



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:07 PM UTC

PDB ID : 2FK0 / pdb_00002fk0
Title : Crystal Structure of a H5N1 influenza virus hemagglutinin.
Authors : Stevens, J.; Wilson, I.A.
Deposited on : 2006-01-03
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

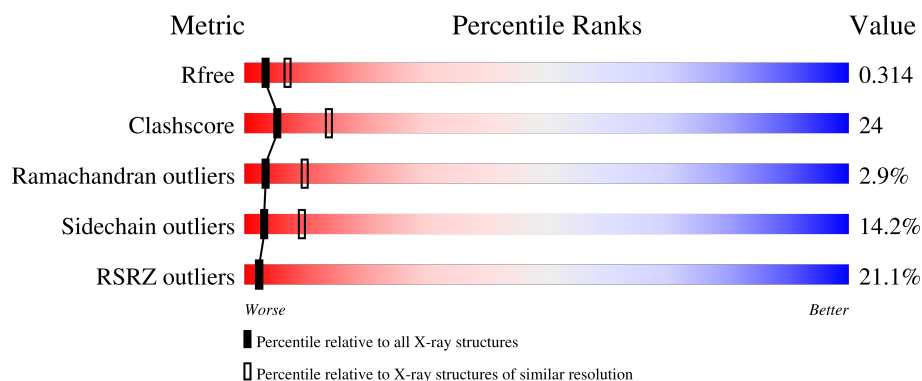
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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

Mol	Chain	Length	Quality of chain
1	A	334	
1	C	334	
1	E	334	
1	G	334	
1	I	334	

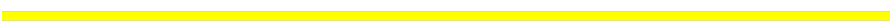
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Mol	Chain	Length	Quality of chain
1	K	334	
1	M	334	
1	O	334	
1	Q	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	
3	S	2	
3	U	2	
3	V	2	
3	W	2	
3	Y	2	
3	a	2	
3	b	2	
3	c	2	
3	d	2	
3	e	2	
3	f	2	
3	g	2	

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Mol	Chain	Length	Quality of chain
3	h	2	 100%
4	T	3	 33% 67%
4	X	3	 67% 33%
4	Z	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	V	1	X	-	-	-
3	NAG	b	1	X	-	-	-
3	NAG	d	1	X	-	-	-
3	NAG	f	1	X	-	-	-
3	NAG	h	1	X	-	-	-
4	NAG	T	1	X	-	-	-
4	NAG	X	1	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36202 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	C	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	E	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	G	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	I	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	K	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	M	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	O	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	Q	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			

There are 36 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called hemagglutinin.

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

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

There are 63 discrepancies between the modelled and reference sequences:

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

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

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



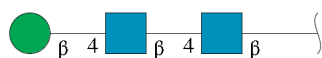
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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

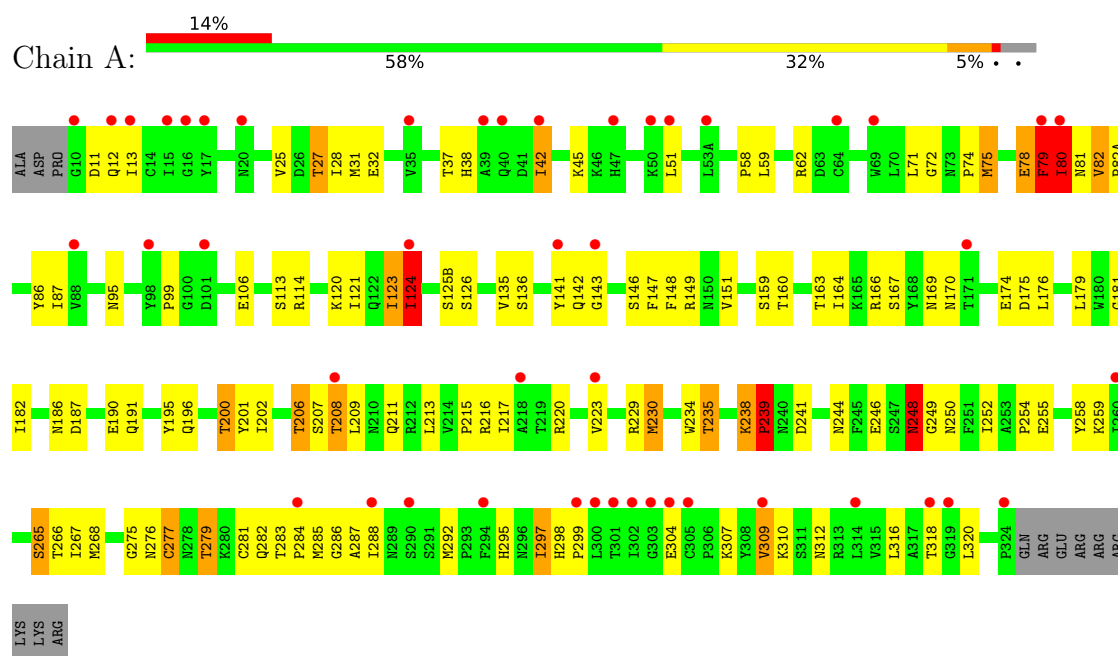


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			

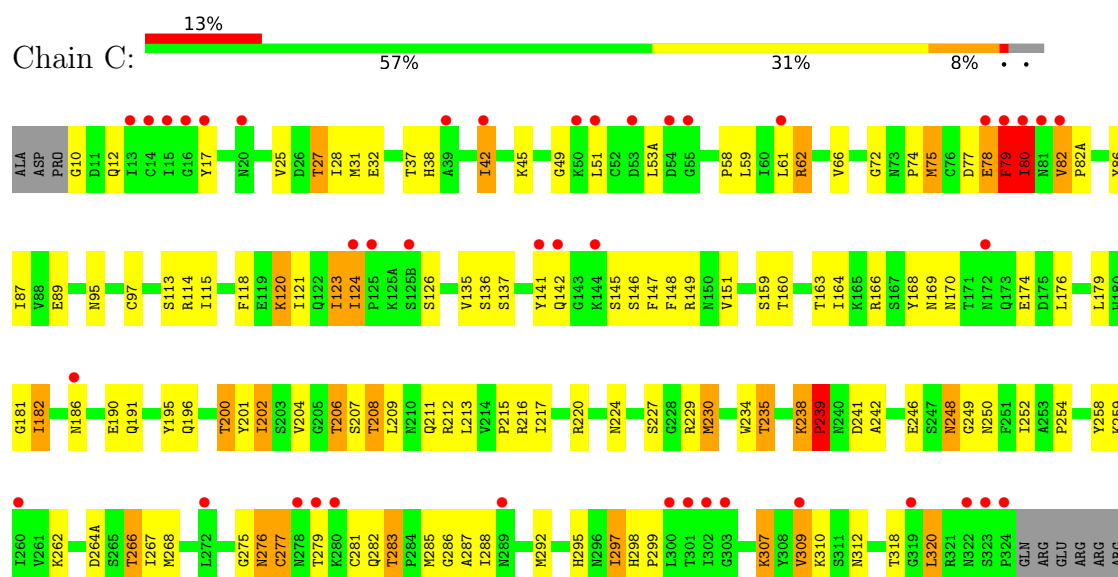
3 Residue-property plots

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

• Molecule 1: hemagglutinin

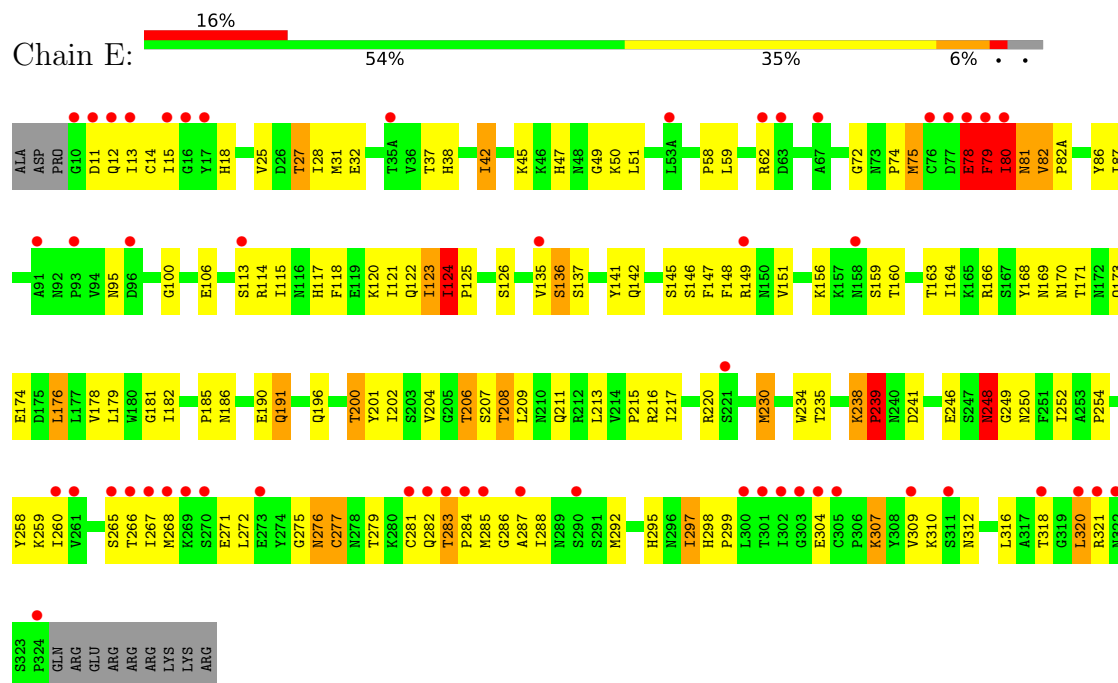


• Molecule 1: hemagglutinin

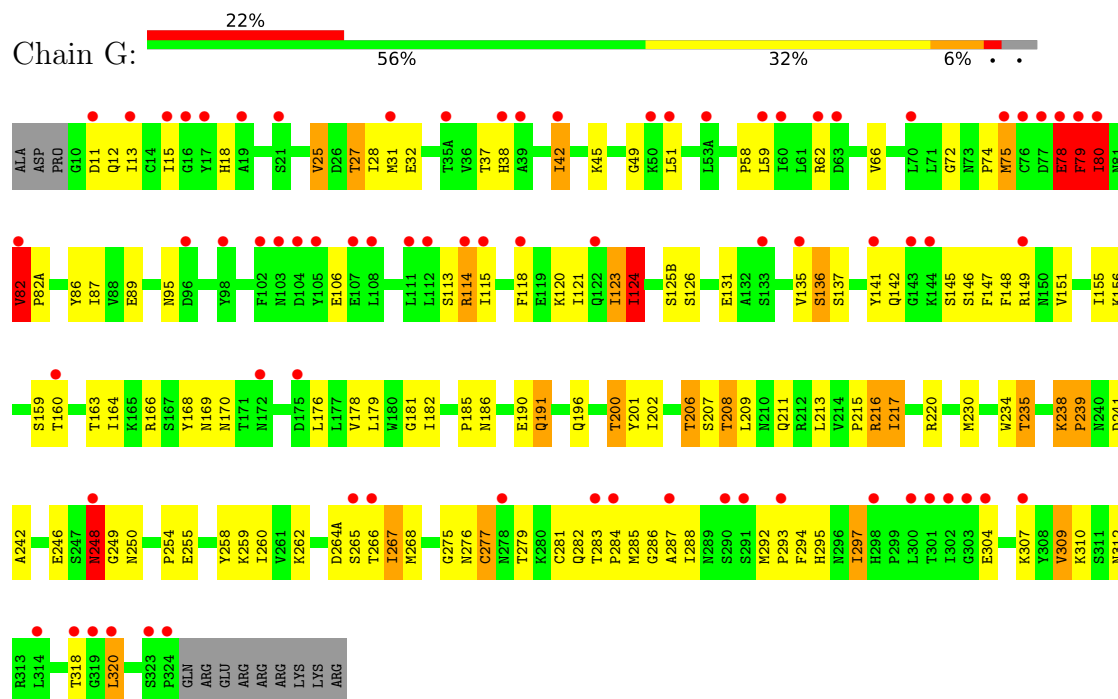


LYS
LYS
LYS
ARG

• Molecule 1: hemagglutinin

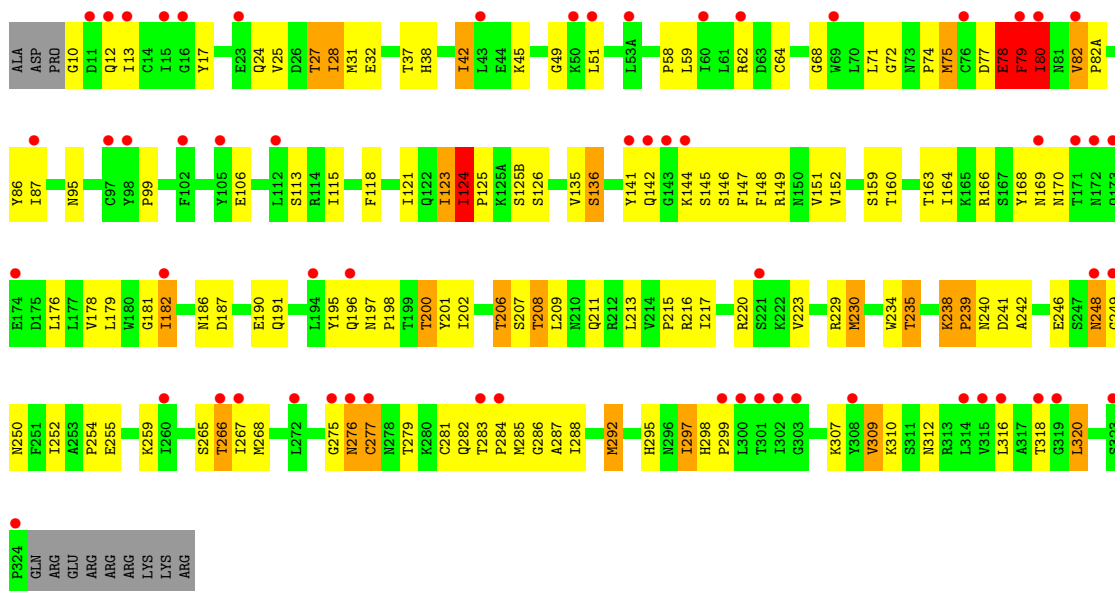


• Molecule 1: hemagglutinin

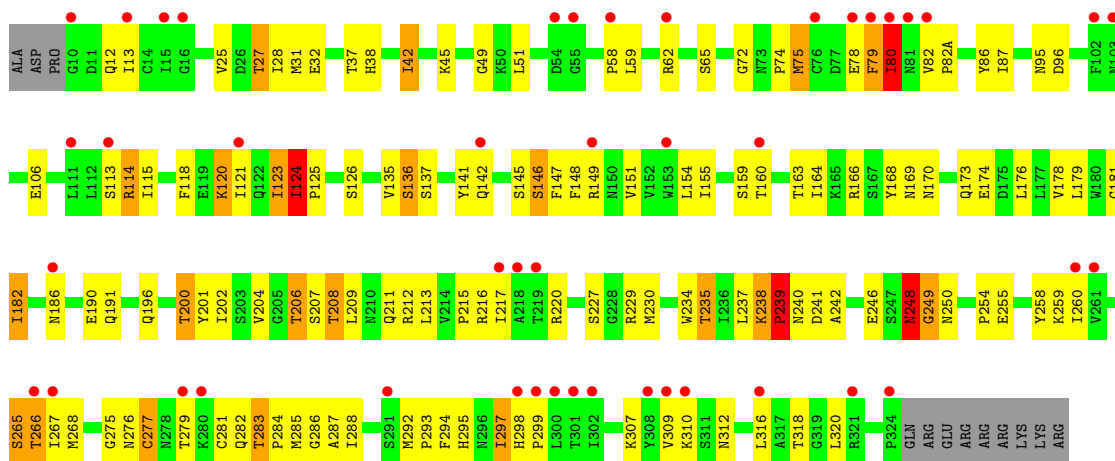


• Molecule 1: hemagglutinin

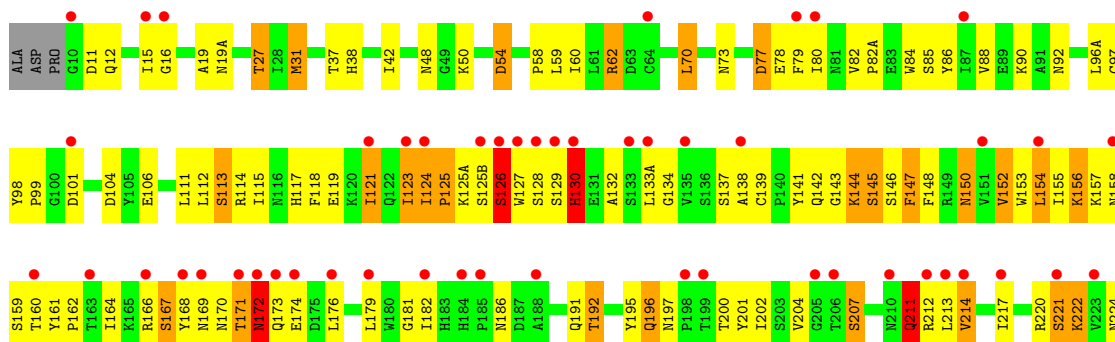


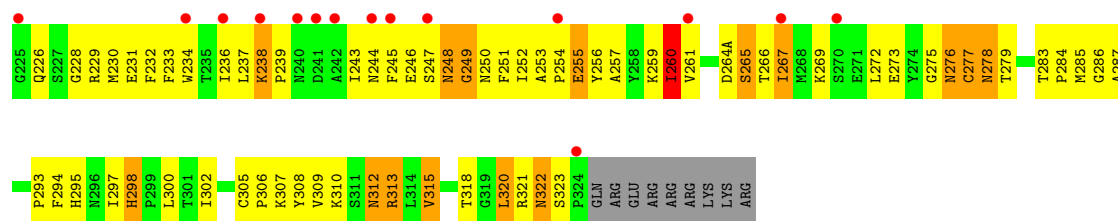


• Molecule 1: hemagglutinin

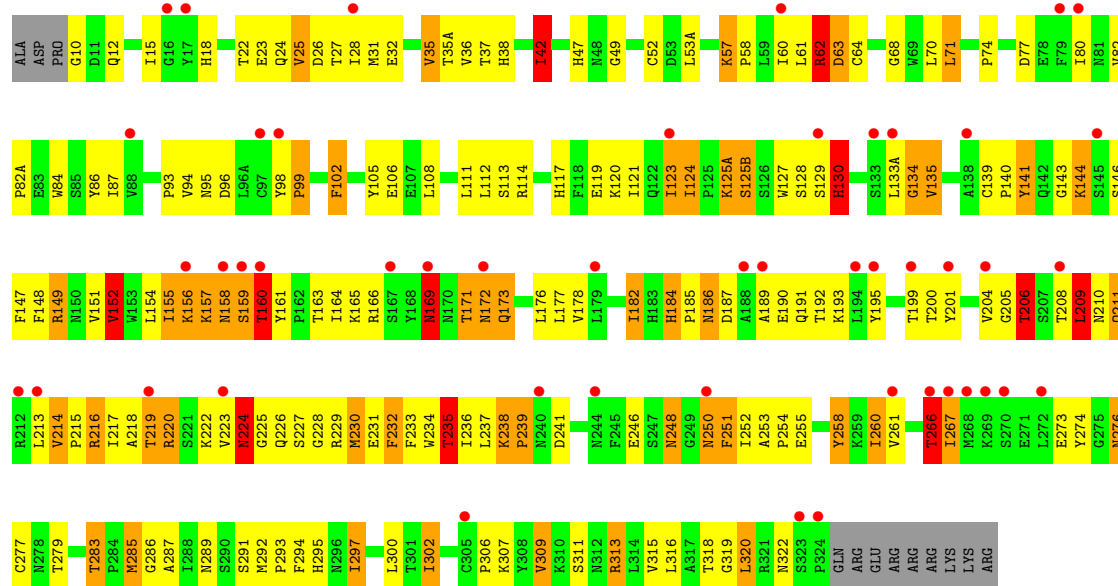


• Molecule 1: hemagglutinin

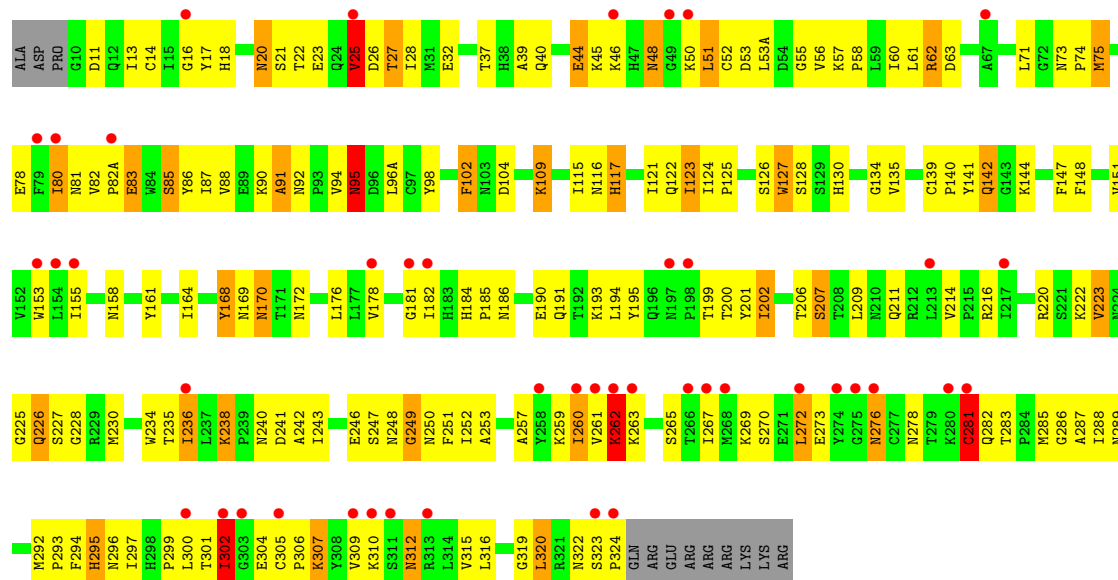




• Molecule 1: hemagglutinin

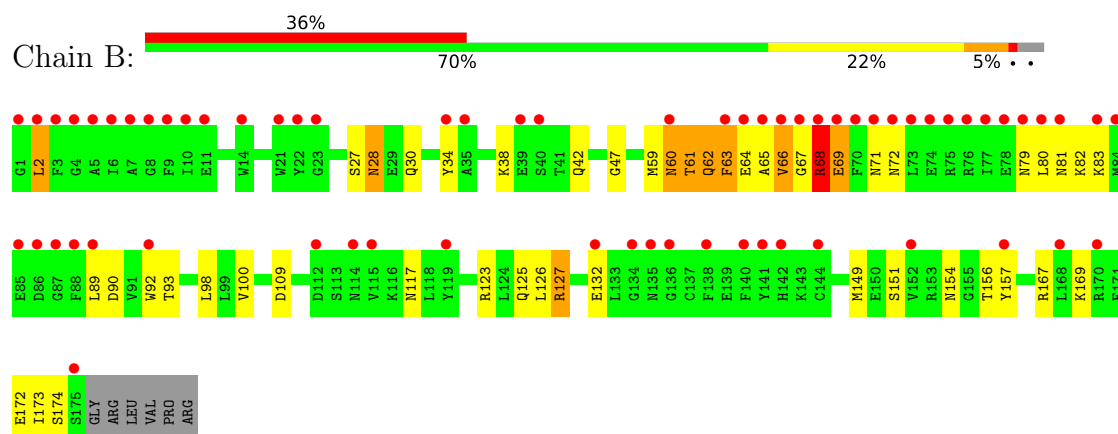


• Molecule 1: hemagglutinin



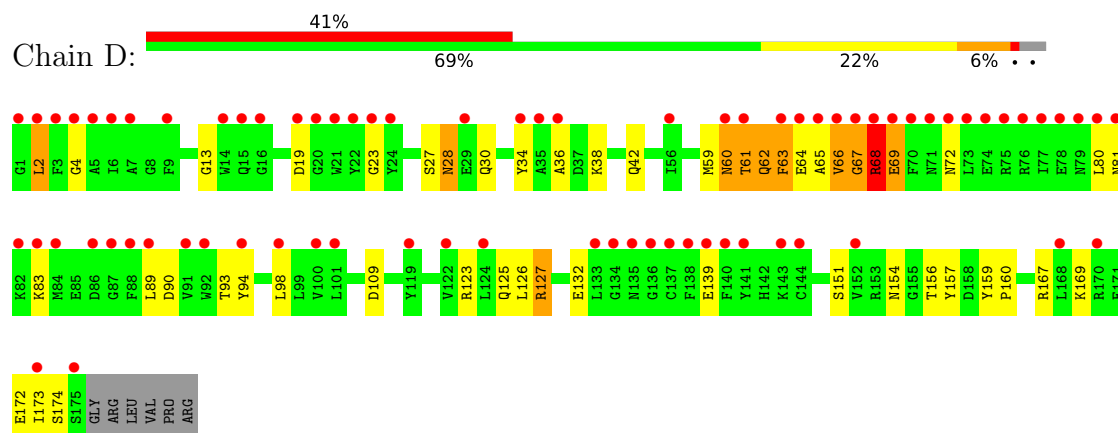
- Molecule 2: hemagglutinin

Chain B:



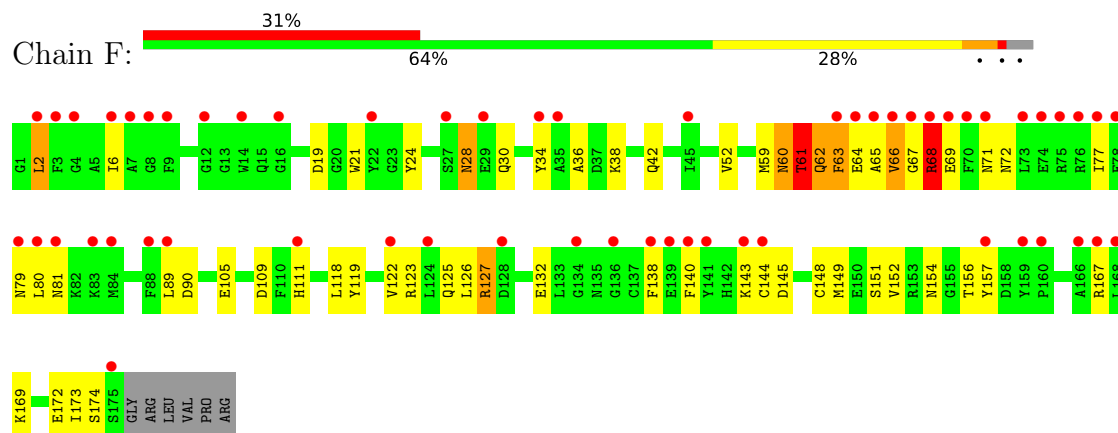
- Molecule 2: hemagglutinin

Chain D:



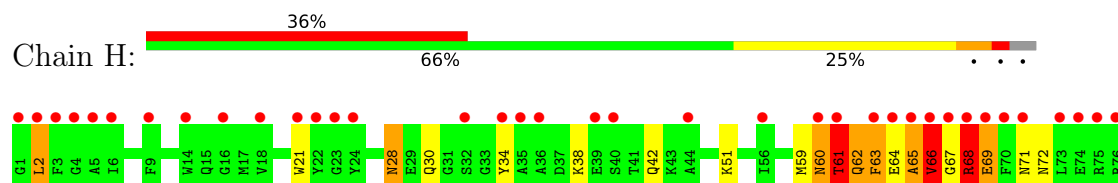
- Molecule 2: hemagglutinin

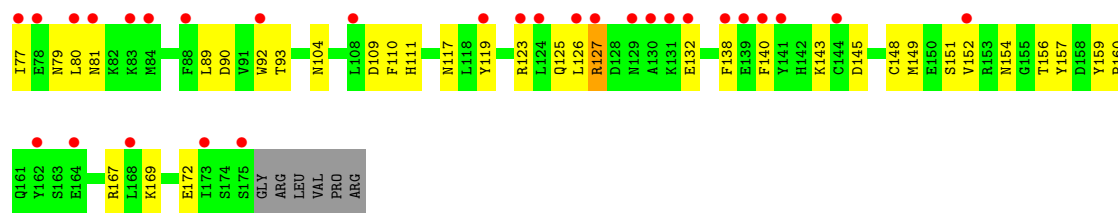
Chain F:



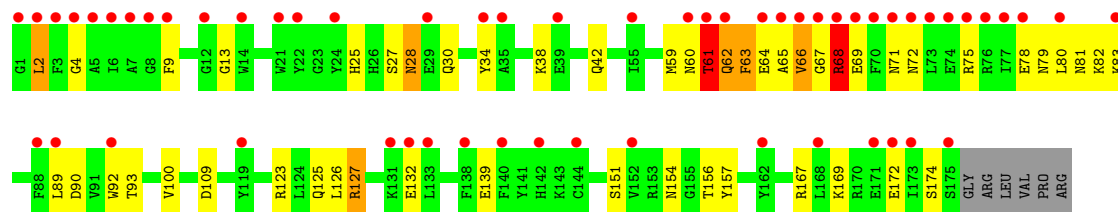
- Molecule 2: hemagglutinin

Chain H:

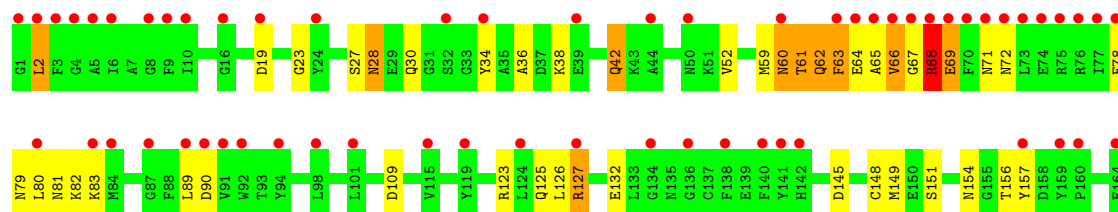




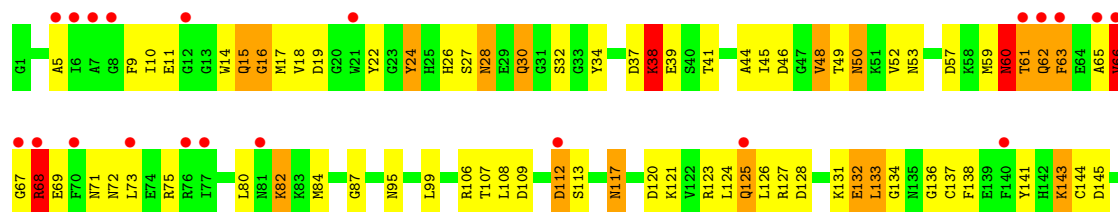
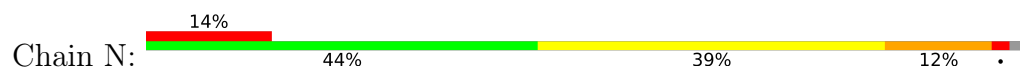
• Molecule 2: hemagglutinin



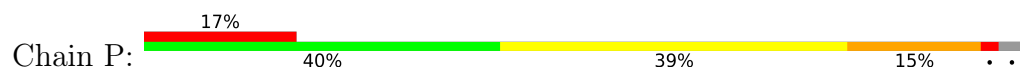
• Molecule 2: hemagglutinin

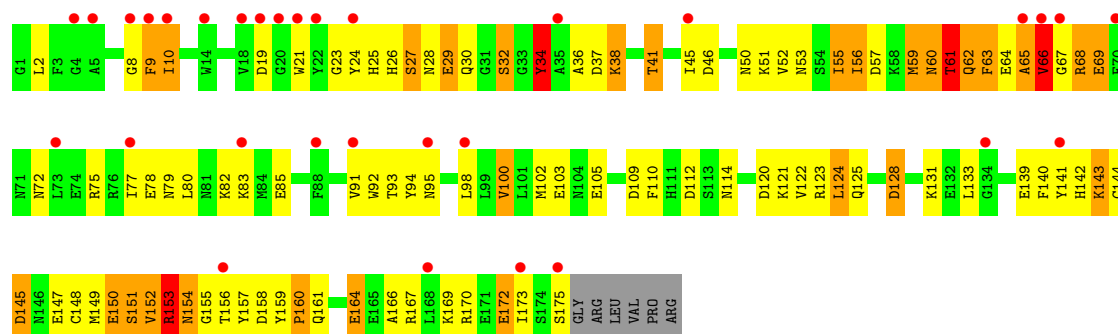


• Molecule 2: hemagglutinin

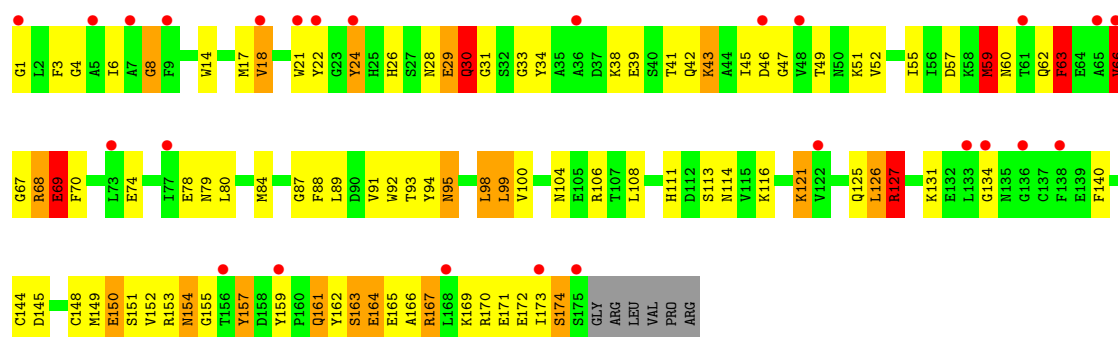
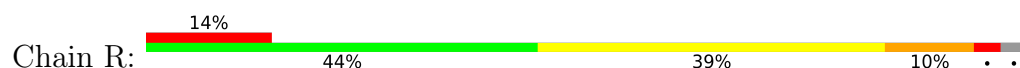


• Molecule 2: hemagglutinin





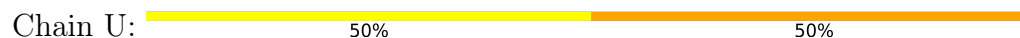
• Molecule 2: hemagglutinin



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



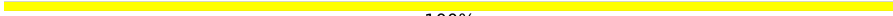
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain W:  100%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain a:  50% 50%

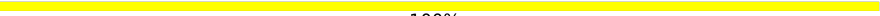
MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  100%

MAG1
MAG2

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

Chain e:  100%

MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

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

Chain g:  100%

MAG1
MAG2

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

Chain h:  100%

MAG1
MAG2

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

Chain T:  33% 67%

MAG1
MAG2
EMA3

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

Chain X:  67% 33%

MAG1
MAG2
EMA3

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

Chain Z:  100%

MAG1
MAG2
EMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	197.94Å 197.94Å 134.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	171.50 – 2.95 171.42 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (171.50-2.95) 98.8 (171.42-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.319 0.266 , 0.314	Depositor DCC
R_{free} test set	1233 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 94.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.008 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	36202	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.94	0/2615	1.10	10/3551 (0.3%)
1	C	1.01	2/2615 (0.1%)	1.13	9/3551 (0.3%)
1	E	1.01	1/2615 (0.0%)	1.13	7/3551 (0.2%)
1	G	1.00	0/2615	1.14	8/3551 (0.2%)
1	I	0.97	1/2615 (0.0%)	1.12	13/3551 (0.4%)
1	K	0.96	3/2615 (0.1%)	1.11	7/3551 (0.2%)
1	M	1.56	23/2615 (0.9%)	1.18	20/3551 (0.6%)
1	O	1.72	27/2615 (1.0%)	1.25	25/3551 (0.7%)
1	Q	1.06	6/2615 (0.2%)	1.05	15/3551 (0.4%)
2	B	0.89	4/1443 (0.3%)	1.05	4/1939 (0.2%)
2	D	0.89	4/1443 (0.3%)	1.05	5/1939 (0.3%)
2	F	0.91	4/1443 (0.3%)	1.04	4/1939 (0.2%)
2	H	0.86	5/1443 (0.3%)	1.02	5/1939 (0.3%)
2	J	0.86	4/1443 (0.3%)	1.03	5/1939 (0.3%)
2	L	0.86	4/1443 (0.3%)	1.04	8/1939 (0.4%)
2	N	1.22	6/1443 (0.4%)	1.14	9/1939 (0.5%)
2	P	1.38	12/1443 (0.8%)	1.14	10/1939 (0.5%)
2	R	0.77	2/1443 (0.1%)	1.03	6/1939 (0.3%)
All	All	1.11	108/36522 (0.3%)	1.11	170/49410 (0.3%)

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

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

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

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	130	HIS	CE1-NE2	46.89	1.79	1.32
1	M	130	HIS	CE1-NE2	43.18	1.75	1.32
1	Q	130	HIS	CE1-NE2	30.81	1.63	1.32
1	M	130	HIS	CG-ND1	29.96	1.71	1.38
2	N	38	LYS	CE-NZ	26.55	2.29	1.49
1	O	130	HIS	CG-ND1	26.09	1.67	1.38
2	P	143	LYS	CE-NZ	23.05	2.18	1.49
1	O	125(B)	SER	CB-OG	22.51	1.87	1.42
2	P	145	ASP	CG-OD1	20.34	1.64	1.25
1	M	166	ARG	C-O	19.40	1.51	1.23
1	O	219	THR	CB-OG1	18.45	1.73	1.43
1	O	157	LYS	CD-CE	18.36	2.07	1.52
1	O	160	THR	CB-OG1	17.54	1.71	1.43
1	Q	130	HIS	CG-ND1	17.50	1.57	1.38
1	O	125(A)	LYS	CE-NZ	15.66	1.96	1.49
2	P	38	LYS	CE-NZ	14.24	1.92	1.49
1	O	157	LYS	CE-NZ	13.67	1.90	1.49
1	M	158	ASN	CG-OD1	13.51	1.49	1.23
1	M	158	ASN	CG-ND2	13.42	1.61	1.33
2	N	38	LYS	CG-CD	13.00	1.91	1.52
2	P	145	ASP	CG-OD2	12.65	1.49	1.25
2	N	38	LYS	CD-CE	12.38	1.89	1.52
1	O	157	LYS	CG-CD	11.79	1.87	1.52
2	P	143	LYS	CD-CE	11.32	1.86	1.52
1	O	125(A)	LYS	CD-CE	10.49	1.83	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	166	ARG	C-N	10.20	1.46	1.33
2	P	125	GLN	CD-NE2	10.04	1.54	1.33
1	M	247	SER	CB-OG	9.54	1.61	1.42
2	F	68	ARG	CA-C	9.51	1.64	1.52
2	B	68	ARG	CA-C	9.37	1.63	1.52
1	O	159	SER	CB-OG	9.24	1.60	1.42
2	F	68	ARG	N-CA	9.24	1.57	1.46
2	P	175	SER	C-O	9.03	1.41	1.23
2	J	68	ARG	CA-C	8.94	1.63	1.52
1	M	172	ASN	CG-OD1	8.69	1.40	1.23
2	L	66	VAL	CA-C	8.68	1.63	1.52
2	D	68	ARG	CA-C	8.66	1.62	1.52
2	H	68	ARG	CA-C	8.63	1.62	1.52
1	M	152	VAL	C-O	8.61	1.34	1.24
2	N	165	GLU	CD-OE2	8.50	1.41	1.25
1	O	156	LYS	CE-NZ	8.49	1.74	1.49
2	L	68	ARG	N-CA	8.29	1.56	1.46
1	O	210	ASN	C-O	8.25	1.33	1.24
2	D	66	VAL	CA-C	8.19	1.63	1.52
1	M	154	LEU	CG-CD1	8.01	1.78	1.52
1	M	159	SER	CB-OG	7.89	1.57	1.42
2	J	66	VAL	CA-C	7.86	1.62	1.52
1	O	128	SER	CB-OG	7.78	1.57	1.42
1	M	172	ASN	CG-ND2	7.78	1.49	1.33
2	D	68	ARG	N-CA	7.47	1.55	1.46
2	P	125	GLN	CG-CD	7.43	1.70	1.52
1	M	166	ARG	CZ-NH1	7.37	1.43	1.32
1	M	130	HIS	CD2-NE2	7.30	1.45	1.37
1	M	126	SER	CB-OG	7.24	1.56	1.42
2	P	125	GLN	CD-OE1	7.21	1.37	1.23
1	Q	130	HIS	CG-CD2	7.12	1.43	1.35
1	M	73	ASN	CG-OD1	7.11	1.37	1.23
1	O	158	ASN	CG-OD1	7.08	1.37	1.23
2	L	68	ARG	CA-C	6.95	1.61	1.52
2	R	150	GLU	CD-OE1	6.93	1.38	1.25
2	H	66	VAL	CA-C	6.93	1.61	1.52
2	H	68	ARG	N-CA	6.87	1.54	1.46
2	B	68	ARG	N-CA	6.86	1.54	1.46
1	M	130	HIS	ND1-CE1	-6.79	1.25	1.32
2	J	68	ARG	N-CA	6.77	1.54	1.46
2	B	66	VAL	N-CA	6.58	1.54	1.46
1	O	128	SER	C-N	6.51	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	66	VAL	CA-C	6.45	1.60	1.52
1	K	260	ILE	CA-CB	-6.36	1.46	1.54
2	F	66	VAL	N-CA	6.33	1.54	1.46
2	B	66	VAL	CA-C	6.33	1.60	1.52
2	R	116	LYS	CD-CE	6.33	1.71	1.52
1	M	186	ASN	CG-ND2	6.24	1.46	1.33
1	M	125	PRO	C-O	6.20	1.32	1.24
1	O	216	ARG	CZ-NH1	6.13	1.41	1.32
1	O	152	VAL	C-O	6.13	1.31	1.24
2	F	66	VAL	CA-C	6.09	1.60	1.52
1	O	10	GLY	N-CA	6.06	1.55	1.45
1	O	165	LYS	CD-CE	6.02	1.70	1.52
1	C	204	VAL	CA-CB	-5.93	1.47	1.54
2	N	66	VAL	CA-C	5.87	1.59	1.52
1	M	186	ASN	CG-OD1	5.83	1.34	1.23
2	H	66	VAL	N-CA	5.78	1.53	1.46
1	E	204	VAL	CA-CB	-5.76	1.47	1.54
2	L	66	VAL	N-CA	5.62	1.53	1.46
2	P	125	GLN	CB-CG	5.62	1.69	1.52
1	O	276	ASN	CG-ND2	5.46	1.44	1.33
2	N	11	GLU	CG-CD	5.44	1.65	1.52
2	J	66	VAL	N-CA	5.42	1.53	1.46
1	M	222	LYS	CE-NZ	5.41	1.65	1.49
1	O	186	ASN	CG-OD1	5.41	1.33	1.23
1	I	64	CYS	CA-C	-5.40	1.46	1.52
2	D	67	GLY	CA-C	5.39	1.57	1.51
1	M	137	SER	CB-OG	5.38	1.52	1.42
1	M	166	ARG	CZ-NH2	5.38	1.40	1.33
1	O	160	THR	CB-CG2	5.35	1.70	1.52
1	Q	126	SER	C-O	5.33	1.30	1.24
1	O	119	GLU	CD-OE2	5.31	1.35	1.25
1	O	130	HIS	C-O	5.29	1.30	1.23
1	K	235	THR	CA-C	-5.29	1.46	1.52
1	Q	302	ILE	CA-CB	5.28	1.60	1.54
1	Q	243	ILE	CA-CB	5.12	1.60	1.53
1	O	276	ASN	CG-OD1	5.08	1.33	1.23
2	P	65	ALA	CA-C	5.05	1.59	1.53
2	H	65	ALA	C-O	-5.04	1.20	1.24
1	C	252	ILE	CA-CB	-5.04	1.47	1.53
1	K	204	VAL	CA-CB	-5.02	1.48	1.54
1	O	219	THR	CB-CG2	5.02	1.69	1.52

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	66	VAL	N-CA-C	11.57	124.77	108.23
2	D	68	ARG	N-CA-C	11.33	128.74	108.69
2	B	68	ARG	N-CA-C	11.04	128.24	108.69
2	L	68	ARG	N-CA-C	11.00	127.61	109.24
2	H	68	ARG	N-CA-C	10.92	128.01	108.69
2	J	68	ARG	N-CA-C	10.68	127.21	109.06
2	F	68	ARG	N-CA-C	10.54	126.98	109.06
1	M	158	ASN	OD1-CG-ND2	10.34	132.94	122.60
1	O	157	LYS	CG-CD-CE	-10.24	87.74	111.30
2	N	38	LYS	CD-CE-NZ	-10.15	79.42	111.90
1	O	130	HIS	ND1-CE1-NE2	-9.20	99.20	108.40
2	N	68	ARG	N-CA-C	9.17	123.89	108.13
1	M	130	HIS	ND1-CG-CD2	9.08	115.18	106.10
2	J	66	VAL	N-CA-C	8.57	127.17	109.34
2	N	38	LYS	CG-CD-CE	-8.51	91.74	111.30
1	O	125(A)	LYS	CD-CE-NZ	-8.50	84.70	111.90
2	N	73	LEU	N-CA-C	-8.26	100.72	113.02
2	D	66	VAL	N-CA-C	8.17	126.34	109.34
2	P	143	LYS	CG-CD-CE	-8.10	92.67	111.30
1	O	125(B)	SER	CA-CB-OG	-7.95	95.20	111.10
2	P	125	GLN	CB-CG-CD	-7.95	99.09	112.60
1	Q	276	ASN	N-CA-C	7.93	121.14	110.35
2	B	66	VAL	N-CA-C	7.77	125.50	109.34
2	F	66	VAL	N-CA-C	7.77	125.50	109.34
2	H	66	VAL	N-CA-C	7.63	125.21	109.34
1	O	157	LYS	CB-CG-CD	-7.57	93.90	111.30
2	P	143	LYS	CD-CE-NZ	-7.47	87.98	111.90
2	L	66	VAL	N-CA-C	7.46	124.85	109.34
2	R	41	THR	N-CA-C	-7.42	103.49	112.54
1	M	130	HIS	CG-CD2-NE2	-7.29	99.91	107.20
1	Q	130	HIS	ND1-CG-CD2	7.22	113.32	106.10
2	R	33	GLY	N-CA-C	7.18	122.41	112.57
1	K	80	ILE	N-CA-C	-7.17	94.44	109.34
2	J	2	LEU	N-CA-C	7.12	120.08	111.82
2	N	136	GLY	N-CA-C	-7.11	105.03	115.63
1	M	130	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	E	124	ILE	CA-C-N	7.06	127.03	119.76
1	E	124	ILE	C-N-CA	7.06	127.03	119.76
1	O	42	ILE	N-CA-C	-7.02	106.46	113.20
1	I	248	ASN	N-CA-C	-6.95	105.33	113.88
1	G	124	ILE	CA-C-N	6.93	126.90	119.76
1	G	124	ILE	C-N-CA	6.93	126.90	119.76
1	O	211	GLN	N-CA-C	6.93	119.66	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	69	GLU	N-CA-C	6.90	119.93	110.06
2	P	66	VAL	N-CA-C	6.88	123.64	109.34
1	M	130	HIS	ND1-CE1-NE2	-6.81	101.59	108.40
1	M	154	LEU	CD1-CG-CD2	6.79	125.74	110.80
1	A	124	ILE	CA-C-N	6.65	127.01	119.83
1	A	124	ILE	C-N-CA	6.65	127.01	119.83
1	I	80	ILE	N-CA-C	-6.56	95.70	109.34
1	G	248	ASN	N-CA-C	-6.55	105.83	113.88
1	A	255	GLU	N-CA-C	-6.51	105.22	113.43
1	G	80	ILE	N-CA-C	-6.50	95.83	109.34
2	L	2	LEU	N-CA-C	6.46	119.14	111.71
2	F	2	LEU	N-CA-C	6.46	119.31	111.82
1	M	154	LEU	CB-CG-CD2	6.45	130.05	110.70
1	C	80	ILE	N-CA-C	-6.43	95.97	109.34
1	M	260	ILE	N-CA-C	6.38	117.01	108.27
2	P	68	ARG	N-CA-C	6.37	121.02	107.70
2	B	2	LEU	N-CA-C	6.34	119.00	111.71
2	L	69	GLU	N-CA-C	6.33	122.10	112.54
2	P	30	GLN	N-CA-C	-6.32	106.15	114.31
1	E	78	GLU	N-CA-C	-6.29	105.43	113.23
1	M	207	SER	N-CA-C	-6.29	106.25	114.04
1	K	248	ASN	N-CA-C	-6.27	106.17	113.88
1	A	80	ILE	N-CA-C	-6.26	96.31	109.34
1	M	172	ASN	OD1-CG-ND2	6.23	128.83	122.60
1	G	78	GLU	N-CA-C	-6.18	105.77	113.38
1	E	80	ILE	N-CA-C	-6.18	96.48	109.34
1	I	255	GLU	N-CA-C	-6.18	105.65	113.43
2	J	78	GLU	N-CA-C	-6.17	104.62	111.71
1	Q	94	VAL	N-CA-C	6.16	116.33	110.42
1	A	248	ASN	N-CA-C	-6.13	106.34	113.88
1	Q	273	GLU	N-CA-C	6.12	117.49	108.86
1	O	42	ILE	CB-CA-C	6.12	116.75	110.70
1	C	61	LEU	CA-C-N	-6.10	113.22	121.71
1	C	61	LEU	C-N-CA	-6.10	113.22	121.71
1	Q	95	ASN	N-CA-C	6.05	117.69	109.11
1	K	124	ILE	CA-C-N	5.96	126.26	119.83
1	K	124	ILE	C-N-CA	5.96	126.26	119.83
1	M	166	ARG	NE-CZ-NH2	-5.92	113.88	119.20
1	M	211	GLN	N-CA-C	5.90	118.11	108.55
1	Q	207	SER	N-CA-C	-5.90	105.17	112.72
2	F	77	ILE	N-CA-C	-5.89	105.34	111.58
1	O	84	TRP	N-CA-C	5.89	117.73	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	128	SER	O-C-N	5.88	130.52	122.46
1	M	305	CYS	CA-C-N	5.87	126.21	119.93
1	M	305	CYS	C-N-CA	5.87	126.21	119.93
2	P	65	ALA	N-CA-C	5.85	116.30	108.23
1	I	240	ASN	N-CA-C	5.84	120.27	113.20
1	Q	241	ASP	N-CA-C	5.80	118.35	110.35
1	G	235	THR	CB-CA-C	-5.78	99.83	111.17
1	G	255	GLU	N-CA-C	-5.75	106.19	113.43
1	O	184	HIS	CA-C-N	5.73	126.02	119.83
1	O	184	HIS	C-N-CA	5.73	126.02	119.83
1	O	169	ASN	N-CA-C	-5.72	101.57	110.10
2	N	38	LYS	CB-CG-CD	-5.72	98.14	111.30
2	R	69	GLU	N-CA-C	5.69	122.93	110.80
1	O	311	SER	N-CA-C	5.69	117.43	108.96
1	I	124	ILE	CA-C-N	5.68	125.97	119.83
1	I	124	ILE	C-N-CA	5.68	125.97	119.83
2	P	161	GLN	N-CA-C	5.67	119.81	113.01
1	C	235	THR	CB-CA-C	-5.66	100.08	111.17
1	C	248	ASN	N-CA-CB	-5.66	103.07	110.59
2	H	2	LEU	N-CA-C	5.66	118.38	111.82
2	H	69	GLU	N-CA-C	5.63	122.05	112.99
1	K	255	GLU	N-CA-C	-5.63	106.34	113.43
1	A	195	TYR	N-CA-C	-5.62	100.62	109.50
2	D	69	GLU	N-CA-C	5.61	122.05	113.19
1	Q	214	VAL	CA-C-N	5.59	125.35	119.76
1	Q	214	VAL	C-N-CA	5.59	125.35	119.76
1	O	297	ILE	N-CA-C	5.58	116.36	110.72
1	C	248	ASN	N-CA-C	-5.58	107.02	113.88
1	I	152	VAL	CB-CA-C	-5.56	102.41	110.63
1	O	206	THR	CB-CA-C	-5.55	106.48	114.87
2	D	2	LEU	N-CA-C	5.52	118.22	111.82
1	O	12	GLN	N-CA-C	5.50	117.76	109.23
1	E	248	ASN	N-CA-C	-5.44	107.19	113.88
1	C	202	ILE	CB-CA-C	-5.43	102.59	110.63
2	L	78	GLU	N-CA-C	-5.43	105.36	111.28
1	M	167	SER	N-CA-C	5.41	116.21	108.74
2	R	172	GLU	N-CA-C	-5.41	105.41	112.23
2	D	23	GLY	N-CA-C	5.39	118.41	110.80
2	R	68	ARG	N-CA-C	5.39	116.26	108.34
1	I	195	TYR	N-CA-C	-5.38	100.26	109.24
1	A	71	LEU	N-CA-C	-5.38	102.92	110.50
2	N	11	GLU	CB-CG-CD	-5.36	103.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	34	TYR	N-CA-C	5.36	116.67	107.28
1	K	240	ASN	N-CA-C	5.35	119.68	113.20
1	A	235	THR	CB-CA-C	-5.35	100.68	111.17
2	R	116	LYS	CG-CD-CE	-5.35	99.00	111.30
2	B	69	GLU	N-CA-C	5.34	121.59	112.99
1	O	158	ASN	OD1-CG-ND2	5.34	127.94	122.60
1	O	302	ILE	N-CA-C	-5.34	101.31	108.35
1	Q	62	ARG	N-CA-C	5.33	117.17	111.36
1	M	128	SER	N-CA-C	5.32	117.49	111.11
1	Q	73	ASN	CA-C-N	5.32	125.03	119.82
1	Q	73	ASN	C-N-CA	5.32	125.03	119.82
2	L	66	VAL	CA-C-N	5.30	129.53	122.75
2	L	66	VAL	C-N-CA	5.30	129.53	122.75
1	O	258	TYR	N-CA-C	5.28	117.26	108.02
1	O	35	VAL	N-CA-C	5.26	116.33	108.54
1	Q	209	LEU	N-CA-C	5.25	117.09	108.52
1	E	176	LEU	N-CA-C	5.24	117.99	109.24
1	C	230	MET	CA-C-N	-5.24	115.61	122.99
1	C	230	MET	C-N-CA	-5.24	115.61	122.99
1	O	266	THR	N-CA-C	5.23	115.96	108.74
2	N	124	LEU	N-CA-C	5.22	117.65	111.33
1	M	152	VAL	N-CA-C	5.22	115.82	108.36
1	O	157	LYS	CD-CE-NZ	-5.21	95.24	111.90
2	L	23	GLY	N-CA-C	5.20	118.13	110.80
1	O	209	LEU	N-CA-C	5.19	117.78	108.17
1	G	82	VAL	CB-CA-C	5.18	116.74	110.78
1	K	235	THR	CB-CA-C	-5.17	101.04	111.17
1	M	126	SER	N-CA-C	5.17	117.51	108.52
1	Q	168	TYR	N-CA-C	5.17	117.41	107.44
2	J	9	PHE	N-CA-C	5.14	116.89	111.28
1	I	235	THR	CB-CA-C	-5.13	101.08	110.62
1	O	186	ASN	N-CA-C	5.12	117.59	111.71
1	M	278	ASN	N-CA-C	5.11	117.74	108.69
1	I	78	GLU	N-CA-C	-5.10	106.91	113.23
1	E	271	GLU	N-CA-C	-5.06	106.80	113.17
1	I	292	MET	CA-C-N	-5.06	114.77	120.89
1	I	292	MET	C-N-CA	-5.06	114.77	120.89
1	M	106	GLU	N-CA-C	5.05	117.18	111.02
1	Q	128	SER	N-CA-C	5.03	117.50	111.71
2	H	77	ILE	N-CA-C	-5.01	106.27	111.58
1	I	152	VAL	N-CA-C	5.01	115.12	108.11
1	A	175	ASP	CA-C-N	-5.00	115.03	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	C-N-CA	-5.00	115.03	122.74

There are no chirality outliers.

All (38) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
2	P	61	THR	Peptide
1	Q	240	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2496	122	2
1	C	2553	0	2496	122	3
1	E	2553	0	2496	172	0
1	G	2553	0	2496	136	3
1	I	2553	0	2496	145	0
1	K	2553	0	2496	118	2
1	M	2553	0	2496	177	0
1	O	2553	0	2496	191	0
1	Q	2553	0	2498	139	0
2	B	1416	0	1320	51	0
2	D	1416	0	1320	45	0
2	F	1416	0	1320	73	0
2	H	1416	0	1320	63	0
2	J	1416	0	1320	44	0
2	L	1416	0	1320	40	0
2	N	1416	0	1320	80	0
2	P	1416	0	1320	86	0
2	R	1416	0	1320	86	0
3	S	28	0	25	1	0
3	U	28	0	25	1	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	Y	28	0	25	2	0
3	a	28	0	25	1	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	1	0
3	f	28	0	25	3	0
3	g	28	0	25	2	0
3	h	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	39	0	34	3	0
4	X	39	0	34	3	0
4	Z	39	0	34	0	0
All	All	36202	0	34773	1695	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1695) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:THR:HG21	1:G:250:ASN:OD1	1.49	1.09
1:E:182:ILE:HD12	1:E:202:ILE:HD13	1.34	1.08
1:I:200:THR:HG21	1:I:250:ASN:OD1	1.51	1.07
1:A:75:MET:HB2	1:A:95:ASN:ND2	1.69	1.07
2:P:143:LYS:CE	2:P:143:LYS:NZ	2.18	1.07
1:G:79:PHE:C	1:G:79:PHE:HD1	1.65	1.05
1:A:75:MET:HB2	1:A:95:ASN:HD22	1.21	1.04
1:A:200:THR:HG21	1:A:250:ASN:OD1	1.55	1.04
1:C:75:MET:HB2	1:C:95:ASN:ND2	1.73	1.04
1:I:75:MET:HB2	1:I:95:ASN:ND2	1.73	1.04
1:K:182:ILE:HD12	1:K:202:ILE:HD13	1.38	1.04
1:M:130:HIS:CG	1:M:130:HIS:CE1	2.40	1.04
1:G:182:ILE:HD11	1:G:213:LEU:HD12	1.40	1.03
1:A:79:PHE:HD1	1:A:79:PHE:C	1.68	1.02
1:G:75:MET:HB2	1:G:95:ASN:HD22	1.24	1.02
1:E:75:MET:HB2	1:E:95:ASN:HD22	1.23	1.01
1:I:79:PHE:HD1	1:I:79:PHE:C	1.70	1.00
1:C:200:THR:HG21	1:C:250:ASN:OD1	1.61	0.99
1:E:79:PHE:C	1:E:79:PHE:HD1	1.68	0.99
2:B:59:MET:O	2:B:61:THR:N	1.94	0.99
1:E:13:ILE:CD1	2:F:152:VAL:HG11	1.93	0.98
1:K:75:MET:HB2	1:K:95:ASN:ND2	1.79	0.98
2:P:59:MET:O	2:P:61:THR:N	1.95	0.98
2:R:165:GLU:O	2:R:169:LYS:HB3	1.64	0.98
1:Q:282:GLN:O	1:Q:301:THR:HB	1.64	0.98
1:C:283:THR:HB	1:C:286:GLY:O	1.64	0.97
2:F:59:MET:O	2:F:61:THR:N	1.97	0.97
1:I:283:THR:HB	1:I:286:GLY:O	1.64	0.97
1:C:75:MET:HB2	1:C:95:ASN:HD22	1.29	0.97
1:E:283:THR:HB	1:E:286:GLY:O	1.65	0.97
2:N:150:GLU:O	2:N:154:ASN:HB2	1.64	0.96
1:O:283:THR:HG22	1:O:285:MET:H	1.30	0.96
1:G:182:ILE:HD12	1:G:202:ILE:HD13	1.46	0.96
1:E:182:ILE:HD11	1:E:213:LEU:HD12	1.47	0.96
1:K:79:PHE:HD1	1:K:79:PHE:C	1.74	0.95
2:N:38:LYS:CE	2:N:38:LYS:NZ	2.29	0.95
1:I:182:ILE:HD11	1:I:213:LEU:HD12	1.46	0.95
1:A:182:ILE:HD12	1:A:202:ILE:HD13	1.49	0.95
1:E:11:ASP:OD2	2:F:143:LYS:HA	1.66	0.95
1:O:28:ILE:HD11	2:P:102:MET:HG3	1.47	0.94
1:C:182:ILE:HD12	1:C:202:ILE:HD13	1.44	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:ILE:HD12	1:I:202:ILE:HD13	1.47	0.94
1:I:75:MET:HB2	1:I:95:ASN:HD22	1.32	0.94
1:O:141:TYR:HB2	1:O:146:SER:HB3	1.46	0.94
1:C:79:PHE:HD1	1:C:79:PHE:C	1.76	0.94
1:O:251:PHE:CE1	1:O:253:ALA:HA	2.03	0.93
1:E:272:LEU:HD21	1:M:171:THR:HG21	1.51	0.93
1:G:283:THR:HB	1:G:286:GLY:O	1.69	0.93
1:M:27:THR:HG22	1:M:31:MET:H	1.31	0.93
1:G:275:GLY:O	1:G:277:CYS:HB3	1.69	0.92
1:K:275:GLY:O	1:K:277:CYS:HB3	1.69	0.92
2:J:59:MET:O	2:J:61:THR:N	2.02	0.92
1:Q:206:THR:CG2	1:Q:207:SER:H	1.83	0.92
1:C:182:ILE:HD11	1:C:213:LEU:HD12	1.52	0.92
2:R:30:GLN:HA	2:R:30:GLN:HE21	1.35	0.92
1:E:275:GLY:O	1:E:277:CYS:HB3	1.70	0.91
1:K:79:PHE:C	1:K:79:PHE:CD1	2.46	0.91
2:R:127:ARG:HB2	2:R:127:ARG:HH11	1.36	0.91
1:A:283:THR:HB	1:A:286:GLY:O	1.70	0.91
1:E:79:PHE:C	1:E:79:PHE:CD1	2.42	0.91
1:G:283:THR:HG22	1:G:285:MET:H	1.35	0.90
2:L:59:MET:O	2:L:61:THR:N	2.04	0.90
1:M:50:LYS:HD3	1:M:275:GLY:HA3	1.50	0.90
1:K:182:ILE:HD11	1:K:213:LEU:HD12	1.53	0.90
2:H:59:MET:O	2:H:61:THR:N	2.05	0.90
1:A:182:ILE:HD11	1:A:213:LEU:HD12	1.53	0.90
2:N:145:ASP:O	2:N:148:CYS:HB3	1.72	0.90
2:P:145:ASP:OD1	2:P:148:CYS:HB2	1.71	0.90
1:Q:206:THR:HG22	1:Q:207:SER:N	1.85	0.90
1:M:275:GLY:O	1:M:277:CYS:HB3	1.71	0.89
1:I:79:PHE:O	1:I:80:ILE:HD13	1.72	0.89
2:P:151:SER:HB2	2:P:157:TYR:HA	1.55	0.89
1:C:275:GLY:O	1:C:277:CYS:HB3	1.71	0.89
1:E:13:ILE:HD12	2:F:152:VAL:HG11	1.53	0.89
1:A:275:GLY:O	1:A:277:CYS:HB3	1.73	0.89
1:C:79:PHE:C	1:C:79:PHE:CD1	2.49	0.89
1:I:79:PHE:C	1:I:79:PHE:CD1	2.44	0.88
1:M:201:TYR:H	1:M:248:ASN:HB2	1.38	0.88
1:Q:16:GLY:HA3	2:R:14:TRP:HD1	1.39	0.87
1:O:157:LYS:CD	1:O:157:LYS:CB	2.53	0.87
1:G:79:PHE:C	1:G:79:PHE:CD1	2.39	0.87
1:A:79:PHE:C	1:A:79:PHE:CD1	2.42	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:O	1:A:196:GLN:HG3	1.74	0.86
1:I:283:THR:HG22	1:I:285:MET:H	1.40	0.86
2:H:63:PHE:N	2:H:63:PHE:HD1	1.73	0.86
2:D:59:MET:O	2:D:61:THR:N	2.09	0.85
1:M:200:THR:HA	1:M:248:ASN:HB3	1.57	0.85
1:K:283:THR:HB	1:K:286:GLY:O	1.75	0.84
1:O:135:VAL:HG22	1:O:146:SER:HA	1.58	0.84
1:C:124:ILE:HD11	1:C:254:PRO:O	1.77	0.84
1:I:275:GLY:O	1:I:277:CYS:HB3	1.76	0.84
1:E:283:THR:HG22	1:E:285:MET:H	1.43	0.84
1:M:114:ARG:HB2	1:M:265:SER:HB3	1.59	0.84
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.59	0.83
2:L:63:PHE:N	2:L:63:PHE:HD1	1.73	0.83
2:P:143:LYS:CE	2:P:143:LYS:CG	2.55	0.83
2:P:63:PHE:N	2:P:63:PHE:HD1	1.77	0.83
1:A:283:THR:HG22	1:A:285:MET:H	1.44	0.83
1:M:130:HIS:CE1	1:M:130:HIS:CD2	2.66	0.83
1:M:38:HIS:HB2	1:M:318:THR:HB	1.61	0.83
1:K:75:MET:HB2	1:K:95:ASN:HD22	1.42	0.82
1:K:283:THR:HG22	1:K:285:MET:H	1.44	0.82
1:M:154:LEU:CD1	1:M:154:LEU:CB	2.56	0.82
1:E:27:THR:HG22	1:E:31:MET:H	1.43	0.82
1:E:272:LEU:CD2	1:M:171:THR:HG21	2.10	0.82
1:G:288:ILE:HD11	1:G:297:ILE:HG13	1.60	0.82
2:N:144:CYS:SG	2:N:149:MET:HG3	2.20	0.81
1:E:79:PHE:CG	1:I:144:LYS:HE3	2.16	0.81
1:E:126:SER:HB2	1:E:166:ARG:HH22	1.45	0.81
1:Q:44:GLU:HB2	1:Q:294:PHE:O	1.81	0.81
2:H:63:PHE:N	2:H:63:PHE:CD1	2.45	0.80
1:C:79:PHE:O	1:C:80:ILE:HD13	1.82	0.80
2:J:63:PHE:N	2:J:63:PHE:HD1	1.78	0.80
2:H:61:THR:OG1	1:I:310:LYS:HD3	1.82	0.80
1:O:53(A):LEU:HD11	1:O:302:ILE:HG22	1.62	0.80
1:I:27:THR:HG22	1:I:31:MET:H	1.47	0.80
1:K:79:PHE:O	1:K:80:ILE:HD13	1.81	0.80
1:M:267:ILE:HD12	1:M:267:ILE:H	1.45	0.80
2:D:63:PHE:N	2:D:63:PHE:HD1	1.78	0.80
2:L:63:PHE:N	2:L:63:PHE:CD1	2.44	0.80
2:N:143:LYS:H	2:N:143:LYS:HD3	1.44	0.79
1:K:288:ILE:HD11	1:K:297:ILE:HG13	1.64	0.79
1:C:27:THR:HG22	1:C:31:MET:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:225:GLY:O	1:Q:226:GLN:HB2	1.83	0.79
2:F:63:PHE:N	2:F:63:PHE:HD1	1.80	0.79
1:K:27:THR:HG22	1:K:31:MET:H	1.44	0.79
1:K:126:SER:HB2	1:K:166:ARG:HH22	1.48	0.79
1:E:87:ILE:HD12	1:E:113:SER:HA	1.64	0.79
1:M:266:THR:HG21	2:N:67:GLY:H	1.47	0.78
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.64	0.78
2:R:95:ASN:O	2:R:99:LEU:HB2	1.84	0.78
1:A:288:ILE:HD11	1:A:297:ILE:HG13	1.66	0.78
1:Q:260:ILE:HG23	1:Q:262:LYS:HB3	1.64	0.78
1:C:283:THR:HG22	1:C:285:MET:H	1.49	0.78
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.65	0.78
1:M:265:SER:OG	1:M:266:THR:N	2.15	0.78
2:B:167:ARG:HD3	2:D:174:SER:HA	1.66	0.77
1:E:18:HIS:HB2	2:F:21:TRP:HA	1.65	0.77
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.66	0.77
1:K:179:LEU:HD23	1:K:234:TRP:HB3	1.65	0.77
2:P:63:PHE:N	2:P:63:PHE:CD1	2.48	0.77
1:A:121:ILE:HG22	1:A:123:ILE:HD13	1.64	0.77
1:C:288:ILE:HD11	1:C:297:ILE:HG13	1.66	0.77
1:G:27:THR:HG22	1:G:31:MET:H	1.48	0.77
1:K:141:TYR:CE2	1:K:142:GLN:NE2	2.29	0.77
1:O:238:LYS:HG3	1:O:239:PRO:HD2	1.65	0.77
2:D:63:PHE:N	2:D:63:PHE:CD1	2.50	0.76
1:E:11:ASP:HB2	2:F:140:PHE:HD1	1.51	0.76
1:I:59:LEU:HD11	1:I:80:ILE:HG23	1.67	0.76
2:N:132:GLU:O	2:N:134:GLY:N	2.18	0.76
2:D:167:ARG:HD3	2:F:174:SER:HA	1.67	0.76
1:O:307:LYS:HD2	2:P:92:TRP:CE2	2.21	0.76
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.67	0.75
1:A:282:GLN:HE21	1:A:283:THR:H	1.32	0.75
1:E:282:GLN:HE21	1:E:283:THR:H	1.34	0.75
1:I:79:PHE:O	1:I:79:PHE:CD1	2.39	0.75
1:M:283:THR:HG22	1:M:284:PRO:HD2	1.67	0.75
1:O:300:LEU:HD21	2:P:68:ARG:HH21	1.51	0.75
2:F:63:PHE:N	2:F:63:PHE:CD1	2.52	0.75
1:E:11:ASP:O	2:F:140:PHE:N	2.16	0.75
2:R:4:GLY:HA2	2:R:8:GLY:HA3	1.68	0.75
1:E:47:HIS:HE1	1:M:171:THR:O	1.69	0.75
1:O:293:PRO:HG2	1:O:294:PHE:CD1	2.22	0.75
1:C:181:GLY:C	1:C:182:ILE:HD13	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:PHE:CD1	1:G:79:PHE:O	2.39	0.74
1:K:13:ILE:HD11	2:L:149:MET:HG2	1.68	0.74
1:C:59:LEU:HD11	1:C:80:ILE:HG23	1.69	0.74
1:O:291:SER:HB2	1:O:292:MET:HE2	1.67	0.74
1:Q:16:GLY:HA3	2:R:14:TRP:CD1	2.20	0.74
2:H:65:ALA:C	2:H:66:VAL:HG13	2.11	0.74
2:P:59:MET:C	2:P:61:THR:H	1.95	0.74
1:C:124:ILE:CG1	1:C:254:PRO:O	2.35	0.74
1:G:206:THR:HG22	1:G:207:SER:N	2.02	0.74
1:M:201:TYR:H	1:M:248:ASN:CB	2.00	0.74
1:I:146:SER:OG	1:I:147:PHE:N	2.19	0.74
1:K:80:ILE:O	1:K:80:ILE:HG22	1.88	0.74
1:A:206:THR:HB	1:A:209:LEU:H	1.52	0.74
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.67	0.74
1:G:124:ILE:HD11	1:G:254:PRO:O	1.88	0.74
2:F:65:ALA:C	2:F:66:VAL:HG13	2.13	0.74
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.68	0.74
2:J:63:PHE:N	2:J:63:PHE:CD1	2.50	0.74
1:M:204:VAL:HA	1:M:244:ASN:O	1.88	0.73
1:O:206:THR:HB	1:O:208:THR:H	1.53	0.73
1:G:206:THR:HG22	1:G:208:THR:H	1.54	0.73
1:I:266:THR:HG21	2:J:67:GLY:H	1.53	0.73
2:B:63:PHE:N	2:B:63:PHE:HD1	1.87	0.73
2:P:37:ASP:O	2:P:41:THR:OG1	2.07	0.73
2:P:164:GLU:HA	2:P:167:ARG:HB2	1.69	0.73
1:I:179:LEU:HD23	1:I:234:TRP:HB3	1.70	0.73
1:C:182:ILE:HD13	1:C:182:ILE:N	2.02	0.73
4:T:2:NAG:H5	4:T:2:NAG:HN2	1.54	0.73
1:A:126:SER:HB2	1:A:166:ARG:HH22	1.54	0.73
3:S:1:NAG:H62	3:S:2:NAG:H2	1.70	0.73
1:C:124:ILE:CD1	1:C:254:PRO:O	2.37	0.72
1:E:11:ASP:CB	2:F:140:PHE:HD1	2.02	0.72
1:E:79:PHE:CD1	1:E:79:PHE:O	2.42	0.72
1:I:124:ILE:HD11	1:I:254:PRO:O	1.89	0.72
1:O:219:THR:HG22	1:O:220:ARG:H	1.54	0.72
2:P:25:HIS:HA	2:P:34:TYR:HB3	1.71	0.72
1:A:181:GLY:C	1:A:182:ILE:HD13	2.14	0.72
1:E:272:LEU:HD21	1:M:171:THR:CG2	2.20	0.72
2:R:30:GLN:HA	2:R:30:GLN:NE2	2.04	0.72
1:M:211:GLN:NE2	1:M:213:LEU:HD21	2.05	0.72
1:Q:104:ASP:HB2	1:Q:234:TRP:HE1	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:THR:HG21	1:G:287:ALA:HB1	1.72	0.72
1:C:279:THR:HG21	1:C:287:ALA:HB1	1.72	0.72
1:G:79:PHE:O	1:G:80:ILE:HD13	1.90	0.72
1:I:181:GLY:C	1:I:182:ILE:HD13	2.15	0.72
1:M:37:THR:HB	1:M:320:LEU:H	1.54	0.72
1:E:59:LEU:HD11	1:E:80:ILE:HG23	1.70	0.71
1:E:121:ILE:HG22	1:E:123:ILE:HD13	1.72	0.71
1:A:27:THR:HG22	1:A:31:MET:H	1.55	0.71
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.72	0.71
1:O:134:GLY:HA2	1:O:155:ILE:HD13	1.72	0.71
1:C:307:LYS:NZ	2:D:62:GLN:HB3	2.06	0.71
1:A:79:PHE:CD1	1:A:79:PHE:O	2.42	0.71
1:C:141:TYR:CE2	1:C:142:GLN:NE2	2.18	0.71
1:O:27:THR:HG22	1:O:31:MET:H	1.55	0.71
1:C:159:SER:O	1:C:196:GLN:HG3	1.91	0.71
1:O:200:THR:HG21	1:O:250:ASN:HB2	1.73	0.71
1:Q:56:VAL:O	1:Q:85:SER:OG	2.09	0.71
1:G:159:SER:O	1:G:196:GLN:HG3	1.91	0.71
1:O:27:THR:HB	1:O:32:GLU:HB2	1.73	0.71
1:E:75:MET:CB	1:E:95:ASN:ND2	2.52	0.70
1:I:159:SER:O	1:I:196:GLN:HG3	1.90	0.70
1:K:124:ILE:HD11	1:K:254:PRO:O	1.90	0.70
1:M:123:ILE:HG23	1:M:124:ILE:HG12	1.72	0.70
1:C:80:ILE:O	1:C:80:ILE:HG22	1.90	0.70
1:O:62:ARG:HD2	1:O:63:ASP:HB2	1.74	0.70
1:E:11:ASP:HB2	2:F:140:PHE:CD1	2.26	0.70
1:G:59:LEU:HD11	1:G:80:ILE:HG23	1.71	0.70
1:O:125(A):LYS:CE	1:O:125(A):LYS:CG	2.70	0.70
1:Q:87:ILE:HD11	1:Q:267:ILE:HA	1.73	0.70
1:M:200:THR:HA	1:M:248:ASN:CB	2.21	0.70
1:K:307:LYS:NZ	2:L:62:GLN:HB3	2.06	0.70
1:A:72:GLY:O	1:A:148:PHE:HA	1.92	0.70
1:A:206:THR:HG22	1:A:208:THR:H	1.56	0.70
1:C:126:SER:HB2	1:C:166:ARG:HH22	1.56	0.70
1:I:182:ILE:HD13	1:I:182:ILE:N	2.07	0.70
1:E:206:THR:HG22	1:E:207:SER:N	2.07	0.70
1:G:11:ASP:OD2	2:H:143:LYS:HA	1.92	0.70
1:O:223:VAL:O	1:O:224:ASN:HB2	1.91	0.70
1:C:206:THR:HG22	1:C:207:SER:N	2.06	0.70
1:E:206:THR:HB	1:E:209:LEU:H	1.57	0.70
1:K:159:SER:O	1:K:196:GLN:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD11	1:A:80:ILE:HG23	1.72	0.69
2:N:37:ASP:O	2:N:39:GLU:N	2.24	0.69
1:Q:181:GLY:O	1:Q:182:ILE:HD13	1.92	0.69
1:G:121:ILE:HG22	1:G:123:ILE:HD13	1.72	0.69
2:N:38:LYS:CD	2:N:38:LYS:CB	2.69	0.69
2:B:63:PHE:N	2:B:63:PHE:CD1	2.59	0.69
1:O:125(A):LYS:CD	1:O:125(A):LYS:NZ	2.56	0.69
1:Q:16:GLY:CA	2:R:14:TRP:HD1	2.04	0.69
1:G:206:THR:CG2	1:G:207:SER:N	2.55	0.69
1:M:202:ILE:HB	1:M:213:LEU:HD12	1.74	0.69
1:C:141:TYR:CD2	1:C:142:GLN:HG3	2.28	0.69
1:M:243:ILE:HG12	1:M:245:PHE:CE1	2.27	0.69
1:C:87:ILE:HD12	1:C:113:SER:HA	1.75	0.69
1:E:124:ILE:HD11	1:E:254:PRO:O	1.92	0.69
1:I:124:ILE:CG1	1:I:254:PRO:O	2.40	0.69
1:M:279:THR:HG21	1:M:287:ALA:HB1	1.73	0.69
1:I:282:GLN:HE21	1:I:283:THR:H	1.40	0.69
2:N:117:ASN:O	2:N:121:LYS:HG2	1.93	0.69
1:M:114:ARG:HH11	1:M:265:SER:HB2	1.59	0.68
1:A:206:THR:HG22	1:A:208:THR:N	2.09	0.68
1:A:206:THR:HG22	1:A:207:SER:N	2.08	0.68
1:I:206:THR:HG22	1:I:207:SER:N	2.08	0.68
1:O:291:SER:CB	1:O:292:MET:HE2	2.24	0.68
1:C:206:THR:CG2	1:C:207:SER:N	2.56	0.68
1:I:38:HIS:HB2	1:I:318:THR:HB	1.75	0.68
1:G:206:THR:HB	1:G:209:LEU:H	1.57	0.68
1:O:295:HIS:HD2	1:O:297:ILE:H	1.39	0.68
1:I:121:ILE:HG22	1:I:123:ILE:HD13	1.75	0.68
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.73	0.68
1:E:18:HIS:N	2:F:21:TRP:O	2.25	0.68
1:K:181:GLY:C	1:K:182:ILE:HD13	2.17	0.68
1:I:126:SER:HB2	1:I:166:ARG:HH22	1.59	0.68
1:Q:172:ASN:ND2	1:Q:259:LYS:HE2	2.09	0.68
1:G:72:GLY:O	1:G:148:PHE:HA	1.94	0.67
1:I:72:GLY:O	1:I:148:PHE:HA	1.94	0.67
1:A:75:MET:CB	1:A:95:ASN:ND2	2.54	0.67
1:A:124:ILE:HD13	1:A:254:PRO:HG2	1.76	0.67
1:A:229:ARG:HH21	1:E:207:SER:HA	1.59	0.67
1:E:307:LYS:NZ	2:F:62:GLN:HB3	2.08	0.67
1:G:13:ILE:CD1	2:H:152:VAL:HG11	2.24	0.67
1:E:124:ILE:HD13	1:E:254:PRO:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:202:ILE:HA	1:M:246:GLU:O	1.94	0.67
1:O:182:ILE:HG23	1:O:215:PRO:HB3	1.77	0.67
1:C:79:PHE:CD1	1:C:79:PHE:O	2.48	0.67
1:K:124:ILE:HD13	1:K:254:PRO:HG2	1.76	0.67
1:A:124:ILE:CG1	1:A:254:PRO:O	2.42	0.67
1:A:124:ILE:HD11	1:A:254:PRO:O	1.95	0.67
1:C:206:THR:HG22	1:C:208:THR:H	1.59	0.67
1:G:126:SER:HB2	1:G:166:ARG:HH22	1.60	0.67
1:K:59:LEU:HD11	1:K:80:ILE:HG23	1.76	0.67
1:O:211:GLN:NE2	1:O:213:LEU:HD11	2.09	0.67
1:E:126:SER:CB	1:E:166:ARG:HH22	2.06	0.66
1:I:27:THR:HG22	1:I:32:GLU:H	1.60	0.66
1:K:121:ILE:HG22	1:K:123:ILE:HD13	1.75	0.66
1:K:206:THR:HG22	1:K:207:SER:N	2.11	0.66
2:N:120:ASP:OD1	2:N:123:ARG:NH1	2.28	0.66
1:Q:14:CYS:O	2:R:24:TYR:HB3	1.95	0.66
1:K:282:GLN:HE21	1:K:283:THR:H	1.41	0.66
1:M:172:ASN:HD22	1:M:172:ASN:H	1.43	0.66
1:E:72:GLY:O	1:E:148:PHE:HA	1.95	0.66
1:I:206:THR:CG2	1:I:207:SER:N	2.58	0.66
1:G:266:THR:HG21	2:H:67:GLY:H	1.60	0.66
1:K:206:THR:CG2	1:K:207:SER:N	2.58	0.66
2:N:38:LYS:CE	2:N:38:LYS:CG	2.73	0.66
2:P:27:SER:HA	2:P:32:SER:HB2	1.76	0.66
2:N:59:MET:O	2:N:61:THR:N	2.29	0.66
1:C:72:GLY:O	1:C:148:PHE:HA	1.96	0.66
1:C:282:GLN:HE21	1:C:283:THR:H	1.42	0.66
1:I:206:THR:HB	1:I:209:LEU:H	1.61	0.66
2:P:63:PHE:HD1	2:P:63:PHE:H	1.43	0.66
1:K:279:THR:HG21	1:K:287:ALA:HB1	1.78	0.66
2:B:90:ASP:OD1	2:F:63:PHE:HE1	1.79	0.65
1:E:206:THR:CG2	1:E:207:SER:N	2.59	0.65
1:G:282:GLN:HE21	1:G:283:THR:H	1.42	0.65
1:K:206:THR:HG22	1:K:208:THR:N	2.11	0.65
2:N:166:ALA:HA	2:N:169:LYS:HB3	1.78	0.65
1:G:181:GLY:C	1:G:182:ILE:HD13	2.22	0.65
1:O:157:LYS:CG	1:O:157:LYS:CE	2.74	0.65
2:P:80:LEU:HD12	2:P:83:LYS:HE3	1.78	0.65
1:A:141:TYR:CE2	1:A:142:GLN:NE2	2.22	0.65
1:O:58:PRO:HB3	1:O:86:TYR:CE2	2.30	0.65
1:I:206:THR:HG22	1:I:208:THR:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:HIS:HB2	1:C:318:THR:HB	1.77	0.65
1:O:27:THR:HG23	2:P:105:GLU:HB2	1.79	0.65
4:T:2:NAG:H5	4:T:2:NAG:N2	2.08	0.65
1:G:75:MET:CB	1:G:95:ASN:ND2	2.55	0.65
1:G:206:THR:HG22	1:G:208:THR:N	2.10	0.65
2:R:166:ALA:HB1	2:R:170:ARG:HD3	1.78	0.65
1:E:79:PHE:O	1:E:80:ILE:HD13	1.96	0.65
1:K:186:ASN:HB3	1:K:190:GLU:OE2	1.97	0.65
1:O:123:ILE:N	1:O:255:GLU:O	2.27	0.65
2:P:65:ALA:C	2:P:66:VAL:HG13	2.22	0.65
1:A:27:THR:HG22	1:A:32:GLU:H	1.61	0.65
1:C:27:THR:HG22	1:C:32:GLU:H	1.62	0.65
1:I:206:THR:HG22	1:I:208:THR:N	2.12	0.65
1:M:277:CYS:SG	1:M:278:ASN:N	2.69	0.65
2:N:37:ASP:C	2:N:39:GLU:H	2.04	0.65
2:N:133:LEU:HB2	2:N:137:CYS:O	1.97	0.65
2:P:128:ASP:HB3	2:P:170:ARG:HH12	1.62	0.65
2:B:62:GLN:CD	2:B:62:GLN:N	2.51	0.65
1:E:126:SER:HB3	1:I:79:PHE:CZ	2.32	0.65
1:O:38:HIS:HD2	1:O:319:GLY:HA3	1.62	0.65
1:C:141:TYR:CE2	1:C:142:GLN:HG3	2.32	0.64
2:P:59:MET:C	2:P:61:THR:N	2.55	0.64
1:Q:200:THR:HG23	1:Q:249:GLY:H	1.62	0.64
1:A:275:GLY:O	1:A:277:CYS:CB	2.45	0.64
2:B:174:SER:HA	2:F:167:ARG:HD3	1.77	0.64
1:K:79:PHE:CD1	1:K:79:PHE:O	2.50	0.64
1:O:177:LEU:HD23	1:O:258:TYR:HD1	1.62	0.64
1:A:79:PHE:O	1:A:80:ILE:HD13	1.97	0.64
2:N:57:ASP:O	2:N:60:ASN:HB2	1.98	0.64
2:H:66:VAL:HG21	2:J:79:ASN:HD21	1.63	0.64
1:I:80:ILE:HG22	1:I:80:ILE:O	1.96	0.64
1:M:221:SER:O	1:M:229:ARG:NH2	2.29	0.64
1:A:12:GLN:HB2	2:B:27:SER:OG	1.98	0.64
2:N:63:PHE:CD1	2:N:63:PHE:N	2.62	0.64
2:P:133:LEU:HD21	2:P:139:GLU:HB2	1.78	0.64
1:A:206:THR:CG2	1:A:207:SER:N	2.61	0.64
1:M:123:ILE:HG22	1:M:255:GLU:C	2.23	0.64
2:N:151:SER:HB2	2:N:156:THR:O	1.98	0.64
1:Q:80:ILE:C	1:Q:82:VAL:H	2.06	0.64
1:Q:320:LEU:HD12	2:R:6:ILE:HG21	1.80	0.64
1:A:266:THR:HG21	2:B:67:GLY:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:ARG:O	2:H:68:ARG:HG3	1.96	0.64
1:Q:53(A):LEU:O	1:Q:278:ASN:HA	1.98	0.64
1:O:57:LYS:CD	1:O:57:LYS:H	2.11	0.64
1:Q:22:THR:CG2	1:Q:324:PRO:HD3	2.27	0.64
1:K:38:HIS:HB2	1:K:318:THR:HB	1.80	0.64
2:P:59:MET:CE	2:P:62:GLN:HG3	2.28	0.64
1:O:172:ASN:N	1:O:172:ASN:ND2	2.47	0.63
1:G:38:HIS:HB2	1:G:318:THR:HB	1.80	0.63
1:C:206:THR:HB	1:C:209:LEU:H	1.63	0.63
1:C:307:LYS:HZ1	2:D:62:GLN:HB3	1.61	0.63
1:I:79:PHE:O	1:I:80:ILE:CD1	2.46	0.63
2:D:62:GLN:N	2:D:62:GLN:CD	2.53	0.63
1:Q:104:ASP:CB	1:Q:234:TRP:HE1	2.11	0.63
1:E:171:THR:HB	1:I:121:ILE:HD13	1.81	0.63
1:K:182:ILE:HD13	1:K:182:ILE:N	2.12	0.63
1:E:47:HIS:CE1	1:M:171:THR:O	2.51	0.63
1:E:50:LYS:HZ2	1:M:121:ILE:HG23	1.63	0.63
1:E:266:THR:HG21	2:F:67:GLY:H	1.64	0.63
1:G:206:THR:HG23	1:G:241:ASP:OD2	1.99	0.63
1:M:172:ASN:HD22	1:M:172:ASN:N	1.97	0.63
1:K:141:TYR:CD2	1:K:142:GLN:HG3	2.32	0.63
1:O:38:HIS:HB2	1:O:318:THR:HB	1.81	0.63
1:C:206:THR:HG22	1:C:208:THR:N	2.14	0.62
1:M:228:GLY:O	1:M:229:ARG:NH1	2.32	0.62
1:E:38:HIS:HB2	1:E:318:THR:HB	1.81	0.62
1:O:102:PHE:HB3	1:O:105:TYR:HB2	1.81	0.62
1:O:214:VAL:O	1:O:216:ARG:HD3	2.00	0.62
2:F:62:GLN:CD	2:F:62:GLN:N	2.58	0.62
1:Q:11:ASP:HB2	2:R:140:PHE:HD1	1.65	0.62
1:I:182:ILE:HD11	1:I:213:LEU:CD1	2.28	0.62
1:K:126:SER:CB	1:K:166:ARG:HH22	2.11	0.62
1:K:201:TYR:CE2	1:K:248:ASN:HB2	2.34	0.62
1:M:114:ARG:NH1	1:M:265:SER:HB2	2.14	0.62
1:M:170:ASN:ND2	1:M:239:PRO:HA	2.14	0.62
2:H:63:PHE:HE1	2:J:90:ASP:OD1	1.81	0.62
1:I:27:THR:CG2	1:I:31:MET:H	2.12	0.62
1:O:313:ARG:HB3	1:O:315:VAL:HG23	1.81	0.62
1:Q:90:LYS:HD3	1:Q:270:SER:O	2.00	0.62
1:Q:63:ASP:HB3	1:Q:95:ASN:HD21	1.65	0.62
1:I:141:TYR:CD2	1:I:142:GLN:HG3	2.35	0.61
1:K:27:THR:HG22	1:K:32:GLU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:63:PHE:H	2:N:63:PHE:HD1	1.48	0.61
1:Q:316:LEU:HD13	2:R:100:VAL:HG22	1.82	0.61
1:C:124:ILE:HG12	1:C:254:PRO:O	2.00	0.61
1:E:206:THR:HG22	1:E:208:THR:N	2.14	0.61
1:K:141:TYR:CE2	1:K:142:GLN:HG3	2.35	0.61
1:K:307:LYS:HZ1	2:L:62:GLN:HB3	1.63	0.61
1:C:27:THR:CG2	1:C:31:MET:H	2.11	0.61
1:M:313:ARG:HD2	1:M:315:VAL:HG21	1.82	0.61
2:R:95:ASN:O	2:R:99:LEU:N	2.31	0.61
1:A:182:ILE:HD13	1:A:182:ILE:N	2.16	0.61
1:G:87:ILE:HD12	1:G:113:SER:HA	1.83	0.61
1:M:167:SER:HB2	1:M:243:ILE:O	2.00	0.61
1:M:182:ILE:CD1	1:M:202:ILE:HD13	2.30	0.61
1:G:170:ASN:O	1:G:239:PRO:O	2.18	0.61
2:N:63:PHE:N	2:N:63:PHE:HD1	1.99	0.61
1:K:206:THR:HG22	1:K:208:THR:H	1.66	0.61
1:A:38:HIS:HB2	1:A:318:THR:HB	1.83	0.61
1:E:15:ILE:HD13	2:F:119:TYR:HA	1.82	0.61
2:F:59:MET:C	2:F:61:THR:N	2.59	0.61
1:G:283:THR:HG22	1:G:285:MET:N	2.14	0.61
1:A:282:GLN:NE2	1:A:283:THR:H	1.97	0.61
1:C:206:THR:CG2	1:C:207:SER:H	2.14	0.61
1:E:117:HIS:CD2	1:I:125(B):SER:HB3	2.35	0.61
1:E:179:LEU:CD2	1:E:234:TRP:HB3	2.30	0.61
1:G:80:ILE:HG22	1:G:80:ILE:O	2.01	0.61
1:Q:127:TRP:HA	1:Q:127:TRP:CE3	2.35	0.61
1:G:11:ASP:HB2	2:H:140:PHE:HD1	1.66	0.61
1:M:171:THR:H	1:M:172:ASN:HD22	1.49	0.61
2:N:59:MET:HE3	2:N:62:GLN:HG3	1.81	0.61
1:O:172:ASN:H	1:O:172:ASN:HD22	1.49	0.61
2:R:145:ASP:O	2:R:148:CYS:HB3	2.00	0.61
1:E:27:THR:CG2	1:E:31:MET:H	2.12	0.60
2:N:164:GLU:HA	2:N:167:ARG:HB2	1.83	0.60
1:O:127:TRP:CZ3	1:O:154:LEU:HD11	2.36	0.60
1:E:320:LEU:HB3	2:F:111:HIS:CD2	2.34	0.60
1:G:179:LEU:CD2	1:G:234:TRP:HB3	2.31	0.60
2:J:167:ARG:HD3	2:L:174:SER:HA	1.83	0.60
1:C:79:PHE:O	1:C:80:ILE:CD1	2.49	0.60
1:M:123:ILE:HD13	1:M:257:ALA:HB3	1.83	0.60
1:Q:53:ASP:HB2	1:Q:276:ASN:ND2	2.16	0.60
1:E:141:TYR:CE2	1:E:142:GLN:NE2	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:ILE:CG1	1:G:254:PRO:O	2.49	0.60
1:K:72:GLY:O	1:K:148:PHE:HA	2.02	0.60
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.83	0.60
1:M:283:THR:HG22	1:M:284:PRO:CD	2.31	0.60
2:D:65:ALA:C	2:D:66:VAL:HG13	2.26	0.60
1:E:282:GLN:NE2	1:E:283:THR:H	1.98	0.60
1:G:79:PHE:HD1	1:G:79:PHE:O	1.79	0.60
1:K:182:ILE:HD11	1:K:213:LEU:CD1	2.30	0.60
1:A:230:MET:SD	1:A:252:ILE:HD11	2.42	0.60
1:E:146:SER:OG	1:E:147:PHE:N	2.26	0.60
1:I:124:ILE:CD1	1:I:254:PRO:O	2.49	0.60
1:O:172:ASN:N	1:O:172:ASN:HD22	1.99	0.60
1:O:177:LEU:HD23	1:O:258:TYR:CD1	2.36	0.60
1:A:80:ILE:C	1:A:82:VAL:H	2.10	0.60
1:A:310:LYS:HD3	2:F:61:THR:OG1	2.01	0.60
1:C:275:GLY:O	1:C:277:CYS:CB	2.48	0.60
1:G:121:ILE:HG13	1:G:259:LYS:HE3	1.84	0.60
1:G:124:ILE:CD1	1:G:254:PRO:O	2.50	0.60
1:G:141:TYR:CD2	1:G:142:GLN:HG3	2.36	0.60
2:L:59:MET:O	2:L:61:THR:C	2.45	0.60
1:O:283:THR:HB	1:O:286:GLY:O	2.02	0.60
1:A:268:MET:HE3	1:A:284:PRO:HA	1.84	0.60
1:E:206:THR:HG22	1:E:208:THR:H	1.67	0.60
1:Q:262:LYS:O	1:Q:262:LYS:HG3	2.02	0.60
1:G:59:LEU:HD11	1:G:80:ILE:CG2	2.32	0.60
1:M:152:VAL:HG23	1:M:255:GLU:HG3	1.82	0.60
2:D:81:ASN:HD22	2:F:80:LEU:HD13	1.66	0.59
2:R:164:GLU:HA	2:R:167:ARG:HD2	1.83	0.59
2:B:59:MET:C	2:B:61:THR:H	2.10	0.59
1:E:141:TYR:CD2	1:E:142:GLN:HG3	2.37	0.59
1:E:179:LEU:HD23	1:E:234:TRP:CB	2.32	0.59
1:G:307:LYS:NZ	2:H:62:GLN:HB3	2.17	0.59
1:M:15:ILE:HD12	1:M:15:ILE:H	1.68	0.59
1:M:172:ASN:N	1:M:172:ASN:ND2	2.49	0.59
1:G:27:THR:HG22	1:G:32:GLU:H	1.66	0.59
1:O:218:ALA:HB3	1:O:220:ARG:HH21	1.66	0.59
1:Q:147:PHE:CE1	1:Q:230:MET:HE3	2.37	0.59
1:E:159:SER:O	1:E:196:GLN:HG3	2.02	0.59
1:G:13:ILE:HD12	2:H:152:VAL:HG11	1.84	0.59
1:A:124:ILE:CD1	1:A:254:PRO:HG2	2.31	0.59
1:E:182:ILE:HD11	1:E:213:LEU:CD1	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:222:LYS:N	1:O:222:LYS:HD2	2.18	0.59
2:D:61:THR:OG1	1:E:310:LYS:HD3	2.02	0.59
1:K:206:THR:HB	1:K:209:LEU:H	1.66	0.59
1:M:313:ARG:HD2	1:M:315:VAL:CG2	2.33	0.59
1:O:184:HIS:HB2	1:O:220:ARG:HH12	1.67	0.59
1:O:222:LYS:HA	1:O:226:GLN:O	2.03	0.59
1:O:295:HIS:HD2	1:O:297:ILE:N	2.00	0.59
2:P:120:ASP:OD1	2:P:123:ARG:NH1	2.36	0.59
1:K:51:LEU:HD22	1:K:268:MET:HE1	1.83	0.59
2:N:159:TYR:N	2:N:160:PRO:HD2	2.18	0.59
1:M:101:ASP:HB3	1:M:231:GLU:HG3	1.84	0.59
2:R:93:THR:HG22	2:R:93:THR:O	2.03	0.59
1:G:51:LEU:HD22	1:G:268:MET:HE1	1.85	0.59
1:I:124:ILE:HD13	1:I:254:PRO:HG2	1.84	0.59
1:Q:260:ILE:O	1:Q:260:ILE:HG22	2.02	0.59
1:Q:320:LEU:HA	2:R:108:LEU:HD23	1.85	0.59
1:O:124:ILE:HD11	1:O:254:PRO:HG2	1.84	0.58
2:P:9:PHE:HD1	2:P:10:ILE:HG13	1.67	0.58
2:B:61:THR:OG1	1:C:310:LYS:HD3	2.04	0.58
1:G:80:ILE:C	1:G:82:VAL:H	2.12	0.58
1:M:161:TYR:CZ	1:M:249:GLY:HA2	2.39	0.58
1:O:146:SER:OG	1:O:147:PHE:N	2.32	0.58
2:P:29:GLU:H	2:P:29:GLU:CD	2.11	0.58
1:Q:53:ASP:HB2	1:Q:276:ASN:HD22	1.68	0.58
2:D:63:PHE:HE1	2:F:90:ASP:OD1	1.87	0.58
1:G:310:LYS:HD3	2:L:61:THR:OG1	2.02	0.58
1:M:27:THR:HG22	1:M:31:MET:N	2.10	0.58
1:O:15:ILE:HD11	2:P:122:VAL:HG21	1.84	0.58
1:Q:282:GLN:H	1:Q:302:ILE:HG22	1.67	0.58
2:B:59:MET:O	2:B:61:THR:C	2.46	0.58
1:E:18:HIS:CB	2:F:21:TRP:HA	2.33	0.58
1:G:275:GLY:O	1:G:277:CYS:CB	2.49	0.58
1:I:179:LEU:CD2	1:I:234:TRP:HB3	2.32	0.58
2:J:62:GLN:CD	2:J:62:GLN:N	2.61	0.58
1:C:266:THR:HG21	2:D:67:GLY:H	1.68	0.58
2:B:2:LEU:HB2	2:B:109:ASP:OD2	2.04	0.58
1:K:206:THR:HG23	1:K:241:ASP:OD2	2.04	0.58
1:M:27:THR:CG2	1:M:31:MET:H	2.11	0.58
1:A:126:SER:CB	1:A:166:ARG:HH22	2.16	0.58
2:D:59:MET:O	2:D:61:THR:O	2.22	0.58
1:A:87:ILE:HD12	1:A:113:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:24:TYR:CE1	2:P:153:ARG:HB3	2.39	0.58
1:Q:296:ASN:HB3	1:Q:309:VAL:O	2.03	0.58
1:K:74:PRO:HB3	1:K:141:TYR:HD1	1.69	0.58
1:M:169:ASN:HB3	1:M:171:THR:HG23	1.86	0.58
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.65	0.58
2:P:150:GLU:HA	2:P:153:ARG:CZ	2.33	0.58
1:Q:200:THR:HG21	1:Q:250:ASN:HB2	1.85	0.58
1:E:13:ILE:HD13	2:F:152:VAL:HG11	1.80	0.57
1:K:124:ILE:CG1	1:K:254:PRO:O	2.52	0.57
1:M:147:PHE:HZ	1:M:230:MET:HE3	1.68	0.57
1:C:124:ILE:HD13	1:C:254:PRO:HG2	1.86	0.57
1:E:81:ASN:HB2	1:I:144:LYS:NZ	2.19	0.57
2:L:2:LEU:HB2	2:L:109:ASP:OD2	2.04	0.57
2:B:59:MET:C	2:B:61:THR:N	2.60	0.57
1:G:11:ASP:O	2:H:140:PHE:N	2.30	0.57
1:M:114:ARG:HH11	1:M:265:SER:CB	2.17	0.57
1:M:293:PRO:HG2	1:M:294:PHE:CD1	2.39	0.57
1:A:141:TYR:CD2	1:A:142:GLN:HG3	2.39	0.57
1:G:75:MET:HB2	1:G:95:ASN:HD21	1.64	0.57
2:H:65:ALA:C	2:H:66:VAL:CG1	2.76	0.57
2:J:59:MET:C	2:J:61:THR:N	2.63	0.57
1:O:178:VAL:O	1:O:234:TRP:HA	2.04	0.57
2:P:128:ASP:CB	2:P:170:ARG:HH12	2.16	0.57
1:Q:74:PRO:HG3	1:Q:139:CYS:HB3	1.86	0.57
2:R:87:GLY:O	2:R:91:VAL:HG23	2.04	0.57
1:E:74:PRO:HB3	1:E:141:TYR:HD1	1.68	0.57
1:E:206:THR:CG2	1:E:207:SER:H	2.18	0.57
1:K:266:THR:HG21	2:L:67:GLY:H	1.69	0.57
1:M:125:PRO:HB2	1:M:126:SER:OG	2.05	0.57
1:Q:11:ASP:H	2:R:140:PHE:HB2	1.69	0.57
1:A:27:THR:CG2	1:A:31:MET:H	2.16	0.57
1:C:146:SER:OG	1:C:147:PHE:N	2.34	0.57
1:C:201:TYR:HE1	1:C:246:GLU:HG2	1.69	0.57
1:E:141:TYR:CE2	1:E:142:GLN:HG3	2.40	0.57
1:O:141:TYR:HB2	1:O:146:SER:CB	2.27	0.57
2:F:59:MET:O	2:F:61:THR:C	2.48	0.57
1:K:316:LEU:HD23	2:L:52:VAL:HG22	1.86	0.57
2:D:59:MET:O	2:D:61:THR:C	2.48	0.57
1:G:42:ILE:O	1:G:292:MET:HB3	2.05	0.57
1:G:206:THR:CG2	1:G:207:SER:H	2.17	0.57
1:O:124:ILE:HG21	1:O:166:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:LEU:HD23	1:G:234:TRP:CB	2.33	0.57
1:K:27:THR:CG2	1:K:31:MET:H	2.13	0.57
2:B:65:ALA:C	2:B:66:VAL:HG13	2.30	0.57
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.05	0.57
1:E:59:LEU:HD11	1:E:80:ILE:CG2	2.35	0.57
1:E:268:MET:HE3	1:E:284:PRO:HA	1.87	0.57
2:J:59:MET:C	2:J:61:THR:H	2.13	0.57
1:M:320:LEU:H	1:M:320:LEU:HD23	1.69	0.57
2:P:38:LYS:NZ	2:P:38:LYS:CD	2.68	0.57
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.87	0.57
1:C:126:SER:CB	1:C:166:ARG:HH22	2.18	0.56
1:M:90:LYS:O	1:M:269:LYS:HD3	2.04	0.56
1:O:87:ILE:HD11	1:O:112:LEU:O	2.04	0.56
2:D:2:LEU:HB2	2:D:109:ASP:OD2	2.05	0.56
2:B:68:ARG:HG3	2:B:68:ARG:O	2.05	0.56
2:J:2:LEU:HB2	2:J:109:ASP:OD2	2.05	0.56
2:L:59:MET:O	2:L:61:THR:O	2.22	0.56
2:L:151:SER:HA	2:L:154:ASN:HB2	1.88	0.56
1:M:59:LEU:HD11	1:M:80:ILE:HG21	1.86	0.56
1:M:144:LYS:HD2	1:M:145:SER:OG	2.05	0.56
2:N:109:ASP:HA	2:N:112:ASP:HB2	1.87	0.56
1:O:24:GLN:HE22	3:g:1:NAG:H61	1.71	0.56
2:P:79:ASN:ND2	2:P:83:LYS:HE2	2.20	0.56
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.45	0.56
1:A:186:ASN:HB3	1:A:190:GLU:OE2	2.06	0.56
1:C:262:LYS:NZ	1:C:264(A):ASP:OD1	2.33	0.56
2:H:151:SER:HA	2:H:154:ASN:HB2	1.88	0.56
2:N:38:LYS:CD	2:N:38:LYS:NZ	2.69	0.56
1:O:87:ILE:HD12	1:O:113:SER:HA	1.86	0.56
1:O:266:THR:HG21	2:P:67:GLY:H	1.70	0.56
1:Q:13:ILE:HD13	2:R:152:VAL:HG11	1.87	0.56
2:R:63:PHE:N	2:R:63:PHE:CD1	2.73	0.56
1:C:186:ASN:HB3	1:C:190:GLU:OE2	2.06	0.56
1:E:307:LYS:HZ1	2:F:62:GLN:HB3	1.68	0.56
1:O:151:VAL:HG23	1:O:254:PRO:HA	1.88	0.56
1:E:121:ILE:HG13	1:E:259:LYS:HE3	1.86	0.56
1:G:182:ILE:HD11	1:G:213:LEU:CD1	2.27	0.56
1:I:282:GLN:NE2	1:I:283:THR:H	2.02	0.56
1:M:266:THR:CG2	1:M:302:ILE:HD11	2.36	0.56
2:P:82:LYS:O	2:P:83:LYS:C	2.49	0.56
1:Q:251:PHE:CE2	1:Q:253:ALA:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:CD1	1:A:254:PRO:O	2.54	0.56
1:E:27:THR:HG22	1:E:32:GLU:H	1.71	0.56
1:I:121:ILE:HG13	1:I:259:LYS:HE3	1.87	0.56
1:K:282:GLN:NE2	1:K:283:THR:H	2.04	0.56
2:L:59:MET:C	2:L:61:THR:N	2.64	0.56
1:O:291:SER:HB2	1:O:292:MET:CE	2.35	0.56
1:E:80:ILE:C	1:E:82:VAL:H	2.13	0.56
1:G:141:TYR:CE2	1:G:142:GLN:HG3	2.41	0.56
1:I:75:MET:HB2	1:I:95:ASN:HD21	1.68	0.56
1:I:126:SER:CB	1:I:166:ARG:HH22	2.18	0.56
1:I:141:TYR:CE2	1:I:142:GLN:NE2	2.21	0.56
1:K:75:MET:HB2	1:K:95:ASN:HD21	1.68	0.56
1:M:220:ARG:O	1:M:222:LYS:NZ	2.32	0.56
2:B:79:ASN:HD21	2:F:66:VAL:HG21	1.70	0.56
1:G:268:MET:HE3	1:G:284:PRO:HA	1.88	0.56
1:K:307:LYS:HG3	2:L:59:MET:SD	2.46	0.56
1:O:307:LYS:HD2	2:P:92:TRP:CZ2	2.41	0.56
1:Q:155:ILE:HG12	1:Q:194:LEU:HD22	1.88	0.56
1:C:170:ASN:O	1:C:239:PRO:O	2.24	0.55
1:E:14:CYS:O	2:F:24:TYR:HA	2.06	0.55
2:F:59:MET:C	2:F:61:THR:H	2.14	0.55
1:G:207:SER:HA	1:I:229:ARG:HH21	1.72	0.55
2:H:59:MET:O	2:H:61:THR:O	2.23	0.55
1:K:275:GLY:O	1:K:277:CYS:CB	2.50	0.55
1:M:212:ARG:O	1:M:213:LEU:HD23	2.06	0.55
1:O:204:VAL:HG12	1:O:205:GLY:N	2.21	0.55
1:C:295:HIS:HD2	1:C:297:ILE:H	1.52	0.55
1:E:79:PHE:HD1	1:E:79:PHE:O	1.81	0.55
1:E:80:ILE:O	1:E:80:ILE:HG22	2.06	0.55
1:E:124:ILE:CD1	1:E:254:PRO:HG2	2.36	0.55
1:G:282:GLN:NE2	1:G:283:THR:H	2.04	0.55
1:I:141:TYR:CE2	1:I:142:GLN:HG3	2.41	0.55
1:I:206:THR:HG23	1:I:241:ASP:OD2	2.07	0.55
2:F:65:ALA:C	2:F:66:VAL:CG1	2.78	0.55
2:H:59:MET:C	2:H:61:THR:N	2.64	0.55
1:Q:98:TYR:CD2	1:Q:230:MET:HB2	2.41	0.55
1:Q:301:THR:OG1	1:Q:305:CYS:SG	2.61	0.55
1:C:121:ILE:HG22	1:C:123:ILE:HD13	1.86	0.55
1:E:272:LEU:HD21	1:M:171:THR:CB	2.37	0.55
1:G:27:THR:CG2	1:G:31:MET:H	2.16	0.55
2:J:66:VAL:HG21	2:L:79:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:65:ALA:C	2:L:66:VAL:HG13	2.32	0.55
1:M:19:ALA:HB1	1:M:322:ASN:ND2	2.21	0.55
1:G:120:LYS:HG3	1:G:258:TYR:CE2	2.42	0.55
1:I:206:THR:CG2	1:I:207:SER:H	2.18	0.55
1:K:124:ILE:CD1	1:K:254:PRO:HG2	2.36	0.55
3:f:1:NAG:O6	3:f:2:NAG:N2	2.40	0.55
1:C:121:ILE:HG13	1:C:259:LYS:HE3	1.88	0.55
1:G:106:GLU:OE2	2:H:71:ASN:HB3	2.07	0.55
1:G:126:SER:CB	1:G:166:ARG:HH22	2.19	0.55
2:H:80:LEU:HD13	2:L:81:ASN:HD22	1.71	0.55
1:Q:293:PRO:HB2	1:Q:294:PHE:CD1	2.42	0.55
2:H:59:MET:O	2:H:61:THR:C	2.49	0.55
2:J:59:MET:O	2:J:61:THR:C	2.50	0.55
1:K:295:HIS:HD2	1:K:297:ILE:H	1.53	0.55
1:O:141:TYR:CB	1:O:146:SER:HB3	2.31	0.55
2:P:23:GLY:HA2	2:P:36:ALA:HA	1.89	0.55
1:Q:127:TRP:HA	1:Q:127:TRP:HE3	1.72	0.55
2:R:127:ARG:NH1	2:R:159:TYR:OH	2.40	0.55
2:B:80:LEU:HD13	2:F:81:ASN:HD22	1.71	0.55
2:J:65:ALA:C	2:J:66:VAL:HG13	2.32	0.55
1:M:283:THR:CG2	1:M:298:HIS:HB3	2.37	0.55
1:A:11:ASP:OD1	2:B:28:ASN:HA	2.07	0.55
1:E:124:ILE:CG1	1:E:254:PRO:O	2.55	0.55
2:F:68:ARG:HG3	2:F:68:ARG:O	2.06	0.55
1:G:79:PHE:O	1:G:80:ILE:CD1	2.55	0.55
1:A:141:TYR:CE2	1:A:142:GLN:HG3	2.42	0.54
1:E:15:ILE:HG23	2:F:118:LEU:HD23	1.90	0.54
1:I:74:PRO:HB3	1:I:141:TYR:HD1	1.71	0.54
1:O:125(B):SER:OG	1:O:125(B):SER:CA	2.53	0.54
2:R:14:TRP:HB3	2:R:34:TYR:HE2	1.72	0.54
2:R:94:TYR:O	2:R:98:LEU:HB2	2.07	0.54
1:G:123:ILE:HD11	1:G:168:TYR:CZ	2.42	0.54
1:G:141:TYR:CE2	1:G:142:GLN:NE2	2.20	0.54
1:G:320:LEU:HB3	2:H:111:HIS:CD2	2.43	0.54
1:O:71:LEU:H	1:O:71:LEU:HD23	1.72	0.54
1:I:27:THR:HG22	1:I:32:GLU:N	2.22	0.54
1:I:106:GLU:OE2	2:J:71:ASN:HB3	2.08	0.54
1:I:216:ARG:O	1:I:220:ARG:NH2	2.41	0.54
2:J:59:MET:O	2:J:61:THR:O	2.25	0.54
2:N:159:TYR:OH	2:N:167:ARG:NH2	2.40	0.54
2:N:166:ALA:C	2:N:168:LEU:H	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:LEU:CD2	1:K:234:TRP:HB3	2.35	0.54
1:O:206:THR:HG22	1:O:241:ASP:OD2	2.07	0.54
2:P:65:ALA:C	2:P:66:VAL:CG1	2.80	0.54
1:Q:55:GLY:HA2	4:X:3:BMA:H62	1.88	0.54
1:C:27:THR:HG22	1:C:32:GLU:N	2.23	0.54
1:O:211:GLN:HE22	1:O:213:LEU:HD11	1.72	0.54
2:P:9:PHE:CD1	2:P:10:ILE:HG13	2.42	0.54
2:R:52:VAL:HA	2:R:55:ILE:HD12	1.89	0.54
1:M:212:ARG:C	1:M:213:LEU:HD23	2.32	0.54
1:O:135:VAL:CG2	1:O:146:SER:HA	2.32	0.54
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.07	0.54
1:K:124:ILE:CD1	1:K:254:PRO:O	2.55	0.54
1:Q:109:LYS:HE3	1:Q:267:ILE:HG12	1.90	0.54
2:R:165:GLU:O	2:R:169:LYS:CB	2.49	0.54
1:A:124:ILE:HG12	1:A:254:PRO:O	2.07	0.54
2:N:141:TYR:HB3	2:N:169:LYS:HG2	1.88	0.54
2:D:59:MET:C	2:D:61:THR:N	2.66	0.54
1:M:320:LEU:HD23	1:M:320:LEU:N	2.22	0.54
1:O:125(B):SER:OG	1:O:125(B):SER:N	2.40	0.54
1:O:209:LEU:HD12	1:O:211:GLN:HB3	1.90	0.54
1:O:238:LYS:HG3	1:O:239:PRO:CD	2.36	0.54
2:B:151:SER:HA	2:B:154:ASN:HB2	1.90	0.54
1:E:42:ILE:O	1:E:292:MET:HB3	2.07	0.54
1:G:124:ILE:HD13	1:G:254:PRO:HG2	1.89	0.54
1:M:267:ILE:HD12	1:M:267:ILE:N	2.20	0.54
1:Q:121:ILE:HD11	1:Q:259:LYS:HE3	1.90	0.54
1:E:124:ILE:CD1	1:E:254:PRO:O	2.56	0.53
2:F:151:SER:HA	2:F:154:ASN:HB2	1.89	0.53
1:I:78:GLU:O	1:I:80:ILE:N	2.40	0.53
1:M:37:THR:HB	1:M:320:LEU:N	2.21	0.53
1:M:295:HIS:CE1	1:M:308:TYR:HB2	2.43	0.53
1:Q:223:VAL:C	1:Q:225:GLY:H	2.15	0.53
1:E:206:THR:HB	1:E:209:LEU:HB3	1.90	0.53
2:J:61:THR:OG1	1:K:310:LYS:HD3	2.07	0.53
2:P:52:VAL:O	2:P:55:ILE:HG22	2.08	0.53
1:Q:320:LEU:HD12	2:R:6:ILE:CG2	2.38	0.53
1:C:59:LEU:HD11	1:C:80:ILE:CG2	2.36	0.53
2:F:2:LEU:HB2	2:F:109:ASP:OD2	2.07	0.53
1:M:141:TYR:HB3	1:M:146:SER:HB2	1.90	0.53
1:O:53(A):LEU:HD11	1:O:302:ILE:CG2	2.35	0.53
2:P:94:TYR:O	2:P:95:ASN:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:90:LYS:O	1:Q:92:ASN:N	2.42	0.53
2:R:100:VAL:O	2:R:104:ASN:HB2	2.09	0.53
1:A:106:GLU:OE2	2:B:71:ASN:HB3	2.08	0.53
1:C:282:GLN:NE2	1:C:283:THR:H	2.06	0.53
1:G:182:ILE:HD13	1:G:182:ILE:N	2.23	0.53
1:I:59:LEU:HD11	1:I:80:ILE:CG2	2.36	0.53
1:A:42:ILE:O	1:A:292:MET:HB3	2.08	0.53
1:A:146:SER:OG	1:A:147:PHE:N	2.41	0.53
2:D:151:SER:HA	2:D:154:ASN:HB2	1.90	0.53
1:E:79:PHE:O	1:E:80:ILE:CD1	2.56	0.53
1:E:164:ILE:O	1:E:246:GLU:HA	2.07	0.53
1:G:181:GLY:O	1:G:182:ILE:HD13	2.08	0.53
1:I:309:VAL:HG22	2:J:93:THR:HA	1.91	0.53
2:P:153:ARG:O	2:P:155:GLY:N	2.41	0.53
1:A:121:ILE:HG13	1:A:259:LYS:HE3	1.89	0.53
1:C:75:MET:CB	1:C:95:ASN:ND2	2.61	0.53
1:G:18:HIS:HB2	2:H:21:TRP:HA	1.91	0.53
1:G:279:THR:HB	1:G:281:CYS:H	1.74	0.53
2:H:117:ASN:HD21	2:J:4:GLY:N	2.05	0.53
1:M:152:VAL:CG2	1:M:255:GLU:HG3	2.39	0.53
1:M:191:GLN:HE21	1:M:195:TYR:HB2	1.74	0.53
1:O:18:HIS:HB2	2:P:21:TRP:HA	1.90	0.53
1:Q:190:GLU:HA	1:Q:193:LYS:HB2	1.90	0.53
1:G:124:ILE:CG1	1:G:124:ILE:O	2.56	0.53
1:M:312:ASN:N	1:M:312:ASN:ND2	2.57	0.53
1:Q:78:GLU:O	1:Q:78:GLU:HG2	2.09	0.53
1:Q:260:ILE:O	1:Q:260:ILE:CG2	2.57	0.53
2:R:59:MET:HE3	2:R:92:TRP:CZ3	2.43	0.53
1:G:146:SER:OG	1:G:147:PHE:N	2.41	0.53
1:K:206:THR:CG2	1:K:207:SER:H	2.21	0.53
1:A:59:LEU:HD11	1:A:80:ILE:CG2	2.37	0.53
2:H:62:GLN:CD	2:H:62:GLN:N	2.67	0.53
1:K:283:THR:HG22	1:K:285:MET:N	2.18	0.53
1:Q:22:THR:HG21	1:Q:324:PRO:HD3	1.89	0.53
1:A:279:THR:HB	1:A:281:CYS:H	1.73	0.53
1:C:74:PRO:HB3	1:C:141:TYR:HD1	1.73	0.53
1:C:201:TYR:CE2	1:C:248:ASN:HB2	2.44	0.53
1:E:238:LYS:O	1:E:239:PRO:C	2.50	0.53
2:H:79:ASN:HD21	2:L:66:VAL:HG21	1.74	0.53
2:J:151:SER:HA	2:J:154:ASN:HB2	1.91	0.53
1:M:156:LYS:O	1:M:156:LYS:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:ILE:HD11	1:M:202:ILE:HD13	1.90	0.53
1:O:200:THR:HG21	1:O:250:ASN:CB	2.39	0.53
1:O:309:VAL:HG22	2:P:93:THR:HA	1.91	0.53
2:P:153:ARG:O	2:P:154:ASN:C	2.52	0.53
1:I:24:GLN:OE1	3:a:1:NAG:H61	2.08	0.52
1:O:57:LYS:H	1:O:57:LYS:HD2	1.73	0.52
2:R:63:PHE:N	2:R:63:PHE:HD1	2.07	0.52
2:R:144:CYS:SG	2:R:149:MET:HG3	2.49	0.52
1:A:206:THR:CG2	1:A:207:SER:H	2.22	0.52
1:E:216:ARG:O	1:E:220:ARG:NH2	2.42	0.52
1:M:156:LYS:HB3	1:M:161:TYR:HB2	1.90	0.52
2:N:71:ASN:C	2:N:71:ASN:OD1	2.52	0.52
1:O:157:LYS:CD	1:O:157:LYS:HB3	2.37	0.52
1:Q:16:GLY:CA	2:R:14:TRP:CD1	2.88	0.52
2:B:47:GLY:O	1:C:31:MET:HG2	2.09	0.52
1:E:181:GLY:C	1:E:182:ILE:HD13	2.35	0.52
2:L:68:ARG:HG3	2:L:68:ARG:O	2.08	0.52
1:I:279:THR:HB	1:I:281:CYS:H	1.73	0.52
1:O:151:VAL:HG22	1:O:252:ILE:HG22	1.90	0.52
1:E:13:ILE:HD11	2:F:149:MET:HG2	1.91	0.52
1:I:42:ILE:O	1:I:292:MET:HB3	2.10	0.52
2:N:68:ARG:HG3	2:N:68:ARG:O	2.09	0.52
1:O:74:PRO:HG2	1:O:139:CYS:HB3	1.92	0.52
1:O:143:GLY:O	1:O:144:LYS:C	2.51	0.52
1:Q:44:GLU:OE1	1:Q:292:MET:HB2	2.09	0.52
1:A:51:LEU:HD22	1:A:268:MET:HE1	1.90	0.52
2:B:59:MET:O	2:B:61:THR:O	2.26	0.52
1:E:11:ASP:OD2	2:F:143:LYS:CA	2.48	0.52
2:H:51:LYS:HA	1:I:28:ILE:O	2.09	0.52
1:K:58:PRO:HB3	1:K:86:TYR:CZ	2.44	0.52
1:O:140:PRO:O	1:O:141:TYR:C	2.51	0.52
1:I:298:HIS:ND1	1:I:299:PRO:HD2	2.25	0.52
1:Q:82:VAL:C	1:Q:83:GLU:H	2.17	0.52
1:C:80:ILE:O	1:C:80:ILE:CG2	2.58	0.52
1:G:13:ILE:HD11	2:H:149:MET:HG2	1.91	0.52
2:J:81:ASN:HD22	2:L:80:LEU:HD13	1.75	0.52
2:P:150:GLU:C	2:P:154:ASN:HB2	2.34	0.52
1:Q:25:VAL:HG13	1:Q:26:ASP:N	2.23	0.52
2:R:84:MET:HE3	2:R:88:PHE:CD1	2.45	0.52
1:C:10:GLY:HA3	2:D:139:GLU:OE2	2.09	0.52
2:D:66:VAL:HG21	2:F:79:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:TYR:HE1	1:K:246:GLU:HG2	1.75	0.52
1:M:297:ILE:O	1:M:298:HIS:HB2	2.10	0.52
1:A:170:ASN:O	1:A:239:PRO:O	2.28	0.52
1:E:122:GLN:OE1	1:I:77:ASP:HB2	2.09	0.52
1:G:74:PRO:HB3	1:G:141:TYR:HD1	1.75	0.52
1:O:220:ARG:HG2	1:O:229:ARG:NH2	2.25	0.52
1:O:228:GLY:O	1:O:229:ARG:NH1	2.42	0.52
2:P:59:MET:HE1	2:P:62:GLN:HG3	1.90	0.52
2:H:2:LEU:HB2	2:H:109:ASP:OD2	2.10	0.51
1:I:170:ASN:O	1:I:239:PRO:O	2.28	0.51
1:K:115:ILE:HG21	1:K:118:PHE:HB2	1.92	0.51
1:M:176:LEU:HD23	1:M:237:LEU:HD23	1.91	0.51
2:P:149:MET:HA	2:P:152:VAL:CG2	2.40	0.51
2:B:63:PHE:HE1	2:D:90:ASP:OD1	1.93	0.51
1:E:279:THR:CG2	1:E:287:ALA:HB1	2.38	0.51
1:I:283:THR:HG22	1:I:285:MET:N	2.18	0.51
1:K:42:ILE:O	1:K:292:MET:HB3	2.10	0.51
2:L:59:MET:C	2:L:61:THR:H	2.19	0.51
2:N:24:TYR:CE1	2:N:153:ARG:HG2	2.45	0.51
1:O:123:ILE:HG23	1:O:124:ILE:HG12	1.91	0.51
1:Q:22:THR:HG22	1:Q:324:PRO:HD3	1.90	0.51
2:R:42:GLN:HA	2:R:45:ILE:HD12	1.92	0.51
1:C:42:ILE:O	1:C:292:MET:HB3	2.10	0.51
1:M:295:HIS:HD2	1:M:297:ILE:HG12	1.75	0.51
1:M:321:ARG:HB3	1:M:321:ARG:HH11	1.75	0.51
1:Q:147:PHE:HE1	1:Q:230:MET:HE3	1.73	0.51
1:A:200:THR:HG22	1:A:215:PRO:CD	2.40	0.51
1:I:72:GLY:HA3	1:I:149:ARG:HB2	1.91	0.51
1:I:164:ILE:O	1:I:246:GLU:HA	2.10	0.51
1:K:179:LEU:HD23	1:K:234:TRP:CB	2.36	0.51
1:Q:123:ILE:HG12	1:Q:257:ALA:HB3	1.92	0.51
1:A:27:THR:HG22	1:A:32:GLU:N	2.24	0.51
1:A:164:ILE:O	1:A:246:GLU:HA	2.11	0.51
2:B:62:GLN:CD	2:B:62:GLN:H	2.18	0.51
1:C:279:THR:HB	1:C:281:CYS:H	1.75	0.51
1:M:200:THR:HA	1:M:248:ASN:CG	2.36	0.51
1:M:200:THR:HG21	1:M:250:ASN:HB2	1.93	0.51
1:O:200:THR:HG21	1:O:250:ASN:OD1	2.10	0.51
1:Q:91:ALA:HA	1:Q:269:LYS:HD2	1.93	0.51
1:E:81:ASN:HB2	1:I:144:LYS:HZ2	1.76	0.51
1:E:122:GLN:HE22	1:I:77:ASP:CB	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:THR:HB	1:E:281:CYS:H	1.75	0.51
1:I:10:GLY:HA3	2:J:139:GLU:OE2	2.10	0.51
1:M:70:LEU:HD13	1:M:179:LEU:HD11	1.92	0.51
1:M:192:THR:HG23	1:M:196:GLN:HA	1.92	0.51
1:G:72:GLY:HA3	1:G:149:ARG:HB2	1.92	0.51
2:H:68:ARG:HB2	2:H:68:ARG:HH11	1.76	0.51
1:M:156:LYS:HG2	1:M:196:GLN:HG2	1.93	0.51
2:N:27:SER:HA	2:N:32:SER:HB3	1.92	0.51
1:Q:182:ILE:HD11	1:Q:202:ILE:HG21	1.93	0.51
1:Q:225:GLY:O	1:Q:226:GLN:CB	2.57	0.51
2:J:68:ARG:O	2:J:68:ARG:HG3	2.10	0.51
1:K:80:ILE:O	1:K:80:ILE:CG2	2.58	0.51
1:O:52:CYS:HA	1:O:277:CYS:HB3	1.93	0.51
1:I:124:ILE:HG12	1:I:254:PRO:O	2.09	0.51
1:Q:182:ILE:HD11	1:Q:202:ILE:HG12	1.92	0.51
2:D:62:GLN:CD	2:D:62:GLN:H	2.17	0.51
1:M:16:GLY:HA3	2:N:14:TRP:NE1	2.26	0.51
2:N:59:MET:O	2:N:61:THR:C	2.54	0.51
1:A:238:LYS:HG3	1:A:239:PRO:HD2	1.92	0.50
1:C:238:LYS:HG3	1:C:239:PRO:HD2	1.93	0.50
1:E:124:ILE:CG1	1:E:124:ILE:O	2.58	0.50
1:G:295:HIS:HD2	1:G:297:ILE:H	1.58	0.50
2:H:59:MET:C	2:H:61:THR:H	2.19	0.50
1:I:49:GLY:HA2	1:I:285:MET:O	2.11	0.50
1:K:87:ILE:HD12	1:K:113:SER:HA	1.92	0.50
1:M:182:ILE:HD12	1:M:202:ILE:HD13	1.93	0.50
1:M:283:THR:CG2	1:M:284:PRO:HD2	2.40	0.50
3:U:1:NAG:O3	3:U:1:NAG:C7	2.60	0.50
1:A:79:PHE:O	1:A:80:ILE:CD1	2.59	0.50
1:C:51:LEU:HD22	1:C:268:MET:HE1	1.93	0.50
1:C:216:ARG:O	1:C:220:ARG:NH2	2.44	0.50
1:E:238:LYS:HG3	1:E:239:PRO:HD2	1.93	0.50
2:F:59:MET:O	2:F:61:THR:O	2.29	0.50
1:K:238:LYS:HG3	1:K:239:PRO:HD2	1.93	0.50
1:M:125(A):LYS:O	1:M:125(B):SER:C	2.53	0.50
2:N:158:ASP:OD1	2:N:161:GLN:HG3	2.11	0.50
1:O:156:LYS:NZ	1:O:156:LYS:CD	2.69	0.50
2:P:150:GLU:HA	2:P:153:ARG:NH1	2.26	0.50
2:R:47:GLY:O	2:R:51:LYS:HB3	2.11	0.50
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.46	0.50
1:C:276:ASN:O	1:C:277:CYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.46	0.50
1:E:283:THR:HG22	1:E:285:MET:N	2.19	0.50
1:G:124:ILE:HG12	1:G:254:PRO:O	2.11	0.50
1:I:51:LEU:HD22	1:I:268:MET:HE1	1.93	0.50
1:I:146:SER:HG	1:I:147:PHE:H	1.59	0.50
1:M:275:GLY:O	1:M:276:ASN:C	2.53	0.50
1:E:11:ASP:H	2:F:140:PHE:HB2	1.76	0.50
1:E:298:HIS:ND1	1:E:299:PRO:HD2	2.26	0.50
2:F:125:GLN:HG2	2:F:157:TYR:HB3	1.94	0.50
1:G:45:LYS:HE2	1:G:312:ASN:O	2.12	0.50
1:I:179:LEU:HD23	1:I:234:TRP:CB	2.38	0.50
2:J:59:MET:HE3	2:J:62:GLN:HG3	1.93	0.50
1:O:74:PRO:HB3	1:O:141:TYR:HA	1.94	0.50
2:P:140:PHE:C	2:P:142:HIS:H	2.20	0.50
1:Q:92:ASN:ND2	1:Q:92:ASN:O	2.45	0.50
1:G:216:ARG:HG2	1:K:212:ARG:HB2	1.92	0.50
1:I:282:GLN:HG3	1:I:283:THR:N	2.25	0.50
1:O:226:GLN:HE22	1:O:228:GLY:H	1.59	0.50
1:O:292:MET:HB3	1:O:293:PRO:CD	2.41	0.50
2:P:34:TYR:N	2:P:34:TYR:CD1	2.79	0.50
1:A:283:THR:HG22	1:A:285:MET:N	2.19	0.50
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.47	0.50
1:E:27:THR:HG22	1:E:31:MET:N	2.19	0.50
1:O:232:PHE:N	1:O:232:PHE:CD1	2.78	0.50
1:O:320:LEU:N	1:O:320:LEU:HD23	2.27	0.50
2:D:68:ARG:HG3	2:D:68:ARG:O	2.11	0.50
2:J:63:PHE:HE1	2:L:90:ASP:OD1	1.94	0.50
1:M:124:ILE:O	1:M:125:PRO:C	2.54	0.50
1:O:23:GLU:O	1:O:35(A):THR:HA	2.12	0.50
3:f:2:NAG:H3	3:f:2:NAG:H83	1.92	0.50
1:A:179:LEU:CD2	1:A:234:TRP:HB3	2.40	0.50
1:E:114:ARG:HH11	1:E:265:SER:HB3	1.77	0.50
2:J:38:LYS:O	2:J:42:GLN:HB2	2.12	0.50
1:K:216:ARG:O	1:K:220:ARG:NH2	2.45	0.50
1:O:189:ALA:O	1:O:193:LYS:N	2.36	0.50
1:C:283:THR:HG22	1:C:285:MET:N	2.22	0.50
1:I:201:TYR:HE1	1:I:246:GLU:HG2	1.76	0.50
1:I:279:THR:CG2	1:I:287:ALA:HB1	2.38	0.50
1:M:179:LEU:O	1:M:254:PRO:HB3	2.12	0.50
2:N:68:ARG:HA	2:N:69:GLU:OE1	2.11	0.50
1:O:52:CYS:SG	1:O:287:ALA:HB2	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:68:GLY:O	1:O:71:LEU:O	2.29	0.50
1:O:190:GLU:C	1:O:192:THR:H	2.20	0.50
1:O:195:TYR:CZ	1:O:250:ASN:HA	2.47	0.50
1:O:295:HIS:CD2	1:O:297:ILE:H	2.26	0.50
2:R:171:GLU:HA	2:R:174:SER:HB3	1.93	0.50
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.48	0.49
1:E:81:ASN:H	1:I:144:LYS:HZ2	1.59	0.49
1:E:182:ILE:CD1	1:E:202:ILE:HD13	2.24	0.49
1:I:80:ILE:C	1:I:82:VAL:H	2.20	0.49
2:J:125:GLN:HG2	2:J:157:TYR:HB3	1.94	0.49
1:K:79:PHE:O	1:K:80:ILE:CD1	2.54	0.49
1:K:164:ILE:O	1:K:246:GLU:HA	2.12	0.49
2:N:65:ALA:C	2:N:66:VAL:CG1	2.85	0.49
2:N:166:ALA:C	2:N:168:LEU:N	2.70	0.49
2:R:30:GLN:HE21	2:R:30:GLN:CA	2.17	0.49
1:O:37:THR:OG1	1:O:320:LEU:N	2.45	0.49
1:A:201:TYR:HE1	1:A:246:GLU:HG2	1.77	0.49
1:E:72:GLY:HA3	1:E:149:ARG:HB2	1.94	0.49
1:E:206:THR:HG23	1:E:241:ASP:OD2	2.13	0.49
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.49
1:M:295:HIS:CD2	1:M:297:ILE:H	2.29	0.49
1:O:37:THR:HG1	1:O:320:LEU:H	1.60	0.49
1:A:307:LYS:HD2	2:B:92:TRP:CE2	2.47	0.49
2:D:59:MET:C	2:D:61:THR:H	2.20	0.49
2:L:62:GLN:N	2:L:62:GLN:CD	2.68	0.49
1:Q:267:ILE:H	1:Q:267:ILE:HD12	1.78	0.49
3:Y:1:NAG:H62	3:Y:2:NAG:HN2	1.78	0.49
1:C:75:MET:HB2	1:C:95:ASN:HD21	1.71	0.49
1:E:45:LYS:HE2	1:E:312:ASN:O	2.12	0.49
1:E:321:ARG:HD2	2:F:6:ILE:HD12	1.94	0.49
1:O:120:LYS:HE3	1:O:258:TYR:HE2	1.77	0.49
1:O:157:LYS:O	1:O:159:SER:N	2.46	0.49
2:P:150:GLU:O	2:P:154:ASN:HB2	2.12	0.49
1:Q:223:VAL:C	1:Q:225:GLY:N	2.70	0.49
1:Q:234:TRP:HZ3	1:Q:236:ILE:HG13	1.78	0.49
1:I:307:LYS:NZ	2:J:62:GLN:HB3	2.28	0.49
2:N:37:ASP:C	2:N:39:GLU:N	2.70	0.49
1:Q:37:THR:HB	1:Q:319:GLY:HA3	1.95	0.49
1:Q:98:TYR:HD2	1:Q:230:MET:HB2	1.77	0.49
2:R:38:LYS:O	2:R:42:GLN:HG2	2.12	0.49
1:E:170:ASN:O	1:E:239:PRO:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:ARG:HB2	2:H:68:ARG:NH1	2.28	0.49
1:I:27:THR:HG22	1:I:31:MET:N	2.22	0.49
1:K:146:SER:OG	1:K:147:PHE:N	2.27	0.49
1:M:139:CYS:O	1:M:146:SER:O	2.31	0.49
1:O:94:VAL:HG12	1:O:95:ASN:OD1	2.12	0.49
1:A:201:TYR:CE2	1:A:248:ASN:HB2	2.47	0.49
1:E:200:THR:HG22	1:E:215:PRO:CD	2.42	0.49
1:E:201:TYR:CE2	1:E:248:ASN:HB2	2.48	0.49
1:E:295:HIS:HD2	1:E:297:ILE:H	1.60	0.49
2:H:38:LYS:O	2:H:42:GLN:HB2	2.13	0.49
1:I:268:MET:HE3	1:I:284:PRO:HA	1.94	0.49
1:K:121:ILE:HG13	1:K:259:LYS:HE3	1.93	0.49
2:P:19:ASP:HB2	2:P:36:ALA:HB2	1.95	0.49
1:Q:316:LEU:HD12	2:R:104:ASN:OD1	2.13	0.49
1:A:74:PRO:HB3	1:A:141:TYR:HD1	1.77	0.49
1:A:143:GLY:HA3	1:Q:285:MET:HG2	1.94	0.49
1:C:179:LEU:HD23	1:C:234:TRP:CB	2.39	0.49
1:G:58:PRO:HB3	1:G:86:TYR:CZ	2.48	0.49
1:K:45:LYS:HE2	1:K:312:ASN:O	2.12	0.49
1:O:279:THR:OG1	1:O:287:ALA:HB1	2.12	0.49
1:Q:53:ASP:HA	1:Q:58:PRO:HD3	1.95	0.49
1:Q:222:LYS:HG2	1:Q:227:SER:HB2	1.95	0.49
1:G:238:LYS:HG3	1:G:239:PRO:HD2	1.94	0.49
1:I:45:LYS:HE2	1:I:312:ASN:O	2.13	0.49
1:I:201:TYR:CE2	1:I:248:ASN:HB2	2.48	0.49
1:M:307:LYS:NZ	2:N:59:MET:HE1	2.27	0.49
1:Q:200:THR:HG21	1:Q:250:ASN:N	2.27	0.49
2:B:117:ASN:HD21	2:D:4:GLY:N	2.11	0.48
1:E:79:PHE:O	1:E:80:ILE:CG1	2.61	0.48
1:E:304:GLU:HG2	2:F:63:PHE:HA	1.95	0.48
1:K:298:HIS:ND1	1:K:299:PRO:HD2	2.28	0.48
1:O:123:ILE:HD12	1:O:123:ILE:HA	1.68	0.48
1:Q:27:THR:CG2	1:Q:28:ILE:N	2.76	0.48
1:Q:82:VAL:O	1:Q:83:GLU:N	2.33	0.48
1:A:27:THR:HG22	1:A:31:MET:N	2.26	0.48
1:E:122:GLN:OE1	1:E:125:PRO:HB3	2.13	0.48
1:E:275:GLY:O	1:E:277:CYS:CB	2.52	0.48
1:Q:109:LYS:NZ	1:Q:267:ILE:HG21	2.28	0.48
1:A:13:ILE:HD11	2:B:149:MET:HG2	1.95	0.48
2:J:28:ASN:HD22	2:J:28:ASN:H	1.62	0.48
1:M:202:ILE:H	1:M:213:LEU:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:MET:CB	1:E:95:ASN:HD21	2.24	0.48
2:H:90:ASP:OD1	2:L:63:PHE:HE1	1.95	0.48
1:I:12:GLN:HB2	2:J:27:SER:OG	2.12	0.48
2:L:63:PHE:HD1	2:L:63:PHE:H	1.57	0.48
1:O:164:ILE:O	1:O:246:GLU:HA	2.14	0.48
1:Q:116:ASN:O	1:Q:117:HIS:HB2	2.12	0.48
1:Q:168:TYR:O	1:Q:242:ALA:HA	2.13	0.48
1:Q:200:THR:HA	1:Q:248:ASN:HB3	1.95	0.48
1:A:120:LYS:HG3	1:A:258:TYR:CE2	2.48	0.48
1:C:179:LEU:CD2	1:C:234:TRP:HB3	2.40	0.48
2:D:28:ASN:HD22	2:D:28:ASN:H	1.61	0.48
1:G:87:ILE:HB	1:G:267:ILE:HG13	1.96	0.48
1:I:206:THR:HB	1:I:209:LEU:HB3	1.95	0.48
1:O:169:ASN:HB3	1:O:171:THR:HG23	1.96	0.48
3:g:1:NAG:H62	3:g:2:NAG:HN2	1.79	0.48
1:E:126:SER:CB	1:I:79:PHE:CZ	2.77	0.48
1:G:279:THR:CG2	1:G:287:ALA:HB1	2.42	0.48
1:I:238:LYS:HG3	1:I:239:PRO:HD2	1.96	0.48
1:M:230:MET:HG2	1:M:232:PHE:CZ	2.49	0.48
2:N:46:ASP:O	2:N:50:ASN:HB2	2.14	0.48
2:N:150:GLU:O	2:N:154:ASN:CB	2.51	0.48
1:O:23:GLU:HA	1:O:23:GLU:OE2	2.14	0.48
1:A:45:LYS:HE2	1:A:312:ASN:O	2.13	0.48
2:D:63:PHE:HD1	2:D:63:PHE:H	1.60	0.48
1:E:51:LEU:HD22	1:E:268:MET:HE1	1.95	0.48
1:Q:55:GLY:C	4:X:3:BMA:O4	2.57	0.48
2:R:14:TRP:HB3	2:R:34:TYR:CE2	2.49	0.48
1:A:143:GLY:O	1:Q:272:LEU:HG	2.14	0.48
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.28	0.48
1:I:58:PRO:HB3	1:I:86:TYR:CZ	2.48	0.48
1:K:124:ILE:CG1	1:K:124:ILE:O	2.62	0.48
1:M:147:PHE:CZ	1:M:230:MET:HE3	2.49	0.48
1:Q:53(A):LEU:HG	1:Q:282:GLN:HB2	1.96	0.48
1:Q:220:ARG:NH1	1:Q:228:GLY:HA2	2.28	0.48
2:H:62:GLN:C	2:H:63:PHE:HD1	2.22	0.48
2:H:81:ASN:HD22	2:J:80:LEU:HD13	1.79	0.48
1:I:123:ILE:HD11	1:I:168:TYR:CZ	2.48	0.48
2:R:166:ALA:O	2:R:170:ARG:HB2	2.13	0.48
1:A:304:GLU:HG2	2:B:63:PHE:HA	1.95	0.47
2:N:123:ARG:HG3	2:N:138:PHE:HZ	1.78	0.47
2:P:72:ASN:HB2	2:P:75:ARG:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:155:GLY:C	2:R:157:TYR:H	2.22	0.47
1:A:80:ILE:HG22	1:A:80:ILE:O	2.14	0.47
2:B:28:ASN:HD22	2:B:28:ASN:H	1.62	0.47
2:B:68:ARG:HH11	2:B:68:ARG:HB2	1.78	0.47
2:F:59:MET:HE3	2:F:62:GLN:HG3	1.95	0.47
1:G:136:SER:O	1:G:145:SER:HB2	2.13	0.47
1:O:206:THR:HB	1:O:208:THR:N	2.24	0.47
2:B:90:ASP:OD1	2:F:63:PHE:CE1	2.62	0.47
1:C:309:VAL:HG22	2:D:93:THR:HA	1.96	0.47
1:K:170:ASN:O	1:K:239:PRO:O	2.32	0.47
2:N:131:LYS:C	2:N:133:LEU:H	2.21	0.47
2:P:2:LEU:HB2	2:P:109:ASP:OD2	2.14	0.47
2:P:9:PHE:HD1	2:P:10:ILE:N	2.12	0.47
1:Q:11:ASP:HB2	2:R:140:PHE:CD1	2.48	0.47
1:Q:247:SER:OG	1:Q:251:PHE:HB2	2.13	0.47
2:R:59:MET:HE2	2:R:59:MET:O	2.13	0.47
1:M:60:ILE:HG23	1:M:88:VAL:HB	1.97	0.47
1:O:201:TYR:CE2	1:O:248:ASN:ND2	2.82	0.47
1:O:316:LEU:HD13	2:P:100:VAL:HG22	1.97	0.47
1:Q:292:MET:HB3	1:Q:293:PRO:HD2	1.96	0.47
2:R:24:TYR:CE2	2:R:153:ARG:HG2	2.50	0.47
2:R:169:LYS:HG3	2:R:169:LYS:O	2.14	0.47
2:H:125:GLN:HG2	2:H:157:TYR:HB3	1.96	0.47
1:I:42:ILE:HD13	1:I:42:ILE:HA	1.68	0.47
1:K:27:THR:HG22	1:K:31:MET:N	2.21	0.47
1:M:307:LYS:HA	1:M:307:LYS:HD3	1.56	0.47
1:O:226:GLN:NE2	1:O:228:GLY:H	2.11	0.47
1:A:174:GLU:N	1:A:174:GLU:OE2	2.45	0.47
2:B:125:GLN:HG2	2:B:157:TYR:HB3	1.95	0.47
1:C:62:ARG:H	1:C:62:ARG:HD3	1.80	0.47
1:G:114:ARG:HH11	1:G:265:SER:HB3	1.79	0.47
2:P:149:MET:HA	2:P:152:VAL:HG23	1.97	0.47
2:B:68:ARG:HB2	2:B:68:ARG:NH1	2.30	0.47
2:B:81:ASN:HD22	2:D:80:LEU:HD13	1.79	0.47
1:C:12:GLN:HB2	2:D:27:SER:OG	2.15	0.47
2:D:123:ARG:HD2	2:D:132:GLU:OE1	2.15	0.47
1:E:49:GLY:HA2	1:E:285:MET:O	2.15	0.47
1:I:307:LYS:HD2	2:J:92:TRP:CE2	2.49	0.47
1:I:316:LEU:HD13	2:J:100:VAL:HG22	1.95	0.47
1:K:27:THR:HG22	1:K:32:GLU:N	2.29	0.47
1:K:123:ILE:HA	1:K:123:ILE:HD12	1.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:MET:HE3	2:L:62:GLN:HG3	1.96	0.47
1:M:154:LEU:HD12	1:M:251:PHE:HB3	1.97	0.47
1:O:64:CYS:SG	1:O:95:ASN:HB2	2.54	0.47
1:O:124:ILE:HD12	1:O:127:TRP:HZ2	1.80	0.47
2:R:28:ASN:HB3	2:R:31:GLY:CA	2.45	0.47
2:R:169:LYS:O	2:R:169:LYS:CG	2.62	0.47
2:B:38:LYS:O	2:B:42:GLN:HB2	2.14	0.47
1:C:45:LYS:HE2	1:C:312:ASN:O	2.14	0.47
1:E:123:ILE:HD11	1:E:168:TYR:CZ	2.49	0.47
1:K:72:GLY:HA3	1:K:149:ARG:H	1.79	0.47
1:K:279:THR:HB	1:K:281:CYS:H	1.80	0.47
2:P:59:MET:HE3	2:P:62:GLN:HG3	1.97	0.47
1:A:59:LEU:CD1	1:A:80:ILE:HG23	2.42	0.47
1:O:220:ARG:HH11	1:O:229:ARG:HG2	1.79	0.47
1:Q:312:ASN:OD1	1:Q:312:ASN:N	2.47	0.47
1:C:72:GLY:HA3	1:C:149:ARG:HB2	1.97	0.47
1:O:47:HIS:HB3	1:O:297:ILE:CD1	2.45	0.47
2:P:41:THR:O	2:P:45:ILE:HG13	2.14	0.47
1:Q:18:HIS:CE1	2:R:18:VAL:HA	2.50	0.47
1:A:216:ARG:O	1:A:220:ARG:NH2	2.48	0.46
1:E:137:SER:HA	1:E:145:SER:HB2	1.97	0.46
1:G:159:SER:C	1:G:196:GLN:HG3	2.40	0.46
2:L:28:ASN:HD22	2:L:28:ASN:H	1.63	0.46
1:M:172:ASN:OD1	1:M:259:LYS:HD3	2.15	0.46
1:M:236:ILE:H	1:M:236:ILE:HD12	1.80	0.46
1:O:36:VAL:HG12	1:O:38:HIS:H	1.78	0.46
1:O:134:GLY:CA	1:O:155:ILE:HD13	2.45	0.46
3:Y:1:NAG:H62	3:Y:2:NAG:N2	2.30	0.46
1:A:230:MET:SD	1:A:252:ILE:CD1	3.02	0.46
1:C:123:ILE:HA	1:C:123:ILE:HD12	1.32	0.46
1:C:181:GLY:O	1:C:182:ILE:HD13	2.15	0.46
1:C:279:THR:CG2	1:C:287:ALA:HB1	2.41	0.46
1:E:27:THR:HG22	1:E:32:GLU:N	2.30	0.46
2:N:30:GLN:HE22	2:N:145:ASP:HB2	1.80	0.46
1:O:27:THR:HG22	1:O:28:ILE:N	2.31	0.46
1:O:60:ILE:CD1	1:O:274:TYR:HB2	2.45	0.46
1:O:124:ILE:HD12	1:O:127:TRP:CZ2	2.51	0.46
1:O:279:THR:HG21	1:O:287:ALA:HB1	1.97	0.46
2:P:169:LYS:HA	2:P:172:GLU:HB2	1.97	0.46
1:Q:262:LYS:O	1:Q:262:LYS:CG	2.63	0.46
1:A:238:LYS:O	1:A:239:PRO:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:THR:HG22	1:C:31:MET:N	2.23	0.46
2:D:63:PHE:CE1	2:F:90:ASP:OD1	2.67	0.46
1:E:182:ILE:HD13	1:E:182:ILE:N	2.30	0.46
2:H:65:ALA:O	2:H:66:VAL:CG1	2.64	0.46
2:L:62:GLN:C	2:L:63:PHE:HD1	2.24	0.46
2:B:83:LYS:HD3	2:F:66:VAL:HG22	1.96	0.46
2:F:65:ALA:O	2:F:66:VAL:CG1	2.64	0.46
2:H:28:ASN:H	2:H:28:ASN:HD22	1.63	0.46
1:I:86:TYR:HA	1:I:113:SER:O	2.15	0.46
1:M:117:HIS:HB3	1:M:261:VAL:HG23	1.98	0.46
1:A:181:GLY:O	1:A:182:ILE:HD13	2.13	0.46
1:G:12:GLN:HA	2:H:138:PHE:O	2.16	0.46
1:M:96(A):LEU:HB3	1:M:98:TYR:O	2.15	0.46
1:O:71:LEU:HD23	1:O:71:LEU:N	2.31	0.46
1:O:129:SER:HA	1:O:157:LYS:HD2	1.97	0.46
1:O:219:THR:HG22	1:O:220:ARG:N	2.27	0.46
1:G:66:VAL:HG23	1:G:89:GLU:OE2	2.16	0.46
1:I:75:MET:CB	1:I:95:ASN:ND2	2.63	0.46
1:K:123:ILE:HD11	1:K:168:TYR:CZ	2.51	0.46
1:O:149:ARG:HH11	1:O:149:ARG:HB3	1.80	0.46
2:P:91:VAL:HG12	2:P:92:TRP:N	2.30	0.46
2:P:141:TYR:O	2:P:169:LYS:HG2	2.15	0.46
1:E:295:HIS:CD2	1:E:297:ILE:H	2.33	0.46
1:G:200:THR:HG22	1:G:215:PRO:CD	2.46	0.46
2:H:63:PHE:CE1	2:J:90:ASP:OD1	2.66	0.46
1:I:124:ILE:CD1	1:I:254:PRO:HG2	2.44	0.46
1:K:206:THR:HB	1:K:209:LEU:HB3	1.97	0.46
1:K:295:HIS:CD2	1:K:297:ILE:H	2.32	0.46
2:R:151:SER:HA	2:R:154:ASN:HB2	1.98	0.46
1:A:249:GLY:O	1:A:250:ASN:OD1	2.34	0.46
2:B:59:MET:HE3	2:B:62:GLN:HG3	1.97	0.46
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.98	0.46
1:E:124:ILE:HG12	1:E:254:PRO:O	2.16	0.46
2:F:68:ARG:HB2	2:F:68:ARG:HH11	1.81	0.46
1:G:309:VAL:HG22	2:H:93:THR:HA	1.98	0.46
1:I:17:TYR:CD1	2:J:13:GLY:HA3	2.51	0.46
1:I:136:SER:O	1:I:145:SER:HB2	2.15	0.46
1:K:238:LYS:O	1:K:239:PRO:C	2.58	0.46
1:E:186:ASN:HB3	1:E:190:GLU:OE2	2.16	0.46
1:K:136:SER:O	1:K:145:SER:HB2	2.16	0.46
2:N:49:THR:HG22	2:N:53:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:59:MET:CE	2:N:62:GLN:HG3	2.44	0.46
2:N:132:GLU:C	2:N:134:GLY:H	2.23	0.46
2:R:111:HIS:HA	2:R:114:ASN:ND2	2.31	0.46
1:G:11:ASP:HB2	2:H:140:PHE:CD1	2.48	0.46
1:G:123:ILE:HA	1:G:123:ILE:HD12	1.36	0.46
1:I:178:VAL:O	1:I:234:TRP:HA	2.15	0.46
1:O:251:PHE:CZ	1:O:253:ALA:HA	2.51	0.46
1:Q:39:ALA:O	1:Q:40:GLN:HB2	2.16	0.46
1:A:279:THR:CG2	1:A:287:ALA:HB1	2.43	0.45
1:I:187:ASP:C	1:I:187:ASP:OD2	2.60	0.45
1:K:87:ILE:HB	1:K:267:ILE:HG13	1.98	0.45
1:M:230:MET:SD	1:M:252:ILE:CD1	3.04	0.45
1:O:147:PHE:O	1:O:148:PHE:C	2.59	0.45
1:O:251:PHE:CD1	1:O:251:PHE:C	2.94	0.45
2:P:53:ASN:O	2:P:57:ASP:N	2.46	0.45
2:P:110:PHE:O	2:P:114:ASN:OD1	2.34	0.45
1:Q:50:LYS:O	1:Q:286:GLY:HA2	2.17	0.45
1:Q:51:LEU:HD11	1:Q:88:VAL:HG21	1.98	0.45
1:Q:80:ILE:C	1:Q:82:VAL:N	2.74	0.45
1:A:179:LEU:HD23	1:A:234:TRP:CB	2.43	0.45
1:C:212:ARG:HB2	1:E:216:ARG:HG2	1.97	0.45
1:I:87:ILE:HD12	1:I:113:SER:HA	1.98	0.45
2:L:125:GLN:HG2	2:L:157:TYR:HB3	1.97	0.45
2:N:44:ALA:O	2:N:45:ILE:C	2.57	0.45
1:O:220:ARG:HB3	1:O:227:SER:HB2	1.98	0.45
1:A:79:PHE:HD1	1:A:79:PHE:O	1.84	0.45
2:H:51:LYS:HG3	1:I:28:ILE:HG23	1.97	0.45
1:O:42:ILE:O	1:O:293:PRO:HD2	2.16	0.45
1:Q:161:TYR:CD2	1:Q:161:TYR:C	2.95	0.45
1:Q:281:CYS:SG	1:Q:288:ILE:HD12	2.55	0.45
1:A:316:LEU:HD13	2:B:100:VAL:HG22	1.98	0.45
1:C:49:GLY:HA2	1:C:285:MET:O	2.17	0.45
1:I:80:ILE:O	1:I:80:ILE:CG2	2.63	0.45
1:M:58:PRO:HB3	1:M:86:TYR:CE2	2.52	0.45
1:M:222:LYS:HA	1:M:226:GLN:O	2.17	0.45
1:A:72:GLY:HA3	1:A:149:ARG:HB2	1.98	0.45
1:C:241:ASP:CG	1:C:242:ALA:H	2.25	0.45
1:E:125:PRO:HG3	1:I:79:PHE:HA	1.12	0.45
1:G:201:TYR:CE2	1:G:248:ASN:HB2	2.51	0.45
1:M:62:ARG:NH2	1:M:77:ASP:OD1	2.49	0.45
1:Q:13:ILE:HD11	2:R:149:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:1:NAG:H3	3:e:2:NAG:O5	2.17	0.45
1:A:114:ARG:HH11	1:A:265:SER:HB3	1.82	0.45
1:C:78:GLU:O	1:C:80:ILE:N	2.49	0.45
1:G:137:SER:HA	1:G:145:SER:HB2	1.99	0.45
1:G:216:ARG:O	1:G:220:ARG:NH2	2.49	0.45
1:O:176:LEU:HD12	1:O:258:TYR:C	2.41	0.45
1:K:59:LEU:HD11	1:K:80:ILE:CG2	2.44	0.45
1:M:15:ILE:HD12	1:M:15:ILE:N	2.31	0.45
2:N:26:HIS:O	2:N:32:SER:HB2	2.16	0.45
2:N:65:ALA:C	2:N:66:VAL:HG13	2.41	0.45
1:O:161:TYR:OH	1:O:164:ILE:HD11	2.16	0.45
2:D:65:ALA:C	2:D:66:VAL:CG1	2.89	0.45
1:M:134:GLY:O	1:M:153:TRP:HB3	2.17	0.45
1:M:232:PHE:C	1:M:233:PHE:CD1	2.94	0.45
2:N:159:TYR:HB3	2:N:160:PRO:CD	2.46	0.45
1:O:185:PRO:O	1:O:217:ILE:HG23	2.17	0.45
1:O:251:PHE:HE1	1:O:253:ALA:HA	1.75	0.45
1:Q:320:LEU:HA	2:R:108:LEU:CD2	2.46	0.45
2:R:1:GLY:C	2:R:3:PHE:H	2.25	0.45
1:A:75:MET:HB2	1:A:95:ASN:HD21	1.72	0.45
1:E:78:GLU:O	1:E:80:ILE:N	2.49	0.45
1:K:137:SER:HA	1:K:145:SER:HB2	1.98	0.45
1:M:283:THR:HG23	1:M:298:HIS:HB3	1.97	0.45
1:O:49:GLY:HA2	1:O:285:MET:O	2.17	0.45
1:E:201:TYR:HE1	1:E:246:GLU:HG2	1.82	0.45
1:E:282:GLN:HG3	1:E:283:THR:N	2.32	0.45
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.99	0.45
1:O:42:ILE:HD13	1:O:42:ILE:HA	1.48	0.45
1:O:200:THR:CG2	1:O:250:ASN:HB2	2.45	0.45
1:Q:102:PHE:C	1:Q:102:PHE:CD2	2.95	0.45
1:Q:206:THR:CG2	1:Q:207:SER:N	2.54	0.45
1:C:80:ILE:C	1:C:82:VAL:H	2.24	0.44
2:F:38:LYS:O	2:F:42:GLN:HB2	2.17	0.44
1:K:227:SER:HA	1:K:229:ARG:HH12	1.82	0.44
1:K:279:THR:CG2	1:K:287:ALA:HB1	2.45	0.44
1:M:129:SER:HA	1:M:157:LYS:HD3	2.00	0.44
1:M:202:ILE:HD12	1:M:202:ILE:N	2.32	0.44
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.18	0.44
1:E:316:LEU:HD23	2:F:52:VAL:HG22	1.99	0.44
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.52	0.44
1:G:27:THR:HG22	1:G:32:GLU:N	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:ASN:HB3	1:G:190:GLU:OE2	2.17	0.44
2:L:38:LYS:O	2:L:42:GLN:HB2	2.18	0.44
4:T:1:NAG:H61	4:T:2:NAG:C1	2.48	0.44
1:G:307:LYS:HZ1	2:H:62:GLN:HB3	1.83	0.44
1:I:206:THR:HB	1:I:209:LEU:CB	2.47	0.44
2:J:123:ARG:HD2	2:J:132:GLU:OE1	2.18	0.44
1:M:85:SER:O	1:M:114:ARG:NH1	2.51	0.44
2:P:77:ILE:O	2:P:78:GLU:C	2.60	0.44
1:Q:48:ASN:OD1	1:Q:287:ALA:N	2.50	0.44
1:Q:139:CYS:SG	1:Q:147:PHE:HA	2.57	0.44
2:R:95:ASN:O	2:R:99:LEU:CB	2.60	0.44
1:C:59:LEU:CD1	1:C:80:ILE:HG23	2.44	0.44
1:E:124:ILE:HA	1:E:125:PRO:HD2	1.68	0.44
1:G:27:THR:HG22	1:G:31:MET:N	2.25	0.44
2:H:59:MET:HE3	2:H:62:GLN:HG3	1.99	0.44
2:J:72:ASN:HB2	2:J:75:ARG:HD2	1.99	0.44
1:M:283:THR:HB	1:M:286:GLY:H	1.81	0.44
1:O:70:LEU:HD23	1:O:70:LEU:HA	1.68	0.44
1:Q:201:TYR:CD2	1:Q:248:ASN:HB2	2.53	0.44
1:A:307:LYS:NZ	2:B:62:GLN:HB3	2.32	0.44
1:E:171:THR:CB	1:I:121:ILE:HD13	2.47	0.44
1:G:206:THR:HB	1:G:209:LEU:HB3	2.00	0.44
1:I:124:ILE:CG1	1:I:124:ILE:O	2.65	0.44
1:I:186:ASN:HB3	1:I:190:GLU:OE2	2.17	0.44
1:I:230:MET:SD	1:I:252:ILE:HD11	2.57	0.44
1:M:306:PRO:O	1:M:307:LYS:C	2.57	0.44
2:N:59:MET:CE	2:N:62:GLN:CG	2.95	0.44
1:O:25:VAL:CG1	1:O:26:ASP:N	2.80	0.44
1:O:234:TRP:O	1:O:235:THR:CB	2.64	0.44
2:P:159:TYR:O	2:P:160:PRO:C	2.60	0.44
1:A:78:GLU:O	1:A:80:ILE:N	2.50	0.44
2:B:66:VAL:HG22	2:D:83:LYS:HD3	2.00	0.44
1:C:182:ILE:HD11	1:C:213:LEU:CD1	2.35	0.44
2:D:38:LYS:O	2:D:42:GLN:HB2	2.18	0.44
1:K:241:ASP:CG	1:K:242:ALA:H	2.26	0.44
1:M:104:ASP:HB2	1:M:234:TRP:HE1	1.83	0.44
1:M:144:LYS:HB3	1:M:144:LYS:HE3	1.80	0.44
1:O:185:PRO:HG2	1:O:217:ILE:HG23	1.99	0.44
1:Q:142:GLN:C	1:Q:144:LYS:H	2.26	0.44
2:B:81:ASN:O	2:B:82:LYS:C	2.58	0.44
1:C:174:GLU:N	1:C:174:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:200:THR:HG22	1:K:215:PRO:CD	2.48	0.44
1:M:152:VAL:N	1:M:253:ALA:O	2.38	0.44
2:P:62:GLN:CD	2:P:62:GLN:N	2.76	0.44
1:Q:182:ILE:CD1	1:Q:202:ILE:HG12	2.48	0.44
2:R:57:ASP:O	2:R:59:MET:N	2.47	0.44
1:A:123:ILE:HG22	1:A:124:ILE:HG23	1.99	0.44
1:A:124:ILE:CG1	1:A:124:ILE:O	2.65	0.44
1:A:159:SER:O	1:A:196:GLN:CG	2.58	0.44
2:F:19:ASP:HB3	2:F:36:ALA:HB3	2.00	0.44
2:F:123:ARG:HD2	2:F:132:GLU:OE1	2.17	0.44
1:G:11:ASP:CB	2:H:140:PHE:HD1	2.28	0.44
1:M:11:ASP:OD2	1:M:11:ASP:N	2.51	0.44
1:M:37:THR:HG22	1:M:38:HIS:CD2	2.52	0.44
1:O:52:CYS:CA	1:O:277:CYS:HB3	2.45	0.44
1:Q:295:HIS:HD2	1:Q:297:ILE:HG12	1.82	0.44
2:R:148:CYS:O	2:R:151:SER:OG	2.35	0.44
1:C:17:TYR:CD1	2:D:13:GLY:HA3	2.53	0.44
1:E:79:PHE:O	1:E:80:ILE:HG12	2.18	0.44
1:G:79:PHE:O	1:G:80:ILE:CG1	2.66	0.44
1:M:97:CYS:HB2	1:M:138:ALA:O	2.18	0.44
1:M:245:PHE:N	1:M:245:PHE:CD1	2.85	0.44
1:O:112:LEU:HD23	1:O:112:LEU:HA	1.67	0.44
1:Q:104:ASP:HB2	1:Q:234:TRP:NE1	2.27	0.44
1:C:124:ILE:CD1	1:C:254:PRO:HG2	2.47	0.43
2:F:145:ASP:O	2:F:148:CYS:HB3	2.17	0.43
1:K:154:LEU:O	1:K:155:ILE:HD12	2.17	0.43
1:M:134:GLY:CA	1:M:153:TRP:HB3	2.48	0.43
1:Q:283:THR:HB	1:Q:286:GLY:O	2.18	0.43
2:R:45:ILE:H	2:R:45:ILE:HG13	1.63	0.43
1:C:120:LYS:HG3	1:C:258:TYR:CE2	2.52	0.43
1:G:293:PRO:HG2	1:G:294:PHE:CE1	2.53	0.43
1:I:121:ILE:HD13	1:I:121:ILE:HA	1.89	0.43
1:M:284:PRO:C	1:M:285:MET:HE2	2.43	0.43
2:N:5:ALA:HA	2:N:9:PHE:CD1	2.53	0.43
1:O:302:ILE:HA	2:P:65:ALA:O	2.18	0.43
1:Q:20:ASN:OD1	1:Q:20:ASN:N	2.38	0.43
2:R:52:VAL:O	2:R:55:ILE:HB	2.18	0.43
1:A:79:PHE:O	1:A:80:ILE:CG1	2.66	0.43
1:A:295:HIS:HD2	1:A:297:ILE:H	1.66	0.43
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.33	0.43
1:C:53(A):LEU:HD23	1:C:53(A):LEU:HA	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:CYS:O	1:C:224:ASN:ND2	2.50	0.43
1:C:115:ILE:HG21	1:C:118:PHE:HB2	2.01	0.43
1:E:307:LYS:HZ3	2:F:62:GLN:HB3	1.82	0.43
1:G:307:LYS:HZ3	2:H:62:GLN:HB3	1.83	0.43
1:I:320:LEU:N	1:I:320:LEU:HD23	2.33	0.43
1:K:114:ARG:HH11	1:K:265:SER:HB3	1.83	0.43
1:O:149:ARG:HH11	1:O:149:ARG:CG	2.32	0.43
1:O:182:ILE:CG2	1:O:215:PRO:HB3	2.48	0.43
1:O:285:MET:CE	1:O:285:MET:HA	2.49	0.43
2:P:145:ASP:OD1	2:P:148:CYS:CB	2.54	0.43
1:A:159:SER:C	1:A:196:GLN:HG3	2.41	0.43
1:E:120:LYS:HG3	1:E:258:TYR:CE2	2.54	0.43
1:I:59:LEU:CD1	1:I:80:ILE:HG23	2.44	0.43
1:M:84:TRP:NE1	1:M:112:LEU:O	2.50	0.43
2:N:82:LYS:C	2:N:84:MET:N	2.75	0.43
2:P:144:CYS:SG	2:P:149:MET:HG2	2.58	0.43
1:Q:86:TYR:HA	1:Q:265:SER:CB	2.49	0.43
2:R:28:ASN:HB3	2:R:31:GLY:HA3	2.00	0.43
1:C:206:THR:HB	1:C:209:LEU:HB3	2.00	0.43
1:E:230:MET:SD	1:E:252:ILE:HD11	2.58	0.43
1:I:200:THR:HG22	1:I:215:PRO:CD	2.48	0.43
1:Q:142:GLN:HG3	1:Q:142:GLN:O	2.19	0.43
1:Q:200:THR:HG23	1:Q:249:GLY:N	2.29	0.43
1:Q:295:HIS:CD2	1:Q:297:ILE:H	2.37	0.43
2:R:151:SER:O	2:R:154:ASN:HB2	2.18	0.43
2:F:28:ASN:H	2:F:28:ASN:HD22	1.67	0.43
2:N:30:GLN:NE2	2:N:145:ASP:HB2	2.33	0.43
2:P:143:LYS:CD	2:P:143:LYS:NZ	2.82	0.43
1:O:230:MET:HB3	1:O:232:PHE:CE1	2.53	0.43
2:P:59:MET:HE2	2:P:59:MET:HB3	1.73	0.43
1:Q:261:VAL:C	1:Q:263:LYS:H	2.27	0.43
2:R:127:ARG:HD3	2:R:127:ARG:H	1.84	0.43
1:G:25:VAL:HG13	2:H:104:ASN:ND2	2.33	0.43
1:G:124:ILE:CD1	1:G:254:PRO:HG2	2.47	0.43
1:M:230:MET:SD	1:M:252:ILE:HD11	2.58	0.43
1:Q:102:PHE:C	1:Q:102:PHE:HD2	2.27	0.43
2:R:18:VAL:O	2:R:18:VAL:HG12	2.18	0.43
2:R:88:PHE:O	2:R:92:TRP:HD1	2.01	0.43
1:A:147:PHE:CE1	1:A:230:MET:HE3	2.53	0.43
1:C:297:ILE:H	1:C:297:ILE:HG12	1.70	0.43
1:G:201:TYR:HE1	1:G:246:GLU:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:ARG:HD3	2:J:174:SER:HA	2.01	0.43
1:K:65:SER:OG	1:K:96:ASP:HA	2.19	0.43
1:M:279:THR:CG2	1:M:287:ALA:HB1	2.44	0.43
2:N:141:TYR:CD1	2:N:166:ALA:HB1	2.53	0.43
1:Q:305:CYS:O	1:Q:307:LYS:N	2.51	0.43
1:A:187:ASP:C	1:A:187:ASP:OD2	2.62	0.43
1:E:115:ILE:HG21	1:E:118:PHE:HB2	2.01	0.43
1:E:174:GLU:OE2	1:E:174:GLU:N	2.47	0.43
1:G:307:LYS:HD2	2:H:92:TRP:CE2	2.53	0.43
1:M:118:PHE:CE1	1:M:260:ILE:HD11	2.54	0.43
1:M:141:TYR:O	1:M:143:GLY:N	2.52	0.43
1:M:147:PHE:CG	1:M:148:PHE:N	2.86	0.43
1:M:181:GLY:HA3	1:M:252:ILE:HB	2.01	0.43
1:M:202:ILE:HG12	1:M:251:PHE:HD1	1.84	0.43
1:O:285:MET:HA	1:O:285:MET:HE3	2.01	0.43
2:P:140:PHE:HB3	2:P:142:HIS:O	2.18	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.19	0.42
1:M:195:TYR:C	1:M:196:GLN:HG2	2.44	0.42
1:O:231:GLU:O	1:O:233:PHE:CE1	2.72	0.42
1:O:260:ILE:HG23	1:O:261:VAL:N	2.34	0.42
1:O:266:THR:HG22	1:O:302:ILE:HD11	2.01	0.42
2:R:70:PHE:HB2	2:R:78:GLU:HB2	2.01	0.42
2:R:99:LEU:HD12	2:R:99:LEU:HA	1.86	0.42
1:C:200:THR:HG23	1:C:201:TYR:N	2.34	0.42
2:D:125:GLN:HG2	2:D:157:TYR:HB3	2.00	0.42
1:G:207:SER:HA	1:I:229:ARG:NH2	2.34	0.42
1:M:19:ALA:HB1	1:M:322:ASN:HD21	1.84	0.42
1:O:42:ILE:HD12	2:P:56:ILE:HD11	2.01	0.42
1:O:52:CYS:HB3	1:O:277:CYS:HB3	1.82	0.42
1:O:220:ARG:HD2	1:O:229:ARG:HG2	2.01	0.42
2:P:26:HIS:CE1	2:P:32:SER:HA	2.54	0.42
1:Q:55:GLY:HA2	1:Q:278:ASN:HD21	1.84	0.42
1:Q:75:MET:HE1	1:Q:140:PRO:HD2	2.01	0.42
3:f:1:NAG:C6	3:f:2:NAG:HN2	2.31	0.42
1:A:123:ILE:CG2	1:A:124:ILE:HG23	2.49	0.42
1:C:206:THR:HG23	1:C:207:SER:H	1.84	0.42
1:G:178:VAL:O	1:G:234:TRP:HA	2.18	0.42
1:M:168:TYR:O	1:M:243:ILE:HG22	2.18	0.42
1:O:220:ARG:HH11	1:O:229:ARG:CG	2.33	0.42
1:Q:122:GLN:HE21	1:Q:125:PRO:HA	1.84	0.42
1:C:137:SER:HA	1:C:145:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LYS:HZ1	2:D:62:GLN:CB	2.31	0.42
2:H:123:ARG:HD2	2:H:132:GLU:OE1	2.20	0.42
1:I:238:LYS:O	1:I:239:PRO:C	2.60	0.42
1:M:12:GLN:HB2	2:N:27:SER:OG	2.19	0.42
2:N:84:MET:O	2:N:87:GLY:N	2.53	0.42
1:O:173:GLN:HE21	1:O:173:GLN:HB2	1.55	0.42
1:C:195:TYR:CE1	1:C:250:ASN:ND2	2.87	0.42
2:D:19:ASP:HB3	2:D:36:ALA:HB3	2.02	0.42
1:E:12:GLN:HG2	2:F:138:PHE:O	2.19	0.42
1:E:106:GLU:OE2	2:F:71:ASN:HB3	2.20	0.42
1:E:136:SER:O	1:E:145:SER:HB2	2.20	0.42
1:I:13:ILE:HA	2:J:25:HIS:O	2.20	0.42
1:I:241:ASP:CG	1:I:242:ALA:H	2.28	0.42
1:I:276:ASN:O	1:I:277:CYS:HB2	2.19	0.42
1:K:106:GLU:OE2	2:L:71:ASN:HB3	2.19	0.42
1:M:114:ARG:HD2	1:M:264(A):ASP:O	2.20	0.42
1:M:118:PHE:HE1	1:M:260:ILE:HD11	1.84	0.42
1:M:238:LYS:O	1:M:239:PRO:C	2.62	0.42
1:O:186:ASN:HB2	1:O:227:SER:O	2.19	0.42
2:B:173:ILE:O	2:F:167:ARG:NH1	2.53	0.42
1:K:59:LEU:CD1	1:K:80:ILE:HG23	2.46	0.42
1:M:19(A):ASN:OD1	1:M:19(A):ASN:C	2.63	0.42
1:O:38:HIS:HB2	1:O:319:GLY:H	1.84	0.42
1:Q:293:PRO:HB2	1:Q:294:PHE:HD1	1.84	0.42
2:R:68:ARG:C	2:R:69:GLU:HG3	2.44	0.42
1:A:80:ILE:C	1:A:82:VAL:N	2.77	0.42
1:A:229:ARG:NH2	1:E:207:SER:HA	2.29	0.42
1:E:171:THR:HB	1:I:121:ILE:CD1	2.48	0.42
1:E:178:VAL:O	1:E:234:TRP:HA	2.19	0.42
1:I:115:ILE:HG21	1:I:118:PHE:HB2	2.01	0.42
1:K:124:ILE:HA	1:K:125:PRO:HD2	1.87	0.42
1:M:77:ASP:HB2	1:M:79:PHE:H	1.82	0.42
1:M:123:ILE:HG23	1:M:124:ILE:N	2.35	0.42
2:N:28:ASN:H	2:N:28:ASN:HD22	1.67	0.42
1:O:32:GLU:HB3	1:O:35:VAL:HG21	2.01	0.42
1:O:61:LEU:HB3	1:O:64:CYS:O	2.18	0.42
1:O:146:SER:HG	1:O:147:PHE:H	1.64	0.42
2:R:84:MET:HE3	2:R:88:PHE:CE1	2.54	0.42
2:R:155:GLY:C	2:R:157:TYR:N	2.77	0.42
1:A:206:THR:HB	1:A:209:LEU:N	2.28	0.42
2:B:59:MET:HG3	2:D:94:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ARG:NH1	2:D:173:ILE:O	2.52	0.42
1:C:79:PHE:O	1:C:80:ILE:CG1	2.68	0.42
2:F:68:ARG:HB2	2:F:68:ARG:NH1	2.35	0.42
1:G:15:ILE:HD13	2:H:119:TYR:HA	2.02	0.42
1:G:115:ILE:HG21	1:G:118:PHE:HB2	2.01	0.42
1:G:304:GLU:HG2	2:H:63:PHE:HA	2.01	0.42
1:K:174:GLU:OE2	1:K:174:GLU:N	2.52	0.42
1:K:268:MET:HE3	1:K:284:PRO:HA	2.02	0.42
2:L:123:ARG:HD2	2:L:132:GLU:OE1	2.19	0.42
1:M:115:ILE:HG21	1:M:118:PHE:HB2	2.02	0.42
1:M:170:ASN:OD1	1:M:171:THR:N	2.53	0.42
2:N:17:MET:HG3	2:N:34:TYR:HB3	2.02	0.42
2:N:38:LYS:NZ	2:N:38:LYS:HD2	2.34	0.42
1:Q:295:HIS:CD2	1:Q:297:ILE:HG12	2.55	0.42
1:A:297:ILE:H	1:A:297:ILE:HG12	1.71	0.42
1:C:227:SER:HA	1:C:229:ARG:HH12	1.85	0.42
1:E:11:ASP:OD2	2:F:144:CYS:N	2.52	0.42
1:E:156:LYS:HD2	1:E:196:GLN:HG2	2.02	0.42
1:G:49:GLY:HA2	1:G:285:MET:O	2.20	0.42
1:M:27:THR:C	1:M:31:MET:H	2.26	0.42
1:O:108:LEU:HD22	1:O:234:TRP:CD1	2.55	0.42
1:Q:60:ILE:HA	1:Q:88:VAL:HB	2.01	0.42
1:A:75:MET:CB	1:A:95:ASN:HD21	2.30	0.42
2:B:65:ALA:C	2:B:66:VAL:CG1	2.93	0.42
1:C:159:SER:C	1:C:196:GLN:HG3	2.45	0.42
1:E:87:ILE:HB	1:E:267:ILE:HG13	2.01	0.42
1:G:72:GLY:HA3	1:G:149:ARG:H	1.84	0.42
1:G:295:HIS:CD2	1:G:297:ILE:H	2.36	0.42
2:H:59:MET:HE2	2:H:59:MET:HB3	1.81	0.42
1:K:206:THR:HG23	1:K:207:SER:H	1.84	0.42
1:M:27:THR:C	1:M:31:MET:N	2.76	0.42
1:M:141:TYR:CB	1:M:146:SER:HB2	2.49	0.42
1:M:294:PHE:HA	1:M:307:LYS:O	2.20	0.42
2:N:95:ASN:O	2:N:99:LEU:HB2	2.20	0.42
2:N:128:ASP:O	2:N:170:ARG:NH1	2.53	0.42
1:O:292:MET:HB3	1:O:293:PRO:HD2	2.01	0.42
1:Q:184:HIS:HA	1:Q:185:PRO:HD3	1.63	0.42
1:Q:220:ARG:HD2	1:Q:227:SER:O	2.20	0.42
2:R:121:LYS:O	2:R:125:GLN:HB2	2.20	0.42
1:G:18:HIS:N	2:H:21:TRP:O	2.48	0.41
1:K:159:SER:C	1:K:196:GLN:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:VAL:O	1:K:234:TRP:HA	2.20	0.41
1:Q:170:ASN:ND2	1:Q:238:LYS:O	2.52	0.41
2:D:167:ARG:NH1	2:F:173:ILE:O	2.53	0.41
1:E:123:ILE:HD12	1:E:123:ILE:HA	1.46	0.41
1:K:120:LYS:HG3	1:K:258:TYR:CE2	2.54	0.41
1:K:201:TYR:CE1	1:K:246:GLU:HG2	2.54	0.41
1:O:190:GLU:OE2	1:O:190:GLU:HA	2.20	0.41
2:P:155:GLY:O	2:P:157:TYR:N	2.49	0.41
1:Q:251:PHE:HE2	1:Q:253:ALA:HB2	1.83	0.41
1:A:309:VAL:HG22	2:B:93:THR:HA	2.01	0.41
2:H:117:ASN:ND2	2:J:4:GLY:CA	2.84	0.41
1:I:124:ILE:HA	1:I:125:PRO:HD2	1.82	0.41
2:L:82:LYS:O	2:L:83:LYS:C	2.63	0.41
1:M:125(A):LYS:HG3	1:M:132:ALA:HB1	2.02	0.41
1:M:161:TYR:CE2	1:M:249:GLY:HA2	2.55	0.41
2:N:143:LYS:HD3	2:N:143:LYS:N	2.22	0.41
1:E:185:PRO:HG3	1:E:191:GLN:HG2	2.02	0.41
2:L:145:ASP:O	2:L:148:CYS:HB3	2.20	0.41
1:O:98:TYR:O	1:O:99:PRO:C	2.62	0.41
1:Q:75:MET:H	1:Q:75:MET:HG2	1.51	0.41
2:R:1:GLY:HA3	2:R:8:GLY:H	1.85	0.41
2:D:81:ASN:HD22	2:F:80:LEU:CD1	2.30	0.41
1:G:80:ILE:C	1:G:82:VAL:N	2.78	0.41
1:G:241:ASP:CG	1:G:242:ALA:H	2.28	0.41
1:I:68:GLY:O	1:I:71:LEU:O	2.39	0.41
1:K:49:GLY:HA2	1:K:285:MET:O	2.20	0.41
1:M:144:LYS:HG2	1:M:145:SER:N	2.36	0.41
1:M:161:TYR:HB2	1:M:196:GLN:HG3	2.02	0.41
2:N:117:ASN:HD22	2:N:117:ASN:HA	1.65	0.41
2:N:143:LYS:H	2:N:143:LYS:CD	2.21	0.41
1:O:42:ILE:CD1	2:P:56:ILE:HD11	2.51	0.41
1:Q:278:ASN:HD21	4:X:3:BMA:H62	1.86	0.41
1:A:99:PRO:HB3	1:A:223:VAL:CG1	2.51	0.41
1:A:206:THR:HB	1:A:209:LEU:HB3	2.02	0.41
1:C:201:TYR:CE1	1:C:246:GLU:HG2	2.52	0.41
1:G:266:THR:HB	2:H:66:VAL:HB	2.02	0.41
1:K:86:TYR:HA	1:K:113:SER:O	2.21	0.41
1:M:266:THR:HG23	1:M:302:ILE:HD11	2.01	0.41
1:Q:147:PHE:CG	1:Q:148:PHE:N	2.89	0.41
2:R:24:TYR:CD1	2:R:24:TYR:N	2.89	0.41
2:R:43:LYS:HA	2:R:46:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TYR:HA	1:A:113:SER:O	2.20	0.41
1:C:66:VAL:HG23	1:C:89:GLU:OE2	2.21	0.41
2:F:59:MET:O	2:F:61:THR:CA	2.66	0.41
1:M:99:PRO:HD2	1:M:226:GLN:HG3	2.02	0.41
1:O:152:VAL:N	1:O:253:ALA:O	2.54	0.41
2:R:26:HIS:CD2	2:R:153:ARG:HH22	2.39	0.41
2:R:38:LYS:C	2:R:42:GLN:HE21	2.28	0.41
1:E:11:ASP:HB2	2:F:140:PHE:HB2	2.02	0.41
1:E:276:ASN:O	1:E:277:CYS:HB2	2.20	0.41
2:J:66:VAL:HG22	2:L:83:LYS:HD3	2.03	0.41
1:K:72:GLY:HA3	1:K:149:ARG:HB2	2.02	0.41
1:M:48:ASN:HD21	1:M:287:ALA:HB3	1.85	0.41
1:M:112:LEU:O	1:M:113:SER:C	2.63	0.41
2:N:72:ASN:HA	2:N:75:ARG:HG3	2.02	0.41
2:N:80:LEU:HD12	2:N:80:LEU:HA	1.92	0.41
2:B:82:LYS:O	2:B:83:LYS:C	2.63	0.41
1:C:86:TYR:HA	1:C:113:SER:O	2.20	0.41
1:C:141:TYR:CE2	1:C:142:GLN:CG	3.03	0.41
1:C:320:LEU:HD23	1:C:320:LEU:N	2.36	0.41
1:E:206:THR:HB	1:E:209:LEU:CB	2.50	0.41
1:G:185:PRO:HG3	1:G:191:GLN:HG2	2.03	0.41
1:G:185:PRO:HG2	1:G:217:ILE:HG13	2.02	0.41
2:H:63:PHE:HD1	2:H:63:PHE:H	1.59	0.41
2:H:110:PHE:CD1	2:J:2:LEU:HD21	2.56	0.41
1:I:159:SER:C	1:I:196:GLN:HG3	2.44	0.41
1:I:197:ASN:HA	1:I:198:PRO:HD3	1.96	0.41
1:I:275:GLY:O	1:I:277:CYS:CB	2.58	0.41
1:I:295:HIS:HD2	1:I:297:ILE:H	1.68	0.41
1:I:297:ILE:H	1:I:297:ILE:HG12	1.64	0.41
1:K:293:PRO:HG2	1:K:294:PHE:CE1	2.56	0.41
1:M:119:GLU:O	1:M:259:LYS:N	2.53	0.41
1:M:176:LEU:O	1:M:237:LEU:N	2.54	0.41
1:M:293:PRO:HG2	1:M:294:PHE:CE1	2.56	0.41
1:M:295:HIS:CD2	1:M:297:ILE:HG12	2.56	0.41
2:N:59:MET:O	2:N:61:THR:O	2.38	0.41
2:N:125:GLN:HE21	2:N:125:GLN:HB2	1.71	0.41
1:O:70:LEU:O	1:O:258:TYR:OH	2.37	0.41
1:O:86:TYR:HA	1:O:113:SER:O	2.21	0.41
1:O:117:HIS:H	1:O:261:VAL:HB	1.86	0.41
1:O:127:TRP:HZ3	1:O:164:ILE:HD13	1.86	0.41
1:O:184:HIS:HA	1:O:185:PRO:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:266:THR:HG23	1:O:267:ILE:N	2.36	0.41
2:P:21:TRP:HB2	2:P:41:THR:HG23	2.02	0.41
1:Q:141:TYR:CG	1:Q:142:GLN:N	2.85	0.41
1:Q:161:TYR:C	1:Q:161:TYR:HD2	2.28	0.41
2:R:66:VAL:HB	2:R:67:GLY:H	1.62	0.41
1:A:167:SER:CB	1:A:244:ASN:OD1	2.69	0.41
1:E:100:GLY:HA3	1:E:230:MET:O	2.21	0.41
1:E:149:ARG:NH1	1:I:142:GLN:OE1	2.54	0.41
1:G:75:MET:CB	1:G:95:ASN:HD21	2.28	0.41
1:I:72:GLY:HA3	1:I:149:ARG:H	1.86	0.41
1:M:130:HIS:NE2	1:M:162:PRO:HD2	2.35	0.41
2:N:15:GLN:HA	2:N:15:GLN:HE21	1.86	0.41
2:N:28:ASN:HB2	2:N:144:CYS:O	2.20	0.41
2:N:52:VAL:O	2:N:53:ASN:C	2.62	0.41
2:P:98:LEU:HD23	2:P:98:LEU:HA	1.77	0.41
2:R:29:GLU:O	2:R:30:GLN:CB	2.69	0.41
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.84	0.40
2:D:159:TYR:N	2:D:160:PRO:HD2	2.37	0.40
1:E:27:THR:HG23	2:F:105:GLU:HB2	2.04	0.40
1:E:266:THR:HB	2:F:66:VAL:HB	2.03	0.40
2:F:65:ALA:O	2:F:66:VAL:HG13	2.21	0.40
1:G:59:LEU:CD1	1:G:80:ILE:HG23	2.45	0.40
1:G:131:GLU:HB2	1:G:155:ILE:O	2.19	0.40
1:G:262:LYS:NZ	1:G:264(A):ASP:OD1	2.29	0.40
1:O:155:ILE:CG2	1:O:156:LYS:N	2.84	0.40
2:P:50:ASN:O	2:P:51:LYS:C	2.64	0.40
2:R:63:PHE:HD1	2:R:63:PHE:H	1.68	0.40
2:R:140:PHE:HE1	2:R:149:MET:HE2	1.86	0.40
1:C:77:ASP:CG	1:C:79:PHE:HB3	2.46	0.40
1:E:59:LEU:CD1	1:E:80:ILE:HG23	2.45	0.40
2:H:145:ASP:O	2:H:148:CYS:HB3	2.21	0.40
1:I:206:THR:HG23	1:I:207:SER:H	1.86	0.40
2:L:19:ASP:HB3	2:L:36:ALA:HB3	2.03	0.40
2:N:48:VAL:O	2:N:49:THR:C	2.65	0.40
1:O:27:THR:HG23	2:P:105:GLU:CB	2.50	0.40
2:P:120:ASP:O	2:P:124:LEU:HD12	2.22	0.40
2:P:141:TYR:HB2	2:P:166:ALA:HB1	2.02	0.40
1:Q:109:LYS:HZ1	2:R:69:GLU:HG2	1.87	0.40
1:E:125:PRO:C	1:I:79:PHE:HD2	2.29	0.40
2:J:82:LYS:O	2:J:83:LYS:C	2.63	0.40
1:K:249:GLY:O	1:K:250:ASN:OD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:145:ASP:H	2:L:148:CYS:HB3	1.86	0.40
1:M:150:ASN:HA	1:M:256:TYR:HD1	1.86	0.40
1:O:295:HIS:HB3	1:O:306:PRO:HG2	2.04	0.40
2:R:126:LEU:HD12	2:R:126:LEU:O	2.21	0.40
2:R:127:ARG:HB2	2:R:127:ARG:NH1	2.18	0.40
2:B:62:GLN:H	2:B:62:GLN:NE2	2.19	0.40
1:E:272:LEU:HD23	1:M:171:THR:HG21	1.98	0.40
2:H:159:TYR:N	2:H:160:PRO:HD2	2.36	0.40
1:I:31:MET:HE2	1:I:31:MET:HB2	1.91	0.40
1:I:99:PRO:HB3	1:I:223:VAL:CG1	2.52	0.40
1:I:307:LYS:HD2	2:J:92:TRP:CZ2	2.57	0.40
1:K:12:GLN:HB2	2:L:27:SER:OG	2.22	0.40
1:K:237:LEU:CD1	1:K:241:ASP:HB3	2.52	0.40
1:M:62:ARG:HH11	1:M:62:ARG:H	1.69	0.40
1:M:126:SER:O	1:M:127:TRP:CD1	2.75	0.40
2:N:16:GLY:HA3	2:N:34:TYR:CZ	2.56	0.40
1:O:182:ILE:HD13	1:O:182:ILE:HA	1.93	0.40
2:B:98:LEU:HD23	2:B:98:LEU:HA	1.91	0.40
2:B:123:ARG:HD2	2:B:132:GLU:OE1	2.22	0.40
1:C:200:THR:HG22	1:C:215:PRO:CD	2.51	0.40
1:M:284:PRO:HD3	1:M:300:LEU:O	2.22	0.40
2:N:107:THR:O	2:N:108:LEU:C	2.65	0.40
1:Q:58:PRO:HG2	1:Q:60:ILE:HD11	2.03	0.40
2:R:150:GLU:O	2:R:154:ASN:CG	2.65	0.40
2:R:162:TYR:O	2:R:163:SER:HB3	2.21	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
2	B	127	ARG
2	D	60	ASN
2	D	127	ARG

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

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Mol	Chain	Res	Type
2	P	152	VAL
1	Q	71	LEU
1	Q	96(A)	LEU
1	Q	142	GLN
1	Q	158	ASN
1	Q	249	GLY
1	Q	281	CYS
2	R	8	GLY
2	R	30	GLN
2	R	39	GLU
2	R	59	MET
2	R	154	ASN
2	R	157	TYR
1	C	277	CYS
1	E	277	CYS
1	G	277	CYS
1	M	144	LYS
1	M	249	GLY
1	M	276	ASN
2	N	167	ARG
1	O	96	ASP
1	O	133(A)	LEU
2	P	150	GLU
1	Q	81	ASN
1	Q	82(A)	PRO
1	Q	83	GLU
1	Q	299	PRO
1	Q	306	PRO
2	R	60	ASN
2	R	161	GLN
2	R	174	SER
1	A	277	CYS
1	I	80	ILE
1	I	277	CYS
1	K	277	CYS
1	M	214	VAL
1	O	62	ARG
1	O	141	TYR
1	Q	45	LYS
1	Q	80	ILE
1	E	81	ASN
1	I	265	SER

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Mol	Chain	Res	Type
1	K	146	SER
1	K	265	SER
1	M	54	ASP
2	N	132	GLU
1	O	99	PRO
1	O	106	GLU
1	O	224	ASN
1	O	236	ILE
1	O	289	ASN
1	Q	21	SER
1	Q	117	HIS
1	Q	262	LYS
2	R	29	GLU
1	A	81	ASN
1	A	239	PRO
1	A	265	SER
1	C	239	PRO
1	I	239	PRO
2	P	156	THR
2	R	17	MET
2	R	49	THR
2	R	66	VAL
2	R	127	ARG
2	R	134	GLY
1	E	239	PRO
2	P	8	GLY
1	K	239	PRO
2	N	16	GLY
1	Q	25	VAL
1	E	249	GLY
1	M	298	HIS
2	P	66	VAL
1	G	249	GLY
2	H	66	VAL
1	M	123	ILE
1	O	93	PRO
2	R	18	VAL
2	R	173	ILE
1	I	249	GLY
2	P	160	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/300 (96%)	253 (88%)	36 (12%)	4	13
1	C	289/300 (96%)	248 (86%)	41 (14%)	3	9
1	E	289/300 (96%)	252 (87%)	37 (13%)	4	13
1	G	289/300 (96%)	252 (87%)	37 (13%)	4	13
1	I	289/300 (96%)	253 (88%)	36 (12%)	4	13
1	K	289/300 (96%)	249 (86%)	40 (14%)	3	10
1	M	289/300 (96%)	240 (83%)	49 (17%)	2	5
1	O	289/300 (96%)	235 (81%)	54 (19%)	1	4
1	Q	289/300 (96%)	234 (81%)	55 (19%)	1	3
2	B	149/155 (96%)	134 (90%)	15 (10%)	7	20
2	D	149/155 (96%)	134 (90%)	15 (10%)	7	20
2	F	149/155 (96%)	134 (90%)	15 (10%)	7	20
2	H	149/155 (96%)	133 (89%)	16 (11%)	6	18
2	J	149/155 (96%)	135 (91%)	14 (9%)	8	22
2	L	149/155 (96%)	134 (90%)	15 (10%)	7	20
2	N	149/155 (96%)	120 (80%)	29 (20%)	1	3
2	P	149/155 (96%)	118 (79%)	31 (21%)	1	3
2	R	149/155 (96%)	124 (83%)	25 (17%)	2	6
All	All	3942/4095 (96%)	3382 (86%)	560 (14%)	3	9

All (560) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	27	THR
1	A	28	ILE
1	A	37	THR
1	A	42	ILE
1	A	62	ARG

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Mol	Chain	Res	Type
1	A	75	MET
1	A	78	GLU
1	A	79	PHE
1	A	80	ILE
1	A	82	VAL
1	A	82(A)	PRO
1	A	123	ILE
1	A	124	ILE
1	A	135	VAL
1	A	136	SER
1	A	151	VAL
1	A	160	THR
1	A	163	THR
1	A	169	ASN
1	A	176	LEU
1	A	191	GLN
1	A	200	THR
1	A	206	THR
1	A	208	THR
1	A	211	GLN
1	A	217	ILE
1	A	230	MET
1	A	235	THR
1	A	238	LYS
1	A	239	PRO
1	A	267	ILE
1	A	279	THR
1	A	297	ILE
1	A	309	VAL
1	A	320	LEU
2	B	28	ASN
2	B	30	GLN
2	B	34	TYR
2	B	62	GLN
2	B	63	PHE
2	B	64	GLU
2	B	68	ARG
2	B	69	GLU
2	B	72	ASN
2	B	89	LEU
2	B	126	LEU
2	B	127	ARG

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Mol	Chain	Res	Type
2	B	156	THR
2	B	169	LYS
2	B	172	GLU
1	C	25	VAL
1	C	27	THR
1	C	28	ILE
1	C	37	THR
1	C	42	ILE
1	C	62	ARG
1	C	75	MET
1	C	78	GLU
1	C	79	PHE
1	C	80	ILE
1	C	82	VAL
1	C	82(A)	PRO
1	C	114	ARG
1	C	120	LYS
1	C	123	ILE
1	C	124	ILE
1	C	135	VAL
1	C	136	SER
1	C	151	VAL
1	C	160	THR
1	C	163	THR
1	C	169	ASN
1	C	176	LEU
1	C	182	ILE
1	C	191	GLN
1	C	200	THR
1	C	206	THR
1	C	208	THR
1	C	211	GLN
1	C	217	ILE
1	C	230	MET
1	C	235	THR
1	C	238	LYS
1	C	239	PRO
1	C	266	THR
1	C	267	ILE
1	C	283	THR
1	C	297	ILE
1	C	307	LYS

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Mol	Chain	Res	Type
1	C	309	VAL
1	C	320	LEU
2	D	28	ASN
2	D	30	GLN
2	D	34	TYR
2	D	62	GLN
2	D	63	PHE
2	D	64	GLU
2	D	68	ARG
2	D	69	GLU
2	D	72	ASN
2	D	89	LEU
2	D	126	LEU
2	D	127	ARG
2	D	156	THR
2	D	169	LYS
2	D	172	GLU
1	E	25	VAL
1	E	27	THR
1	E	28	ILE
1	E	37	THR
1	E	42	ILE
1	E	62	ARG
1	E	75	MET
1	E	78	GLU
1	E	79	PHE
1	E	82	VAL
1	E	82(A)	PRO
1	E	123	ILE
1	E	124	ILE
1	E	135	VAL
1	E	136	SER
1	E	151	VAL
1	E	160	THR
1	E	163	THR
1	E	169	ASN
1	E	173	GLN
1	E	176	LEU
1	E	191	GLN
1	E	200	THR
1	E	206	THR
1	E	208	THR

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Mol	Chain	Res	Type
1	E	211	GLN
1	E	217	ILE
1	E	230	MET
1	E	235	THR
1	E	238	LYS
1	E	239	PRO
1	E	260	ILE
1	E	283	THR
1	E	297	ILE
1	E	307	LYS
1	E	309	VAL
1	E	320	LEU
2	F	28	ASN
2	F	30	GLN
2	F	34	TYR
2	F	61	THR
2	F	62	GLN
2	F	63	PHE
2	F	64	GLU
2	F	69	GLU
2	F	72	ASN
2	F	89	LEU
2	F	126	LEU
2	F	127	ARG
2	F	156	THR
2	F	169	LYS
2	F	172	GLU
1	G	25	VAL
1	G	27	THR
1	G	28	ILE
1	G	37	THR
1	G	42	ILE
1	G	62	ARG
1	G	75	MET
1	G	78	GLU
1	G	79	PHE
1	G	82	VAL
1	G	82(A)	PRO
1	G	114	ARG
1	G	123	ILE
1	G	124	ILE
1	G	135	VAL

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Mol	Chain	Res	Type
1	G	136	SER
1	G	151	VAL
1	G	160	THR
1	G	163	THR
1	G	169	ASN
1	G	176	LEU
1	G	191	GLN
1	G	200	THR
1	G	206	THR
1	G	208	THR
1	G	211	GLN
1	G	216	ARG
1	G	217	ILE
1	G	230	MET
1	G	235	THR
1	G	238	LYS
1	G	239	PRO
1	G	260	ILE
1	G	267	ILE
1	G	297	ILE
1	G	309	VAL
1	G	320	LEU
2	H	28	ASN
2	H	30	GLN
2	H	34	TYR
2	H	61	THR
2	H	62	GLN
2	H	63	PHE
2	H	64	GLU
2	H	68	ARG
2	H	69	GLU
2	H	72	ASN
2	H	89	LEU
2	H	126	LEU
2	H	127	ARG
2	H	156	THR
2	H	169	LYS
2	H	172	GLU
1	I	25	VAL
1	I	27	THR
1	I	28	ILE
1	I	37	THR

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Mol	Chain	Res	Type
1	I	42	ILE
1	I	62	ARG
1	I	75	MET
1	I	78	GLU
1	I	79	PHE
1	I	80	ILE
1	I	82	VAL
1	I	82(A)	PRO
1	I	123	ILE
1	I	124	ILE
1	I	135	VAL
1	I	136	SER
1	I	151	VAL
1	I	160	THR
1	I	163	THR
1	I	169	ASN
1	I	176	LEU
1	I	182	ILE
1	I	191	GLN
1	I	200	THR
1	I	206	THR
1	I	208	THR
1	I	211	GLN
1	I	217	ILE
1	I	230	MET
1	I	235	THR
1	I	238	LYS
1	I	266	THR
1	I	267	ILE
1	I	297	ILE
1	I	309	VAL
1	I	320	LEU
2	J	28	ASN
2	J	30	GLN
2	J	34	TYR
2	J	61	THR
2	J	62	GLN
2	J	63	PHE
2	J	64	GLU
2	J	69	GLU
2	J	89	LEU
2	J	126	LEU

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Mol	Chain	Res	Type
2	J	127	ARG
2	J	156	THR
2	J	169	LYS
2	J	172	GLU
1	K	25	VAL
1	K	27	THR
1	K	28	ILE
1	K	37	THR
1	K	42	ILE
1	K	62	ARG
1	K	75	MET
1	K	78	GLU
1	K	79	PHE
1	K	80	ILE
1	K	82	VAL
1	K	82(A)	PRO
1	K	114	ARG
1	K	120	LYS
1	K	123	ILE
1	K	124	ILE
1	K	135	VAL
1	K	136	SER
1	K	151	VAL
1	K	160	THR
1	K	163	THR
1	K	169	ASN
1	K	173	GLN
1	K	176	LEU
1	K	182	ILE
1	K	191	GLN
1	K	200	THR
1	K	206	THR
1	K	208	THR
1	K	211	GLN
1	K	217	ILE
1	K	230	MET
1	K	235	THR
1	K	238	LYS
1	K	239	PRO
1	K	266	THR
1	K	283	THR
1	K	297	ILE

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Mol	Chain	Res	Type
1	K	309	VAL
1	K	320	LEU
2	L	28	ASN
2	L	30	GLN
2	L	34	TYR
2	L	42	GLN
2	L	62	GLN
2	L	63	PHE
2	L	64	GLU
2	L	69	GLU
2	L	72	ASN
2	L	89	LEU
2	L	126	LEU
2	L	127	ARG
2	L	156	THR
2	L	169	LYS
2	L	172	GLU
1	M	27	THR
1	M	31	MET
1	M	42	ILE
1	M	54	ASP
1	M	62	ARG
1	M	70	LEU
1	M	77	ASP
1	M	78	GLU
1	M	82	VAL
1	M	82(A)	PRO
1	M	92	ASN
1	M	111	LEU
1	M	121	ILE
1	M	124	ILE
1	M	126	SER
1	M	155	ILE
1	M	156	LYS
1	M	160	THR
1	M	164	ILE
1	M	171	THR
1	M	172	ASN
1	M	173	GLN
1	M	174	GLU
1	M	192	THR
1	M	196	GLN

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Mol	Chain	Res	Type
1	M	197	ASN
1	M	207	SER
1	M	211	GLN
1	M	214	VAL
1	M	217	ILE
1	M	221	SER
1	M	224	ASN
1	M	238	LYS
1	M	248	ASN
1	M	255	GLU
1	M	260	ILE
1	M	265	SER
1	M	267	ILE
1	M	272	LEU
1	M	273	GLU
1	M	277	CYS
1	M	309	VAL
1	M	310	LYS
1	M	312	ASN
1	M	313	ARG
1	M	315	VAL
1	M	320	LEU
1	M	322	ASN
1	M	323	SER
2	N	10	ILE
2	N	15	GLN
2	N	18	VAL
2	N	19	ASP
2	N	22	TYR
2	N	24	TYR
2	N	28	ASN
2	N	30	GLN
2	N	41	THR
2	N	48	VAL
2	N	50	ASN
2	N	60	ASN
2	N	62	GLN
2	N	63	PHE
2	N	66	VAL
2	N	82	LYS
2	N	106	ARG
2	N	112	ASP

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Mol	Chain	Res	Type
2	N	113	SER
2	N	117	ASN
2	N	125	GLN
2	N	126	LEU
2	N	127	ARG
2	N	143	LYS
2	N	149	MET
2	N	156	THR
2	N	158	ASP
2	N	164	GLU
2	N	174	SER
1	O	22	THR
1	O	25	VAL
1	O	42	ILE
1	O	57	LYS
1	O	62	ARG
1	O	63	ASP
1	O	71	LEU
1	O	77	ASP
1	O	80	ILE
1	O	82	VAL
1	O	82(A)	PRO
1	O	102	PHE
1	O	111	LEU
1	O	114	ARG
1	O	121	ILE
1	O	123	ILE
1	O	124	ILE
1	O	130	HIS
1	O	135	VAL
1	O	149	ARG
1	O	152	VAL
1	O	155	ILE
1	O	160	THR
1	O	163	THR
1	O	169	ASN
1	O	171	THR
1	O	172	ASN
1	O	173	GLN
1	O	182	ILE
1	O	187	ASP
1	O	191	GLN

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Mol	Chain	Res	Type
1	O	199	THR
1	O	206	THR
1	O	209	LEU
1	O	214	VAL
1	O	220	ARG
1	O	224	ASN
1	O	230	MET
1	O	232	PHE
1	O	235	THR
1	O	237	LEU
1	O	238	LYS
1	O	248	ASN
1	O	250	ASN
1	O	251	PHE
1	O	260	ILE
1	O	266	THR
1	O	267	ILE
1	O	273	GLU
1	O	283	THR
1	O	285	MET
1	O	309	VAL
1	O	320	LEU
1	O	322	ASN
2	P	9	PHE
2	P	10	ILE
2	P	27	SER
2	P	28	ASN
2	P	29	GLU
2	P	32	SER
2	P	34	TYR
2	P	41	THR
2	P	46	ASP
2	P	55	ILE
2	P	56	ILE
2	P	59	MET
2	P	61	THR
2	P	62	GLN
2	P	63	PHE
2	P	64	GLU
2	P	69	GLU
2	P	85	GLU
2	P	100	VAL

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Mol	Chain	Res	Type
2	P	103	GLU
2	P	112	ASP
2	P	121	LYS
2	P	124	LEU
2	P	128	ASP
2	P	131	LYS
2	P	147	GLU
2	P	153	ARG
2	P	158	ASP
2	P	164	GLU
2	P	172	GLU
2	P	173	ILE
1	Q	17	TYR
1	Q	20	ASN
1	Q	23	GLU
1	Q	25	VAL
1	Q	27	THR
1	Q	32	GLU
1	Q	44	GLU
1	Q	46	LYS
1	Q	48	ASN
1	Q	51	LEU
1	Q	52	CYS
1	Q	57	LYS
1	Q	61	LEU
1	Q	62	ARG
1	Q	75	MET
1	Q	85	SER
1	Q	95	ASN
1	Q	102	PHE
1	Q	109	LYS
1	Q	115	ILE
1	Q	123	ILE
1	Q	124	ILE
1	Q	127	TRP
1	Q	135	VAL
1	Q	151	VAL
1	Q	169	ASN
1	Q	170	ASN
1	Q	176	LEU
1	Q	178	VAL
1	Q	186	ASN

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Mol	Chain	Res	Type
1	Q	191	GLN
1	Q	195	TYR
1	Q	199	THR
1	Q	202	ILE
1	Q	211	GLN
1	Q	216	ARG
1	Q	223	VAL
1	Q	235	THR
1	Q	236	ILE
1	Q	238	LYS
1	Q	260	ILE
1	Q	262	LYS
1	Q	272	LEU
1	Q	281	CYS
1	Q	289	ASN
1	Q	295	HIS
1	Q	300	LEU
1	Q	302	ILE
1	Q	304	GLU
1	Q	310	LYS
1	Q	312	ASN
1	Q	315	VAL
1	Q	320	LEU
1	Q	322	ASN
1	Q	323	SER
2	R	21	TRP
2	R	22	TYR
2	R	24	TYR
2	R	30	GLN
2	R	43	LYS
2	R	59	MET
2	R	62	GLN
2	R	63	PHE
2	R	66	VAL
2	R	69	GLU
2	R	79	ASN
2	R	80	LEU
2	R	89	LEU
2	R	95	ASN
2	R	98	LEU
2	R	99	LEU
2	R	106	ARG

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Mol	Chain	Res	Type
2	R	113	SER
2	R	121	LYS
2	R	126	LEU
2	R	127	ARG
2	R	131	LYS
2	R	161	GLN
2	R	164	GLU
2	R	167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	92	ASN
1	A	110	HIS
1	A	197	ASN
2	B	25	HIS
2	B	26	HIS
2	B	50	ASN
2	B	79	ASN
2	B	81	ASN
2	B	117	ASN
1	C	38	HIS
1	C	81	ASN
1	C	110	HIS
1	C	197	ASN
2	D	15	GLN
2	D	25	HIS
2	D	42	GLN
2	D	50	ASN
2	D	79	ASN
2	D	81	ASN
2	D	117	ASN
1	E	47	HIS
1	E	197	ASN
1	E	210	ASN
1	E	295	HIS
2	F	25	HIS
2	F	79	ASN
2	F	81	ASN
2	F	117	ASN
2	F	142	HIS

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Mol	Chain	Res	Type
1	G	197	ASN
1	G	295	HIS
2	H	25	HIS
2	H	79	ASN
2	H	81	ASN
2	H	117	ASN
1	I	38	HIS
1	I	81	ASN
1	I	92	ASN
1	I	110	HIS
1	I	197	ASN
2	J	15	GLN
2	J	25	HIS
2	J	50	ASN
2	J	79	ASN
2	J	81	ASN
2	J	117	ASN
1	K	110	HIS
1	K	158	ASN
1	K	197	ASN
1	K	210	ASN
1	K	226	GLN
1	K	295	HIS
2	L	25	HIS
2	L	50	ASN
2	L	79	ASN
2	L	81	ASN
1	M	12	GLN
1	M	48	ASN
1	M	81	ASN
1	M	95	ASN
1	M	117	HIS
1	M	172	ASN
1	M	191	GLN
1	M	295	HIS
1	M	312	ASN
2	N	15	GLN
2	N	26	HIS
2	N	30	GLN
2	N	53	ASN
2	N	79	ASN
2	N	117	ASN

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Mol	Chain	Res	Type
2	N	125	GLN
2	N	142	HIS
1	O	38	HIS
1	O	117	HIS
1	O	172	ASN
1	O	173	GLN
1	O	196	GLN
1	O	226	GLN
1	O	322	ASN
2	P	15	GLN
2	P	53	ASN
2	P	79	ASN
2	P	81	ASN
2	P	117	ASN
2	P	129	ASN
2	P	135	ASN
1	Q	18	HIS
1	Q	19(A)	ASN
1	Q	24	GLN
1	Q	38	HIS
1	Q	81	ASN
1	Q	92	ASN
1	Q	95	ASN
1	Q	116	ASN
1	Q	122	GLN
1	Q	130	HIS
1	Q	150	ASN
1	Q	170	ASN
1	Q	211	GLN
1	Q	276	ASN
1	Q	278	ASN
1	Q	295	HIS
2	R	15	GLN
2	R	25	HIS
2	R	26	HIS
2	R	30	GLN
2	R	42	GLN
2	R	81	ASN
2	R	114	ASN
2	R	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

35 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	S	1	3,1	14,14,15	0.63	0	17,19,21	1.48	3 (17%)
3	NAG	S	2	3	14,14,15	0.98	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	T	1	4,1	14,14,15	0.71	0	17,19,21	1.77	3 (17%)
4	NAG	T	2	4	14,14,15	0.76	0	17,19,21	1.78	5 (29%)
4	BMA	T	3	4	11,11,12	0.68	0	15,15,17	1.33	1 (6%)
3	NAG	U	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	2.73	6 (35%)
3	NAG	U	2	3	14,14,15	0.61	0	17,19,21	1.63	3 (17%)
3	NAG	V	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	2.35	6 (35%)
3	NAG	V	2	3	14,14,15	0.59	0	17,19,21	1.80	4 (23%)
3	NAG	W	1	3,1	14,14,15	0.62	0	17,19,21	1.80	5 (29%)
3	NAG	W	2	3	14,14,15	0.97	1 (7%)	17,19,21	1.75	2 (11%)
4	NAG	X	1	4,1	14,14,15	0.66	0	17,19,21	1.39	2 (11%)
4	NAG	X	2	4	14,14,15	0.58	0	17,19,21	1.37	3 (17%)
4	BMA	X	3	4	11,11,12	0.84	0	15,15,17	2.26	4 (26%)
3	NAG	Y	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	1.23	1 (5%)
3	NAG	Y	2	3	14,14,15	1.06	1 (7%)	17,19,21	1.46	2 (11%)
4	NAG	Z	1	4,1	14,14,15	0.79	0	17,19,21	2.47	5 (29%)
4	NAG	Z	2	4	14,14,15	0.76	0	17,19,21	1.50	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	Z	3	4	11,11,12	0.55	0	15,15,17	2.47	2 (13%)
3	NAG	a	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	2.88	7 (41%)
3	NAG	a	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.63	4 (23%)
3	NAG	b	1	3,1	14,14,15	0.86	1 (7%)	17,19,21	1.62	5 (29%)
3	NAG	b	2	3	14,14,15	0.65	0	17,19,21	1.54	3 (17%)
3	NAG	c	1	3,1	14,14,15	0.79	0	17,19,21	2.15	5 (29%)
3	NAG	c	2	3	14,14,15	1.08	1 (7%)	17,19,21	2.65	6 (35%)
3	NAG	d	1	3,1	14,14,15	0.74	0	17,19,21	1.90	4 (23%)
3	NAG	d	2	3	14,14,15	0.54	0	17,19,21	1.34	2 (11%)
3	NAG	e	1	3,1	14,14,15	0.84	0	17,19,21	1.70	3 (17%)
3	NAG	e	2	3	14,14,15	0.99	1 (7%)	17,19,21	1.14	1 (5%)
3	NAG	f	1	3,1	14,14,15	0.95	1 (7%)	17,19,21	1.86	4 (23%)
3	NAG	f	2	3	14,14,15	0.90	1 (7%)	17,19,21	2.08	5 (29%)
3	NAG	g	1	3,1	14,14,15	0.95	1 (7%)	17,19,21	2.02	6 (35%)
3	NAG	g	2	3	14,14,15	1.29	1 (7%)	17,19,21	1.89	3 (17%)
3	NAG	h	1	3,1	14,14,15	0.74	0	17,19,21	2.67	7 (41%)
3	NAG	h	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.37	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	S	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
4	NAG	T	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	T	2	4	-	4/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	NAG	V	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	W	2	3	-	4/6/23/26	0/1/1/1
4	NAG	X	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	1/2/19/22	0/1/1/1
3	NAG	Y	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	6/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
3	NAG	a	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	c	2	3	-	1/6/23/26	0/1/1/1
3	NAG	d	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	4/6/23/26	0/1/1/1
3	NAG	e	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	3/6/23/26	0/1/1/1
3	NAG	g	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	g	2	3	-	4/6/23/26	0/1/1/1
3	NAG	h	1	3,1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	5/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	NAG	C1-C2	4.01	1.57	1.52
3	S	2	NAG	C1-C2	3.08	1.56	1.52
3	e	2	NAG	C1-C2	2.99	1.56	1.52
3	Y	2	NAG	C1-C2	2.98	1.56	1.52
3	g	1	NAG	C1-C2	2.98	1.56	1.52
3	c	2	NAG	C1-C2	2.84	1.56	1.52
3	f	1	NAG	C1-C2	2.74	1.56	1.52
3	W	2	NAG	C1-C2	2.71	1.56	1.52
3	h	2	NAG	C1-C2	2.47	1.55	1.52
3	a	1	NAG	C1-C2	2.46	1.55	1.52
3	b	1	NAG	C1-C2	2.35	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	2	NAG	C1-C2	2.28	1.55	1.52
3	Y	1	NAG	C1-C2	2.12	1.55	1.52
3	V	1	NAG	O5-C1	-2.09	1.40	1.43
3	U	1	NAG	C1-C2	2.07	1.55	1.52
3	f	2	NAG	C1-C2	2.00	1.55	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	3	BMA	C1-O5-C5	8.78	123.95	112.19
3	U	1	NAG	C1-O5-C5	8.61	123.73	112.19
3	a	1	NAG	C1-O5-C5	8.31	123.33	112.19
4	Z	1	NAG	O5-C1-C2	-6.53	101.19	111.29
3	c	2	NAG	C1-O5-C5	6.33	120.66	112.19
3	V	1	NAG	C1-O5-C5	-5.81	104.40	112.19
3	h	1	NAG	C4-C3-C2	-5.77	102.56	111.02
4	X	3	BMA	C1-C2-C3	5.54	117.71	109.64
3	h	1	NAG	C1-O5-C5	5.40	119.42	112.19
4	T	1	NAG	O5-C1-C2	-5.26	103.15	111.29
3	c	1	NAG	C1-O5-C5	5.18	119.12	112.19
4	X	3	BMA	C1-O5-C5	5.08	119.00	112.19
3	V	2	NAG	C2-N2-C7	-5.03	116.16	122.90
3	f	1	NAG	O5-C1-C2	-5.01	103.54	111.29
3	W	2	NAG	C2-N2-C7	4.88	129.44	122.90
3	f	2	NAG	C2-N2-C7	4.86	129.41	122.90
4	Z	1	NAG	C1-O5-C5	4.78	118.59	112.19
3	h	1	NAG	O5-C1-C2	-4.75	103.95	111.29
3	a	1	NAG	O5-C1-C2	4.64	118.48	111.29
3	g	2	NAG	C1-O5-C5	4.60	118.36	112.19
3	V	1	NAG	C2-N2-C7	-4.60	116.73	122.90
4	T	2	NAG	C1-O5-C5	-4.52	106.13	112.19
3	d	1	NAG	C2-N2-C7	4.41	128.81	122.90
3	U	2	NAG	C3-C4-C5	4.36	118.15	110.23
3	W	1	NAG	C2-N2-C7	-4.36	117.06	122.90
3	f	2	NAG	C4-C3-C2	4.22	117.20	111.02
3	c	2	NAG	C3-C4-C5	4.20	117.85	110.23
3	c	1	NAG	C4-C3-C2	4.04	116.93	111.02
4	T	3	BMA	C1-O5-C5	3.97	117.51	112.19
3	W	2	NAG	C4-C3-C2	3.96	116.82	111.02
3	a	2	NAG	C1-O5-C5	3.94	117.46	112.19
3	c	2	NAG	C4-C3-C2	3.93	116.78	111.02
3	c	2	NAG	O5-C5-C6	3.92	115.29	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	1	NAG	C3-C4-C5	-3.91	103.15	110.23
3	W	1	NAG	C1-O5-C5	3.89	117.40	112.19
3	e	1	NAG	C2-N2-C7	3.86	128.07	122.90
4	X	1	NAG	O5-C1-C2	-3.86	105.32	111.29
4	Z	2	NAG	C4-C3-C2	3.77	116.54	111.02
3	U	1	NAG	C4-C3-C2	-3.72	105.57	111.02
3	h	2	NAG	C4-C3-C2	3.69	116.42	111.02
3	h	1	NAG	C2-N2-C7	-3.61	118.06	122.90
3	d	2	NAG	C1-O5-C5	3.57	116.97	112.19
3	c	2	NAG	C2-N2-C7	3.56	127.67	122.90
3	a	1	NAG	C4-C3-C2	-3.49	105.91	111.02
4	X	2	NAG	C4-C3-C2	3.48	116.12	111.02
3	V	2	NAG	C1-O5-C5	3.40	116.75	112.19
3	c	2	NAG	O5-C1-C2	3.38	116.52	111.29
3	c	1	NAG	C3-C4-C5	3.37	116.33	110.23
3	g	2	NAG	O5-C1-C2	3.36	116.49	111.29
3	g	2	NAG	C2-N2-C7	3.33	127.36	122.90
3	S	1	NAG	C4-C3-C2	-3.25	106.26	111.02
3	V	1	NAG	C8-C7-N2	3.23	121.47	116.12
3	b	1	NAG	C2-N2-C7	3.23	127.22	122.90
3	g	1	NAG	C4-C3-C2	-3.22	106.30	111.02
3	d	1	NAG	C1-O5-C5	3.18	116.45	112.19
3	g	1	NAG	C1-C2-N2	3.17	115.43	110.43
4	Z	2	NAG	C2-N2-C7	-3.14	118.70	122.90
3	f	2	NAG	C1-O5-C5	-3.10	108.03	112.19
3	b	2	NAG	O5-C5-C4	-3.08	103.33	110.83
3	Y	2	NAG	C2-N2-C7	3.06	127.01	122.90
3	U	2	NAG	O5-C1-C2	-3.03	106.60	111.29
3	f	2	NAG	C3-C4-C5	3.03	115.72	110.23
3	c	1	NAG	O5-C5-C6	2.97	113.45	107.66
3	b	1	NAG	O5-C1-C2	-2.96	106.70	111.29
4	T	1	NAG	C1-O5-C5	-2.95	108.23	112.19
3	f	1	NAG	C3-C4-C5	-2.94	104.91	110.23
3	e	1	NAG	C1-O5-C5	2.93	116.11	112.19
3	h	1	NAG	O4-C4-C5	2.92	116.50	109.32
3	b	2	NAG	C1-C2-N2	-2.91	105.84	110.43
3	e	1	NAG	C4-C3-C2	2.90	115.27	111.02
3	d	1	NAG	C1-C2-N2	-2.89	105.88	110.43
3	S	2	NAG	O5-C1-C2	2.86	115.72	111.29
4	X	1	NAG	C1-O5-C5	2.84	116.00	112.19
3	Y	1	NAG	C1-O5-C5	2.80	115.94	112.19
3	S	1	NAG	C1-O5-C5	2.80	115.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	1	NAG	O5-C5-C4	-2.75	104.13	110.83
3	a	1	NAG	O4-C4-C3	2.74	116.83	110.38
4	Z	2	NAG	C1-C2-N2	-2.72	106.15	110.43
3	a	2	NAG	C4-C3-C2	2.71	114.98	111.02
3	b	2	NAG	C3-C4-C5	-2.67	105.39	110.23
3	g	1	NAG	C1-O5-C5	2.66	115.76	112.19
4	Z	1	NAG	C2-N2-C7	-2.63	119.38	122.90
3	b	1	NAG	C3-C4-C5	2.59	114.94	110.23
3	g	1	NAG	O4-C4-C5	2.59	115.71	109.32
3	U	1	NAG	O3-C3-C2	2.55	114.71	109.40
4	T	2	NAG	O3-C3-C2	-2.50	104.20	109.40
3	f	1	NAG	C1-C2-N2	2.48	114.35	110.43
4	X	3	BMA	O5-C1-C2	2.48	116.70	110.79
4	T	2	NAG	O5-C5-C4	-2.48	104.80	110.83
3	c	1	NAG	O4-C4-C5	-2.46	103.26	109.32
3	U	1	NAG	O4-C4-C5	2.46	115.38	109.32
3	a	2	NAG	O5-C1-C2	2.45	115.08	111.29
4	Z	3	BMA	O5-C5-C4	2.42	116.72	110.83
4	X	2	NAG	C3-C4-C5	2.42	114.62	110.23
3	a	2	NAG	C3-C4-C5	2.39	114.57	110.23
4	Z	1	NAG	C1-C2-N2	-2.38	106.67	110.43
3	a	1	NAG	C1-C2-N2	2.36	114.16	110.43
3	V	2	NAG	O5-C1-C2	2.34	114.91	111.29
3	h	1	NAG	C1-C2-N2	2.33	114.10	110.43
3	U	1	NAG	C3-C4-C5	-2.32	106.03	110.23
3	b	1	NAG	C1-C2-N2	2.31	114.07	110.43
3	S	1	NAG	C2-N2-C7	2.31	125.99	122.90
3	V	1	NAG	O5-C1-C2	-2.30	107.73	111.29
4	Z	1	NAG	O5-C5-C6	-2.30	103.19	107.66
3	d	1	NAG	O5-C1-C2	-2.29	107.75	111.29
3	d	2	NAG	O4-C4-C5	2.28	114.95	109.32
4	X	3	BMA	C2-C3-C4	2.28	114.87	110.86
4	T	2	NAG	O5-C5-C6	2.26	112.07	107.66
3	W	1	NAG	C3-C4-C5	-2.25	106.15	110.23
4	X	2	NAG	C1-O5-C5	2.24	115.19	112.19
3	W	1	NAG	O5-C5-C6	2.22	111.98	107.66
3	U	2	NAG	C4-C3-C2	2.22	114.27	111.02
3	W	1	NAG	O5-C1-C2	-2.21	107.87	111.29
3	U	1	NAG	C1-C2-N2	2.21	113.92	110.43
3	e	2	NAG	C4-C3-C2	2.21	114.25	111.02
3	b	1	NAG	O7-C7-C8	-2.14	118.25	122.05
3	Y	2	NAG	O5-C5-C6	2.10	111.74	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	1	NAG	O4-C4-C5	2.09	114.47	109.32
3	V	2	NAG	C3-C4-C5	2.07	113.99	110.23
3	f	1	NAG	O5-C5-C6	2.06	111.68	107.66
3	f	2	NAG	C8-C7-N2	2.06	119.53	116.12
3	V	1	NAG	O7-C7-N2	-2.05	118.36	121.98
4	T	2	NAG	O5-C1-C2	2.05	114.46	111.29
3	a	1	NAG	C3-C4-C5	-2.04	106.53	110.23
3	a	1	NAG	O7-C7-C8	-2.04	118.42	122.05
3	g	1	NAG	O5-C1-C2	-2.03	108.15	111.29
3	h	1	NAG	O5-C5-C4	2.01	115.71	110.83

All (7) chirality outliers are listed below:

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

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C3-C2-N2-C7
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C3-C2-N2-C7
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C3-C2-N2-C7
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2

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

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

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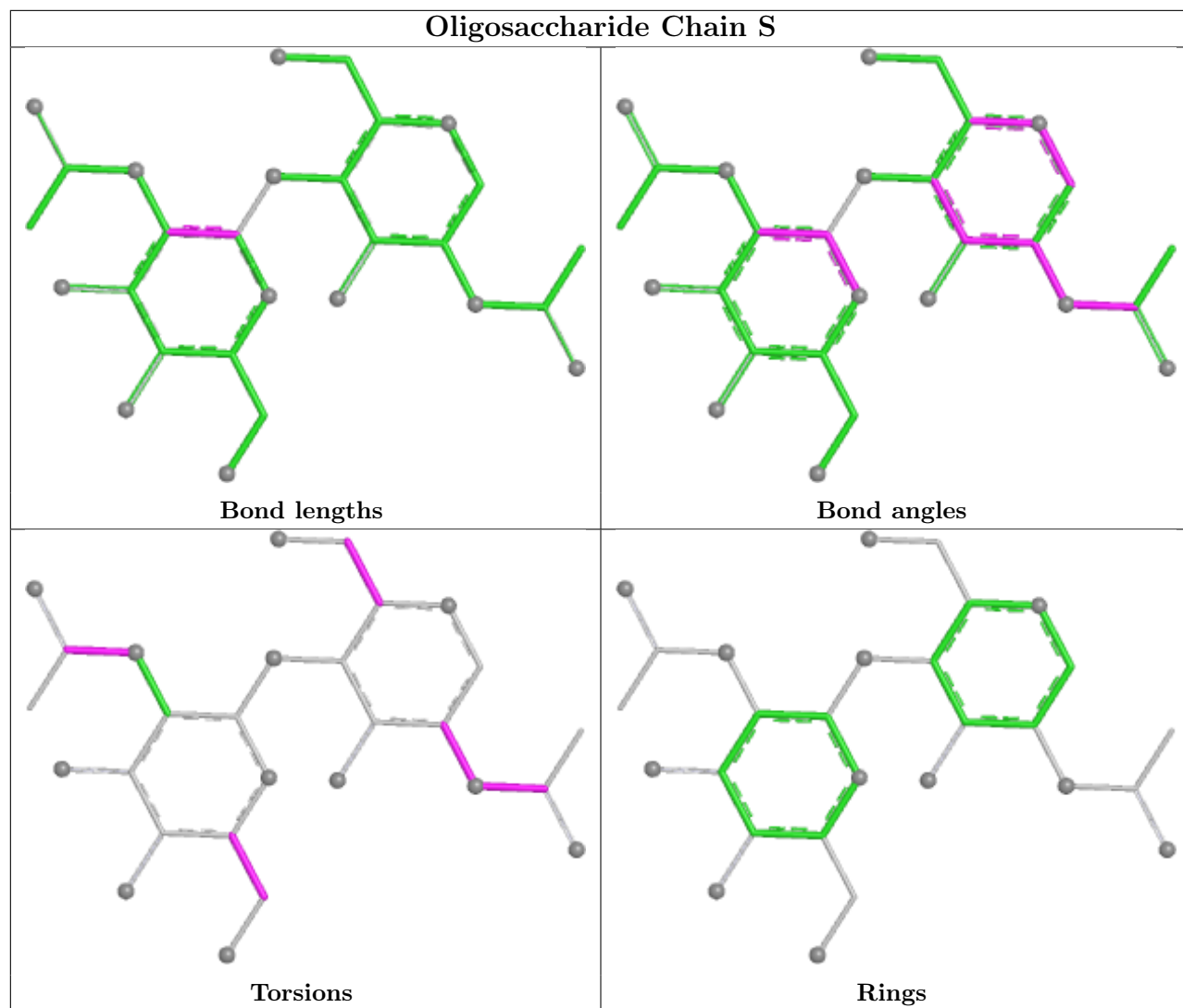
Mol	Chain	Res	Type	Atoms
3	h	2	NAG	O5-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6

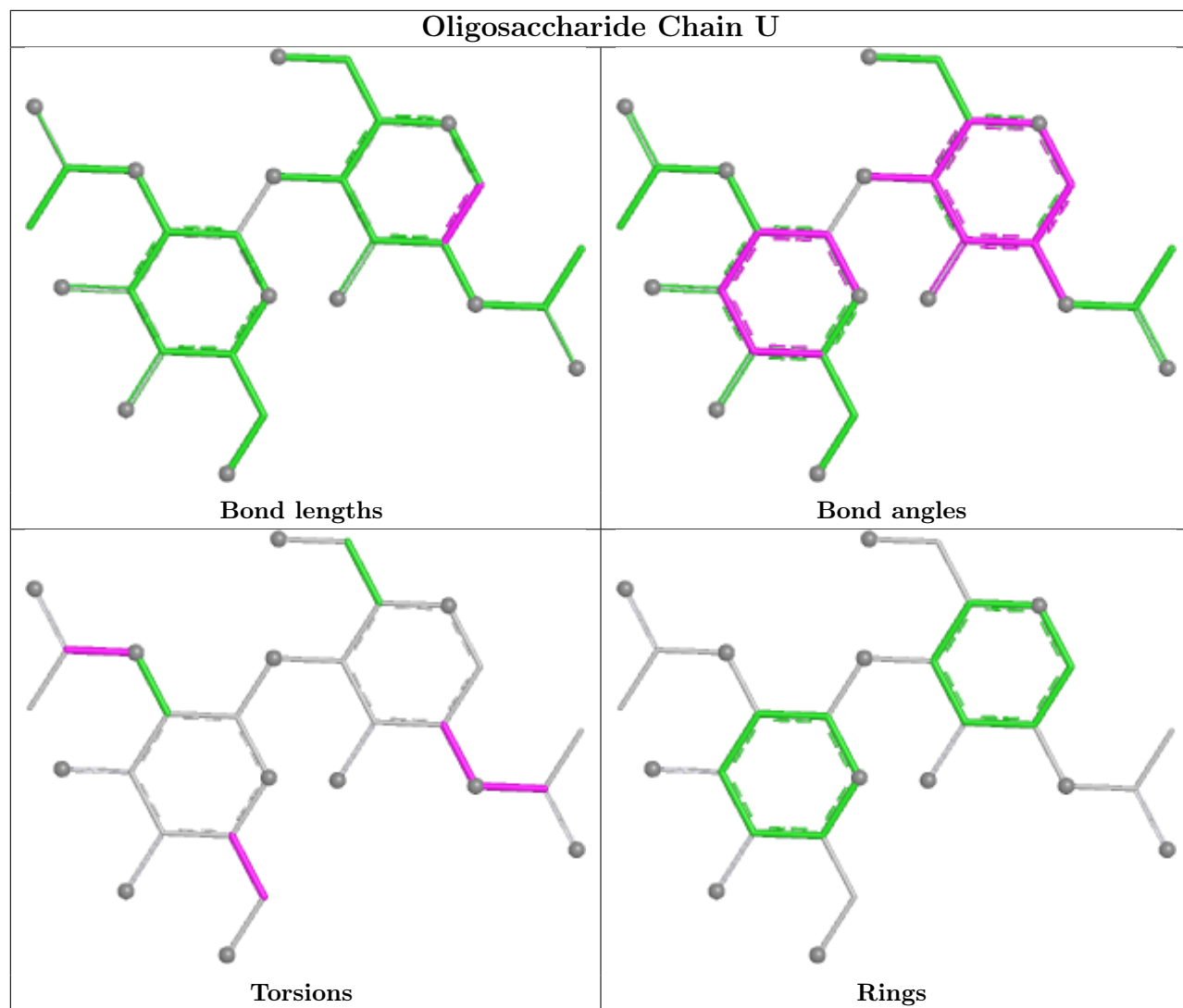
There are no ring outliers.

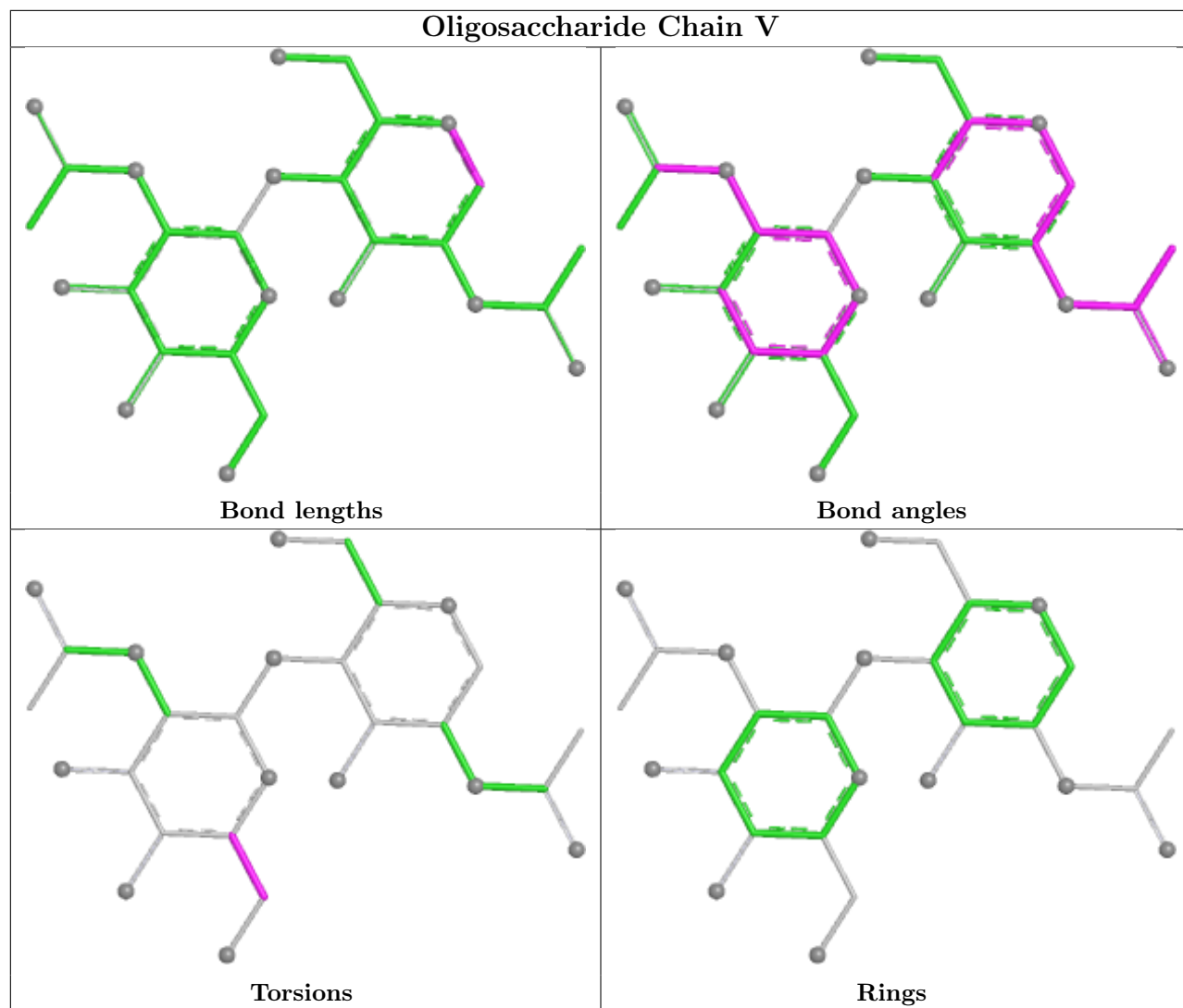
15 monomers are involved in 17 short contacts:

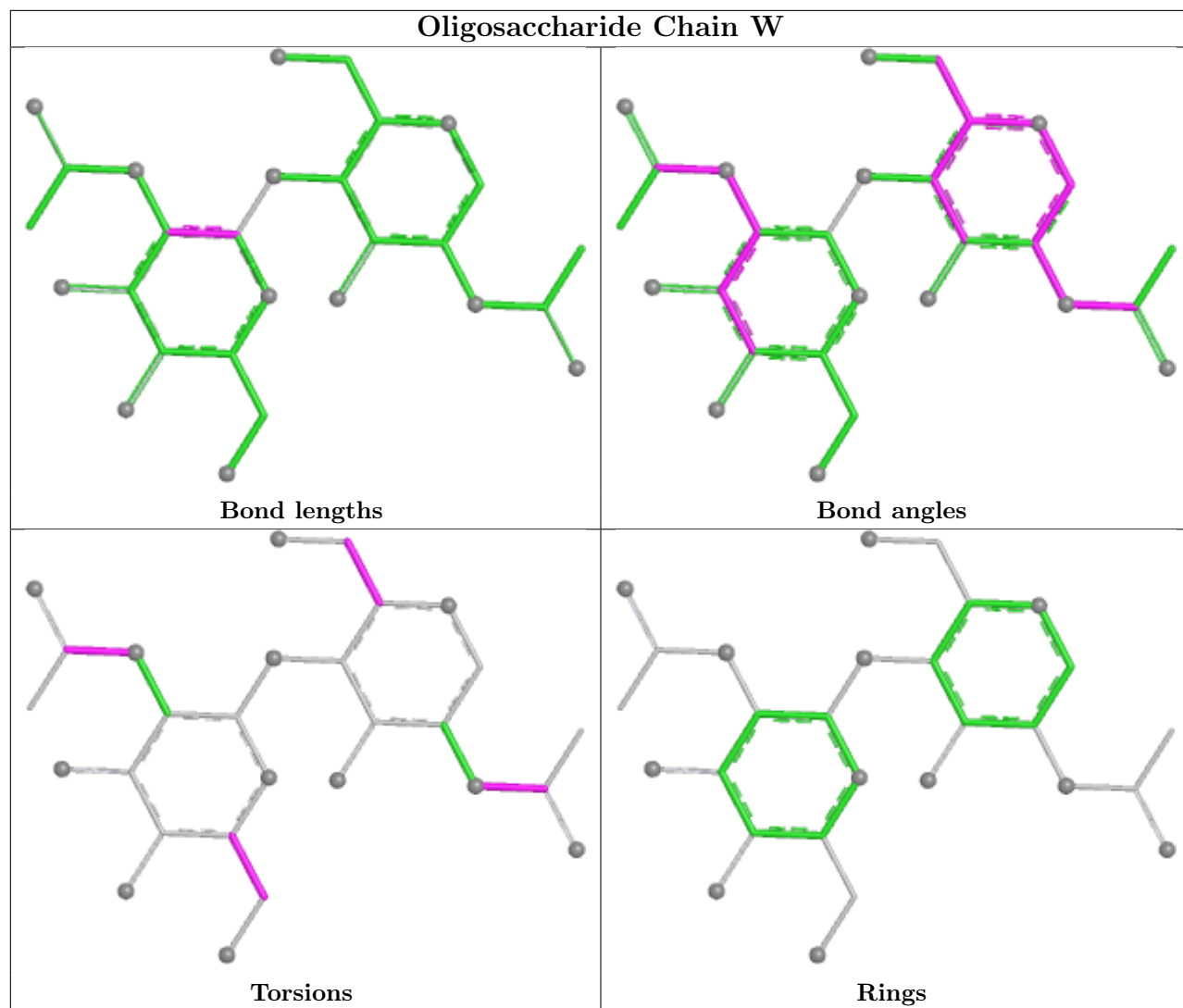
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	e	1	NAG	1	0
3	U	1	NAG	1	0
3	g	2	NAG	1	0
3	S	1	NAG	1	0
3	f	2	NAG	3	0
3	Y	2	NAG	2	0
3	f	1	NAG	2	0
4	X	3	BMA	3	0
3	g	1	NAG	2	0
4	T	1	NAG	1	0
4	T	2	NAG	3	0
3	Y	1	NAG	2	0
3	S	2	NAG	1	0
3	e	2	NAG	1	0
3	a	1	NAG	1	0

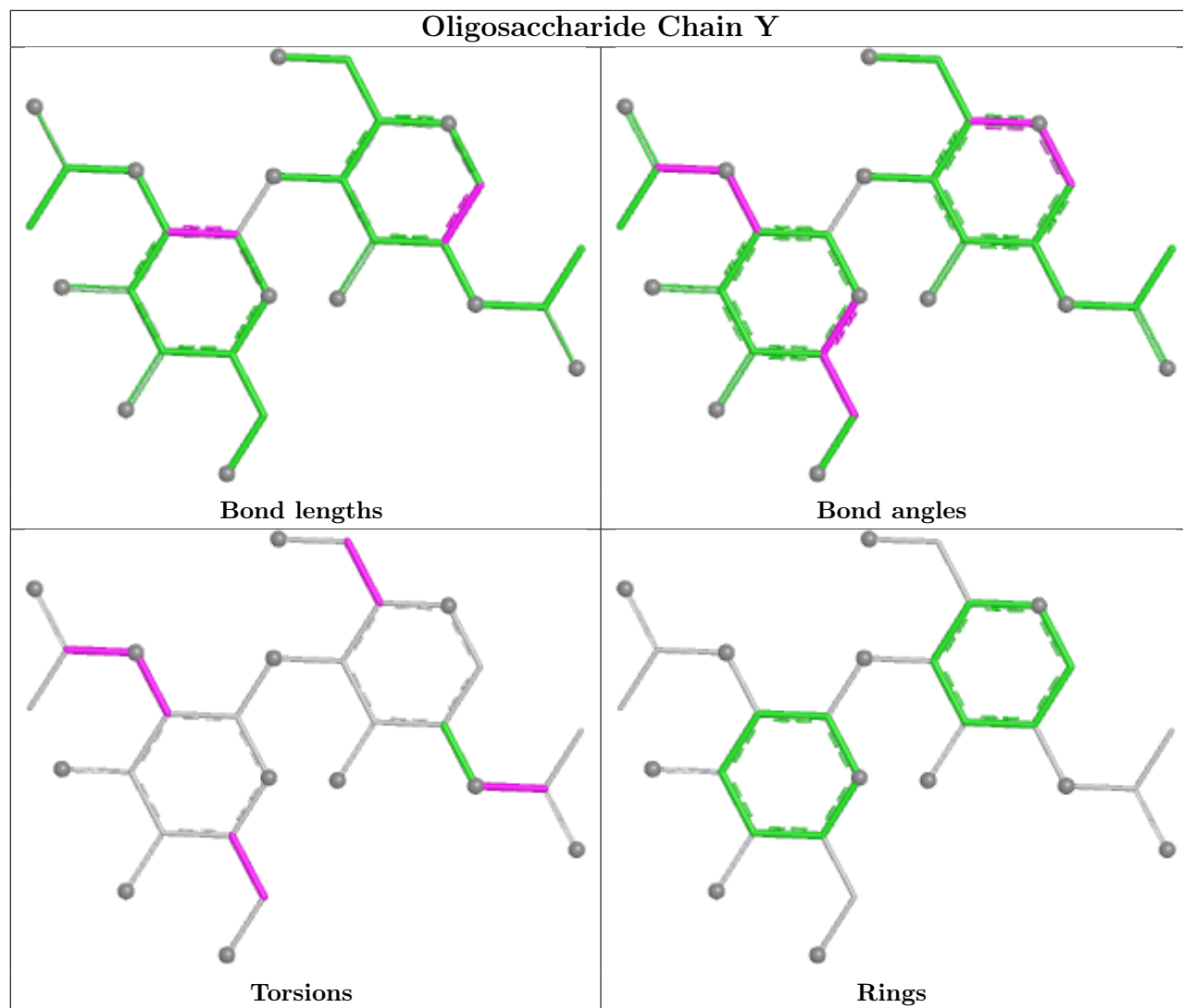
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

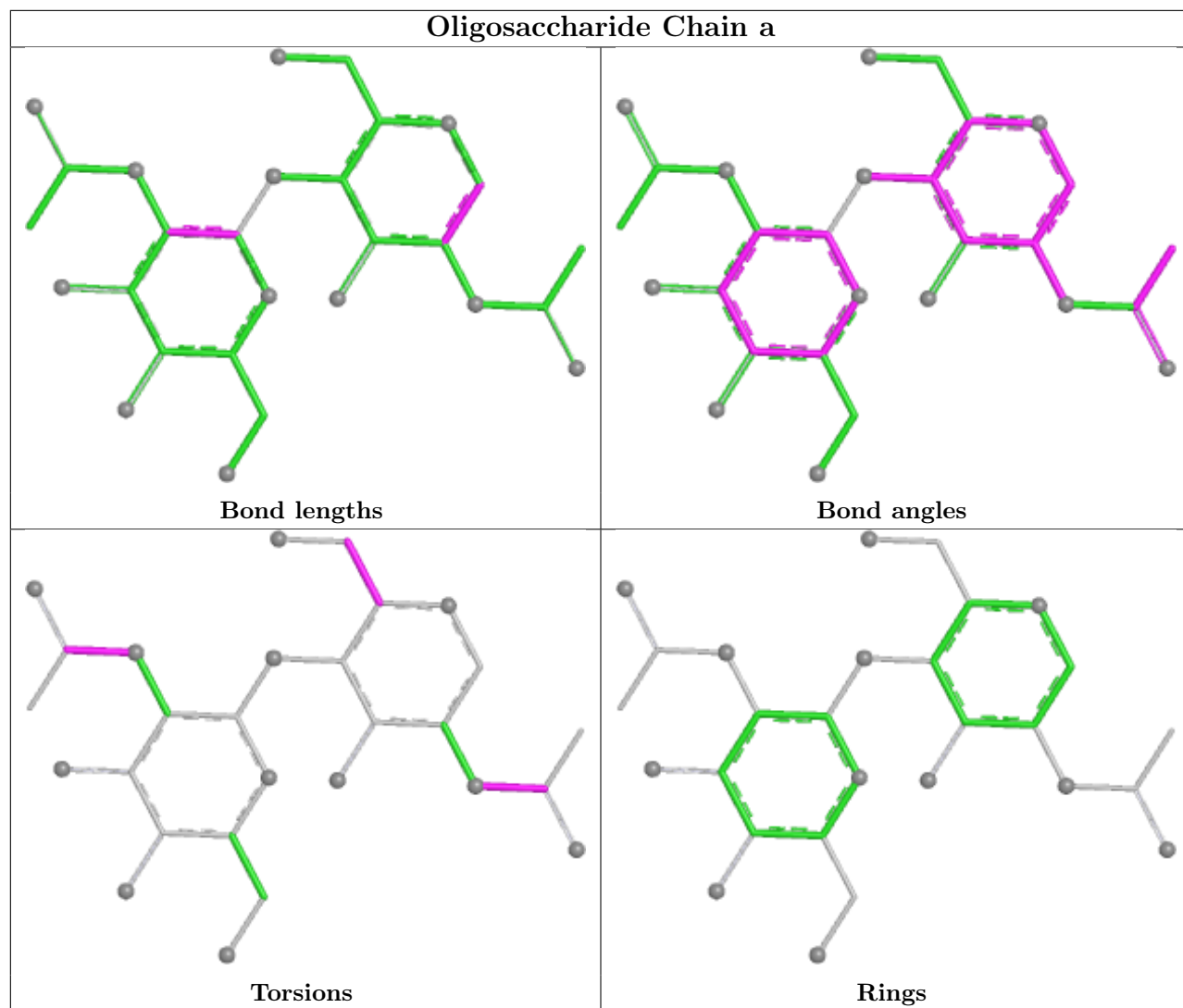


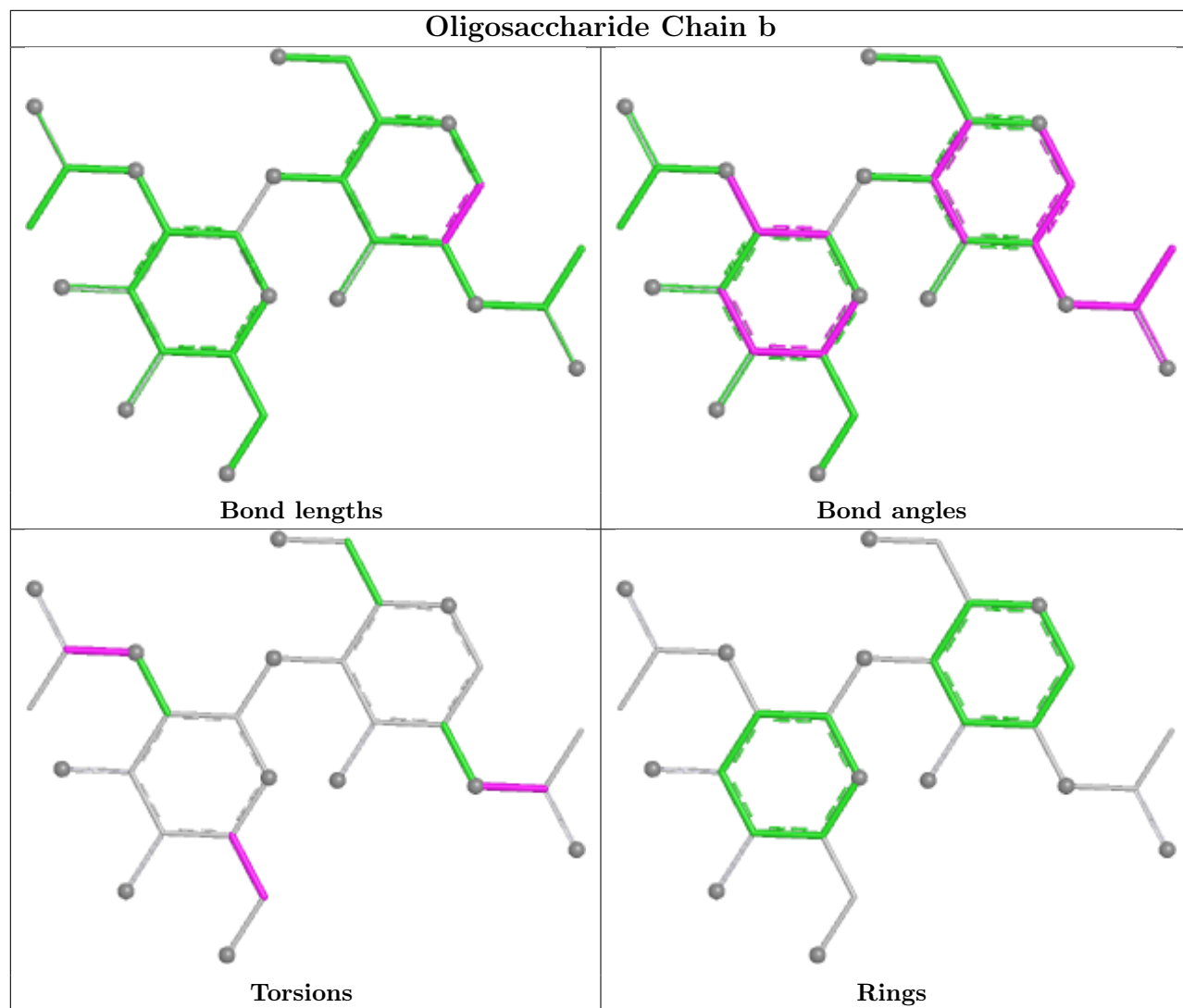


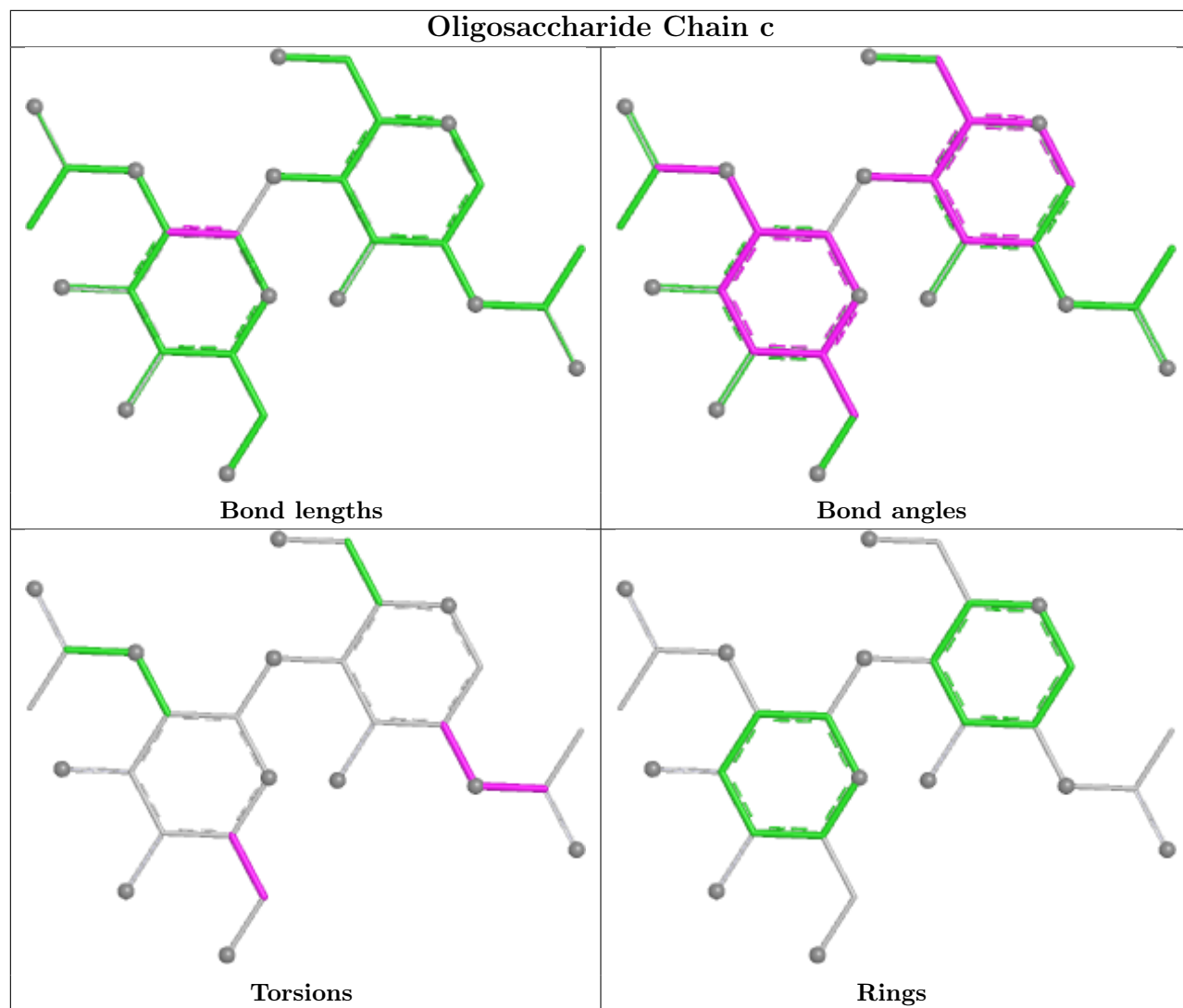


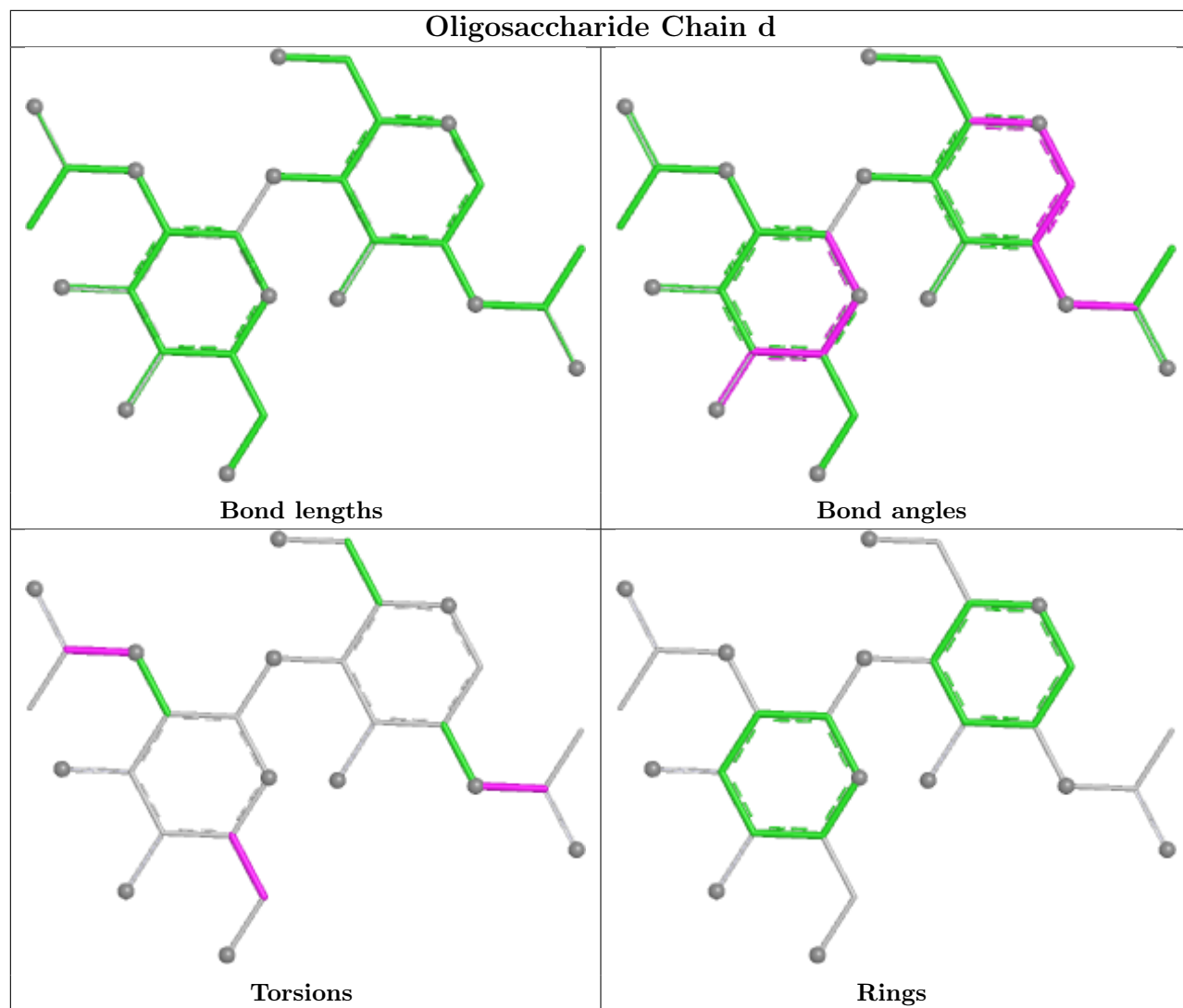


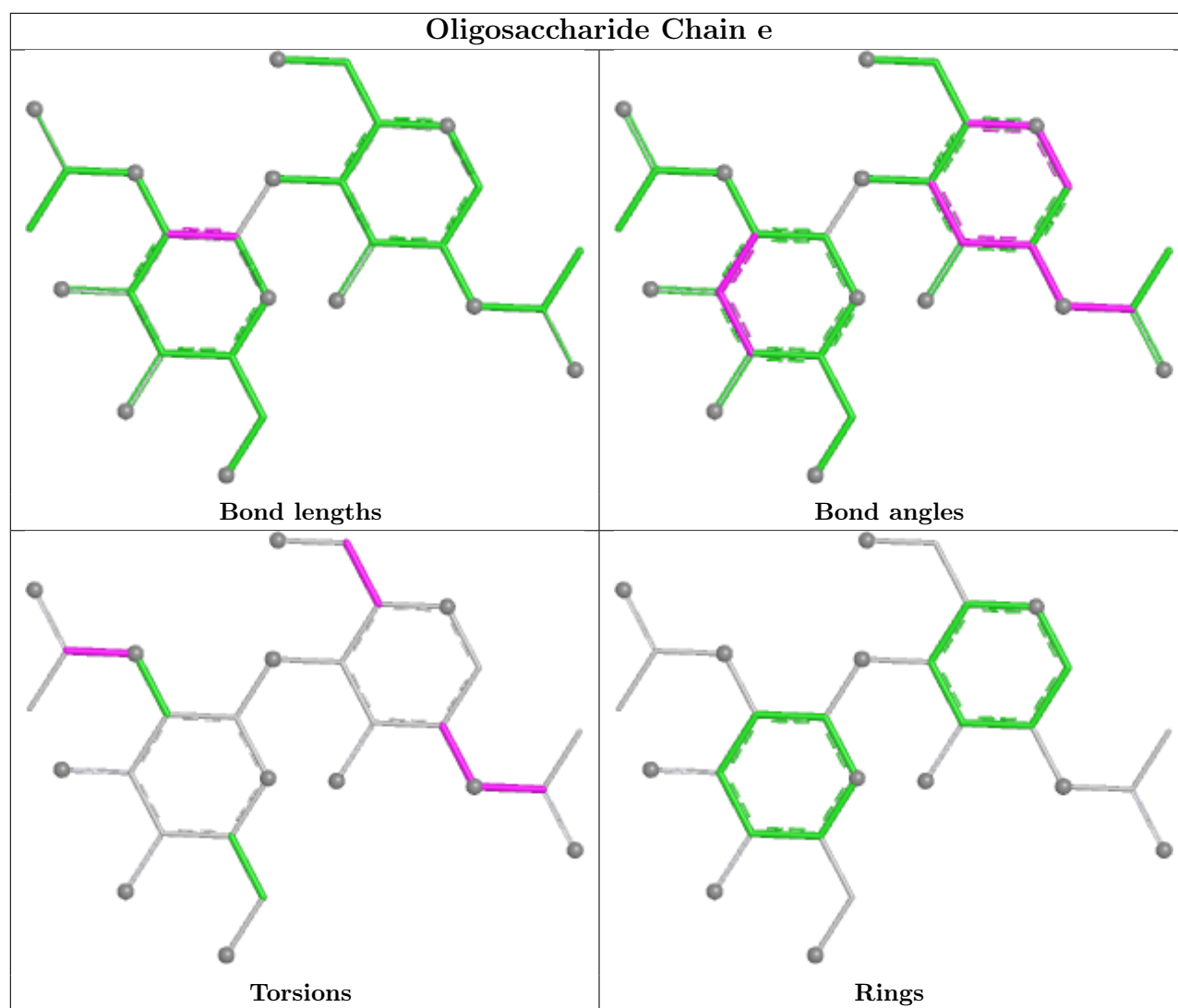


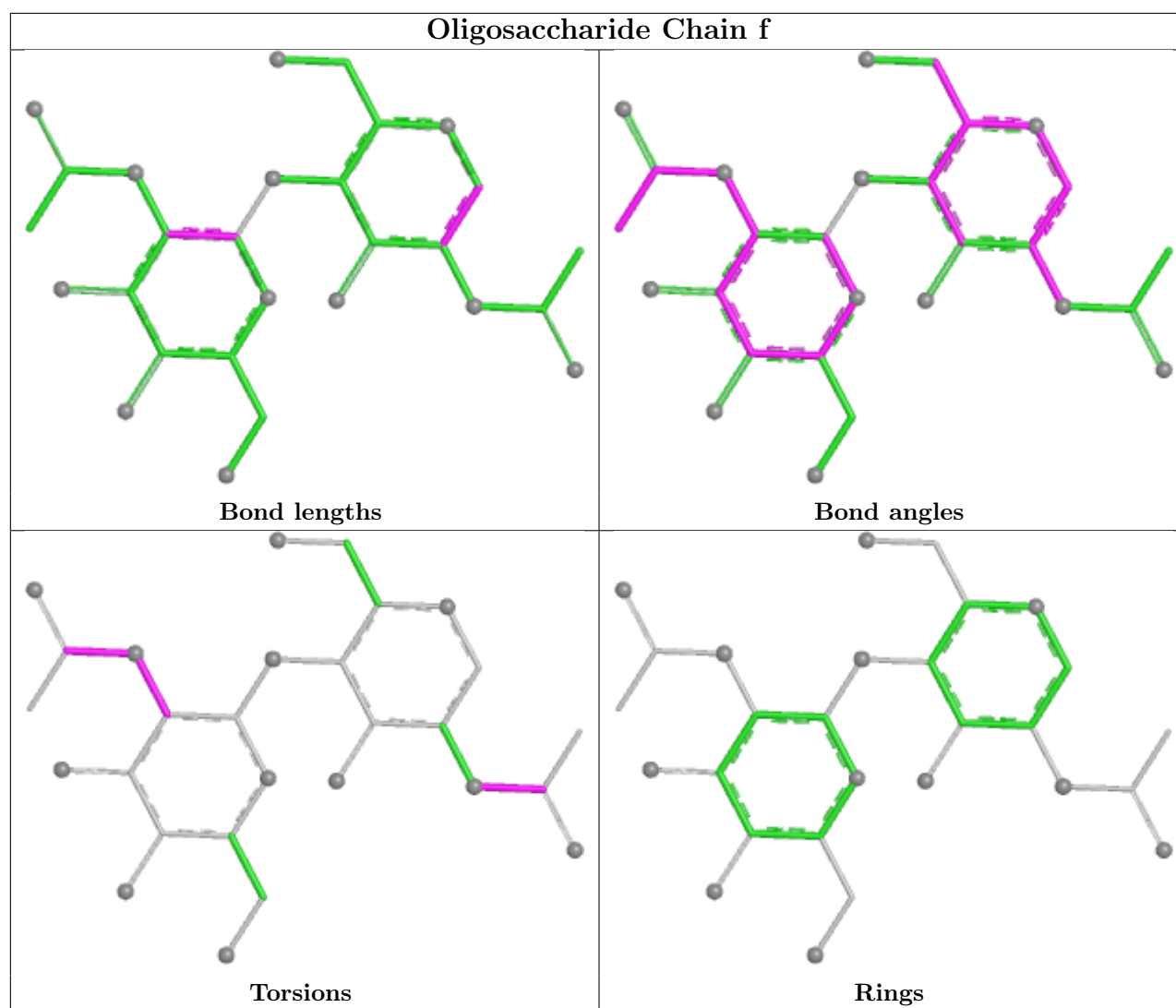


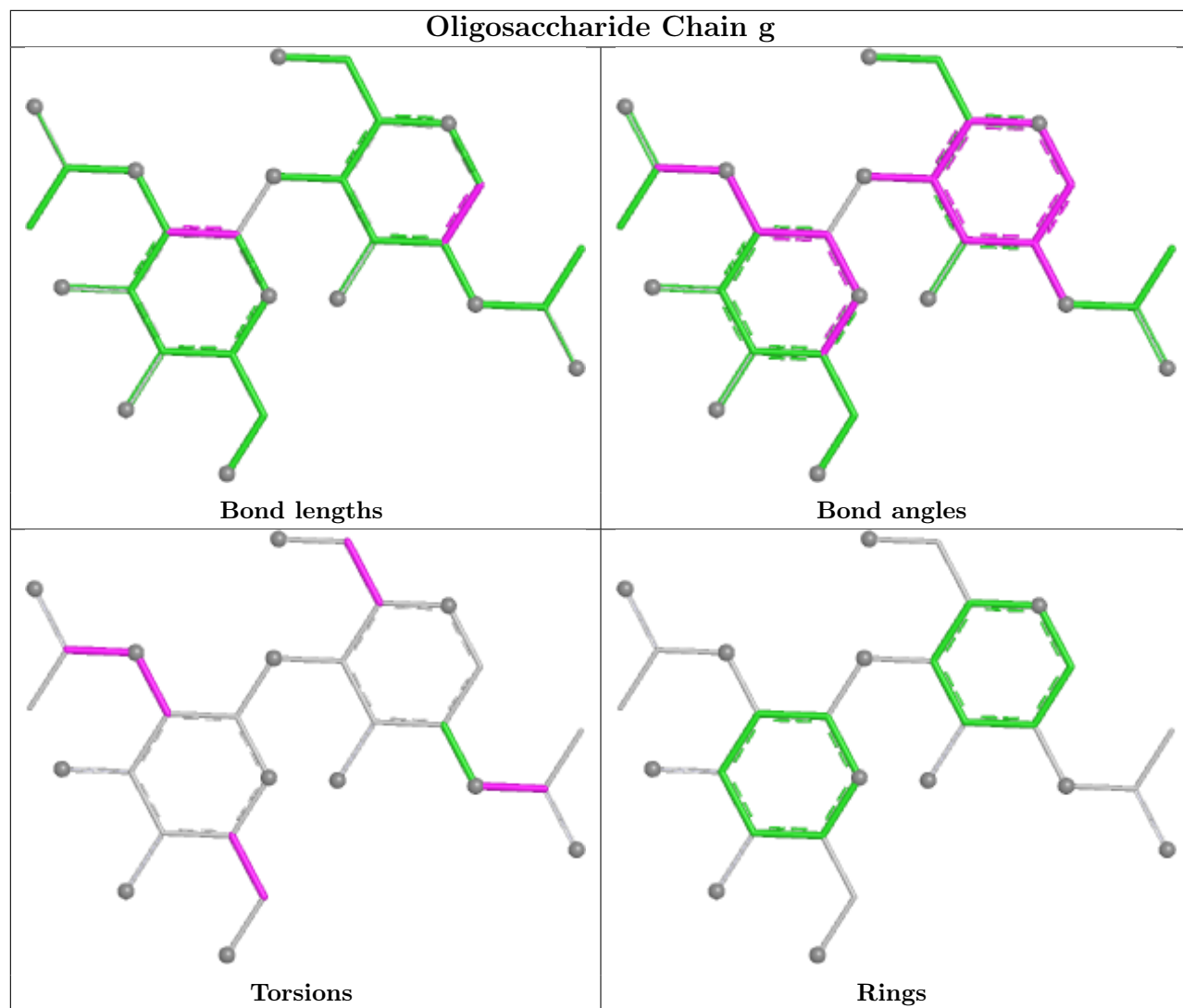


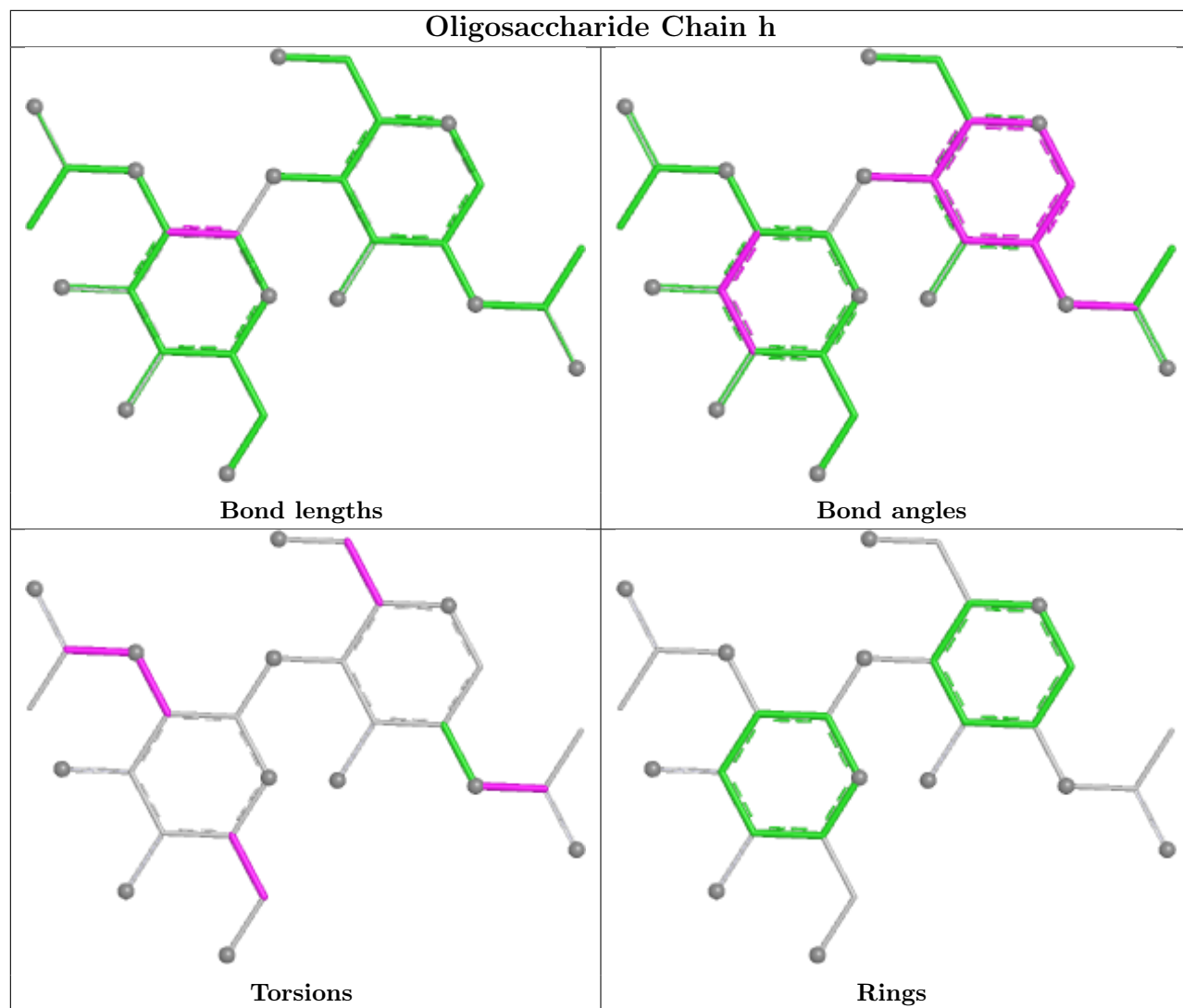


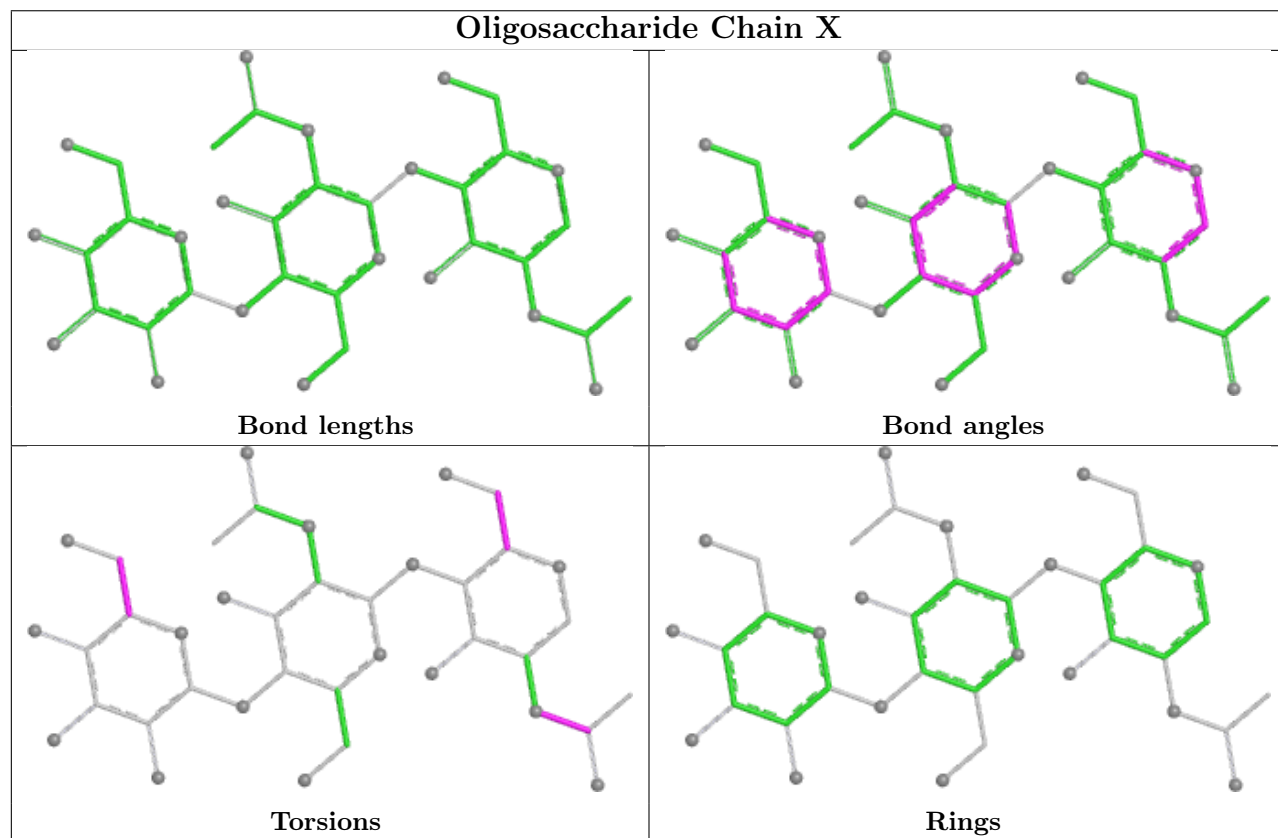
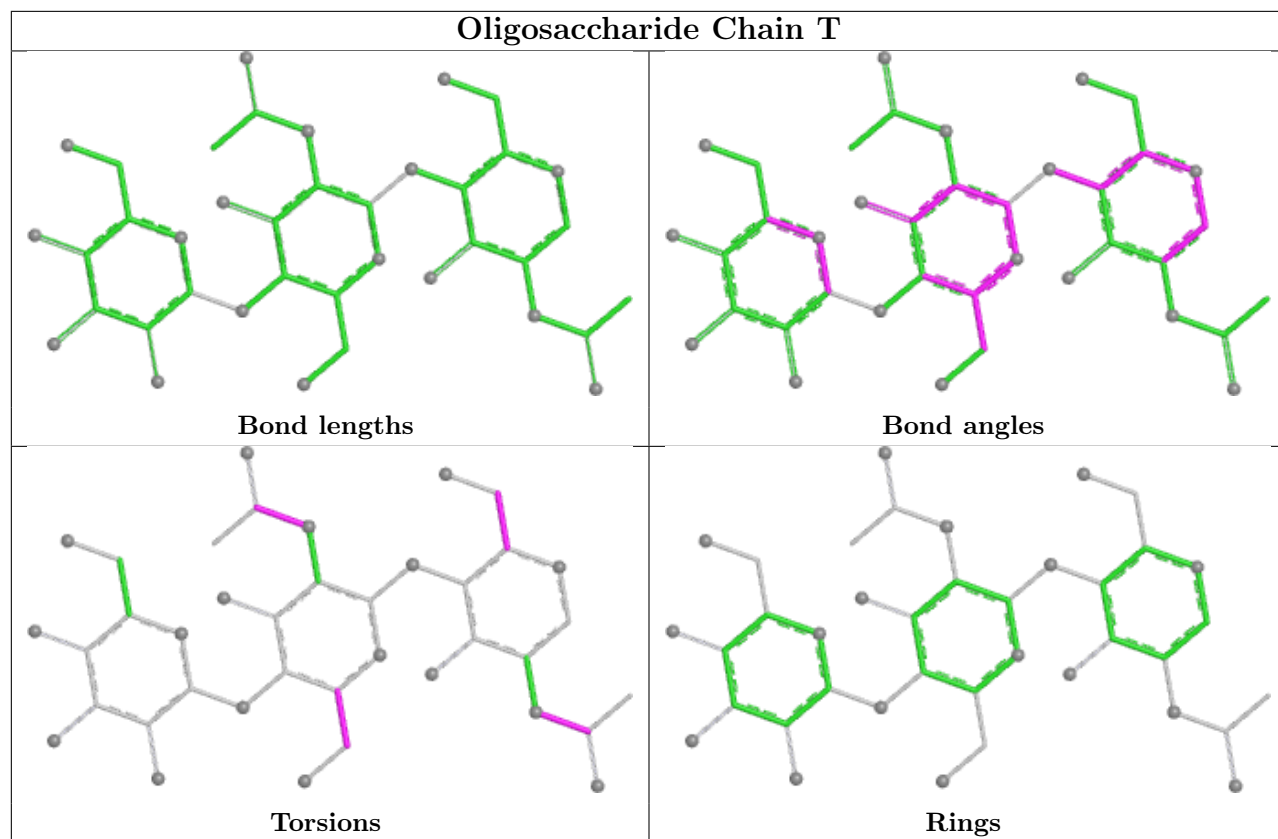


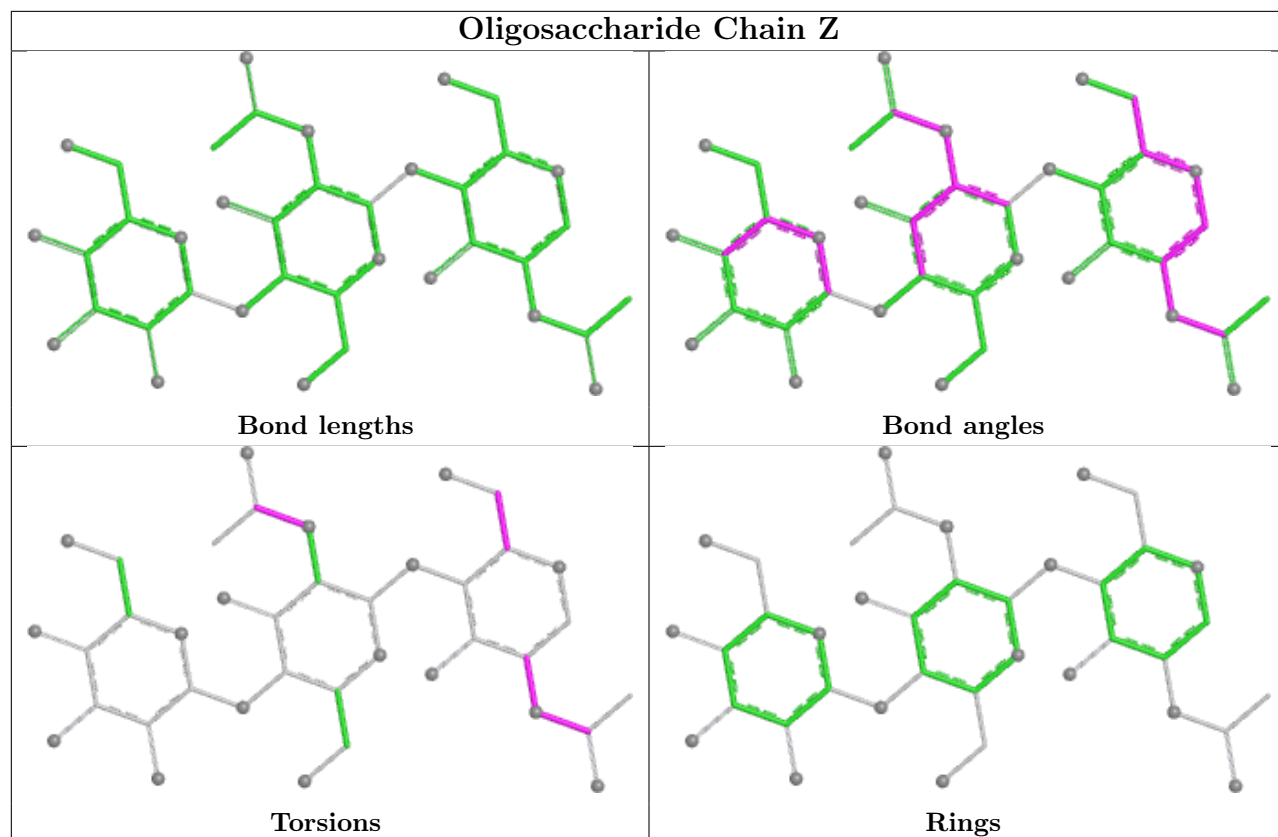












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/334 (96%)	1.29	46 (14%) 6 6	70, 71, 72, 73	0
1	C	322/334 (96%)	1.18	42 (13%) 7 7	70, 71, 72, 73	0
1	E	322/334 (96%)	1.39	54 (16%) 4 4	70, 71, 72, 73	0
1	G	322/334 (96%)	1.40	73 (22%) 2 2	70, 71, 72, 73	0
1	I	322/334 (96%)	1.36	60 (18%) 3 3	70, 71, 72, 73	0
1	K	322/334 (96%)	1.26	45 (13%) 6 6	70, 71, 72, 74	0
1	M	322/334 (96%)	1.26	65 (20%) 3 2	54, 67, 75, 84	0
1	O	322/334 (96%)	1.18	48 (14%) 5 5	57, 68, 76, 83	0
1	Q	322/334 (96%)	1.26	44 (13%) 6 6	63, 72, 81, 86	0
2	B	175/181 (96%)	1.91	65 (37%) 1 1	70, 71, 72, 73	0
2	D	175/181 (96%)	1.94	75 (42%) 0 0	70, 71, 72, 73	0
2	F	175/181 (96%)	1.68	57 (32%) 1 1	70, 71, 72, 73	0
2	H	175/181 (96%)	1.90	66 (37%) 1 0	70, 71, 72, 73	0
2	J	175/181 (96%)	1.66	57 (32%) 1 1	70, 71, 72, 73	0
2	L	175/181 (96%)	1.77	64 (36%) 1 1	70, 71, 72, 73	0
2	N	175/181 (96%)	1.20	26 (14%) 5 5	55, 71, 82, 87	0
2	P	175/181 (96%)	1.14	31 (17%) 4 3	58, 68, 80, 82	0
2	R	175/181 (96%)	1.28	26 (14%) 5 5	60, 70, 85, 87	0
All	All	4473/4635 (96%)	1.40	944 (21%) 2 2	54, 71, 77, 87	0

All (944) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	13	ILE	8.7
2	D	175	SER	8.0
2	F	140	PHE	7.8

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Mol	Chain	Res	Type	RSRZ
1	E	80	ILE	6.0
2	B	1	GLY	5.9
2	H	73	LEU	5.8
2	H	5	ALA	5.7
2	H	76	ARG	5.7
2	D	5	ALA	5.7
1	C	16	GLY	5.6
1	E	16	GLY	5.5
2	D	66	VAL	5.5
1	O	272	LEU	5.5
2	B	2	LEU	5.3
2	D	73	LEU	5.3
2	H	66	VAL	5.3
2	F	175	SER	5.3
2	B	175	SER	5.2
2	J	65	ALA	5.2
2	H	175	SER	5.2
2	L	70	PHE	5.2
1	E	78	GLU	5.2
2	D	77	ILE	5.2
2	H	22	TYR	5.2
2	B	73	LEU	5.1
1	E	15	ILE	5.1
1	G	319	GLY	5.1
1	C	324	PRO	5.1
1	G	80	ILE	5.0
2	H	77	ILE	5.0
1	I	141	TYR	5.0
1	E	79	PHE	4.9
2	B	8	GLY	4.9
2	B	65	ALA	4.9
1	A	80	ILE	4.9
1	G	78	GLU	4.9
2	F	65	ALA	4.9
1	K	79	PHE	4.9
2	H	18	VAL	4.8
2	B	77	ILE	4.8
2	D	80	LEU	4.8
2	H	80	LEU	4.8
2	D	76	ARG	4.8
2	B	70	PHE	4.8
1	Q	324	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
2	J	73	LEU	4.8
2	L	65	ALA	4.8
2	B	6	ILE	4.7
2	J	175	SER	4.7
1	I	142	GLN	4.7
1	A	15	ILE	4.7
2	D	9	PHE	4.6
2	J	168	LEU	4.6
2	B	5	ALA	4.6
2	F	73	LEU	4.6
1	G	79	PHE	4.6
2	D	65	ALA	4.5
1	Q	261	VAL	4.5
2	H	65	ALA	4.5
2	B	67	GLY	4.5
2	J	1	GLY	4.5
2	L	9	PHE	4.5
2	R	175	SER	4.5
2	B	7	ALA	4.4
2	J	66	VAL	4.4
2	D	138	PHE	4.4
1	A	300	LEU	4.4
2	H	6	ILE	4.4
1	G	16	GLY	4.3
2	B	80	LEU	4.3
1	I	79	PHE	4.3
2	L	138	PHE	4.3
2	L	77	ILE	4.3
2	D	134	GLY	4.3
2	D	67	GLY	4.3
2	J	133	LEU	4.2
1	Q	274	TYR	4.2
2	L	80	LEU	4.2
2	D	1	GLY	4.2
2	F	29	GLU	4.2
1	G	302	ILE	4.2
1	G	318	THR	4.1
2	H	124	LEU	4.1
2	H	69	GLU	4.1
2	F	66	VAL	4.1
2	J	67	GLY	4.1
2	L	73	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	Q	80	ILE	4.1
2	J	6	ILE	4.1
2	B	66	VAL	4.0
2	J	7	ALA	4.0
1	Q	302	ILE	4.0
2	H	34	TYR	4.0
1	C	79	PHE	4.0
2	D	144	CYS	4.0
1	E	77	ASP	4.0
1	G	76	CYS	4.0
1	A	301	THR	4.0
2	J	76	ARG	4.0
2	R	18	VAL	4.0
2	R	65	ALA	3.9
2	H	16	GLY	3.9
1	I	302	ILE	3.9
2	H	70	PHE	3.9
2	F	143	LYS	3.9
1	I	60	ILE	3.9
2	L	67	GLY	3.9
2	D	69	GLU	3.9
1	K	81	ASN	3.9
1	O	268	MET	3.9
2	H	141	TYR	3.9
2	P	175	SER	3.9
1	I	16	GLY	3.9
2	D	4	GLY	3.9
2	H	64	GLU	3.9
1	A	284	PRO	3.9
1	A	302	ILE	3.9
1	K	15	ILE	3.9
2	R	134	GLY	3.8
1	G	53(A)	LEU	3.8
1	E	302	ILE	3.8
2	F	76	ARG	3.8
2	L	141	TYR	3.8
2	H	67	GLY	3.8
2	L	76	ARG	3.8
1	C	80	ILE	3.8
1	C	17	TYR	3.8
2	B	168	LEU	3.8
2	H	1	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	70	PHE	3.8
1	C	15	ILE	3.8
1	E	11	ASP	3.8
1	Q	275	GLY	3.8
1	C	302	ILE	3.7
1	O	269	LYS	3.7
2	N	7	ALA	3.7
2	B	60	ASN	3.7
2	D	72	ASN	3.7
2	B	71	ASN	3.7
2	J	172	GLU	3.7
2	L	91	VAL	3.7
2	N	77	ILE	3.7
1	M	242	ALA	3.7
2	L	71	ASN	3.7
2	H	138	PHE	3.7
2	F	77	ILE	3.7
2	F	141	TYR	3.7
1	K	82	VAL	3.7
2	B	74	GLU	3.6
2	L	60	ASN	3.6
1	A	53(A)	LEU	3.6
2	L	175	SER	3.6
2	P	66	VAL	3.6
2	R	156	THR	3.6
2	F	124	LEU	3.6
1	K	218	ALA	3.6
2	D	83	LYS	3.6
2	D	136	GLY	3.6
2	P	67	GLY	3.6
2	H	173	ILE	3.6
2	J	173	ILE	3.6
1	I	82	VAL	3.6
1	Q	263	LYS	3.6
2	N	65	ALA	3.6
2	D	23	GLY	3.6
1	K	80	ILE	3.6
2	F	139	GLU	3.6
1	Q	25	VAL	3.5
2	R	133	LEU	3.5
2	R	168	LEU	3.5
1	Q	67	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	N	125	GLN	3.5
2	F	138	PHE	3.5
1	I	51	LEU	3.5
2	L	168	LEU	3.5
1	G	284	PRO	3.5
2	B	68	ARG	3.5
1	E	76	CYS	3.5
2	J	70	PHE	3.5
1	O	223	VAL	3.5
2	B	64	GLU	3.5
1	C	141	TYR	3.5
1	I	15	ILE	3.5
1	E	10	GLY	3.5
2	D	75	ARG	3.5
1	M	217	ILE	3.4
1	Q	268	MET	3.4
2	B	83	LYS	3.4
2	L	1	GLY	3.4
1	C	300	LEU	3.4
2	B	69	GLU	3.4
2	D	119	TYR	3.4
2	B	3	PHE	3.4
1	M	179	LEU	3.4
1	A	288	ILE	3.4
2	B	88	PHE	3.4
2	B	138	PHE	3.4
2	B	76	ARG	3.4
1	O	188	ALA	3.4
1	C	13	ILE	3.4
2	F	80	LEU	3.3
1	C	81	ASN	3.3
2	L	66	VAL	3.3
2	J	80	LEU	3.3
2	N	66	VAL	3.3
1	O	80	ILE	3.3
1	O	267	ILE	3.3
2	J	77	ILE	3.3
2	L	134	GLY	3.3
1	G	324	PRO	3.3
1	A	51	LEU	3.3
1	I	276	ASN	3.3
1	Q	310	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	188	ALA	3.3
2	B	115	VAL	3.3
1	O	160	THR	3.3
2	F	69	GLU	3.2
2	F	78	GLU	3.2
2	J	132	GLU	3.2
2	L	64	GLU	3.2
2	D	6	ILE	3.2
2	D	7	ALA	3.2
2	F	4	GLY	3.2
1	Q	262	LYS	3.2
2	B	14	TRP	3.2
1	G	17	TYR	3.2
1	G	15	ILE	3.2
1	E	281	CYS	3.2
1	Q	305	CYS	3.2
1	I	308	TYR	3.2
2	R	173	ILE	3.2
2	J	74	GLU	3.2
1	M	127	TRP	3.2
1	K	302	ILE	3.2
2	D	22	TYR	3.2
2	J	119	TYR	3.2
1	G	104	ASP	3.2
2	H	168	LEU	3.2
2	F	6	ILE	3.2
2	H	2	LEU	3.1
1	K	309	VAL	3.1
1	I	319	GLY	3.1
2	F	64	GLU	3.1
2	D	124	LEU	3.1
2	N	73	LEU	3.1
2	H	140	PHE	3.1
2	D	122	VAL	3.1
1	M	173	GLN	3.1
2	J	4	GLY	3.1
1	G	13	ILE	3.1
1	I	300	LEU	3.1
2	H	68	ARG	3.1
2	F	83	LYS	3.1
2	P	65	ALA	3.1
2	R	5	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	3	PHE	3.1
1	C	319	GLY	3.1
1	M	80	ILE	3.1
1	M	174	GLU	3.1
1	C	14	CYS	3.1
2	D	60	ASN	3.1
1	I	80	ILE	3.1
1	G	149	ARG	3.1
1	I	171	THR	3.1
2	L	83	LYS	3.1
1	Q	258	TYR	3.0
2	D	91	VAL	3.0
1	C	20	ASN	3.0
1	G	103	ASN	3.0
1	I	221	SER	3.0
1	O	129	SER	3.0
2	D	71	ASN	3.0
2	N	175	SER	3.0
1	K	55	GLY	3.0
2	F	134	GLY	3.0
2	L	136	GLY	3.0
2	D	143	LYS	3.0
1	O	324	PRO	3.0
1	E	266	THR	3.0
2	R	122	VAL	3.0
1	Q	276	ASN	3.0
1	E	267	ILE	3.0
2	D	68	ARG	3.0
2	L	4	GLY	3.0
2	J	64	GLU	3.0
1	O	16	GLY	3.0
2	J	68	ARG	3.0
2	L	19	ASP	3.0
2	R	73	LEU	3.0
2	H	74	GLU	3.0
2	H	164	GLU	3.0
2	F	22	TYR	3.0
1	Q	155	ILE	3.0
1	C	55	GLY	3.0
1	K	219	THR	3.0
2	D	88	PHE	3.0
2	F	70	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	236	ILE	2.9
1	E	17	TYR	2.9
1	E	53(A)	LEU	2.9
1	G	300	LEU	2.9
1	I	12	GLN	2.9
1	G	50	LYS	2.9
2	H	83	LYS	2.9
1	G	314	LEU	2.9
1	K	300	LEU	2.9
2	D	168	LEU	2.9
2	L	2	LEU	2.9
1	G	105	TYR	2.9
2	B	136	GLY	2.9
2	H	4	GLY	2.9
2	P	8	GLY	2.9
1	G	77	ASP	2.9
2	H	71	ASN	2.9
2	F	166	ALA	2.9
1	Q	266	THR	2.9
2	B	9	PHE	2.9
2	H	63	PHE	2.9
1	I	316	LEU	2.9
1	C	303	GLY	2.9
2	H	14	TRP	2.9
1	G	304	GLU	2.9
2	D	135	ASN	2.9
2	H	81	ASN	2.9
1	O	79	PHE	2.9
2	F	3	PHE	2.9
2	L	3	PHE	2.9
2	N	70	PHE	2.9
1	O	219	THR	2.9
1	I	267	ILE	2.9
2	D	78	GLU	2.9
1	C	289	ASN	2.9
2	F	71	ASN	2.9
1	C	309	VAL	2.9
1	M	261	VAL	2.9
2	B	140	PHE	2.9
2	J	9	PHE	2.9
2	B	78	GLU	2.8
2	J	22	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	24	TYR	2.8
1	Q	313	ARG	2.8
2	J	35	ALA	2.8
2	P	18	VAL	2.8
1	I	102	PHE	2.8
2	D	140	PHE	2.8
2	N	63	PHE	2.8
1	E	96	ASP	2.8
1	O	270	SER	2.8
1	Q	311	SER	2.8
1	A	318	THR	2.8
2	D	2	LEU	2.8
1	I	249	GLY	2.8
1	M	10	GLY	2.8
2	J	8	GLY	2.8
1	A	40	GLN	2.8
1	E	282	GLN	2.8
1	C	39	ALA	2.8
2	R	138	PHE	2.8
1	K	298	HIS	2.8
1	O	213	LEU	2.8
1	G	283	THR	2.8
1	G	323	SER	2.8
2	B	4	GLY	2.8
2	H	84	MET	2.8
1	M	238	LYS	2.8
1	E	12	GLN	2.8
1	M	151	VAL	2.8
2	L	119	TYR	2.8
2	L	127	ARG	2.8
2	F	7	ALA	2.8
1	C	322	ASN	2.8
2	B	79	ASN	2.8
1	G	266	THR	2.8
1	Q	323	SER	2.8
1	I	144	LYS	2.8
2	F	74	GLU	2.8
1	K	62	ARG	2.8
2	B	75	ARG	2.8
1	A	79	PHE	2.8
1	G	141	TYR	2.8
2	H	44	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	88	PHE	2.8
1	Q	213	LEU	2.8
1	Q	217	ILE	2.8
1	M	172	ASN	2.8
2	J	72	ASN	2.8
1	A	101	ASP	2.8
2	D	61	THR	2.8
1	M	225	GLY	2.8
2	B	23	GLY	2.8
2	D	74	GLU	2.7
2	H	9	PHE	2.7
1	C	260	ILE	2.7
1	M	124	ILE	2.7
1	M	182	ILE	2.7
2	F	157	TYR	2.7
2	H	56	ILE	2.7
2	J	162	TYR	2.7
1	C	278	ASN	2.7
1	G	248	ASN	2.7
1	M	101	ASP	2.7
1	C	51	LEU	2.7
1	I	97	CYS	2.7
1	M	138	ALA	2.7
1	C	301	THR	2.7
2	B	87	GLY	2.7
1	E	321	ARG	2.7
1	G	62	ARG	2.7
2	J	78	GLU	2.7
2	L	69	GLU	2.7
1	K	111	LEU	2.7
2	J	138	PHE	2.7
2	L	173	ILE	2.7
1	A	305	CYS	2.7
1	K	76	CYS	2.7
1	I	105	TYR	2.7
1	E	35(A)	THR	2.7
1	E	158	ASN	2.7
2	L	16	GLY	2.7
2	L	39	GLU	2.7
1	G	111	LEU	2.7
1	M	245	PHE	2.7
2	F	88	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	153	TRP	2.7
2	L	94	TYR	2.7
1	I	266	THR	2.7
1	I	284	PRO	2.7
1	K	324	PRO	2.7
2	F	12	GLY	2.7
1	G	11	ASP	2.7
1	M	123	ILE	2.6
1	Q	154	LEU	2.7
2	J	5	ALA	2.6
1	A	10	GLY	2.6
2	L	8	GLY	2.6
2	J	60	ASN	2.6
2	P	168	LEU	2.6
1	A	290	SER	2.6
1	O	167	SER	2.6
2	D	21	TRP	2.6
2	H	144	CYS	2.6
1	M	324	PRO	2.6
2	D	16	GLY	2.6
2	P	4	GLY	2.6
1	E	269	LYS	2.6
1	I	315	VAL	2.6
2	D	173	ILE	2.6
1	M	79	PHE	2.6
2	L	5	ALA	2.6
2	J	75	ARG	2.6
2	D	92	TRP	2.6
1	E	303	GLY	2.6
1	K	16	GLY	2.6
1	M	205	GLY	2.6
1	I	76	CYS	2.6
1	O	156	LYS	2.6
1	Q	281	CYS	2.6
1	M	133(A)	LEU	2.6
1	M	213	LEU	2.6
1	M	223	VAL	2.6
2	R	61	THR	2.6
1	G	75	MET	2.6
1	G	118	PHE	2.6
2	H	32	SER	2.6
2	F	167	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	68	ARG	2.6
1	A	319	GLY	2.6
1	G	143	GLY	2.6
2	B	22	TYR	2.6
2	B	34	TYR	2.6
2	L	124	LEU	2.6
1	A	13	ILE	2.6
1	A	309	VAL	2.6
1	M	214	VAL	2.6
1	O	123	ILE	2.6
2	H	152	VAL	2.6
1	K	78	GLU	2.6
2	D	139	GLU	2.6
2	H	78	GLU	2.6
2	L	75	ARG	2.5
1	E	270	SER	2.5
1	M	247	SER	2.5
1	A	303	GLY	2.5
1	G	70	LEU	2.5
1	G	303	GLY	2.5
1	I	275	GLY	2.5
2	N	173	ILE	2.5
2	P	77	ILE	2.5
1	E	304	GLU	2.5
1	I	283	THR	2.5
1	K	160	THR	2.5
1	G	287	ALA	2.5
2	J	140	PHE	2.5
2	P	5	ALA	2.5
1	O	172	ASN	2.5
1	O	244	ASN	2.5
2	D	79	ASN	2.5
1	Q	272	LEU	2.5
2	L	160	PRO	2.5
2	J	14	TRP	2.5
2	P	14	TRP	2.5
1	G	60	ILE	2.5
1	I	13	ILE	2.5
1	I	260	ILE	2.5
1	Q	267	ILE	2.5
2	B	141	TYR	2.5
2	D	141	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	34	TYR	2.5
1	E	318	THR	2.5
1	I	173	GLN	2.5
1	O	208	THR	2.5
2	L	63	PHE	2.5
1	A	39	ALA	2.5
1	Q	280	LYS	2.5
2	D	82	LYS	2.5
1	I	323	SER	2.5
1	E	320	LEU	2.5
2	D	133	LEU	2.5
2	N	6	ILE	2.5
1	A	35	VAL	2.5
2	J	21	TRP	2.5
1	I	318	THR	2.5
2	N	62	GLN	2.5
1	A	20	ASN	2.5
1	I	50	LYS	2.5
1	I	277	CYS	2.5
2	B	72	ASN	2.5
2	J	71	ASN	2.5
2	D	101	LEU	2.5
2	F	89	LEU	2.5
1	O	159	SER	2.5
1	Q	303	GLY	2.5
2	N	21	TRP	2.5
1	C	78	GLU	2.5
1	G	107	GLU	2.5
2	D	63	PHE	2.5
2	L	140	PHE	2.5
1	G	301	THR	2.5
2	N	61	THR	2.5
2	R	7	ALA	2.5
1	C	144	LYS	2.5
2	J	131	LYS	2.5
1	K	186	ASN	2.5
2	J	144	CYS	2.5
1	M	176	LEU	2.4
2	B	112	ASP	2.4
2	D	98	LEU	2.4
2	J	2	LEU	2.4
1	E	284	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	324	PRO	2.4
1	C	82	VAL	2.4
1	Q	49	GLY	2.4
2	F	136	GLY	2.4
1	M	126	SER	2.4
2	H	132	GLU	2.4
2	H	139	GLU	2.4
2	L	170	ARG	2.4
1	K	308	TYR	2.4
2	B	157	TYR	2.4
1	M	210	ASN	2.4
2	F	2	LEU	2.4
2	P	98	LEU	2.4
1	M	15	ILE	2.4
2	B	152	VAL	2.4
2	L	87	GLY	2.4
2	P	20	GLY	2.4
1	E	311	SER	2.4
1	G	114	ARG	2.4
2	F	68	ARG	2.4
2	N	174	SER	2.4
2	H	131	LYS	2.4
2	J	29	GLU	2.4
2	J	69	GLU	2.4
2	J	83	LYS	2.4
2	R	9	PHE	2.4
1	A	98	TYR	2.4
2	D	34	TYR	2.4
2	F	34	TYR	2.4
2	F	159	TYR	2.4
1	A	208	THR	2.4
1	G	38	HIS	2.4
1	G	320	LEU	2.4
2	F	84	MET	2.4
1	A	143	GLY	2.4
1	E	309	VAL	2.4
2	B	39	GLU	2.4
2	B	85	GLU	2.4
2	P	70	PHE	2.4
1	E	91	ALA	2.4
2	L	159	TYR	2.4
2	P	141	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	R	24	TYR	2.4
1	E	268	MET	2.4
1	O	133(A)	LEU	2.4
2	H	108	LEU	2.4
2	P	73	LEU	2.4
1	I	87	ILE	2.4
1	K	217	ILE	2.4
1	K	260	ILE	2.4
1	M	121	ILE	2.4
2	J	55	ILE	2.4
1	A	16	GLY	2.4
2	D	87	GLY	2.4
2	N	67	GLY	2.4
2	R	136	GLY	2.4
2	L	68	ARG	2.4
2	J	171	GLU	2.4
1	G	39	ALA	2.4
1	G	291	SER	2.4
1	M	129	SER	2.4
1	A	69	TRP	2.4
1	O	195	TYR	2.4
2	L	157	TYR	2.4
2	P	22	TYR	2.4
1	I	43	LEU	2.4
1	M	87	ILE	2.4
1	M	185	PRO	2.4
1	C	172	ASN	2.3
1	I	62	ARG	2.3
1	M	135	VAL	2.3
2	D	152	VAL	2.3
2	N	76	ARG	2.3
1	G	102	PHE	2.3
1	Q	79	PHE	2.3
2	B	86	ASP	2.3
2	B	144	CYS	2.3
2	D	19	ASP	2.3
2	L	44	ALA	2.3
1	G	122	GLN	2.3
1	G	133	SER	2.3
1	G	59	LEU	2.3
1	K	316	LEU	2.3
1	M	171	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	89	LEU	2.3
2	F	160	PRO	2.3
2	N	170	ARG	2.3
1	M	244	ASN	2.3
2	L	72	ASN	2.3
2	P	88	PHE	2.3
1	E	63	ASP	2.3
2	L	164	GLU	2.3
2	N	112	ASP	2.3
1	G	51	LEU	2.3
2	L	32	SER	2.3
2	L	142	HIS	2.3
1	G	160	THR	2.3
1	O	98	TYR	2.3
1	Q	198	PRO	2.3
2	D	170	ARG	2.3
1	G	82	VAL	2.3
2	F	67	GLY	2.3
1	C	186	ASN	2.3
1	E	322	ASN	2.3
2	B	114	ASN	2.3
2	D	81	ASN	2.3
2	N	140	PHE	2.3
1	A	304	GLU	2.3
1	E	273	GLU	2.3
1	G	96	ASP	2.3
2	F	144	CYS	2.3
1	C	50	LYS	2.3
1	C	323	SER	2.3
1	E	113	SER	2.3
2	B	10	ILE	2.3
1	K	279	THR	2.3
1	M	160	THR	2.3
1	A	141	TYR	2.3
1	K	103	ASN	2.3
2	B	135	ASN	2.3
2	F	9	PHE	2.3
2	H	129	ASN	2.3
1	E	300	LEU	2.3
1	I	112	LEU	2.3
1	C	42	ILE	2.3
1	G	115	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	121	ILE	2.3
1	I	301	THR	2.3
1	K	113	SER	2.3
1	K	321	ARG	2.3
1	M	199	THR	2.3
2	F	14	TRP	2.3
1	E	93	PRO	2.3
1	M	198	PRO	2.3
2	F	8	GLY	2.3
2	F	16	GLY	2.3
1	O	189	ALA	2.2
1	O	240	ASN	2.2
2	H	35	ALA	2.2
2	F	168	LEU	2.2
2	L	101	LEU	2.2
1	Q	46	LYS	2.2
1	M	241	ASP	2.2
1	A	42	ILE	2.2
1	A	124	ILE	2.2
2	L	6	ILE	2.2
1	A	47	HIS	2.2
1	E	149	ARG	2.2
2	J	142	HIS	2.2
1	E	305	CYS	2.2
1	C	125	PRO	2.2
1	K	266	THR	2.2
1	M	163	THR	2.2
2	H	61	THR	2.2
2	P	21	TRP	2.2
1	G	98	TYR	2.2
1	M	133	SER	2.2
1	M	221	SER	2.2
1	O	133	SER	2.2
1	Q	16	GLY	2.2
2	H	23	GLY	2.2
2	J	12	GLY	2.2
2	N	12	GLY	2.2
2	J	88	PHE	2.2
2	P	9	PHE	2.2
1	A	218	ALA	2.2
1	O	138	ALA	2.2
2	B	11	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	50	LYS	2.2
2	B	81	ASN	2.2
1	A	260	ILE	2.2
1	K	142	GLN	2.2
1	K	267	ILE	2.2
1	M	267	ILE	2.2
1	Q	260	ILE	2.2
2	D	56	ILE	2.2
2	P	10	ILE	2.2
2	P	45	ILE	2.2
2	R	77	ILE	2.2
1	M	130	HIS	2.2
2	B	170	ARG	2.2
1	A	171	THR	2.2
1	O	97	CYS	2.2
2	B	92	TRP	2.2
1	E	290	SER	2.2
2	H	40	SER	2.2
2	R	1	GLY	2.2
1	E	287	ALA	2.2
2	D	35	ALA	2.2
2	D	36	ALA	2.2
2	N	168	LEU	2.2
1	M	169	ASN	2.2
2	F	79	ASN	2.2
1	O	28	ILE	2.2
2	H	75	ARG	2.2
2	H	127	ARG	2.2
1	G	63	ASP	2.2
2	L	90	ASP	2.2
1	A	324	PRO	2.2
1	E	283	THR	2.2
2	J	61	THR	2.2
1	E	265	SER	2.2
2	L	24	TYR	2.2
2	H	3	PHE	2.2
1	I	272	LEU	2.2
1	O	179	LEU	2.2
1	Q	300	LEU	2.2
2	H	126	LEU	2.2
1	I	174	GLU	2.2
2	D	64	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	62	ARG	2.2
1	E	260	ILE	2.2
1	I	182	ILE	2.2
1	O	212	ARG	2.2
1	G	278	ASN	2.2
2	F	81	ASN	2.2
2	J	62	GLN	2.2
1	G	175	ASP	2.2
1	K	58	PRO	2.2
1	O	88	VAL	2.2
1	O	261	VAL	2.2
2	D	100	VAL	2.2
2	R	66	VAL	2.2
1	K	301	THR	2.2
1	M	206	THR	2.2
1	O	199	THR	2.2
1	I	69	TRP	2.2
1	K	310	LYS	2.2
1	O	17	TYR	2.2
2	D	137	CYS	2.2
1	C	272	LEU	2.2
2	B	40	SER	2.2
2	J	89	LEU	2.2
2	L	98	LEU	2.2
2	L	74	GLU	2.2
1	K	13	ILE	2.1
1	Q	182	ILE	2.1
1	C	142	GLN	2.1
2	D	15	GLN	2.1
1	M	240	ASN	2.1
2	B	142	HIS	2.1
2	N	81	ASN	2.1
1	A	88	VAL	2.1
1	E	261	VAL	2.1
1	G	293	PRO	2.1
1	Q	82(A)	PRO	2.1
2	F	122	VAL	2.1
2	L	115	VAL	2.1
1	I	11	ASP	2.1
2	D	84	MET	2.1
1	A	50	LYS	2.1
1	C	279	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	144	LYS	2.1
2	D	20	GLY	2.1
2	N	8	GLY	2.1
2	B	21	TRP	2.1
2	R	21	TRP	2.1
2	B	89	LEU	2.1
2	F	63	PHE	2.1
1	G	290	SER	2.1
2	B	35	ALA	2.1
1	K	149	ARG	2.1
2	B	132	GLU	2.1
2	D	29	GLU	2.1
1	C	124	ILE	2.1
2	F	111	HIS	2.1
1	Q	197	ASN	2.1
1	Q	309	VAL	2.1
1	I	143	GLY	2.1
2	P	134	GLY	2.1
1	G	108	LEU	2.1
2	H	21	TRP	2.1
2	L	92	TRP	2.1
1	A	17	TYR	2.1
1	G	19	ALA	2.1
1	I	98	TYR	2.1
2	P	35	ALA	2.1
2	R	36	ALA	2.1
1	M	128	SER	2.1
1	O	305	CYS	2.1
1	G	298	HIS	2.1
1	A	299	PRO	2.1
1	I	169	ASN	2.1
1	I	172	ASN	2.1
1	I	248	ASN	2.1
1	I	299	PRO	2.1
1	O	169	ASN	2.1
2	H	60	ASN	2.1
1	A	314	LEU	2.1
1	C	61	LEU	2.1
1	I	303	GLY	2.1
2	D	86	ASP	2.1
2	L	89	LEU	2.1
1	K	102	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	46	ASP	2.1
2	D	14	TRP	2.1
2	H	92	TRP	2.1
2	B	119	TYR	2.1
2	H	162	TYR	2.1
2	J	34	TYR	2.1
2	L	10	ILE	2.1
2	L	172	GLU	2.1
2	P	173	ILE	2.1
1	G	265	SER	2.1
2	F	27	SER	2.1
1	M	184	HIS	2.1
1	A	223	VAL	2.1
1	C	280	LYS	2.1
1	G	135	VAL	2.1
1	M	254	PRO	2.1
2	P	95	ASN	2.1
1	G	112	LEU	2.1
1	I	53(A)	LEU	2.1
1	I	314	LEU	2.1
1	M	154	LEU	2.1
1	A	294	PHE	2.1
1	K	10	GLY	2.1
2	H	123	ARG	2.1
1	M	236	ILE	2.1
2	J	92	TRP	2.1
2	H	39	GLU	2.1
1	O	201	TYR	2.1
2	J	24	TYR	2.1
1	C	125(B)	SER	2.0
1	K	280	LYS	2.0
1	K	291	SER	2.0
1	Q	178	VAL	2.0
1	E	324	PRO	2.0
1	K	299	PRO	2.0
1	G	172	ASN	2.0
1	I	194	LEU	2.0
1	O	158	ASN	2.0
2	L	50	ASN	2.0
1	M	212	ARG	2.0
2	B	63	PHE	2.0
2	B	134	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	75	ARG	2.0
1	G	35(A)	THR	2.0
2	P	156	THR	2.0
1	C	53	ASP	2.0
1	E	67	ALA	2.0
2	H	36	ALA	2.0
2	N	5	ALA	2.0
2	P	19	ASP	2.0
1	K	153	TRP	2.0
2	L	78	GLU	2.0
1	G	307	LYS	2.0
1	M	168	TYR	2.0
2	D	24	TYR	2.0
2	D	94	TYR	2.0
2	R	22	TYR	2.0
1	E	285	MET	2.0
1	G	31	MET	2.0
2	L	84	MET	2.0
1	A	12	GLN	2.0
1	E	221	SER	2.0
1	G	21	SER	2.0
1	I	196	GLN	2.0
1	K	261	VAL	2.0
1	M	125(B)	SER	2.0
1	M	270	SER	2.0
1	O	145	SER	2.0
1	O	204	VAL	2.0
1	O	323	SER	2.0
2	P	91	VAL	2.0
1	A	64	CYS	2.0
1	M	64	CYS	2.0
1	O	194	LEU	2.0
1	M	158	ASN	2.0
1	M	166	ARG	2.0
1	O	250	ASN	2.0
1	M	16	GLY	2.0
1	Q	181	GLY	2.0
2	D	3	PHE	2.0
1	G	42	ILE	2.0
1	O	60	ILE	2.0
2	F	45	ILE	2.0
1	E	301	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	266	THR	2.0
2	F	35	ALA	2.0
2	H	130	ALA	2.0
1	C	54	ASP	2.0
1	I	23	GLU	2.0
1	K	54	ASP	2.0
2	F	128	ASP	2.0
2	J	39	GLU	2.0
2	P	83	LYS	2.0
1	M	234	TRP	2.0
2	B	84	MET	2.0
2	H	24	TYR	2.0
2	H	119	TYR	2.0
2	R	159	TYR	2.0
1	E	135	VAL	2.0
2	J	152	VAL	2.0
2	R	48	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	W	2	14/15	0.15	0.25	108,111,113,113	0
4	BMA	Z	3	11/12	0.33	0.20	94,96,97,97	0
4	BMA	T	3	11/12	0.35	0.21	96,100,101,102	0
3	NAG	Y	2	14/15	0.35	0.22	103,106,107,108	0
3	NAG	S	2	14/15	0.41	0.20	97,100,103,104	0
4	BMA	X	3	11/12	0.43	0.18	105,106,107,107	0
4	NAG	X	2	14/15	0.46	0.21	94,97,100,103	0
3	NAG	S	1	14/15	0.47	0.19	87,93,97,98	0
3	NAG	U	1	14/15	0.51	0.19	85,91,92,94	0
3	NAG	U	2	14/15	0.58	0.18	94,95,97,97	0
3	NAG	a	1	14/15	-	-	90,97,100,103	0

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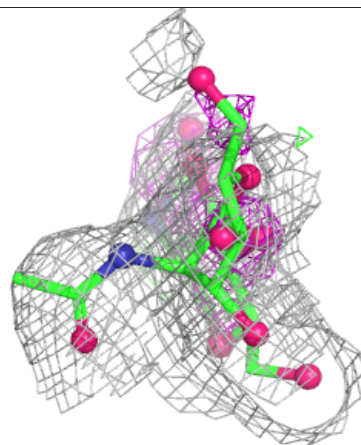
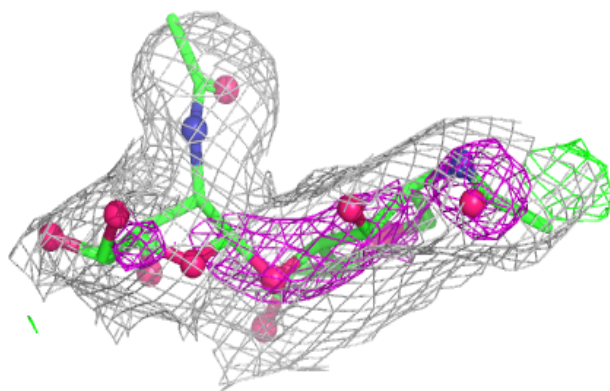
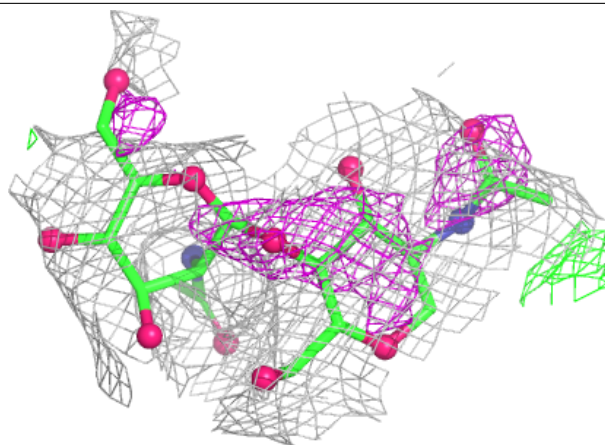
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	a	2	14/15	-	-	107,108,109,110	0
3	NAG	b	1	14/15	-	-	64,72,76,79	0
3	NAG	b	2	14/15	-	-	82,85,88,88	0
3	NAG	c	1	14/15	-	-	90,97,100,106	0
3	NAG	c	2	14/15	-	-	109,112,114,115	0
3	NAG	d	1	14/15	-	-	61,71,74,80	0
3	NAG	d	2	14/15	-	-	82,84,85,87	0
3	NAG	e	1	14/15	-	-	92,98,102,105	0
3	NAG	e	2	14/15	-	-	109,110,110,110	0
3	NAG	f	1	14/15	-	-	82,85,87,89	0
3	NAG	f	2	14/15	-	-	92,93,94,94	0
3	NAG	g	1	14/15	-	-	99,104,107,113	0
3	NAG	g	2	14/15	-	-	115,117,118,118	0
3	NAG	h	1	14/15	-	-	87,91,94,99	0
3	NAG	h	2	14/15	-	-	104,106,111,112	0
3	NAG	W	1	14/15	0.60	0.18	87,91,96,102	0
4	NAG	T	2	14/15	0.62	0.21	80,84,88,92	0
3	NAG	Y	1	14/15	0.64	0.17	87,91,94,100	0
3	NAG	V	2	14/15	0.67	0.19	80,82,86,86	0
4	NAG	Z	2	14/15	0.69	0.18	82,85,88,91	0
3	NAG	V	1	14/15	0.73	0.17	70,73,77,78	0
4	NAG	X	1	14/15	0.77	0.20	79,81,84,89	0
4	NAG	T	1	14/15	0.85	0.14	57,64,69,75	0
4	NAG	Z	1	14/15	0.85	0.15	67,69,73,78	0

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

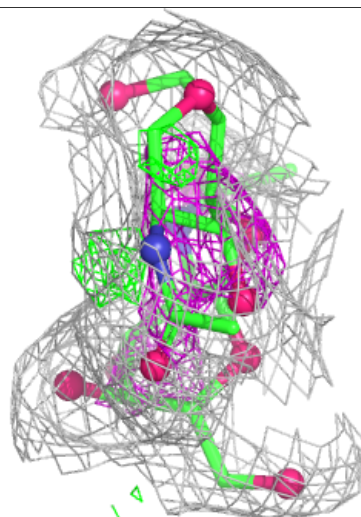
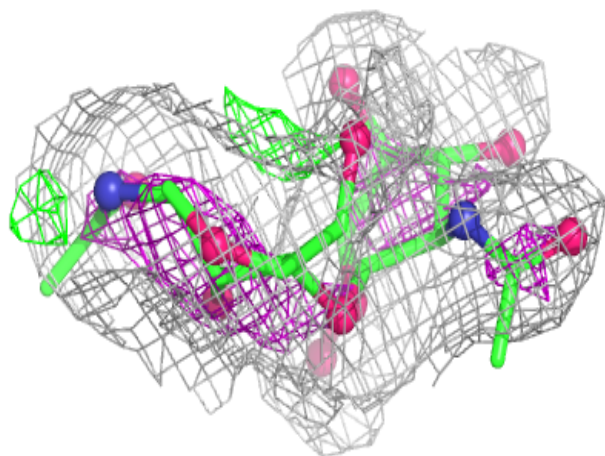
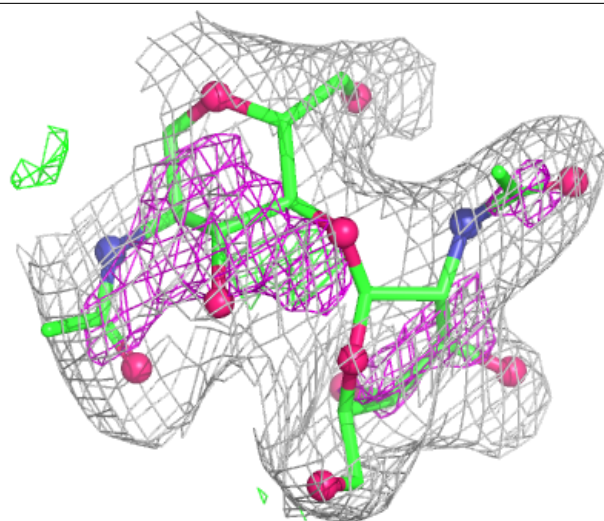
Electron density around Chain S:

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



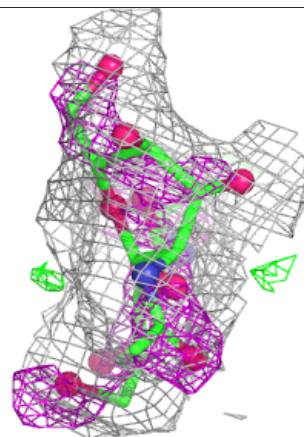
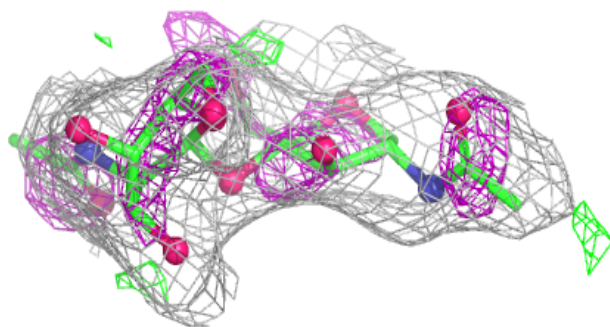
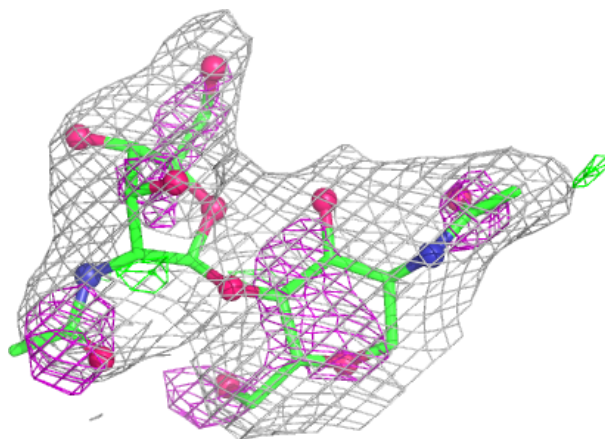
Electron density around Chain U:

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



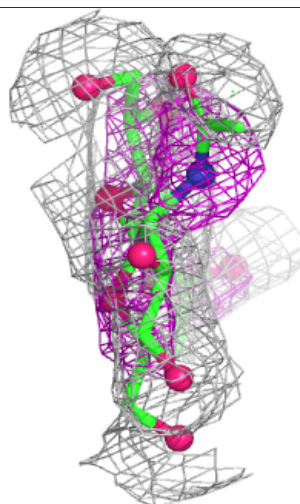
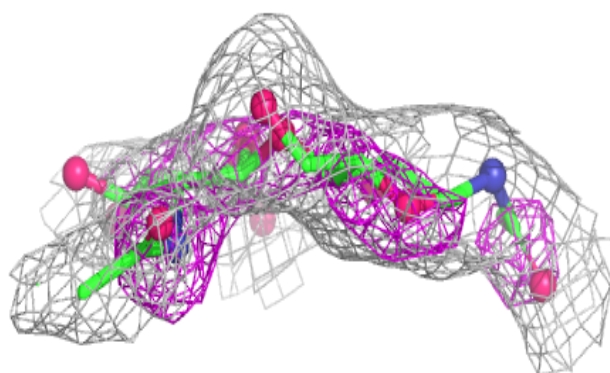
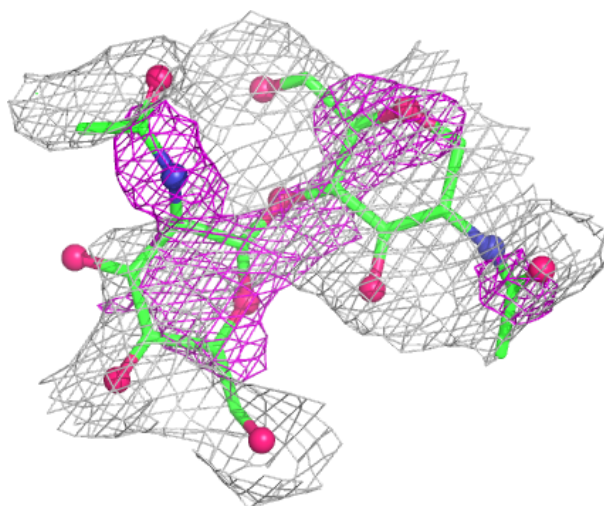
Electron density around Chain V:

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



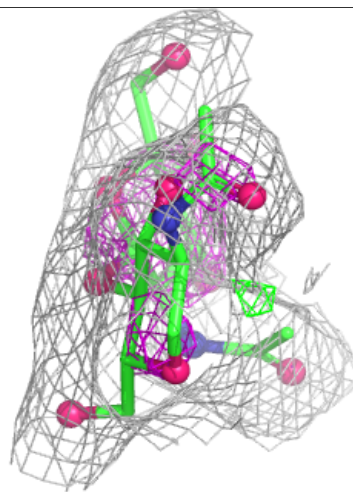
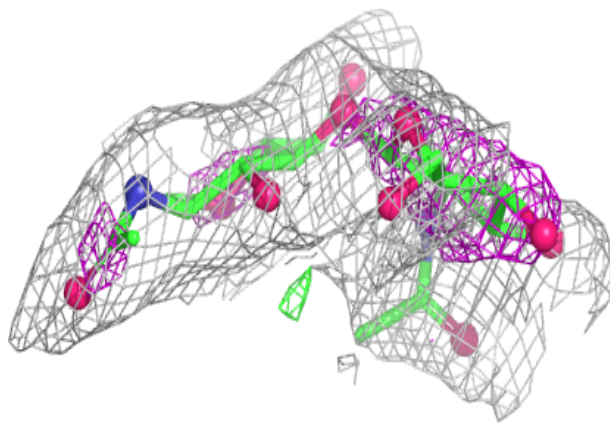
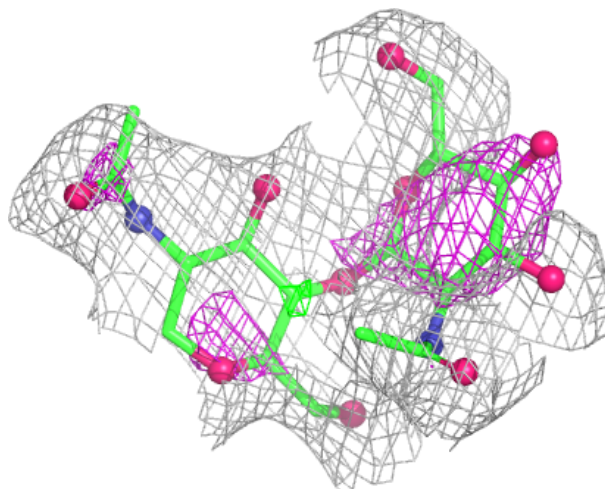
Electron density around Chain W:

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



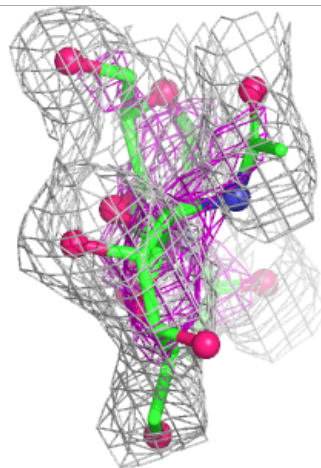
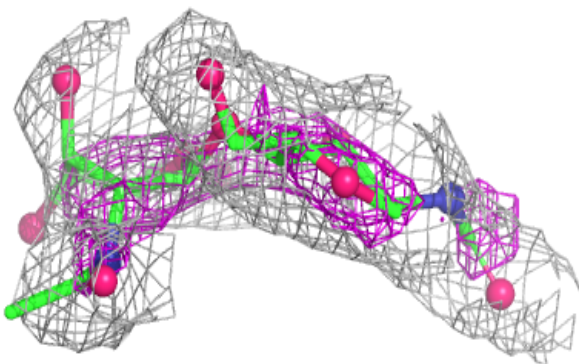
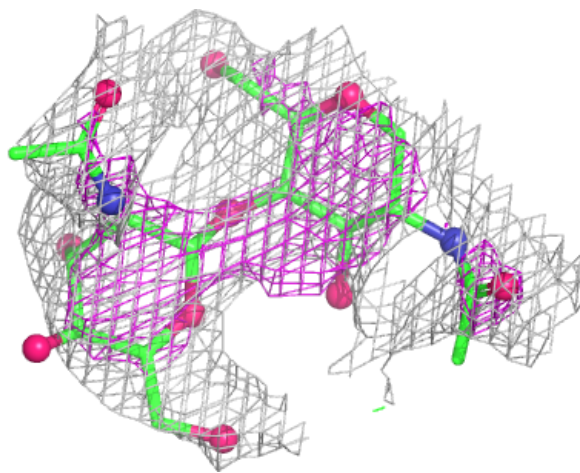
Electron density around Chain Y:

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



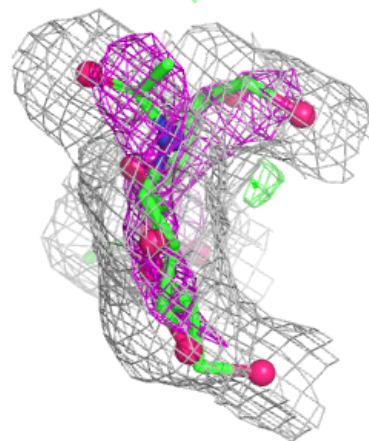
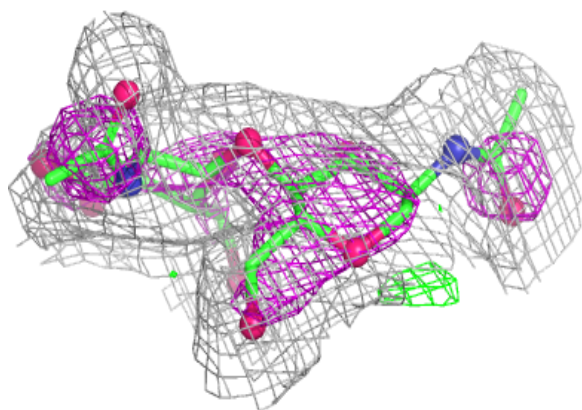
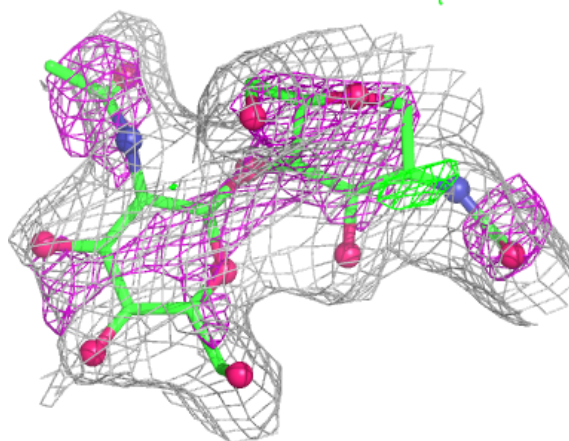
Electron density around Chain a:

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



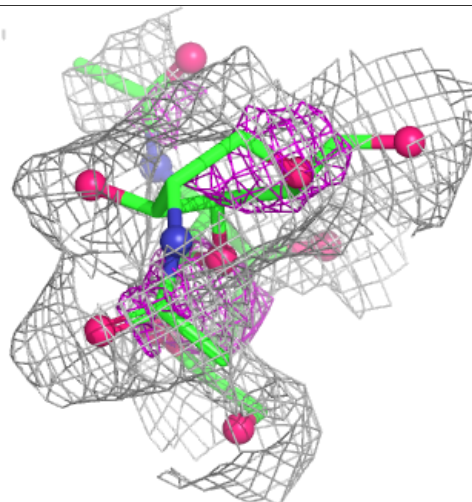
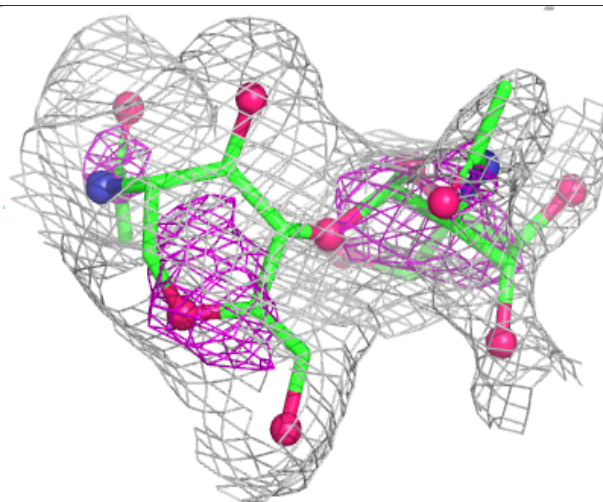
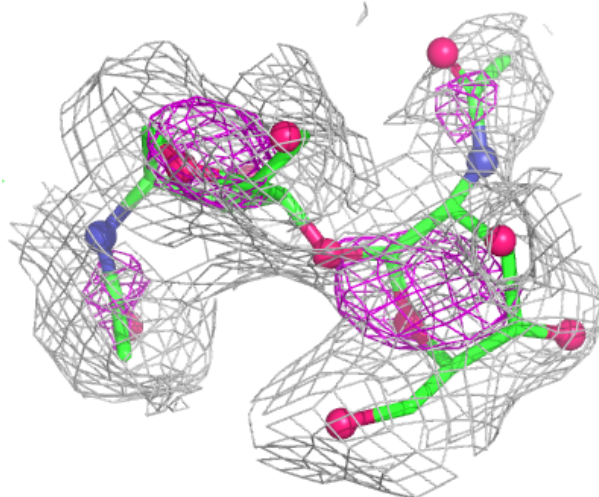
Electron density around Chain b:

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



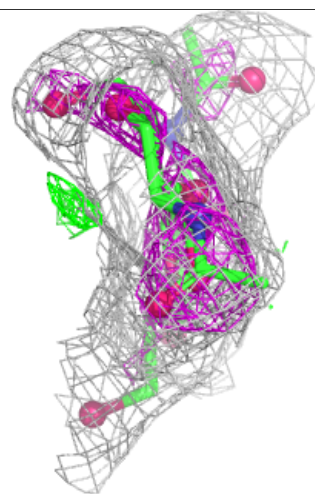
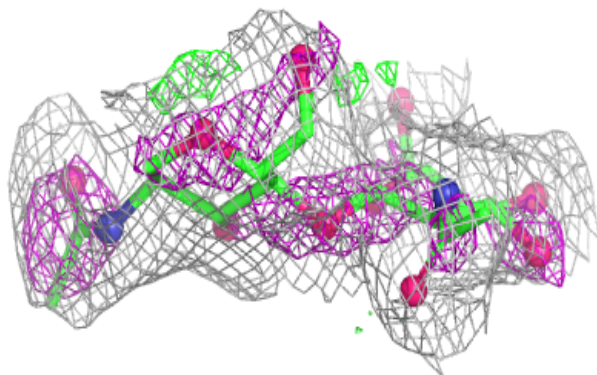
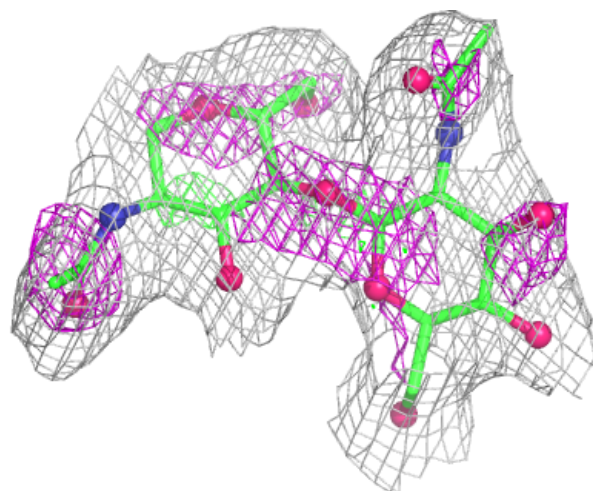
Electron density around Chain c:

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



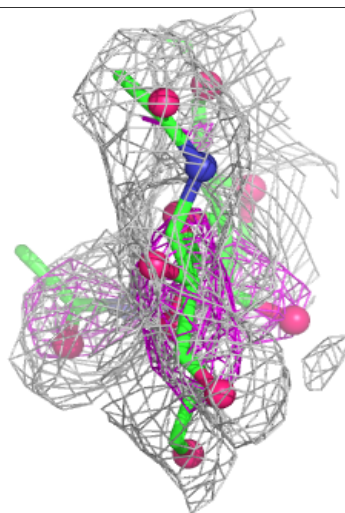
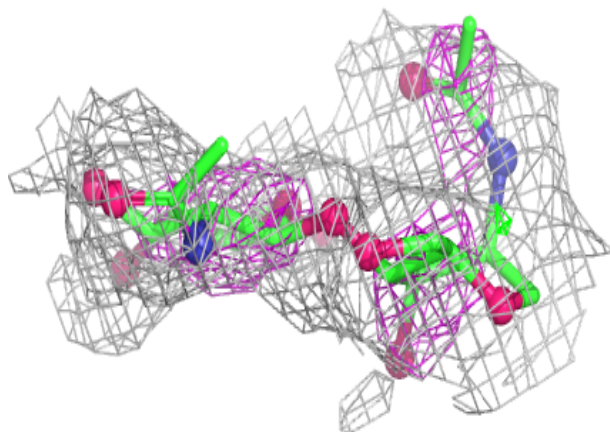
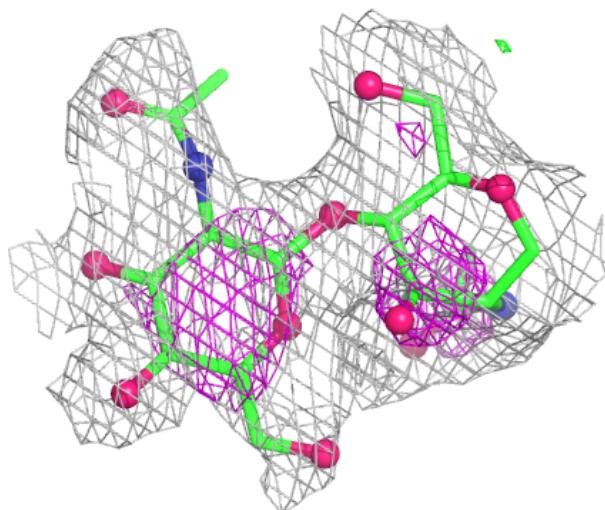
Electron density around Chain d:

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



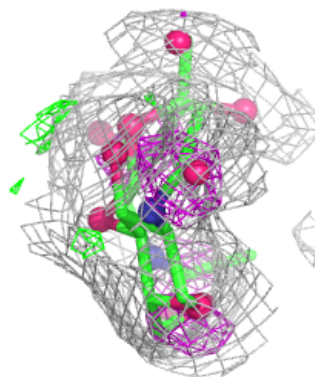
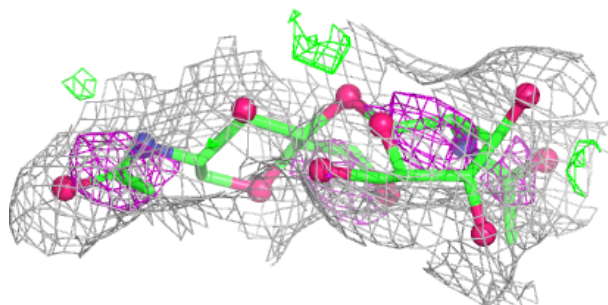
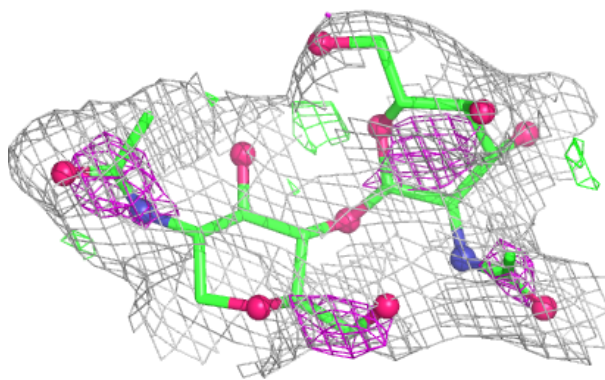
Electron density around Chain e:

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



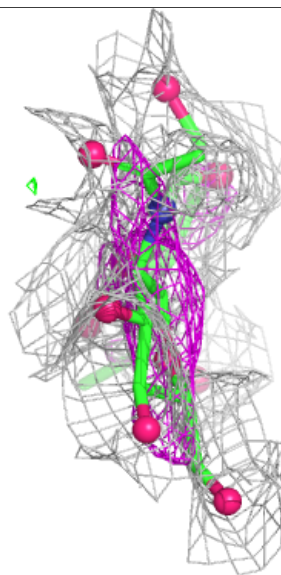
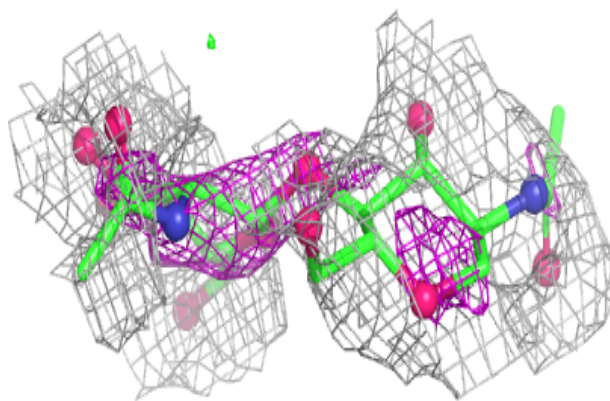
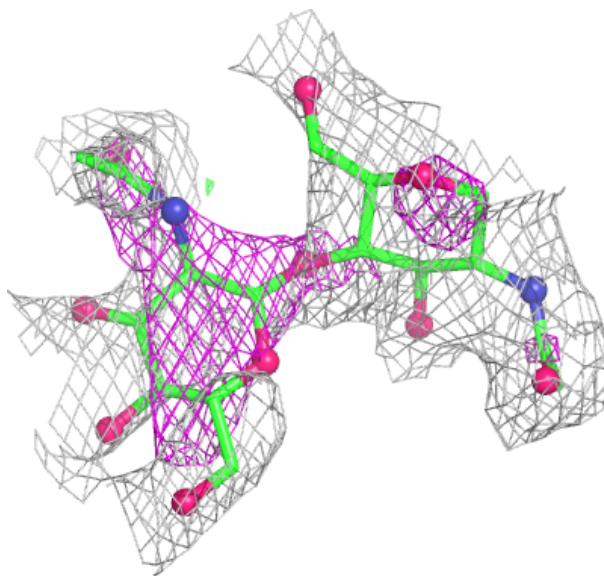
Electron density around Chain f:

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



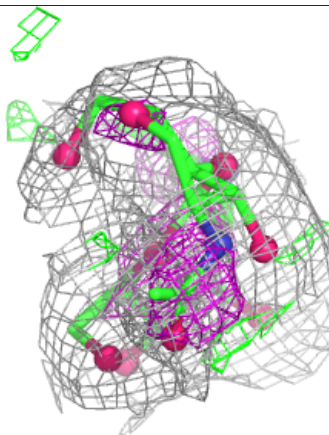
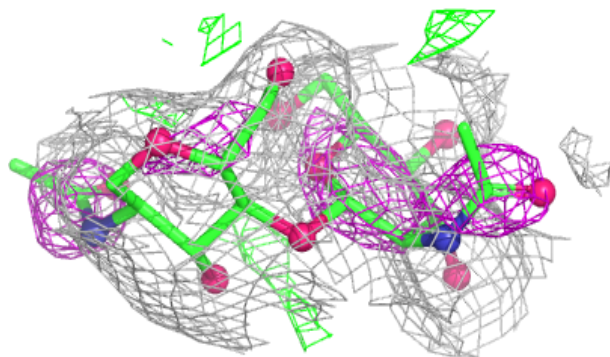
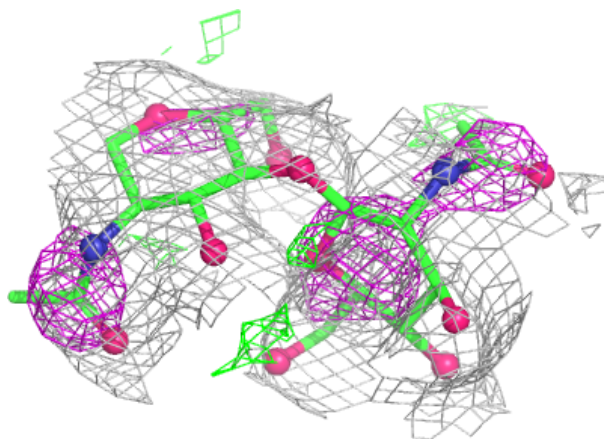
Electron density around Chain g:

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

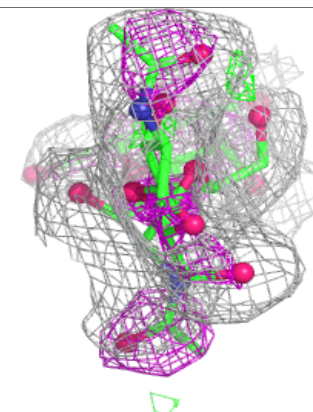
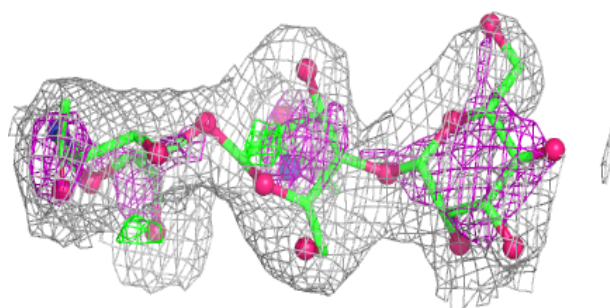
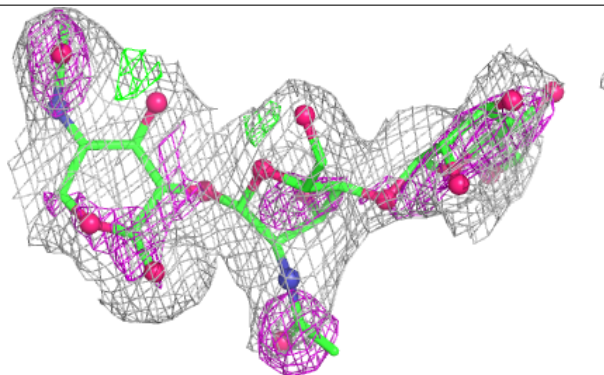


Electron density around Chain h:

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

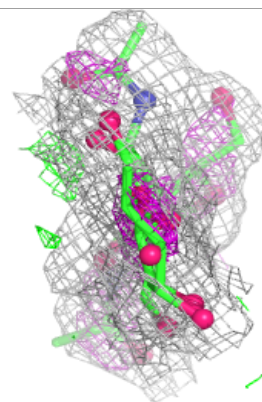
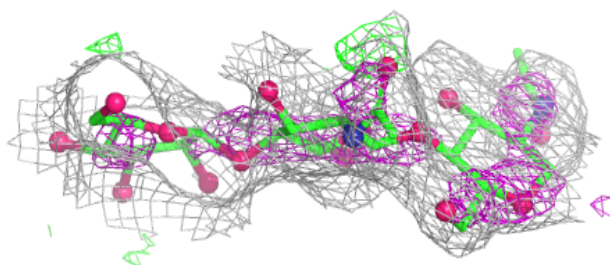
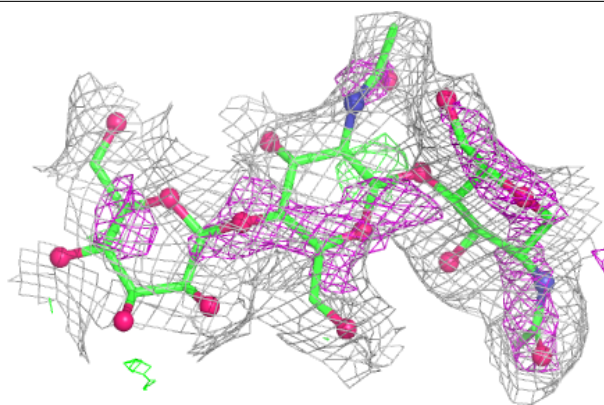
**Electron density around Chain T:**

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

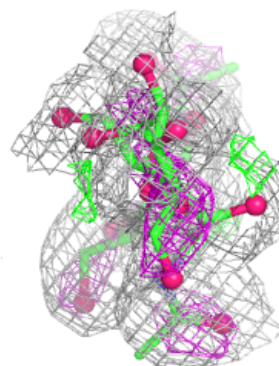
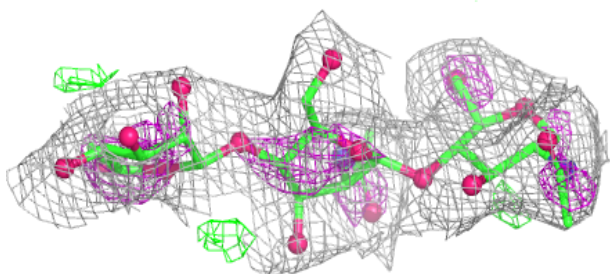
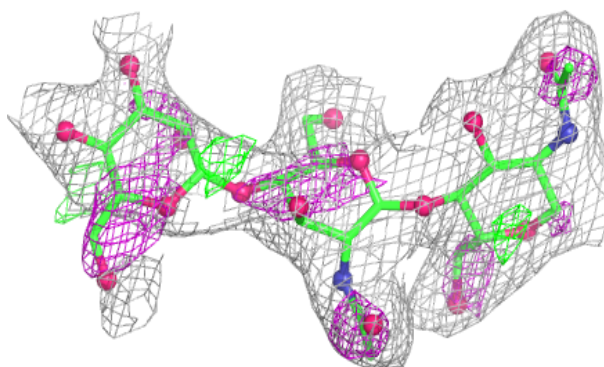


Electron density around Chain X:

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

**Electron density around Chain Z:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.