 (15%) 2 1	70, 71, 72, 73	0
1	K	322/334 (96%)	1.38	60 (18%) 1 0	70, 71, 72, 74	0
1	M	322/334 (96%)	2.22	153 (47%) 0 0	54, 67, 75, 84	0
1	O	322/334 (96%)	2.08	140 (43%) 0 0	57, 68, 76, 83	0
1	Q	322/334 (96%)	3.58	228 (70%) 0 0	63, 72, 81, 86	0
2	B	175/181 (96%)	2.27	70 (40%) 0 0	70, 71, 72, 73	0
2	D	175/181 (96%)	2.62	89 (50%) 0 0	70, 71, 72, 73	0
2	F	175/181 (96%)	2.56	75 (42%) 0 0	70, 71, 72, 73	0
2	H	175/181 (96%)	2.81	90 (51%) 0 0	70, 71, 72, 73	0
2	J	175/181 (96%)	2.54	84 (48%) 0 0	70, 71, 72, 73	0
2	L	175/181 (96%)	2.80	88 (50%) 0 0	70, 71, 72, 73	0
2	N	175/181 (96%)	2.06	68 (38%) 0 0	55, 71, 82, 87	0
2	P	175/181 (96%)	2.13	65 (37%) 0 0	58, 68, 80, 82	0
2	R	175/181 (96%)	3.94	122 (69%) 0 0	60, 70, 85, 87	0
All	All	4473/4635 (96%)	2.06	1566 (35%) 0 0	54, 71, 77, 87	0

All (1566) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	134	GLY	20.5
1	G	324	PRO	20.3
1	I	16	GLY	18.5

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Mol	Chain	Res	Type	RSRZ
1	Q	324	PRO	18.4
1	Q	323	SER	15.6
1	A	324	PRO	14.8
1	K	16	GLY	14.7
2	F	160	PRO	14.4
2	R	175	SER	14.0
2	L	138	PHE	13.7
2	J	8	GLY	13.6
2	L	175	SER	13.0
2	J	142	HIS	12.6
2	D	138	PHE	12.5
2	H	164	GLU	12.5
2	R	64	GLU	12.3
2	L	160	PRO	12.0
2	R	65	ALA	12.0
1	Q	267	ILE	11.9
1	E	13	ILE	11.8
2	H	22	TYR	11.7
2	F	167	ARG	11.5
2	J	157	TYR	11.1
2	D	29	GLU	11.0
2	H	6	ILE	11.0
2	F	140	PHE	10.7
1	E	324	PRO	10.7
2	R	133	LEU	10.7
2	H	140	PHE	10.7
2	F	175	SER	10.6
1	Q	281	CYS	10.6
1	E	10	GLY	10.5
1	C	324	PRO	10.5
1	O	324	PRO	10.3
2	D	139	GLU	10.3
2	B	8	GLY	10.2
2	F	159	TYR	10.2
1	Q	198	PRO	10.1
1	Q	276	ASN	10.1
1	Q	309	VAL	10.0
2	R	35	ALA	10.0
2	L	19	ASP	10.0
2	J	29	GLU	9.9
1	G	14	CYS	9.8
2	R	168	LEU	9.7

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Mol	Chain	Res	Type	RSRZ
2	J	7	ALA	9.6
2	R	63	PHE	9.6
2	R	129	ASN	9.6
2	R	130	ALA	9.6
1	Q	60	ILE	9.5
2	P	174	SER	9.2
1	Q	303	GLY	9.1
1	M	324	PRO	9.1
2	B	2	LEU	9.1
1	Q	82(A)	PRO	9.1
1	M	189	ALA	9.0
2	N	174	SER	9.0
1	Q	262	LYS	9.0
2	R	147	GLU	9.0
1	O	188	ALA	8.9
2	R	156	THR	8.9
2	R	19	ASP	8.8
1	Q	322	ASN	8.8
1	Q	254	PRO	8.7
2	R	160	PRO	8.7
2	L	157	TYR	8.7
2	R	17	MET	8.6
1	Q	26	ASP	8.6
2	R	158	ASP	8.6
2	B	29	GLU	8.6
2	D	167	ARG	8.5
2	L	156	THR	8.5
2	R	144	CYS	8.5
2	L	139	GLU	8.5
2	F	139	GLU	8.5
2	H	18	VAL	8.4
2	J	23	GLY	8.4
2	F	29	GLU	8.3
2	R	27	SER	8.3
1	Q	167	SER	8.2
1	Q	304	GLU	8.2
2	L	25	HIS	8.2
2	P	175	SER	8.1
2	R	143	LYS	8.1
2	L	174	SER	8.1
1	Q	256	TYR	8.0
2	F	142	HIS	8.0

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Mol	Chain	Res	Type	RSRZ
1	E	80	ILE	8.0
1	O	51	LEU	8.0
2	H	141	TYR	8.0
2	J	174	SER	8.0
2	R	174	SER	8.0
1	Q	176	LEU	8.0
2	R	138	PHE	8.0
2	D	170	ARG	7.9
2	P	5	ALA	7.9
1	I	15	ILE	7.8
1	Q	296	ASN	7.8
2	L	141	TYR	7.8
1	Q	133(A)	LEU	7.8
1	Q	151	VAL	7.7
2	R	14	TRP	7.7
2	H	8	GLY	7.7
1	Q	125(B)	SER	7.7
2	H	157	TYR	7.7
2	D	23	GLY	7.7
2	B	147	GLU	7.6
1	A	16	GLY	7.6
2	H	16	GLY	7.6
1	Q	61	LEU	7.5
1	O	192	THR	7.5
2	R	125	GLN	7.5
1	M	166	ARG	7.4
2	H	32	SER	7.4
1	Q	133	SER	7.4
2	H	147	GLU	7.4
1	Q	76	CYS	7.4
2	R	146	ASN	7.4
1	K	55	GLY	7.3
2	R	73	LEU	7.3
2	L	1	GLY	7.3
2	P	173	ILE	7.3
2	H	1	GLY	7.3
2	R	28	ASN	7.3
2	R	135	ASN	7.2
2	J	173	ILE	7.2
1	Q	64	CYS	7.2
1	Q	302	ILE	7.1
2	F	22	TYR	7.1

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Mol	Chain	Res	Type	RSRZ
1	K	79	PHE	7.1
1	Q	52	CYS	7.0
1	Q	38	HIS	7.0
1	Q	58	PRO	7.0
2	D	1	GLY	7.0
2	B	1	GLY	7.0
1	M	174	GLU	7.0
1	E	12	GLN	7.0
2	F	8	GLY	7.0
1	Q	18	HIS	6.9
1	Q	150	ASN	6.9
1	Q	188	ALA	6.9
1	M	10	GLY	6.9
1	Q	68	GLY	6.9
2	R	145	ASP	6.9
2	R	23	GLY	6.9
2	B	144	CYS	6.9
1	C	79	PHE	6.9
2	H	9	PHE	6.8
1	Q	282	GLN	6.8
2	F	138	PHE	6.8
1	M	199	THR	6.8
1	O	248	ASN	6.8
1	Q	82	VAL	6.8
2	F	143	LYS	6.8
2	N	173	ILE	6.8
1	Q	118	PHE	6.7
1	Q	170	ASN	6.7
1	O	10	GLY	6.7
2	H	5	ALA	6.7
1	Q	129	SER	6.7
2	H	138	PHE	6.7
2	H	132	GLU	6.7
2	H	163	SER	6.7
2	L	140	PHE	6.7
1	Q	79	PHE	6.6
2	H	21	TRP	6.6
2	L	4	GLY	6.6
2	R	29	GLU	6.6
2	J	1	GLY	6.6
1	O	127	TRP	6.6
2	P	28	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
1	O	156	LYS	6.6
1	Q	155	ILE	6.6
1	O	152	VAL	6.6
1	K	324	PRO	6.5
2	J	175	SER	6.5
2	F	141	TYR	6.5
1	Q	253	ALA	6.5
2	R	7	ALA	6.5
2	J	6	ILE	6.5
2	H	10	ILE	6.4
1	M	12	GLN	6.4
1	M	55	GLY	6.4
1	O	80	ILE	6.4
2	P	166	ALA	6.4
2	P	156	THR	6.4
1	M	188	ALA	6.4
1	G	13	ILE	6.3
2	L	24	TYR	6.3
2	F	148	CYS	6.3
1	G	12	GLN	6.3
2	L	22	TYR	6.3
1	Q	25	VAL	6.3
2	N	125	GLN	6.3
2	R	148	CYS	6.2
2	N	7	ALA	6.2
1	Q	288	ILE	6.2
2	D	35	ALA	6.2
2	L	32	SER	6.2
2	N	175	SER	6.2
2	J	168	LEU	6.2
1	E	17	TYR	6.2
1	Q	13	ILE	6.1
1	Q	144	LYS	6.1
2	N	172	GLU	6.1
1	Q	258	TYR	6.1
2	H	29	GLU	6.1
2	L	130	ALA	6.1
1	K	15	ILE	6.1
2	L	167	ARG	6.1
1	Q	237	LEU	6.1
2	P	145	ASP	6.0
2	J	27	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	76	CYS	6.0
1	O	79	PHE	6.0
2	D	9	PHE	6.0
1	K	12	GLN	6.0
2	B	60	ASN	6.0
1	Q	305	CYS	6.0
2	R	163	SER	6.0
2	N	139	GLU	6.0
2	B	18	VAL	6.0
2	D	25	HIS	6.0
1	Q	219	THR	5.9
1	E	78	GLU	5.9
2	P	168	LEU	5.9
1	Q	194	LEU	5.9
1	A	323	SER	5.9
1	O	141	TYR	5.9
2	B	30	GLN	5.9
2	J	3	PHE	5.9
2	B	28	ASN	5.9
1	I	324	PRO	5.9
1	Q	131	GLU	5.9
2	F	174	SER	5.9
2	H	137	CYS	5.9
1	Q	171	THR	5.9
2	R	132	GLU	5.8
2	L	28	ASN	5.8
1	M	154	LEU	5.8
2	L	149	MET	5.8
2	R	150	GLU	5.8
2	D	155	GLY	5.8
2	F	144	CYS	5.8
2	H	17	MET	5.8
2	F	161	GLN	5.7
1	I	12	GLN	5.7
2	N	27	SER	5.7
2	J	131	LYS	5.7
2	L	166	ALA	5.7
1	O	158	ASN	5.7
1	Q	128	SER	5.7
2	N	162	TYR	5.7
2	N	145	ASP	5.7
2	J	139	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	15	ILE	5.7
2	L	8	GLY	5.7
2	J	28	ASN	5.6
1	G	15	ILE	5.6
2	R	18	VAL	5.6
1	Q	130	HIS	5.6
1	Q	62	ARG	5.6
2	B	23	GLY	5.6
2	J	143	LYS	5.6
2	L	9	PHE	5.6
2	H	142	HIS	5.6
2	H	36	ALA	5.6
1	Q	263	LYS	5.6
2	F	145	ASP	5.6
1	M	79	PHE	5.5
2	F	157	TYR	5.5
1	M	209	LEU	5.5
2	L	164	GLU	5.5
2	J	25	HIS	5.5
1	Q	63	ASP	5.5
1	M	64	CYS	5.5
2	D	22	TYR	5.5
2	L	163	SER	5.5
2	R	8	GLY	5.5
2	H	143	LYS	5.5
2	H	167	ARG	5.5
1	C	322	ASN	5.5
2	H	139	GLU	5.5
1	Q	252	ILE	5.4
2	D	132	GLU	5.4
1	M	200	THR	5.4
2	P	142	HIS	5.4
2	D	174	SER	5.4
2	L	27	SER	5.4
1	E	318	THR	5.4
2	F	26	HIS	5.4
1	O	133(A)	LEU	5.4
2	B	7	ALA	5.4
2	L	137	CYS	5.4
2	F	16	GLY	5.4
1	K	13	ILE	5.4
1	O	252	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
2	J	18	VAL	5.4
1	M	81	ASN	5.4
1	M	158	ASN	5.4
2	L	170	ARG	5.4
2	R	5	ALA	5.3
1	M	129	SER	5.3
2	D	163	SER	5.3
2	D	124	LEU	5.3
1	M	192	THR	5.3
1	M	128	SER	5.3
2	H	175	SER	5.3
2	P	8	GLY	5.3
2	R	20	GLY	5.3
1	M	256	TYR	5.3
2	L	171	GLU	5.3
2	R	12	GLY	5.3
1	Q	307	LYS	5.3
1	E	11	ASP	5.3
1	K	11	ASP	5.3
2	R	4	GLY	5.3
1	M	322	ASN	5.3
2	B	168	LEU	5.3
1	K	276	ASN	5.2
1	Q	310	LYS	5.2
2	P	141	TYR	5.2
1	Q	260	ILE	5.2
1	O	68	GLY	5.2
1	O	253	ALA	5.2
2	D	141	TYR	5.2
1	A	14	CYS	5.2
1	K	17	TYR	5.2
2	P	139	GLU	5.2
1	Q	318	THR	5.2
2	J	132	GLU	5.1
1	G	17	TYR	5.1
2	H	14	TRP	5.1
1	I	11	ASP	5.1
2	D	19	ASP	5.1
1	Q	286	GLY	5.1
1	A	290	SER	5.1
2	N	5	ALA	5.1
2	H	173	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
2	R	149	MET	5.1
1	I	20	ASN	5.1
1	K	81	ASN	5.1
1	Q	46	LYS	5.1
1	I	323	SER	5.1
1	Q	285	MET	5.1
2	L	7	ALA	5.1
1	O	48	ASN	5.1
1	M	77	ASP	5.1
1	Q	308	TYR	5.0
1	O	13	ILE	5.0
1	G	78	GLU	5.0
2	D	27	SER	5.0
1	C	289	ASN	5.0
1	Q	88	VAL	5.0
2	H	31	GLY	5.0
1	Q	291	SER	5.0
1	M	198	PRO	5.0
2	L	142	HIS	5.0
2	R	141	TYR	5.0
2	D	168	LEU	5.0
2	R	170	ARG	5.0
1	M	17	TYR	4.9
1	M	205	GLY	4.9
2	D	34	TYR	4.9
1	K	14	CYS	4.9
2	L	29	GLU	4.9
2	N	17	MET	4.9
2	L	162	TYR	4.9
1	G	318	THR	4.9
2	B	146	ASN	4.9
2	F	149	MET	4.9
1	Q	152	VAL	4.9
1	O	98	TYR	4.9
1	Q	229	ARG	4.9
1	Q	236	ILE	4.9
2	R	157	TYR	4.8
1	A	22	THR	4.8
1	G	10	GLY	4.8
1	Q	42	ILE	4.8
2	J	162	TYR	4.8
2	R	40	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	16	GLY	4.8
1	M	187	ASP	4.8
2	D	131	LYS	4.8
2	R	159	TYR	4.8
2	R	162	TYR	4.8
1	Q	255	GLU	4.8
2	F	170	ARG	4.8
1	Q	244	ASN	4.8
2	J	2	LEU	4.8
2	H	26	HIS	4.8
2	P	147	GLU	4.8
1	Q	197	ASN	4.8
1	C	14	CYS	4.8
2	R	3	PHE	4.8
1	M	201	TYR	4.8
1	Q	84	TRP	4.7
1	M	91	ALA	4.7
2	F	156	THR	4.7
2	J	144	CYS	4.7
2	D	159	TYR	4.7
2	D	171	GLU	4.7
2	P	125	GLN	4.7
1	Q	53	ASP	4.7
2	D	60	ASN	4.7
2	H	155	GLY	4.7
1	Q	83	GLU	4.7
2	R	128	ASP	4.7
2	R	123	ARG	4.7
2	D	3	PHE	4.7
1	M	194	LEU	4.7
1	I	21	SER	4.7
2	N	28	ASN	4.6
1	M	122	GLN	4.6
2	R	21	TRP	4.6
1	Q	230	MET	4.6
1	M	225	GLY	4.6
1	Q	228	GLY	4.6
2	F	128	ASP	4.6
1	O	160	THR	4.6
1	O	81	ASN	4.6
2	N	144	CYS	4.6
2	P	18	VAL	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Q	195	TYR	4.6
2	L	60	ASN	4.6
2	N	140	PHE	4.6
2	B	31	GLY	4.6
2	N	1	GLY	4.6
1	O	129	SER	4.6
2	D	143	LYS	4.6
2	H	35	ALA	4.6
2	J	137	CYS	4.6
2	R	49	THR	4.6
1	O	201	TYR	4.6
2	L	144	CYS	4.6
2	D	144	CYS	4.5
2	P	45	ILE	4.5
1	M	184	HIS	4.5
2	B	22	TYR	4.5
2	R	16	GLY	4.5
1	C	13	ILE	4.5
2	F	27	SER	4.5
1	M	133(A)	LEU	4.5
2	L	5	ALA	4.5
1	O	283	THR	4.5
2	F	3	PHE	4.5
2	H	161	GLN	4.5
1	C	15	ILE	4.5
1	Q	127	TRP	4.5
1	Q	266	THR	4.5
2	R	136	GLY	4.5
2	B	162	TYR	4.5
2	D	175	SER	4.5
2	L	152	VAL	4.5
2	R	173	ILE	4.5
1	I	322	ASN	4.5
1	Q	274	TYR	4.5
1	O	322	ASN	4.4
1	Q	19(A)	ASN	4.4
2	F	2	LEU	4.4
1	C	323	SER	4.4
1	A	13	ILE	4.4
1	G	80	ILE	4.4
2	F	164	GLU	4.4
2	P	30	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	20	ASN	4.4
1	M	48	ASN	4.4
1	Q	113	SER	4.4
2	L	127	ARG	4.4
1	O	54	ASP	4.4
2	R	46	ASP	4.4
1	O	117	HIS	4.4
2	H	165	GLU	4.4
1	Q	208	THR	4.4
2	R	11	GLU	4.4
2	F	12	GLY	4.4
2	P	134	GLY	4.4
2	R	22	TYR	4.4
1	Q	157	LYS	4.4
1	Q	23	GLU	4.4
1	O	67	ALA	4.4
1	I	51	LEU	4.4
2	H	172	GLU	4.4
2	R	31	GLY	4.4
2	P	167	ARG	4.3
1	K	323	SER	4.3
1	O	112	LEU	4.3
2	J	133	LEU	4.3
1	Q	15	ILE	4.3
2	R	50	ASN	4.3
2	D	164	GLU	4.3
1	Q	77	ASP	4.3
1	M	76	CYS	4.3
1	Q	290	SER	4.3
2	R	126	LEU	4.3
2	R	45	ILE	4.3
2	N	133	LEU	4.3
1	A	143	GLY	4.3
1	M	221	SER	4.3
2	J	4	GLY	4.3
1	O	225	GLY	4.3
1	O	163	THR	4.3
2	R	172	GLU	4.3
1	M	283	THR	4.3
1	K	20	ASN	4.3
2	N	45	ILE	4.3
2	F	28	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	21	SER	4.3
2	B	38	LYS	4.3
2	B	5	ALA	4.2
2	N	154	ASN	4.2
1	O	251	PHE	4.2
2	N	132	GLU	4.2
2	P	35	ALA	4.2
1	O	132	ALA	4.2
1	O	189	ALA	4.2
2	L	148	CYS	4.2
2	R	41	THR	4.2
2	R	127	ARG	4.2
2	R	161	GLN	4.2
2	F	147	GLU	4.2
1	C	16	GLY	4.2
1	Q	265	SER	4.2
2	D	156	THR	4.2
2	R	61	THR	4.2
1	Q	261	VAL	4.2
2	N	134	GLY	4.2
2	D	31	GLY	4.2
2	J	166	ALA	4.2
2	F	158	ASP	4.2
1	A	322	ASN	4.2
1	M	210	ASN	4.2
1	Q	193	LYS	4.2
1	Q	269	LYS	4.2
2	H	160	PRO	4.2
1	Q	168	TYR	4.2
2	H	144	CYS	4.2
1	M	41	ASP	4.2
1	M	116	ASN	4.2
1	Q	75	MET	4.2
2	L	36	ALA	4.2
1	I	79	PHE	4.2
1	O	199	THR	4.2
2	D	4	GLY	4.2
1	O	161	TYR	4.2
1	K	19(A)	ASN	4.1
1	Q	81	ASN	4.1
2	J	135	ASN	4.1
2	J	136	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	130	ALA	4.1
2	J	172	GLU	4.1
2	R	118	LEU	4.1
1	E	79	PHE	4.1
1	Q	97	CYS	4.1
1	Q	39	ALA	4.1
1	Q	24	GLN	4.1
2	J	30	GLN	4.1
2	P	46	ASP	4.1
1	Q	49	GLY	4.1
2	H	34	TYR	4.1
2	D	122	VAL	4.1
1	Q	182	ILE	4.1
1	Q	292	MET	4.1
1	M	246	GLU	4.1
1	Q	279	THR	4.1
1	Q	143	GLY	4.1
1	Q	319	GLY	4.1
2	N	8	GLY	4.1
1	A	23	GLU	4.1
2	D	24	TYR	4.1
2	N	34	TYR	4.1
1	C	55	GLY	4.1
1	G	76	CYS	4.1
1	O	184	HIS	4.0
2	J	22	TYR	4.0
2	B	157	TYR	4.0
2	P	144	CYS	4.0
2	R	56	ILE	4.0
1	Q	191	GLN	4.0
2	N	141	TYR	4.0
2	H	156	THR	4.0
1	O	140	PRO	4.0
2	N	160	PRO	4.0
1	I	141	TYR	4.0
2	D	61	THR	4.0
2	J	138	PHE	4.0
1	Q	189	ALA	4.0
2	R	137	CYS	4.0
2	D	8	GLY	4.0
1	E	186	ASN	4.0
1	O	77	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	132	ALA	4.0
1	O	285	MET	4.0
2	L	16	GLY	4.0
2	B	145	ASP	4.0
2	D	28	ASN	4.0
1	Q	153	TRP	4.0
1	M	242	ALA	4.0
2	H	23	GLY	4.0
1	M	190	GLU	4.0
2	R	53	ASN	4.0
1	M	143	GLY	4.0
2	B	131	LYS	3.9
2	B	158	ASP	3.9
2	B	6	ILE	3.9
1	Q	67	ALA	3.9
2	B	3	PHE	3.9
1	Q	242	ALA	3.9
1	Q	174	GLU	3.9
2	F	60	ASN	3.9
2	J	171	GLU	3.9
1	O	75	MET	3.9
2	F	38	LYS	3.9
2	D	2	LEU	3.9
1	A	21	SER	3.9
1	O	159	SER	3.9
2	F	163	SER	3.9
2	N	163	SER	3.9
2	B	4	GLY	3.9
2	B	155	GLY	3.9
2	D	146	ASN	3.9
1	Q	295	HIS	3.9
2	B	143	LYS	3.9
2	R	58	LYS	3.9
1	C	12	GLN	3.9
2	B	173	ILE	3.9
2	D	173	ILE	3.9
1	Q	259	LYS	3.9
2	B	27	SER	3.9
1	Q	199	THR	3.9
1	I	240	ASN	3.9
2	F	7	ALA	3.9
2	D	158	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	Q	313	ARG	3.9
2	D	134	GLY	3.9
1	I	290	SER	3.9
2	P	159	TYR	3.8
2	H	13	GLY	3.8
2	J	61	THR	3.8
1	Q	270	SER	3.8
2	D	140	PHE	3.8
1	M	51	LEU	3.8
2	R	36	ALA	3.8
1	I	289	ASN	3.8
2	J	117	ASN	3.8
1	M	277	CYS	3.8
1	O	128	SER	3.8
2	P	27	SER	3.8
1	M	186	ASN	3.8
2	R	72	ASN	3.8
1	Q	47	HIS	3.8
2	R	37	ASP	3.8
1	G	159	SER	3.8
2	D	32	SER	3.8
2	B	138	PHE	3.8
2	H	19	ASP	3.8
2	P	140	PHE	3.8
2	R	171	GLU	3.8
1	E	141	TYR	3.8
1	M	86	TYR	3.8
2	H	131	LYS	3.8
2	H	148	CYS	3.8
1	Q	80	ILE	3.8
1	M	208	THR	3.8
1	Q	126	SER	3.8
2	R	154	ASN	3.8
1	O	206	THR	3.8
2	F	14	TRP	3.8
2	H	33	GLY	3.8
1	M	14	CYS	3.7
2	J	147	GLU	3.7
2	J	26	HIS	3.7
1	C	17	TYR	3.7
2	B	165	GLU	3.7
2	R	32	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	R	155	GLY	3.7
1	Q	173	GLN	3.7
1	M	278	ASN	3.7
2	P	162	TYR	3.7
2	B	136	GLY	3.7
2	L	159	TYR	3.7
1	M	219	THR	3.7
2	N	161	GLN	3.7
1	O	214	VAL	3.7
2	D	137	CYS	3.7
1	O	310	LYS	3.7
1	Q	45	LYS	3.7
2	R	113	SER	3.7
1	Q	111	LEU	3.7
2	F	133	LEU	3.7
2	P	133	LEU	3.7
2	L	21	TRP	3.7
1	Q	102	PHE	3.7
1	Q	56	VAL	3.7
1	C	141	TYR	3.7
1	O	155	ILE	3.7
1	M	67	ALA	3.7
2	H	133	LEU	3.7
2	R	89	LEU	3.7
1	E	21	SER	3.7
1	O	133	SER	3.7
1	M	59	LEU	3.6
1	O	194	LEU	3.6
1	Q	85	SER	3.6
1	Q	211	GLN	3.6
2	P	164	GLU	3.6
2	P	21	TRP	3.6
2	F	18	VAL	3.6
1	K	10	GLY	3.6
1	Q	43	LEU	3.6
2	P	160	PRO	3.6
2	L	41	THR	3.6
1	Q	53(A)	LEU	3.6
2	D	135	ASN	3.6
2	L	117	ASN	3.6
2	N	168	LEU	3.6
2	N	16	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	109	ASP	3.6
2	F	17	MET	3.6
1	M	257	ALA	3.6
2	D	130	ALA	3.6
1	M	254	PRO	3.6
1	O	153	TRP	3.6
2	N	42	GLN	3.6
2	P	42	GLN	3.6
1	I	60	ILE	3.6
1	Q	300	LEU	3.6
1	E	54	ASP	3.6
2	P	14	TRP	3.6
2	N	32	SER	3.6
1	M	121	ILE	3.6
2	B	172	GLU	3.6
2	L	168	LEU	3.6
2	F	6	ILE	3.6
2	D	72	ASN	3.6
2	J	167	ARG	3.6
1	Q	165	LYS	3.5
1	M	145	SER	3.5
1	M	227	SER	3.5
2	L	33	GLY	3.5
1	Q	27	THR	3.5
2	R	107	THR	3.5
1	C	186	ASN	3.5
1	Q	241	ASP	3.5
2	P	158	ASP	3.5
2	P	34	TYR	3.5
1	K	292	MET	3.5
1	K	21	SER	3.5
1	O	71	LEU	3.5
2	F	168	LEU	3.5
1	E	14	CYS	3.5
1	Q	20	ASN	3.5
2	B	141	TYR	3.5
2	D	157	TYR	3.5
1	A	292	MET	3.5
2	B	175	SER	3.5
1	K	160	THR	3.5
2	H	159	TYR	3.5
2	P	24	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
2	P	126	LEU	3.5
2	J	120	ASP	3.5
2	J	12	GLY	3.5
1	M	142	GLN	3.5
2	R	52	VAL	3.5
2	P	172	GLU	3.5
2	R	140	PHE	3.5
1	C	20	ASN	3.5
1	O	154	LEU	3.5
2	B	10	ILE	3.5
1	M	159	SER	3.5
1	Q	283	THR	3.5
1	G	317	ALA	3.5
2	D	5	ALA	3.5
2	N	3	PHE	3.5
1	Q	72	GLY	3.5
2	B	21	TRP	3.5
2	B	142	HIS	3.5
1	O	66	VAL	3.5
2	P	13	GLY	3.4
2	F	137	CYS	3.4
1	M	108	LEU	3.4
1	Q	158	ASN	3.4
1	Q	192	THR	3.4
2	P	165	GLU	3.4
1	C	19(A)	ASN	3.4
1	C	22	THR	3.4
1	G	31	MET	3.4
1	M	230	MET	3.4
2	P	111	HIS	3.4
1	Q	116	ASN	3.4
1	Q	138	ALA	3.4
2	D	166	ALA	3.4
1	M	323	SER	3.4
1	O	95	ASN	3.4
1	Q	212	ARG	3.4
2	J	109	ASP	3.4
1	A	33	LYS	3.4
2	F	132	GLU	3.4
1	O	41	ASP	3.4
2	L	151	SER	3.4
1	Q	94	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	142	HIS	3.4
2	H	4	GLY	3.4
2	P	161	GLN	3.4
1	Q	117	HIS	3.4
2	R	1	GLY	3.4
2	P	19	ASP	3.4
1	O	62	ARG	3.4
2	H	7	ALA	3.4
2	F	9	PHE	3.4
1	O	256	TYR	3.4
1	G	11	ASP	3.4
1	Q	35(A)	THR	3.4
2	L	145	ASP	3.4
2	N	21	TRP	3.4
2	N	41	THR	3.4
2	L	165	GLU	3.4
2	P	4	GLY	3.4
2	J	60	ASN	3.4
2	R	79	ASN	3.4
2	L	161	GLN	3.3
1	Q	140	PRO	3.3
1	Q	55	GLY	3.3
2	F	152	VAL	3.3
1	G	323	SER	3.3
1	M	240	ASN	3.3
1	M	37	THR	3.3
1	M	127	TRP	3.3
2	H	118	LEU	3.3
2	L	2	LEU	3.3
1	Q	321	ARG	3.3
1	M	101	ASP	3.3
2	J	38	LYS	3.3
2	R	121	LYS	3.3
1	Q	12	GLN	3.3
1	G	33	LYS	3.3
2	J	106	ARG	3.3
2	N	170	ARG	3.3
1	Q	137	SER	3.3
1	Q	184	HIS	3.3
2	H	158	ASP	3.3
2	H	168	LEU	3.3
1	A	318	THR	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	10	GLY	3.3
2	N	6	ILE	3.3
2	D	160	PRO	3.3
1	O	174	GLU	3.3
2	L	147	GLU	3.3
2	P	26	HIS	3.3
2	H	60	ASN	3.3
2	J	165	GLU	3.3
1	E	322	ASN	3.3
1	O	224	ASN	3.3
1	Q	57	LYS	3.3
2	H	2	LEU	3.3
1	Q	264	GLY	3.3
1	A	80	ILE	3.3
1	Q	115	ILE	3.3
2	F	10	ILE	3.3
1	M	163	THR	3.3
1	M	241	ASP	3.3
1	Q	312	ASN	3.3
2	N	60	ASN	3.3
1	M	13	ILE	3.3
2	L	3	PHE	3.3
2	N	61	THR	3.3
2	R	116	LYS	3.3
2	F	1	GLY	3.3
2	J	24	TYR	3.3
2	N	159	TYR	3.3
2	N	147	GLU	3.3
1	A	24	GLN	3.3
1	O	205	GLY	3.3
2	J	155	GLY	3.3
1	Q	11	ASP	3.2
1	E	290	SER	3.2
1	M	193	LYS	3.2
2	R	26	HIS	3.2
2	H	28	ASN	3.2
1	Q	246	GLU	3.2
2	L	169	LYS	3.2
1	C	290	SER	3.2
1	E	276	ASN	3.2
1	M	217	ILE	3.2
1	O	151	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	40	GLN	3.2
1	I	292	MET	3.2
2	B	156	THR	3.2
2	B	25	HIS	3.2
1	C	145	SER	3.2
1	Q	169	ASN	3.2
2	H	171	GLU	3.2
2	F	127	ARG	3.2
2	J	140	PHE	3.2
1	O	65	SER	3.2
2	D	151	SER	3.2
2	N	36	ALA	3.2
1	A	101	ASP	3.2
2	H	127	ARG	3.2
2	F	166	ALA	3.2
2	N	25	HIS	3.2
1	M	291	SER	3.2
1	Q	65	SER	3.2
1	Q	311	SER	3.2
1	O	212	ARG	3.2
1	E	77	ASP	3.2
1	K	142	GLN	3.2
1	K	290	SER	3.2
2	D	33	GLY	3.2
2	R	139	GLU	3.2
1	I	142	GLN	3.2
1	K	322	ASN	3.2
2	J	113	SER	3.2
1	Q	297	ILE	3.1
1	I	14	CYS	3.1
1	K	25	VAL	3.1
2	H	146	ASN	3.1
1	M	54	ASP	3.1
2	P	170	ARG	3.1
1	M	214	VAL	3.1
2	H	166	ALA	3.1
1	O	275	GLY	3.1
1	E	158	ASN	3.1
2	P	40	SER	3.1
2	D	128	ASP	3.1
2	H	153	ARG	3.1
2	R	9	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	157	LYS	3.1
1	K	80	ILE	3.1
1	Q	287	ALA	3.1
2	J	5	ALA	3.1
2	H	111	HIS	3.1
1	Q	78	GLU	3.1
1	I	291	SER	3.1
1	M	20	ASN	3.1
1	M	290	SER	3.1
1	Q	203	SER	3.1
2	B	114	ASN	3.1
1	Q	132	ALA	3.1
2	D	161	GLN	3.1
2	N	167	ARG	3.1
1	O	241	ASP	3.1
1	O	284	PRO	3.1
1	M	60	ILE	3.1
1	O	191	GLN	3.1
1	A	141	TYR	3.1
2	L	34	TYR	3.1
2	P	72	ASN	3.1
2	R	119	TYR	3.1
2	N	4	GLY	3.1
1	K	132	ALA	3.1
2	R	39	GLU	3.1
2	F	25	HIS	3.1
1	M	95	ASN	3.1
1	O	86	TYR	3.1
2	R	24	TYR	3.1
2	R	42	GLN	3.1
2	N	148	CYS	3.1
2	B	9	PHE	3.1
1	M	125(B)	SER	3.1
1	O	166	ARG	3.1
2	F	33	GLY	3.1
1	M	191	GLN	3.1
2	L	14	TRP	3.1
2	L	37	ASP	3.1
1	E	20	ASN	3.1
1	I	81	ASN	3.1
2	F	124	LEU	3.0
1	M	183	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	21	TRP	3.0
1	A	15	ILE	3.0
1	Q	163	THR	3.0
2	J	32	SER	3.0
2	J	34	TYR	3.0
1	C	80	ILE	3.0
2	R	66	VAL	3.0
1	Q	227	SER	3.0
2	B	106	ARG	3.0
2	D	152	VAL	3.0
1	C	276	ASN	3.0
1	M	287	ALA	3.0
2	L	35	ALA	3.0
2	P	60	ASN	3.0
2	F	32	SER	3.0
1	M	87	ILE	3.0
1	O	60	ILE	3.0
2	R	84	MET	3.0
2	H	152	VAL	3.0
1	K	46	LYS	3.0
1	Q	240	ASN	3.0
2	N	26	HIS	3.0
1	M	139	CYS	3.0
1	E	320	LEU	3.0
1	Q	145	SER	3.0
1	O	216	ARG	3.0
1	M	11	ASP	3.0
2	B	112	ASP	3.0
2	B	125	GLN	3.0
2	N	46	ASP	3.0
1	M	119	GLU	3.0
2	B	17	MET	3.0
2	B	35	ALA	3.0
2	R	151	SER	3.0
1	Q	196	GLN	3.0
1	O	185	PRO	2.9
1	K	173	GLN	2.9
1	G	25	VAL	2.9
2	F	155	GLY	2.9
2	R	30	GLN	2.9
1	O	40	GLN	2.9
2	L	146	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	45	ILE	2.9
2	R	86	ASP	2.9
2	J	149	MET	2.9
1	M	52	CYS	2.9
2	F	35	ALA	2.9
2	L	26	HIS	2.9
1	M	175	ASP	2.9
2	F	111	HIS	2.9
2	N	165	GLU	2.9
2	P	22	TYR	2.9
1	Q	178	VAL	2.9
1	Q	214	VAL	2.9
2	H	170	ARG	2.9
2	R	62	GLN	2.9
1	K	52	CYS	2.9
1	E	25	VAL	2.9
1	O	219	THR	2.9
2	D	119	TYR	2.9
1	M	267	ILE	2.9
1	I	315	VAL	2.9
1	O	14	CYS	2.9
2	J	11	GLU	2.9
2	N	171	GLU	2.9
1	Q	271	GLU	2.8
2	R	164	GLU	2.8
1	O	146	SER	2.8
1	O	193	LYS	2.8
2	J	163	SER	2.8
1	C	199	THR	2.8
2	J	164	GLU	2.8
2	L	23	GLY	2.8
1	M	152	VAL	2.8
2	H	117	ASN	2.8
2	D	101	LEU	2.8
1	A	75	MET	2.8
2	R	44	ALA	2.8
1	I	26	ASP	2.8
1	O	76	CYS	2.8
2	F	125	GLN	2.8
1	E	323	SER	2.8
2	H	27	SER	2.8
1	K	283	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	202	ILE	2.8
1	C	144	LYS	2.8
1	O	144	LYS	2.8
1	M	92	ASN	2.8
1	O	52	CYS	2.8
1	Q	70	LEU	2.8
1	A	142	GLN	2.8
2	L	30	GLN	2.8
2	D	45	ILE	2.8
1	Q	187	ASP	2.8
2	J	112	ASP	2.8
1	O	82	VAL	2.8
2	R	124	LEU	2.8
1	O	246	GLU	2.8
1	G	281	CYS	2.8
2	N	33	GLY	2.8
1	Q	273	GLU	2.8
2	B	34	TYR	2.8
2	F	34	TYR	2.8
1	Q	224	ASN	2.8
2	P	146	ASN	2.8
1	O	134	GLY	2.8
1	M	167	SER	2.8
1	Q	301	THR	2.8
1	K	186	ASN	2.8
1	O	210	ASN	2.8
2	J	21	TRP	2.8
2	H	12	GLY	2.8
1	C	282	GLN	2.7
2	H	30	GLN	2.7
2	N	30	GLN	2.7
1	Q	86	TYR	2.7
2	H	24	TYR	2.7
1	K	275	GLY	2.7
1	O	186	ASN	2.7
1	Q	34	ASN	2.7
2	H	38	LYS	2.7
1	I	241	ASP	2.7
1	O	237	LEU	2.7
1	Q	207	SER	2.7
1	C	279	THR	2.7
1	K	266	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	280	LYS	2.7
2	F	24	TYR	2.7
1	M	204	VAL	2.7
1	O	142	GLN	2.7
1	I	27	THR	2.7
1	K	141	TYR	2.7
2	D	136	GLY	2.7
2	L	155	GLY	2.7
1	I	276	ASN	2.7
2	B	117	ASN	2.7
1	C	94	VAL	2.7
1	G	316	LEU	2.7
1	Q	235	THR	2.7
1	O	176	LEU	2.7
1	O	69	TRP	2.7
2	J	170	ARG	2.7
2	L	136	GLY	2.7
1	M	141	TYR	2.7
1	A	87	ILE	2.7
1	M	160	THR	2.7
2	H	114	ASN	2.7
2	P	15	GLN	2.7
1	I	174	GLU	2.7
1	G	18	HIS	2.7
1	O	183	HIS	2.7
1	Q	201	TYR	2.7
2	N	119	TYR	2.7
1	I	87	ILE	2.7
2	L	18	VAL	2.7
2	R	74	GLU	2.7
2	R	142	HIS	2.7
1	G	149	ARG	2.7
2	D	162	TYR	2.7
2	L	119	TYR	2.7
1	A	35(A)	THR	2.7
1	A	158	ASN	2.7
1	E	35	VAL	2.7
1	M	213	LEU	2.7
2	D	30	GLN	2.7
2	H	66	VAL	2.7
1	O	218	ALA	2.7
2	B	174	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	138	PHE	2.6
1	I	23	GLU	2.6
2	H	11	GLU	2.6
1	A	314	LEU	2.6
1	O	20	ASN	2.6
2	L	43	LYS	2.6
2	P	25	HIS	2.6
2	H	119	TYR	2.6
1	O	101	ASP	2.6
1	A	27	THR	2.6
1	O	116	ASN	2.6
2	B	129	ASN	2.6
2	N	130	ALA	2.6
2	B	11	GLU	2.6
2	L	11	GLU	2.6
2	R	54	SER	2.6
2	F	120	ASP	2.6
1	M	93	PRO	2.6
1	M	80	ILE	2.6
1	Q	202	ILE	2.6
1	O	113	SER	2.6
1	O	226	GLN	2.6
2	J	31	GLY	2.6
2	N	156	THR	2.6
1	Q	147	PHE	2.6
1	E	18	HIS	2.6
1	I	17	TYR	2.6
1	M	100	GLY	2.6
2	F	4	GLY	2.6
2	F	134	GLY	2.6
1	O	63	ASP	2.6
2	B	109	ASP	2.6
1	M	231	GLU	2.6
1	O	250	ASN	2.6
1	Q	103	ASN	2.6
1	Q	317	ALA	2.6
2	F	146	ASN	2.6
2	N	81	ASN	2.6
1	I	22	THR	2.6
2	J	102	MET	2.6
2	R	6	ILE	2.6
1	M	68	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	272	LEU	2.6
2	J	101	LEU	2.6
2	F	171	GLU	2.6
2	B	154	ASN	2.6
2	F	5	ALA	2.6
1	E	35(A)	THR	2.6
1	M	144	LYS	2.6
2	L	10	ILE	2.6
2	D	13	GLY	2.6
1	E	128	SER	2.6
1	G	141	TYR	2.6
1	O	17	TYR	2.6
2	H	37	ASP	2.6
1	I	19(A)	ASN	2.6
1	Q	233	PHE	2.6
2	P	6	ILE	2.6
2	P	29	GLU	2.6
1	I	277	CYS	2.5
1	I	279	THR	2.5
1	M	112	LEU	2.5
2	N	142	HIS	2.5
2	R	131	LYS	2.5
1	K	291	SER	2.5
1	O	227	SER	2.5
2	H	3	PHE	2.5
1	E	16	GLY	2.5
1	C	177	LEU	2.5
1	M	179	LEU	2.5
2	L	132	GLU	2.5
1	O	200	THR	2.5
1	Q	114	ARG	2.5
1	O	187	ASP	2.5
1	K	288	ILE	2.5
1	M	47	HIS	2.5
1	O	204	VAL	2.5
2	F	66	VAL	2.5
1	E	317	ALA	2.5
1	M	137	SER	2.5
2	B	113	SER	2.5
2	P	163	SER	2.5
1	M	269	LYS	2.5
1	O	12	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	50	LYS	2.5
1	E	19(A)	ASN	2.5
1	Q	73	ASN	2.5
2	P	154	ASN	2.5
2	R	71	ASN	2.5
1	M	82	VAL	2.5
1	K	41	ASP	2.5
2	D	120	ASP	2.5
2	J	19	ASP	2.5
2	J	111	HIS	2.5
2	N	138	PHE	2.5
1	K	287	ALA	2.5
2	H	162	TYR	2.5
1	I	52	CYS	2.5
1	M	133	SER	2.5
1	O	215	PRO	2.5
2	D	6	ILE	2.5
1	I	82	VAL	2.5
2	H	149	MET	2.5
1	E	291	SER	2.5
1	M	185	PRO	2.5
1	Q	48	ASN	2.5
2	B	149	MET	2.5
1	M	168	TYR	2.5
1	M	195	TYR	2.5
1	Q	239	PRO	2.5
1	M	32	GLU	2.5
1	Q	121	ILE	2.5
1	A	48	ASN	2.5
1	M	135	VAL	2.5
1	C	69	TRP	2.5
1	E	33	LYS	2.5
1	M	134	GLY	2.5
1	Q	142	GLN	2.5
2	J	116	LYS	2.5
2	L	61	THR	2.5
1	E	304	GLU	2.4
2	P	106	ARG	2.4
1	C	158	ASN	2.4
1	M	232	PHE	2.4
2	J	110	PHE	2.4
2	L	38	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	16	GLY	2.4
2	H	108	LEU	2.4
1	G	289	ASN	2.4
1	K	82	VAL	2.4
1	K	53	ASP	2.4
2	R	166	ALA	2.4
1	O	97	CYS	2.4
1	O	137	SER	2.4
1	O	290	SER	2.4
1	Q	277	CYS	2.4
1	G	73	ASN	2.4
1	I	173	GLN	2.4
1	K	24	GLN	2.4
1	M	218	ALA	2.4
2	D	36	ALA	2.4
2	N	166	ALA	2.4
1	M	115	ILE	2.4
1	M	84	TRP	2.4
1	O	208	THR	2.4
2	B	14	TRP	2.4
2	J	145	ASP	2.4
1	O	287	ALA	2.4
1	A	28	ILE	2.4
1	I	13	ILE	2.4
1	K	194	LEU	2.4
2	B	140	PHE	2.4
2	D	66	VAL	2.4
1	K	122	GLN	2.4
1	K	282	GLN	2.4
1	M	103	ASN	2.4
1	O	190	GLU	2.4
1	K	166	ARG	2.4
1	M	35(A)	THR	2.4
2	J	9	PHE	2.4
2	R	94	TYR	2.4
1	Q	69	TRP	2.4
1	Q	275	GLY	2.4
2	F	21	TRP	2.4
1	E	142	GLN	2.4
1	Q	119	GLU	2.4
1	M	202	ILE	2.4
2	B	137	CYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	O	99	PRO	2.4
1	Q	107	GLU	2.4
1	M	244	ASN	2.4
1	G	320	LEU	2.4
1	M	176	LEU	2.4
2	D	10	ILE	2.4
1	C	130	HIS	2.4
1	M	165	LYS	2.4
1	K	94	VAL	2.4
1	O	82(A)	PRO	2.4
1	O	139	CYS	2.4
2	N	157	TYR	2.4
1	C	31	MET	2.4
1	K	279	THR	2.4
1	Q	264(A)	ASP	2.4
1	E	81	ASN	2.4
1	M	207	SER	2.4
1	M	265	SER	2.4
2	L	101	LEU	2.4
2	R	169	LYS	2.4
1	Q	245	PHE	2.3
1	M	94	VAL	2.3
1	M	22	THR	2.3
1	M	156	LYS	2.3
1	C	81	ASN	2.3
2	J	146	ASN	2.3
2	N	164	GLU	2.3
1	A	319	GLY	2.3
1	Q	16	GLY	2.3
1	A	40	GLN	2.3
2	D	106	ARG	2.3
1	A	291	SER	2.3
2	L	40	SER	2.3
2	H	110	PHE	2.3
1	Q	222	LYS	2.3
2	R	91	VAL	2.3
1	I	105	TYR	2.3
1	M	104	ASP	2.3
1	E	292	MET	2.3
1	Q	87	ILE	2.3
2	B	107	THR	2.3
2	D	172	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	10	ILE	2.3
2	L	113	SER	2.3
1	O	55	GLY	2.3
1	O	277	CYS	2.3
1	Q	156	LYS	2.3
1	O	282	GLN	2.3
2	D	123	ARG	2.3
1	Q	179	LEU	2.3
2	R	2	LEU	2.3
1	A	232	PHE	2.3
1	Q	220	ARG	2.3
1	A	281	CYS	2.3
1	A	144	LYS	2.3
1	Q	177	LEU	2.3
1	Q	249	GLY	2.3
1	A	19(A)	ASN	2.3
1	E	149	ARG	2.3
1	O	178	VAL	2.3
2	L	121	LYS	2.3
1	K	218	ALA	2.3
2	B	84	MET	2.3
2	D	108	LEU	2.3
1	M	220	ARG	2.3
1	Q	149	ARG	2.3
1	O	36	VAL	2.3
1	A	11	ASP	2.3
1	Q	299	PRO	2.3
1	I	321	ARG	2.3
1	Q	112	LEU	2.3
1	K	303	GLY	2.3
1	O	217	ILE	2.3
1	I	97	CYS	2.3
1	A	282	GLN	2.3
1	G	95	ASN	2.3
1	I	65	SER	2.3
1	M	136	SER	2.3
2	B	115	VAL	2.3
2	L	91	VAL	2.3
2	H	124	LEU	2.3
1	A	217	ILE	2.3
1	C	246	GLU	2.3
1	G	186	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	SER	2.2
1	A	277	CYS	2.2
2	D	107	THR	2.2
1	C	98	TYR	2.2
1	G	124	ILE	2.2
1	M	73	ASN	2.2
2	D	104	ASN	2.2
2	F	95	ASN	2.2
1	C	52	CYS	2.2
2	P	148	CYS	2.2
1	E	140	PRO	2.2
1	K	285	MET	2.2
1	O	267	ILE	2.2
1	A	78	GLU	2.2
2	J	150	GLU	2.2
2	L	39	GLU	2.2
2	R	48	VAL	2.2
1	I	46	LYS	2.2
2	D	95	ASN	2.2
1	Q	101	ASP	2.2
2	B	111	HIS	2.2
2	R	67	GLY	2.2
2	D	7	ALA	2.2
1	K	88	VAL	2.2
2	R	122	VAL	2.2
1	E	113	SER	2.2
1	A	131	GLU	2.2
1	I	160	THR	2.2
2	D	112	ASP	2.2
2	F	113	SER	2.2
2	B	132	GLU	2.2
2	F	96	ALA	2.2
1	M	173	GLN	2.2
2	J	141	TYR	2.2
1	Q	35	VAL	2.2
1	K	296	ASN	2.2
2	N	29	GLU	2.2
2	N	135	ASN	2.2
1	Q	51	LEU	2.2
1	C	19	ALA	2.2
2	B	15	GLN	2.2
2	J	13	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	34	ASN	2.2
1	I	312	ASN	2.2
2	J	104	ASN	2.2
1	G	22	THR	2.2
2	J	156	THR	2.2
2	H	100	VAL	2.2
2	N	22	TYR	2.2
1	M	125(A)	LYS	2.2
2	N	106	ARG	2.2
2	P	16	GLY	2.2
1	C	277	CYS	2.2
1	Q	96(A)	LEU	2.2
1	C	74	PRO	2.2
1	K	174	GLU	2.2
2	P	11	GLU	2.2
1	M	212	ARG	2.2
1	Q	134	GLY	2.2
1	C	272	LEU	2.2
2	J	10	ILE	2.2
2	L	150	GLU	2.2
1	G	143	GLY	2.1
1	Q	234	TRP	2.1
1	M	282	GLN	2.1
2	J	154	ASN	2.1
1	G	65	SER	2.1
1	M	146	SER	2.1
1	K	286	GLY	2.1
1	A	176	LEU	2.1
1	C	54	ASP	2.1
2	H	128	ASP	2.1
2	N	37	ASP	2.1
1	Q	19	ALA	2.1
2	N	129	ASN	2.1
2	R	81	ASN	2.1
1	O	323	SER	2.1
1	K	22	THR	2.1
1	M	151	VAL	2.1
1	I	144	LYS	2.1
1	O	233	PHE	2.1
1	A	119	GLU	2.1
1	M	132	ALA	2.1
2	D	165	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	289	ASN	2.1
1	M	82(A)	PRO	2.1
2	P	17	MET	2.1
2	H	134	GLY	2.1
2	J	67	GLY	2.1
1	G	125(A)	LYS	2.1
2	D	41	THR	2.1
2	L	94	TYR	2.1
1	K	277	CYS	2.1
1	M	284	PRO	2.1
1	O	198	PRO	2.1
1	Q	268	MET	2.1
1	O	203	SER	2.1
1	C	274	TYR	2.1
2	R	108	LEU	2.1
1	C	40	GLN	2.1
1	E	55	GLY	2.1
1	G	322	ASN	2.1
2	F	31	GLY	2.1
1	M	71	LEU	2.1
2	D	11	GLU	2.1
2	J	94	TYR	2.1
2	J	107	THR	2.1
1	C	142	GLN	2.1
1	M	40	GLN	2.1
1	K	116	ASN	2.1
1	I	25	VAL	2.1
2	N	123	ARG	2.1
1	M	247	SER	2.1
1	O	209	LEU	2.1
2	D	94	TYR	2.1
1	C	39	ALA	2.1
1	A	62	ARG	2.1
1	A	315	VAL	2.1
1	O	278	ASN	2.1
2	B	135	ASN	2.1
1	A	70	LEU	2.1
2	H	25	HIS	2.1
1	I	84	TRP	2.1
1	O	167	SER	2.1
2	J	125	GLN	2.1
2	D	96	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	127	ARG	2.1
2	H	136	GLY	2.1
2	L	17	MET	2.1
2	L	102	MET	2.1
2	L	172	GLU	2.1
1	M	310	LYS	2.1
1	Q	90	LYS	2.1
1	I	272	LEU	2.0
1	M	130	HIS	2.0
1	K	265	SER	2.0
2	H	113	SER	2.0
1	O	87	ILE	2.0
1	Q	164	ILE	2.0
2	R	10	ILE	2.0
1	G	45	LYS	2.0
2	P	149	MET	2.0
1	O	177	LEU	2.0
1	M	113	SER	2.0
1	G	248	ASN	2.0
1	O	53(A)	LEU	2.0
1	O	276	ASN	2.0
2	L	114	ASN	2.0
1	A	18	HIS	2.0
1	G	62	ARG	2.0
1	G	54	ASP	2.0
1	K	302	ILE	2.0
1	Q	175	ASP	2.0
2	B	90	ASP	2.0
2	L	143	LYS	2.0
1	M	273	GLU	2.0
2	L	107	THR	2.0
1	C	292	MET	2.0
1	G	75	MET	2.0
2	J	48	VAL	2.0
1	E	172	ASN	2.0
1	K	176	LEU	2.0
2	H	101	LEU	2.0
1	O	125(A)	LYS	2.0
2	B	43	LYS	2.0
2	N	38	LYS	2.0
1	M	117	HIS	2.0
1	O	47	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	40	SER	2.0
2	J	44	ALA	2.0
1	Q	98	TYR	2.0
2	F	162	TYR	2.0
1	A	160	THR	2.0
1	O	232	PHE	2.0
1	A	61	LEU	2.0
2	D	169	LYS	2.0
1	O	92	ASN	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.

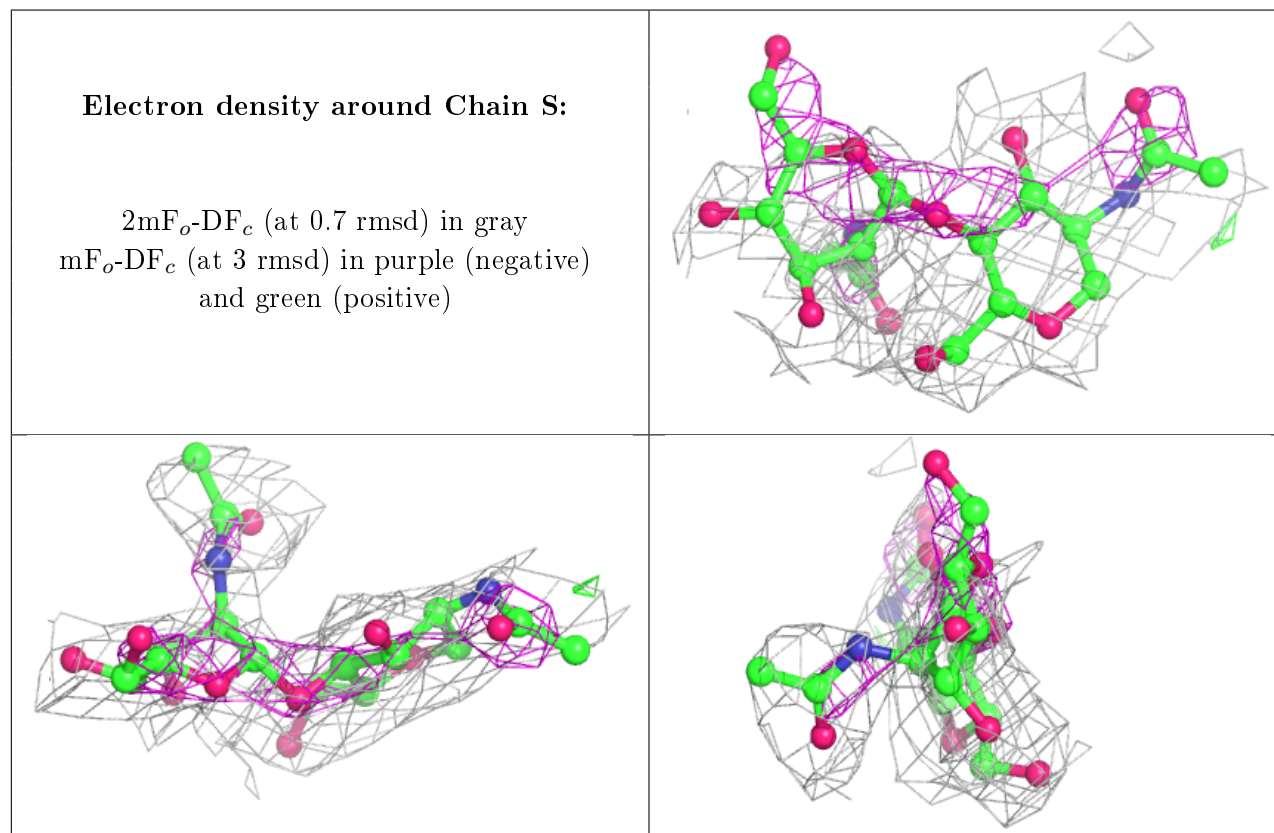
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	g	2	14/15	0.10	0.66	115,117,118,118	0
3	NAG	W	2	14/15	0.29	0.49	108,111,113,113	0
4	BMA	T	3	11/12	0.32	0.57	96,100,101,102	0
3	NAG	h	2	14/15	0.44	0.52	104,106,111,112	0
3	NAG	c	2	14/15	0.47	0.43	109,112,114,115	0
4	BMA	X	3	11/12	0.48	0.47	105,106,107,107	0
4	BMA	Z	3	11/12	0.50	0.60	94,96,97,97	0
3	NAG	f	2	14/15	0.51	0.34	92,93,94,94	0
3	NAG	e	2	14/15	0.59	0.62	109,110,110,110	0
3	NAG	g	1	14/15	0.60	0.41	99,104,107,113	0
3	NAG	a	2	14/15	0.60	0.70	107,108,109,110	0
3	NAG	S	2	14/15	0.61	0.56	97,100,103,104	0
3	NAG	c	1	14/15	0.61	0.45	90,97,100,106	0
4	NAG	X	2	14/15	0.61	0.39	94,97,100,103	0
3	NAG	a	1	14/15	0.62	0.42	90,97,100,103	0
3	NAG	Y	2	14/15	0.62	0.46	103,106,107,108	0
4	NAG	Z	2	14/15	0.65	0.36	82,85,88,91	0
3	NAG	h	1	14/15	0.67	0.49	87,91,94,99	0

*Continued on next page...*

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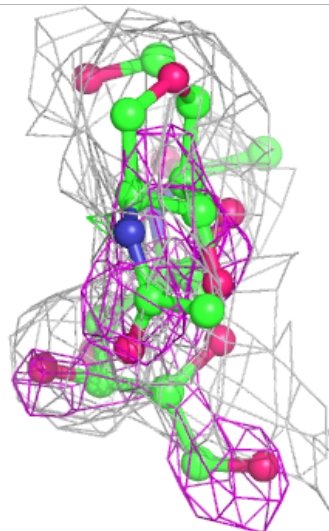
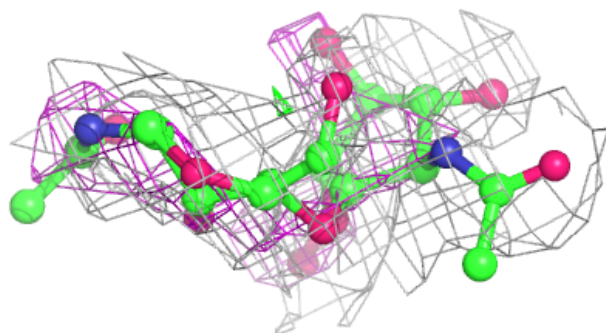
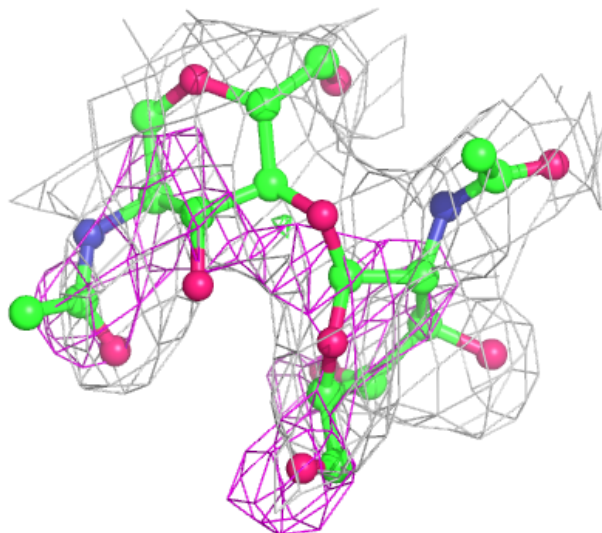
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	b	2	14/15	0.69	0.44	82,85,88,88	0
3	NAG	S	1	14/15	0.69	0.48	87,93,97,98	0
3	NAG	W	1	14/15	0.70	0.36	87,91,96,102	0
4	NAG	T	2	14/15	0.70	0.41	80,84,88,92	0
3	NAG	U	2	14/15	0.71	0.51	94,95,97,97	0
3	NAG	e	1	14/15	0.72	0.52	92,98,102,105	0
3	NAG	V	1	14/15	0.72	0.34	70,73,77,78	0
3	NAG	V	2	14/15	0.75	0.52	80,82,86,86	0
3	NAG	d	2	14/15	0.75	0.48	82,84,85,87	0
3	NAG	U	1	14/15	0.77	0.43	85,91,92,94	0
3	NAG	f	1	14/15	0.78	0.41	82,85,87,89	0
3	NAG	b	1	14/15	0.78	0.31	64,72,76,79	0
3	NAG	Y	1	14/15	0.79	0.35	87,91,94,100	0
4	NAG	X	1	14/15	0.81	0.33	79,81,84,89	0
3	NAG	d	1	14/15	0.83	0.30	61,71,74,80	0
4	NAG	Z	1	14/15	0.85	0.23	67,69,73,78	0
4	NAG	T	1	14/15	0.87	0.20	57,64,69,75	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.



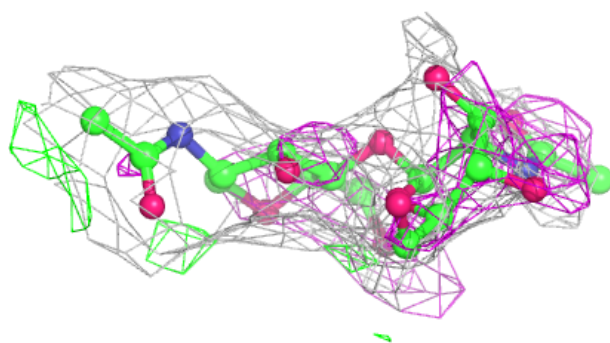
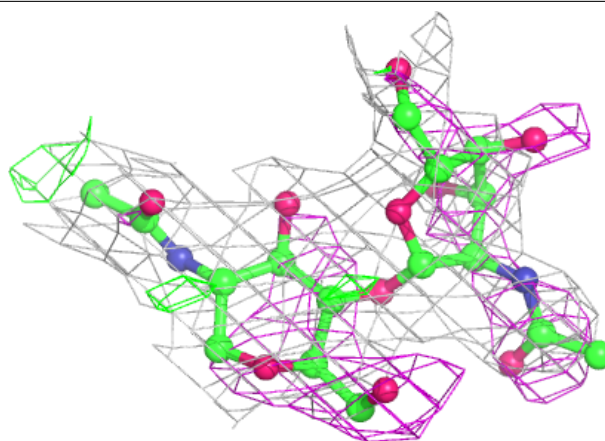
**Electron density around Chain U:**

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



**Electron density around Chain V:**

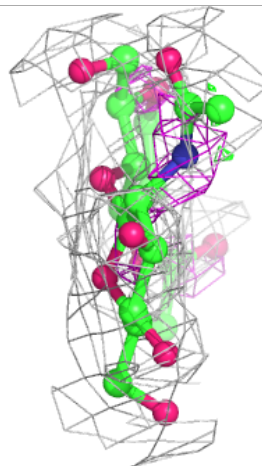
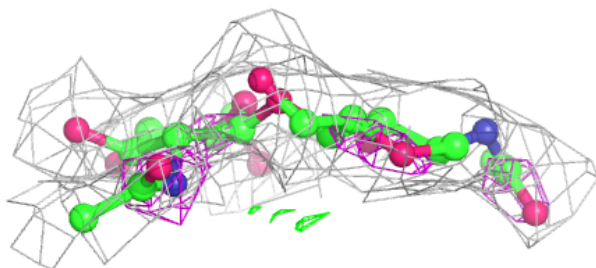
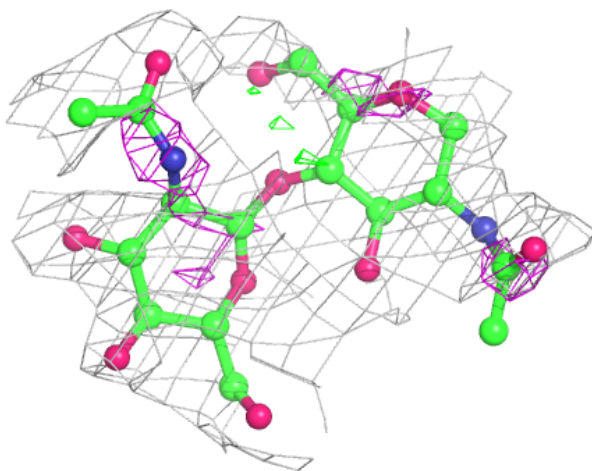
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





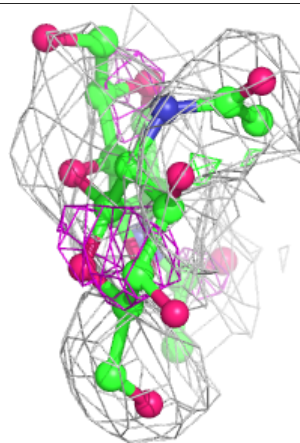
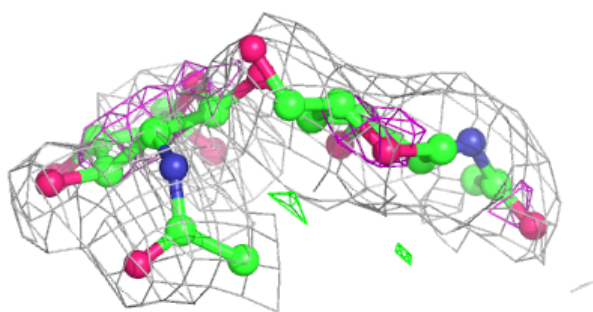
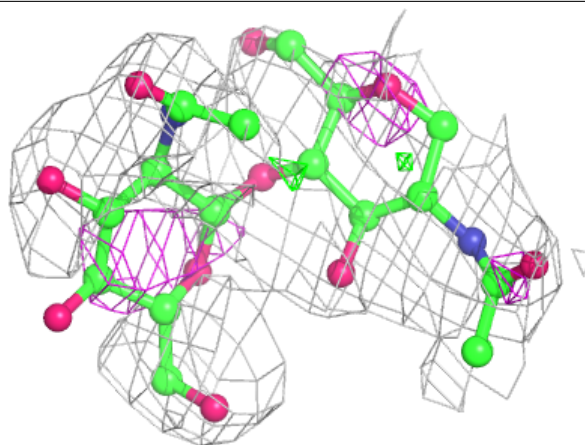
**Electron density around Chain W:**

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



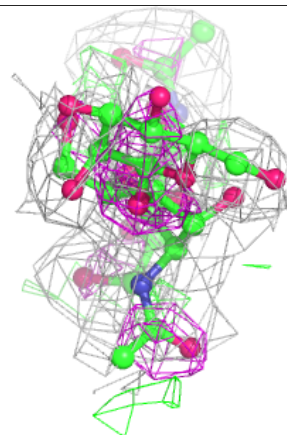
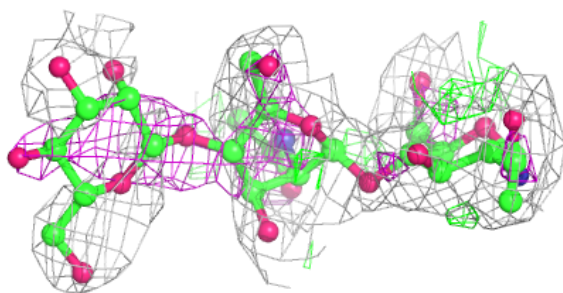
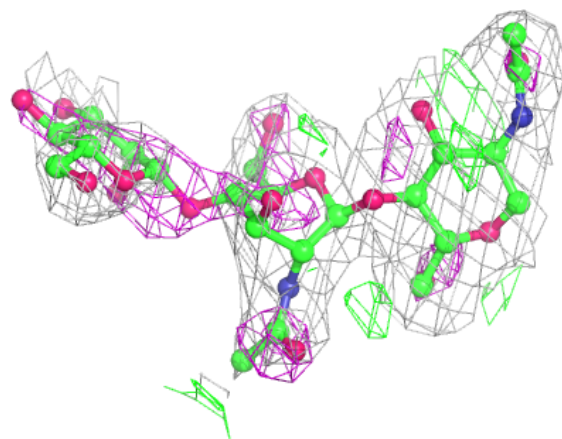
**Electron density around Chain Y:**

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

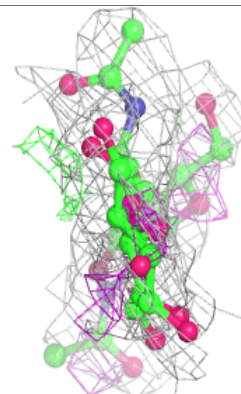
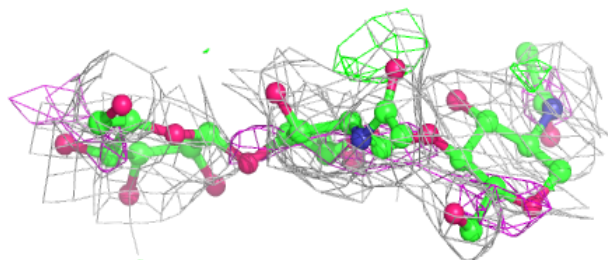
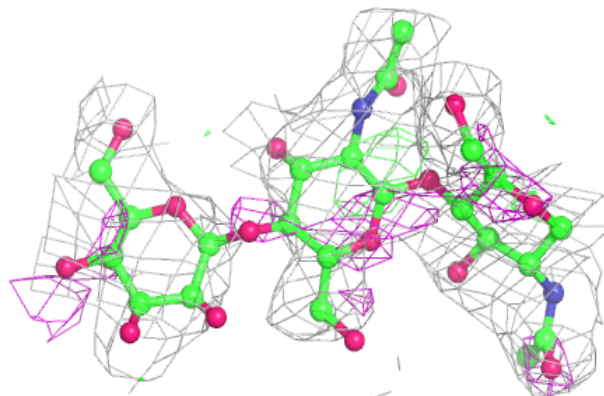


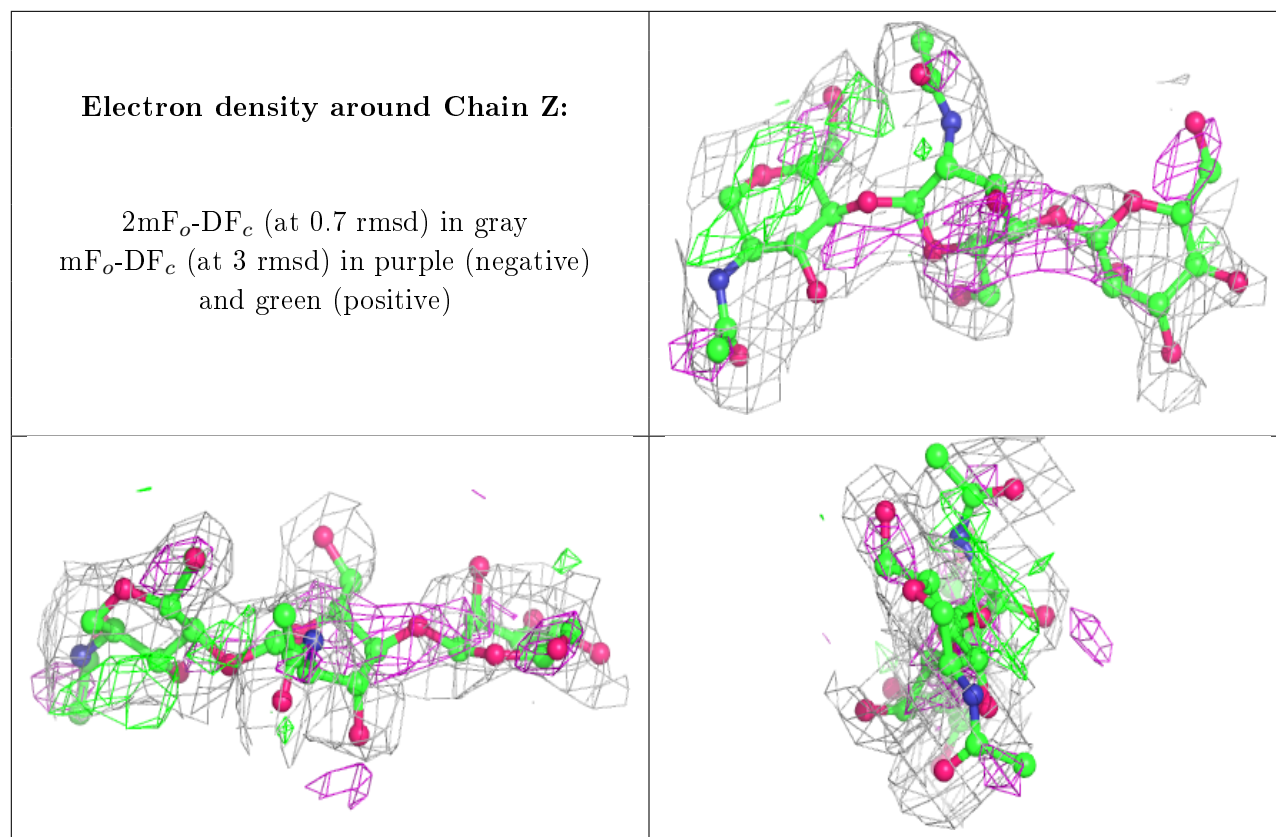
**Electron density around Chain T:**

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

**Electron density around Chain X:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.