



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 04:54 PM EDT

PDB ID : 5V7J  
Title : Crystal Structure at 3.7 Å Resolution of Glycosylated HIV-1 Clade A BG505 SOSIP.664 Prefusion Env Trimer with Four Glycans (N197, N276, N362, and N462) removed in Complex with Neutralizing Antibodies 3H+109L and 35O22.  
Authors : Stewart-Jones, G.B.E.; Zhou, T.; Kwong, P.D.  
Deposited on : 2017-03-20  
Resolution : 2.91 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

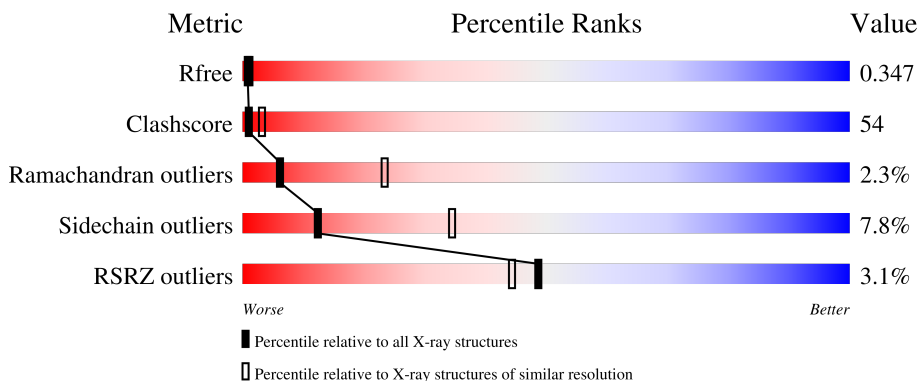
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	G	480	
2	B	153	
3	L	218	
4	H	236	
5	D	240	

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Mol	Chain	Length	Quality of chain
6	E	216	
7	A	6	
8	C	7	
9	F	7	
9	K	7	
10	I	3	
10	S	3	
11	J	8	
11	M	8	
12	N	6	
13	O	10	
14	P	7	
15	Q	2	
15	R	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MAN	M	5	-	-	-	X
7	NAG	A	1	-	-	X	-

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 12436 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	452	3538	2222	625	664	27	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	199	ALA	SER	engineered mutation	UNP Q2N0S6
G	278	ALA	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	365	ALA	SER	engineered mutation	UNP Q2N0S6
G	464	ALA	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	148	1167	739	203	219	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called Antibody 3H+109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	Total 1603	C 1007	N 276	O 315	S 5	0	0	0

- Molecule 4 is a protein called Antibody 3H+109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	231	Total 1744	C 1108	N 283	O 347	S 6	0	0	0

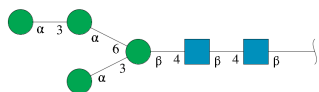
- Molecule 5 is a protein called Antibody 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	240	Total 1813	C 1150	N 303	O 352	S 8	0	0	0

- Molecule 6 is a protein called Antibody 35O22 Fab heavy chain.

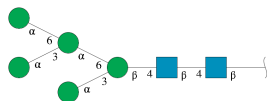
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	213	Total 1615	C 1012	N 267	O 328	S 8	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



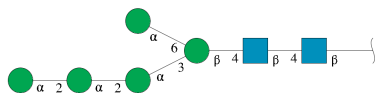
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	A	6	Total 72	C 40	N 2	O 30	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



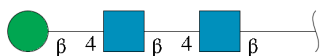
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	C	7	83	46	2	35	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



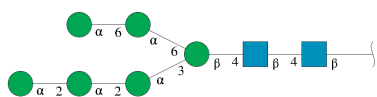
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	F	7	83	46	2	35	0	0	0
9	K	7	83	46	2	35	0	0	0

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



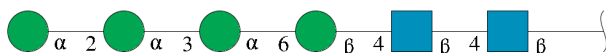
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	3	39	22	2	15	0	0	0
10	S	3	39	22	2	15	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



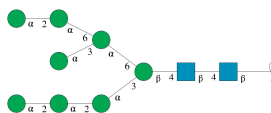
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	8	Total	C	N	O	0	0	0
			94	52	2	40			
11	M	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



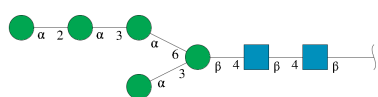
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



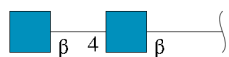
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	O	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



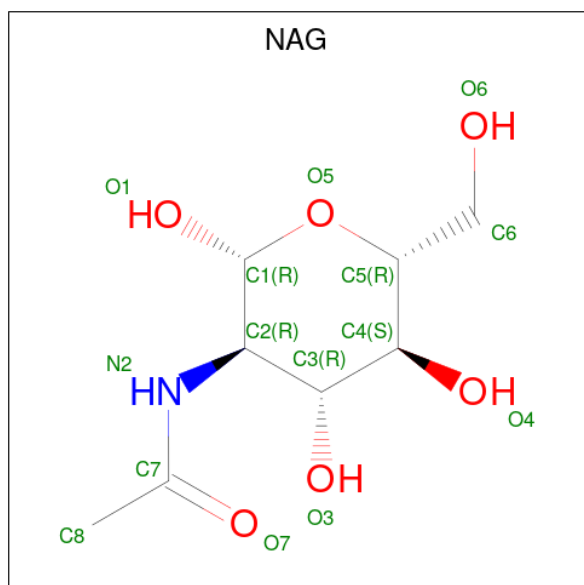
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	P	7	83	46	2	35	0	0	0

- Molecule 15 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
			Total	C	N	O			
15	Q	2	28	16	2	10	0	0	0
15	R	2	28	16	2	10	0	0	0

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



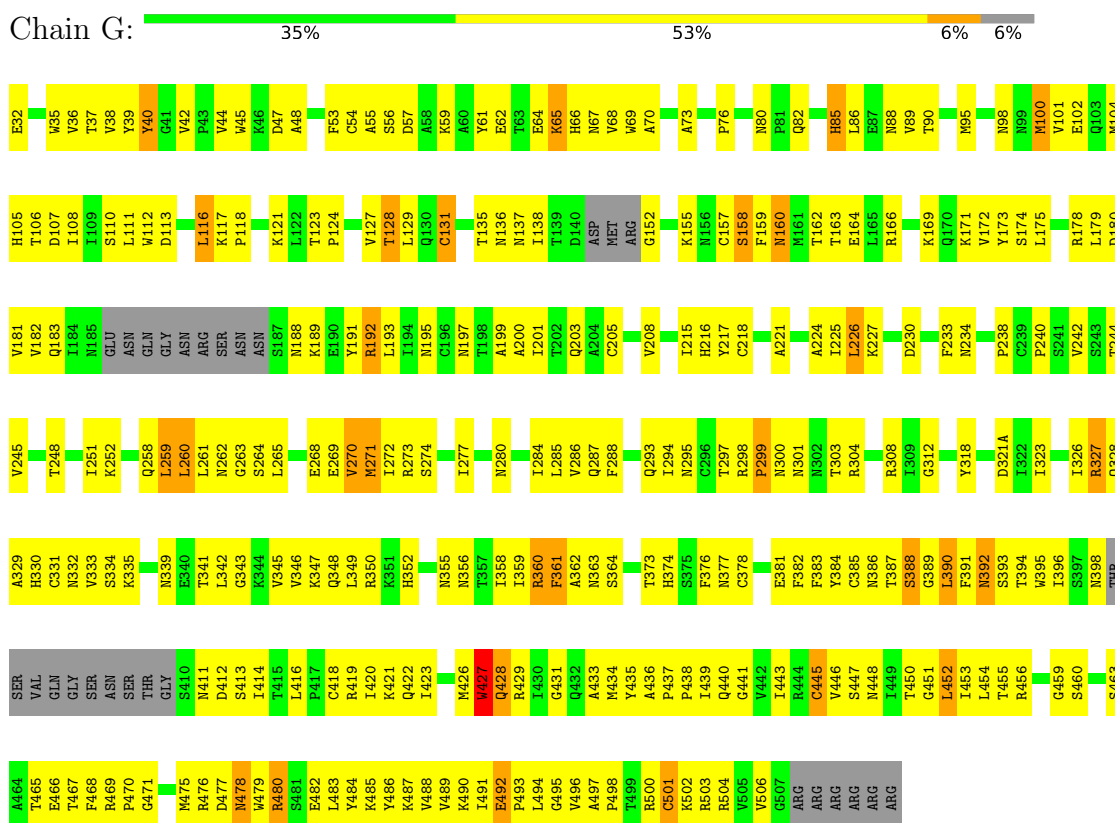
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
16	G	1	14	8	1	5	0	0
16	B	1	14	8	1	5	0	0
16	B	1	14	8	1	5	0	0



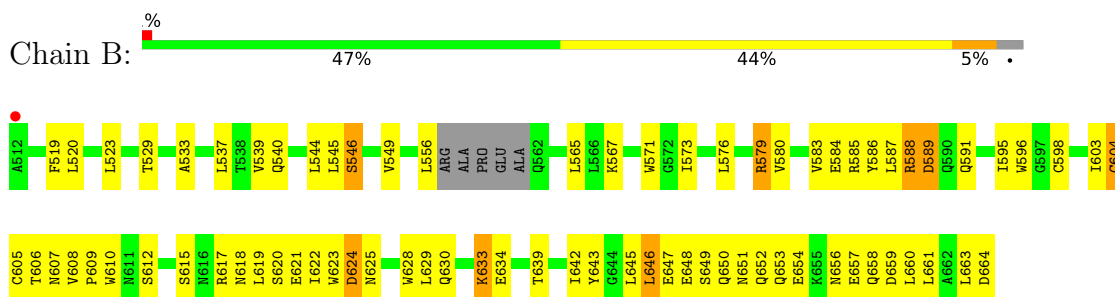
### 3 Residue-property plots

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

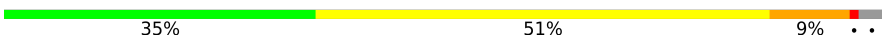
- Molecule 1: Envelope glycoprotein gp160

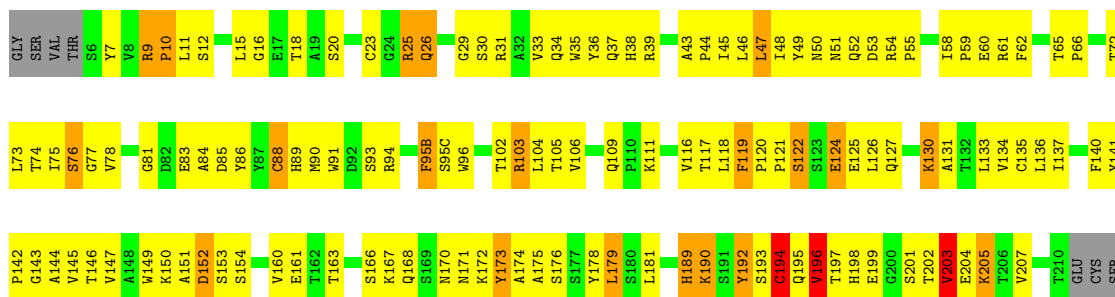


- Molecule 2: Envelope glycoprotein gp160



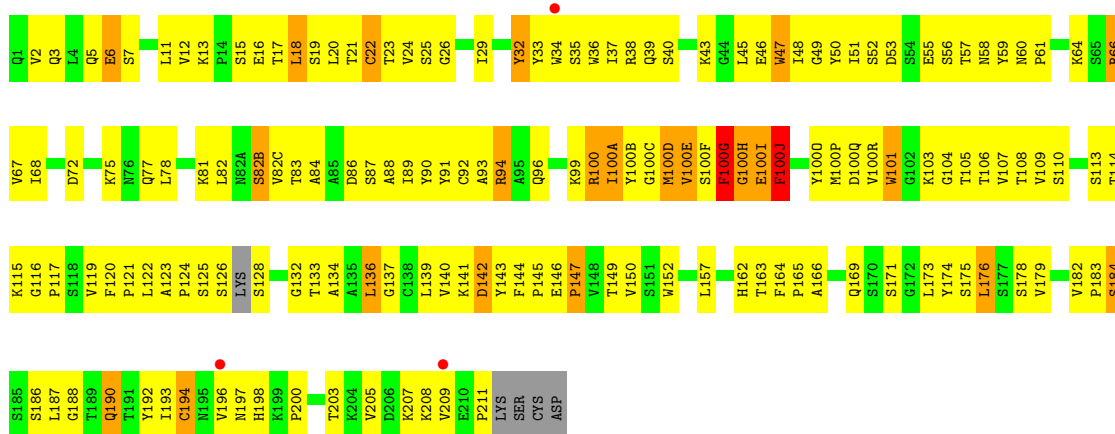
- Molecule 3: Antibody 3H+109L Fab light chain

Chain L: 



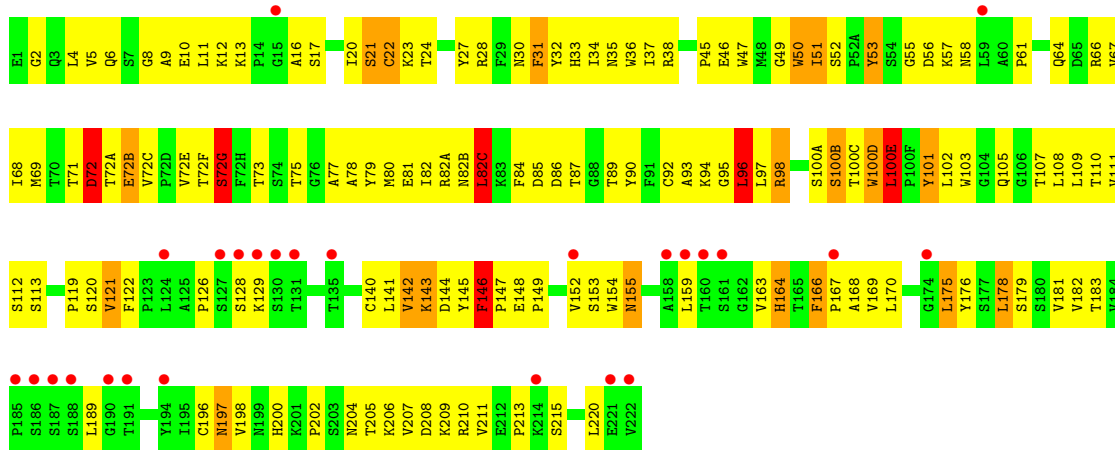
• Molecule 4: Antibody 3H+109L Fab heavy chain

Chain H: 



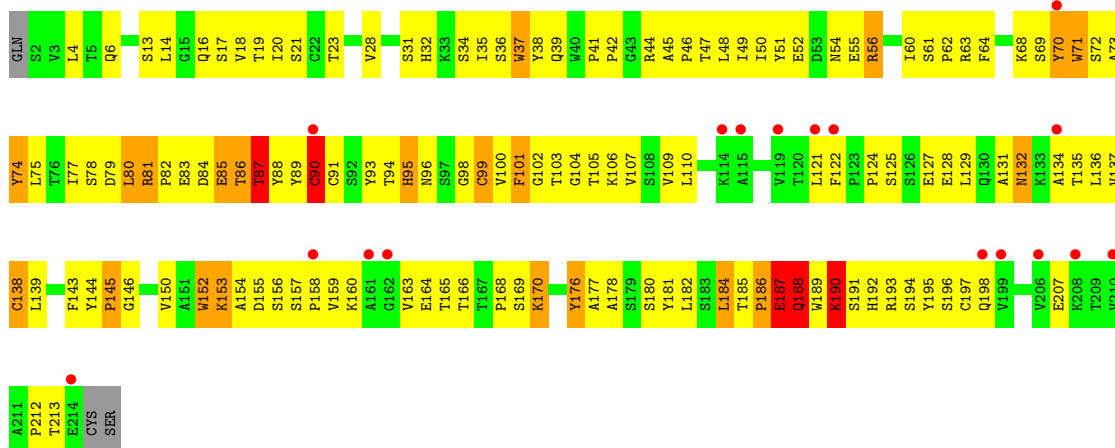
• Molecule 5: Antibody 35O22 Fab light chain

Chain D: 



• Molecule 6: Antibody 35O22 Fab heavy chain

Chain E: 



- Molecule 7:  $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain A:  67%  33%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 8:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain C:  43%  57%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 9:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain F:  43%  57%

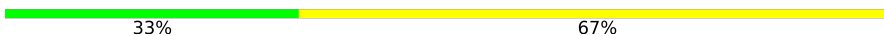
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 9:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain K:  43%  57%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%

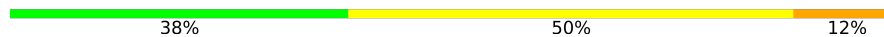
  
MAG1  
MAG2  
BMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  67% 33%

  
MAG1  
MAG2  
BMA3

- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  38% 50% 12%

  
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

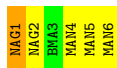
- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  25% 62% 12%

  
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  17% 67% 17%

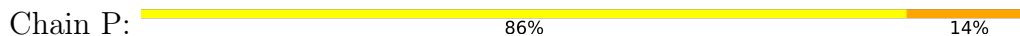
  
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

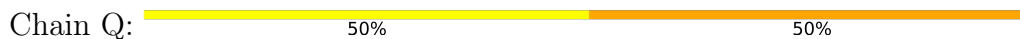
Chain O:  50% 50%



- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.16Å 131.16Å 315.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.42 – 2.91 41.42 – 2.91	Depositor EDS
% Data completeness (in resolution range)	49.9 (41.42-2.91) 49.9 (41.42-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.316 , 0.339 0.320 , 0.347	Depositor DCC
$R_{free}$ test set	1972 reflections (5.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , -9.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.340 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	12436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	G	0.43	2/3611 (0.1%)	0.69	4/4903 (0.1%)
2	B	0.51	2/1186 (0.2%)	0.71	1/1608 (0.1%)
3	L	0.57	1/1646 (0.1%)	0.79	4/2247 (0.2%)
4	H	0.46	0/1787	0.79	5/2436 (0.2%)
5	D	0.51	1/1860 (0.1%)	0.87	8/2533 (0.3%)
6	E	0.68	4/1659 (0.2%)	0.94	8/2269 (0.4%)
All	All	0.52	10/11749 (0.1%)	0.79	30/15996 (0.2%)

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	G	0	3
3	L	0	3
4	H	0	2
5	D	0	4
6	E	0	7
All	All	0	19

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	22	CYS	CB-SG	-11.40	1.62	1.82
2	B	604	CYS	CB-SG	-8.39	1.68	1.82
2	B	598	CYS	CB-SG	-7.02	1.70	1.82
6	E	187	GLU	CA-C	-6.82	1.35	1.52
6	E	85	GLU	CA-C	-6.26	1.36	1.52
6	E	99	CYS	CB-SG	-5.53	1.72	1.81
6	E	90	CYS	CB-SG	-5.46	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	160	ASN	CB-CG	5.42	1.63	1.51
1	G	390	LEU	N-CA	-5.08	1.36	1.46
3	L	194	CYS	CB-SG	-5.06	1.73	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	82(C)	LEU	CB-CG-CD1	-11.09	92.14	111.00
5	D	100(E)	LEU	CA-CB-CG	9.36	136.84	115.30
6	E	85	GLU	N-CA-C	8.28	133.36	111.00
6	E	86	THR	OG1-CB-CG2	-8.02	91.54	110.00
4	H	194	CYS	CA-CB-SG	7.51	127.51	114.00
5	D	82(C)	LEU	CA-CB-CG	7.49	132.52	115.30
1	G	226	LEU	CA-CB-CG	-7.07	99.04	115.30
5	D	22	CYS	CA-CB-SG	6.89	126.40	114.00
6	E	80	LEU	CB-CG-CD2	-6.68	99.64	111.00
6	E	188	GLN	C-N-CA	6.66	138.34	121.70
3	L	20	SER	CB-CA-C	-6.46	97.83	110.10
6	E	184	LEU	CA-CB-CG	6.34	129.89	115.30
4	H	176	LEU	CA-CB-CG	5.94	128.95	115.30
6	E	87	THR	N-CA-C	5.88	126.87	111.00
1	G	390	LEU	CA-CB-CG	5.87	128.79	115.30
5	D	98	ARG	N-CA-C	5.73	126.47	111.00
6	E	190	LYS	N-CA-CB	5.65	120.78	110.60
5	D	98	ARG	NE-CZ-NH2	-5.65	117.47	120.30
4	H	136	LEU	CB-CG-CD2	-5.61	101.46	111.00
3	L	205	LYS	CD-CE-NZ	-5.47	99.12	111.70
4	H	18	LEU	CA-CB-CG	5.38	127.69	115.30
2	B	646	LEU	CA-CB-CG	5.33	127.57	115.30
6	E	188	GLN	CA-CB-CG	5.24	124.92	113.40
3	L	179	LEU	CA-CB-CG	5.23	127.32	115.30
1	G	390	LEU	N-CA-C	5.21	125.06	111.00
4	H	110	SER	N-CA-CB	5.21	118.31	110.50
1	G	116	LEU	CA-CB-CG	5.19	127.23	115.30
5	D	178	LEU	CB-CG-CD1	5.14	119.74	111.00
3	L	196	VAL	N-CA-C	5.10	124.77	111.00
5	D	178	LEU	CD1-CG-CD2	-5.05	95.35	110.50

There are no chirality outliers.

All (19) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
5	D	100(B)	SER	Peptide
5	D	146	PHE	Peptide
5	D	21	SER	Peptide
5	D	96	LEU	Mainchain
6	E	101	PHE	Peptide
6	E	187	GLU	Mainchain
6	E	188	GLN	Mainchain
6	E	28	VAL	Peptide
6	E	34	SER	Peptide
6	E	37	TRP	Peptide
6	E	90	CYS	Peptide
1	G	128	THR	Peptide
1	G	158	SER	Peptide
1	G	492	GLU	Peptide
4	H	100(H)	GLY	Peptide
4	H	100(J)	PHE	Peptide
3	L	119	PHE	Peptide
3	L	202	THR	Peptide
3	L	203	VAL	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3538	0	3469	368	0
2	B	1167	0	1158	117	0
3	L	1603	0	1546	195	0
4	H	1744	0	1710	232	0
5	D	1813	0	1784	243	0
6	E	1615	0	1544	220	0
7	A	72	0	61	9	0
8	C	83	0	70	8	0
9	F	83	0	70	6	0
9	K	83	0	70	8	0
10	I	39	0	34	2	0
10	S	39	0	34	0	0
11	J	94	0	79	1	0
11	M	94	0	79	2	0
12	N	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	O	116	0	97	11	0
14	P	83	0	70	3	0
15	Q	28	0	25	2	0
15	R	28	0	25	0	0
16	B	28	0	26	5	0
16	G	14	0	13	1	0
All	All	12436	0	12025	1323	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (1323) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:ASN:HD21	9:K:1:NAG:C1	1.12	1.60
5:D:22:CYS:O	5:D:23:LYS:HE2	1.42	1.15
4:H:113:SER:O	4:H:144:PHE:CE2	2.01	1.13
5:D:22:CYS:C	5:D:23:LYS:HE2	1.72	1.09
1:G:226:LEU:HD11	1:G:244:THR:HA	1.28	1.08
1:G:456:ARG:HA	1:G:468:PHE:HB2	1.30	1.06
3:L:37:GLN:HA	3:L:86:TYR:HD1	1.20	1.05
5:D:69:MET:HG2	5:D:80:MET:HA	1.38	1.05
1:G:452:LEU:HD12	1:G:454:LEU:HD11	1.36	1.04
5:D:34:ILE:O	5:D:35:ASN:ND2	1.88	1.03
1:G:364:SER:HA	1:G:469:ARG:HD3	1.39	1.03
2:B:618:ASN:HB2	2:B:621:GLU:CD	1.79	1.02
1:G:234:ASN:CG	9:K:1:NAG:C1	2.30	1.00
1:G:385:CYS:SG	1:G:418:CYS:SG	1.18	1.00
5:D:166:PHE:O	5:D:178:LEU:HD22	1.59	1.00
3:L:150:LYS:HB3	3:L:193:SER:HB2	1.43	0.99
6:E:4:LEU:HD11	6:E:102:GLY:HA2	1.45	0.99
6:E:49:ILE:HD11	6:E:64:PHE:HB3	1.43	0.99
2:B:639:THR:O	2:B:643:TYR:CD1	2.17	0.98
4:H:2:VAL:HG23	4:H:26:GLY:HA3	1.45	0.98
1:G:271:MET:C	1:G:272:ILE:HD12	1.84	0.97
6:E:153:LYS:HE2	6:E:159:VAL:H	1.27	0.97
1:G:160:ASN:HB3	7:A:1:NAG:C7	1.96	0.96
4:H:149:THR:HG22	4:H:197:ASN:OD1	1.66	0.96
1:G:100:MET:HB2	1:G:483:LEU:HD21	1.47	0.96
5:D:98:ARG:HH12	5:D:100(C):THR:HA	1.30	0.95
1:G:259:LEU:HD11	1:G:374:HIS:NE2	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:33:TYR:HE1	4:H:53:ASP:H	1.16	0.93
4:H:119:VAL:HG11	4:H:205:VAL:HG11	1.48	0.93
3:L:54:ARG:HH11	3:L:58:ILE:HD13	1.29	0.93
4:H:33:TYR:HB3	4:H:50:TYR:HE2	1.33	0.93
1:G:95:MET:HE2	1:G:484:TYR:HB2	1.50	0.93
1:G:385:CYS:SG	1:G:418:CYS:CB	2.58	0.92
6:E:68:LYS:HE2	6:E:72:SER:HB3	1.52	0.92
1:G:38:VAL:HG12	1:G:496:VAL:HG12	1.51	0.91
1:G:261:LEU:HD11	1:G:447:SER:HB3	1.53	0.91
6:E:49:ILE:HD11	6:E:64:PHE:CB	2.01	0.91
1:G:129:LEU:HG	1:G:159:PHE:HB2	1.50	0.91
3:L:37:GLN:HA	3:L:86:TYR:CD1	2.05	0.90
3:L:54:ARG:NH2	3:L:62:PHE:O	2.05	0.89
1:G:272:ILE:HG12	1:G:286:VAL:HA	1.54	0.89
5:D:122:PHE:O	5:D:141:LEU:HB2	1.71	0.89
1:G:259:LEU:HD11	1:G:374:HIS:CD2	2.08	0.89
4:H:88:ALA:HB3	4:H:90:TYR:HE1	1.34	0.89
5:D:98:ARG:NH1	5:D:100(C):THR:OG1	2.06	0.88
5:D:144:ASP:HB2	5:D:175:LEU:HD13	1.55	0.88
5:D:66:ARG:HH22	5:D:82(C):LEU:HD11	1.37	0.88
1:G:506:VAL:HG21	2:B:658:GLN:HE21	1.39	0.87
5:D:23:LYS:HD2	5:D:77:ALA:HA	1.55	0.87
1:G:361:PHE:CE1	1:G:470:PRO:HD3	2.09	0.87
1:G:234:ASN:OD1	9:K:1:NAG:C1	2.23	0.86
1:G:391:PHE:HE2	1:G:470:PRO:HG3	1.38	0.86
2:B:648:GLU:HA	2:B:652:GLN:HB2	1.57	0.86
5:D:152:VAL:HG12	5:D:198:VAL:HA	1.57	0.86
6:E:14:LEU:HG	6:E:81:ARG:HH12	1.42	0.85
1:G:252:LYS:NZ	1:G:262:ASN:O	2.10	0.85
1:G:385:CYS:CB	1:G:418:CYS:SG	2.64	0.85
3:L:10:PRO:HA	3:L:103:ARG:HB3	1.59	0.85
3:L:54:ARG:NH1	3:L:59:PRO:O	2.10	0.85
5:D:66:ARG:NH2	5:D:82(C):LEU:HD11	1.92	0.85
6:E:137:VAL:HG12	6:E:181:TYR:CB	2.06	0.85
5:D:96:LEU:HD11	5:D:100(E):LEU:N	1.92	0.85
5:D:10:GLU:HG2	5:D:202:PRO:HD3	1.57	0.84
6:E:80:LEU:HD21	6:E:84:ASP:HB2	1.58	0.84
4:H:137:GLY:HA3	4:H:179:VAL:HG22	1.59	0.84
3:L:137:ILE:HD11	3:L:175:ALA:HB3	1.58	0.84
1:G:335:LYS:O	1:G:339:ASN:ND2	2.09	0.84
6:E:143:PHE:CE2	6:E:146:GLY:HA2	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:391:PHE:CE2	1:G:470:PRO:HG3	2.13	0.84
3:L:54:ARG:NH1	3:L:58:ILE:HD13	1.92	0.83
1:G:160:ASN:HB3	7:A:1:NAG:N2	1.92	0.83
5:D:23:LYS:HZ1	5:D:78:ALA:HB3	1.44	0.83
5:D:35:ASN:HB2	5:D:94:LYS:HE3	1.61	0.83
6:E:121:LEU:HG	6:E:138:CYS:HB2	1.60	0.82
3:L:195:GLN:HB3	3:L:204:GLU:HB3	1.61	0.82
2:B:607:ASN:HD21	2:B:650:GLN:HA	1.44	0.82
5:D:93:ALA:HB3	5:D:103:TRP:HA	1.60	0.81
1:G:304:ARG:HH11	1:G:440:GLN:HB3	1.45	0.81
6:E:13:SER:OG	6:E:110:LEU:O	1.96	0.81
1:G:201:ILE:HG13	1:G:433:ALA:HB3	1.63	0.81
2:B:618:ASN:CB	2:B:621:GLU:CD	2.49	0.81
5:D:121:VAL:HG23	5:D:141:LEU:HD12	1.63	0.81
5:D:141:LEU:HD21	5:D:143:LYS:HB3	1.63	0.81
1:G:95:MET:CE	1:G:484:TYR:HB2	2.10	0.81
5:D:35:ASN:HD21	5:D:50:TRP:HB3	1.44	0.81
1:G:203:GLN:HE21	1:G:437:PRO:HG3	1.45	0.80
4:H:115:LYS:HB3	4:H:144:PHE:HE1	1.44	0.80
5:D:12:LYS:NZ	5:D:13:LYS:O	2.14	0.80
1:G:361:PHE:HE1	1:G:470:PRO:HD3	1.47	0.80
1:G:454:LEU:HA	1:G:470:PRO:HA	1.63	0.80
2:B:618:ASN:OD1	16:B:702:NAG:N2	2.15	0.80
2:B:639:THR:O	2:B:643:TYR:HD1	1.60	0.80
1:G:469:ARG:HG3	1:G:470:PRO:HD2	1.64	0.79
1:G:333:VAL:O	1:G:414:ILE:N	2.16	0.79
3:L:143:GLY:HA3	3:L:173:TYR:HD2	1.46	0.79
1:G:386:ASN:HD21	14:P:1:NAG:C7	1.96	0.79
2:B:639:THR:O	2:B:643:TYR:CE1	2.34	0.79
5:D:166:PHE:CE2	6:E:177:ALA:HB3	2.17	0.79
6:E:79:ASP:OD1	6:E:81:ARG:NH2	2.14	0.79
7:A:1:NAG:H83	7:A:1:NAG:H3	1.65	0.79
1:G:476:ARG:HG3	1:G:480:ARG:HH12	1.47	0.78
6:E:176:TYR:HD1	6:E:177:ALA:H	1.31	0.78
3:L:96:TRP:HA	4:H:47:TRP:CZ3	2.18	0.78
3:L:167:LYS:HB2	3:L:173:TYR:HD1	1.48	0.77
5:D:35:ASN:ND2	5:D:50:TRP:HB3	1.99	0.77
6:E:68:LYS:HD3	6:E:74:TYR:HB2	1.64	0.77
1:G:38:VAL:HG22	2:B:604:CYS:HB2	1.66	0.77
2:B:639:THR:HG22	2:B:643:TYR:CE1	2.20	0.77
1:G:381:GLU:OE1	1:G:438:PRO:HA	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:84:ALA:H	3:L:104:LEU:HD11	1.50	0.76
5:D:20:ILE:HG12	5:D:107:THR:HG21	1.66	0.76
4:H:115:LYS:HB3	4:H:144:PHE:CE1	2.21	0.76
6:E:14:LEU:HG	6:E:81:ARG:NH1	2.01	0.76
4:H:113:SER:O	4:H:144:PHE:HE2	1.66	0.76
5:D:121:VAL:HA	5:D:141:LEU:HD12	1.68	0.76
5:D:4:LEU:HD21	5:D:22:CYS:HB3	1.66	0.75
1:G:131:CYS:HB3	1:G:157:CYS:HA	1.67	0.75
1:G:364:SER:CA	1:G:469:ARG:HD3	2.17	0.75
3:L:134:VAL:HG11	3:L:178:TYR:CD2	2.22	0.75
5:D:23:LYS:NZ	5:D:78:ALA:HB3	2.00	0.75
5:D:142:VAL:HG21	5:D:178:LEU:HG	1.67	0.75
1:G:188:ASN:N	1:G:189:LYS:HA	2.01	0.75
1:G:271:MET:O	1:G:272:ILE:HD12	1.86	0.75
3:L:142:PRO:O	3:L:198:HIS:NE2	2.19	0.75
5:D:22:CYS:O	5:D:23:LYS:CE	2.30	0.75
6:E:49:ILE:HG13	6:E:60:ILE:HD13	1.67	0.75
1:G:475:MET:O	1:G:478:ASN:N	2.16	0.75
4:H:134:ALA:N	4:H:182:VAL:O	2.17	0.74
2:B:596:TRP:HE1	2:B:647:GLU:CD	1.90	0.74
2:B:608:VAL:H	2:B:650:GLN:NE2	1.85	0.74
3:L:30:SER:HB3	4:H:100:ARG:HH21	1.52	0.74
4:H:11:LEU:HD12	4:H:108:THR:O	1.86	0.74
5:D:166:PHE:CD2	5:D:167:PRO:HD2	2.23	0.74
5:D:96:LEU:HD11	5:D:100(E):LEU:HB3	1.70	0.74
6:E:155:ASP:HB2	6:E:192:HIS:HB2	1.68	0.74
1:G:452:LEU:HD12	1:G:454:LEU:CD1	2.16	0.74
3:L:35:TRP:HB3	3:L:47:LEU:HD21	1.69	0.74
6:E:86:THR:HG22	6:E:87:THR:HG23	1.69	0.74
1:G:164:GLU:HA	1:G:312:GLY:HA2	1.70	0.73
6:E:42:PRO:HD3	6:E:86:THR:HG21	1.70	0.73
4:H:136:LEU:HD11	4:H:209:VAL:HG11	1.70	0.73
6:E:42:PRO:CD	6:E:86:THR:HG21	2.17	0.73
5:D:72(E):VAL:HB	5:D:73:THR:HG23	1.70	0.73
5:D:36:TRP:HE1	5:D:80:MET:HE3	1.53	0.73
1:G:195:ASN:OD1	1:G:201:ILE:HD11	1.87	0.73
4:H:125:SER:HG	4:H:128:SER:N	1.86	0.73
5:D:119:PRO:HA	5:D:145:TYR:CE1	2.24	0.73
4:H:132:GLY:O	4:H:184:SER:N	2.17	0.73
2:B:596:TRP:HD1	2:B:647:GLU:HB3	1.54	0.73
2:B:606:THR:HG23	2:B:650:GLN:HE22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:ILE:HG12	1:G:465:THR:HA	1.71	0.72
2:B:606:THR:HG23	2:B:650:GLN:NE2	2.04	0.72
5:D:51:ILE:HG13	5:D:52:SER:H	1.52	0.72
6:E:23:THR:HG22	6:E:72:SER:CB	2.18	0.72
3:L:31:ARG:NH2	3:L:65:THR:O	2.22	0.72
3:L:48:ILE:HG22	3:L:54:ARG:HG2	1.71	0.72
2:B:618:ASN:HB3	2:B:621:GLU:OE1	1.89	0.72
1:G:439:ILE:HD12	1:G:443:ILE:HG21	1.71	0.72
4:H:114:THR:HG21	4:H:200:PRO:C	2.09	0.72
3:L:167:LYS:HB2	3:L:173:TYR:CD1	2.24	0.72
6:E:13:SER:CB	6:E:110:LEU:O	2.37	0.72
3:L:38:HIS:O	3:L:84:ALA:HB1	1.90	0.72
6:E:44:ARG:NH1	6:E:45:ALA:O	2.23	0.72
5:D:69:MET:HG2	5:D:80:MET:CA	2.19	0.71
3:L:134:VAL:HG12	3:L:178:TYR:HA	1.72	0.71
2:B:639:THR:HG22	2:B:643:TYR:HE1	1.55	0.71
3:L:150:LYS:NZ	3:L:154:SER:H	1.88	0.71
3:L:54:ARG:HH11	3:L:58:ILE:CD1	2.03	0.71
6:E:189:TRP:O	6:E:192:HIS:ND1	2.23	0.71
2:B:596:TRP:CD1	2:B:647:GLU:HB3	2.25	0.71
6:E:49:ILE:HD11	6:E:64:PHE:CG	2.25	0.71
6:E:137:VAL:HG12	6:E:181:TYR:HB2	1.72	0.71
1:G:171:LYS:HG3	7:A:1:NAG:O7	1.91	0.71
6:E:184:LEU:HA	6:E:189:TRP:CZ2	2.26	0.71
5:D:98:ARG:HH12	5:D:100(C):THR:CA	2.04	0.71
6:E:16:GLN:NE2	6:E:18:VAL:HB	2.06	0.71
5:D:169:VAL:HG22	5:D:170:LEU:H	1.56	0.70
1:G:476:ARG:HG3	1:G:480:ARG:NH1	2.06	0.70
4:H:152:TRP:HB3	4:H:157:LEU:HD21	1.73	0.70
5:D:154:TRP:CE2	5:D:196:CYS:HB3	2.26	0.70
1:G:360:ARG:HG3	1:G:467:THR:HA	1.73	0.70
3:L:189:HIS:HD1	3:L:190:LYS:H	1.38	0.70
5:D:72(C):VAL:N	5:D:75:THR:O	2.21	0.70
4:H:16:GLU:O	4:H:82(B):SER:N	2.23	0.70
4:H:88:ALA:HB3	4:H:90:TYR:CE1	2.23	0.70
2:B:647:GLU:O	2:B:651:ASN:N	2.17	0.70
3:L:124:GLU:O	3:L:127:GLN:NE2	2.21	0.70
4:H:20:LEU:HD12	4:H:36:TRP:HH2	1.55	0.70
4:H:48:ILE:HA	4:H:60:ASN:HB2	1.73	0.70
5:D:51:ILE:HD13	5:D:57:LYS:HE2	1.73	0.70
3:L:121:PRO:HD3	3:L:133:LEU:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:428:GLN:O	1:G:428:GLN:NE2	2.23	0.70
3:L:195:GLN:HE22	3:L:205:LYS:C	1.94	0.70
4:H:35:SER:N	4:H:93:ALA:O	2.22	0.70
5:D:142:VAL:HG21	5:D:178:LEU:CG	2.22	0.70
9:K:1:NAG:H4	9:K:2:NAG:N2	2.06	0.69
1:G:39:TYR:HD2	2:B:603:ILE:HG22	1.57	0.69
2:B:654:GLU:O	2:B:658:GLN:NE2	2.26	0.69
4:H:149:THR:CG2	4:H:197:ASN:OD1	2.39	0.69
5:D:121:VAL:HA	5:D:141:LEU:CD1	2.22	0.69
5:D:69:MET:HG2	5:D:81:GLU:H	1.56	0.69
1:G:69:TRP:HA	1:G:111:LEU:HD11	1.74	0.69
1:G:226:LEU:HD11	1:G:244:THR:CA	2.15	0.69
4:H:3:GLN:OE1	4:H:3:GLN:N	2.26	0.69
3:L:195:GLN:HB3	3:L:204:GLU:CB	2.23	0.69
4:H:99:LYS:HD3	13:O:9:MAN:H62	1.74	0.69
6:E:184:LEU:HA	6:E:189:TRP:CH2	2.27	0.69
3:L:204:GLU:C	3:L:205:LYS:HD3	2.14	0.69
1:G:288:PHE:N	1:G:450:THR:O	2.24	0.69
1:G:121:LYS:HZ1	1:G:201:ILE:H	1.41	0.68
3:L:43:ALA:HA	4:H:91:TYR:CE2	2.29	0.68
4:H:113:SER:O	4:H:144:PHE:CD2	2.46	0.68
6:E:47:THR:C	6:E:48:LEU:HD23	2.14	0.68
3:L:149:TRP:CE3	3:L:194:CYS:HB2	2.28	0.68
9:F:3:BMA:H4	9:F:4:MAN:H2	1.75	0.68
1:G:183:GLN:HB3	1:G:191:TYR:CD1	2.29	0.68
3:L:61:ARG:NH2	3:L:74:THR:O	2.26	0.68
5:D:196:CYS:SG	5:D:209:LYS:HD3	2.34	0.68
1:G:129:LEU:HG	1:G:159:PHE:CB	2.22	0.68
2:B:576:LEU:HA	2:B:579:ARG:HE	1.58	0.68
6:E:96:ASN:HB2	8:C:6:MAN:H2	1.74	0.68
3:L:18:THR:OG1	3:L:76:SER:HA	1.93	0.68
5:D:84:PHE:HE2	5:D:112:SER:HA	1.58	0.68
4:H:59:TYR:HB2	4:H:64:LYS:HE2	1.76	0.68
4:H:100(A):ILE:HG22	4:H:100(J):PHE:HB3	1.75	0.68
1:G:138:ILE:HG23	10:I:1:NAG:H83	1.76	0.67
1:G:303:THR:OG1	1:G:321(A):ASP:O	2.10	0.67
1:G:350:ARG:NH1	1:G:398:ASN:OD1	2.28	0.67
3:L:163:THR:HG21	3:L:175:ALA:HA	1.75	0.67
4:H:20:LEU:HD12	4:H:36:TRP:CH2	2.29	0.67
4:H:100(D):MET:HB3	13:O:2:NAG:H2	1.77	0.67
1:G:152:GLY:HA3	1:G:178:ARG:HE	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:TYR:CD1	2:B:587:LEU:HD23	2.29	0.67
3:L:37:GLN:HB3	3:L:45:ILE:HG13	1.75	0.67
3:L:35:TRP:HE1	3:L:73:LEU:HD11	1.59	0.67
3:L:95(C):SER:O	4:H:47:TRP:HZ3	1.77	0.67
2:B:545:LEU:HD23	2:B:586:TYR:CG	2.29	0.67
4:H:22:CYS:HB3	4:H:78:LEU:HD21	1.77	0.67
6:E:110:LEU:N	6:E:110:LEU:HD12	2.10	0.67
2:B:544:LEU:HD11	2:B:586:TYR:HB2	1.77	0.67
4:H:33:TYR:HE1	4:H:53:ASP:N	1.92	0.67
4:H:207:LYS:NZ	4:H:208:LYS:O	2.28	0.67
1:G:502:LYS:HA	2:B:605:CYS:HB3	1.76	0.66
6:E:49:ILE:CD1	6:E:64:PHE:CD2	2.79	0.66
1:G:106:THR:O	1:G:110:SER:OG	2.12	0.66
3:L:54:ARG:HH12	3:L:59:PRO:C	1.97	0.66
5:D:2:GLY:HA3	5:D:27:TYR:CD1	2.30	0.66
6:E:152:TRP:CZ2	6:E:160:LYS:HA	2.30	0.66
1:G:37:THR:HB	2:B:604:CYS:O	1.96	0.66
1:G:225:ILE:HA	1:G:488:VAL:HA	1.77	0.66
3:L:35:TRP:O	3:L:46:LEU:HD11	1.96	0.66
5:D:93:ALA:CB	5:D:103:TRP:HA	2.24	0.66
5:D:169:VAL:HG23	6:E:166:THR:HG22	1.78	0.66
9:K:1:NAG:H4	9:K:2:NAG:C7	2.26	0.66
5:D:11:LEU:HB2	5:D:147:PRO:HG3	1.78	0.66
5:D:122:PHE:H	5:D:141:LEU:HG	1.61	0.66
7:A:1:NAG:H3	7:A:1:NAG:C8	2.25	0.66
1:G:323:ILE:HD11	12:N:1:NAG:H61	1.76	0.65
2:B:618:ASN:HB2	2:B:621:GLU:OE2	1.95	0.65
6:E:68:LYS:HG2	6:E:73:ALA:HA	1.77	0.65
3:L:44:PRO:HD3	4:H:91:TYR:HE2	1.61	0.65
4:H:117:PRO:HD2	4:H:203:THR:HG21	1.77	0.65
1:G:350:ARG:HG3	1:G:355:ASN:HA	1.77	0.65
1:G:422:GLN:O	1:G:436:ALA:N	2.17	0.65
4:H:100:ARG:NH2	13:O:4:MAN:O6	2.29	0.65
5:D:71:THR:HB	5:D:78:ALA:HA	1.78	0.65
1:G:304:ARG:HH12	1:G:439:ILE:HA	1.59	0.65
4:H:149:THR:HG22	4:H:197:ASN:CG	2.16	0.65
5:D:108:LEU:HD22	5:D:149:PRO:HD3	1.78	0.65
6:E:84:ASP:OD1	6:E:88:TYR:OH	2.15	0.65
3:L:126:LEU:HD23	3:L:127:GLN:H	1.60	0.65
5:D:153:SER:C	5:D:154:TRP:HD1	1.99	0.65
9:K:3:BMA:H62	9:K:7:MAN:H5	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:THR:HG22	2:B:606:THR:HB	1.79	0.65
1:G:386:ASN:ND2	14:P:1:NAG:C7	2.59	0.65
4:H:84:ALA:HA	4:H:109:VAL:HG13	1.78	0.65
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.79	0.65
1:G:112:TRP:CG	1:G:427:TRP:HH2	2.14	0.65
4:H:141:LYS:NZ	4:H:142:ASP:OD1	2.30	0.65
1:G:304:ARG:HH12	1:G:439:ILE:CA	2.10	0.64
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.32	0.64
2:B:618:ASN:CB	2:B:621:GLU:OE1	2.45	0.64
6:E:189:TRP:CD1	6:E:189:TRP:N	2.65	0.64
1:G:271:MET:C	1:G:272:ILE:CD1	2.64	0.64
4:H:59:TYR:HB2	4:H:64:LYS:HB3	1.78	0.64
3:L:104:LEU:HD12	3:L:104:LEU:O	1.98	0.64
1:G:271:MET:SD	1:G:271:MET:N	2.70	0.64
2:B:544:LEU:HD12	2:B:586:TYR:HD2	1.62	0.64
3:L:170:ASN:O	3:L:171:ASN:HB2	1.96	0.64
4:H:123:ALA:HB1	4:H:211:PRO:HA	1.79	0.64
1:G:327:ARG:HH12	4:H:100(C):GLY:HA3	1.63	0.64
6:E:129:LEU:O	6:E:132:ASN:ND2	2.28	0.64
1:G:421:LYS:NZ	1:G:423:ILE:O	2.23	0.64
3:L:35:TRP:HD1	3:L:48:ILE:HG12	1.61	0.64
3:L:195:GLN:NE2	3:L:205:LYS:O	2.30	0.64
5:D:4:LEU:O	5:D:105:GLN:NE2	2.31	0.64
5:D:100(D):TRP:CZ2	6:E:93:TYR:HB2	2.33	0.64
1:G:359:ILE:N	1:G:396:ILE:HD11	2.12	0.64
3:L:25:ARG:NH2	3:L:88:CYS:SG	2.71	0.63
3:L:149:TRP:CZ3	3:L:179:LEU:HG	2.33	0.63
1:G:131:CYS:HB3	1:G:157:CYS:CA	2.28	0.63
4:H:18:LEU:O	4:H:81:LYS:NZ	2.27	0.63
1:G:286:VAL:HB	1:G:452:LEU:HG	1.79	0.63
5:D:168:ALA:HA	5:D:178:LEU:HB3	1.80	0.63
2:B:653:GLN:HG2	2:B:656:ASN:ND2	2.13	0.63
6:E:42:PRO:HD3	6:E:86:THR:CG2	2.27	0.63
6:E:68:LYS:HZ2	6:E:74:TYR:HD2	1.46	0.63
9:K:3:BMA:O4	9:K:7:MAN:O6	2.15	0.63
5:D:5:VAL:HA	5:D:105:GLN:NE2	2.14	0.63
1:G:48:ALA:HB2	1:G:490:LYS:HB2	1.78	0.63
6:E:136:LEU:HD21	6:E:195:TYR:CE2	2.33	0.63
4:H:186:SER:O	4:H:190:GLN:NE2	2.26	0.63
5:D:100(D):TRP:HZ2	6:E:93:TYR:HB2	1.64	0.63
1:G:53:PHE:O	1:G:218:CYS:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:100(D):MET:SD	13:O:1:NAG:H5	2.40	0.62
1:G:65:LYS:HB3	1:G:66:HIS:HD2	1.65	0.62
1:G:270:VAL:O	1:G:272:ILE:HD13	1.99	0.62
4:H:72:ASP:OD1	4:H:75:LYS:N	2.31	0.62
1:G:90:THR:HG22	1:G:240:PRO:HA	1.81	0.62
1:G:270:VAL:C	1:G:272:ILE:HD13	2.20	0.62
4:H:100(D):MET:C	4:H:100(I):GLU:HG3	2.20	0.62
5:D:30:ASN:HD21	5:D:53:TYR:HB2	1.64	0.62
5:D:81:GLU:OE1	5:D:82(A):ARG:NH1	2.31	0.62
5:D:95:GLY:O	5:D:96:LEU:HG	1.99	0.62
8:C:2:NAG:H83	8:C:2:NAG:H3	1.81	0.62
1:G:259:LEU:O	1:G:260:LEU:HG	1.99	0.62
5:D:96:LEU:HD11	5:D:100(E):LEU:CB	2.29	0.62
1:G:57:ASP:O	1:G:59:LYS:NZ	2.33	0.62
1:G:261:LEU:CD1	1:G:447:SER:HB3	2.28	0.62
3:L:58:ILE:HB	3:L:62:PHE:HZ	1.63	0.62
6:E:137:VAL:HG12	6:E:181:TYR:HB3	1.77	0.62
1:G:261:LEU:HG	1:G:448:ASN:C	2.20	0.62
1:G:393:SER:HB3	1:G:395:TRP:NE1	2.15	0.62
3:L:44:PRO:HD3	4:H:91:TYR:CE2	2.35	0.62
4:H:100(D):MET:N	4:H:100(I):GLU:OE2	2.28	0.62
4:H:169:GLN:HG2	4:H:173:LEU:H	1.63	0.62
5:D:168:ALA:HB1	5:D:176:TYR:HB3	1.80	0.62
4:H:133:THR:HA	4:H:183:PRO:HA	1.82	0.62
6:E:6:GLN:HE21	6:E:102:GLY:HA3	1.65	0.62
6:E:20:ILE:HG21	6:E:88:TYR:HB2	1.80	0.62
1:G:121:LYS:HZ1	1:G:200:ALA:HB1	1.65	0.62
1:G:361:PHE:CZ	1:G:470:PRO:HD3	2.35	0.62
3:L:61:ARG:NH2	3:L:76:SER:H	1.98	0.62
4:H:34:TRP:N	4:H:50:TYR:OH	2.26	0.62
1:G:284:ILE:N	1:G:454:LEU:O	2.32	0.62
1:G:298:ARG:HG2	1:G:420:ILE:HD11	1.80	0.62
4:H:100(A):ILE:HD11	13:O:3:BMA:H62	1.81	0.62
1:G:39:TYR:CD2	2:B:603:ILE:HG22	2.35	0.61
1:G:113:ASP:HA	1:G:116:LEU:HG	1.81	0.61
1:G:453:ILE:C	1:G:454:LEU:HD12	2.21	0.61
3:L:39:ARG:NH2	3:L:81:GLY:O	2.33	0.61
4:H:100(P):MET:HB3	4:H:101:TRP:HE1	1.65	0.61
1:G:421:LYS:HE2	1:G:422:GLN:H	1.64	0.61
3:L:25:ARG:NE	3:L:88:CYS:O	2.34	0.61
4:H:143:TYR:OH	4:H:176:LEU:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:140:VAL:HG12	4:H:143:TYR:CD2	2.35	0.61
5:D:120:SER:O	5:D:145:TYR:OH	2.17	0.61
5:D:154:TRP:O	5:D:155:ASN:ND2	2.33	0.61
5:D:164:HIS:H	5:D:182:VAL:HG22	1.65	0.61
5:D:10:GLU:HG2	5:D:202:PRO:CD	2.29	0.61
6:E:37:TRP:HA	6:E:38:TYR:CE2	2.35	0.61
1:G:335:LYS:HB3	1:G:414:ILE:HD11	1.81	0.61
6:E:31:SER:OG	6:E:32:HIS:N	2.34	0.61
5:D:96:LEU:CD1	5:D:100(E):LEU:HB3	2.30	0.61
6:E:41:PRO:HB2	6:E:44:ARG:HB3	1.80	0.61
1:G:101:VAL:HA	1:G:104:MET:HG2	1.81	0.61
6:E:37:TRP:CE2	6:E:90:CYS:HB2	2.36	0.61
1:G:225:ILE:HG21	1:G:486:TYR:HD2	1.65	0.61
4:H:91:TYR:CE1	4:H:104:GLY:HA3	2.35	0.61
6:E:35:ILE:HG23	6:E:91:CYS:O	2.01	0.61
1:G:334:SER:HA	1:G:413:SER:HA	1.83	0.61
3:L:84:ALA:N	3:L:104:LEU:HD11	2.16	0.61
5:D:143:LYS:HG3	5:D:145:TYR:CZ	2.36	0.61
6:E:23:THR:HG22	6:E:72:SER:OG	2.00	0.61
3:L:84:ALA:HB3	3:L:86:TYR:CZ	2.36	0.60
3:L:86:TYR:HE2	3:L:104:LEU:HD21	1.64	0.60
3:L:143:GLY:HA3	3:L:173:TYR:CD2	2.33	0.60
1:G:248:THR:HA	1:G:486:TYR:CE2	2.36	0.60
1:G:393:SER:CB	1:G:395:TRP:HE1	2.14	0.60
6:E:49:ILE:HD11	6:E:64:PHE:CD2	2.35	0.60
3:L:37:GLN:HG3	3:L:86:TYR:HE1	1.65	0.60
3:L:61:ARG:CZ	3:L:75:ILE:HA	2.30	0.60
4:H:33:TYR:HB3	4:H:50:TYR:CE2	2.25	0.60
6:E:50:ILE:HD11	6:E:54:ASN:C	2.21	0.60
1:G:259:LEU:HD21	1:G:374:HIS:CG	2.37	0.60
6:E:50:ILE:HD12	6:E:56:ARG:HB3	1.83	0.60
1:G:359:ILE:H	1:G:396:ILE:HD11	1.67	0.60
5:D:121:VAL:HA	5:D:141:LEU:HG	1.84	0.60
1:G:304:ARG:NH2	1:G:438:PRO:O	2.29	0.60
3:L:61:ARG:NH1	3:L:75:ILE:HA	2.17	0.60
5:D:68:ILE:O	5:D:81:GLU:HG2	2.02	0.60
5:D:96:LEU:HD11	5:D:100(E):LEU:CA	2.32	0.60
6:E:6:GLN:NE2	6:E:102:GLY:HA3	2.17	0.60
3:L:59:PRO:HG2	3:L:62:PHE:HE1	1.66	0.60
6:E:80:LEU:HD21	6:E:84:ASP:CB	2.29	0.60
1:G:362:ALA:C	1:G:469:ARG:HH21	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:189:HIS:HD1	3:L:190:LYS:N	2.00	0.60
4:H:115:LYS:NZ	4:H:142:ASP:OD2	2.29	0.60
1:G:39:TYR:HH	2:B:623:TRP:HH2	1.49	0.60
2:B:544:LEU:HD12	2:B:586:TYR:CD2	2.37	0.60
6:E:36:SER:OG	6:E:51:TYR:HA	2.02	0.60
5:D:53:TYR:CD2	8:C:1:NAG:H5	2.37	0.59
1:G:163:THR:HG22	1:G:164:GLU:H	1.66	0.59
5:D:34:ILE:HD13	5:D:51:ILE:HG23	1.84	0.59
5:D:119:PRO:HD2	5:D:205:THR:HB	1.85	0.59
1:G:295:ASN:OD1	1:G:332:ASN:HB2	2.02	0.59
1:G:363:ASN:ND2	1:G:388:SER:HA	2.17	0.59
4:H:39:GLN:O	4:H:88:ALA:HB1	2.02	0.59
6:E:19:THR:HG21	6:E:75:LEU:HG	1.85	0.59
1:G:127:VAL:C	1:G:129:LEU:HD13	2.23	0.59
6:E:13:SER:O	6:E:16:GLN:HB2	2.02	0.59
6:E:190:LYS:HZ1	6:E:212:PRO:C	2.05	0.59
1:G:327:ARG:HH11	4:H:100(B):TYR:HD2	1.43	0.59
1:G:491:ILE:HG21	2:B:544:LEU:HD23	1.85	0.59
3:L:125:GLU:HG2	3:L:130:LYS:O	2.03	0.59
4:H:150:VAL:HG12	4:H:196:VAL:HG12	1.85	0.59
4:H:190:GLN:HG2	4:H:192:TYR:CE1	2.38	0.59
6:E:143:PHE:HE2	6:E:146:GLY:HA2	1.66	0.59
1:G:39:TYR:CE1	1:G:497:ALA:HB3	2.37	0.59
1:G:363:ASN:HD21	1:G:388:SER:HA	1.68	0.59
2:B:533:ALA:HB3	2:B:628:TRP:HE1	1.66	0.59
5:D:93:ALA:C	5:D:94:LYS:HD2	2.23	0.59
1:G:280:ASN:HA	1:G:456:ARG:HB2	1.84	0.58
3:L:33:VAL:HG22	3:L:90:MET:HA	1.84	0.58
5:D:119:PRO:HA	5:D:145:TYR:CZ	2.37	0.58
3:L:31:ARG:NH1	3:L:51:ASN:OD1	2.37	0.58
5:D:69:MET:CG	5:D:80:MET:HA	2.24	0.58
6:E:37:TRP:HD1	6:E:91:CYS:HB3	1.69	0.58
6:E:176:TYR:HD1	6:E:177:ALA:N	1.99	0.58
5:D:96:LEU:CG	5:D:100(E):LEU:HB3	2.34	0.58
6:E:49:ILE:HD12	6:E:64:PHE:CD2	2.39	0.58
3:L:119:PHE:H	3:L:133:LEU:HD11	1.69	0.58
5:D:12:LYS:HD2	5:D:111:VAL:HG22	1.86	0.58
5:D:72(B):GLU:CD	5:D:72(B):GLU:H	2.06	0.58
6:E:189:TRP:O	6:E:192:HIS:CG	2.56	0.58
5:D:69:MET:HG2	5:D:81:GLU:N	2.18	0.58
5:D:89:THR:HA	5:D:108:LEU:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:164:GLU:N	6:E:164:GLU:OE1	2.36	0.58
6:E:6:GLN:NE2	6:E:103:THR:H	2.02	0.58
6:E:168:PRO:HB2	6:E:176:TYR:CE1	2.39	0.58
2:B:544:LEU:HD13	2:B:544:LEU:C	2.24	0.57
3:L:95(B):PHE:CE1	4:H:47:TRP:HH2	2.22	0.57
4:H:5:GLN:HE21	4:H:5:GLN:HA	1.68	0.57
5:D:51:ILE:HD12	5:D:57:LYS:N	2.18	0.57
1:G:501:CYS:SG	1:G:502:LYS:N	2.78	0.57
3:L:61:ARG:HG2	3:L:61:ARG:HH21	1.68	0.57
3:L:171:ASN:C	3:L:172:LYS:HD3	2.25	0.57
4:H:149:THR:HG22	4:H:197:ASN:H	1.68	0.57
6:E:170:LYS:H	6:E:170:LYS:HD3	1.69	0.57
3:L:12:SER:OG	3:L:103:ARG:NH1	2.37	0.57
4:H:11:LEU:HD11	4:H:108:THR:H	1.69	0.57
4:H:12:VAL:HG23	4:H:16:GLU:OE1	2.03	0.57
4:H:94:ARG:O	4:H:94:ARG:HG3	2.04	0.57
5:D:189:LEU:HD22	5:D:213:PRO:HB2	1.86	0.57
5:D:90:TYR:N	5:D:107:THR:O	2.20	0.57
4:H:18:LEU:HD23	4:H:19:SER:N	2.19	0.57
5:D:9:ALA:CB	5:D:108:LEU:H	2.17	0.57
1:G:469:ARG:HG3	1:G:470:PRO:CD	2.32	0.57
2:B:586:TYR:HD1	2:B:587:LEU:HD23	1.70	0.57
3:L:46:LEU:HD12	3:L:47:LEU:H	1.70	0.57
6:E:36:SER:C	6:E:37:TRP:CD1	2.78	0.57
6:E:68:LYS:HG3	6:E:69:SER:H	1.70	0.57
1:G:36:VAL:HG13	2:B:610:TRP:HB2	1.86	0.57
5:D:6:GLN:H	5:D:105:GLN:HG2	1.70	0.57
13:O:1:NAG:H3	13:O:1:NAG:H83	1.86	0.57
2:B:621:GLU:OE1	2:B:621:GLU:N	2.37	0.57
1:G:116:LEU:HD12	1:G:117:LYS:N	2.20	0.57
2:B:620:SER:OG	5:D:97:LEU:CD2	2.53	0.57
2:B:643:TYR:HA	2:B:646:LEU:CD1	2.35	0.56
3:L:47:LEU:O	3:L:54:ARG:HB3	2.04	0.56
5:D:142:VAL:CG2	5:D:178:LEU:HG	2.34	0.56
7:A:1:NAG:H83	7:A:1:NAG:C3	2.33	0.56
4:H:29:ILE:HA	4:H:34:TRP:CH2	2.39	0.56
4:H:37:ILE:HB	4:H:45:LEU:HD21	1.88	0.56
4:H:144:PHE:HA	4:H:173:LEU:HD11	1.88	0.56
6:E:94:THR:O	6:E:96:ASN:N	2.39	0.56
1:G:127:VAL:HG23	1:G:129:LEU:CD2	2.35	0.56
1:G:159:PHE:CE1	1:G:173:TYR:HA	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ARG:NH1	1:G:440:GLN:N	2.54	0.56
1:G:502:LYS:NZ	1:G:503:ARG:O	2.38	0.56
3:L:195:GLN:CD	3:L:204:GLU:HB3	2.26	0.56
4:H:51:ILE:HD13	4:H:57:THR:HB	1.86	0.56
5:D:109:LEU:CD2	5:D:111:VAL:HG23	2.36	0.56
2:B:629:LEU:HD12	2:B:629:LEU:H	1.71	0.56
5:D:120:SER:N	5:D:145:TYR:OH	2.38	0.56
1:G:363:ASN:OD1	1:G:388:SER:HA	2.05	0.56
4:H:15:SER:HA	4:H:82(B):SER:HA	1.87	0.56
5:D:34:ILE:HD13	5:D:51:ILE:CG2	2.36	0.56
5:D:100(C):THR:HG22	5:D:100(D):TRP:CZ3	2.41	0.56
1:G:271:MET:SD	1:G:348:GLN:OE1	2.63	0.56
1:G:439:ILE:CD1	1:G:443:ILE:HG21	2.35	0.56
5:D:84:PHE:CZ	5:D:111:VAL:HG12	2.41	0.56
5:D:179:SER:HB3	6:E:139:LEU:CD2	2.36	0.56
1:G:506:VAL:HG21	2:B:658:GLN:NE2	2.15	0.56
3:L:109:GLN:OE1	3:L:109:GLN:N	2.36	0.56
5:D:72(A):THR:HG23	5:D:72(B):GLU:OE1	2.06	0.56
5:D:167:PRO:HG3	6:E:169:SER:HB3	1.88	0.56
1:G:102:GLU:O	1:G:106:THR:OG1	2.20	0.56
1:G:181:VAL:HG12	1:G:193:LEU:HA	1.88	0.56
2:B:618:ASN:OD1	16:B:702:NAG:C2	2.52	0.56
5:D:69:MET:CG	5:D:81:GLU:H	2.18	0.56
1:G:362:ALA:HB3	1:G:469:ARG:NH2	2.20	0.55
2:B:523:LEU:HD12	2:B:540:GLN:NE2	2.21	0.55
3:L:86:TYR:CE2	3:L:104:LEU:HD21	2.40	0.55
9:F:3:BMA:O2	9:F:4:MAN:H3	2.07	0.55
1:G:393:SER:HB3	1:G:395:TRP:HE1	1.72	0.55
3:L:149:TRP:CD2	3:L:194:CYS:HB2	2.41	0.55
4:H:115:LYS:HG2	4:H:116:GLY:N	2.20	0.55
6:E:153:LYS:HD2	6:E:157:SER:N	2.22	0.55
1:G:270:VAL:HG13	1:G:287:GLN:O	2.06	0.55
2:B:619:LEU:HD22	2:B:623:TRP:HE1	1.70	0.55
4:H:140:VAL:HG12	4:H:143:TYR:CE2	2.40	0.55
5:D:32:TYR:CD1	5:D:98:ARG:HG3	2.42	0.55
5:D:51:ILE:HG13	5:D:55:GLY:HA2	1.88	0.55
10:I:1:NAG:H62	10:I:2:NAG:N2	2.21	0.55
1:G:427:TRP:HD1	1:G:429:ARG:HB2	1.71	0.55
1:G:188:ASN:H	1:G:189:LYS:HA	1.72	0.55
3:L:146:THR:O	3:L:197:THR:HG23	2.05	0.55
5:D:50:TRP:NE1	5:D:58:ASN:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:387:THR:HG23	1:G:390:LEU:HD12	1.89	0.55
5:D:72:ASP:HB2	5:D:77:ALA:HB3	1.89	0.55
6:E:61:SER:HB3	6:E:62:PRO:CD	2.36	0.55
1:G:259:LEU:CD1	1:G:374:HIS:NE2	2.64	0.55
2:B:656:ASN:HA	2:B:659:ASP:HB3	1.89	0.55
2:B:660:LEU:HA	2:B:663:LEU:HD12	1.89	0.55
3:L:205:LYS:HD3	3:L:205:LYS:N	2.22	0.55
5:D:23:LYS:CE	5:D:23:LYS:HA	2.35	0.55
5:D:38:ARG:HG2	5:D:46:GLU:HB3	1.89	0.55
5:D:67:VAL:HG22	5:D:69:MET:HE1	1.88	0.55
6:E:16:GLN:CD	6:E:18:VAL:H	2.10	0.55
6:E:134:ALA:HB3	6:E:184:LEU:HG	1.89	0.55
4:H:149:THR:HG22	4:H:197:ASN:N	2.21	0.55
5:D:96:LEU:HD11	5:D:100(D):TRP:C	2.28	0.55
2:B:588:ARG:NH1	2:B:589:ASP:OD1	2.40	0.55
2:B:647:GLU:HB2	2:B:652:GLN:OE1	2.07	0.55
4:H:67:VAL:HG12	4:H:82:LEU:HD12	1.89	0.55
6:E:68:LYS:HG3	6:E:69:SER:N	2.22	0.55
1:G:95:MET:CE	1:G:484:TYR:CB	2.83	0.55
1:G:230:ASP:OD1	1:G:233:PHE:HB2	2.07	0.55
3:L:50:ASN:HD21	13:O:5:MAN:H61	1.70	0.55
4:H:16:GLU:OE2	4:H:16:GLU:N	2.40	0.55
4:H:83:THR:O	4:H:109:VAL:HG11	2.07	0.55
1:G:85:HIS:HD1	1:G:86:LEU:N	2.05	0.54
1:G:387:THR:HG22	1:G:387:THR:O	2.06	0.54
2:B:651:ASN:HA	2:B:654:GLU:HB3	1.88	0.54
3:L:58:ILE:HB	3:L:62:PHE:CZ	2.42	0.54
3:L:145:VAL:HG23	3:L:198:HIS:N	2.23	0.54
4:H:145:PRO:HA	4:H:174:TYR:CE1	2.42	0.54
6:E:84:ASP:O	6:E:88:TYR:OH	2.24	0.54
6:E:192:HIS:HD2	6:E:194:SER:N	2.05	0.54
1:G:203:GLN:HB2	1:G:435:TYR:HD2	1.73	0.54
2:B:573:ILE:HG13	2:B:576:LEU:HD22	1.89	0.54
1:G:295:ASN:HA	1:G:445:CYS:O	2.07	0.54
3:L:86:TYR:O	3:L:102:THR:HG22	2.06	0.54
3:L:151:ALA:O	3:L:154:SER:N	2.41	0.54
4:H:100(J):PHE:N	4:H:100(J):PHE:CD1	2.75	0.54
1:G:67:ASN:OD1	1:G:68:VAL:HG12	2.08	0.54
3:L:58:ILE:HD12	3:L:58:ILE:O	2.08	0.54
3:L:15:LEU:HD13	3:L:106:VAL:HG11	1.89	0.54
4:H:100(D):MET:O	4:H:100(I):GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:31:PHE:HA	8:C:1:NAG:O6	2.07	0.54
5:D:121:VAL:CG2	5:D:141:LEU:HD12	2.36	0.54
5:D:121:VAL:HG22	5:D:209:LYS:NZ	2.22	0.54
1:G:65:LYS:HB3	1:G:66:HIS:CD2	2.43	0.54
1:G:287:GLN:HE21	1:G:450:THR:CB	2.21	0.54
2:B:565:LEU:O	2:B:567:LYS:NZ	2.41	0.54
4:H:82:LEU:HD22	4:H:82(C):VAL:HG22	1.90	0.54
4:H:125:SER:O	4:H:126:SER:OG	2.23	0.54
4:H:136:LEU:HD13	4:H:137:GLY:N	2.22	0.54
5:D:23:LYS:HE2	5:D:23:LYS:HA	1.90	0.54
6:E:72:SER:OG	6:E:73:ALA:N	2.40	0.54
1:G:174:SER:OG	1:G:175:LEU:N	2.41	0.54
1:G:395:TRP:O	1:G:396:ILE:HD13	2.08	0.54
3:L:83:GLU:HA	3:L:104:LEU:CD1	2.38	0.54
3:L:150:LYS:NZ	3:L:154:SER:N	2.56	0.54
3:L:167:LYS:HA	3:L:173:TYR:HA	1.89	0.54
6:E:75:LEU:O	6:E:75:LEU:HD12	2.08	0.54
1:G:159:PHE:O	1:G:171:LYS:HA	2.08	0.53
1:G:200:ALA:O	1:G:433:ALA:N	2.24	0.53
2:B:624:ASP:O	5:D:97:LEU:O	2.26	0.53
3:L:96:TRP:HA	4:H:47:TRP:HZ3	1.71	0.53
3:L:116:VAL:HG22	3:L:137:ILE:HG22	1.90	0.53
1:G:121:LYS:NZ	1:G:201:ILE:H	2.06	0.53
3:L:35:TRP:HE1	3:L:73:LEU:CD1	2.20	0.53
3:L:203:VAL:O	3:L:204:GLU:HG3	2.08	0.53
4:H:66:ARG:NH1	4:H:82:LEU:HD21	2.23	0.53
6:E:37:TRP:CD1	6:E:90:CYS:HA	2.43	0.53
1:G:268:GLU:HG2	1:G:269:GLU:H	1.74	0.53
3:L:34:GLN:OE1	3:L:91:TRP:NE1	2.42	0.53
4:H:100(G):PHE:HB3	4:H:100(I):GLU:CG	2.38	0.53
6:E:37:TRP:CZ2	6:E:90:CYS:HB2	2.43	0.53
6:E:63:ARG:HB3	6:E:78:SER:O	2.09	0.53
1:G:183:GLN:HA	1:G:191:TYR:HA	1.91	0.53
1:G:195:ASN:CG	1:G:201:ILE:HD11	2.28	0.53
2:B:617:ARG:HH12	2:B:621:GLU:HB3	1.74	0.53
3:L:199:GLU:CG	3:L:201:SER:HB2	2.39	0.53
6:E:39:GLN:HA	6:E:88:TYR:CD1	2.44	0.53
4:H:139:LEU:HD23	4:H:140:VAL:N	2.23	0.53
6:E:16:GLN:HE22	6:E:18:VAL:HB	1.72	0.53
4:H:11:LEU:HD11	4:H:108:THR:N	2.23	0.53
4:H:152:TRP:HH2	4:H:178:SER:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:150:VAL:HG23	6:E:198:GLN:O	2.09	0.53
1:G:259:LEU:HA	1:G:452:LEU:HA	1.90	0.53
3:L:195:GLN:CB	3:L:204:GLU:HB3	2.36	0.53
6:E:105:THR:O	6:E:106:LYS:HG2	2.08	0.53
6:E:129:LEU:HD21	6:E:134:ALA:HB2	1.89	0.53
1:G:389:GLY:HA2	15:Q:1:NAG:O6	2.08	0.53
3:L:168:GLN:HE22	3:L:173:TYR:C	2.12	0.53
4:H:121:PRO:HB2	4:H:209:VAL:HG13	1.91	0.53
5:D:9:ALA:HB1	5:D:108:LEU:H	1.74	0.53
6:E:39:GLN:HA	6:E:88:TYR:HD1	1.74	0.53
1:G:39:TYR:OH	2:B:623:TRP:HH2	1.92	0.53
3:L:25:ARG:HG3	3:L:90:MET:SD	2.49	0.53
4:H:115:LYS:CB	4:H:144:PHE:CE1	2.92	0.53
5:D:34:ILE:O	5:D:50:TRP:HB3	2.09	0.53
6:E:168:PRO:HB3	6:E:178:ALA:HB2	1.91	0.53
1:G:73:ALA:HB3	2:B:571:TRP:HD1	1.74	0.53
1:G:491:ILE:HG22	1:G:493:PRO:HD3	1.90	0.53
5:D:121:VAL:HG22	5:D:209:LYS:HD2	1.91	0.53
6:E:20:ILE:HB	6:E:105:THR:HG21	1.91	0.53
6:E:36:SER:O	6:E:38:TYR:CZ	2.61	0.53
1:G:121:LYS:NZ	1:G:201:ILE:O	2.34	0.52
2:B:645:LEU:HD23	2:B:648:GLU:HB3	1.90	0.52
4:H:96:GLN:N	4:H:100(O):TYR:O	2.42	0.52
5:D:206:LYS:HE2	5:D:208:ASP:OD1	2.10	0.52
6:E:37:TRP:HA	6:E:38:TYR:CD2	2.44	0.52
1:G:335:LYS:HE2	1:G:412:ASP:HB3	1.91	0.52
2:B:607:ASN:ND2	2:B:650:GLN:HA	2.21	0.52
2:B:625:ASN:HB2	5:D:97:LEU:HG	1.91	0.52
1:G:107:ASP:OD2	1:G:217:TYR:OH	2.22	0.52
1:G:298:ARG:HB3	1:G:329:ALA:HA	1.91	0.52
1:G:342:LEU:O	1:G:346:VAL:HG23	2.08	0.52
5:D:121:VAL:HA	5:D:141:LEU:CG	2.38	0.52
5:D:155:ASN:ND2	5:D:159:LEU:HB3	2.24	0.52
1:G:39:TYR:HE1	1:G:497:ALA:HB3	1.74	0.52
1:G:427:TRP:CD1	1:G:429:ARG:HB2	2.45	0.52
4:H:6:GLU:HB3	4:H:20:LEU:HD11	1.90	0.52
5:D:140:CYS:SG	5:D:209:LYS:HD3	2.49	0.52
6:E:38:TYR:O	6:E:88:TYR:HA	2.09	0.52
2:B:544:LEU:CD1	2:B:586:TYR:HB2	2.39	0.52
2:B:545:LEU:HD23	2:B:586:TYR:CD1	2.44	0.52
3:L:167:LYS:HD2	3:L:171:ASN:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:11:LEU:HD11	5:D:112:SER:HB2	1.90	0.52
6:E:124:PRO:HB2	6:E:128:GLU:OE1	2.09	0.52
1:G:205:CYS:O	1:G:208:VAL:HG22	2.10	0.52
1:G:287:GLN:HA	1:G:450:THR:O	2.10	0.52
5:D:23:LYS:NZ	5:D:78:ALA:CB	2.73	0.52
6:E:68:LYS:HG2	6:E:73:ALA:CA	2.37	0.52
6:E:87:THR:HG22	6:E:106:LYS:HG2	1.92	0.52
6:E:110:LEU:N	6:E:110:LEU:CD1	2.73	0.52
6:E:135:THR:HA	6:E:182:LEU:O	2.10	0.52
3:L:34:GLN:HG2	4:H:100(O):TYR:HB3	1.90	0.52
3:L:86:TYR:HE2	3:L:104:LEU:CD2	2.22	0.52
3:L:119:PHE:CZ	4:H:125:SER:HB3	2.45	0.52
5:D:95:GLY:HA3	5:D:101:TYR:HB3	1.90	0.52
1:G:69:TRP:HA	1:G:111:LEU:CD1	2.40	0.52
1:G:265:LEU:HD11	1:G:288:PHE:HB2	1.92	0.52
1:G:294:ILE:HD13	1:G:333:VAL:HG22	1.90	0.52
3:L:54:ARG:NH1	3:L:60:GLU:HA	2.24	0.52
3:L:122:SER:CB	4:H:120:PHE:HB3	2.40	0.52
3:L:122:SER:HB2	4:H:120:PHE:HB3	1.91	0.52
5:D:121:VAL:CA	5:D:141:LEU:HD12	2.39	0.52
6:E:192:HIS:CE1	6:E:195:TYR:CZ	2.97	0.52
4:H:100(H):GLY:N	4:H:100(I):GLU:HG2	2.25	0.52
5:D:21:SER:HA	5:D:36:TRP:HH2	1.74	0.52
1:G:101:VAL:HG11	1:G:480:ARG:CD	2.40	0.52
1:G:299:PRO:HD2	1:G:327:ARG:HB3	1.90	0.52
3:L:35:TRP:O	3:L:36:TYR:CG	2.63	0.52
4:H:136:LEU:O	4:H:179:VAL:HG13	2.10	0.52
4:H:149:THR:HG22	4:H:197:ASN:CB	2.39	0.52
1:G:181:VAL:HG12	1:G:193:LEU:HG	1.92	0.51
3:L:84:ALA:H	3:L:104:LEU:CD1	2.20	0.51
5:D:9:ALA:HB1	5:D:108:LEU:HB3	1.92	0.51
6:E:99:CYS:HB3	6:E:101:PHE:HE1	1.75	0.51
6:E:153:LYS:HD2	6:E:157:SER:H	1.74	0.51
7:A:1:NAG:C8	7:A:1:NAG:C3	2.87	0.51
1:G:261:LEU:HD21	1:G:448:ASN:H	1.76	0.51
1:G:364:SER:HA	1:G:469:ARG:CD	2.26	0.51
2:B:647:GLU:CG	2:B:652:GLN:HE22	2.23	0.51
4:H:59:TYR:HD2	4:H:64:LYS:HB2	1.74	0.51
5:D:21:SER:OG	5:D:79:TYR:HA	2.10	0.51
6:E:134:ALA:N	6:E:184:LEU:HG	2.25	0.51
1:G:80:ASN:O	1:G:82:GLN:NE2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:MET:HA	1:G:348:GLN:OE1	2.10	0.51
1:G:361:PHE:HE1	1:G:470:PRO:CD	2.21	0.51
3:L:37:GLN:OE1	3:L:45:ILE:HD11	2.10	0.51
4:H:100(B):TYR:CE2	4:H:100(I):GLU:HA	2.45	0.51
4:H:166:ALA:HB2	4:H:176:LEU:HB2	1.92	0.51
5:D:51:ILE:HG13	5:D:52:SER:N	2.21	0.51
1:G:327:ARG:NH1	4:H:100(C):GLY:HA3	2.24	0.51
1:G:376:PHE:CE1	1:G:383:PHE:HB2	2.46	0.51
4:H:145:PRO:HD2	4:H:198:HIS:CE1	2.45	0.51
1:G:62:GLU:OE2	1:G:62:GLU:N	2.41	0.51
1:G:107:ASP:O	1:G:110:SER:N	2.43	0.51
2:B:647:GLU:HG3	2:B:652:GLN:HE22	1.74	0.51
4:H:66:ARG:HH11	4:H:82:LEU:HD11	1.76	0.51
5:D:11:LEU:HD11	5:D:112:SER:CB	2.40	0.51
5:D:98:ARG:CZ	5:D:98:ARG:HA	2.40	0.51
5:D:121:VAL:CG2	5:D:209:LYS:HD2	2.40	0.51
1:G:101:VAL:HG13	1:G:483:LEU:HD23	1.93	0.51
3:L:38:HIS:HB3	3:L:85:ASP:O	2.11	0.51
4:H:5:GLN:HA	4:H:5:GLN:NE2	2.25	0.51
4:H:16:GLU:HG2	4:H:17:THR:N	2.26	0.51
6:E:86:THR:HG22	6:E:87:THR:H	1.75	0.51
6:E:152:TRP:HD1	6:E:152:TRP:O	1.94	0.51
1:G:116:LEU:HD12	1:G:117:LYS:HG2	1.92	0.51
1:G:346:VAL:HG13	1:G:359:ILE:CD1	2.41	0.51
1:G:359:ILE:O	1:G:394:THR:HG23	2.10	0.51
3:L:37:GLN:HE21	3:L:86:TYR:HE1	1.53	0.51
4:H:89:ILE:HD11	4:H:104:GLY:HA3	1.93	0.51
5:D:35:ASN:HD21	5:D:50:TRP:HE3	1.57	0.51
5:D:144:ASP:HA	5:D:176:TYR:O	2.10	0.51
6:E:23:THR:CG2	6:E:72:SER:CB	2.89	0.51
1:G:271:MET:HA	1:G:348:GLN:CD	2.31	0.51
4:H:124:PRO:HD2	4:H:211:PRO:HA	1.93	0.51
5:D:100(A):SER:OG	8:C:7:MAN:H3	2.11	0.51
1:G:363:ASN:O	1:G:469:ARG:NE	2.44	0.51
2:B:576:LEU:HA	2:B:579:ARG:NE	2.24	0.51
2:B:657:GLU:O	2:B:661:LEU:N	2.44	0.51
5:D:163:VAL:HG13	5:D:182:VAL:HG21	1.92	0.51
6:E:13:SER:HB2	6:E:110:LEU:O	2.10	0.51
6:E:100:VAL:C	6:E:101:PHE:HD1	2.14	0.51
6:E:131:ALA:N	6:E:132:ASN:HA	2.26	0.51
1:G:152:GLY:N	1:G:178:ARG:HH21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:117:PRO:HA	4:H:142:ASP:O	2.11	0.51
4:H:164:PHE:O	4:H:176:LEU:HG	2.11	0.51
1:G:44:VAL:HG13	1:G:492:GLU:HB2	1.93	0.50
1:G:327:ARG:NH1	4:H:100(B):TYR:CD2	2.70	0.50
1:G:373:THR:OG1	1:G:385:CYS:O	2.27	0.50
5:D:68:ILE:C	5:D:69:MET:HG3	2.31	0.50
1:G:104:MET:O	1:G:108:ILE:HG13	2.12	0.50
1:G:287:GLN:HE21	1:G:450:THR:HB	1.75	0.50
4:H:100:ARG:O	4:H:100(A):ILE:HG12	2.11	0.50
5:D:142:VAL:HG11	5:D:178:LEU:HD12	1.93	0.50
6:E:37:TRP:CD1	6:E:91:CYS:HB3	2.45	0.50
6:E:68:LYS:HG2	6:E:72:SER:C	2.32	0.50
6:E:185:THR:HG22	6:E:186:PRO:HD2	1.92	0.50
1:G:128:THR:C	1:G:129:LEU:CD1	2.80	0.50
1:G:203:GLN:HE22	1:G:318:TYR:HB2	1.75	0.50
2:B:576:LEU:HA	2:B:579:ARG:HH21	1.76	0.50
6:E:38:TYR:CE2	6:E:101:PHE:CE2	2.99	0.50
3:L:36:TYR:HA	3:L:46:LEU:CD1	2.41	0.50
4:H:117:PRO:HB3	4:H:143:TYR:HB3	1.93	0.50
4:H:149:THR:CG2	4:H:197:ASN:N	2.73	0.50
5:D:103:TRP:CE3	6:E:46:PRO:HD2	2.45	0.50
6:E:49:ILE:HD13	6:E:75:LEU:HD13	1.93	0.50
1:G:40:TYR:HA	1:G:494:LEU:HD22	1.92	0.50
1:G:285:LEU:HD21	1:G:477:ASP:HB3	1.93	0.50
3:L:36:TYR:HA	3:L:46:LEU:HD13	1.91	0.50
1:G:469:ARG:CZ	1:G:469:ARG:HB2	2.41	0.50
3:L:18:THR:HG23	3:L:75:ILE:C	2.32	0.50
3:L:189:HIS:HD2	3:L:192:TYR:CE2	2.30	0.50
4:H:33:TYR:O	4:H:94:ARG:NH2	2.45	0.50
4:H:51:ILE:HA	4:H:56:SER:O	2.12	0.50
2:B:523:LEU:HD12	2:B:540:GLN:HE21	1.77	0.50
2:B:624:ASP:HB3	5:D:97:LEU:HB3	1.93	0.50
3:L:37:GLN:CG	3:L:86:TYR:HE1	2.25	0.50
4:H:198:HIS:NE2	4:H:200:PRO:HG2	2.27	0.50
5:D:17:SER:OG	5:D:82(A):ARG:HD3	2.10	0.50
1:G:127:VAL:HG23	1:G:129:LEU:HD21	1.94	0.50
4:H:149:THR:CG2	4:H:197:ASN:CG	2.80	0.50
5:D:96:LEU:HD21	5:D:100(E):LEU:HB2	1.94	0.50
1:G:350:ARG:CG	1:G:355:ASN:HA	2.41	0.50
6:E:68:LYS:CG	6:E:73:ALA:HA	2.41	0.50
1:G:346:VAL:HG13	1:G:359:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ILE:HA	2:B:576:LEU:HB3	1.94	0.49
3:L:143:GLY:CA	3:L:173:TYR:HD2	2.21	0.49
4:H:113:SER:C	4:H:144:PHE:CE2	2.80	0.49
5:D:31:PHE:CE2	8:C:1:NAG:H4	2.46	0.49
3:L:197:THR:O	3:L:197:THR:OG1	2.28	0.49
5:D:142:VAL:O	5:D:142:VAL:HG13	2.12	0.49
3:L:29:GLY:HA3	3:L:93:SER:OG	2.11	0.49
5:D:11:LEU:HD22	5:D:147:PRO:HD3	1.95	0.49
5:D:96:LEU:HD21	5:D:100(E):LEU:CB	2.42	0.49
6:E:134:ALA:H	6:E:184:LEU:HG	1.77	0.49
4:H:91:TYR:HE1	4:H:104:GLY:HA3	1.77	0.49
4:H:100(D):MET:O	4:H:100(F):SER:N	2.45	0.49
4:H:149:THR:CG2	4:H:197:ASN:H	2.24	0.49
14:P:1:NAG:O3	14:P:2:NAG:O5	2.23	0.49
2:B:608:VAL:HG21	2:B:649:SER:HB3	1.94	0.49
3:L:171:ASN:O	3:L:172:LYS:HD3	2.11	0.49
5:D:71:THR:CB	5:D:78:ALA:HA	2.41	0.49
5:D:93:ALA:HB1	5:D:102:LEU:O	2.12	0.49
1:G:327:ARG:HA	4:H:100(G):PHE:HZ	1.78	0.49
4:H:6:GLU:HG2	4:H:22:CYS:HB2	1.94	0.49
4:H:145:PRO:HB2	4:H:147:PRO:HD2	1.95	0.49
1:G:68:VAL:HG13	1:G:69:TRP:H	1.77	0.49
2:B:591:GLN:O	2:B:595:ILE:HG12	2.13	0.49
6:E:80:LEU:HD22	6:E:81:ARG:N	2.26	0.49
1:G:327:ARG:NH1	4:H:100(I):GLU:OE1	2.46	0.49
3:L:149:TRP:CE3	3:L:179:LEU:HG	2.47	0.49
5:D:155:ASN:HD21	5:D:159:LEU:N	2.11	0.49
6:E:23:THR:CG2	6:E:72:SER:HB2	2.43	0.49
6:E:49:ILE:O	6:E:56:ARG:HB2	2.13	0.49
6:E:192:HIS:HE1	6:E:195:TYR:CZ	2.31	0.49
1:G:216:HIS:ND1	1:G:248:THR:O	2.42	0.49
1:G:227:LYS:HG3	1:G:485:LYS:HB3	1.94	0.49
1:G:274:SER:OG	1:G:277:ILE:HG13	2.13	0.49
1:G:392:ASN:OD1	15:Q:1:NAG:O5	2.21	0.49
2:B:606:THR:CG2	2:B:650:GLN:HE22	2.23	0.49
6:E:49:ILE:HG23	6:E:50:ILE:H	1.78	0.49
1:G:294:ILE:O	1:G:447:SER:HB2	2.13	0.49
3:L:61:ARG:NH1	3:L:62:PHE:HB3	2.28	0.49
4:H:146:GLU:HB2	4:H:174:TYR:CD2	2.48	0.49
5:D:96:LEU:HD13	5:D:98:ARG:HH22	1.77	0.49
5:D:100(E):LEU:HD22	5:D:101:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:197:ASN:HB2	5:D:208:ASP:OD1	2.13	0.49
2:B:642:ILE:O	2:B:646:LEU:HD12	2.12	0.48
3:L:93:SER:OG	3:L:94:ARG:HG3	2.13	0.48
4:H:46:GLU:HG2	4:H:48:ILE:CD1	2.43	0.48
4:H:183:PRO:O	4:H:186:SER:HB3	2.12	0.48
6:E:121:LEU:HD12	6:E:197:CYS:SG	2.53	0.48
1:G:226:LEU:HD11	1:G:245:VAL:H	1.78	0.48
2:B:617:ARG:NH1	2:B:621:GLU:HB3	2.27	0.48
3:L:7:TYR:H	3:L:9:ARG:NH1	2.11	0.48
3:L:7:TYR:H	3:L:9:ARG:HH12	1.61	0.48
3:L:66:PRO:HB3	13:O:5:MAN:O3	2.13	0.48
3:L:160:VAL:N	3:L:161:GLU:OE2	2.46	0.48
4:H:123:ALA:HB1	4:H:124:PRO:HD2	1.95	0.48
5:D:198:VAL:HG12	5:D:207:VAL:H	1.77	0.48
6:E:49:ILE:CD1	6:E:64:PHE:CG	2.96	0.48
1:G:107:ASP:O	1:G:111:LEU:HD23	2.12	0.48
3:L:199:GLU:HG2	3:L:201:SER:HB2	1.94	0.48
4:H:60:ASN:C	4:H:64:LYS:HE3	2.33	0.48
4:H:86:ASP:O	4:H:90:TYR:OH	2.27	0.48
1:G:455:THR:HG23	1:G:471:GLY:HA3	1.95	0.48
3:L:47:LEU:HB2	3:L:62:PHE:CD2	2.48	0.48
3:L:51:ASN:N	3:L:51:ASN:HD22	2.11	0.48
3:L:146:THR:O	3:L:197:THR:N	2.47	0.48
5:D:100(D):TRP:HH2	6:E:94:THR:O	1.96	0.48
5:D:153:SER:C	5:D:154:TRP:CD1	2.83	0.48
6:E:129:LEU:HD13	6:E:132:ASN:HB3	1.95	0.48
1:G:446:VAL:O	11:M:1:NAG:H3	2.14	0.48
2:B:618:ASN:CB	2:B:621:GLU:OE2	2.57	0.48
3:L:50:ASN:C	3:L:52:GLN:H	2.17	0.48
4:H:114:THR:HG21	4:H:200:PRO:O	2.12	0.48
1:G:258:GLN:OE1	1:G:470:PRO:HB2	2.13	0.48
6:E:49:ILE:HG23	6:E:50:ILE:N	2.27	0.48
6:E:188:GLN:HB2	6:E:189:TRP:CD1	2.48	0.48
4:H:25:SER:O	4:H:25:SER:OG	2.32	0.48
1:G:271:MET:HA	1:G:348:GLN:NE2	2.28	0.48
2:B:630:GLN:O	2:B:633:LYS:HE3	2.14	0.48
3:L:48:ILE:HA	3:L:54:ARG:HA	1.96	0.48
3:L:118:LEU:HD12	3:L:133:LEU:HD21	1.94	0.48
5:D:163:VAL:HG22	5:D:182:VAL:HG11	1.95	0.48
6:E:23:THR:HB	6:E:71:TRP:O	2.13	0.48
1:G:485:LYS:HB2	1:G:486:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:23:CYS:HB3	3:L:25:ARG:NH1	2.28	0.48
6:E:74:TYR:HD1	6:E:75:LEU:H	1.60	0.48
1:G:35:TRP:CE3	2:B:609:PRO:HA	2.49	0.48
1:G:62:GLU:HA	1:G:65:LYS:HE3	1.96	0.48
1:G:272:ILE:CG1	1:G:286:VAL:HA	2.36	0.48
3:L:144:ALA:O	3:L:198:HIS:HD2	1.97	0.48
4:H:20:LEU:HD21	4:H:105:THR:HG21	1.94	0.48
5:D:38:ARG:O	5:D:45:PRO:HA	2.14	0.48
5:D:84:PHE:O	5:D:87:THR:HG22	2.14	0.48
5:D:86:ASP:O	5:D:90:TYR:OH	2.18	0.48
6:E:44:ARG:HG2	6:E:45:ALA:N	2.29	0.48
1:G:86:LEU:HD12	1:G:89:VAL:HG21	1.96	0.47
2:B:596:TRP:CH2	2:B:643:TYR:HD2	2.32	0.47
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.95	0.47
1:G:360:ARG:HE	1:G:467:THR:C	2.17	0.47
4:H:100(P):MET:HB2	4:H:101:TRP:HZ2	1.79	0.47
4:H:115:LYS:CB	4:H:144:PHE:HE1	2.21	0.47
5:D:51:ILE:HD13	5:D:57:LYS:CE	2.41	0.47
5:D:152:VAL:CG1	5:D:198:VAL:HA	2.36	0.47
1:G:47:ASP:OD1	1:G:487:LYS:NZ	2.46	0.47
1:G:56:SER:O	1:G:76:PRO:HA	2.13	0.47
1:G:163:THR:HG22	1:G:164:GLU:N	2.28	0.47
1:G:225:ILE:HG22	1:G:226:LEU:N	2.28	0.47
5:D:9:ALA:H	5:D:10:GLU:CD	2.18	0.47
5:D:143:LYS:HG3	5:D:145:TYR:OH	2.14	0.47
6:E:23:THR:HG22	6:E:72:SER:HA	1.96	0.47
6:E:153:LYS:HE2	6:E:159:VAL:N	2.11	0.47
1:G:67:ASN:HD22	1:G:70:ALA:HB3	1.80	0.47
1:G:226:LEU:CD1	1:G:245:VAL:H	2.27	0.47
3:L:117:THR:OG1	3:L:136:LEU:HD23	2.15	0.47
6:E:189:TRP:N	6:E:189:TRP:HD1	2.09	0.47
1:G:347:LYS:HA	1:G:347:LYS:HD3	1.65	0.47
1:G:502:LYS:HE2	2:B:607:ASN:HB2	1.97	0.47
6:E:38:TYR:HD1	6:E:48:LEU:CD2	2.27	0.47
6:E:136:LEU:HD21	6:E:195:TYR:CD2	2.49	0.47
1:G:101:VAL:HG11	1:G:480:ARG:HD3	1.94	0.47
1:G:158:SER:OG	1:G:173:TYR:HB3	2.14	0.47
1:G:37:THR:CG2	2:B:605:CYS:HA	2.44	0.47
1:G:459:GLY:O	1:G:460:SER:OG	2.29	0.47
16:B:702:NAG:H83	6:E:55:GLU:CD	2.34	0.47
4:H:23:THR:HA	4:H:77:GLN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:ILE:HG23	4:H:60:ASN:HB3	1.96	0.47
4:H:50:TYR:CG	4:H:51:ILE:N	2.83	0.47
4:H:100(B):TYR:CZ	4:H:100(I):GLU:HA	2.50	0.47
4:H:100(G):PHE:HD1	4:H:100(G):PHE:O	1.97	0.47
4:H:100(P):MET:HB3	4:H:101:TRP:NE1	2.29	0.47
4:H:150:VAL:HG12	4:H:196:VAL:CG1	2.43	0.47
4:H:157:LEU:H	4:H:157:LEU:HD23	1.80	0.47
4:H:166:ALA:HB1	4:H:175:SER:H	1.80	0.47
5:D:6:GLN:NE2	5:D:22:CYS:SG	2.88	0.47
5:D:12:LYS:HZ1	5:D:16:ALA:N	2.13	0.47
5:D:142:VAL:CG1	5:D:179:SER:HA	2.45	0.47
6:E:63:ARG:O	6:E:78:SER:N	2.48	0.47
6:E:101:PHE:HD1	6:E:101:PHE:N	2.12	0.47
6:E:121:LEU:HA	6:E:138:CYS:HB2	1.96	0.47
1:G:349:LEU:O	1:G:352:HIS:ND1	2.47	0.47
1:G:502:LYS:HE2	2:B:607:ASN:CB	2.45	0.47
2:B:580:VAL:O	2:B:584:GLU:HG3	2.15	0.47
3:L:119:PHE:C	3:L:133:LEU:HD13	2.35	0.47
4:H:94:ARG:O	4:H:100(P):MET:HA	2.14	0.47
2:B:533:ALA:HB3	2:B:628:TRP:NE1	2.29	0.47
4:H:89:ILE:HD12	4:H:105:THR:O	2.14	0.47
4:H:100(J):PHE:N	4:H:100(J):PHE:HD1	2.13	0.47
5:D:78:ALA:HB1	5:D:80:MET:HE1	1.97	0.47
6:E:121:LEU:HG	6:E:138:CYS:CB	2.40	0.47
1:G:112:TRP:CZ2	1:G:426:MET:HE1	2.49	0.47
1:G:304:ARG:HH12	1:G:440:GLN:N	2.13	0.47
6:E:96:ASN:HB2	8:C:6:MAN:C2	2.45	0.47
6:E:135:THR:HG21	6:E:181:TYR:CD1	2.50	0.47
4:H:17:THR:HA	4:H:82:LEU:O	2.15	0.46
5:D:179:SER:HB3	6:E:139:LEU:HD22	1.97	0.46
6:E:125:SER:O	6:E:128:GLU:HB3	2.16	0.46
1:G:287:GLN:HA	1:G:451:GLY:HA2	1.97	0.46
1:G:393:SER:HB2	1:G:395:TRP:HE1	1.80	0.46
4:H:46:GLU:HG2	4:H:48:ILE:HD11	1.96	0.46
5:D:37:ILE:HD11	5:D:103:TRP:CH2	2.50	0.46
5:D:84:PHE:CE2	5:D:111:VAL:HG12	2.50	0.46
5:D:147:PRO:O	5:D:200:HIS:NE2	2.47	0.46
6:E:4:LEU:HD11	6:E:102:GLY:CA	2.31	0.46
1:G:35:TRP:CD1	1:G:502:LYS:HB2	2.50	0.46
1:G:178:ARG:NH1	1:G:419:ARG:HH22	2.14	0.46
1:G:363:ASN:CG	1:G:388:SER:HA	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:377:ASN:ND2	1:G:382:PHE:HE1	2.13	0.46
6:E:56:ARG:HG3	6:E:60:ILE:HD11	1.97	0.46
6:E:190:LYS:HZ1	6:E:213:THR:N	2.12	0.46
1:G:192:ARG:HH21	1:G:197:ASN:HB2	1.81	0.46
3:L:163:THR:HG22	3:L:176:SER:H	1.80	0.46
4:H:33:TYR:H	4:H:94:ARG:HH22	1.62	0.46
5:D:23:LYS:HE2	5:D:23:LYS:CA	2.46	0.46
6:E:101:PHE:N	6:E:101:PHE:CD1	2.84	0.46
1:G:323:ILE:O	1:G:323:ILE:HG13	2.15	0.46
3:L:46:LEU:HD12	3:L:46:LEU:HA	1.41	0.46
4:H:94:ARG:HG2	4:H:100(R):VAL:H	1.80	0.46
5:D:36:TRP:NE1	5:D:80:MET:HG2	2.31	0.46
6:E:37:TRP:HB3	6:E:89:TYR:O	2.16	0.46
2:B:645:LEU:HD23	2:B:648:GLU:CG	2.46	0.46
5:D:31:PHE:CE1	8:C:2:NAG:H82	2.51	0.46
1:G:135:THR:HG1	3:L:94:ARG:HH21	1.61	0.46
1:G:259:LEU:C	1:G:260:LEU:HG	2.35	0.46
4:H:45:LEU:HD23	4:H:46:GLU:N	2.31	0.46
4:H:64:LYS:HE2	4:H:64:LYS:HB3	1.55	0.46
5:D:33:HIS:HE1	5:D:98:ARG:NE	2.13	0.46
5:D:100(B):SER:HB3	6:E:52:GLU:OE1	2.14	0.46
6:E:184:LEU:HD23	6:E:189:TRP:CZ3	2.50	0.46
1:G:200:ALA:C	1:G:201:ILE:HD12	2.35	0.46
1:G:480:ARG:HG2	1:G:480:ARG:HH11	1.81	0.46
3:L:167:LYS:HD3	3:L:173:TYR:CE1	2.51	0.46
5:D:35:ASN:CB	5:D:94:LYS:HE3	2.40	0.46
1:G:62:GLU:HA	1:G:65:LYS:CE	2.45	0.46
4:H:29:ILE:HA	4:H:34:TRP:HH2	1.81	0.46
5:D:72(C):VAL:O	5:D:75:THR:N	2.48	0.46
5:D:96:LEU:HG	5:D:100(E):LEU:HB3	1.97	0.46
6:E:129:LEU:CD2	6:E:134:ALA:HB2	2.46	0.46
1:G:85:HIS:ND1	1:G:242:VAL:O	2.48	0.46
1:G:478:ASN:O	1:G:478:ASN:ND2	2.49	0.46
2:B:545:LEU:HD13	2:B:545:LEU:O	2.16	0.46
3:L:37:GLN:NE2	3:L:86:TYR:CE1	2.76	0.46
3:L:72:THR:C	3:L:73:LEU:HD12	2.35	0.46
4:H:24:VAL:HG22	4:H:26:GLY:H	1.80	0.46
5:D:96:LEU:CD1	5:D:100(D):TRP:C	2.84	0.46
6:E:99:CYS:SG	6:E:100:VAL:N	2.88	0.46
1:G:68:VAL:HG13	1:G:69:TRP:N	2.31	0.45
3:L:137:ILE:HD13	3:L:140:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:47:TRP:CZ2	5:D:49:GLY:HA2	2.51	0.45
5:D:68:ILE:O	5:D:69:MET:HG3	2.15	0.45
5:D:167:PRO:HG3	6:E:169:SER:CB	2.46	0.45
6:E:95:HIS:CE1	6:E:96:ASN:HB3	2.51	0.45
1:G:295:ASN:HD21	9:F:1:NAG:C7	2.28	0.45
1:G:301:ASN:HB3	1:G:441:GLY:HA2	1.98	0.45
3:L:16:GLY:H	3:L:78:VAL:HG23	1.81	0.45
3:L:61:ARG:NH2	3:L:61:ARG:HG2	2.31	0.45
3:L:195:GLN:OE1	3:L:204:GLU:HB3	2.16	0.45
4:H:38:ARG:HE	4:H:38:ARG:HB2	1.59	0.45
4:H:107:VAL:HG23	4:H:107:VAL:O	2.16	0.45
5:D:30:ASN:ND2	5:D:53:TYR:HB2	2.31	0.45
5:D:155:ASN:HD21	5:D:159:LEU:H	1.64	0.45
1:G:335:LYS:HG2	1:G:412:ASP:O	2.15	0.45
3:L:75:ILE:HD13	3:L:78:VAL:CG1	2.46	0.45
3:L:84:ALA:HB3	3:L:86:TYR:CE1	2.51	0.45
5:D:11:LEU:CD1	5:D:110:THR:HG22	2.47	0.45
5:D:72(F):THR:HG22	5:D:72(G):SER:H	1.81	0.45
1:G:42:VAL:HG22	1:G:493:PRO:O	2.16	0.45
1:G:95:MET:HA	1:G:98:ASN:HB2	1.99	0.45
1:G:264:SER:H	1:G:482:GLU:CD	2.20	0.45
4:H:82(C):VAL:HG13	4:H:86:ASP:HB2	1.97	0.45
1:G:272:ILE:HG21	1:G:286:VAL:HA	1.98	0.45
1:G:300:ASN:OD1	1:G:327:ARG:HB2	2.17	0.45
3:L:16:GLY:N	3:L:78:VAL:HG23	2.31	0.45
5:D:36:TRP:NE1	5:D:80:MET:HE3	2.27	0.45
5:D:168:ALA:CB	5:D:176:TYR:HB3	2.46	0.45
6:E:144:TYR:CD1	6:E:145:PRO:HA	2.51	0.45
1:G:221:ALA:HB1	2:B:544:LEU:O	2.16	0.45
1:G:383:PHE:CD1	1:G:383:PHE:N	2.85	0.45
4:H:20:LEU:HD13	4:H:21:THR:N	2.31	0.45
6:E:68:LYS:CB	6:E:73:ALA:HA	2.47	0.45
6:E:152:TRP:O	6:E:152:TRP:CD1	2.69	0.45
6:E:170:LYS:HD3	6:E:170:LYS:N	2.31	0.45
6:E:196:SER:HB3	6:E:207:GLU:OE1	2.16	0.45
1:G:111:LEU:HD23	1:G:111:LEU:H	1.80	0.45
4:H:187:LEU:HA	4:H:188:GLY:HA2	1.67	0.45
6:E:35:ILE:HA	6:E:91:CYS:O	2.16	0.45
1:G:101:VAL:HG21	1:G:480:ARG:NE	2.31	0.45
1:G:181:VAL:CG1	1:G:193:LEU:HG	2.46	0.45
1:G:384:TYR:HE1	1:G:421:LYS:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:539:VAL:HG13	2:B:540:GLN:OE1	2.16	0.45
3:L:83:GLU:HA	3:L:104:LEU:HD11	1.99	0.45
5:D:140:CYS:HB2	5:D:154:TRP:CZ2	2.52	0.45
1:G:304:ARG:HD2	1:G:440:GLN:HB3	1.99	0.45
2:B:650:GLN:O	2:B:654:GLU:HB2	2.16	0.45
6:E:131:ALA:H	6:E:132:ASN:HA	1.81	0.45
1:G:37:THR:HG22	2:B:606:THR:CB	2.46	0.45
1:G:123:THR:HG23	1:G:124:PRO:HD3	1.98	0.45
1:G:128:THR:N	1:G:129:LEU:HD13	2.32	0.45
1:G:335:LYS:C	1:G:339:ASN:HD22	2.16	0.45
3:L:37:GLN:O	3:L:44:PRO:HA	2.17	0.45
1:G:234:ASN:ND2	9:K:1:NAG:O5	2.23	0.44
2:B:519:PHE:HA	2:B:520:LEU:HA	1.52	0.44
2:B:639:THR:O	2:B:642:ILE:HG22	2.17	0.44
3:L:150:LYS:NZ	3:L:153:SER:N	2.65	0.44
4:H:51:ILE:HD12	4:H:56:SER:C	2.37	0.44
4:H:162:HIS:C	4:H:162:HIS:CD2	2.90	0.44
5:D:24:THR:HG23	5:D:27:TYR:CZ	2.52	0.44
5:D:169:VAL:HG22	5:D:170:LEU:N	2.29	0.44
1:G:35:TRP:O	1:G:498:PRO:HA	2.17	0.44
1:G:128:THR:O	1:G:129:LEU:HD12	2.17	0.44
1:G:298:ARG:H	1:G:443:ILE:HD11	1.81	0.44
2:B:639:THR:CG2	2:B:643:TYR:HE1	2.24	0.44
3:L:59:PRO:HG2	3:L:62:PHE:CE1	2.49	0.44
3:L:109:GLN:O	3:L:109:GLN:HG2	2.16	0.44
5:D:6:GLN:CD	5:D:22:CYS:SG	2.96	0.44
1:G:360:ARG:O	1:G:361:PHE:HB2	2.17	0.44
3:L:135:CYS:O	3:L:136:LEU:HD13	2.16	0.44
4:H:87:SER:O	4:H:88:ALA:HB2	2.18	0.44
4:H:146:GLU:N	4:H:147:PRO:HD2	2.32	0.44
5:D:121:VAL:HG22	5:D:209:LYS:HZ2	1.82	0.44
1:G:76:PRO:HG3	2:B:556:LEU:HB3	1.99	0.44
1:G:95:MET:HE1	1:G:484:TYR:CB	2.48	0.44
1:G:238:PRO:HG2	5:D:72(F):THR:HA	2.00	0.44
5:D:61:PRO:HA	5:D:64:GLN:CD	2.38	0.44
5:D:98:ARG:NE	5:D:98:ARG:CA	2.81	0.44
6:E:37:TRP:CG	6:E:90:CYS:HA	2.53	0.44
6:E:165:THR:HB	6:E:180:SER:CB	2.47	0.44
1:G:361:PHE:HD1	1:G:362:ALA:H	1.66	0.44
3:L:96:TRP:HH2	4:H:49:GLY:HA2	1.83	0.44
4:H:23:THR:HA	4:H:77:GLN:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:51:ILE:HG13	4:H:52:SER:N	2.32	0.44
5:D:72(F):THR:HG22	5:D:72(G):SER:N	2.32	0.44
6:E:99:CYS:SG	6:E:101:PHE:HE1	2.41	0.44
6:E:192:HIS:HE1	6:E:195:TYR:CE2	2.36	0.44
1:G:105:HIS:HB3	1:G:479:TRP:NE1	2.32	0.44
1:G:261:LEU:CD2	1:G:448:ASN:H	2.31	0.44
3:L:150:LYS:HZ2	3:L:154:SER:H	1.63	0.44
4:H:66:ARG:NH1	4:H:82:LEU:HD11	2.31	0.44
4:H:99:LYS:O	4:H:100:ARG:HB3	2.18	0.44
4:H:149:THR:CB	4:H:197:ASN:OD1	2.66	0.44
5:D:154:TRP:CD2	5:D:196:CYS:HB3	2.52	0.44
1:G:356:ASN:OD1	16:G:1663:NAG:H2	2.18	0.44
3:L:50:ASN:OD1	3:L:51:ASN:N	2.51	0.44
4:H:5:GLN:NE2	4:H:103:LYS:HE3	2.33	0.44
4:H:57:THR:OG1	4:H:58:ASN:N	2.51	0.44
5:D:121:VAL:HG23	5:D:141:LEU:CD1	2.40	0.44
6:E:23:THR:HG22	6:E:72:SER:CA	2.47	0.44
6:E:37:TRP:CE3	6:E:75:LEU:HD23	2.53	0.44
1:G:48:ALA:HB2	1:G:490:LYS:N	2.33	0.44
1:G:327:ARG:HE	4:H:100(B):TYR:HD2	1.65	0.44
3:L:10:PRO:O	3:L:11:LEU:HD13	2.17	0.44
3:L:46:LEU:HD12	3:L:47:LEU:N	2.32	0.44
5:D:119:PRO:HG2	5:D:205:THR:HB	2.00	0.44
3:L:194:CYS:O	3:L:194:CYS:SG	2.76	0.43
4:H:67:VAL:O	4:H:68:ILE:HG13	2.18	0.43
6:E:85:GLU:OE1	6:E:109:VAL:HG22	2.18	0.43
7:A:2:NAG:O7	7:A:2:NAG:O3	2.34	0.43
5:D:38:ARG:O	5:D:46:GLU:N	2.50	0.43
6:E:185:THR:HB	6:E:188:GLN:HG3	2.00	0.43
1:G:359:ILE:HG12	1:G:396:ILE:HD11	2.00	0.43
1:G:387:THR:HA	1:G:416:LEU:HD21	2.00	0.43
4:H:32:TYR:OH	4:H:96:GLN:HA	2.18	0.43
5:D:11:LEU:HA	5:D:110:THR:O	2.18	0.43
6:E:20:ILE:HD12	6:E:21:SER:H	1.83	0.43
6:E:64:PHE:HD2	6:E:77:ILE:HG22	1.83	0.43
6:E:189:TRP:O	6:E:192:HIS:CE1	2.72	0.43
9:F:5:MAN:H61	9:F:6:MAN:O6	2.19	0.43
1:G:61:TYR:O	1:G:61:TYR:CG	2.72	0.43
1:G:178:ARG:HB3	1:G:179:LEU:HD22	2.00	0.43
1:G:373:THR:HG21	1:G:384:TYR:HB3	2.00	0.43
3:L:43:ALA:HA	4:H:91:TYR:HE2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:141:LYS:HG3	4:H:142:ASP:HB2	1.99	0.43
4:H:173:LEU:HD12	4:H:173:LEU:HA	1.58	0.43
6:E:134:ALA:CB	6:E:184:LEU:HG	2.48	0.43
9:F:3:BMA:C4	9:F:4:MAN:H2	2.46	0.43
5:D:198:VAL:O	5:D:206:LYS:HA	2.19	0.43
6:E:153:LYS:HG3	6:E:156:SER:HA	1.99	0.43
1:G:39:TYR:HD1	1:G:495:GLY:O	2.01	0.43
1:G:102:GLU:HA	1:G:105:HIS:CD2	2.53	0.43
1:G:201:ILE:HD12	1:G:201:ILE:N	2.34	0.43
1:G:360:ARG:NE	1:G:468:PHE:HD1	2.16	0.43
2:B:586:TYR:CE1	2:B:587:LEU:HD23	2.53	0.43
4:H:6:GLU:HA	4:H:22:CYS:HA	2.00	0.43
1:G:55:ALA:O	1:G:216:HIS:HB2	2.19	0.43
1:G:136:ASN:OD1	1:G:137:ASN:N	2.51	0.43
2:B:645:LEU:HD23	2:B:648:GLU:CB	2.48	0.43
4:H:16:GLU:N	4:H:82(B):SER:HA	2.34	0.43
6:E:143:PHE:CD2	6:E:146:GLY:HA2	2.52	0.43
1:G:108:ILE:HD12	1:G:479:TRP:CH2	2.54	0.43
1:G:469:ARG:HH11	1:G:469:ARG:HD2	1.68	0.43
2:B:573:ILE:O	2:B:576:LEU:HB3	2.18	0.43
3:L:131:ALA:O	3:L:181:LEU:HB3	2.18	0.43
4:H:81:LYS:HE3	4:H:81:LYS:HB3	1.77	0.43
4:H:149:THR:CG2	4:H:197:ASN:CB	2.97	0.43
5:D:72(B):GLU:OE1	5:D:72(B):GLU:N	2.48	0.43
5:D:98:ARG:NH1	5:D:100(C):THR:CA	2.79	0.43
1:G:152:GLY:CA	1:G:178:ARG:HE	2.29	0.43
1:G:180:ASP:OD1	1:G:180:ASP:N	2.52	0.43
2:B:546:SER:HB2	2:B:549:VAL:HG12	2.00	0.43
2:B:622:ILE:HG13	2:B:623:TRP:N	2.34	0.43
3:L:152:ASP:OD1	3:L:152:ASP:N	2.51	0.43
4:H:39:GLN:OE1	4:H:91:TYR:CZ	2.71	0.43
6:E:192:HIS:CE1	6:E:195:TYR:CE2	3.07	0.43
1:G:298:ARG:HG3	1:G:443:ILE:HD11	2.01	0.43
3:L:111:LYS:HB3	3:L:141:TYR:O	2.18	0.43
4:H:50:TYR:O	4:H:58:ASN:N	2.52	0.43
5:D:33:HIS:O	5:D:94:LYS:HG3	2.19	0.43
5:D:67:VAL:HG13	5:D:69:MET:HE1	2.01	0.43
1:G:330:HIS:HA	1:G:416:LEU:O	2.19	0.42
2:B:633:LYS:HD2	2:B:634:GLU:N	2.34	0.42
3:L:36:TYR:HE2	3:L:89:HIS:HB2	1.84	0.42
3:L:50:ASN:HB3	3:L:52:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:137:ILE:HD12	3:L:137:ILE:O	2.19	0.42
6:E:6:GLN:NE2	6:E:103:THR:N	2.66	0.42
6:E:84:ASP:O	6:E:107:VAL:HG11	2.19	0.42
1:G:64:GLU:OE2	11:M:4:MAN:O4	2.30	0.42
1:G:172:VAL:HG22	1:G:173:TYR:N	2.35	0.42
3:L:120:PRO:O	4:H:122:LEU:HG	2.19	0.42
5:D:8:GLY:O	5:D:107:THR:OG1	2.25	0.42
5:D:179:SER:HB3	6:E:139:LEU:HD21	2.00	0.42
1:G:469:ARG:HB2	1:G:469:ARG:NH1	2.34	0.42
2:B:618:ASN:OD1	16:B:702:NAG:C7	2.67	0.42
2:B:643:TYR:HA	2:B:646:LEU:HD13	2.02	0.42
6:E:16:GLN:NE2	6:E:18:VAL:H	2.17	0.42
6:E:17:SER:HA	6:E:77:ILE:O	2.19	0.42
6:E:192:HIS:CD2	6:E:193:ARG:N	2.87	0.42
1:G:32:GLU:N	1:G:500:ARG:HH21	2.17	0.42
1:G:128:THR:C	1:G:129:LEU:HD13	2.38	0.42
3:L:119:PHE:HA	3:L:120:PRO:HD3	1.92	0.42
4:H:29:ILE:HG23	4:H:34:TRP:CZ3	2.54	0.42
4:H:136:LEU:HA	4:H:136:LEU:HD22	1.67	0.42
5:D:82(B):ASN:C	5:D:82(C):LEU:HD12	2.39	0.42
1:G:40:TYR:O	2:B:537:LEU:HB3	2.19	0.42
1:G:162:THR:OG1	1:G:166:ARG:NH2	2.31	0.42
1:G:215:ILE:N	1:G:251:ILE:O	2.47	0.42
1:G:224:ALA:O	1:G:489:VAL:N	2.52	0.42
1:G:263:GLY:H	1:G:450:THR:HG21	1.84	0.42
3:L:166:SER:O	3:L:174:ALA:N	2.44	0.42
3:L:172:LYS:HD3	3:L:172:LYS:N	2.33	0.42
5:D:67:VAL:HG23	5:D:82:ILE:HA	2.02	0.42
6:E:68:LYS:HG2	6:E:73:ALA:N	2.34	0.42
6:E:81:ARG:HB2	6:E:83:GLU:OE2	2.20	0.42
6:E:81:ARG:O	6:E:83:GLU:N	2.52	0.42
6:E:188:GLN:O	6:E:191:SER:HB2	2.18	0.42
1:G:155:LYS:NZ	1:G:191:TYR:HE2	2.17	0.42
2:B:608:VAL:H	2:B:650:GLN:HE22	1.62	0.42
3:L:25:ARG:N	11:J:5:MAN:O6	2.53	0.42
3:L:150:LYS:NZ	3:L:153:SER:H	2.17	0.42
4:H:121:PRO:HD3	4:H:207:LYS:HE3	2.02	0.42
5:D:100(C):THR:HG23	5:D:100(C):THR:O	2.19	0.42
5:D:181:VAL:HG21	6:E:122:PHE:CE2	2.54	0.42
6:E:153:LYS:HD3	6:E:154:ALA:N	2.34	0.42
1:G:297:THR:O	1:G:329:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:382:PHE:O	1:G:420:ILE:HA	2.20	0.42
5:D:148:GLU:HB2	5:D:149:PRO:HA	2.02	0.42
5:D:153:SER:O	5:D:154:TRP:HD1	2.03	0.42
6:E:38:TYR:OH	6:E:91:CYS:SG	2.76	0.42
6:E:70:TYR:HD1	6:E:70:TYR:H	1.67	0.42
6:E:144:TYR:HA	6:E:145:PRO:C	2.40	0.42
6:E:152:TRP:HE3	6:E:163:VAL:HG23	1.84	0.42
1:G:298:ARG:NH1	1:G:300:ASN:O	2.53	0.42
1:G:327:ARG:NH1	4:H:100(B):TYR:HD2	2.12	0.42
2:B:544:LEU:HD13	2:B:544:LEU:O	2.19	0.42
3:L:25:ARG:CZ	3:L:88:CYS:SG	3.08	0.42
3:L:95(B):PHE:CE1	4:H:47:TRP:CH2	3.06	0.42
4:H:163:THR:HA	4:H:178:SER:HA	2.02	0.42
5:D:100(D):TRP:CD1	5:D:100(E):LEU:N	2.87	0.42
1:G:328:GLN:H	4:H:100(G):PHE:HZ	1.66	0.42
1:G:385:CYS:HA	1:G:418:CYS:HA	2.02	0.42
1:G:455:THR:CG2	1:G:471:GLY:HA3	2.50	0.42
1:G:493:PRO:C	1:G:494:LEU:HD23	2.40	0.42
4:H:33:TYR:CE1	4:H:52:SER:HA	2.54	0.42
4:H:100(D):MET:HB2	13:O:2:NAG:O7	2.19	0.42
4:H:125:SER:OG	4:H:128:SER:N	2.49	0.42
4:H:193:ILE:HD13	4:H:208:LYS:NZ	2.35	0.42
5:D:33:HIS:C	5:D:94:LYS:HZ2	2.23	0.42
5:D:52:SER:HB2	5:D:56:ASP:OD1	2.20	0.42
5:D:110:THR:HG21	5:D:147:PRO:HB3	2.00	0.42
1:G:128:THR:C	1:G:129:LEU:HD12	2.40	0.42
1:G:411:ASN:OD1	1:G:412:ASP:N	2.53	0.42
2:B:583:VAL:O	2:B:587:LEU:N	2.37	0.42
4:H:6:GLU:HG2	4:H:92:CYS:SG	2.59	0.42
4:H:87:SER:HA	4:H:108:THR:HA	2.02	0.42
4:H:100(D):MET:CB	13:O:2:NAG:H2	2.48	0.42
5:D:10:GLU:HG2	5:D:202:PRO:CG	2.50	0.42
6:E:89:TYR:OH	6:E:104:GLY:HA2	2.19	0.42
1:G:332:ASN:HA	1:G:414:ILE:O	2.20	0.41
4:H:59:TYR:CD2	4:H:64:LYS:HB2	2.52	0.41
4:H:166:ALA:HB1	4:H:175:SER:N	2.35	0.41
5:D:210:ARG:NH1	5:D:211:VAL:O	2.53	0.41
6:E:41:PRO:HG2	6:E:44:ARG:HD3	2.01	0.41
6:E:180:SER:O	6:E:181:TYR:HB3	2.20	0.41
1:G:182:VAL:C	1:G:191:TYR:HB3	2.39	0.41
1:G:226:LEU:N	1:G:487:LYS:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:497:ALA:HA	1:G:498:PRO:HD3	1.89	0.41
5:D:33:HIS:CE1	5:D:98:ARG:CD	3.03	0.41
5:D:153:SER:O	5:D:154:TRP:CD1	2.72	0.41
6:E:99:CYS:SG	6:E:101:PHE:CE1	3.13	0.41
1:G:179:LEU:HD21	1:G:419:ARG:NH2	2.35	0.41
1:G:182:VAL:O	1:G:192:ARG:N	2.44	0.41
1:G:391:PHE:N	1:G:391:PHE:CD1	2.85	0.41
2:B:596:TRP:NE1	2:B:647:GLU:CD	2.67	0.41
3:L:49:TYR:HB2	4:H:100(O):TYR:CG	2.56	0.41
4:H:59:TYR:CB	4:H:64:LYS:HB3	2.46	0.41
4:H:100(D):MET:O	4:H:100(D):MET:HG2	2.20	0.41
5:D:166:PHE:O	5:D:178:LEU:HD13	2.20	0.41
6:E:87:THR:HG22	6:E:105:THR:O	2.20	0.41
1:G:502:LYS:HD2	2:B:607:ASN:HA	2.02	0.41
4:H:40:SER:OG	4:H:43:LYS:HB2	2.21	0.41
4:H:51:ILE:HD11	4:H:55:GLU:HA	2.02	0.41
5:D:72(E):VAL:O	5:D:72(F):THR:OG1	2.33	0.41
6:E:81:ARG:HA	6:E:81:ARG:HD3	1.84	0.41
2:B:576:LEU:HA	2:B:579:ARG:NH2	2.35	0.41
2:B:595:ILE:HG21	2:B:647:GLU:OE2	2.20	0.41
2:B:619:LEU:O	2:B:622:ILE:HG12	2.20	0.41
16:B:702:NAG:C7	16:B:702:NAG:HO3	2.33	0.41
3:L:47:LEU:H	3:L:47:LEU:HD23	1.86	0.41
3:L:52:GLN:OE1	3:L:53:ASP:HB3	2.20	0.41
3:L:96:TRP:CH2	4:H:49:GLY:HA2	2.56	0.41
3:L:106:VAL:O	3:L:109:GLN:NE2	2.52	0.41
4:H:13:LYS:O	4:H:16:GLU:CD	2.58	0.41
5:D:66:ARG:HD2	5:D:66:ARG:HA	1.38	0.41
6:E:138:CYS:N	6:E:139:LEU:HD12	2.36	0.41
6:E:187:GLU:O	6:E:189:TRP:N	2.54	0.41
1:G:104:MET:SD	1:G:479:TRP:HB3	2.60	0.41
3:L:35:TRP:HB3	3:L:47:LEU:CD2	2.45	0.41
4:H:146:GLU:OE1	4:H:165:PRO:HB3	2.20	0.41
4:H:190:GLN:HG2	4:H:192:TYR:CZ	2.56	0.41
5:D:82:ILE:O	5:D:82(A):ARG:HB2	2.21	0.41
5:D:121:VAL:CG2	5:D:141:LEU:HB3	2.51	0.41
6:E:42:PRO:HD2	6:E:86:THR:HG21	2.00	0.41
1:G:423:ILE:HA	1:G:434:MET:O	2.20	0.41
1:G:460:SER:HB2	1:G:466:GLU:OE1	2.20	0.41
1:G:503:ARG:HD3	1:G:503:ARG:HA	1.88	0.41
2:B:580:VAL:O	2:B:583:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:72(C):VAL:HB	5:D:75:THR:HB	2.01	0.41
5:D:96:LEU:HD13	5:D:98:ARG:NH2	2.34	0.41
6:E:17:SER:O	6:E:17:SER:OG	2.23	0.41
6:E:23:THR:HG21	6:E:72:SER:HB2	2.03	0.41
6:E:192:HIS:CD2	6:E:194:SER:N	2.88	0.41
1:G:117:LYS:N	1:G:118:PRO:HD2	2.36	0.41
1:G:178:ARG:CZ	1:G:419:ARG:HH22	2.34	0.41
1:G:271:MET:HG3	1:G:348:GLN:OE1	2.20	0.41
3:L:50:ASN:OD1	13:O:5:MAN:O4	2.37	0.41
3:L:133:LEU:HG	3:L:134:VAL:N	2.36	0.41
3:L:147:VAL:HA	3:L:196:VAL:HA	2.03	0.41
4:H:7:SER:O	4:H:20:LEU:HD22	2.20	0.41
5:D:37:ILE:HD11	5:D:103:TRP:CZ3	2.56	0.41
1:G:272:ILE:HG23	1:G:285:LEU:O	2.21	0.41
1:G:293:GLN:OE1	9:F:1:NAG:H3	2.20	0.41
1:G:363:ASN:HD22	1:G:363:ASN:N	2.19	0.41
3:L:120:PRO:HG3	3:L:207:VAL:HG21	2.02	0.41
3:L:167:LYS:HD3	3:L:173:TYR:CD1	2.56	0.41
4:H:100(A):ILE:HA	4:H:100(I):GLU:O	2.20	0.41
5:D:34:ILE:O	5:D:35:ASN:CG	2.52	0.41
5:D:50:TRP:CH2	6:E:98:GLY:HA2	2.56	0.41
5:D:72:ASP:OD1	5:D:72:ASP:N	2.53	0.41
6:E:49:ILE:HD13	6:E:49:ILE:HG21	1.86	0.41
6:E:87:THR:HB	6:E:89:TYR:HE1	1.86	0.41
6:E:190:LYS:HA	6:E:190:LYS:HD2	1.25	0.41
6:E:192:HIS:HD2	6:E:193:ARG:C	2.24	0.41
1:G:171:LYS:CG	7:A:1:NAG:O7	2.65	0.41
1:G:199:ALA:HB1	1:G:431:GLY:O	2.21	0.41
1:G:298:ARG:N	1:G:443:ILE:HD11	2.36	0.41
1:G:343:GLY:O	1:G:346:VAL:HB	2.21	0.41
3:L:37:GLN:NE2	3:L:86:TYR:HE1	2.18	0.41
3:L:199:GLU:HG2	3:L:201:SER:H	1.86	0.41
4:H:34:TRP:N	4:H:50:TYR:CZ	2.89	0.41
5:D:129:LYS:NZ	5:D:183:THR:HG21	2.36	0.41
6:E:190:LYS:NZ	6:E:212:PRO:HB2	2.36	0.41
1:G:271:MET:CG	1:G:348:GLN:OE1	2.68	0.40
2:B:656:ASN:C	2:B:656:ASN:OD1	2.59	0.40
3:L:76:SER:OG	3:L:77:GLY:N	2.54	0.40
1:G:45:TRP:HB2	1:G:489:VAL:HG22	2.04	0.40
1:G:162:THR:HG1	1:G:166:ARG:HH22	1.60	0.40
1:G:421:LYS:HD2	1:G:421:LYS:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:TRP:CE3	3:L:35:TRP:HA	2.56	0.40
3:L:103:ARG:CZ	3:L:105:THR:HG22	2.51	0.40
3:L:189:HIS:ND1	3:L:190:LYS:N	2.67	0.40
4:H:100(E):VAL:HG23	4:H:100(F):SER:N	2.37	0.40
5:D:100(B):SER:HA	6:E:93:TYR:CE1	2.57	0.40
6:E:127:GLU:H	6:E:127:GLU:CD	2.24	0.40
1:G:166:ARG:HH21	1:G:169:LYS:NZ	2.20	0.40
2:B:529:THR:HB	2:B:623:TRP:O	2.21	0.40
4:H:13:LYS:HB2	4:H:13:LYS:HE3	1.89	0.40
4:H:38:ARG:CZ	4:H:90:TYR:CZ	3.05	0.40
4:H:50:TYR:HD1	4:H:50:TYR:HA	1.63	0.40
4:H:115:LYS:HG2	4:H:116:GLY:H	1.87	0.40
4:H:157:LEU:HD23	4:H:157:LEU:N	2.36	0.40
5:D:37:ILE:HG22	5:D:47:TRP:HA	2.04	0.40
1:G:127:VAL:HG23	1:G:129:LEU:CD1	2.52	0.40
1:G:269:GLU:HB2	1:G:271:MET:CE	2.50	0.40
1:G:326:ILE:O	1:G:327:ARG:HG2	2.21	0.40
1:G:360:ARG:HE	1:G:467:THR:CA	2.34	0.40
3:L:145:VAL:CG2	3:L:196:VAL:HB	2.51	0.40
5:D:94:LYS:HA	5:D:94:LYS:HE2	2.04	0.40
1:G:113:ASP:N	1:G:113:ASP:OD1	2.55	0.40
1:G:274:SER:OG	1:G:277:ILE:N	2.53	0.40
1:G:341:THR:O	1:G:345:VAL:HG23	2.21	0.40
1:G:362:ALA:CA	1:G:469:ARG:HH21	2.35	0.40
5:D:85:ASP:N	5:D:85:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	444/480 (92%)	378 (85%)	62 (14%)	4 (1%)	<b>17</b> 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	144/153 (94%)	127 (88%)	16 (11%)	1 (1%)	22	54
3	L	209/218 (96%)	171 (82%)	34 (16%)	4 (2%)	8	28
4	H	227/236 (96%)	184 (81%)	35 (15%)	8 (4%)	3	14
5	D	238/240 (99%)	190 (80%)	36 (15%)	12 (5%)	2	7
6	E	211/216 (98%)	177 (84%)	29 (14%)	5 (2%)	6	22
All	All	1473/1543 (96%)	1227 (83%)	212 (14%)	34 (2%)	6	23

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	88	ASN
4	H	100	ARG
4	H	100(E)	VAL
4	H	100(G)	PHE
5	D	72(B)	GLU
5	D	100(E)	LEU
6	E	95	HIS
1	G	427	TRP
4	H	100(A)	ILE
5	D	51	ILE
5	D	92	CYS
5	D	100(D)	TRP
5	D	142	VAL
5	D	204	ASN
2	B	546	SER
3	L	26	GLN
4	H	100(Q)	ASP
5	D	72	ASP
5	D	72(G)	SER
4	H	100(I)	GLU
5	D	121	VAL
5	D	155	ASN
6	E	145	PRO
6	E	158	PRO
3	L	203	VAL
4	H	82(B)	SER
5	D	146	PHE
6	E	186	PRO
6	E	82	PRO
3	L	55	PRO

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Mol	Chain	Res	Type
4	H	147	PRO
1	G	270	VAL
1	G	299	PRO
3	L	10	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	397/424 (94%)	369 (93%)	28 (7%)	14	40
2	B	126/129 (98%)	117 (93%)	9 (7%)	14	40
3	L	175/181 (97%)	157 (90%)	18 (10%)	7	22
4	H	200/205 (98%)	183 (92%)	17 (8%)	10	31
5	D	203/203 (100%)	187 (92%)	16 (8%)	12	34
6	E	186/189 (98%)	173 (93%)	13 (7%)	15	41
All	All	1287/1331 (97%)	1186 (92%)	101 (8%)	12	34

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	40	TYR
1	G	54	CYS
1	G	65	LYS
1	G	85	HIS
1	G	100	MET
1	G	131	CYS
1	G	192	ARG
1	G	259	LEU
1	G	260	LEU
1	G	271	MET
1	G	273	ARG
1	G	308	ARG
1	G	327	ARG
1	G	331	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	360	ARG
1	G	361	PHE
1	G	378	CYS
1	G	388	SER
1	G	392	ASN
1	G	427	TRP
1	G	428	GLN
1	G	445	CYS
1	G	452	LEU
1	G	463	SER
1	G	478	ASN
1	G	480	ARG
1	G	501	CYS
1	G	504	ARG
2	B	579	ARG
2	B	585	ARG
2	B	588	ARG
2	B	589	ASP
2	B	612	SER
2	B	615	SER
2	B	624	ASP
2	B	633	LYS
2	B	664	ASP
3	L	9	ARG
3	L	25	ARG
3	L	26	GLN
3	L	47	LEU
3	L	76	SER
3	L	88	CYS
3	L	95(B)	PHE
3	L	103	ARG
3	L	122	SER
3	L	124	GLU
3	L	130	LYS
3	L	152	ASP
3	L	173	TYR
3	L	189	HIS
3	L	190	LYS
3	L	192	TYR
3	L	194	CYS
3	L	196	VAL
4	H	6	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	H	22	CYS
4	H	32	TYR
4	H	47	TRP
4	H	61	PRO
4	H	66	ARG
4	H	94	ARG
4	H	100(D)	MET
4	H	100(G)	PHE
4	H	100(J)	PHE
4	H	101	TRP
4	H	106	THR
4	H	142	ASP
4	H	171	SER
4	H	184	SER
4	H	190	GLN
4	H	194	CYS
5	D	28	ARG
5	D	31	PHE
5	D	50	TRP
5	D	53	TYR
5	D	72	ASP
5	D	72(G)	SER
5	D	82(C)	LEU
5	D	96	LEU
5	D	101	TYR
5	D	113	SER
5	D	143	LYS
5	D	146	PHE
5	D	164	HIS
5	D	166	PHE
5	D	175	LEU
5	D	197	ASN
6	E	56	ARG
6	E	70	TYR
6	E	71	TRP
6	E	74	TYR
6	E	81	ARG
6	E	87	THR
6	E	132	ASN
6	E	138	CYS
6	E	152	TRP
6	E	153	LYS

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Mol	Chain	Res	Type
6	E	170	LYS
6	E	176	TYR
6	E	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	66	HIS
1	G	203	GLN
1	G	287	GLN
1	G	339	ASN
1	G	478	ASN
2	B	607	ASN
2	B	653	GLN
2	B	658	GLN
3	L	168	GLN
3	L	195	GLN
4	H	5	GLN
4	H	97	GLN
4	H	162	HIS
4	H	198	HIS
5	D	33	HIS
5	D	35	ASN
5	D	64	GLN
5	D	105	GLN
5	D	155	ASN
6	E	192	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

76 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
7	NAG	A	1	7,1	14,14,15	2.57	2 (14%)	17,19,21	1.71	3 (17%)
7	NAG	A	2	7	14,14,15	1.47	2 (14%)	17,19,21	0.93	1 (5%)
7	BMA	A	3	7	11,11,12	1.68	4 (36%)	15,15,17	1.84	4 (26%)
7	MAN	A	4	7	11,11,12	1.08	1 (9%)	15,15,17	0.92	0
7	MAN	A	5	7	11,11,12	0.80	0	15,15,17	0.98	1 (6%)
7	MAN	A	6	7	11,11,12	0.75	0	15,15,17	0.89	1 (6%)
8	NAG	C	1	8,1	14,14,15	1.14	1 (7%)	17,19,21	1.65	2 (11%)
8	NAG	C	2	8	14,14,15	1.04	2 (14%)	17,19,21	1.29	2 (11%)
8	BMA	C	3	8	11,11,12	0.93	1 (9%)	15,15,17	0.99	1 (6%)
8	MAN	C	4	8	11,11,12	1.00	1 (9%)	15,15,17	1.30	3 (20%)
8	MAN	C	5	8	11,11,12	0.59	0	15,15,17	1.01	2 (13%)
8	MAN	C	6	8	11,11,12	0.94	1 (9%)	15,15,17	1.51	3 (20%)
8	MAN	C	7	8	11,11,12	0.89	1 (9%)	15,15,17	1.19	2 (13%)
9	NAG	F	1	9,1	14,14,15	0.22	0	17,19,21	0.53	0
9	NAG	F	2	9	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
9	BMA	F	3	9	11,11,12	1.91	2 (18%)	15,15,17	1.23	2 (13%)
9	MAN	F	4	9	11,11,12	2.09	3 (27%)	15,15,17	1.58	3 (20%)
9	MAN	F	5	9	11,11,12	1.19	2 (18%)	15,15,17	1.68	3 (20%)
9	MAN	F	6	9	11,11,12	0.75	0	15,15,17	1.01	2 (13%)
9	MAN	F	7	9	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
10	NAG	I	1	10,1	14,14,15	0.32	0	17,19,21	0.67	0
10	NAG	I	2	10	14,14,15	0.26	0	17,19,21	0.54	0
10	BMA	I	3	10	11,11,12	0.50	0	15,15,17	0.81	0
11	NAG	J	1	11,1	14,14,15	0.20	0	17,19,21	0.51	0
11	NAG	J	2	11	14,14,15	0.22	0	17,19,21	0.44	0
11	BMA	J	3	11	11,11,12	0.52	0	15,15,17	0.86	0
11	MAN	J	4	11	11,11,12	0.69	0	15,15,17	1.31	2 (13%)
11	MAN	J	5	11	11,11,12	0.78	0	15,15,17	1.20	2 (13%)
11	MAN	J	6	11	11,11,12	0.81	0	15,15,17	1.05	2 (13%)
11	MAN	J	7	11	11,11,12	0.67	0	15,15,17	1.19	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	J	8	11	11,11,12	0.73	0	15,15,17	0.88	1 (6%)
9	NAG	K	1	9,1	14,14,15	0.71	1 (7%)	17,19,21	0.43	0
9	NAG	K	2	9	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)
9	BMA	K	3	9	11,11,12	0.34	0	15,15,17	1.74	2 (13%)
9	MAN	K	4	9	11,11,12	1.35	2 (18%)	15,15,17	1.53	4 (26%)
9	MAN	K	5	9	11,11,12	1.07	0	15,15,17	1.64	3 (20%)
9	MAN	K	6	9	11,11,12	0.98	1 (9%)	15,15,17	1.11	2 (13%)
9	MAN	K	7	9	11,11,12	0.34	0	15,15,17	1.11	2 (13%)
11	NAG	M	1	11,1	14,14,15	0.22	0	17,19,21	0.55	0
11	NAG	M	2	11	14,14,15	0.20	0	17,19,21	0.41	0
11	BMA	M	3	11	11,11,12	0.59	0	15,15,17	0.76	0
11	MAN	M	4	11	11,11,12	0.81	0	15,15,17	1.27	2 (13%)
11	MAN	M	5	11	11,11,12	0.69	0	15,15,17	1.19	2 (13%)
11	MAN	M	6	11	11,11,12	0.82	1 (9%)	15,15,17	0.92	1 (6%)
11	MAN	M	7	11	11,11,12	0.79	1 (9%)	15,15,17	1.13	2 (13%)
11	MAN	M	8	11	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
12	NAG	N	1	12,1	14,14,15	1.87	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	N	2	12	14,14,15	0.40	0	17,19,21	0.67	1 (5%)
12	BMA	N	3	12	11,11,12	0.76	0	15,15,17	0.87	0
12	MAN	N	4	12	11,11,12	0.82	1 (9%)	15,15,17	1.12	2 (13%)
12	MAN	N	5	12	11,11,12	1.41	1 (9%)	15,15,17	1.41	2 (13%)
12	MAN	N	6	12	11,11,12	0.92	1 (9%)	15,15,17	1.54	2 (13%)
13	NAG	O	1	13,1	14,14,15	0.92	1 (7%)	17,19,21	1.41	2 (11%)
13	MAN	O	10	13	11,11,12	0.58	0	15,15,17	1.10	2 (13%)
13	NAG	O	2	13	14,14,15	0.34	0	17,19,21	0.51	0
13	BMA	O	3	13	11,11,12	1.02	1 (9%)	15,15,17	1.07	1 (6%)
13	MAN	O	4	13	11,11,12	0.86	1 (9%)	15,15,17	1.20	2 (13%)
13	MAN	O	5	13	11,11,12	0.97	2 (18%)	15,15,17	1.21	1 (6%)
13	MAN	O	6	13	11,11,12	1.00	1 (9%)	15,15,17	0.83	1 (6%)
13	MAN	O	7	13	11,11,12	0.57	0	15,15,17	1.16	2 (13%)
13	MAN	O	8	13	11,11,12	0.76	1 (9%)	15,15,17	1.06	1 (6%)
13	MAN	O	9	13	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
14	NAG	P	1	14,1	14,14,15	2.16	4 (28%)	17,19,21	1.01	0
14	NAG	P	2	14	14,14,15	0.36	0	17,19,21	0.59	0
14	BMA	P	3	14	11,11,12	0.61	0	15,15,17	1.71	3 (20%)
14	MAN	P	4	14	11,11,12	0.94	1 (9%)	15,15,17	1.42	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	MAN	P	5	14	11,11,12	1.12	1 (9%)	15,15,17	1.41	3 (20%)
14	MAN	P	6	14	11,11,12	1.09	1 (9%)	15,15,17	1.02	2 (13%)
14	MAN	P	7	14	11,11,12	1.08	1 (9%)	15,15,17	0.89	1 (6%)
15	NAG	Q	1	15,1	14,14,15	0.56	0	17,19,21	1.07	1 (5%)
15	NAG	Q	2	15	14,14,15	0.63	1 (7%)	17,19,21	0.98	1 (5%)
15	NAG	R	1	15,1	14,14,15	0.15	0	17,19,21	0.79	1 (5%)
15	NAG	R	2	15	14,14,15	0.33	0	17,19,21	0.51	0
10	NAG	S	1	2,10	14,14,15	0.44	0	17,19,21	0.60	0
10	NAG	S	2	10	14,14,15	0.24	0	17,19,21	0.55	0
10	BMA	S	3	10	11,11,12	0.53	0	15,15,17	1.16	1 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,1	-	5/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
8	MAN	C	5	8	-	0/2/19/22	0/1/1/1
8	MAN	C	6	8	-	0/2/19/22	0/1/1/1
8	MAN	C	7	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
9	MAN	F	6	9	-	0/2/19/22	0/1/1/1
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
10	NAG	I	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	BMA	J	3	11	-	2/2/19/22	0/1/1/1
11	MAN	J	4	11	-	1/2/19/22	0/1/1/1
11	MAN	J	5	11	-	0/2/19/22	0/1/1/1
11	MAN	J	6	11	-	0/2/19/22	0/1/1/1
11	MAN	J	7	11	-	2/2/19/22	0/1/1/1
11	MAN	J	8	11	-	0/2/19/22	0/1/1/1
9	NAG	K	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	BMA	K	3	9	-	2/2/19/22	0/1/1/1
9	MAN	K	4	9	-	0/2/19/22	0/1/1/1
9	MAN	K	5	9	-	2/2/19/22	0/1/1/1
9	MAN	K	6	9	-	0/2/19/22	0/1/1/1
9	MAN	K	7	9	-	0/2/19/22	0/1/1/1
11	NAG	M	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	M	2	11	-	0/6/23/26	0/1/1/1
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	1/2/19/22	0/1/1/1
11	MAN	M	5	11	-	2/2/19/22	0/1/1/1
11	MAN	M	6	11	-	0/2/19/22	0/1/1/1
11	MAN	M	7	11	-	0/2/19/22	0/1/1/1
11	MAN	M	8	11	-	0/2/19/22	0/1/1/1
12	NAG	N	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1
12	MAN	N	4	12	-	0/2/19/22	0/1/1/1
12	MAN	N	5	12	-	1/2/19/22	0/1/1/1
12	MAN	N	6	12	-	2/2/19/22	0/1/1/1
13	NAG	O	1	13,1	-	3/6/23/26	0/1/1/1
13	MAN	O	10	13	-	0/2/19/22	0/1/1/1
13	NAG	O	2	13	-	2/6/23/26	0/1/1/1
13	BMA	O	3	13	-	0/2/19/22	0/1/1/1
13	MAN	O	4	13	-	2/2/19/22	0/1/1/1
13	MAN	O	5	13	-	0/2/19/22	0/1/1/1
13	MAN	O	6	13	-	0/2/19/22	0/1/1/1
13	MAN	O	7	13	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	O	8	13	-	2/2/19/22	0/1/1/1
13	MAN	O	9	13	-	1/2/19/22	0/1/1/1
14	NAG	P	1	14,1	-	2/6/23/26	0/1/1/1
14	NAG	P	2	14	-	2/6/23/26	0/1/1/1
14	BMA	P	3	14	-	2/2/19/22	0/1/1/1
14	MAN	P	4	14	-	0/2/19/22	0/1/1/1
14	MAN	P	5	14	-	0/2/19/22	0/1/1/1
14	MAN	P	6	14	-	0/2/19/22	0/1/1/1
14	MAN	P	7	14	-	0/2/19/22	0/1/1/1
15	NAG	Q	1	15,1	-	0/6/23/26	0/1/1/1
15	NAG	Q	2	15	-	2/6/23/26	0/1/1/1
15	NAG	R	1	15,1	-	2/6/23/26	0/1/1/1
15	NAG	R	2	15	-	2/6/23/26	0/1/1/1
10	NAG	S	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	NAG	O5-C1	9.12	1.58	1.43
12	N	1	NAG	O5-C1	6.33	1.53	1.43
14	P	1	NAG	O5-C1	5.17	1.52	1.43
14	P	1	NAG	C1-C2	-4.93	1.45	1.52
9	F	4	MAN	O2-C2	4.65	1.53	1.43
7	A	2	NAG	O5-C1	4.39	1.50	1.43
9	F	3	BMA	O3-C3	4.37	1.53	1.43
9	F	4	MAN	C1-C2	3.95	1.61	1.52
9	F	3	BMA	C2-C3	3.71	1.58	1.52
8	C	1	NAG	O5-C1	3.65	1.49	1.43
7	A	3	BMA	O5-C1	3.43	1.49	1.43
13	O	1	NAG	O5-C1	-3.31	1.38	1.43
12	N	5	MAN	O5-C1	-3.16	1.38	1.43
9	F	4	MAN	C2-C3	3.04	1.57	1.52
8	C	6	MAN	C1-C2	2.99	1.59	1.52
14	P	6	MAN	O5-C1	-2.95	1.39	1.43
9	K	4	MAN	C1-C2	2.95	1.58	1.52
14	P	7	MAN	O5-C1	-2.88	1.39	1.43
13	O	6	MAN	O5-C1	-2.88	1.39	1.43
8	C	2	NAG	C1-C2	2.84	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2	NAG	C1-C2	2.74	1.56	1.52
8	C	4	MAN	C1-C2	2.68	1.58	1.52
7	A	3	BMA	O5-C5	2.62	1.48	1.43
9	K	2	NAG	C1-C2	2.58	1.56	1.52
9	K	4	MAN	C2-C3	2.56	1.56	1.52
7	A	1	NAG	C3-C2	2.55	1.57	1.52
9	K	6	MAN	O5-C1	-2.48	1.39	1.43
14	P	4	MAN	C1-C2	2.45	1.57	1.52
8	C	2	NAG	O5-C1	2.44	1.47	1.43
11	M	7	MAN	C1-C2	2.42	1.57	1.52
9	K	1	NAG	O5-C1	-2.32	1.40	1.43
8	C	7	MAN	C1-C2	2.31	1.57	1.52
13	O	4	MAN	C1-C2	2.28	1.57	1.52
9	F	5	MAN	O5-C1	-2.27	1.40	1.43
11	M	6	MAN	O5-C1	-2.27	1.40	1.43
7	A	3	BMA	C1-C2	2.24	1.57	1.52
14	P	5	MAN	O5-C1	-2.21	1.40	1.43
8	C	3	BMA	C1-C2	2.20	1.57	1.52
14	P	1	NAG	O7-C7	2.18	1.28	1.23
12	N	6	MAN	C1-C2	2.17	1.57	1.52
9	F	5	MAN	C1-C2	2.17	1.57	1.52
14	P	1	NAG	C8-C7	-2.15	1.46	1.50
15	Q	2	NAG	C1-C2	2.15	1.55	1.52
13	O	5	MAN	C1-C2	2.14	1.57	1.52
13	O	5	MAN	O5-C1	-2.09	1.40	1.43
13	O	8	MAN	C1-C2	2.09	1.57	1.52
7	A	4	MAN	C2-C3	2.08	1.55	1.52
12	N	4	MAN	O5-C1	-2.06	1.40	1.43
7	A	3	BMA	C2-C3	2.02	1.55	1.52
13	O	3	BMA	C2-C3	2.02	1.55	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1	NAG	C1-O5-C5	5.34	119.43	112.19
12	N	6	MAN	C1-O5-C5	4.87	118.79	112.19
7	A	1	NAG	C2-N2-C7	4.80	129.74	122.90
9	K	3	BMA	C1-O5-C5	4.67	118.52	112.19
7	A	3	BMA	O3-C3-C2	4.54	118.68	109.99
13	O	1	NAG	C2-N2-C7	4.45	129.24	122.90
9	F	5	MAN	O2-C2-C1	4.39	118.13	109.15
12	N	5	MAN	C1-C2-C3	-4.22	104.48	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	3	BMA	C1-O5-C5	4.04	117.66	112.19
9	K	5	MAN	O2-C2-C3	-4.03	102.06	110.14
8	C	2	NAG	C2-N2-C7	3.86	128.40	122.90
11	M	4	MAN	C1-O5-C5	3.85	117.41	112.19
15	Q	2	NAG	C1-O5-C5	3.80	117.34	112.19
9	F	5	MAN	O2-C2-C3	-3.75	102.62	110.14
14	P	4	MAN	C1-O5-C5	3.70	117.20	112.19
14	P	3	BMA	O3-C3-C2	3.64	116.97	109.99
11	J	7	MAN	C1-O5-C5	3.56	117.02	112.19
7	A	3	BMA	C1-C2-C3	-3.55	105.30	109.67
9	K	3	BMA	C1-C2-C3	3.54	114.02	109.67
8	C	6	MAN	C1-O5-C5	3.51	116.95	112.19
9	F	4	MAN	O2-C2-C1	3.42	116.15	109.15
13	O	7	MAN	C1-O5-C5	3.37	116.76	112.19
13	O	5	MAN	O2-C2-C3	-3.33	103.47	110.14
7	A	2	NAG	C1-O5-C5	3.31	116.68	112.19
14	P	5	MAN	C1-C2-C3	-3.31	105.60	109.67
13	O	9	MAN	C1-O5-C5	3.28	116.64	112.19
9	F	3	BMA	O3-C3-C4	3.17	117.68	110.35
14	P	5	MAN	O2-C2-C3	-3.13	103.87	110.14
13	O	10	MAN	C1-O5-C5	3.07	116.35	112.19
8	C	6	MAN	C1-C2-C3	3.05	113.42	109.67
11	M	5	MAN	C1-O5-C5	3.05	116.32	112.19
9	K	5	MAN	C1-C2-C3	-3.04	105.93	109.67
10	S	3	BMA	C1-O5-C5	2.96	116.21	112.19
9	K	4	MAN	C1-C2-C3	2.95	113.30	109.67
8	C	4	MAN	C1-O5-C5	2.92	116.15	112.19
9	K	2	NAG	C1-O5-C5	2.88	116.10	112.19
9	K	5	MAN	C1-O5-C5	2.88	116.09	112.19
14	P	3	BMA	O5-C1-C2	2.87	115.20	110.77
9	K	4	MAN	O2-C2-C1	2.87	115.03	109.15
13	O	3	BMA	C1-C2-C3	2.87	113.19	109.67
9	F	4	MAN	O3-C3-C2	2.76	115.28	109.99
9	K	4	MAN	C1-O5-C5	2.75	115.91	112.19
11	M	5	MAN	O2-C2-C3	-2.73	104.67	110.14
11	J	4	MAN	O2-C2-C3	-2.65	104.82	110.14
11	J	5	MAN	O2-C2-C3	-2.64	104.86	110.14
12	N	5	MAN	O3-C3-C2	2.60	114.97	109.99
8	C	4	MAN	C1-C2-C3	2.60	112.86	109.67
11	M	7	MAN	C1-O5-C5	2.60	115.71	112.19
11	J	4	MAN	C1-O5-C5	2.58	115.69	112.19
9	F	2	NAG	O4-C4-C3	-2.57	104.40	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	1	NAG	C1-O5-C5	2.56	115.66	112.19
15	Q	1	NAG	O5-C1-C2	-2.56	107.25	111.29
11	M	8	MAN	C1-O5-C5	2.56	115.65	112.19
8	C	7	MAN	O2-C2-C3	-2.52	105.09	110.14
12	N	1	NAG	O5-C5-C6	2.49	111.11	107.20
12	N	4	MAN	O2-C2-C3	-2.48	105.17	110.14
7	A	3	BMA	O5-C5-C6	2.47	111.08	107.20
9	F	7	MAN	C1-O5-C5	2.46	115.52	112.19
9	F	6	MAN	O2-C2-C3	-2.45	105.23	110.14
11	M	6	MAN	O2-C2-C3	-2.43	105.27	110.14
13	O	7	MAN	O2-C2-C3	-2.43	105.27	110.14
9	F	6	MAN	C1-O5-C5	2.42	115.47	112.19
9	K	7	MAN	C1-C2-C3	2.41	112.63	109.67
9	F	3	BMA	O3-C3-C2	2.41	114.61	109.99
13	O	9	MAN	O2-C2-C3	-2.41	105.32	110.14
12	N	2	NAG	C1-O5-C5	2.37	115.40	112.19
11	J	5	MAN	C1-C2-C3	-2.34	106.79	109.67
8	C	2	NAG	C1-C2-N2	2.34	114.49	110.49
14	P	7	MAN	O2-C2-C3	-2.34	105.45	110.14
8	C	5	MAN	O2-C2-C3	-2.34	105.45	110.14
13	O	6	MAN	O2-C2-C3	-2.34	105.45	110.14
13	O	1	NAG	C1-C2-N2	2.33	114.47	110.49
13	O	8	MAN	C1-O5-C5	2.33	115.35	112.19
14	P	6	MAN	O2-C2-C3	-2.31	105.50	110.14
7	A	6	MAN	O2-C2-C3	-2.31	105.51	110.14
9	F	7	MAN	O2-C2-C3	-2.31	105.51	110.14
11	J	7	MAN	O2-C2-C3	-2.31	105.51	110.14
9	K	6	MAN	O2-C2-C3	-2.31	105.51	110.14
9	F	5	MAN	C1-O5-C5	2.30	115.31	112.19
13	O	10	MAN	O2-C2-C3	-2.30	105.53	110.14
11	J	6	MAN	C1-O5-C5	2.30	115.30	112.19
11	J	6	MAN	O2-C2-C3	-2.29	105.55	110.14
7	A	3	BMA	O5-C1-C2	-2.29	107.23	110.77
11	J	8	MAN	O2-C2-C3	-2.29	105.55	110.14
7	A	5	MAN	O2-C2-C3	-2.29	105.55	110.14
11	M	7	MAN	O2-C2-C3	-2.29	105.56	110.14
9	K	7	MAN	O5-C1-C2	-2.28	107.25	110.77
9	F	4	MAN	O2-C2-C3	2.25	114.65	110.14
8	C	4	MAN	O2-C2-C3	-2.23	105.66	110.14
9	K	6	MAN	C1-O5-C5	2.21	115.19	112.19
12	N	6	MAN	O2-C2-C3	-2.20	105.72	110.14
8	C	5	MAN	C1-O5-C5	2.17	115.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	6	MAN	O2-C2-C3	-2.17	105.80	110.14
13	O	4	MAN	O2-C2-C3	-2.13	105.87	110.14
11	M	8	MAN	O2-C2-C3	-2.12	105.89	110.14
7	A	1	NAG	C1-C2-N2	2.11	114.08	110.49
8	C	7	MAN	C1-O5-C5	2.10	115.04	112.19
12	N	4	MAN	C3-C4-C5	2.10	113.98	110.24
9	K	4	MAN	O5-C1-C2	2.09	114.00	110.77
11	M	4	MAN	O2-C2-C3	-2.09	105.95	110.14
13	O	4	MAN	O2-C2-C1	2.08	113.41	109.15
14	P	6	MAN	C1-C2-C3	-2.08	107.11	109.67
8	C	1	NAG	O6-C6-C5	2.07	118.39	111.29
8	C	3	BMA	O3-C3-C2	2.06	113.94	109.99
7	A	1	NAG	C8-C7-N2	2.06	119.58	116.10
14	P	5	MAN	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C3-C2-N2-C7
8	C	1	NAG	O5-C5-C6-O6
11	J	1	NAG	O5-C5-C6-O6
14	P	1	NAG	C4-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6
14	P	1	NAG	O5-C5-C6-O6
11	J	3	BMA	C4-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
11	J	7	MAN	O5-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
13	O	4	MAN	O5-C5-C6-O6
13	O	8	MAN	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
12	N	2	NAG	C4-C5-C6-O6
14	P	2	NAG	O5-C5-C6-O6
11	J	1	NAG	C4-C5-C6-O6
11	J	3	BMA	O5-C5-C6-O6
12	N	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	N	1	NAG	C4-C5-C6-O6
13	O	4	MAN	C4-C5-C6-O6
13	O	2	NAG	O5-C5-C6-O6
9	K	3	BMA	C4-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
9	K	5	MAN	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
11	J	7	MAN	C4-C5-C6-O6
14	P	2	NAG	C4-C5-C6-O6
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
8	C	2	NAG	C8-C7-N2-C2
8	C	2	NAG	O7-C7-N2-C2
10	I	2	NAG	C8-C7-N2-C2
10	I	2	NAG	O7-C7-N2-C2
13	O	1	NAG	C8-C7-N2-C2
13	O	1	NAG	O7-C7-N2-C2
15	R	1	NAG	C8-C7-N2-C2
15	R	1	NAG	O7-C7-N2-C2
9	F	4	MAN	C4-C5-C6-O6
11	M	5	MAN	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
15	Q	2	NAG	C4-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
13	O	2	NAG	C4-C5-C6-O6
9	K	3	BMA	O5-C5-C6-O6
12	N	6	MAN	O5-C5-C6-O6
15	R	2	NAG	O5-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
13	O	8	MAN	O5-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
9	K	5	MAN	C4-C5-C6-O6
11	J	4	MAN	O5-C5-C6-O6
15	Q	2	NAG	O5-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
14	P	3	BMA	C4-C5-C6-O6
9	F	3	BMA	C4-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
11	M	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	O	7	MAN	C4-C5-C6-O6
9	F	3	BMA	O5-C5-C6-O6
15	R	2	NAG	C4-C5-C6-O6
9	K	1	NAG	C1-C2-N2-C7
14	P	3	BMA	O5-C5-C6-O6
8	C	2	NAG	C3-C2-N2-C7
13	O	1	NAG	C3-C2-N2-C7
13	O	7	MAN	O5-C5-C6-O6
11	M	1	NAG	O5-C5-C6-O6
12	N	6	MAN	C4-C5-C6-O6
11	M	4	MAN	C4-C5-C6-O6
10	I	1	NAG	C1-C2-N2-C7
13	O	9	MAN	C4-C5-C6-O6
11	M	5	MAN	C4-C5-C6-O6
12	N	5	MAN	C4-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7

There are no ring outliers.

30 monomers are involved in 53 short contacts:

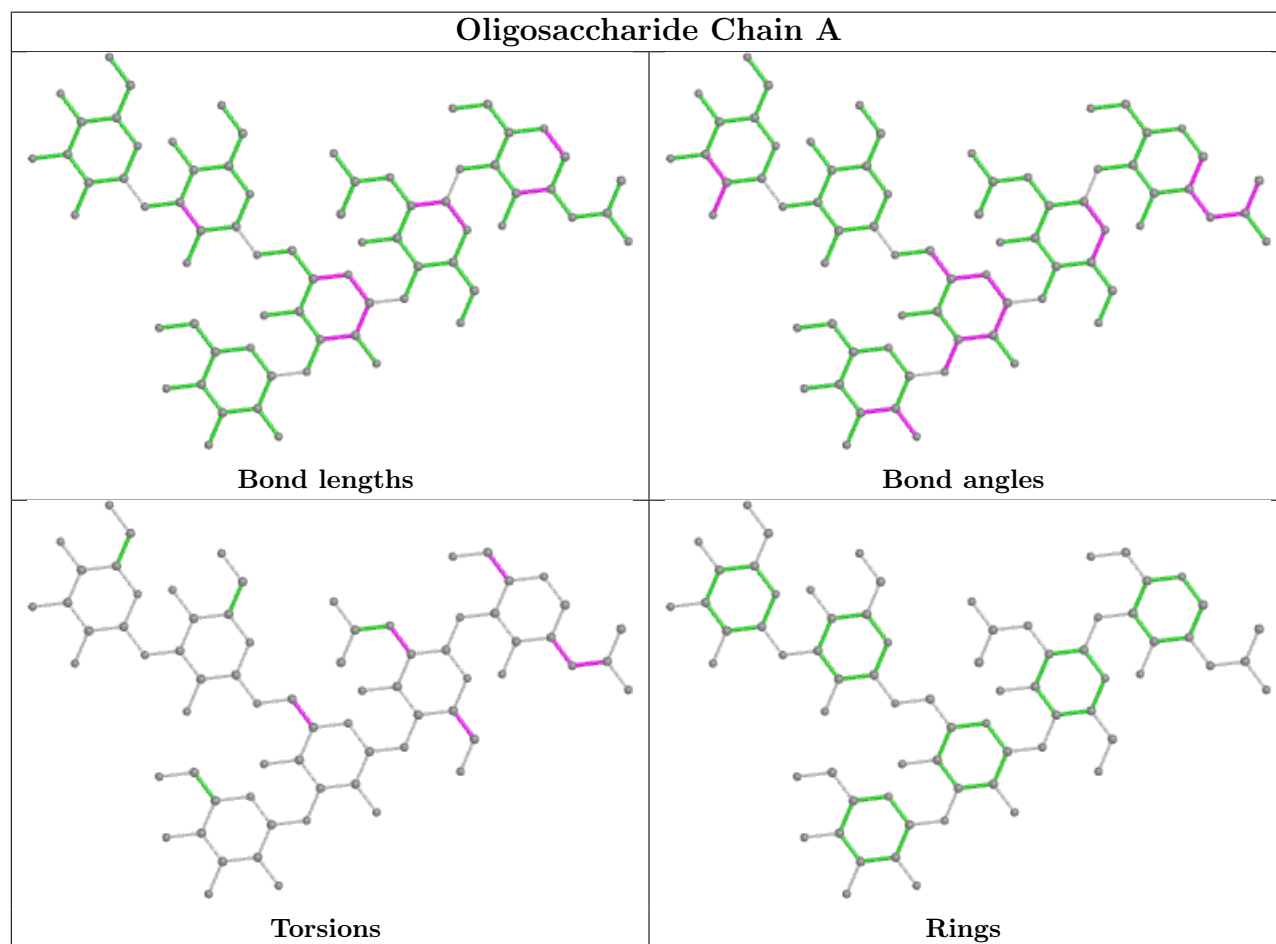
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	1	NAG	6	0
9	F	6	MAN	1	0
7	A	2	NAG	1	0
9	K	2	NAG	2	0
10	I	2	NAG	1	0
11	M	1	NAG	1	0
9	K	7	MAN	2	0
9	F	5	MAN	1	0
9	F	4	MAN	3	0
13	O	1	NAG	2	0
8	C	7	MAN	1	0
14	P	1	NAG	3	0
13	O	5	MAN	3	0
12	N	1	NAG	1	0
9	F	3	BMA	3	0
14	P	2	NAG	1	0
13	O	3	BMA	1	0
11	J	5	MAN	1	0
13	O	4	MAN	1	0
8	C	1	NAG	3	0
9	F	1	NAG	2	0

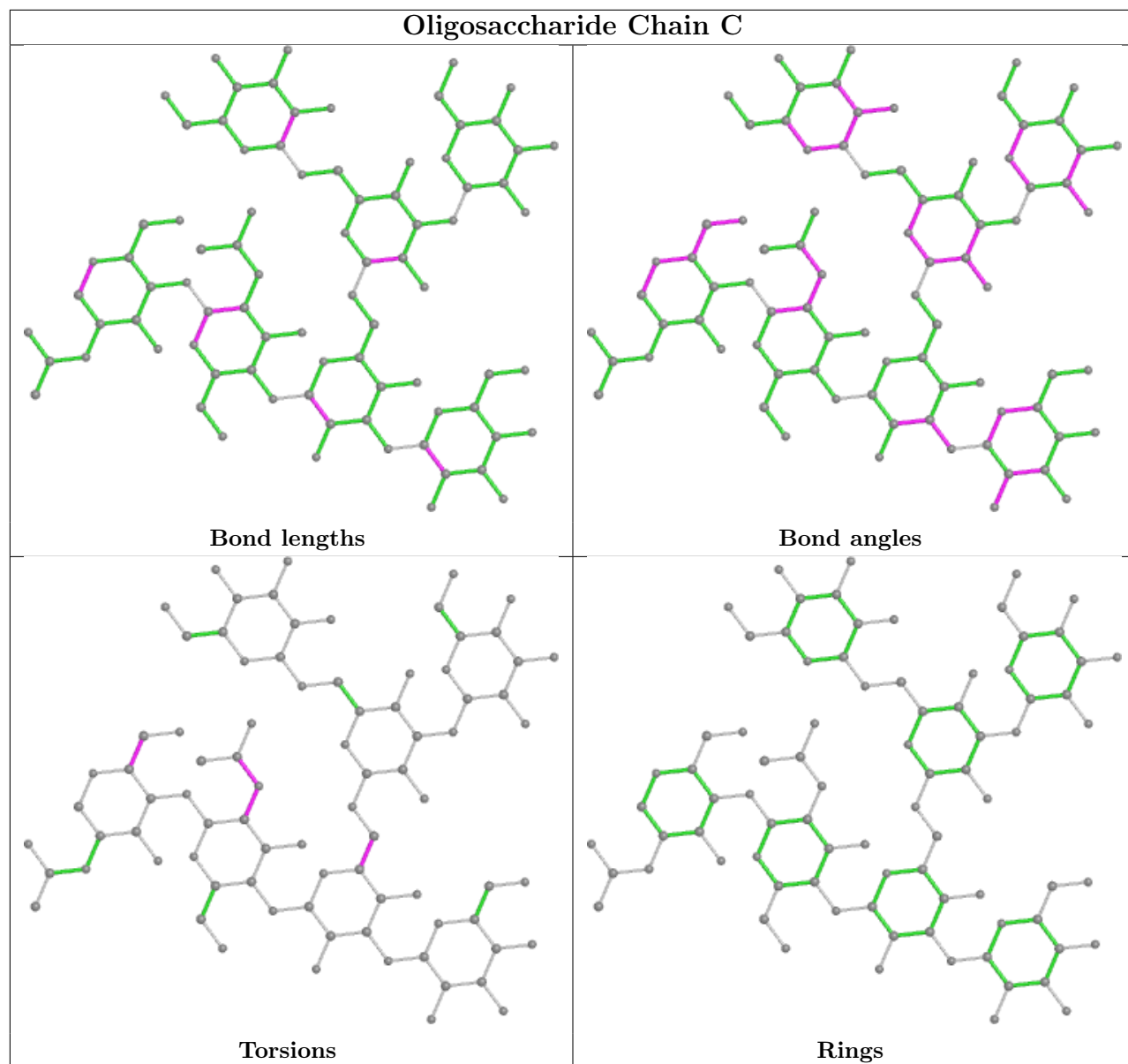
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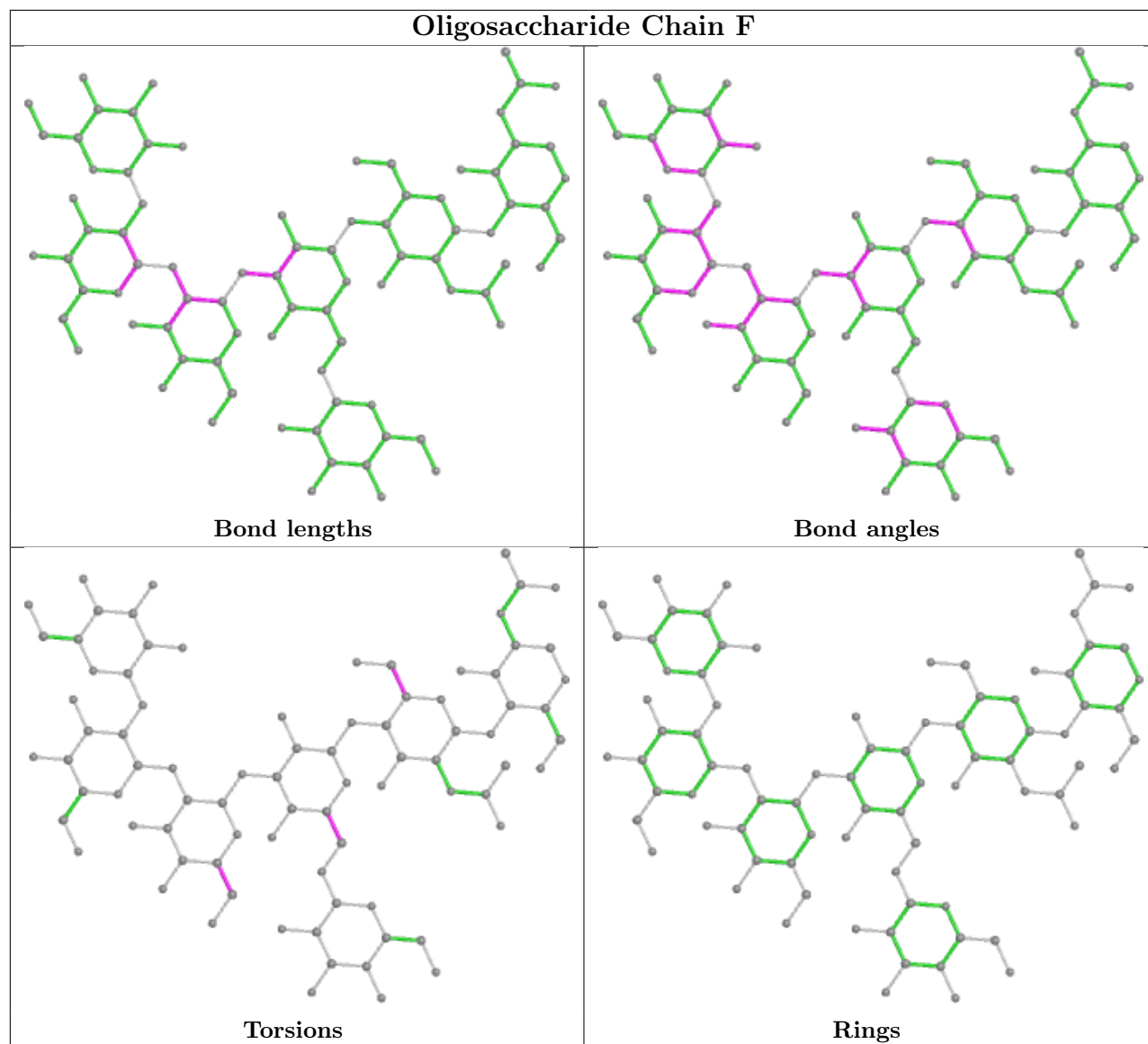
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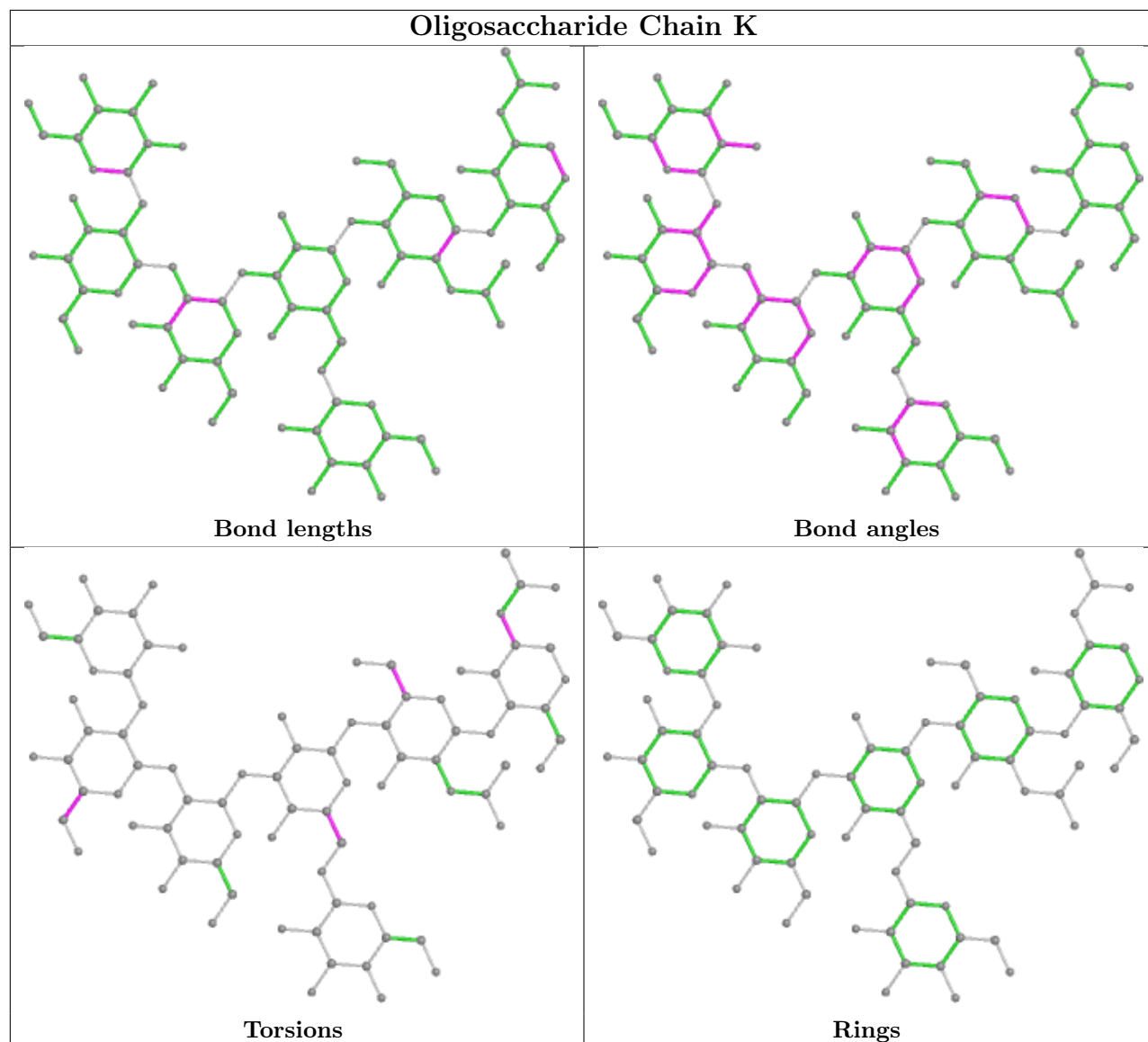
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	1	NAG	2	0
7	A	1	NAG	8	0
8	C	2	NAG	2	0
13	O	2	NAG	3	0
15	Q	1	NAG	2	0
13	O	9	MAN	1	0
11	M	4	MAN	1	0
9	K	3	BMA	2	0
8	C	6	MAN	2	0

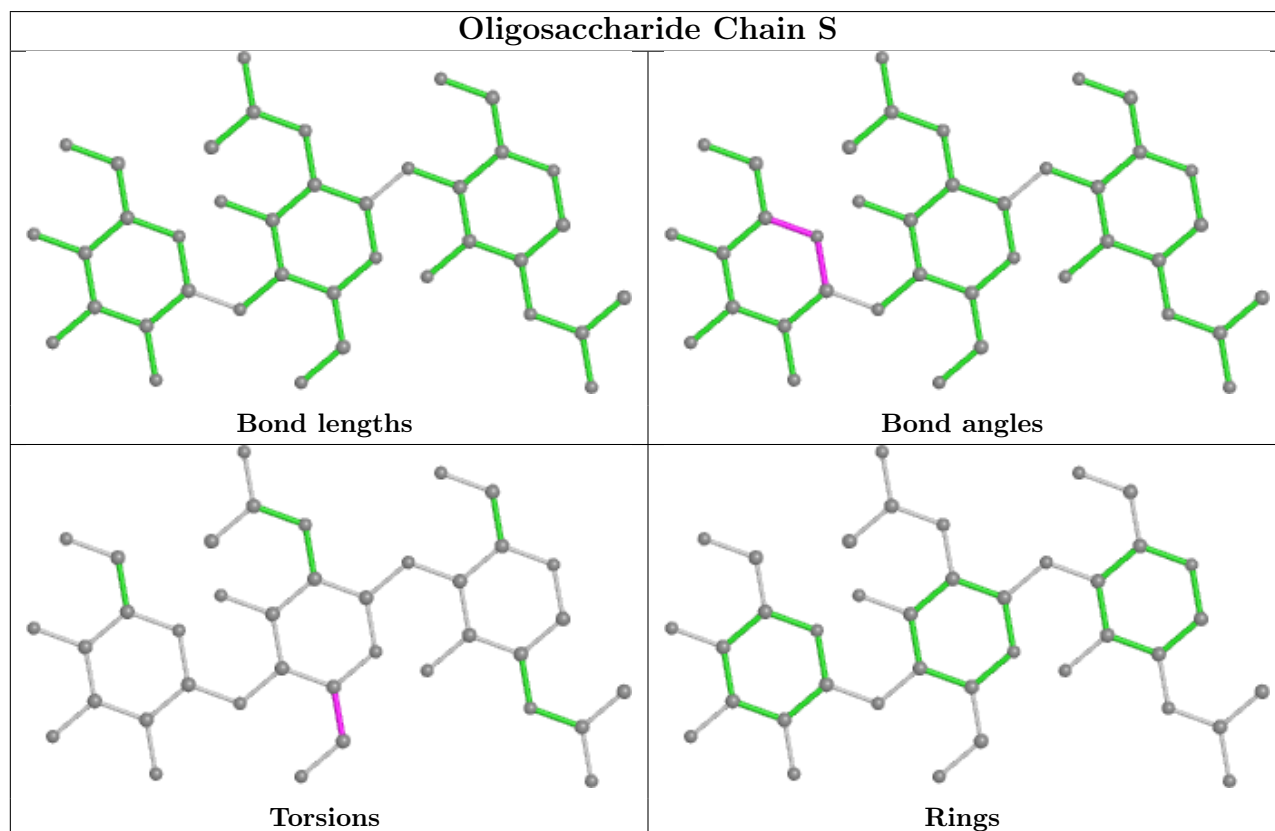
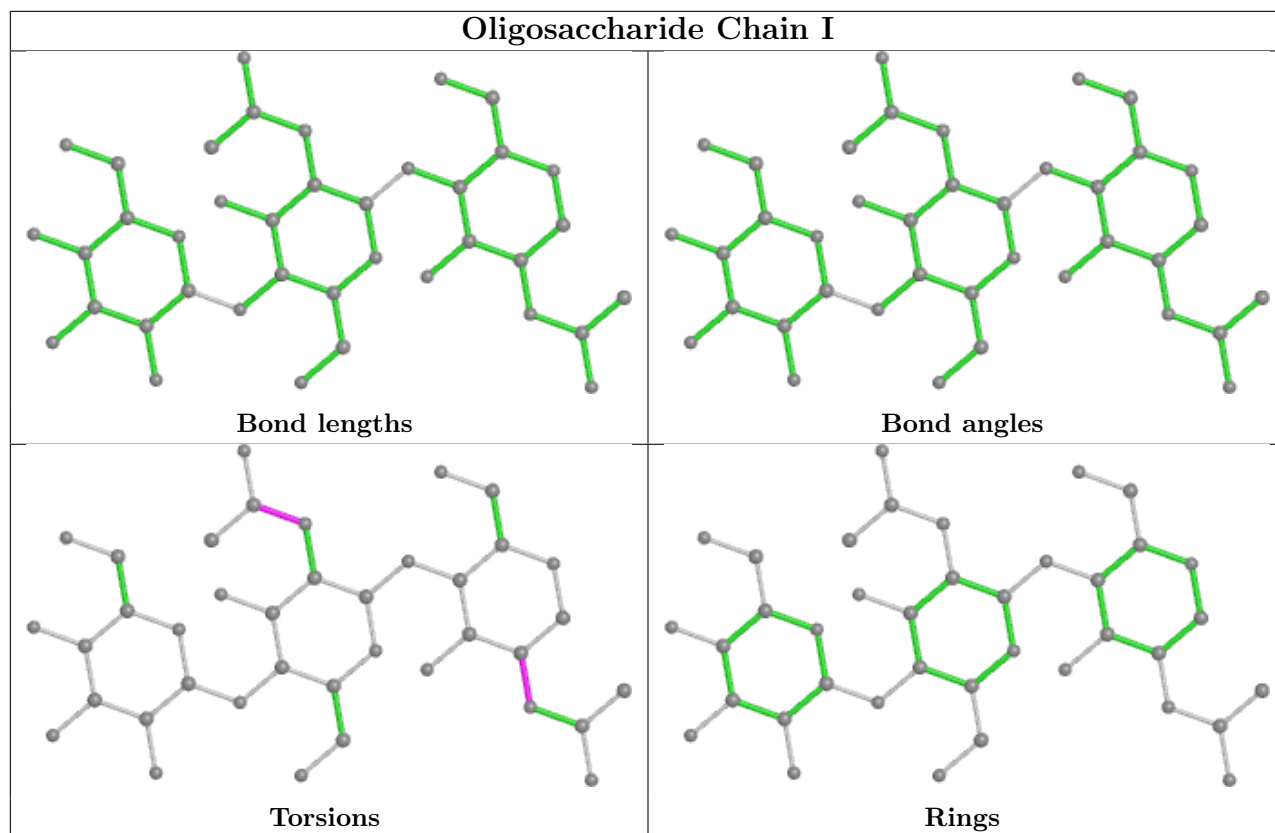
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

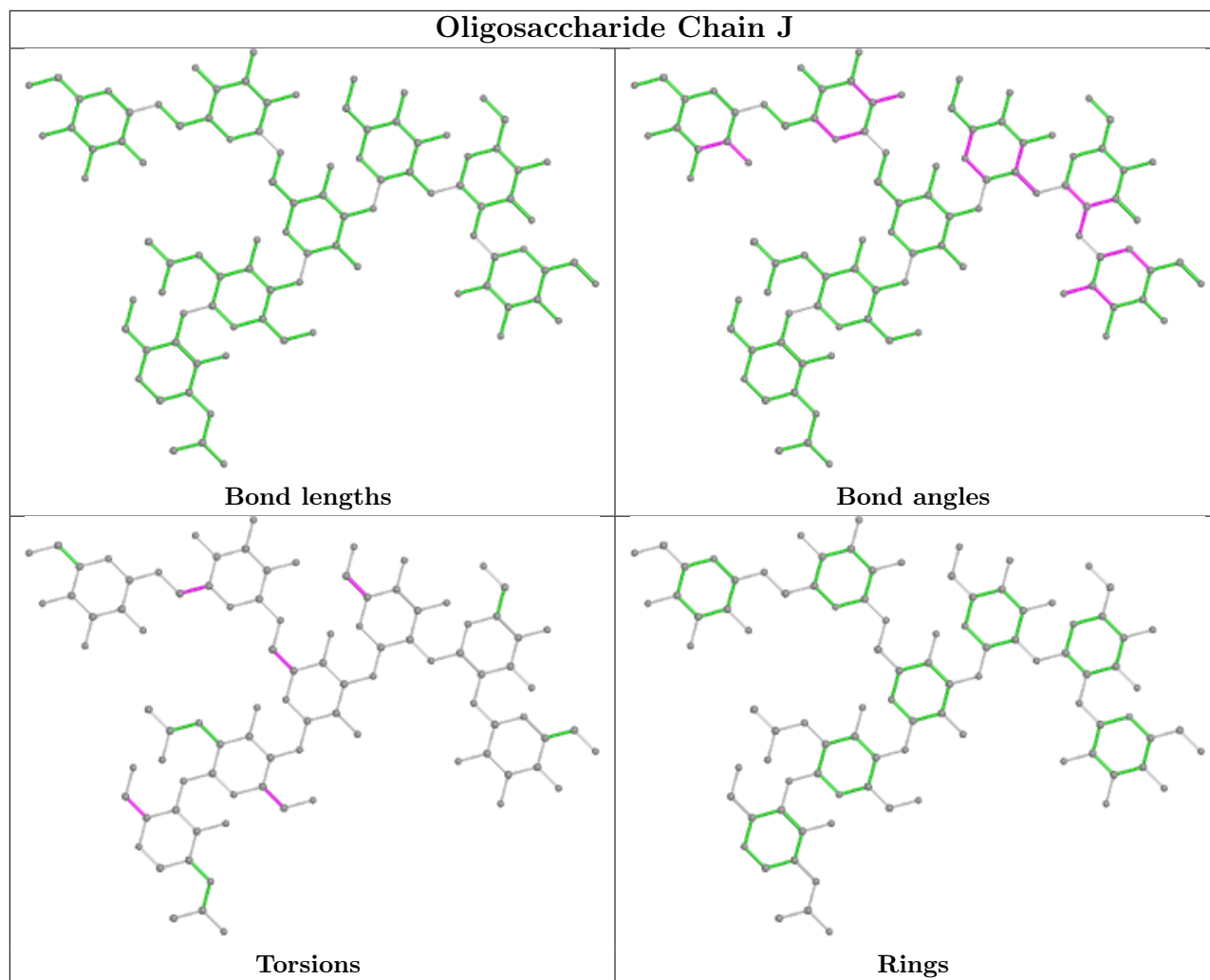




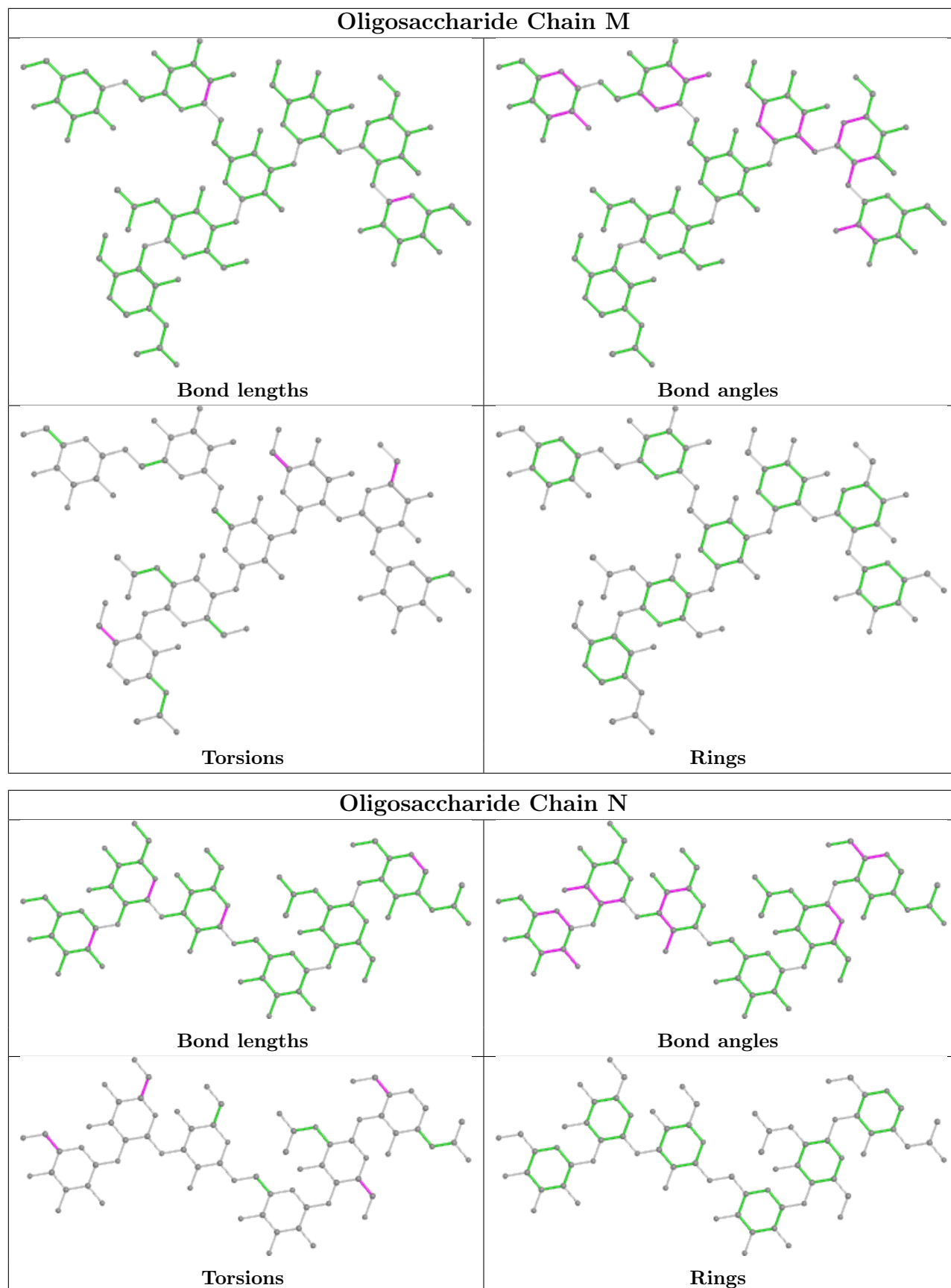


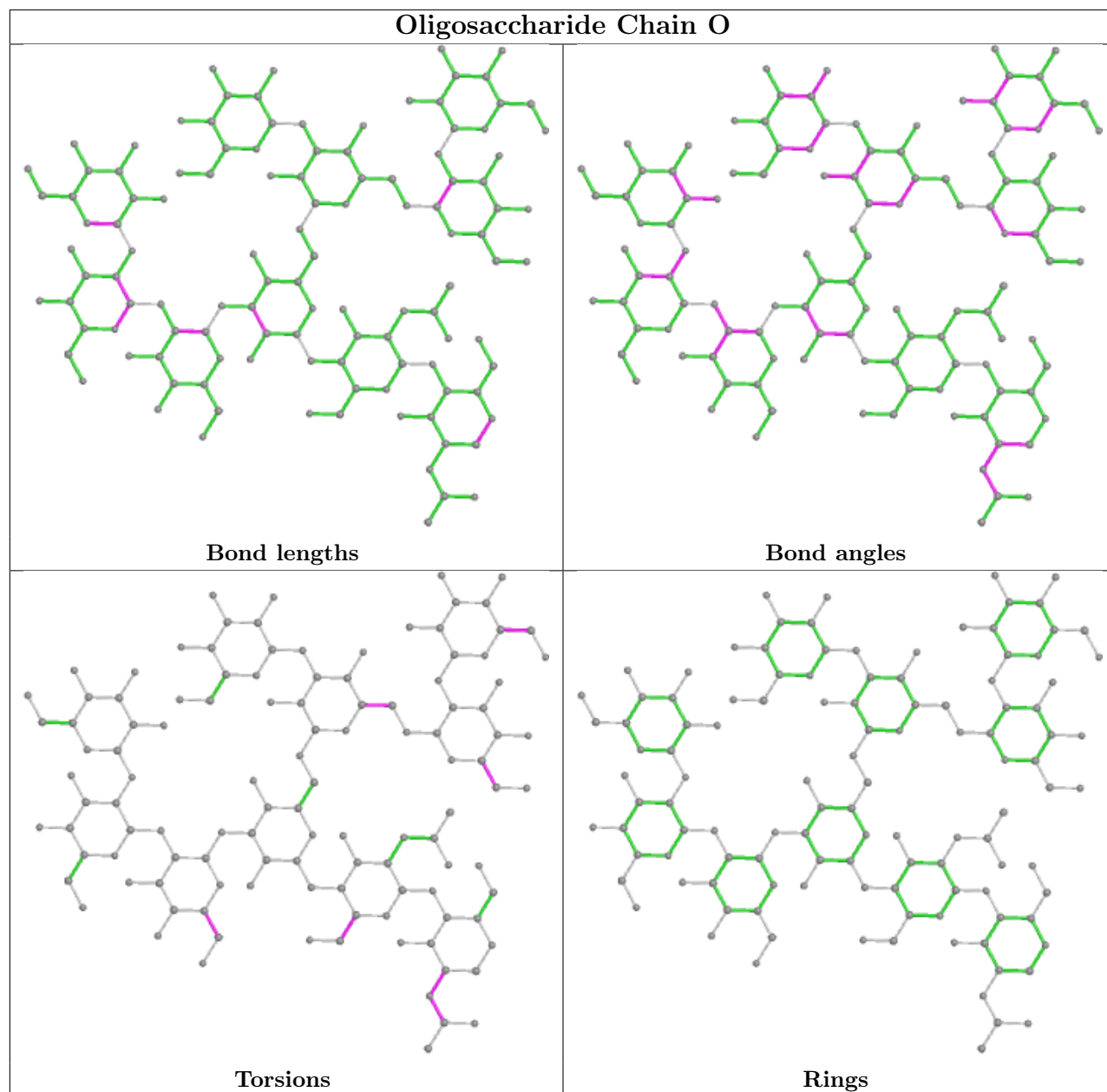


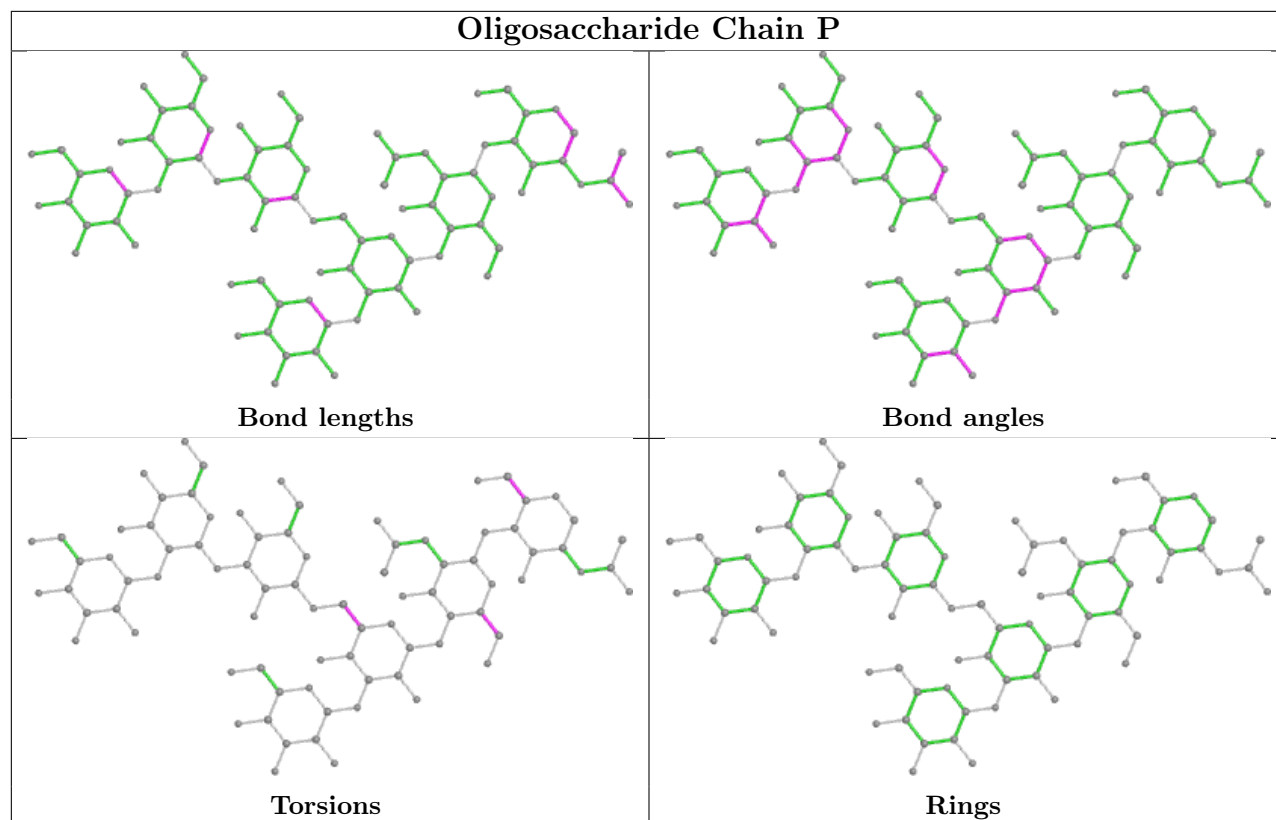


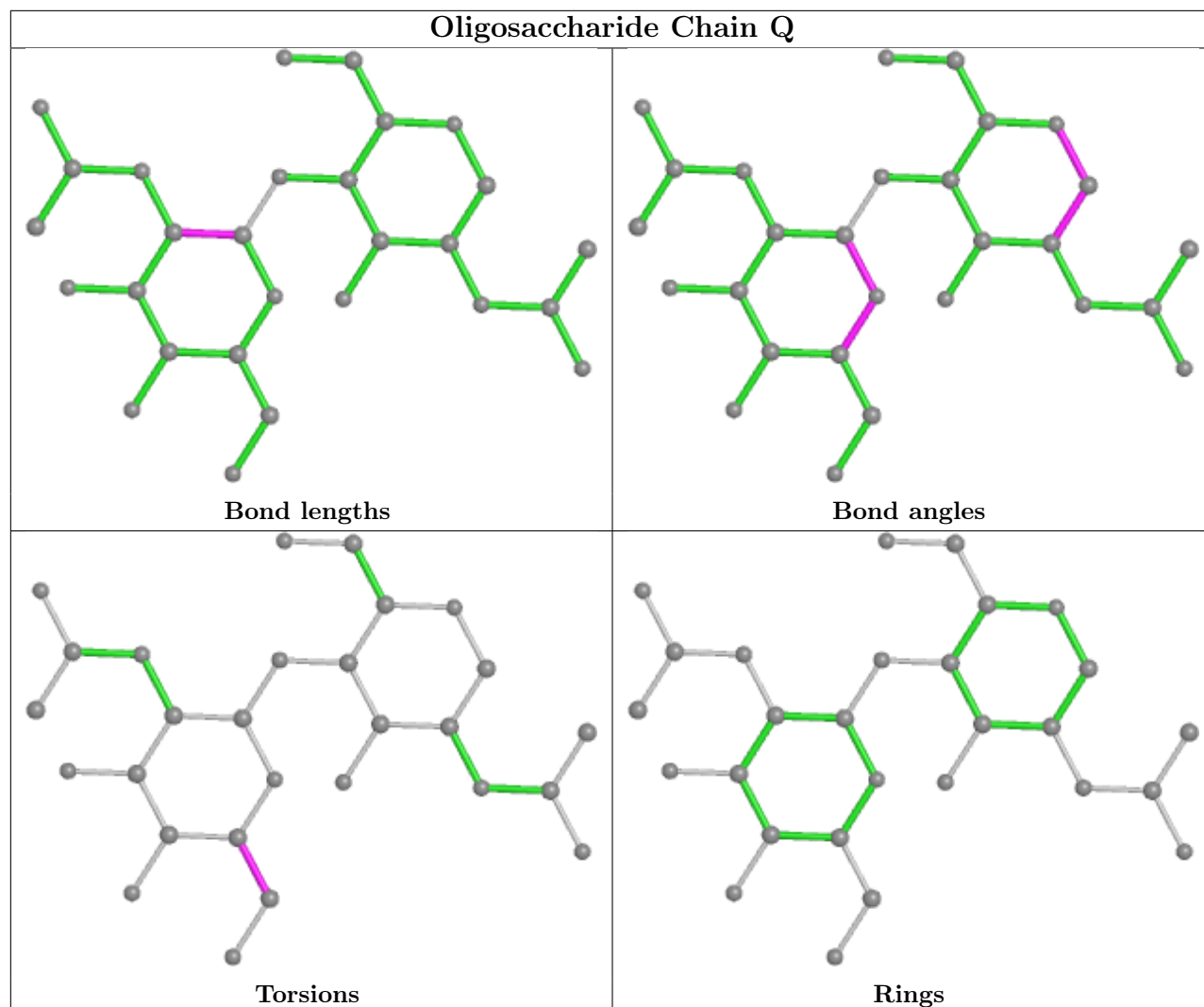


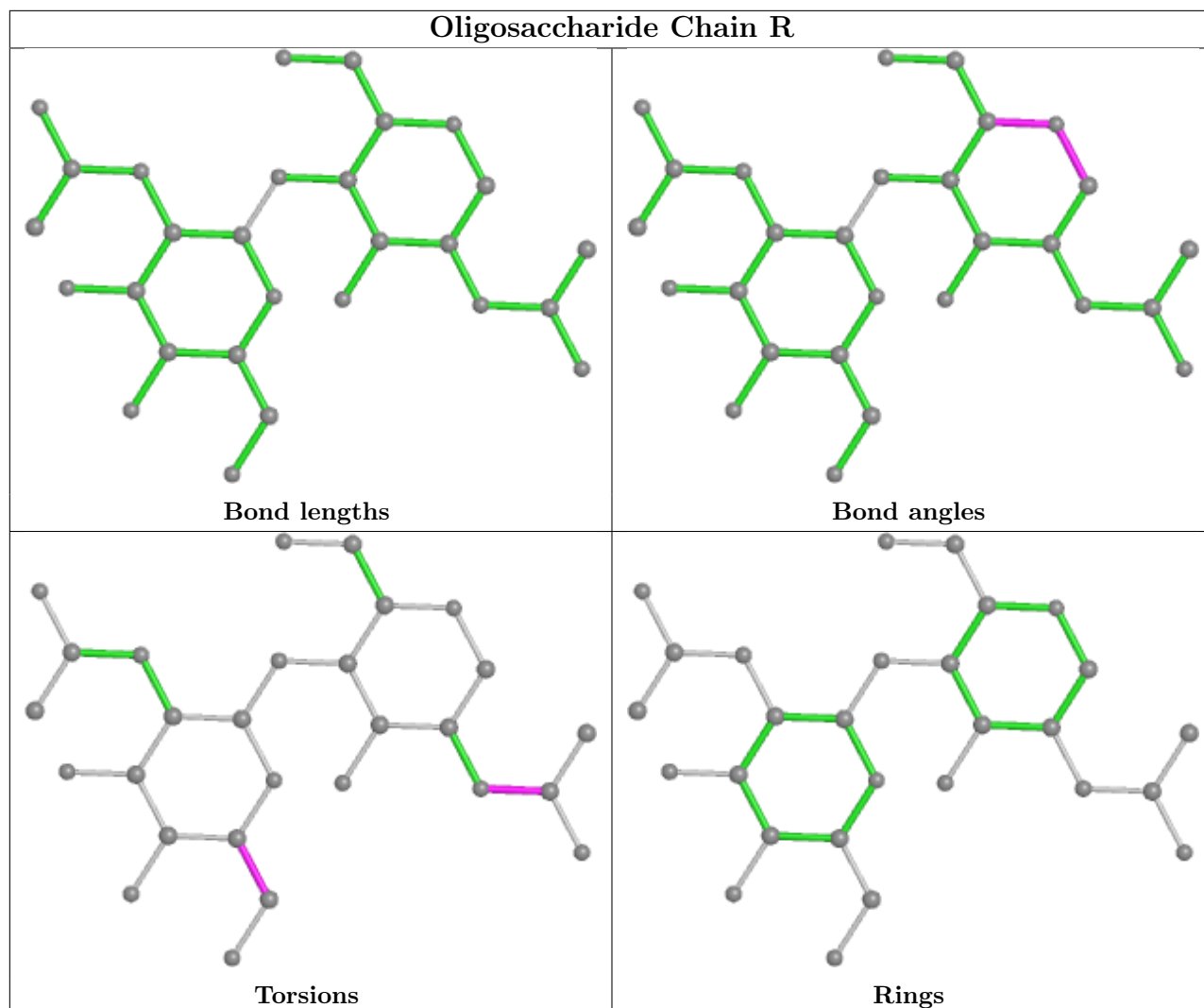












## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
16	NAG	G	1663	1	14,14,15	0.44	0	17,19,21	0.57	0
16	NAG	B	701	-	14,14,15	0.76	1 (7%)	17,19,21	0.37	0
16	NAG	B	702	2	14,14,15	2.37	2 (14%)	17,19,21	1.58	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	G	1663	1	-	2/6/23/26	0/1/1/1
16	NAG	B	701	-	-	0/6/23/26	0/1/1/1
16	NAG	B	702	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	702	NAG	C1-C2	-6.82	1.42	1.52
16	B	702	NAG	O5-C1	5.29	1.52	1.43
16	B	701	NAG	O5-C1	-2.80	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	702	NAG	C1-O5-C5	5.11	119.11	112.19
16	B	702	NAG	O5-C5-C4	-2.10	105.72	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	702	NAG	C4-C5-C6-O6
16	B	702	NAG	O5-C5-C6-O6
16	G	1663	NAG	O5-C5-C6-O6
16	G	1663	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1663	NAG	1	0
16	B	702	NAG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	G	452/480 (94%)	-0.65	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	10, 33, 73, 120	0
2	B	148/153 (96%)	-0.46	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">87</span>	9, 37, 109, 192	0
3	L	211/218 (96%)	-0.69	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	19, 44, 79, 104	0
4	H	231/236 (97%)	-0.62	3 (1%) <span style="border: 1px solid blue; padding: 2px;">77</span> <span style="border: 1px solid blue; padding: 2px;">77</span>	32, 62, 91, 228	0
5	D	240/240 (100%)	-0.02	26 (10%) <span style="border: 1px solid red; padding: 2px;">5</span> <span style="border: 1px solid red; padding: 2px;">4</span>	36, 97, 226, 263	0
6	E	213/216 (98%)	-0.04	17 (7%) <span style="border: 1px solid red; padding: 2px;">12</span> <span style="border: 1px solid red; padding: 2px;">9</span>	55, 115, 172, 202	0
All	All	1495/1543 (96%)	-0.45	47 (3%) <span style="border: 1px solid gray; padding: 2px;">49</span> <span style="border: 1px solid gray; padding: 2px;">44</span>	9, 55, 165, 263	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	222	VAL	9.3
5	D	129	LYS	8.7
6	E	214	GLU	6.8
5	D	160	THR	6.7
6	E	198	GLN	6.1
5	D	187	SER	5.9
5	D	188	SER	5.7
6	E	199	VAL	4.8
6	E	161	ALA	4.6
5	D	214	LYS	4.3
4	H	209	VAL	4.2
6	E	119	VAL	4.0
5	D	159	LEU	3.7
5	D	128	SER	3.1
5	D	124	LEU	3.1
6	E	114	LYS	3.1
5	D	167	PRO	3.1
5	D	185	PRO	3.0
5	D	135	THR	3.0

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Mol	Chain	Res	Type	RSRZ
5	D	131	THR	2.9
6	E	158	PRO	2.9
6	E	208	LYS	2.9
5	D	190	GLY	2.8
5	D	15	GLY	2.8
6	E	206	VAL	2.8
6	E	115	ALA	2.7
6	E	70	TYR	2.7
4	H	196	VAL	2.6
2	B	512	ALA	2.6
5	D	130	SER	2.6
6	E	210	VAL	2.5
5	D	152	VAL	2.4
6	E	121	LEU	2.4
5	D	191	THR	2.2
5	D	194	TYR	2.2
5	D	186	SER	2.2
6	E	90	CYS	2.2
5	D	221	GLU	2.1
6	E	122	PHE	2.1
6	E	162	GLY	2.1
5	D	158	ALA	2.1
5	D	161	SER	2.1
5	D	174	GLY	2.1
5	D	127	SER	2.0
6	E	134	ALA	2.0
4	H	34	TRP	2.0
5	D	59	LEU	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( $\text{\AA}^2$ )	Q<0.9
10	NAG	I	2	14/15	0.52	0.21	213,239,249,255	0
7	NAG	A	1	14/15	0.56	0.30	142,152,164,166	0
14	BMA	P	3	11/12	0.62	0.14	235,247,263,263	0
14	MAN	P	7	11/12	0.67	0.35	262,267,270,273	0
12	BMA	N	3	11/12	0.69	0.40	212,225,229,231	0
11	MAN	M	5	11/12	0.71	0.42	267,278,283,284	0
9	NAG	F	2	14/15	0.71	0.28	146,153,166,167	0
11	MAN	M	6	11/12	0.73	0.18	246,261,264,268	0
8	NAG	C	1	14/15	0.73	0.19	134,135,138,145	0
11	MAN	J	7	11/12	0.74	0.15	241,243,257,260	0
10	NAG	S	2	14/15	0.74	0.40	191,196,215,219	0
11	MAN	M	7	11/12	0.77	0.22	150,181,209,210	0
14	MAN	P	6	11/12	0.77	0.38	201,208,212,213	0
11	MAN	J	8	11/12	0.77	0.17	263,269,274,275	0
11	MAN	M	4	11/12	0.78	0.23	243,244,255,265	0
7	MAN	A	6	11/12	0.79	0.30	160,167,172,173	0
10	BMA	S	3	11/12	0.79	0.19	181,186,191,191	0
8	NAG	C	2	14/15	0.79	0.25	135,141,146,148	0
10	NAG	S	1	14/15	0.79	0.40	143,170,181,191	0
15	NAG	R	2	14/15	0.79	0.21	176,181,183,186	0
8	MAN	C	4	11/12	0.80	0.16	170,172,183,187	0
9	NAG	F	1	14/15	0.81	0.19	122,130,140,142	0
9	MAN	F	7	11/12	0.81	0.37	160,171,179,190	0
9	BMA	K	3	11/12	0.81	0.09	231,234,240,242	0
8	BMA	C	3	11/12	0.82	0.11	127,140,157,159	0
10	BMA	I	3	11/12	0.82	0.20	263,271,276,280	0
14	MAN	P	5	11/12	0.83	0.23	209,221,224,226	0
12	NAG	N	2	14/15	0.83	0.22	181,190,208,215	0
9	MAN	K	7	11/12	0.83	0.45	233,243,248,257	0
8	MAN	C	5	11/12	0.83	0.17	165,172,184,185	0
12	MAN	N	4	11/12	0.84	0.13	191,199,207,208	0
14	NAG	P	1	14/15	0.84	0.20	178,191,199,199	0
9	NAG	K	2	14/15	0.84	0.33	231,240,257,259	0
15	NAG	R	1	14/15	0.84	0.13	154,165,171,171	0
14	MAN	P	4	11/12	0.84	0.14	228,240,254,255	0
9	MAN	F	6	11/12	0.85	0.16	98,102,105,106	0
13	NAG	O	2	14/15	0.85	0.24	127,131,150,172	0
11	MAN	J	6	11/12	0.86	0.16	209,227,238,239	0
11	BMA	M	3	11/12	0.86	0.21	214,223,228,232	0
14	NAG	P	2	14/15	0.86	0.17	204,213,217,225	0
15	NAG	Q	2	14/15	0.86	0.34	201,214,223,228	0
9	MAN	K	4	11/12	0.86	0.16	202,211,230,239	0
12	MAN	N	6	11/12	0.86	0.19	223,225,234,237	0

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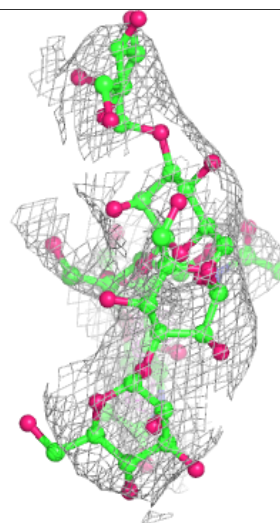
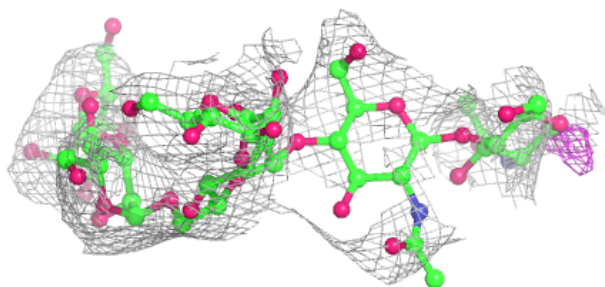
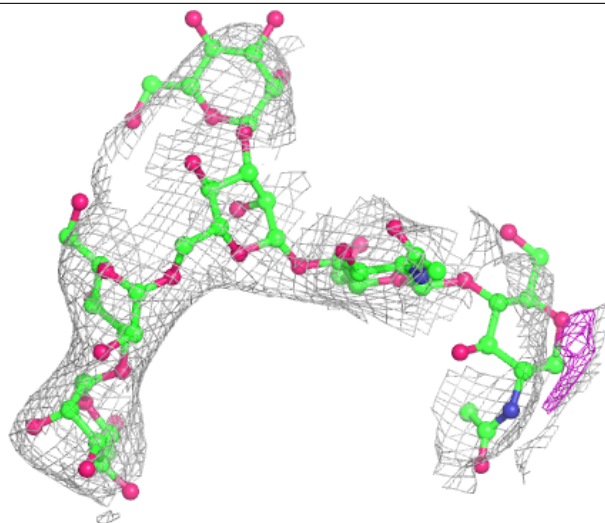
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	BMA	J	3	11/12	0.87	0.12	209,215,228,233	0
11	NAG	M	2	14/15	0.87	0.21	177,196,201,205	0
11	MAN	J	5	11/12	0.87	0.16	213,225,232,239	0
7	MAN	A	4	11/12	0.87	0.23	136,139,144,148	0
7	NAG	A	2	14/15	0.87	0.16	171,175,181,186	0
12	MAN	N	5	11/12	0.87	0.25	204,211,226,227	0
11	MAN	J	4	11/12	0.88	0.18	216,217,221,222	0
12	NAG	N	1	14/15	0.88	0.28	133,150,161,169	0
7	BMA	A	3	11/12	0.88	0.12	150,162,167,168	0
13	NAG	O	1	14/15	0.89	0.14	132,137,140,141	0
10	NAG	I	1	14/15	0.89	0.23	203,222,253,261	0
13	MAN	O	4	11/12	0.89	0.18	101,102,106,109	0
13	MAN	O	5	11/12	0.89	0.11	103,107,113,114	0
13	MAN	O	6	11/12	0.89	0.12	123,125,129,139	0
15	NAG	Q	1	14/15	0.89	0.19	152,164,180,193	0
13	MAN	O	9	11/12	0.89	0.16	152,157,169,174	0
8	MAN	C	7	11/12	0.89	0.14	117,120,133,134	0
9	BMA	F	3	11/12	0.89	0.10	160,165,168,172	0
9	MAN	F	5	11/12	0.90	0.10	108,116,127,131	0
11	NAG	J	1	14/15	0.90	0.14	165,173,182,184	0
13	MAN	O	7	11/12	0.90	0.13	149,154,159,163	0
11	NAG	J	2	14/15	0.90	0.23	182,193,199,201	0
7	MAN	A	5	11/12	0.90	0.20	133,137,149,150	0
9	MAN	K	5	11/12	0.91	0.12	187,195,205,208	0
11	NAG	M	1	14/15	0.91	0.22	181,187,211,221	0
11	MAN	M	8	11/12	0.91	0.13	99,118,144,152	0
9	MAN	F	4	11/12	0.92	0.12	136,155,161,171	0
8	MAN	C	6	11/12	0.92	0.10	184,191,198,199	0
9	NAG	K	1	14/15	0.92	0.28	168,198,226,229	0
13	MAN	O	8	11/12	0.92	0.08	146,151,154,154	0
13	MAN	O	10	11/12	0.93	0.12	165,174,180,184	0
9	MAN	K	6	11/12	0.93	0.23	219,223,235,238	0
13	BMA	O	3	11/12	0.94	0.10	119,126,138,145	0

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

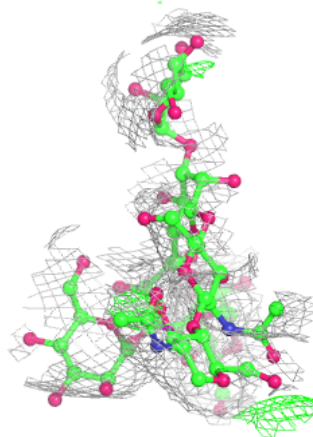
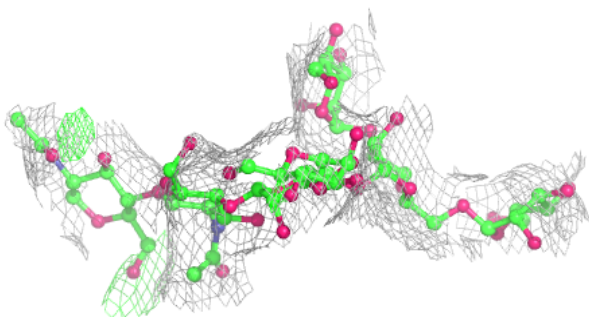
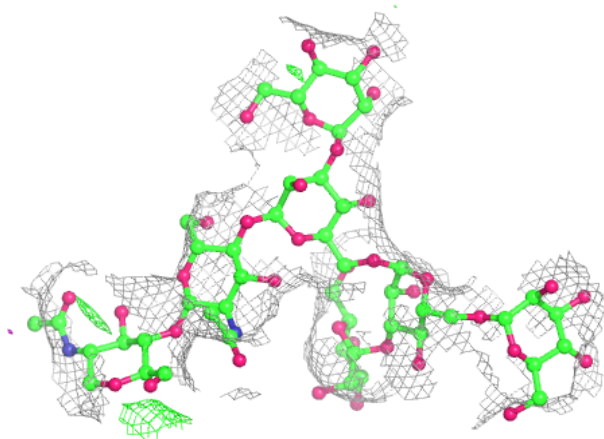
**Electron density around Chain A:**

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

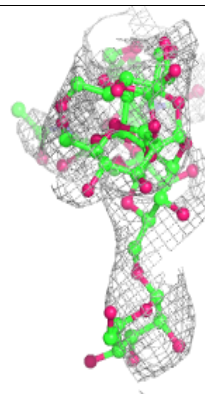
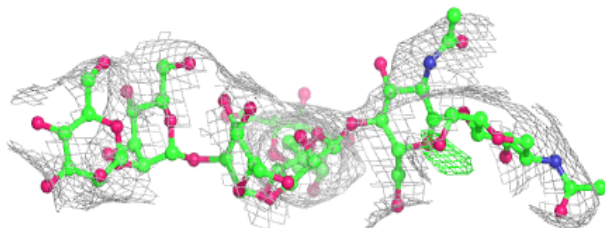
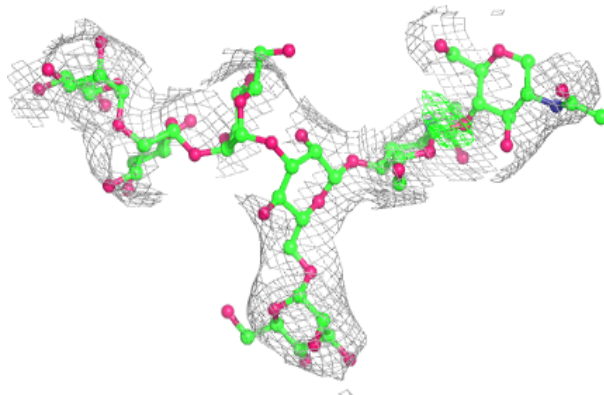


**Electron density around Chain C:**

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

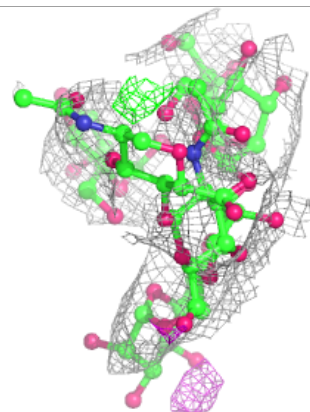
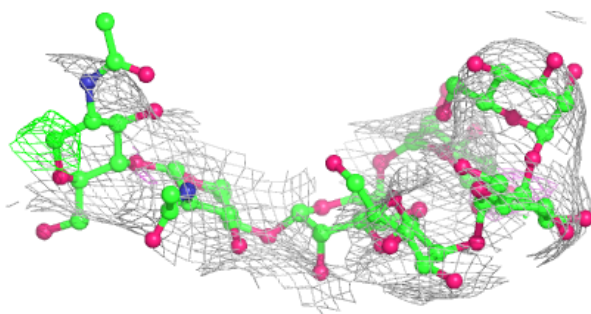
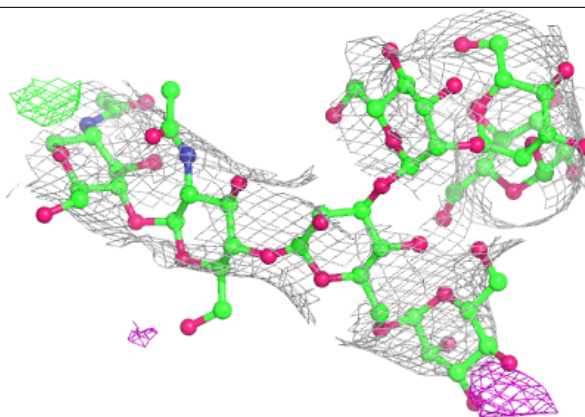
**Electron density around Chain F:**

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

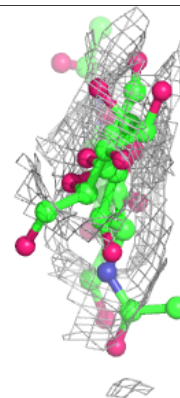
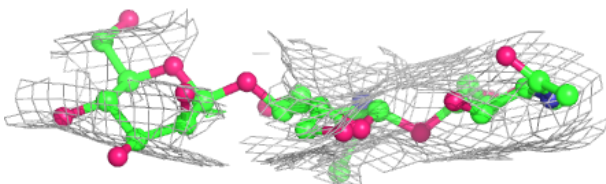
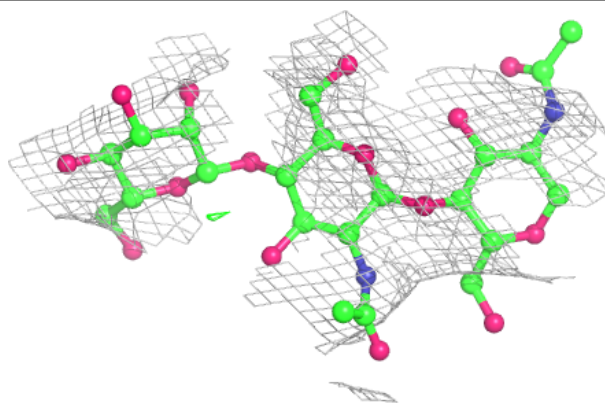


**Electron density around Chain K:**

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

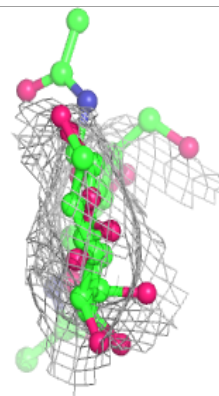
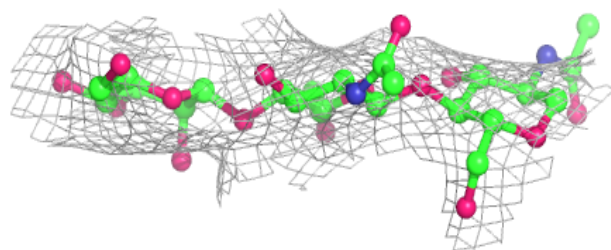
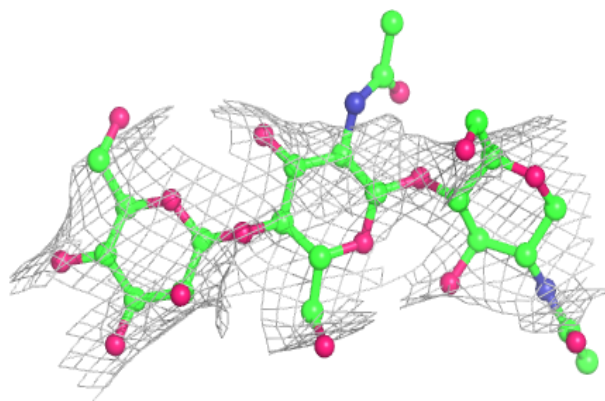
**Electron density around Chain I:**

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

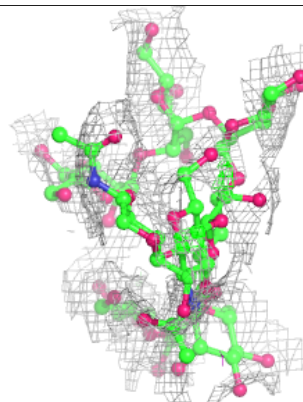
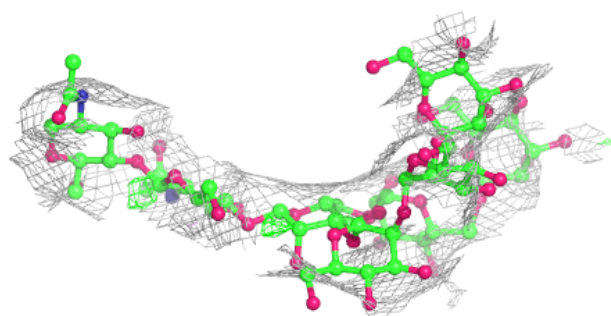
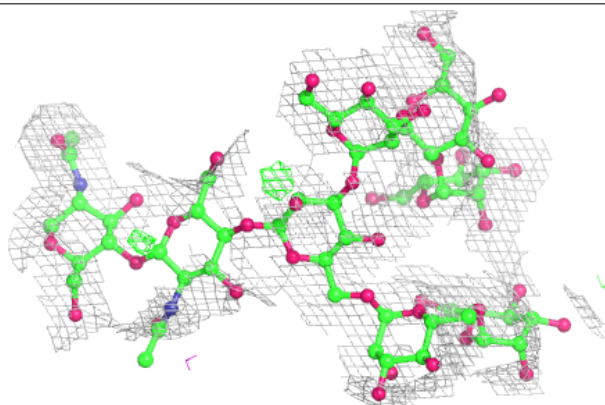


**Electron density around Chain S:**

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

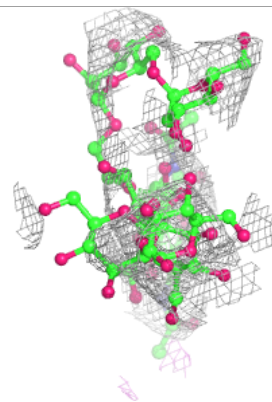
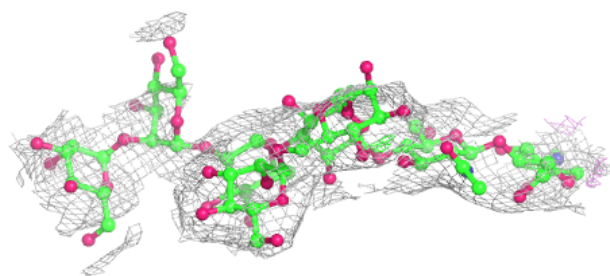
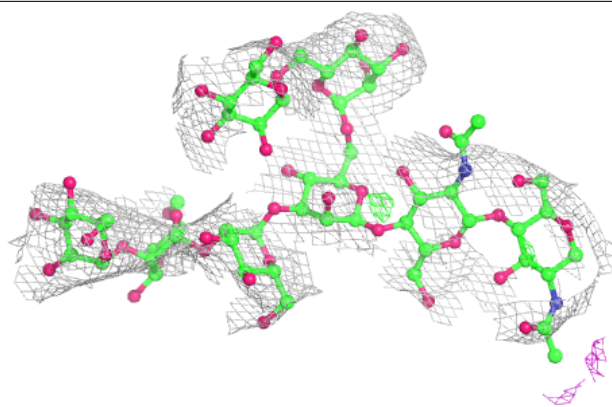
**Electron density around Chain J:**

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

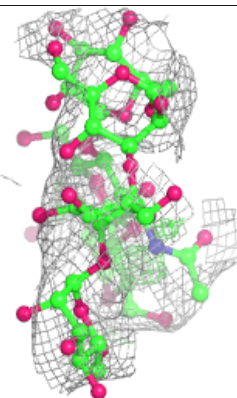
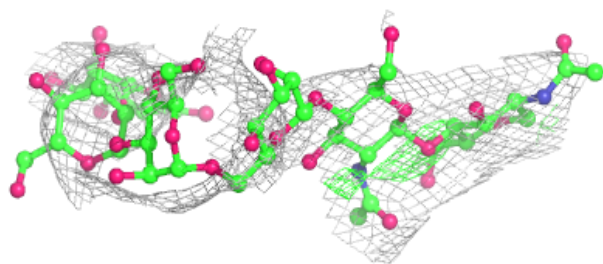
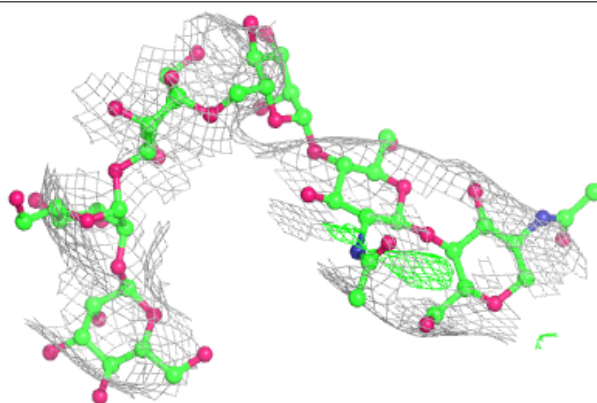


**Electron density around Chain M:**

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

**Electron density around Chain N:**

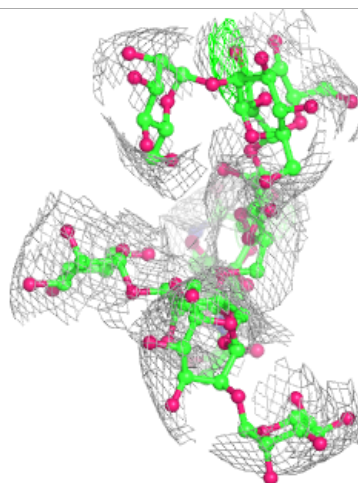
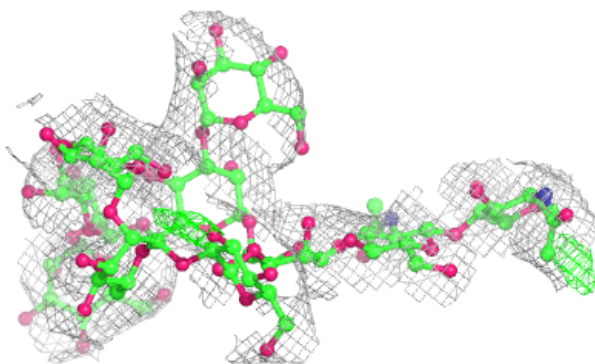
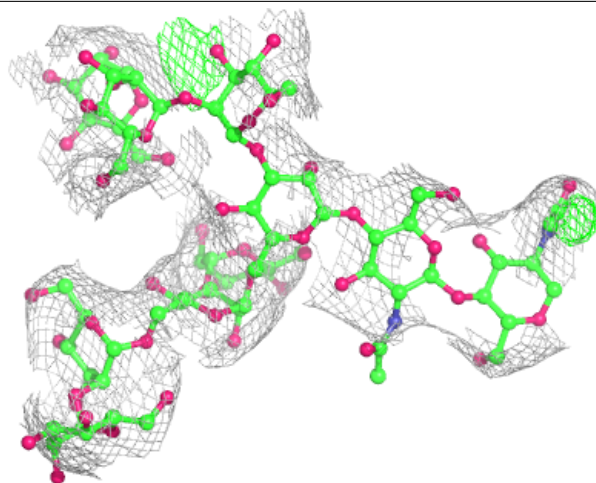
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





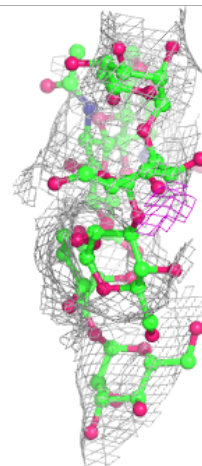
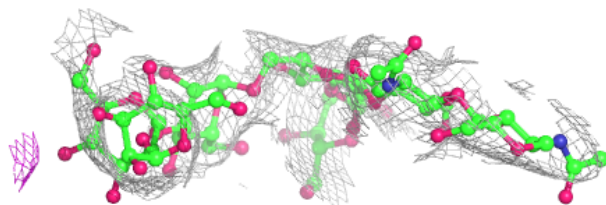
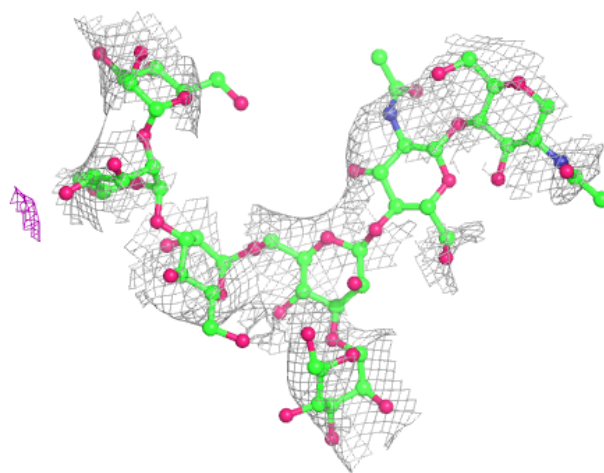
**Electron density around Chain O:**

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



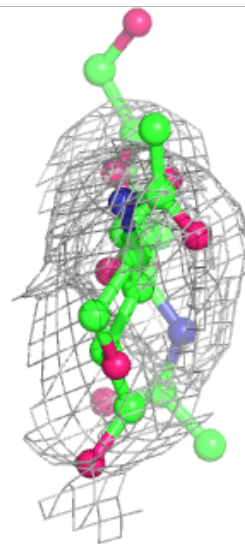
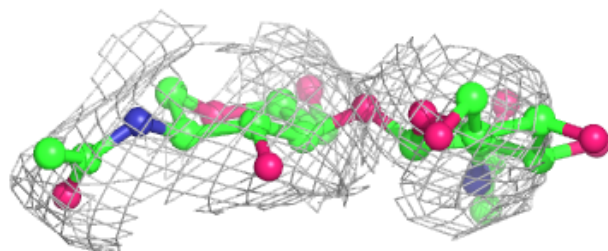
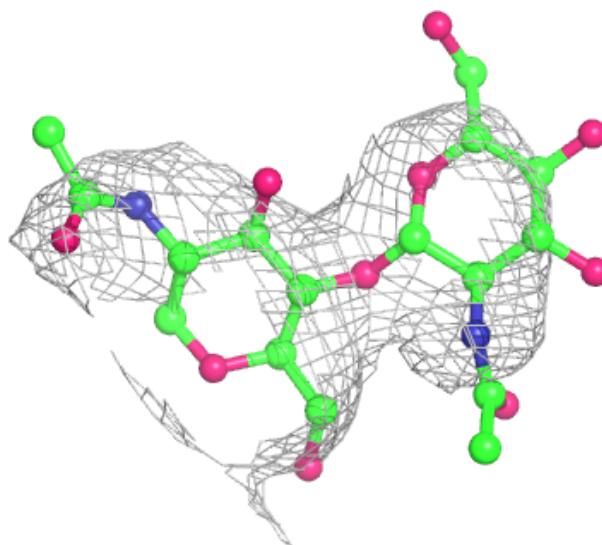
**Electron density around Chain P:**

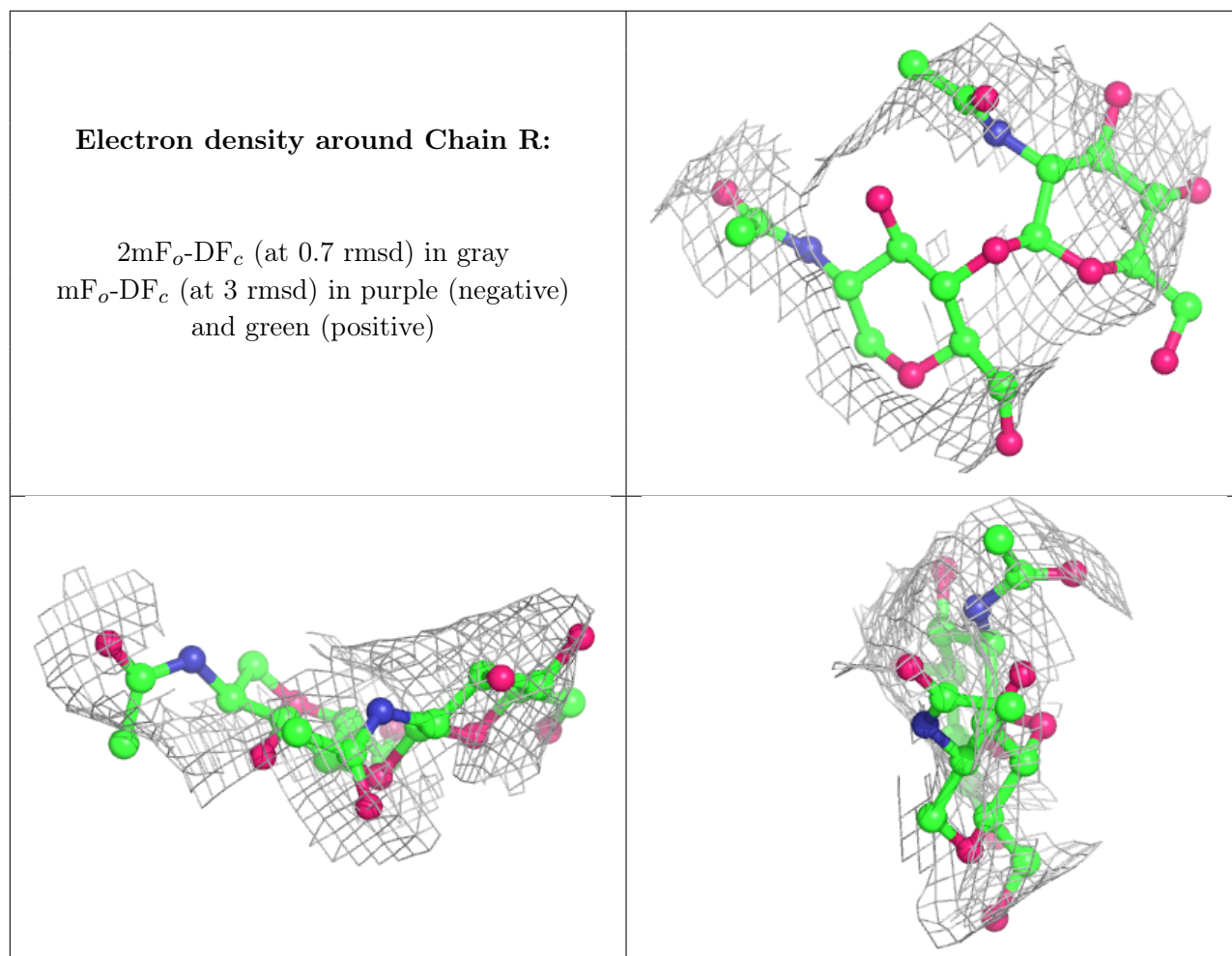
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain Q:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	NAG	B	701	14/15	0.77	0.28	169,185,194,204	0
16	NAG	B	702	14/15	0.86	0.23	212,220,224,225	0
16	NAG	G	1663	14/15	0.88	0.22	134,144,154,161	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.