



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:04 PM UTC

PDB ID : 1XFD / pdb_00001xfg
Title : Structure of a human A-type Potassium Channel Accelerating factor DPPX,
a member of the dipeptidyl aminopeptidase family
Authors : Strop, P.; Bankovich, A.J.; Hansen, K.C.; Garcia, K.C.; Brunger, A.T.
Deposited on : 2004-09-14
Resolution : 3.00 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

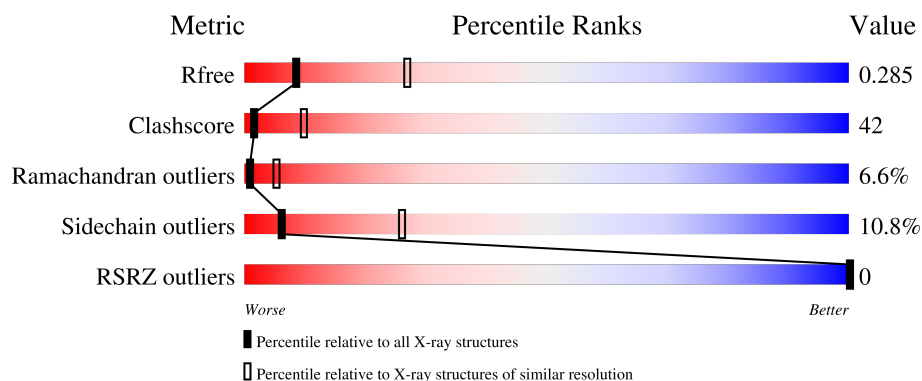
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



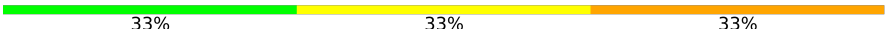
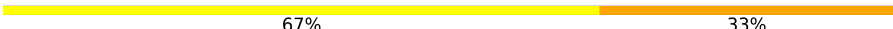
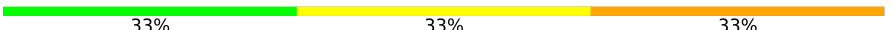
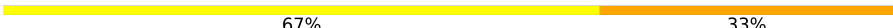
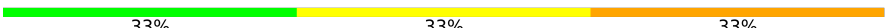
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	723	
1	B	723	
1	C	723	
1	D	723	
2	E	3	

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Mol	Chain	Length	Quality of chain
2	G	3	
2	I	3	
2	K	3	
2	N	3	
2	Q	3	
2	T	3	
2	V	3	
2	Y	3	
2	Z	3	
3	F	4	
4	H	4	
5	J	2	
5	M	2	
5	O	2	
5	P	2	
5	S	2	
5	U	2	
6	L	3	
6	R	3	
6	W	3	
7	X	4	

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
2	NAG	E	1	X	-	-	-
2	NAG	G	1	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	2	-	-	X	-
2	NAG	I	1	X	-	-	-
2	NAG	K	1	X	-	-	-
2	NAG	Q	1	X	-	-	-
2	NAG	V	1	X	-	-	-
2	NAG	Z	1	X	-	-	-
3	NAG	F	1	X	-	-	-
4	BMA	H	3	-	-	X	-
5	NAG	J	1	X	-	-	-
5	NAG	M	1	X	-	-	-
5	NAG	O	1	X	-	-	-
5	NAG	S	1	X	-	-	-
5	NAG	U	1	X	-	-	-
6	NAG	L	1	X	-	-	-
6	NAG	R	1	X	-	-	-
6	NAG	W	1	X	-	-	-
7	NAG	X	1	X	-	-	-
7	MAN	X	4	-	-	X	-

2 Entry composition [i](#)

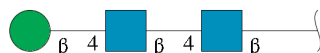
There are 8 unique types of molecules in this entry. The entry contains 24224 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl aminopeptidase-like protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			
1	B	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			
1	C	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			
1	D	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			

- Molecule 2 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
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	V	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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



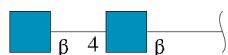
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-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	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



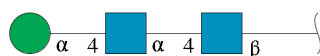
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	W	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	13	Total	O	0	0
			13	13		

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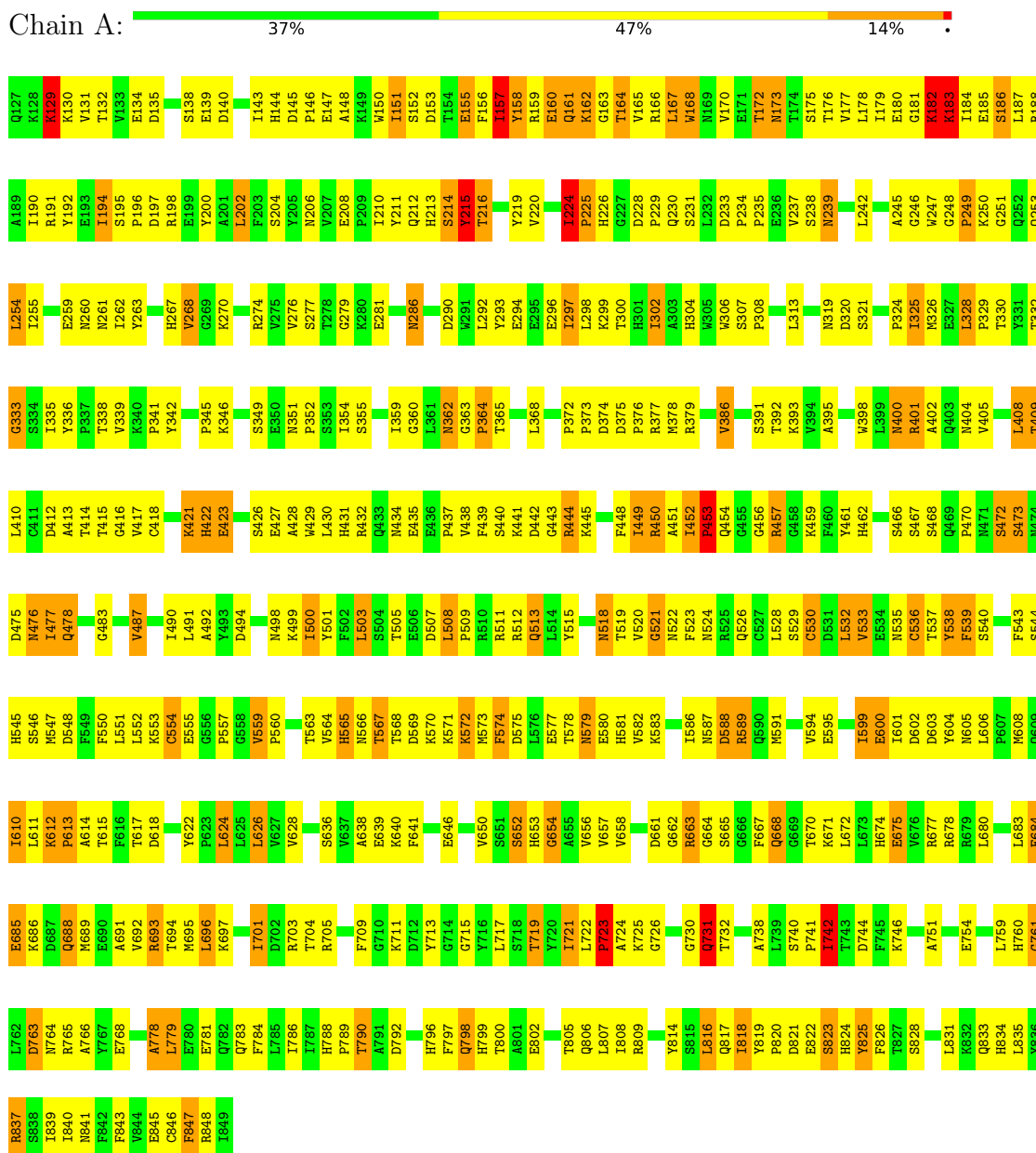
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	14	Total 14	O 14	0	0
8	C	14	Total 14	O 14	0	0
8	D	10	Total 10	O 10	0	0

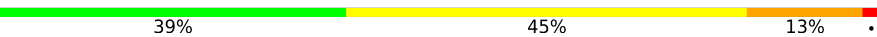
3 Residue-property plots

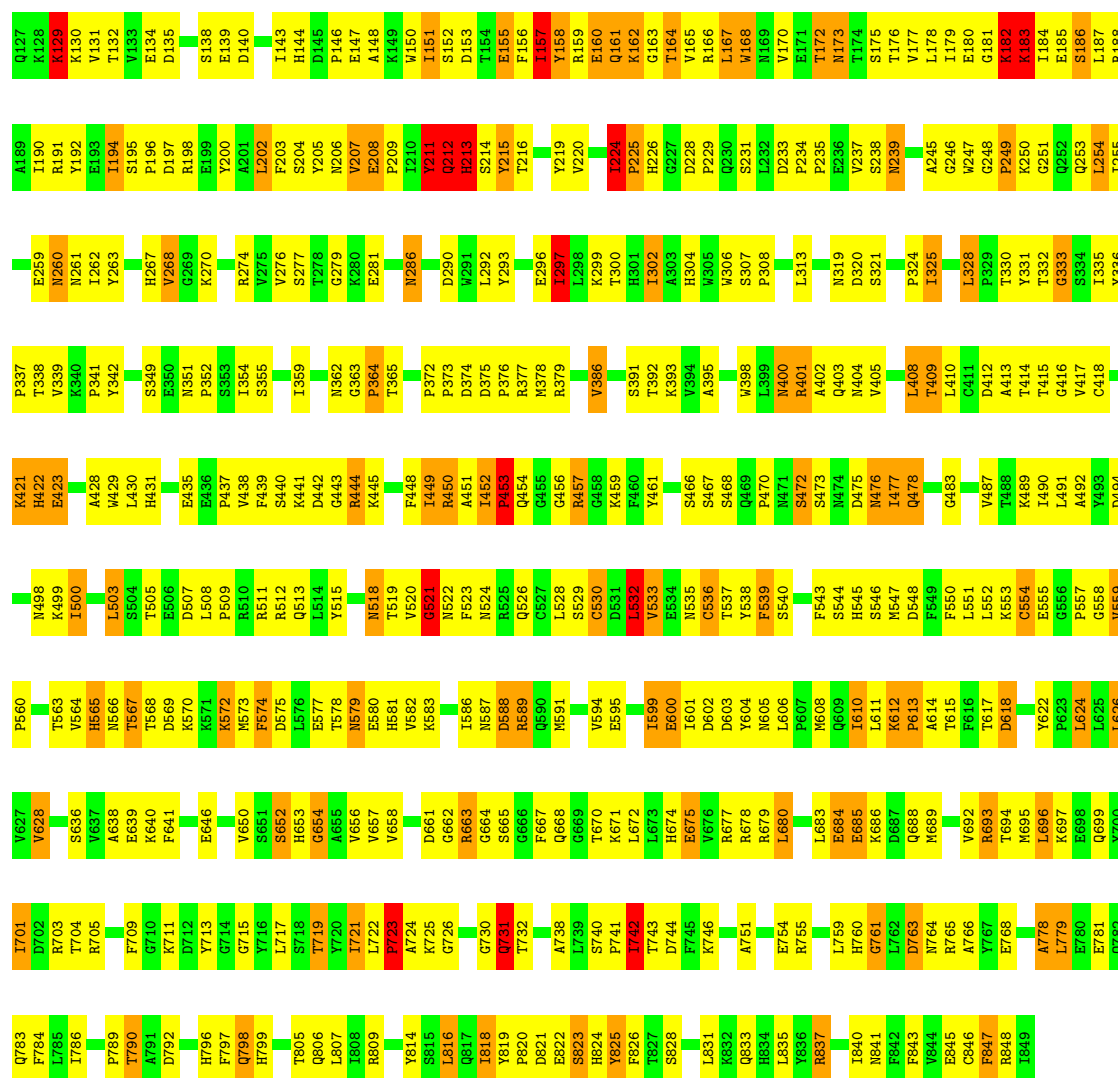
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Dipeptidyl aminopeptidase-like protein 6

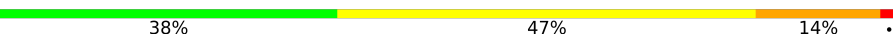


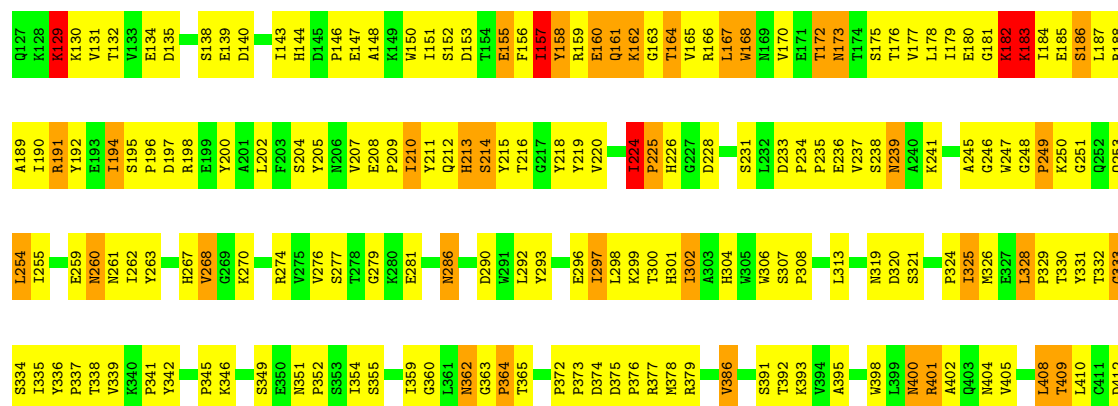
- Molecule 1: Dipeptidyl aminopeptidase-like protein 6

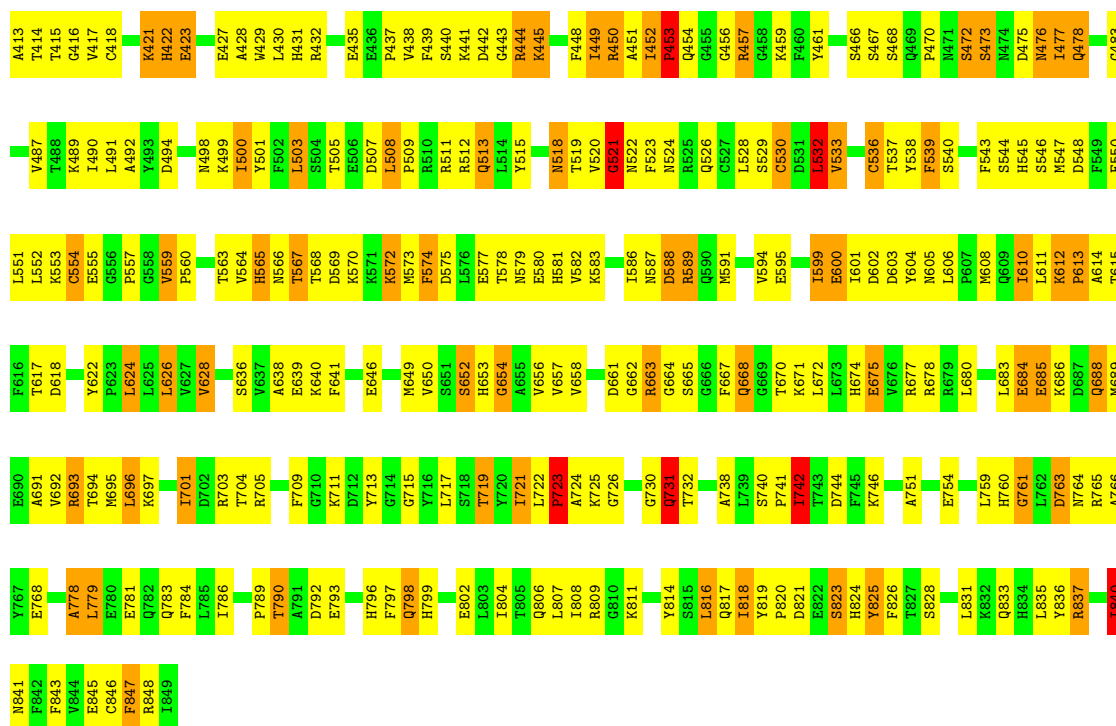
Chain B:  39% 45% 13%



• Molecule 1: Dipeptidyl aminopeptidase-like protein 6

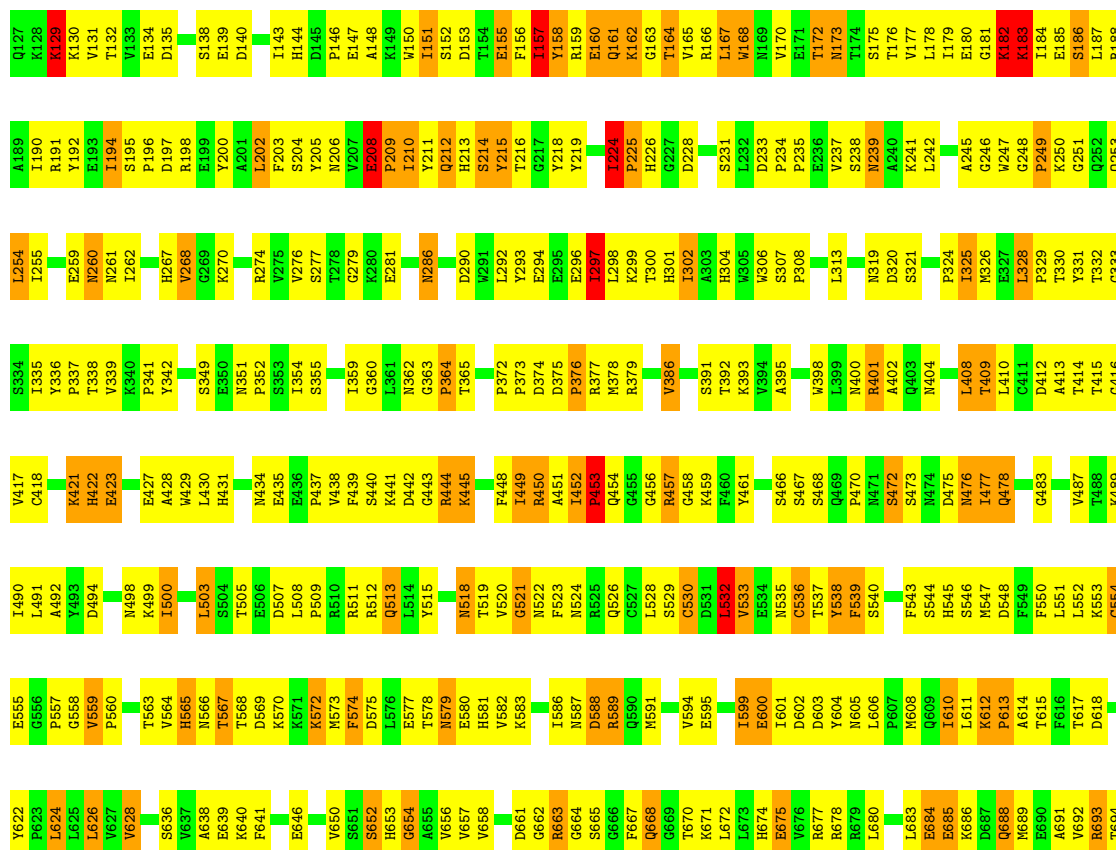
Chain C:  38% 47% 14%

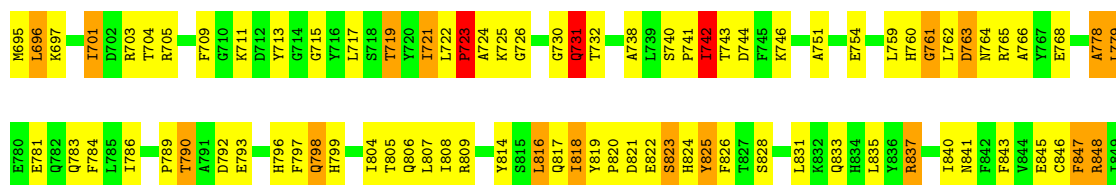




• Molecule 1: Dipeptidyl aminopeptidase-like protein 6

Chain D: 38% 46% 14%





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



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



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



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



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



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





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

Chain T: 67% 33%



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

Chain V: 33% 67%



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

Chain Y: 33% 67%



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

Chain Z: 33% 33% 33%



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

Chain F: 25% 75%



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

Chain H: 25% 75%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%

MAG1
MAG2

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

Chain L:  100%

MAG1
NDG2
MAN3

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

Chain R:  33% 67%

MAG1
NDG2
MAN3

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

Chain W:  100%

MAG1
NDG2
MAN3

- Molecule 7: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.98Å 170.23Å 159.32Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (15.00-3.00) 81.7 (15.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.280 0.255 , 0.285	Depositor DCC
R_{free} test set	3338 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	70.9	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24224	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	23/5987 (0.4%)	1.06	50/8118 (0.6%)
1	B	0.60	19/5987 (0.3%)	1.08	56/8118 (0.7%)
1	C	0.64	26/5987 (0.4%)	1.08	55/8118 (0.7%)
1	D	0.59	21/5987 (0.4%)	1.07	56/8118 (0.7%)
All	All	0.60	89/23948 (0.4%)	1.07	217/32472 (0.7%)

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	ARG	CD-NE	-9.54	1.32	1.46
1	C	191	ARG	NE-CZ	-9.48	1.22	1.33
1	C	191	ARG	CZ-NH2	-8.99	1.21	1.33
1	C	840	ILE	CB-CG2	-8.08	1.25	1.52
1	C	840	ILE	CB-CG1	-5.52	1.42	1.53
1	A	206	ASN	CG-OD1	5.42	1.33	1.23
1	D	653	HIS	ND1-CE1	5.41	1.38	1.32
1	A	212	GLN	CD-OE1	5.38	1.33	1.23
1	B	653	HIS	ND1-CE1	5.37	1.38	1.32
1	B	213	HIS	ND1-CE1	5.35	1.37	1.32
1	A	653	HIS	ND1-CE1	5.34	1.37	1.32
1	C	783	GLN	CD-OE1	5.32	1.33	1.23
1	A	400	ASN	CG-OD1	5.32	1.33	1.23
1	B	783	GLN	CD-OE1	5.31	1.33	1.23
1	C	653	HIS	ND1-CE1	5.31	1.37	1.32
1	C	817	GLN	CD-OE1	5.30	1.33	1.23
1	D	760	HIS	ND1-CE1	5.30	1.37	1.32
1	C	526	GLN	CD-OE1	5.28	1.33	1.23
1	B	587	ASN	CG-OD1	5.28	1.33	1.23
1	C	212	GLN	CD-OE1	5.28	1.33	1.23
1	A	817	GLN	CD-OE1	5.27	1.33	1.23
1	B	565	HIS	ND1-CE1	5.27	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	799	HIS	ND1-CE1	5.26	1.37	1.32
1	A	760	HIS	ND1-CE1	5.26	1.37	1.32
1	C	760	HIS	ND1-CE1	5.25	1.37	1.32
1	D	526	GLN	CD-OE1	5.25	1.33	1.23
1	A	688	GLN	CD-OE1	5.25	1.33	1.23
1	A	526	GLN	CD-OE1	5.25	1.33	1.23
1	D	260	ASN	CG-OD1	5.25	1.33	1.23
1	A	513	GLN	CD-OE1	5.24	1.33	1.23
1	B	760	HIS	ND1-CE1	5.24	1.37	1.32
1	A	587	ASN	CG-OD1	5.24	1.33	1.23
1	D	304	HIS	ND1-CE1	5.24	1.37	1.32
1	D	668	GLN	CD-OE1	5.23	1.33	1.23
1	C	565	HIS	ND1-CE1	5.23	1.37	1.32
1	B	260	ASN	CG-OD1	5.23	1.33	1.23
1	A	304	HIS	ND1-CE1	5.22	1.37	1.32
1	B	699	GLN	CD-OE1	5.21	1.33	1.23
1	B	304	HIS	ND1-CE1	5.21	1.37	1.32
1	D	565	HIS	ND1-CE1	5.21	1.37	1.32
1	D	783	GLN	CD-OE1	5.21	1.33	1.23
1	B	579	ASN	CG-OD1	5.20	1.33	1.23
1	C	799	HIS	ND1-CE1	5.19	1.37	1.32
1	A	731	GLN	CD-OE1	5.19	1.33	1.23
1	C	513	GLN	CD-OE1	5.19	1.33	1.23
1	B	731	GLN	CD-OE1	5.18	1.33	1.23
1	D	798	GLN	CD-OE1	5.18	1.33	1.23
1	A	783	GLN	CD-OE1	5.18	1.33	1.23
1	D	518	ASN	CG-OD1	5.18	1.33	1.23
1	C	731	GLN	CD-OE1	5.17	1.33	1.23
1	B	798	GLN	CD-OE1	5.16	1.33	1.23
1	C	304	HIS	ND1-CE1	5.16	1.37	1.32
1	C	518	ASN	CG-OD1	5.15	1.33	1.23
1	C	668	GLN	CD-OE1	5.14	1.33	1.23
1	C	688	GLN	CD-OE1	5.14	1.33	1.23
1	D	587	ASN	CG-OD1	5.14	1.33	1.23
1	B	526	GLN	CD-OE1	5.14	1.33	1.23
1	A	579	ASN	CG-OD1	5.13	1.33	1.23
1	C	587	ASN	CG-OD1	5.13	1.33	1.23
1	D	817	GLN	CD-OE1	5.13	1.33	1.23
1	A	668	GLN	CD-OE1	5.13	1.33	1.23
1	B	799	HIS	ND1-CE1	5.13	1.37	1.32
1	C	400	ASN	CG-OD1	5.12	1.33	1.23
1	C	260	ASN	CG-OD1	5.12	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	ASN	CG-OD1	5.12	1.33	1.23
1	A	565	HIS	ND1-CE1	5.11	1.37	1.32
1	C	362	ASN	CG-OD1	5.11	1.33	1.23
1	D	212	GLN	CD-OE1	5.11	1.33	1.23
1	C	161	GLN	CD-OE1	5.11	1.33	1.23
1	A	798	GLN	CD-OE1	5.10	1.33	1.23
1	C	798	GLN	CD-OE1	5.10	1.33	1.23
1	D	731	GLN	CD-OE1	5.09	1.33	1.23
1	B	476	ASN	CG-OD1	5.09	1.33	1.23
1	D	476	ASN	CG-OD1	5.09	1.33	1.23
1	D	799	HIS	ND1-CE1	5.09	1.37	1.32
1	A	476	ASN	CG-OD1	5.08	1.33	1.23
1	B	161	GLN	CD-OE1	5.08	1.33	1.23
1	C	476	ASN	CG-OD1	5.08	1.33	1.23
1	D	400	ASN	CG-OD1	5.07	1.33	1.23
1	A	161	GLN	CD-OE1	5.07	1.33	1.23
1	D	513	GLN	CD-OE1	5.07	1.33	1.23
1	B	400	ASN	CG-OD1	5.06	1.33	1.23
1	D	161	GLN	CD-OE1	5.06	1.33	1.23
1	B	518	ASN	CG-OD1	5.04	1.33	1.23
1	A	518	ASN	CG-OD1	5.03	1.33	1.23
1	A	351	ASN	CG-OD1	5.03	1.33	1.23
1	D	579	ASN	CG-OD1	5.02	1.33	1.23
1	D	688	GLN	CD-OE1	5.00	1.33	1.23
1	B	351	ASN	CG-OD1	5.00	1.33	1.23

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	766	ALA	N-CA-C	-11.87	99.00	114.31
1	A	766	ALA	N-CA-C	-11.87	99.00	114.31
1	D	825	TYR	N-CA-C	11.86	127.17	112.23
1	B	825	TYR	N-CA-C	11.84	127.15	112.23
1	C	825	TYR	N-CA-C	11.80	127.10	112.23
1	A	825	TYR	N-CA-C	11.78	127.07	112.23
1	C	766	ALA	N-CA-C	-11.78	99.11	114.31
1	D	766	ALA	N-CA-C	-11.77	99.12	114.31
1	D	532	LEU	N-CA-C	-9.94	97.70	110.53
1	A	532	LEU	N-CA-C	-9.81	97.87	110.53
1	C	532	LEU	N-CA-C	-9.71	98.00	110.53
1	D	208	GLU	CA-C-N	9.40	129.98	119.92
1	D	208	GLU	C-N-CA	9.40	129.98	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	ASN	N-CA-C	-9.15	102.04	113.02
1	D	476	ASN	N-CA-C	-9.12	102.08	113.02
1	C	476	ASN	N-CA-C	-9.11	102.08	113.02
1	A	476	ASN	N-CA-C	-9.06	102.15	113.02
1	B	790	THR	N-CA-C	9.06	121.15	111.28
1	C	790	THR	N-CA-C	8.97	121.06	111.28
1	A	790	THR	N-CA-C	8.88	120.96	111.28
1	B	532	LEU	N-CA-C	-8.85	97.76	110.59
1	D	790	THR	N-CA-C	8.84	120.92	111.28
1	D	664	GLY	N-CA-C	-8.56	103.58	114.37
1	B	212	GLN	N-CA-C	-8.43	92.85	110.80
1	B	664	GLY	N-CA-C	-8.29	103.93	114.37
1	C	840	ILE	CB-CA-C	-8.21	101.37	111.88
1	C	191	ARG	CD-NE-CZ	-8.14	113.01	124.40
1	A	664	GLY	N-CA-C	-8.12	104.14	114.37
1	C	664	GLY	N-CA-C	-8.10	104.16	114.37
1	D	612	LYS	CA-C-N	7.79	129.58	119.84
1	D	612	LYS	C-N-CA	7.79	129.58	119.84
1	A	612	LYS	CA-C-N	7.77	129.56	119.84
1	A	612	LYS	C-N-CA	7.77	129.56	119.84
1	C	612	LYS	CA-C-N	7.73	129.51	119.84
1	C	612	LYS	C-N-CA	7.73	129.51	119.84
1	B	612	LYS	CA-C-N	7.71	129.48	119.84
1	B	612	LYS	C-N-CA	7.71	129.48	119.84
1	C	214	SER	N-CA-C	7.43	120.29	107.28
1	C	182	LYS	N-CA-C	-7.40	103.84	113.17
1	D	182	LYS	N-CA-C	-7.39	103.86	113.17
1	B	182	LYS	N-CA-C	-7.37	103.89	113.17
1	A	290	ASP	N-CA-C	-7.31	99.13	110.17
1	C	290	ASP	N-CA-C	-7.31	99.13	110.17
1	A	182	LYS	N-CA-C	-7.31	103.96	113.17
1	B	290	ASP	N-CA-C	-7.23	99.25	110.17
1	B	213	HIS	CB-CG-CD2	-7.22	121.82	131.20
1	D	290	ASP	N-CA-C	-7.20	99.30	110.17
1	B	297	ILE	N-CA-C	7.17	119.18	111.58
1	A	224	ILE	CA-C-N	-7.15	110.90	119.84
1	A	224	ILE	C-N-CA	-7.15	110.90	119.84
1	C	191	ARG	NE-CZ-NH2	-7.12	112.79	119.20
1	D	224	ILE	CA-C-N	-7.07	111.00	119.84
1	D	224	ILE	C-N-CA	-7.07	111.00	119.84
1	C	224	ILE	CA-C-N	-7.01	111.07	119.84
1	C	224	ILE	C-N-CA	-7.01	111.07	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ILE	CA-C-N	-6.99	111.10	119.84
1	B	224	ILE	C-N-CA	-6.99	111.10	119.84
1	A	157	ILE	N-CA-C	6.92	118.52	110.62
1	B	157	ILE	N-CA-C	6.91	118.50	110.62
1	C	157	ILE	N-CA-C	6.91	118.49	110.62
1	D	157	ILE	N-CA-C	6.90	118.48	110.62
1	D	615	THR	N-CA-C	-6.84	102.23	111.87
1	B	615	THR	N-CA-C	-6.82	102.25	111.87
1	C	615	THR	N-CA-C	-6.82	102.25	111.87
1	D	487	VAL	N-CA-C	-6.82	98.50	108.87
1	B	559	VAL	CA-C-N	6.81	126.80	119.78
1	B	559	VAL	C-N-CA	6.81	126.80	119.78
1	A	487	VAL	N-CA-C	-6.77	98.58	108.87
1	A	615	THR	N-CA-C	-6.71	102.41	111.87
1	C	487	VAL	N-CA-C	-6.68	98.71	108.87
1	D	214	SER	N-CA-C	6.68	120.34	107.44
1	B	760	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	D	760	HIS	CB-CG-CD2	-6.65	122.56	131.20
1	A	559	VAL	CA-C-N	6.65	126.63	119.78
1	A	559	VAL	C-N-CA	6.65	126.63	119.78
1	B	487	VAL	N-CA-C	-6.65	98.77	108.87
1	C	760	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	A	760	HIS	CB-CG-CD2	-6.61	122.60	131.20
1	D	799	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	C	653	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	D	653	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	D	559	VAL	CA-C-N	6.57	126.54	119.78
1	D	559	VAL	C-N-CA	6.57	126.54	119.78
1	C	799	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	B	653	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	C	559	VAL	CA-C-N	6.54	126.52	119.78
1	C	559	VAL	C-N-CA	6.54	126.52	119.78
1	A	653	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	B	799	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	C	304	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	A	799	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	304	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	C	840	ILE	CG1-CB-CG2	-6.45	91.37	110.70
1	B	304	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	D	304	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	C	452	ILE	CA-C-N	6.35	127.78	119.84
1	C	452	ILE	C-N-CA	6.35	127.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ILE	CA-C-N	6.34	127.77	119.84
1	A	452	ILE	C-N-CA	6.34	127.77	119.84
1	C	565	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	A	565	HIS	CB-CG-CD2	-6.32	122.99	131.20
1	D	452	ILE	CA-C-N	6.32	127.73	119.84
1	D	452	ILE	C-N-CA	6.32	127.73	119.84
1	B	565	HIS	CB-CG-CD2	-6.31	122.99	131.20
1	D	565	HIS	CB-CG-CD2	-6.30	123.00	131.20
1	C	191	ARG	NH1-CZ-NH2	6.29	127.48	119.30
1	D	600	GLU	N-CA-C	6.25	117.90	108.46
1	B	600	GLU	N-CA-C	6.22	117.85	108.46
1	A	600	GLU	N-CA-C	6.20	117.83	108.46
1	A	184	ILE	N-CA-C	-6.20	104.30	110.62
1	B	213	HIS	CB-CG-ND1	6.20	132.00	122.70
1	C	600	GLU	N-CA-C	6.20	117.81	108.46
1	D	184	ILE	N-CA-C	-6.04	104.46	110.62
1	B	452	ILE	CA-C-N	6.04	127.39	119.84
1	B	452	ILE	C-N-CA	6.04	127.39	119.84
1	D	742	ILE	N-CA-C	-6.01	99.92	108.58
1	B	211	TYR	N-CA-C	5.99	119.09	107.71
1	C	416	GLY	N-CA-C	-5.99	106.83	115.27
1	C	184	ILE	N-CA-C	-5.96	104.54	110.62
1	A	416	GLY	N-CA-C	-5.94	106.90	115.27
1	A	742	ILE	N-CA-C	-5.91	99.88	108.87
1	B	416	GLY	N-CA-C	-5.91	106.94	115.27
1	B	184	ILE	N-CA-C	-5.88	104.63	110.62
1	D	539	PHE	N-CA-C	5.86	118.09	109.24
1	C	224	ILE	N-CA-C	5.84	121.50	108.88
1	A	539	PHE	N-CA-C	5.82	118.03	109.24
1	D	416	GLY	N-CA-C	-5.80	107.09	115.27
1	C	296	GLU	N-CA-C	5.79	120.63	112.93
1	C	742	ILE	N-CA-C	-5.79	100.24	108.58
1	B	207	VAL	N-CA-C	-5.77	101.58	109.55
1	A	224	ILE	N-CA-C	5.77	121.35	108.88
1	A	760	HIS	CB-CG-ND1	5.77	131.35	122.70
1	B	296	GLU	N-CA-C	5.77	120.60	112.93
1	C	760	HIS	CB-CG-ND1	5.76	131.35	122.70
1	C	472	SER	N-CA-C	5.76	123.07	110.80
1	D	760	HIS	CB-CG-ND1	5.76	131.34	122.70
1	D	224	ILE	N-CA-C	5.75	121.29	108.88
1	B	760	HIS	CB-CG-ND1	5.73	131.30	122.70
1	D	296	GLU	N-CA-C	5.72	120.53	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ILE	N-CA-C	5.71	121.22	108.88
1	B	539	PHE	N-CA-C	5.71	117.86	109.24
1	A	296	GLU	N-CA-C	5.71	120.52	112.93
1	D	301	HIS	N-CA-C	-5.70	106.16	113.23
1	D	183	LYS	N-CA-C	-5.68	104.70	111.69
1	A	472	SER	N-CA-C	5.67	122.88	110.80
1	D	653	HIS	CB-CG-ND1	5.67	131.20	122.70
1	A	653	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	713	TYR	N-CA-C	-5.66	105.64	112.54
1	C	653	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	653	HIS	CB-CG-ND1	5.65	131.17	122.70
1	C	183	LYS	N-CA-C	-5.64	104.75	111.69
1	B	472	SER	N-CA-C	5.63	122.80	110.80
1	C	799	HIS	CB-CG-ND1	5.63	131.15	122.70
1	C	539	PHE	N-CA-C	5.63	117.74	109.24
1	D	799	HIS	CB-CG-ND1	5.62	131.13	122.70
1	A	713	TYR	N-CA-C	-5.60	105.70	112.54
1	C	304	HIS	CB-CG-ND1	5.60	131.10	122.70
1	A	183	LYS	N-CA-C	-5.60	104.81	111.69
1	B	799	HIS	CB-CG-ND1	5.58	131.07	122.70
1	D	472	SER	N-CA-C	5.58	122.69	110.80
1	B	304	HIS	CB-CG-ND1	5.58	131.07	122.70
1	A	304	HIS	CB-CG-ND1	5.57	131.05	122.70
1	A	799	HIS	CB-CG-ND1	5.56	131.04	122.70
1	D	304	HIS	CB-CG-ND1	5.55	131.03	122.70
1	B	742	ILE	N-CA-C	-5.54	100.45	108.87
1	D	139	GLU	N-CA-C	-5.51	106.39	113.01
1	D	652	SER	N-CA-C	5.51	118.21	111.82
1	A	214	SER	N-CA-C	5.49	117.65	107.60
1	C	565	HIS	CB-CG-ND1	5.48	130.92	122.70
1	D	565	HIS	CB-CG-ND1	5.47	130.90	122.70
1	B	565	HIS	CB-CG-ND1	5.45	130.88	122.70
1	A	565	HIS	CB-CG-ND1	5.44	130.86	122.70
1	C	307	SER	N-CA-C	-5.43	102.38	110.20
1	A	652	SER	N-CA-C	5.42	118.11	111.82
1	B	183	LYS	N-CA-C	-5.42	105.03	111.69
1	B	652	SER	N-CA-C	5.42	118.10	111.82
1	D	209	PRO	N-CA-C	5.41	119.72	111.34
1	D	307	SER	N-CA-C	-5.40	102.43	110.20
1	C	713	TYR	N-CA-C	-5.39	105.97	112.54
1	B	307	SER	N-CA-C	-5.37	102.47	110.20
1	C	139	GLU	N-CA-C	-5.36	106.58	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	GLU	N-CA-C	5.34	117.19	108.76
1	D	155	GLU	N-CA-C	5.33	117.18	108.76
1	B	139	GLU	N-CA-C	-5.31	106.64	113.01
1	C	652	SER	N-CA-C	5.30	117.97	111.82
1	A	155	GLU	N-CA-C	5.29	117.12	108.76
1	A	746	LYS	N-CA-C	-5.29	105.56	112.23
1	B	155	GLU	N-CA-C	5.28	117.09	108.76
1	A	307	SER	N-CA-C	-5.26	102.62	110.20
1	B	151	ILE	N-CA-C	-5.26	108.38	113.53
1	D	713	TYR	N-CA-C	-5.24	105.99	112.38
1	D	151	ILE	N-CA-C	-5.24	108.40	113.53
1	B	628	VAL	N-CA-C	5.23	116.11	108.53
1	A	139	GLU	N-CA-C	-5.22	106.75	113.01
1	D	704	THR	N-CA-C	5.15	117.80	111.82
1	C	628	VAL	N-CA-C	5.15	116.00	108.53
1	D	628	VAL	N-CA-C	5.15	116.00	108.53
1	A	151	ILE	N-CA-C	-5.13	108.50	113.53
1	C	158	TYR	N-CA-C	-5.13	104.34	111.52
1	A	704	THR	N-CA-C	5.12	117.77	111.82
1	C	191	ARG	CG-CD-NE	-5.12	100.75	112.00
1	B	158	TYR	N-CA-C	-5.10	104.37	111.52
1	D	746	LYS	N-CA-C	-5.10	105.81	112.23
1	C	704	THR	N-CA-C	5.09	117.73	111.82
1	D	158	TYR	N-CA-C	-5.08	104.41	111.52
1	B	618	ASP	N-CA-C	-5.07	108.37	114.75
1	D	434	ASN	N-CA-C	-5.06	106.88	113.16
1	B	704	THR	N-CA-C	5.06	117.69	111.82
1	D	297	ILE	N-CA-C	5.06	119.48	112.35
1	A	158	TYR	N-CA-C	-5.05	104.44	111.52
1	C	746	LYS	N-CA-C	-5.05	105.87	112.23
1	D	538	TYR	N-CA-C	-5.04	101.50	109.76
1	A	538	TYR	N-CA-C	-5.03	101.51	109.76
1	B	746	LYS	N-CA-C	-5.03	105.89	112.23
1	A	434	ASN	N-CA-C	-5.02	106.94	113.16
1	B	521	GLY	N-CA-C	5.02	125.07	113.18
1	C	521	GLY	N-CA-C	5.00	125.04	113.18

There are no chirality outliers.

There are no planarity outliers.

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	5837	0	5677	497	1
1	B	5837	0	5678	497	1
1	C	5837	0	5679	509	1
1	D	5837	0	5679	495	1
2	E	39	0	34	2	0
2	G	39	0	34	10	0
2	I	39	0	34	1	0
2	K	39	0	34	2	0
2	N	39	0	34	3	0
2	Q	39	0	34	1	0
2	T	39	0	34	3	0
2	V	39	0	34	3	0
2	Y	39	0	34	5	0
2	Z	39	0	34	2	0
3	F	50	0	42	2	0
4	H	50	0	43	9	0
5	J	28	0	25	4	0
5	M	28	0	25	1	0
5	O	28	0	25	3	0
5	P	28	0	25	3	0
5	S	28	0	25	4	0
5	U	28	0	25	0	0
6	L	39	0	33	6	0
6	R	39	0	33	4	0
6	W	39	0	33	4	0
7	X	50	0	43	10	0
8	A	13	0	0	2	0
8	B	14	0	0	8	0
8	C	14	0	0	2	0
8	D	10	0	0	2	0
All	All	24224	0	23430	2015	2

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 42.

All (2015) 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:D:617:THR:HG22	1:D:618:ASP:H	1.01	1.17
1:A:498:ASN:HA	1:A:519:THR:HG22	1.31	1.11
1:C:498:ASN:HA	1:C:519:THR:HG22	1.32	1.10
1:D:498:ASN:HA	1:D:519:THR:HG22	1.33	1.09
1:B:617:THR:HG22	1:B:618:ASP:H	1.07	1.09
1:C:617:THR:HG22	1:C:618:ASP:H	1.06	1.09
1:B:146:PRO:O	1:B:159:ARG:HB3	1.55	1.07
1:B:498:ASN:HA	1:B:519:THR:HG22	1.34	1.07
1:A:617:THR:HG22	1:A:618:ASP:H	1.07	1.06
1:D:146:PRO:O	1:D:159:ARG:HB3	1.55	1.06
1:C:724:ALA:HB1	1:C:730:GLY:HA2	1.36	1.06
1:A:146:PRO:O	1:A:159:ARG:HB3	1.55	1.05
1:C:146:PRO:O	1:C:159:ARG:HB3	1.55	1.04
1:A:724:ALA:HB1	1:A:730:GLY:HA2	1.37	1.04
4:H:3:BMA:O3	4:H:4:MAN:H3	1.57	1.02
7:X:3:MAN:C5	7:X:4:MAN:H2	1.86	1.01
7:X:3:MAN:H5	7:X:4:MAN:C2	1.86	1.01
1:D:724:ALA:HB1	1:D:730:GLY:HA2	1.37	1.01
1:B:724:ALA:HB1	1:B:730:GLY:HA2	1.37	1.00
1:A:599:ILE:HB	1:A:608:MET:HE3	1.48	0.95
1:D:498:ASN:HB3	1:D:520:VAL:HG23	1.47	0.95
1:C:498:ASN:HB3	1:C:520:VAL:HG23	1.48	0.94
1:D:617:THR:HG22	1:D:618:ASP:N	1.80	0.94
1:A:557:PRO:HG3	1:A:639:GLU:HB3	1.47	0.94
1:A:498:ASN:HB3	1:A:520:VAL:HG23	1.47	0.94
1:B:498:ASN:HB3	1:B:520:VAL:HG23	1.48	0.93
1:B:557:PRO:HG3	1:B:639:GLU:HB3	1.47	0.93
1:B:599:ILE:HB	1:B:608:MET:HE3	1.48	0.93
1:C:520:VAL:HG12	1:C:521:GLY:H	1.34	0.93
1:C:557:PRO:HG3	1:C:639:GLU:HB3	1.48	0.93
1:A:520:VAL:HG12	1:A:521:GLY:H	1.35	0.92
1:C:599:ILE:HB	1:C:608:MET:HE3	1.48	0.92
1:D:599:ILE:HB	1:D:608:MET:HE3	1.48	0.92
4:H:2:NAG:C3	4:H:3:BMA:H2	2.01	0.91
1:D:520:VAL:HG12	1:D:521:GLY:H	1.36	0.91
1:D:557:PRO:HG3	1:D:639:GLU:HB3	1.50	0.91
1:D:159:ARG:HG3	1:D:192:TYR:OH	1.70	0.91
1:A:159:ARG:HG3	1:A:192:TYR:OH	1.71	0.90
1:B:520:VAL:HG12	1:B:521:GLY:H	1.35	0.90
1:B:159:ARG:HG3	1:B:192:TYR:OH	1.70	0.90
1:B:617:THR:HG22	1:B:618:ASP:N	1.86	0.90
1:C:564:VAL:HG12	1:C:573:MET:HE3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:VAL:HG12	1:D:573:MET:HE3	1.54	0.89
1:A:564:VAL:HG12	1:A:573:MET:HE3	1.55	0.89
1:B:564:VAL:HG12	1:B:573:MET:HE3	1.54	0.89
1:C:694:THR:HA	1:C:697:LYS:HE2	1.55	0.89
1:B:325:ILE:HD11	1:B:341:PRO:HB2	1.55	0.89
1:C:159:ARG:HG3	1:C:192:TYR:OH	1.71	0.89
1:C:326:MET:HE1	1:D:337:PRO:HD2	1.55	0.89
1:C:176:THR:HG22	1:C:177:VAL:H	1.38	0.89
1:D:694:THR:HA	1:D:697:LYS:HE2	1.55	0.88
1:A:498:ASN:CA	1:A:519:THR:HG22	2.03	0.88
1:C:498:ASN:CA	1:C:519:THR:HG22	2.03	0.88
1:B:694:THR:HA	1:B:697:LYS:HE2	1.55	0.88
1:A:617:THR:HG22	1:A:618:ASP:N	1.86	0.88
7:X:3:MAN:H5	7:X:4:MAN:H2	0.93	0.88
1:B:498:ASN:CA	1:B:519:THR:HG22	2.05	0.87
1:D:498:ASN:CA	1:D:519:THR:HG22	2.05	0.87
5:P:1:NAG:H3	5:P:1:NAG:H83	1.55	0.87
1:A:176:THR:HG22	1:A:177:VAL:H	1.39	0.87
1:B:421:LYS:HE2	1:B:470:PRO:HD2	1.55	0.87
1:A:694:THR:HA	1:A:697:LYS:HE2	1.56	0.87
1:C:617:THR:HG22	1:C:618:ASP:N	1.86	0.87
1:D:325:ILE:HD11	1:D:341:PRO:HB2	1.57	0.87
1:B:207:VAL:HG12	1:B:208:GLU:HG2	1.57	0.87
1:D:176:THR:HG22	1:D:177:VAL:H	1.38	0.87
1:C:214:SER:HB2	8:C:20:HOH:O	1.75	0.86
4:H:2:NAG:H3	4:H:3:BMA:H2	1.57	0.86
1:D:532:LEU:HD23	1:D:533:VAL:H	1.40	0.86
1:A:532:LEU:HD23	1:A:533:VAL:H	1.39	0.86
1:B:537:THR:H	1:B:557:PRO:HD3	1.41	0.86
1:B:176:THR:HG22	1:B:177:VAL:H	1.38	0.86
1:C:537:THR:H	1:C:557:PRO:HD3	1.41	0.85
1:A:325:ILE:HD11	1:A:341:PRO:HB2	1.56	0.85
1:C:325:ILE:HD11	1:C:341:PRO:HB2	1.56	0.85
1:A:214:SER:O	1:A:216:THR:HG22	1.76	0.85
1:A:537:THR:H	1:A:557:PRO:HD3	1.42	0.85
1:C:724:ALA:HB1	1:C:730:GLY:CA	2.07	0.85
1:A:837:ARG:HB3	1:A:837:ARG:HH11	1.41	0.85
1:C:532:LEU:HD23	1:C:533:VAL:H	1.41	0.84
1:A:759:LEU:H	1:A:759:LEU:HD12	1.42	0.84
1:B:532:LEU:HD23	1:B:533:VAL:H	1.41	0.84
1:C:677:ARG:HG3	1:C:678:ARG:HG3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:677:ARG:HG3	1:D:678:ARG:HG3	1.58	0.84
1:C:191:ARG:NH2	1:C:215:TYR:CG	2.46	0.84
1:C:759:LEU:H	1:C:759:LEU:HD12	1.43	0.83
1:D:444:ARG:C	1:D:468:SER:HB2	2.04	0.83
1:D:421:LYS:HE2	1:D:470:PRO:HD2	1.58	0.83
1:A:724:ALA:HB1	1:A:730:GLY:CA	2.08	0.83
1:A:421:LYS:HE2	1:A:470:PRO:HD2	1.59	0.83
1:B:320:ASP:OD1	1:B:352:PRO:HB3	1.79	0.83
1:B:444:ARG:C	1:B:468:SER:HB2	2.04	0.83
1:B:837:ARG:HB3	1:B:837:ARG:HH11	1.43	0.83
1:C:442:ASP:OD2	1:C:444:ARG:HB2	1.79	0.83
1:C:837:ARG:HB3	1:C:837:ARG:HH11	1.44	0.83
1:D:442:ASP:OD2	1:D:444:ARG:HB2	1.78	0.83
5:P:1:NAG:H62	5:P:2:NAG:O5	1.79	0.83
1:A:442:ASP:OD2	1:A:444:ARG:HB2	1.79	0.83
1:A:444:ARG:C	1:A:468:SER:HB2	2.04	0.83
1:C:320:ASP:OD1	1:C:352:PRO:HB3	1.79	0.83
1:A:409:THR:HG21	1:A:418:CYS:HB3	1.61	0.82
1:A:677:ARG:HG3	1:A:678:ARG:HG3	1.60	0.82
1:B:724:ALA:HB1	1:B:730:GLY:CA	2.08	0.82
1:C:444:ARG:C	1:C:468:SER:HB2	2.03	0.82
1:D:537:THR:H	1:D:557:PRO:HD3	1.42	0.82
1:D:724:ALA:HB1	1:D:730:GLY:CA	2.08	0.82
1:B:442:ASP:OD2	1:B:444:ARG:HB2	1.80	0.82
1:D:837:ARG:HB3	1:D:837:ARG:HH11	1.43	0.82
1:B:759:LEU:H	1:B:759:LEU:HD12	1.43	0.82
1:C:624:LEU:HD23	1:C:656:VAL:HG23	1.62	0.82
1:B:677:ARG:HG3	1:B:678:ARG:HG3	1.60	0.82
1:D:759:LEU:H	1:D:759:LEU:HD12	1.43	0.81
1:C:715:GLY:O	1:C:719:THR:HG23	1.79	0.81
1:D:320:ASP:OD1	1:D:352:PRO:HB3	1.78	0.81
1:A:611:LEU:HB2	1:A:657:VAL:HG22	1.63	0.81
1:C:421:LYS:HE2	1:C:470:PRO:HD2	1.60	0.81
1:B:611:LEU:HB2	1:B:657:VAL:HG22	1.63	0.81
1:C:409:THR:HG21	1:C:418:CYS:HB3	1.63	0.81
7:X:1:NAG:H83	7:X:2:NAG:H83	1.63	0.81
1:B:196:PRO:HG2	1:B:251:GLY:O	1.81	0.80
1:A:196:PRO:HG2	1:A:251:GLY:O	1.80	0.80
1:A:624:LEU:HD23	1:A:656:VAL:HG23	1.63	0.80
1:C:721:ILE:C	1:C:723:PRO:HD3	2.06	0.80
1:D:409:THR:HG21	1:D:418:CYS:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:NH2	1:C:215:TYR:HB3	1.96	0.80
1:D:196:PRO:HG2	1:D:251:GLY:O	1.81	0.80
1:B:833:GLN:O	1:B:837:ARG:HG3	1.81	0.80
1:C:611:LEU:HB2	1:C:657:VAL:HG22	1.64	0.80
1:A:320:ASP:OD1	1:A:352:PRO:HB3	1.80	0.80
1:B:672:LEU:HD21	8:B:36:HOH:O	1.81	0.80
1:D:624:LEU:HD23	1:D:656:VAL:HG23	1.64	0.80
1:D:715:GLY:O	1:D:719:THR:HG23	1.79	0.80
1:B:624:LEU:HD23	1:B:656:VAL:HG23	1.64	0.80
1:B:721:ILE:C	1:B:723:PRO:HD3	2.07	0.80
1:A:191:ARG:NH2	1:A:215:TYR:HD2	1.80	0.80
1:D:427:GLU:HA	7:X:1:NAG:O7	1.81	0.80
1:D:611:LEU:HB2	1:D:657:VAL:HG22	1.64	0.80
1:B:409:THR:HG21	1:B:418:CYS:HB3	1.61	0.79
1:B:599:ILE:CD1	1:B:600:GLU:H	1.94	0.79
1:A:599:ILE:CD1	1:A:600:GLU:H	1.96	0.79
1:C:415:THR:HG22	1:C:417:VAL:HG23	1.65	0.79
1:D:721:ILE:C	1:D:723:PRO:HD3	2.08	0.79
1:A:326:MET:HE1	1:B:337:PRO:HD2	1.65	0.79
1:C:599:ILE:CD1	1:C:600:GLU:H	1.96	0.79
1:C:833:GLN:O	1:C:837:ARG:HG3	1.83	0.79
1:C:224:ILE:HG22	1:C:225:PRO:HD3	1.65	0.79
1:A:715:GLY:O	1:A:719:THR:HG23	1.81	0.78
1:D:599:ILE:CD1	1:D:600:GLU:H	1.95	0.78
1:A:721:ILE:C	1:A:723:PRO:HD3	2.08	0.78
1:B:715:GLY:O	1:B:719:THR:HG23	1.82	0.78
1:C:210:ILE:HG13	1:C:216:THR:HG21	1.65	0.78
4:H:2:NAG:H3	4:H:3:BMA:C2	2.12	0.78
1:C:196:PRO:HG2	1:C:251:GLY:O	1.83	0.78
1:A:224:ILE:HG22	1:A:225:PRO:HD3	1.65	0.78
1:A:415:THR:HG22	1:A:417:VAL:HG23	1.66	0.78
1:A:833:GLN:O	1:A:837:ARG:HG3	1.84	0.77
1:D:833:GLN:O	1:D:837:ARG:HG3	1.83	0.77
1:D:262:ILE:HB	1:D:276:VAL:HG12	1.64	0.77
1:D:191:ARG:HG2	1:D:192:TYR:N	2.00	0.77
1:D:302:ILE:HD13	1:D:302:ILE:C	2.10	0.77
1:A:569:ASP:OD2	5:J:1:NAG:H5	1.84	0.77
1:A:694:THR:HG22	8:A:17:HOH:O	1.85	0.77
1:C:262:ILE:HB	1:C:276:VAL:HG12	1.67	0.76
1:D:475:ASP:HB2	1:D:477:ILE:HG12	1.67	0.76
1:D:415:THR:HG22	1:D:417:VAL:HG23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:HIS:C	1:D:573:MET:HE2	2.10	0.76
1:A:262:ILE:HB	1:A:276:VAL:HG12	1.66	0.76
1:A:302:ILE:C	1:A:302:ILE:HD13	2.10	0.76
1:C:475:ASP:HB2	1:C:477:ILE:HG12	1.66	0.76
1:D:224:ILE:HG22	1:D:225:PRO:HD3	1.66	0.76
1:A:566:ASN:OD1	1:A:569:ASP:HB3	1.84	0.76
1:B:475:ASP:HB2	1:B:477:ILE:HG12	1.68	0.76
1:A:475:ASP:HB2	1:A:477:ILE:HG12	1.67	0.76
1:A:565:HIS:C	1:A:573:MET:HE2	2.10	0.76
1:B:224:ILE:HG22	1:B:225:PRO:HD3	1.67	0.76
1:B:302:ILE:HD13	1:B:302:ILE:C	2.11	0.76
1:C:302:ILE:C	1:C:302:ILE:HD13	2.10	0.76
1:C:565:HIS:C	1:C:573:MET:HE2	2.11	0.75
1:B:554:CYS:O	1:B:555:GLU:HB2	1.85	0.75
1:B:262:ILE:HB	1:B:276:VAL:HG12	1.66	0.75
1:B:421:LYS:CE	1:B:470:PRO:HD2	2.17	0.75
1:C:532:LEU:HD22	1:C:533:VAL:HG13	1.68	0.75
1:B:191:ARG:HG2	1:B:192:TYR:N	2.00	0.75
1:B:565:HIS:C	1:B:573:MET:HE2	2.12	0.75
1:A:182:LYS:O	1:A:185:GLU:HB3	1.87	0.75
1:A:191:ARG:HG2	1:A:192:TYR:N	2.00	0.75
1:B:409:THR:CG2	1:B:418:CYS:HB3	2.17	0.75
1:B:532:LEU:HD22	1:B:533:VAL:HG13	1.68	0.75
1:D:554:CYS:O	1:D:555:GLU:HB2	1.86	0.75
1:A:532:LEU:HD22	1:A:533:VAL:HG13	1.67	0.74
1:B:415:THR:HG22	1:B:417:VAL:HG23	1.69	0.74
1:D:617:THR:CG2	1:D:618:ASP:H	1.87	0.74
1:B:566:ASN:OD1	1:B:569:ASP:HB3	1.87	0.74
1:A:191:ARG:NH2	1:A:215:TYR:CD2	2.56	0.74
1:C:554:CYS:O	1:C:555:GLU:HB2	1.86	0.74
1:D:297:ILE:C	1:D:297:ILE:HD12	2.12	0.74
1:D:532:LEU:HD22	1:D:533:VAL:HG13	1.68	0.74
1:C:566:ASN:OD1	1:C:569:ASP:HB3	1.88	0.74
1:A:554:CYS:O	1:A:555:GLU:HB2	1.86	0.74
1:D:409:THR:CG2	1:D:418:CYS:HB3	2.18	0.74
1:C:234:PRO:HG2	1:C:237:VAL:HB	1.69	0.74
1:B:444:ARG:CA	1:B:468:SER:HB2	2.18	0.73
1:A:444:ARG:CA	1:A:468:SER:HB2	2.18	0.73
1:A:409:THR:CG2	1:A:418:CYS:HB3	2.18	0.73
1:C:444:ARG:CA	1:C:468:SER:HB2	2.18	0.73
1:A:613:PRO:HA	1:A:650:VAL:HG12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:HH21	1:C:215:TYR:HB3	1.54	0.73
1:D:214:SER:OG	1:D:216:THR:HG22	1.88	0.73
1:D:421:LYS:CE	1:D:470:PRO:HD2	2.19	0.73
1:D:444:ARG:CA	1:D:468:SER:HB2	2.18	0.72
1:B:444:ARG:HA	1:B:468:SER:HB2	1.71	0.72
1:C:375:ASP:HB3	1:C:377:ARG:NH1	2.04	0.72
1:C:409:THR:CG2	1:C:418:CYS:HB3	2.19	0.72
1:C:444:ARG:HA	1:C:468:SER:HB2	1.70	0.72
1:D:444:ARG:HA	1:D:468:SER:HB2	1.71	0.72
1:A:375:ASP:HB3	1:A:377:ARG:NH1	2.04	0.72
1:D:182:LYS:O	1:D:185:GLU:HB3	1.88	0.72
1:C:613:PRO:HA	1:C:650:VAL:HG12	1.70	0.72
1:B:234:PRO:HG2	1:B:237:VAL:HB	1.70	0.72
1:B:617:THR:CG2	1:B:618:ASP:H	1.90	0.72
1:C:192:TYR:HA	1:C:202:LEU:O	1.90	0.72
1:A:297:ILE:C	1:A:297:ILE:HD12	2.14	0.72
1:C:182:LYS:O	1:C:185:GLU:HB3	1.90	0.72
1:D:566:ASN:OD1	1:D:569:ASP:HB3	1.89	0.72
1:C:297:ILE:C	1:C:297:ILE:HD12	2.14	0.72
1:A:234:PRO:HG2	1:A:237:VAL:HB	1.72	0.71
1:A:444:ARG:HA	1:A:468:SER:HB2	1.71	0.71
1:B:297:ILE:C	1:B:297:ILE:HD12	2.15	0.71
1:B:613:PRO:HA	1:B:650:VAL:HG12	1.71	0.71
1:A:759:LEU:HD12	1:A:759:LEU:N	2.04	0.71
1:B:765:ARG:HD2	1:B:765:ARG:O	1.91	0.71
1:A:421:LYS:CE	1:A:470:PRO:HD2	2.21	0.71
1:A:374:ASP:O	1:A:375:ASP:C	2.34	0.71
1:C:176:THR:HG22	1:C:177:VAL:N	2.06	0.70
1:A:346:LYS:HG2	1:B:335:ILE:HG23	1.73	0.70
1:B:182:LYS:O	1:B:185:GLU:HB3	1.91	0.70
1:B:176:THR:HG22	1:B:177:VAL:N	2.07	0.70
1:B:759:LEU:HD12	1:B:759:LEU:N	2.06	0.70
1:A:191:ARG:HH21	1:A:215:TYR:HB3	1.57	0.70
1:B:332:THR:HB	1:B:821:ASP:OD2	1.92	0.70
1:A:765:ARG:HD2	1:A:765:ARG:O	1.91	0.70
1:D:176:THR:HG22	1:D:177:VAL:N	2.07	0.70
1:D:375:ASP:HB3	1:D:377:ARG:NH1	2.05	0.70
1:D:759:LEU:HD12	1:D:759:LEU:N	2.05	0.70
1:C:759:LEU:HD12	1:C:759:LEU:N	2.05	0.70
1:A:176:THR:HG22	1:A:177:VAL:N	2.07	0.70
1:A:498:ASN:O	1:A:518:ASN:HA	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ASP:O	1:B:375:ASP:C	2.35	0.70
1:D:234:PRO:HG2	1:D:237:VAL:HB	1.72	0.70
1:D:613:PRO:HA	1:D:650:VAL:HG12	1.73	0.70
1:B:376:PRO:HA	1:B:379:ARG:HD3	1.74	0.70
1:C:210:ILE:H	1:C:214:SER:HB3	1.57	0.70
1:C:374:ASP:O	1:C:375:ASP:C	2.34	0.70
1:B:520:VAL:HG12	1:B:521:GLY:N	2.07	0.70
1:B:438:VAL:HG21	1:B:490:ILE:HG21	1.74	0.69
1:C:421:LYS:CE	1:C:470:PRO:HD2	2.21	0.69
1:D:374:ASP:O	1:D:375:ASP:C	2.35	0.69
1:A:520:VAL:HG12	1:A:521:GLY:N	2.07	0.69
1:B:375:ASP:HB3	1:B:377:ARG:NH1	2.06	0.69
1:D:520:VAL:HG12	1:D:521:GLY:N	2.07	0.69
1:D:765:ARG:HD2	1:D:765:ARG:O	1.92	0.69
1:C:376:PRO:HA	1:C:379:ARG:HD3	1.74	0.69
1:D:498:ASN:O	1:D:518:ASN:HA	1.91	0.69
1:C:600:GLU:HB3	1:C:605:ASN:HA	1.75	0.69
1:D:129:LYS:HD3	8:D:41:HOH:O	1.93	0.69
1:A:600:GLU:HB3	1:A:605:ASN:HA	1.75	0.69
1:B:157:ILE:HG22	1:B:159:ARG:N	2.08	0.69
1:B:600:GLU:HB3	1:B:605:ASN:HA	1.75	0.69
1:D:167:LEU:HD21	1:D:198:ARG:HH21	1.56	0.69
1:D:332:THR:HB	1:D:821:ASP:OD2	1.93	0.69
1:D:376:PRO:HA	1:D:379:ARG:HD3	1.74	0.69
1:B:513:GLN:HB2	1:B:515:TYR:CE1	2.28	0.69
1:D:157:ILE:HG22	1:D:159:ARG:N	2.08	0.69
1:A:438:VAL:HG21	1:A:490:ILE:HG21	1.75	0.68
1:A:513:GLN:HB2	1:A:515:TYR:CE1	2.28	0.68
1:A:599:ILE:HD12	1:A:600:GLU:H	1.58	0.68
1:A:724:ALA:HB2	1:A:731:GLN:H	1.58	0.68
1:B:190:ILE:HD13	1:B:205:TYR:HA	1.74	0.68
1:C:724:ALA:HB2	1:C:731:GLN:H	1.57	0.68
1:D:438:VAL:HG21	1:D:490:ILE:HG21	1.75	0.68
1:D:762:LEU:CD2	7:X:4:MAN:O2	2.42	0.68
1:B:599:ILE:HD12	1:B:600:GLU:H	1.57	0.68
1:B:797:PHE:CE1	1:B:818:ILE:HD11	2.28	0.68
1:C:332:THR:HB	1:C:821:ASP:OD2	1.93	0.68
1:D:536:CYS:HA	1:D:557:PRO:HD2	1.76	0.68
1:A:157:ILE:HG22	1:A:159:ARG:N	2.08	0.68
1:C:498:ASN:O	1:C:518:ASN:HA	1.92	0.68
1:C:765:ARG:O	1:C:765:ARG:HD2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:NAG:H4	2:G:2:NAG:H82	1.75	0.68
1:A:249:PRO:HD2	1:A:253:GLN:OE1	1.94	0.68
1:C:157:ILE:HG22	1:C:159:ARG:N	2.09	0.68
1:C:668:GLN:HB2	1:C:672:LEU:HD23	1.75	0.68
1:B:724:ALA:HB2	1:B:731:GLN:H	1.57	0.68
1:C:346:LYS:HG2	1:D:335:ILE:HG23	1.76	0.68
1:C:513:GLN:HB2	1:C:515:TYR:CE1	2.29	0.68
1:C:599:ILE:HD12	1:C:600:GLU:H	1.59	0.68
1:D:599:ILE:HD12	1:D:600:GLU:H	1.57	0.68
1:D:797:PHE:CE1	1:D:818:ILE:HD11	2.29	0.68
1:A:332:THR:HB	1:A:821:ASP:OD2	1.94	0.68
1:A:498:ASN:HA	1:A:519:THR:CG2	2.19	0.68
1:D:600:GLU:HB3	1:D:605:ASN:HA	1.76	0.68
1:C:438:VAL:HG21	1:C:490:ILE:HG21	1.75	0.68
1:C:158:TYR:CD2	1:C:166:ARG:HB2	2.30	0.67
1:D:158:TYR:CD2	1:D:166:ARG:HB2	2.29	0.67
1:D:668:GLN:HB2	1:D:672:LEU:HD23	1.75	0.67
1:A:167:LEU:HD21	1:A:198:ARG:HH21	1.59	0.67
1:A:191:ARG:HH11	1:A:191:ARG:HG3	1.60	0.67
1:B:547:MET:O	1:B:567:THR:HB	1.93	0.67
1:C:167:LEU:HD21	1:C:198:ARG:HH21	1.59	0.67
1:D:513:GLN:HB2	1:D:515:TYR:CE1	2.29	0.67
1:D:724:ALA:HB2	1:D:731:GLN:H	1.58	0.67
4:H:2:NAG:O3	4:H:3:BMA:H2	1.95	0.67
1:A:668:GLN:HB2	1:A:672:LEU:HD23	1.75	0.67
1:B:167:LEU:HD21	1:B:198:ARG:HH21	1.60	0.67
1:A:376:PRO:HA	1:A:379:ARG:HD3	1.75	0.67
1:C:520:VAL:HG12	1:C:521:GLY:N	2.06	0.67
1:A:693:ARG:HH21	1:A:725:LYS:HD3	1.60	0.67
1:C:191:ARG:NH2	1:C:215:TYR:CB	2.58	0.67
1:C:547:MET:O	1:C:567:THR:HB	1.94	0.67
1:D:152:SER:HG	1:D:155:GLU:HG2	1.59	0.67
1:D:547:MET:O	1:D:567:THR:HB	1.94	0.67
2:Y:1:NAG:H83	2:Y:1:NAG:H3	1.77	0.67
1:A:158:TYR:CD2	1:A:166:ARG:HB2	2.30	0.67
1:A:802:GLU:OE2	1:B:332:THR:HG23	1.95	0.67
1:B:194:ILE:H	1:B:194:ILE:HD12	1.59	0.67
1:C:249:PRO:HD2	1:C:253:GLN:OE1	1.94	0.67
1:B:536:CYS:HA	1:B:557:PRO:HD2	1.77	0.66
1:C:505:THR:HB	1:C:509:PRO:HA	1.76	0.66
1:C:536:CYS:HA	1:C:557:PRO:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:LYS:HD2	1:D:726:GLY:H	1.60	0.66
1:A:254:LEU:HD12	1:A:254:LEU:C	2.21	0.66
1:B:158:TYR:CD2	1:B:166:ARG:HB2	2.29	0.66
1:C:693:ARG:HH21	1:C:725:LYS:HD3	1.61	0.66
1:A:547:MET:O	1:A:567:THR:HB	1.94	0.66
1:B:693:ARG:HH21	1:B:725:LYS:HD3	1.60	0.66
1:C:498:ASN:HA	1:C:519:THR:CG2	2.19	0.66
1:A:725:LYS:HD2	1:A:726:GLY:H	1.61	0.66
1:A:797:PHE:CE1	1:A:818:ILE:HD11	2.30	0.66
1:B:468:SER:C	1:B:470:PRO:HD3	2.21	0.66
1:A:536:CYS:HA	1:A:557:PRO:HD2	1.77	0.66
1:D:249:PRO:HD2	1:D:253:GLN:OE1	1.95	0.66
1:D:254:LEU:C	1:D:254:LEU:HD12	2.21	0.66
1:D:135:ASP:HA	1:D:138:SER:OG	1.96	0.66
1:B:254:LEU:C	1:B:254:LEU:HD12	2.21	0.66
1:B:498:ASN:O	1:B:518:ASN:HA	1.94	0.66
1:D:260:ASN:O	1:D:286:ASN:ND2	2.28	0.66
1:C:194:ILE:H	1:C:194:ILE:HD12	1.60	0.66
1:D:161:GLN:O	1:D:162:LYS:HG3	1.96	0.66
1:D:313:LEU:HB3	1:D:359:ILE:HD11	1.77	0.66
1:C:725:LYS:HD2	1:C:726:GLY:H	1.60	0.66
1:C:797:PHE:CE1	1:C:818:ILE:HD11	2.31	0.66
1:A:468:SER:C	1:A:470:PRO:HD3	2.21	0.65
1:B:845:GLU:C	1:B:847:PHE:H	2.04	0.65
1:C:468:SER:C	1:C:470:PRO:HD3	2.21	0.65
1:C:260:ASN:O	1:C:286:ASN:ND2	2.29	0.65
1:D:468:SER:C	1:D:470:PRO:HD3	2.22	0.65
1:D:845:GLU:C	1:D:847:PHE:H	2.05	0.65
1:A:617:THR:CG2	1:A:618:ASP:H	1.90	0.65
1:B:191:ARG:HG3	1:B:191:ARG:HH11	1.60	0.65
1:B:668:GLN:HB2	1:B:672:LEU:HD23	1.78	0.65
1:C:214:SER:O	1:C:216:THR:HG22	1.96	0.65
1:D:204:SER:HB3	1:D:219:TYR:CE2	2.31	0.65
1:D:498:ASN:CB	1:D:519:THR:HG22	2.27	0.65
1:A:571:LYS:HE2	5:J:1:NAG:H61	1.78	0.65
1:B:313:LEU:HB3	1:B:359:ILE:HD11	1.79	0.65
1:C:135:ASP:HA	1:C:138:SER:OG	1.96	0.65
1:C:254:LEU:C	1:C:254:LEU:HD12	2.21	0.65
1:D:191:ARG:HH11	1:D:191:ARG:HG3	1.60	0.65
1:B:498:ASN:CB	1:B:519:THR:HG22	2.27	0.65
1:B:670:THR:HG23	1:B:674:HIS:CE1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:CYS:HA	1:D:557:PRO:CD	2.26	0.65
1:D:693:ARG:HH21	1:D:725:LYS:HD3	1.62	0.65
1:A:498:ASN:CB	1:A:519:THR:HG22	2.27	0.65
1:D:670:THR:HG23	1:D:674:HIS:CE1	2.32	0.65
1:A:435:GLU:CG	1:A:449:ILE:HG23	2.27	0.65
1:B:536:CYS:HA	1:B:557:PRO:CD	2.27	0.65
1:C:536:CYS:HA	1:C:557:PRO:CD	2.27	0.65
1:C:670:THR:HG23	1:C:674:HIS:CE1	2.32	0.65
1:A:194:ILE:HD12	1:A:194:ILE:H	1.60	0.65
1:C:498:ASN:CB	1:C:519:THR:HG22	2.26	0.65
1:A:845:GLU:C	1:A:847:PHE:H	2.05	0.65
1:B:161:GLN:O	1:B:162:LYS:HG3	1.97	0.65
1:C:845:GLU:C	1:C:847:PHE:H	2.05	0.65
1:C:214:SER:OG	1:C:216:THR:HG22	1.97	0.64
1:C:689:MET:HE1	1:C:732:THR:HG21	1.79	0.64
1:A:260:ASN:O	1:A:286:ASN:ND2	2.29	0.64
1:A:313:LEU:HB3	1:A:359:ILE:HD11	1.79	0.64
1:C:313:LEU:HB3	1:C:359:ILE:HD11	1.79	0.64
1:D:191:ARG:HG3	1:D:191:ARG:NH1	2.13	0.64
1:B:135:ASP:HA	1:B:138:SER:OG	1.97	0.64
1:D:505:THR:HB	1:D:509:PRO:HA	1.78	0.64
1:D:599:ILE:HG23	1:D:600:GLU:N	2.12	0.64
1:C:204:SER:HB3	1:C:219:TYR:CE2	2.33	0.64
1:C:293:TYR:CE2	1:C:354:ILE:HD12	2.32	0.64
2:N:1:NAG:H83	2:N:1:NAG:H3	1.79	0.64
1:A:191:ARG:HG3	1:A:191:ARG:NH1	2.13	0.64
1:B:505:THR:HB	1:B:509:PRO:HA	1.78	0.64
1:C:435:GLU:CG	1:C:449:ILE:HG23	2.28	0.64
1:D:816:LEU:HD13	1:D:818:ILE:HD13	1.79	0.64
1:A:532:LEU:CD2	1:A:533:VAL:H	2.11	0.64
1:A:536:CYS:HA	1:A:557:PRO:CD	2.28	0.64
1:B:178:LEU:O	1:B:179:ILE:HD13	1.98	0.64
1:B:249:PRO:HD2	1:B:253:GLN:OE1	1.98	0.64
1:A:505:THR:HB	1:A:509:PRO:HA	1.78	0.64
1:A:761:GLY:C	1:A:763:ASP:H	2.05	0.64
1:B:260:ASN:O	1:B:286:ASN:ND2	2.31	0.64
1:C:161:GLN:O	1:C:162:LYS:HG3	1.98	0.64
1:B:599:ILE:HG23	1:B:600:GLU:N	2.12	0.63
1:A:437:PRO:HB3	1:A:448:PHE:HD1	1.63	0.63
1:D:178:LEU:O	1:D:179:ILE:HD13	1.97	0.63
1:D:293:TYR:CE2	1:D:354:ILE:HD12	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:789:PRO:HA	1:D:819:TYR:HB2	1.80	0.63
1:B:789:PRO:HA	1:B:819:TYR:HB2	1.80	0.63
1:C:153:ASP:HB2	1:C:546:SER:HB2	1.80	0.63
1:A:689:MET:HE1	1:A:732:THR:HG21	1.80	0.63
1:B:293:TYR:CE2	1:B:354:ILE:HD12	2.33	0.63
1:A:161:GLN:O	1:A:162:LYS:HG3	1.98	0.63
1:A:670:THR:HG23	1:A:674:HIS:CE1	2.33	0.63
1:B:191:ARG:HG3	1:B:191:ARG:NH1	2.13	0.63
1:D:437:PRO:HB3	1:D:448:PHE:HD1	1.64	0.63
1:C:789:PRO:HA	1:C:819:TYR:HB2	1.81	0.63
1:A:135:ASP:HA	1:A:138:SER:OG	1.99	0.63
1:A:427:GLU:HA	2:G:1:NAG:O7	1.98	0.63
1:B:437:PRO:HB3	1:B:448:PHE:HD1	1.62	0.63
1:B:725:LYS:HD2	1:B:726:GLY:H	1.61	0.63
1:D:194:ILE:HD12	1:D:194:ILE:H	1.63	0.63
1:B:152:SER:OG	1:B:155:GLU:HG2	1.99	0.63
1:B:435:GLU:CG	1:B:449:ILE:HG23	2.28	0.63
1:C:451:ALA:HB1	1:C:459:LYS:HG3	1.81	0.63
1:D:498:ASN:HA	1:D:519:THR:CG2	2.21	0.63
1:A:599:ILE:HG23	1:A:600:GLU:N	2.12	0.62
1:A:789:PRO:HA	1:A:819:TYR:HB2	1.81	0.62
1:A:797:PHE:HD2	1:B:331:TYR:CE2	2.16	0.62
1:A:152:SER:OG	1:A:155:GLU:HG2	1.99	0.62
1:A:548:ASP:O	1:A:567:THR:HG22	1.99	0.62
1:B:451:ALA:HB1	1:B:459:LYS:HG3	1.82	0.62
1:B:548:ASP:O	1:B:567:THR:HG22	1.99	0.62
1:B:761:GLY:C	1:B:763:ASP:H	2.06	0.62
1:B:194:ILE:H	1:B:194:ILE:CD1	2.13	0.62
1:A:451:ALA:HB1	1:A:459:LYS:HG3	1.81	0.62
1:C:180:GLU:C	1:C:182:LYS:H	2.08	0.62
1:A:293:TYR:CE2	1:A:354:ILE:HD12	2.34	0.62
1:B:569:ASP:O	1:B:570:LYS:HB2	2.00	0.62
1:C:761:GLY:C	1:C:763:ASP:H	2.06	0.62
1:D:435:GLU:CG	1:D:449:ILE:HG23	2.28	0.62
1:A:511:ARG:O	1:A:512:ARG:HD2	2.00	0.62
1:B:498:ASN:HA	1:B:519:THR:CG2	2.21	0.62
1:C:599:ILE:HG23	1:C:600:GLU:N	2.13	0.62
1:A:180:GLU:C	1:A:182:LYS:H	2.08	0.62
1:B:402:ALA:CB	1:B:759:LEU:HD11	2.30	0.62
1:C:437:PRO:HB3	1:C:448:PHE:HD1	1.64	0.62
1:C:513:GLN:HB2	1:C:515:TYR:HE1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:HB2	1:A:546:SER:HB2	1.82	0.61
1:B:613:PRO:HG3	1:B:622:TYR:CE2	2.35	0.61
1:B:401:ARG:HD2	1:B:754:GLU:OE1	2.00	0.61
1:C:548:ASP:O	1:C:567:THR:HG22	2.00	0.61
1:D:180:GLU:C	1:D:182:LYS:H	2.08	0.61
1:D:761:GLY:C	1:D:763:ASP:H	2.06	0.61
1:B:689:MET:HE1	1:B:732:THR:HG21	1.82	0.61
1:D:401:ARG:HD2	1:D:754:GLU:OE1	1.99	0.61
1:B:180:GLU:C	1:B:182:LYS:H	2.07	0.61
1:D:152:SER:OG	1:D:155:GLU:HG2	2.00	0.61
1:D:513:GLN:HB2	1:D:515:TYR:HE1	1.64	0.61
1:B:546:SER:C	1:B:547:MET:HG2	2.26	0.61
1:D:210:ILE:HG13	1:D:216:THR:HG21	1.81	0.61
1:D:451:ALA:HB1	1:D:459:LYS:HG3	1.83	0.61
1:D:613:PRO:HG3	1:D:622:TYR:CE2	2.36	0.61
1:B:166:ARG:HD2	1:B:176:THR:O	2.01	0.61
1:C:725:LYS:HD2	1:C:726:GLY:N	2.16	0.61
1:D:454:GLN:NE2	1:D:483:GLY:H	1.98	0.61
1:A:454:GLN:NE2	1:A:483:GLY:H	1.99	0.61
1:B:454:GLN:NE2	1:B:483:GLY:H	1.98	0.61
1:C:152:SER:OG	1:C:155:GLU:HG2	2.01	0.61
1:D:721:ILE:HG22	1:D:721:ILE:O	2.01	0.61
1:C:178:LEU:O	1:C:179:ILE:HD13	2.01	0.61
1:C:511:ARG:O	1:C:512:ARG:HD2	2.01	0.61
1:C:613:PRO:HG3	1:C:622:TYR:CE2	2.35	0.61
1:B:153:ASP:HB2	1:B:546:SER:HB2	1.82	0.61
1:B:724:ALA:CB	1:B:731:GLN:H	2.14	0.61
1:C:454:GLN:NE2	1:C:483:GLY:H	1.99	0.61
1:D:725:LYS:HD2	1:D:726:GLY:N	2.15	0.61
1:A:513:GLN:HB2	1:A:515:TYR:HE1	1.64	0.60
1:A:725:LYS:HD2	1:A:726:GLY:N	2.16	0.60
1:D:567:THR:HG23	1:D:568:THR:N	2.15	0.60
1:C:567:THR:HG23	1:C:568:THR:N	2.16	0.60
1:C:569:ASP:O	1:C:570:LYS:HB2	2.00	0.60
1:C:724:ALA:CB	1:C:731:GLN:H	2.14	0.60
1:D:759:LEU:H	1:D:759:LEU:CD1	2.14	0.60
1:A:178:LEU:O	1:A:179:ILE:HD13	2.01	0.60
1:A:663:ARG:HB2	1:A:675:GLU:HB3	1.83	0.60
1:B:511:ARG:O	1:B:512:ARG:HD2	2.01	0.60
1:C:215:TYR:CD1	1:C:301:HIS:NE2	2.63	0.60
1:C:663:ARG:HB2	1:C:675:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:HG22	1:D:211:TYR:N	2.16	0.60
1:A:401:ARG:HD2	1:A:754:GLU:OE1	2.01	0.60
1:B:540:SER:HB3	1:B:553:LYS:HG3	1.83	0.60
1:C:215:TYR:CE1	1:C:301:HIS:NE2	2.69	0.60
1:C:797:PHE:HD2	1:D:331:TYR:CE2	2.18	0.60
1:D:511:ARG:O	1:D:512:ARG:HD2	2.01	0.60
1:A:759:LEU:H	1:A:759:LEU:CD1	2.13	0.60
1:D:153:ASP:HB2	1:D:546:SER:HB2	1.82	0.60
1:D:402:ALA:CB	1:D:759:LEU:HD11	2.31	0.60
1:D:569:ASP:O	1:D:570:LYS:HB2	2.01	0.60
1:B:567:THR:HG23	1:B:568:THR:N	2.15	0.60
1:D:166:ARG:HD2	1:D:176:THR:O	2.01	0.60
1:B:475:ASP:CB	1:B:477:ILE:HG23	2.32	0.60
1:B:513:GLN:HB2	1:B:515:TYR:HE1	1.64	0.60
1:C:401:ARG:HD2	1:C:754:GLU:OE1	2.02	0.60
1:A:724:ALA:CB	1:A:731:GLN:H	2.15	0.60
1:C:166:ARG:HD2	1:C:176:THR:O	2.01	0.60
1:C:402:ALA:CB	1:C:759:LEU:HD11	2.32	0.60
1:D:546:SER:C	1:D:547:MET:HG2	2.26	0.60
1:D:548:ASP:O	1:D:567:THR:HG22	2.01	0.60
1:A:166:ARG:HD2	1:A:176:THR:O	2.02	0.60
1:B:759:LEU:H	1:B:759:LEU:CD1	2.14	0.60
1:C:190:ILE:HD13	1:C:207:VAL:HG23	1.83	0.60
1:C:194:ILE:HG22	1:C:224:ILE:HD11	1.84	0.60
1:A:194:ILE:HG22	1:A:224:ILE:HD11	1.84	0.60
1:A:248:GLY:HA3	1:A:253:GLN:HG3	1.84	0.60
1:B:194:ILE:HG22	1:B:224:ILE:HD11	1.84	0.60
1:C:326:MET:HE1	1:D:337:PRO:CD	2.28	0.60
1:D:689:MET:HE1	1:D:732:THR:HG21	1.83	0.60
1:C:475:ASP:CB	1:C:477:ILE:HG23	2.32	0.59
1:A:402:ALA:CB	1:A:759:LEU:HD11	2.33	0.59
1:A:624:LEU:HD21	1:A:658:VAL:HG23	1.84	0.59
1:C:339:VAL:HG11	1:D:339:VAL:CG1	2.32	0.59
1:C:717:LEU:O	1:C:721:ILE:HG13	2.02	0.59
1:A:816:LEU:HD13	1:A:818:ILE:HD13	1.83	0.59
1:A:825:TYR:O	1:A:826:PHE:HB2	2.03	0.59
1:B:194:ILE:HD12	1:B:194:ILE:N	2.16	0.59
1:D:475:ASP:CB	1:D:477:ILE:HG23	2.32	0.59
1:B:274:ARG:NE	1:B:277:SER:HB3	2.17	0.59
1:B:717:LEU:O	1:B:721:ILE:HG13	2.02	0.59
1:B:725:LYS:HD2	1:B:726:GLY:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HG22	1:C:211:TYR:N	2.17	0.59
1:C:274:ARG:NE	1:C:277:SER:HB3	2.18	0.59
1:C:591:MET:O	1:C:614:ALA:HB2	2.02	0.59
1:D:194:ILE:HG22	1:D:224:ILE:HD11	1.85	0.59
1:D:378:MET:HE1	1:D:398:TRP:HB3	1.84	0.59
1:A:613:PRO:HG3	1:A:622:TYR:CE2	2.37	0.59
1:A:709:PHE:HB2	1:A:843:PHE:CZ	2.37	0.59
1:B:663:ARG:HB2	1:B:675:GLU:HB3	1.83	0.59
1:B:722:LEU:N	1:B:723:PRO:HD3	2.18	0.59
1:C:617:THR:CG2	1:C:618:ASP:H	1.89	0.59
1:C:722:LEU:N	1:C:723:PRO:HD3	2.17	0.59
1:D:663:ARG:HB2	1:D:675:GLU:HB3	1.83	0.59
1:B:573:MET:O	1:B:574:PHE:HB3	2.03	0.59
1:C:540:SER:HB3	1:C:553:LYS:HG3	1.83	0.59
1:C:546:SER:C	1:C:547:MET:HG2	2.27	0.59
1:C:759:LEU:H	1:C:759:LEU:CD1	2.14	0.59
1:D:452:ILE:HG13	1:D:452:ILE:O	2.03	0.59
1:D:540:SER:HB3	1:D:553:LYS:HG3	1.83	0.59
1:A:532:LEU:HD23	1:A:533:VAL:N	2.15	0.59
1:C:709:PHE:HB2	1:C:843:PHE:CZ	2.37	0.59
2:G:1:NAG:H4	2:G:2:NAG:N2	2.17	0.59
1:A:194:ILE:HD12	1:A:194:ILE:N	2.17	0.59
1:A:546:SER:C	1:A:547:MET:HG2	2.28	0.59
1:B:816:LEU:HD13	1:B:818:ILE:HD13	1.84	0.59
1:C:528:LEU:HD12	1:C:528:LEU:N	2.18	0.59
1:D:709:PHE:HB2	1:D:843:PHE:CZ	2.37	0.59
1:D:717:LEU:O	1:D:721:ILE:HG13	2.03	0.59
1:D:724:ALA:CB	1:D:731:GLN:H	2.15	0.59
1:A:608:MET:O	1:A:608:MET:HG3	2.03	0.59
1:A:722:LEU:N	1:A:723:PRO:HD3	2.17	0.59
1:C:248:GLY:HA3	1:C:253:GLN:HG3	1.85	0.59
1:A:475:ASP:CB	1:A:477:ILE:HG23	2.33	0.59
1:A:567:THR:HG23	1:A:568:THR:N	2.16	0.59
1:B:250:LYS:O	1:B:253:GLN:HG2	2.02	0.59
1:C:339:VAL:HG11	1:D:339:VAL:HG11	1.85	0.59
1:C:378:MET:HE1	1:C:398:TRP:HB3	1.85	0.59
1:C:816:LEU:HD13	1:C:818:ILE:HD13	1.85	0.59
1:B:709:PHE:HB2	1:B:843:PHE:CZ	2.37	0.58
1:D:528:LEU:HD12	1:D:528:LEU:N	2.18	0.58
1:D:573:MET:O	1:D:574:PHE:HB3	2.03	0.58
1:A:717:LEU:O	1:A:721:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:O	1:B:182:LYS:N	2.35	0.58
1:B:183:LYS:HG2	1:B:203:PHE:HE1	1.67	0.58
1:C:582:VAL:O	1:C:586:ILE:HG22	2.03	0.58
1:C:721:ILE:O	1:C:721:ILE:HG22	2.03	0.58
1:A:569:ASP:O	1:A:570:LYS:HB2	2.01	0.58
1:D:248:GLY:HA3	1:D:253:GLN:HG3	1.84	0.58
1:D:437:PRO:HG2	1:D:439:PHE:HE1	1.69	0.58
1:D:624:LEU:HD21	1:D:658:VAL:HG23	1.84	0.58
1:A:528:LEU:HD12	1:A:528:LEU:N	2.18	0.58
1:C:608:MET:HG3	1:C:608:MET:O	2.03	0.58
1:D:591:MET:O	1:D:614:ALA:HB2	2.03	0.58
1:D:722:LEU:N	1:D:723:PRO:HD3	2.18	0.58
1:A:624:LEU:HD21	1:A:658:VAL:CG2	2.33	0.58
1:A:636:SER:HB2	1:A:661:ASP:OD2	2.03	0.58
1:A:701:ILE:HD13	1:A:701:ILE:C	2.28	0.58
1:B:192:TYR:HA	1:B:202:LEU:O	2.04	0.58
1:C:180:GLU:O	1:C:182:LYS:N	2.36	0.58
1:A:721:ILE:HG22	1:A:721:ILE:O	2.04	0.58
1:D:532:LEU:HD23	1:D:533:VAL:N	2.15	0.58
1:D:825:TYR:O	1:D:826:PHE:HB2	2.03	0.58
1:B:402:ALA:HB2	1:B:759:LEU:HD11	1.86	0.58
1:B:610:ILE:HD12	1:B:611:LEU:N	2.19	0.58
1:C:302:ILE:HD13	1:C:302:ILE:O	2.04	0.58
1:C:624:LEU:HD21	1:C:658:VAL:HG23	1.85	0.58
1:D:129:LYS:HG2	1:D:589:ARG:CZ	2.34	0.58
1:D:192:TYR:HA	1:D:202:LEU:O	2.04	0.58
1:A:274:ARG:NE	1:A:277:SER:HB3	2.19	0.58
1:A:346:LYS:HD3	1:B:336:TYR:CZ	2.38	0.58
1:B:528:LEU:N	1:B:528:LEU:HD12	2.18	0.58
1:D:572:LYS:HD2	1:D:575:ASP:OD1	2.04	0.58
1:A:688:GLN:O	1:A:692:VAL:HG23	2.04	0.58
1:B:359:ILE:HD12	1:B:359:ILE:O	2.04	0.58
1:D:532:LEU:CD2	1:D:533:VAL:H	2.13	0.58
1:A:437:PRO:HG2	1:A:439:PHE:HE1	1.69	0.58
1:B:582:VAL:O	1:B:586:ILE:HG22	2.04	0.58
1:B:721:ILE:O	1:B:721:ILE:HG22	2.03	0.58
1:C:825:TYR:O	1:C:826:PHE:HB2	2.03	0.58
1:D:624:LEU:HD21	1:D:658:VAL:CG2	2.33	0.58
1:A:573:MET:O	1:A:574:PHE:HB3	2.03	0.57
1:C:339:VAL:CG1	1:D:339:VAL:HG11	2.34	0.57
1:C:520:VAL:CG1	1:C:521:GLY:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:ILE:HD13	1:C:600:GLU:H	1.68	0.57
1:B:520:VAL:CG1	1:B:521:GLY:H	2.14	0.57
1:C:194:ILE:HD12	1:C:194:ILE:N	2.17	0.57
1:D:167:LEU:HD21	1:D:198:ARG:NH2	2.19	0.57
1:D:466:SER:HA	1:D:476:ASN:HB2	1.86	0.57
1:B:636:SER:HB2	1:B:661:ASP:OD2	2.05	0.57
1:D:701:ILE:HD13	1:D:701:ILE:C	2.30	0.57
1:D:816:LEU:CD1	1:D:818:ILE:HD13	2.35	0.57
1:A:582:VAL:O	1:A:586:ILE:HG22	2.04	0.57
1:B:532:LEU:CD2	1:B:533:VAL:HG13	2.34	0.57
1:B:599:ILE:HD13	1:B:600:GLU:H	1.68	0.57
1:C:129:LYS:HG2	1:C:589:ARG:CZ	2.35	0.57
1:C:573:MET:O	1:C:574:PHE:HB3	2.03	0.57
1:C:624:LEU:HD21	1:C:658:VAL:CG2	2.34	0.57
1:D:180:GLU:O	1:D:182:LYS:N	2.37	0.57
1:C:532:LEU:O	1:C:533:VAL:C	2.48	0.57
1:C:636:SER:HB2	1:C:661:ASP:OD2	2.05	0.57
1:D:194:ILE:HD12	1:D:194:ILE:N	2.19	0.57
1:A:192:TYR:HA	1:A:202:LEU:O	2.04	0.57
1:A:250:LYS:O	1:A:253:GLN:HG2	2.04	0.57
1:A:599:ILE:HD13	1:A:600:GLU:H	1.69	0.57
1:B:608:MET:HG3	1:B:608:MET:O	2.04	0.57
1:B:825:TYR:O	1:B:826:PHE:HB2	2.02	0.57
1:C:437:PRO:HG2	1:C:439:PHE:HE1	1.69	0.57
1:C:532:LEU:CD2	1:C:533:VAL:H	2.13	0.57
1:C:701:ILE:C	1:C:701:ILE:HD13	2.29	0.57
2:G:1:NAG:H4	2:G:2:NAG:C8	2.35	0.57
1:A:166:ARG:O	1:A:178:LEU:HD22	2.05	0.57
1:A:540:SER:HB3	1:A:553:LYS:HG3	1.85	0.57
1:B:466:SER:HA	1:B:476:ASN:HB2	1.87	0.57
1:C:250:LYS:O	1:C:253:GLN:HG2	2.04	0.57
1:A:426:SER:O	2:G:1:NAG:O7	2.23	0.57
1:A:591:MET:O	1:A:614:ALA:HB2	2.04	0.57
1:A:802:GLU:CD	1:B:332:THR:HG23	2.29	0.57
1:B:129:LYS:HG2	1:B:589:ARG:CZ	2.35	0.57
1:B:248:GLY:HA3	1:B:253:GLN:HG3	1.85	0.57
1:B:532:LEU:HD23	1:B:533:VAL:N	2.16	0.57
1:B:532:LEU:CD2	1:B:533:VAL:H	2.14	0.57
1:B:591:MET:O	1:B:614:ALA:HB2	2.05	0.57
1:B:604:TYR:OH	1:B:671:LYS:HG2	2.05	0.57
1:B:624:LEU:HD21	1:B:658:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:ASP:N	1:D:547:MET:HE2	2.20	0.57
2:T:2:NAG:H3	2:T:3:BMA:H2	1.87	0.57
1:A:452:ILE:O	1:A:452:ILE:HG13	2.05	0.56
1:D:188:ARG:HH11	1:D:188:ARG:HG3	1.70	0.56
1:A:466:SER:HA	1:A:476:ASN:HB2	1.86	0.56
1:C:624:LEU:HD23	1:C:656:VAL:CG2	2.34	0.56
1:C:182:LYS:O	1:C:182:LYS:HD3	2.06	0.56
1:C:210:ILE:CG1	1:C:216:THR:HG21	2.34	0.56
1:C:444:ARG:HA	1:C:468:SER:CB	2.35	0.56
4:H:3:BMA:O3	4:H:4:MAN:C3	2.43	0.56
1:A:339:VAL:HG11	1:B:339:VAL:HG11	1.87	0.56
1:A:604:TYR:OH	1:A:671:LYS:HG2	2.06	0.56
1:B:158:TYR:CD2	1:B:168:TRP:HD1	2.23	0.56
1:B:378:MET:HE1	1:B:398:TRP:HB3	1.87	0.56
1:B:452:ILE:O	1:B:454:GLN:HG2	2.05	0.56
1:C:452:ILE:O	1:C:454:GLN:HG2	2.06	0.56
1:D:158:TYR:CD2	1:D:168:TRP:HD1	2.23	0.56
1:D:402:ALA:HB2	1:D:759:LEU:HD11	1.88	0.56
1:D:608:MET:HG3	1:D:608:MET:O	2.06	0.56
1:A:412:ASP:C	1:A:414:THR:H	2.14	0.56
1:A:452:ILE:O	1:A:454:GLN:HG2	2.05	0.56
1:B:494:ASP:N	1:B:547:MET:HE2	2.21	0.56
1:B:532:LEU:O	1:B:533:VAL:C	2.48	0.56
1:B:701:ILE:C	1:B:701:ILE:HD13	2.30	0.56
1:C:158:TYR:CD2	1:C:168:TRP:HD1	2.23	0.56
1:D:452:ILE:O	1:D:454:GLN:HG2	2.05	0.56
1:A:359:ILE:O	1:A:359:ILE:HD12	2.06	0.56
1:A:498:ASN:HB2	1:A:519:THR:N	2.19	0.56
1:B:421:LYS:HG3	1:B:470:PRO:HG2	1.88	0.56
1:C:334:SER:HB2	8:C:7:HOH:O	2.05	0.56
1:A:129:LYS:HG2	1:A:589:ARG:CZ	2.35	0.56
1:A:346:LYS:HG2	1:B:335:ILE:CG2	2.34	0.56
1:C:166:ARG:O	1:C:178:LEU:HD22	2.06	0.56
1:C:529:SER:O	1:C:530:CYS:C	2.48	0.56
1:D:582:VAL:O	1:D:586:ILE:HG22	2.05	0.56
1:C:204:SER:HA	1:C:218:TYR:O	2.05	0.56
1:C:402:ALA:HB2	1:C:759:LEU:HD11	1.88	0.56
1:D:250:LYS:O	1:D:253:GLN:HG2	2.06	0.56
1:D:274:ARG:NE	1:D:277:SER:HB3	2.19	0.56
1:D:404:ASN:HA	1:D:430:LEU:HD23	1.88	0.56
1:D:599:ILE:HD13	1:D:600:GLU:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:ILE:HD12	1:D:611:LEU:N	2.21	0.56
1:A:158:TYR:CD2	1:A:168:TRP:HD1	2.23	0.56
1:A:610:ILE:HD12	1:A:611:LEU:N	2.21	0.56
1:B:183:LYS:HG2	1:B:203:PHE:CE1	2.40	0.56
1:B:188:ARG:HH11	1:B:188:ARG:HG3	1.71	0.56
1:B:529:SER:O	1:B:530:CYS:C	2.48	0.56
1:D:302:ILE:HD13	1:D:302:ILE:O	2.06	0.56
1:A:444:ARG:HA	1:A:468:SER:CB	2.36	0.56
1:A:494:ASP:N	1:A:547:MET:HE2	2.21	0.56
1:A:571:LYS:HE2	5:J:1:NAG:C6	2.36	0.56
1:B:168:TRP:HH2	6:L:1:NAG:C1	2.19	0.56
1:C:452:ILE:O	1:C:452:ILE:HG13	2.05	0.56
1:C:532:LEU:CD2	1:C:533:VAL:HG13	2.35	0.56
1:A:195:SER:HB2	1:A:196:PRO:HD2	1.88	0.55
1:A:378:MET:HE1	1:A:398:TRP:HB3	1.88	0.55
1:A:532:LEU:CD2	1:A:533:VAL:HG13	2.34	0.55
1:A:532:LEU:O	1:A:533:VAL:C	2.48	0.55
1:A:624:LEU:HD23	1:A:656:VAL:CG2	2.36	0.55
1:D:319:ASN:OD1	1:D:321:SER:HB3	2.06	0.55
1:B:452:ILE:O	1:B:452:ILE:HG13	2.06	0.55
1:B:624:LEU:HD23	1:B:656:VAL:CG2	2.35	0.55
1:B:624:LEU:HD21	1:B:658:VAL:CG2	2.35	0.55
1:C:359:ILE:HD12	1:C:359:ILE:O	2.07	0.55
1:C:494:ASP:N	1:C:547:MET:HE2	2.20	0.55
1:D:532:LEU:CD2	1:D:533:VAL:HG13	2.35	0.55
1:A:837:ARG:HH11	1:A:837:ARG:CB	2.18	0.55
1:B:572:LYS:HD2	1:B:575:ASP:OD1	2.06	0.55
1:C:412:ASP:C	1:C:414:THR:H	2.15	0.55
1:D:421:LYS:HG3	1:D:470:PRO:HG2	1.89	0.55
1:D:498:ASN:HB2	1:D:519:THR:N	2.21	0.55
5:O:2:NAG:H83	5:O:2:NAG:O3	2.07	0.55
1:A:231:SER:HB3	1:A:233:ASP:OD1	2.07	0.55
1:A:402:ALA:HB2	1:A:759:LEU:HD11	1.88	0.55
1:B:167:LEU:HD21	1:B:198:ARG:NH2	2.21	0.55
1:C:572:LYS:HD2	1:C:575:ASP:OD1	2.06	0.55
1:D:166:ARG:O	1:D:178:LEU:HD22	2.06	0.55
1:D:182:LYS:O	1:D:182:LYS:HD3	2.07	0.55
1:D:604:TYR:OH	1:D:671:LYS:HG2	2.07	0.55
1:D:778:ALA:O	1:D:779:LEU:O	2.25	0.55
1:B:456:GLY:O	1:B:457:ARG:HB2	2.07	0.55
1:C:191:ARG:HB3	1:C:204:SER:OG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LYS:HG3	1:C:470:PRO:HG2	1.88	0.55
1:C:610:ILE:HD12	1:C:611:LEU:N	2.22	0.55
1:D:532:LEU:O	1:D:533:VAL:C	2.50	0.55
2:Q:2:NAG:H83	2:Q:2:NAG:O3	2.06	0.55
2:Y:1:NAG:C8	2:Y:1:NAG:C1	2.84	0.55
1:C:604:TYR:OH	1:C:671:LYS:HG2	2.06	0.55
1:D:231:SER:HB3	1:D:233:ASP:OD1	2.06	0.55
1:D:529:SER:O	1:D:530:CYS:C	2.49	0.55
1:A:204:SER:HB3	1:A:219:TYR:CE2	2.41	0.55
1:A:302:ILE:HD13	1:A:302:ILE:O	2.06	0.55
1:A:572:LYS:HD2	1:A:575:ASP:OD1	2.06	0.55
1:B:166:ARG:O	1:B:178:LEU:HD22	2.06	0.55
1:B:412:ASP:C	1:B:414:THR:H	2.15	0.55
1:B:696:LEU:HA	1:B:701:ILE:HD12	1.89	0.55
1:C:319:ASN:OD1	1:C:321:SER:HB3	2.06	0.55
1:D:444:ARG:HA	1:D:468:SER:CB	2.36	0.55
1:B:372:PRO:HB3	1:B:398:TRP:CZ3	2.41	0.55
1:C:613:PRO:O	1:C:614:ALA:HB3	2.07	0.55
2:Y:1:NAG:C1	2:Y:1:NAG:H82	2.36	0.55
1:A:167:LEU:HD21	1:A:198:ARG:NH2	2.20	0.55
1:B:444:ARG:HA	1:B:468:SER:CB	2.36	0.55
1:C:194:ILE:H	1:C:194:ILE:CD1	2.14	0.55
1:D:599:ILE:CB	1:D:608:MET:HE3	2.31	0.55
1:A:319:ASN:OD1	1:A:321:SER:HB3	2.07	0.55
1:B:421:LYS:HE2	1:B:470:PRO:CD	2.35	0.55
1:B:742:ILE:HD12	1:B:744:ASP:H	1.72	0.55
1:C:778:ALA:O	1:C:779:LEU:O	2.24	0.55
1:D:624:LEU:HD23	1:D:656:VAL:CG2	2.36	0.55
1:B:206:ASN:ND2	1:B:216:THR:O	2.39	0.54
1:B:778:ALA:O	1:B:779:LEU:O	2.25	0.54
1:D:412:ASP:C	1:D:414:THR:H	2.15	0.54
1:A:182:LYS:O	1:A:182:LYS:HD3	2.07	0.54
1:A:808:ILE:HD13	1:B:819:TYR:CD1	2.42	0.54
1:B:195:SER:HB2	1:B:196:PRO:HD2	1.89	0.54
1:C:167:LEU:HD21	1:C:198:ARG:NH2	2.21	0.54
1:D:191:ARG:HH21	1:D:215:TYR:HB3	1.73	0.54
1:D:195:SER:HB2	1:D:196:PRO:HD2	1.89	0.54
1:A:778:ALA:O	1:A:779:LEU:O	2.24	0.54
1:B:293:TYR:CE2	1:B:297:ILE:HD11	2.42	0.54
1:B:437:PRO:HG2	1:B:439:PHE:HE1	1.71	0.54
1:C:188:ARG:HH11	1:C:188:ARG:HG3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:GLY:O	1:C:457:ARG:HB2	2.08	0.54
1:C:518:ASN:O	1:C:523:PHE:HD1	1.91	0.54
1:D:636:SER:HB2	1:D:661:ASP:OD2	2.07	0.54
1:A:293:TYR:CE2	1:A:297:ILE:HD11	2.42	0.54
1:B:613:PRO:O	1:B:614:ALA:HB3	2.07	0.54
1:A:326:MET:HE1	1:B:337:PRO:CD	2.36	0.54
1:B:182:LYS:O	1:B:182:LYS:HD3	2.07	0.54
1:C:377:ARG:HG2	1:C:377:ARG:HH11	1.72	0.54
1:C:466:SER:HA	1:C:476:ASN:HB2	1.87	0.54
1:C:492:ALA:HB1	1:C:547:MET:HE1	1.90	0.54
1:D:372:PRO:HB3	1:D:398:TRP:CZ3	2.42	0.54
1:D:554:CYS:O	1:D:555:GLU:CB	2.56	0.54
1:D:696:LEU:HA	1:D:701:ILE:HD12	1.89	0.54
1:D:806:GLN:HE22	1:D:809:ARG:HH11	1.55	0.54
7:X:1:NAG:H4	7:X:2:NAG:N2	2.22	0.54
1:A:188:ARG:HG3	1:A:188:ARG:HH11	1.72	0.54
1:A:372:PRO:HB3	1:A:398:TRP:CZ3	2.42	0.54
1:A:529:SER:O	1:A:530:CYS:C	2.49	0.54
1:A:613:PRO:O	1:A:614:ALA:HB3	2.07	0.54
1:D:166:ARG:NE	1:D:177:VAL:HG22	2.23	0.54
1:A:845:GLU:O	1:A:847:PHE:N	2.41	0.54
1:C:172:THR:O	1:C:173:ASN:C	2.51	0.54
1:C:498:ASN:HB2	1:C:519:THR:N	2.21	0.54
1:A:172:THR:O	1:A:173:ASN:C	2.50	0.54
1:B:319:ASN:OD1	1:B:321:SER:HB3	2.06	0.54
1:B:498:ASN:HB2	1:B:519:THR:N	2.22	0.54
1:B:816:LEU:CD1	1:B:818:ILE:HD13	2.38	0.54
1:C:166:ARG:NE	1:C:177:VAL:HG22	2.23	0.54
1:C:195:SER:HB2	1:C:196:PRO:HD2	1.90	0.54
1:C:539:PHE:CE1	1:C:552:LEU:HD11	2.42	0.54
1:D:823:SER:OG	1:D:824:HIS:N	2.41	0.54
1:A:404:ASN:HA	1:A:430:LEU:HD23	1.90	0.54
1:A:539:PHE:CE1	1:A:552:LEU:HD11	2.42	0.54
1:B:302:ILE:HD13	1:B:302:ILE:O	2.07	0.54
1:C:688:GLN:O	1:C:692:VAL:HG23	2.07	0.54
1:A:422:HIS:CD2	1:A:423:GLU:H	2.26	0.54
1:B:475:ASP:HB2	1:B:477:ILE:HG23	1.90	0.54
1:B:823:SER:OG	1:B:824:HIS:N	2.41	0.54
1:C:176:THR:CG2	1:C:177:VAL:H	2.17	0.54
1:A:421:LYS:HG3	1:A:470:PRO:HG2	1.89	0.53
1:A:520:VAL:CG1	1:A:521:GLY:H	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:HB3	1:B:204:SER:OG	2.08	0.53
1:B:539:PHE:CE1	1:B:552:LEU:HD11	2.43	0.53
1:C:210:ILE:HB	1:C:214:SER:CB	2.38	0.53
1:C:210:ILE:CD1	1:C:216:THR:HG21	2.38	0.53
1:B:231:SER:HB3	1:B:233:ASP:OD1	2.08	0.53
1:D:742:ILE:HD12	1:D:744:ASP:H	1.73	0.53
1:B:166:ARG:NE	1:B:177:VAL:HG22	2.23	0.53
1:B:492:ALA:HB1	1:B:547:MET:HE1	1.89	0.53
5:S:1:NAG:H4	5:S:2:NAG:H82	1.91	0.53
1:B:518:ASN:O	1:B:523:PHE:HD1	1.91	0.53
1:B:695:MET:O	1:B:701:ILE:HG21	2.07	0.53
1:A:168:TRP:HH2	3:F:1:NAG:C1	2.22	0.53
1:A:806:GLN:HE22	1:A:809:ARG:HH11	1.55	0.53
1:B:404:ASN:HA	1:B:430:LEU:HD23	1.91	0.53
1:C:475:ASP:HB2	1:C:477:ILE:HG23	1.91	0.53
1:C:696:LEU:HA	1:C:701:ILE:HD12	1.89	0.53
1:D:293:TYR:CE2	1:D:297:ILE:HD11	2.43	0.53
1:D:359:ILE:O	1:D:359:ILE:HD12	2.08	0.53
1:D:456:GLY:O	1:D:457:ARG:HB2	2.08	0.53
1:A:293:TYR:HA	1:A:297:ILE:HG13	1.90	0.53
1:B:688:GLN:O	1:B:692:VAL:HG23	2.08	0.53
1:B:806:GLN:HE22	1:B:809:ARG:HH11	1.57	0.53
1:C:404:ASN:HA	1:C:430:LEU:HD23	1.91	0.53
1:C:695:MET:O	1:C:701:ILE:HG21	2.09	0.53
1:C:816:LEU:CD1	1:C:818:ILE:HD13	2.39	0.53
1:D:539:PHE:CE1	1:D:552:LEU:HD11	2.44	0.53
1:A:492:ALA:HB1	1:A:547:MET:HE1	1.91	0.53
1:A:661:ASP:HB3	1:A:665:SER:OG	2.09	0.53
1:B:500:ILE:CG2	1:B:500:ILE:O	2.57	0.53
1:B:554:CYS:O	1:B:555:GLU:CB	2.56	0.53
1:C:302:ILE:C	1:C:302:ILE:CD1	2.81	0.53
1:D:183:LYS:HG2	1:D:203:PHE:HE1	1.74	0.53
1:D:492:ALA:HB1	1:D:547:MET:HE1	1.89	0.53
1:A:200:TYR:CZ	1:A:268:VAL:HG11	2.44	0.53
1:A:456:GLY:O	1:A:457:ARG:HB2	2.07	0.53
1:B:172:THR:O	1:B:173:ASN:C	2.51	0.53
1:C:532:LEU:HD23	1:C:533:VAL:N	2.16	0.53
1:C:786:ILE:O	1:C:816:LEU:HD23	2.08	0.53
1:D:475:ASP:HB2	1:D:477:ILE:HG23	1.91	0.53
1:D:688:GLN:O	1:D:692:VAL:HG23	2.09	0.53
1:A:166:ARG:NE	1:A:177:VAL:HG22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LYS:CD	1:B:470:PRO:HD2	2.39	0.53
1:C:215:TYR:N	1:C:215:TYR:CD2	2.75	0.53
1:C:742:ILE:HD12	1:C:744:ASP:H	1.74	0.53
1:C:802:GLU:OE2	1:D:332:THR:HG23	2.09	0.53
1:A:422:HIS:ND1	1:A:450:ARG:NH1	2.57	0.53
1:B:422:HIS:CD2	1:B:423:GLU:H	2.27	0.53
1:B:693:ARG:HH21	1:B:725:LYS:CD	2.22	0.53
1:B:845:GLU:O	1:B:847:PHE:N	2.41	0.53
1:C:168:TRP:CD1	1:C:175:SER:HB3	2.44	0.53
1:C:200:TYR:CZ	1:C:268:VAL:HG11	2.44	0.53
1:C:231:SER:HB3	1:C:233:ASP:OD1	2.08	0.53
1:C:293:TYR:HA	1:C:297:ILE:HG13	1.91	0.53
1:A:168:TRP:CD1	1:A:175:SER:HB3	2.45	0.52
1:A:176:THR:CG2	1:A:177:VAL:H	2.18	0.52
1:A:518:ASN:O	1:A:523:PHE:HD1	1.92	0.52
1:B:422:HIS:ND1	1:B:450:ARG:NH1	2.56	0.52
1:D:422:HIS:CD2	1:D:423:GLU:H	2.27	0.52
1:A:386:VAL:HA	1:A:395:ALA:O	2.10	0.52
1:A:786:ILE:O	1:A:816:LEU:HD23	2.09	0.52
1:B:183:LYS:HB2	1:B:183:LYS:NZ	2.25	0.52
1:C:560:PRO:HD3	1:C:641:PHE:CD2	2.44	0.52
1:D:191:ARG:HE	1:D:215:TYR:HB3	1.74	0.52
1:D:440:SER:O	1:D:443:GLY:N	2.43	0.52
1:D:518:ASN:O	1:D:523:PHE:HD1	1.92	0.52
1:A:442:ASP:CG	1:A:444:ARG:HB2	2.35	0.52
1:A:560:PRO:HD3	1:A:641:PHE:CD2	2.45	0.52
1:B:254:LEU:HD12	1:B:254:LEU:O	2.09	0.52
1:B:538:TYR:O	1:B:554:CYS:O	2.28	0.52
1:C:372:PRO:HB3	1:C:398:TRP:CZ3	2.44	0.52
1:D:500:ILE:O	1:D:500:ILE:CG2	2.56	0.52
1:D:786:ILE:O	1:D:816:LEU:HD23	2.10	0.52
1:A:335:ILE:HG22	1:A:336:TYR:CD1	2.45	0.52
1:A:475:ASP:HB2	1:A:477:ILE:HG23	1.91	0.52
1:A:816:LEU:CD1	1:A:818:ILE:HD13	2.40	0.52
1:B:293:TYR:HA	1:B:297:ILE:HG13	1.92	0.52
1:B:386:VAL:HA	1:B:395:ALA:O	2.09	0.52
1:B:566:ASN:HD21	1:B:569:ASP:HB2	1.72	0.52
1:C:166:ARG:CD	1:C:177:VAL:HG22	2.38	0.52
1:C:719:THR:HB	1:C:784:PHE:CZ	2.45	0.52
1:D:520:VAL:CG1	1:D:521:GLY:H	2.15	0.52
1:A:155:GLU:HB2	1:A:168:TRP:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:TYR:CD2	1:A:297:ILE:HD11	2.45	0.52
1:C:823:SER:OG	1:C:824:HIS:N	2.42	0.52
1:D:613:PRO:O	1:D:614:ALA:HB3	2.08	0.52
1:B:661:ASP:HB3	1:B:665:SER:OG	2.10	0.52
1:C:293:TYR:CE2	1:C:297:ILE:HD11	2.44	0.52
1:D:267:HIS:HB3	1:D:270:LYS:HB2	1.91	0.52
1:D:422:HIS:ND1	1:D:450:ARG:NH1	2.57	0.52
1:D:695:MET:O	1:D:701:ILE:HG21	2.10	0.52
1:D:837:ARG:HH11	1:D:837:ARG:CB	2.18	0.52
1:A:166:ARG:CD	1:A:177:VAL:HG22	2.39	0.52
1:A:494:ASP:HB2	1:A:547:MET:HE2	1.92	0.52
1:A:823:SER:OG	1:A:824:HIS:N	2.41	0.52
1:B:537:THR:HA	8:B:38:HOH:O	2.09	0.52
1:D:172:THR:O	1:D:173:ASN:C	2.52	0.52
1:D:293:TYR:HA	1:D:297:ILE:HG13	1.92	0.52
1:D:617:THR:CG2	1:D:618:ASP:N	2.55	0.52
1:D:661:ASP:HB3	1:D:665:SER:OG	2.09	0.52
1:A:346:LYS:HE3	1:B:335:ILE:O	2.10	0.52
1:B:155:GLU:HB2	1:B:168:TRP:O	2.10	0.52
1:B:260:ASN:O	1:B:279:GLY:HA3	2.10	0.52
1:C:185:GLU:O	1:C:187:LEU:N	2.42	0.52
1:C:845:GLU:O	1:C:847:PHE:N	2.42	0.52
1:D:190:ILE:N	1:D:190:ILE:HD12	2.25	0.52
1:D:386:VAL:HA	1:D:395:ALA:O	2.09	0.52
1:A:180:GLU:O	1:A:182:LYS:N	2.35	0.52
1:A:191:ARG:NH2	1:A:215:TYR:HB3	2.23	0.52
1:A:695:MET:O	1:A:701:ILE:HG21	2.09	0.52
1:B:166:ARG:CD	1:B:177:VAL:HG22	2.40	0.52
1:B:185:GLU:O	1:B:187:LEU:N	2.41	0.52
1:B:267:HIS:HB3	1:B:270:LYS:HB2	1.91	0.52
1:B:293:TYR:CD2	1:B:297:ILE:HD11	2.45	0.52
1:D:155:GLU:HB2	1:D:168:TRP:O	2.10	0.52
1:D:166:ARG:CD	1:D:177:VAL:HG22	2.40	0.52
1:A:693:ARG:HH21	1:A:725:LYS:CD	2.21	0.52
1:C:155:GLU:HB2	1:C:168:TRP:O	2.10	0.52
1:C:444:ARG:HH11	1:C:444:ARG:HG2	1.75	0.52
1:A:191:ARG:HB3	1:A:204:SER:OG	2.11	0.51
1:B:594:VAL:O	1:B:595:GLU:HG3	2.10	0.51
1:C:186:SER:O	1:C:187:LEU:C	2.53	0.51
1:C:260:ASN:O	1:C:279:GLY:HA3	2.10	0.51
1:D:377:ARG:HG2	1:D:377:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LEU:CD2	1:D:533:VAL:N	2.73	0.51
1:D:594:VAL:O	1:D:595:GLU:HG3	2.10	0.51
1:D:845:GLU:O	1:D:847:PHE:N	2.42	0.51
1:A:564:VAL:HG21	1:A:574:PHE:CZ	2.46	0.51
1:A:841:ASN:O	1:A:845:GLU:HG2	2.11	0.51
1:C:599:ILE:CB	1:C:608:MET:HE3	2.30	0.51
1:C:806:GLN:HE22	1:C:809:ARG:HH11	1.57	0.51
1:D:194:ILE:H	1:D:194:ILE:CD1	2.15	0.51
1:D:200:TYR:CZ	1:D:268:VAL:HG11	2.45	0.51
1:D:421:LYS:O	1:D:422:HIS:HB2	2.11	0.51
1:D:442:ASP:CG	1:D:444:ARG:HB2	2.34	0.51
2:K:2:NAG:H83	2:K:2:NAG:O3	2.10	0.51
1:A:211:TYR:HD2	1:A:294:GLU:OE1	1.93	0.51
1:A:260:ASN:O	1:A:279:GLY:HA3	2.11	0.51
1:A:339:VAL:HG11	1:B:339:VAL:CG1	2.40	0.51
1:B:183:LYS:NZ	1:B:183:LYS:CB	2.73	0.51
1:B:299:LYS:HE2	1:B:299:LYS:HA	1.91	0.51
1:B:440:SER:O	1:B:443:GLY:N	2.43	0.51
1:B:442:ASP:CG	1:B:444:ARG:HB2	2.35	0.51
1:C:442:ASP:CG	1:C:444:ARG:HB2	2.35	0.51
1:B:168:TRP:CD1	1:B:175:SER:HB3	2.45	0.51
1:B:595:GLU:OE2	1:B:612:LYS:HD2	2.10	0.51
1:C:422:HIS:CD2	1:C:423:GLU:H	2.28	0.51
1:C:532:LEU:CD2	1:C:533:VAL:N	2.74	0.51
1:A:500:ILE:O	1:A:500:ILE:CG2	2.58	0.51
1:A:532:LEU:CD2	1:A:533:VAL:N	2.72	0.51
1:B:560:PRO:HD3	1:B:641:PHE:CD2	2.46	0.51
1:B:841:ASN:O	1:B:845:GLU:HG2	2.10	0.51
1:C:346:LYS:HE3	1:D:335:ILE:O	2.10	0.51
1:C:386:VAL:HA	1:C:395:ALA:O	2.10	0.51
1:C:500:ILE:O	1:C:500:ILE:CG2	2.57	0.51
1:A:719:THR:HB	1:A:784:PHE:CZ	2.45	0.51
1:A:742:ILE:HD12	1:A:744:ASP:H	1.75	0.51
1:B:828:SER:HB3	1:B:831:LEU:HB2	1.93	0.51
1:C:346:LYS:HG2	1:D:335:ILE:CG2	2.41	0.51
1:D:168:TRP:CD1	1:D:175:SER:HB3	2.45	0.51
1:D:566:ASN:HD21	1:D:569:ASP:HB2	1.76	0.51
1:A:377:ARG:HG2	1:A:377:ARG:HH11	1.75	0.51
1:A:494:ASP:HB3	1:A:499:LYS:HB2	1.93	0.51
1:A:696:LEU:HA	1:A:701:ILE:HD12	1.92	0.51
1:B:214:SER:O	1:B:216:THR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:HIS:ND1	1:C:450:ARG:NH1	2.58	0.51
1:C:440:SER:O	1:C:443:GLY:N	2.43	0.51
1:C:594:VAL:O	1:C:595:GLU:HG3	2.10	0.51
5:P:2:NAG:H83	5:P:2:NAG:O3	2.10	0.51
1:D:421:LYS:CD	1:D:470:PRO:HD2	2.41	0.51
1:A:220:VAL:HG13	1:A:230:GLN:H	1.76	0.51
1:A:339:VAL:CG1	1:B:339:VAL:HG11	2.41	0.51
1:B:190:ILE:HD12	1:B:190:ILE:N	2.26	0.51
1:C:259:GLU:HA	1:C:281:GLU:OE1	2.11	0.51
1:C:841:ASN:O	1:C:845:GLU:HG2	2.11	0.51
1:D:185:GLU:O	1:D:187:LEU:N	2.41	0.51
1:D:191:ARG:NH2	1:D:215:TYR:HD1	2.09	0.51
1:A:421:LYS:CD	1:A:470:PRO:HD2	2.41	0.51
1:A:564:VAL:C	1:A:565:HIS:CD2	2.89	0.51
1:B:837:ARG:HH11	1:B:837:ARG:CB	2.19	0.51
1:C:190:ILE:HD12	1:C:190:ILE:N	2.26	0.51
1:C:494:ASP:HB3	1:C:499:LYS:HB2	1.94	0.51
1:D:437:PRO:HG2	1:D:439:PHE:CE1	2.46	0.51
1:D:564:VAL:C	1:D:565:HIS:CD2	2.89	0.51
1:A:594:VAL:O	1:A:595:GLU:HG3	2.12	0.50
1:B:377:ARG:HG2	1:B:377:ARG:HH11	1.76	0.50
1:B:719:THR:HB	1:B:784:PHE:CZ	2.45	0.50
1:C:262:ILE:H	1:C:276:VAL:CG1	2.24	0.50
1:C:421:LYS:CD	1:C:470:PRO:HD2	2.40	0.50
1:D:210:ILE:H	1:D:214:SER:CB	2.24	0.50
1:D:560:PRO:HD3	1:D:641:PHE:CD2	2.47	0.50
1:D:693:ARG:HH21	1:D:725:LYS:CD	2.24	0.50
1:A:267:HIS:HB3	1:A:270:LYS:HB2	1.92	0.50
1:A:802:GLU:OE1	1:B:332:THR:HG23	2.11	0.50
1:B:532:LEU:CD2	1:B:533:VAL:N	2.74	0.50
1:C:606:LEU:HD22	1:C:662:GLY:HA2	1.94	0.50
1:D:494:ASP:HB3	1:D:499:LYS:HB2	1.92	0.50
1:A:190:ILE:N	1:A:190:ILE:HD12	2.26	0.50
1:A:220:VAL:HG11	1:A:229:PRO:HB2	1.93	0.50
1:A:392:THR:HG23	1:A:393:LYS:HG3	1.93	0.50
1:B:200:TYR:CZ	1:B:268:VAL:HG11	2.45	0.50
1:D:183:LYS:HB2	1:D:183:LYS:NZ	2.26	0.50
1:D:262:ILE:H	1:D:276:VAL:CG1	2.25	0.50
1:B:421:LYS:O	1:B:422:HIS:HB2	2.11	0.50
1:B:444:ARG:HG2	1:B:444:ARG:HH11	1.75	0.50
1:C:595:GLU:OE2	1:C:612:LYS:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:ARG:HH21	1:C:725:LYS:CD	2.23	0.50
1:D:186:SER:O	1:D:187:LEU:C	2.54	0.50
1:D:219:TYR:CD1	1:D:242:LEU:HB2	2.47	0.50
1:D:293:TYR:CD2	1:D:297:ILE:HD11	2.47	0.50
1:A:444:ARG:O	1:A:468:SER:HB2	2.12	0.50
1:A:453:PRO:HA	1:A:459:LYS:HB3	1.94	0.50
1:A:565:HIS:O	1:A:573:MET:HE2	2.12	0.50
1:B:786:ILE:O	1:B:816:LEU:HD23	2.11	0.50
1:C:715:GLY:O	1:C:719:THR:CG2	2.57	0.50
1:C:818:ILE:HG23	1:C:820:PRO:HD3	1.94	0.50
1:A:444:ARG:HG2	1:A:444:ARG:HH11	1.77	0.50
1:A:563:THR:HG22	1:A:564:VAL:N	2.27	0.50
1:D:328:LEU:HD13	1:D:342:TYR:HE2	1.77	0.50
1:D:595:GLU:OE2	1:D:612:LYS:HD2	2.12	0.50
1:A:160:GLU:HG2	1:A:163:GLY:O	2.11	0.50
1:A:210:ILE:HG22	1:A:211:TYR:N	2.26	0.50
1:A:262:ILE:H	1:A:276:VAL:CG1	2.25	0.50
1:A:437:PRO:HG2	1:A:439:PHE:CE1	2.46	0.50
1:B:186:SER:O	1:B:187:LEU:C	2.55	0.50
1:B:220:VAL:HG11	1:B:229:PRO:HB2	1.94	0.50
1:B:564:VAL:HG21	1:B:574:PHE:CZ	2.47	0.50
1:B:599:ILE:CB	1:B:608:MET:HE3	2.30	0.50
1:C:160:GLU:HG2	1:C:163:GLY:O	2.12	0.50
1:C:375:ASP:HB3	1:C:377:ARG:HH11	1.76	0.50
1:C:738:ALA:HB1	1:C:741:PRO:HB3	1.94	0.50
1:D:260:ASN:O	1:D:279:GLY:HA3	2.12	0.50
1:D:375:ASP:HB3	1:D:377:ARG:HH11	1.77	0.50
1:A:183:LYS:HB2	1:A:183:LYS:NZ	2.27	0.50
1:A:183:LYS:NZ	1:A:183:LYS:CB	2.75	0.50
1:A:185:GLU:O	1:A:187:LEU:N	2.44	0.50
1:A:354:ILE:HG12	1:A:355:SER:N	2.27	0.50
1:A:599:ILE:CD1	1:A:600:GLU:N	2.73	0.50
1:C:299:LYS:HE2	1:C:299:LYS:HA	1.93	0.50
1:C:346:LYS:HD3	1:D:336:TYR:CZ	2.46	0.50
1:D:205:TYR:CE1	1:D:218:TYR:HB2	2.46	0.50
1:D:841:ASN:O	1:D:845:GLU:HG2	2.12	0.50
1:A:254:LEU:HD12	1:A:254:LEU:O	2.10	0.50
1:A:328:LEU:HD13	1:A:342:TYR:HE2	1.77	0.50
1:A:421:LYS:O	1:A:422:HIS:HB2	2.11	0.50
1:A:828:SER:HB3	1:A:831:LEU:HB2	1.94	0.50
1:B:249:PRO:HD3	1:B:306:TRP:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLU:HA	1:B:281:GLU:OE1	2.12	0.50
1:C:183:LYS:HB2	1:C:183:LYS:HZ2	1.77	0.50
1:C:564:VAL:C	1:C:565:HIS:CD2	2.89	0.50
1:C:661:ASP:HB3	1:C:665:SER:OG	2.11	0.50
1:D:494:ASP:HB2	1:D:547:MET:HE2	1.94	0.50
1:D:563:THR:HG22	1:D:564:VAL:N	2.27	0.50
1:D:848:ARG:NH2	8:D:47:HOH:O	2.32	0.50
4:H:1:NAG:H3	4:H:1:NAG:H83	1.94	0.50
1:C:267:HIS:HB3	1:C:270:LYS:HB2	1.93	0.49
1:D:538:TYR:O	1:D:554:CYS:O	2.30	0.49
1:A:249:PRO:HD3	1:A:306:TRP:CD2	2.47	0.49
1:A:375:ASP:HB3	1:A:377:ARG:HH11	1.75	0.49
1:B:190:ILE:N	1:B:204:SER:O	2.45	0.49
1:B:533:VAL:HG23	1:B:533:VAL:O	2.12	0.49
1:C:566:ASN:HD21	1:C:569:ASP:HB2	1.77	0.49
1:D:159:ARG:O	1:D:160:GLU:C	2.55	0.49
1:D:247:TRP:CZ3	1:D:254:LEU:HD23	2.47	0.49
1:D:565:HIS:O	1:D:573:MET:HE2	2.12	0.49
1:D:719:THR:HB	1:D:784:PHE:CZ	2.48	0.49
1:A:693:ARG:NH2	1:A:725:LYS:HD3	2.28	0.49
1:C:335:ILE:HG22	1:C:336:TYR:CD1	2.47	0.49
1:D:606:LEU:HD22	1:D:662:GLY:HA2	1.93	0.49
1:A:738:ALA:HB1	1:A:741:PRO:HB3	1.94	0.49
1:B:132:THR:HG22	1:B:135:ASP:OD2	2.11	0.49
1:B:363:GLY:O	1:B:365:THR:HG23	2.12	0.49
1:B:494:ASP:HB2	1:B:547:MET:HE2	1.95	0.49
1:B:535:ASN:ND2	5:O:1:NAG:H83	2.27	0.49
1:B:564:VAL:C	1:B:565:HIS:CD2	2.90	0.49
1:C:132:THR:HG22	1:C:135:ASP:OD2	2.12	0.49
1:C:183:LYS:NZ	1:C:183:LYS:CB	2.75	0.49
1:C:437:PRO:HG2	1:C:439:PHE:CE1	2.46	0.49
1:D:528:LEU:HD12	1:D:528:LEU:H	1.77	0.49
1:A:249:PRO:HD3	1:A:306:TRP:CE3	2.47	0.49
1:B:325:ILE:HD11	1:B:341:PRO:CB	2.37	0.49
1:C:183:LYS:HB2	1:C:183:LYS:NZ	2.27	0.49
1:C:293:TYR:CD2	1:C:297:ILE:HD11	2.48	0.49
1:C:494:ASP:HB2	1:C:547:MET:HE2	1.95	0.49
1:D:183:LYS:NZ	1:D:183:LYS:CB	2.75	0.49
1:D:444:ARG:HG2	1:D:444:ARG:HH11	1.77	0.49
1:A:259:GLU:HA	1:A:281:GLU:OE1	2.12	0.49
1:A:440:SER:O	1:A:443:GLY:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:TYR:O	1:B:212:GLN:O	2.31	0.49
1:B:249:PRO:HD3	1:B:306:TRP:CE3	2.48	0.49
1:B:845:GLU:C	1:B:847:PHE:N	2.71	0.49
1:C:190:ILE:HB	1:C:207:VAL:HG21	1.93	0.49
1:C:431:HIS:HB3	1:C:461:TYR:OH	2.13	0.49
1:C:453:PRO:HA	1:C:459:LYS:HB3	1.94	0.49
1:C:837:ARG:HH11	1:C:837:ARG:CB	2.19	0.49
1:D:444:ARG:O	1:D:468:SER:HB2	2.12	0.49
1:D:738:ALA:HB1	1:D:741:PRO:HB3	1.94	0.49
1:A:299:LYS:HA	1:A:299:LYS:HE2	1.93	0.49
1:B:445:LYS:NZ	8:B:6:HOH:O	2.46	0.49
1:B:528:LEU:HD12	1:B:528:LEU:H	1.77	0.49
1:A:363:GLY:O	1:A:365:THR:HG23	2.13	0.49
1:B:176:THR:CG2	1:B:177:VAL:H	2.17	0.49
1:B:214:SER:OG	1:B:216:THR:HG22	2.13	0.49
1:B:721:ILE:O	1:B:722:LEU:HD12	2.12	0.49
1:C:214:SER:OG	1:C:216:THR:CG2	2.61	0.49
1:C:329:PRO:HG3	1:D:331:TYR:CE2	2.48	0.49
1:C:392:THR:HG23	1:C:393:LYS:HG3	1.94	0.49
1:C:554:CYS:O	1:C:555:GLU:CB	2.56	0.49
1:C:563:THR:HG22	1:C:564:VAL:N	2.28	0.49
1:D:626:LEU:C	1:D:626:LEU:CD2	2.86	0.49
1:A:538:TYR:O	1:A:554:CYS:O	2.30	0.49
1:C:363:GLY:O	1:C:365:THR:HG23	2.13	0.49
1:C:564:VAL:HG21	1:C:574:PHE:CZ	2.48	0.49
1:D:132:THR:HG22	1:D:135:ASP:OD2	2.13	0.49
1:D:159:ARG:O	1:D:160:GLU:O	2.31	0.49
1:D:564:VAL:HG21	1:D:574:PHE:CZ	2.47	0.49
1:B:202:LEU:HD11	1:B:245:ALA:HB1	1.95	0.49
1:B:328:LEU:HD13	1:B:342:TYR:HE2	1.78	0.49
1:B:375:ASP:C	1:B:377:ARG:N	2.71	0.49
1:B:494:ASP:HB3	1:B:499:LYS:HB2	1.93	0.49
1:C:528:LEU:HD12	1:C:528:LEU:H	1.76	0.49
1:D:168:TRP:HH2	6:W:1:NAG:C1	2.25	0.49
1:D:538:TYR:CD2	1:D:640:LYS:HG3	2.48	0.49
1:D:845:GLU:C	1:D:847:PHE:N	2.71	0.49
1:A:626:LEU:C	1:A:626:LEU:CD2	2.86	0.48
1:B:262:ILE:H	1:B:276:VAL:CG1	2.25	0.48
1:B:437:PRO:HG2	1:B:439:PHE:CE1	2.48	0.48
1:C:533:VAL:HG23	1:C:533:VAL:O	2.12	0.48
1:C:808:ILE:HD13	1:D:819:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LEU:HD12	1:D:254:LEU:O	2.12	0.48
1:D:299:LYS:HA	1:D:299:LYS:HE2	1.94	0.48
2:T:2:NAG:C3	2:T:3:BMA:H2	2.43	0.48
2:V:2:NAG:H62	2:V:3:BMA:C1	2.43	0.48
1:A:538:TYR:CD2	1:A:640:LYS:HG3	2.48	0.48
1:A:602:ASP:C	1:A:604:TYR:H	2.22	0.48
1:B:444:ARG:O	1:B:468:SER:HB2	2.11	0.48
1:B:606:LEU:HD22	1:B:662:GLY:HA2	1.94	0.48
1:C:130:LYS:HD3	1:C:652:SER:HA	1.95	0.48
1:D:335:ILE:HG22	1:D:336:TYR:CD1	2.48	0.48
2:Y:2:NAG:H3	2:Y:3:BMA:H2	1.94	0.48
1:A:186:SER:O	1:A:187:LEU:C	2.55	0.48
1:A:247:TRP:CZ3	1:A:254:LEU:HD23	2.48	0.48
1:A:330:THR:HB	1:A:338:THR:O	2.13	0.48
1:A:503:LEU:N	1:A:503:LEU:HD22	2.28	0.48
1:A:595:GLU:OE2	1:A:612:LYS:HD2	2.12	0.48
1:A:765:ARG:O	1:A:765:ARG:CD	2.60	0.48
1:B:577:GLU:HG3	1:B:579:ASN:ND2	2.28	0.48
1:B:668:GLN:HB2	1:B:672:LEU:CD2	2.44	0.48
1:C:421:LYS:O	1:C:422:HIS:HB2	2.11	0.48
1:C:444:ARG:O	1:C:468:SER:HB2	2.12	0.48
1:C:565:HIS:O	1:C:573:MET:HE2	2.13	0.48
2:G:1:NAG:H2	2:G:2:NAG:C8	2.43	0.48
6:L:1:NAG:HO6	6:L:2:NDG:C1	2.26	0.48
1:A:159:ARG:O	1:A:160:GLU:C	2.55	0.48
1:A:255:ILE:HG23	1:A:306:TRP:CH2	2.49	0.48
1:A:528:LEU:HD12	1:A:528:LEU:H	1.77	0.48
1:A:818:ILE:HG23	1:A:820:PRO:HD3	1.95	0.48
1:B:563:THR:HG22	1:B:564:VAL:N	2.28	0.48
1:C:159:ARG:O	1:C:160:GLU:C	2.56	0.48
1:C:538:TYR:CD2	1:C:640:LYS:HG3	2.49	0.48
1:C:626:LEU:C	1:C:626:LEU:CD2	2.87	0.48
1:D:255:ILE:HG23	1:D:306:TRP:CH2	2.48	0.48
1:A:302:ILE:C	1:A:302:ILE:CD1	2.81	0.48
1:B:453:PRO:HA	1:B:459:LYS:HB3	1.94	0.48
1:C:192:TYR:CD1	1:C:192:TYR:C	2.92	0.48
1:C:395:ALA:HA	1:C:409:THR:O	2.13	0.48
1:C:544:SER:C	1:C:546:SER:H	2.22	0.48
1:C:617:THR:CG2	1:C:618:ASP:N	2.58	0.48
5:M:1:NAG:H4	5:M:2:NAG:N2	2.26	0.48
1:A:606:LEU:HD22	1:A:662:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLU:HG2	1:B:163:GLY:O	2.12	0.48
1:B:180:GLU:C	1:B:182:LYS:N	2.72	0.48
1:B:626:LEU:C	1:B:626:LEU:CD2	2.86	0.48
1:C:249:PRO:HD3	1:C:306:TRP:CE3	2.48	0.48
1:C:324:PRO:HB2	1:D:336:TYR:CZ	2.48	0.48
1:C:503:LEU:HD22	1:C:503:LEU:N	2.29	0.48
1:C:522:ASN:CB	1:C:524:ASN:OD1	2.62	0.48
1:D:192:TYR:CD1	1:D:192:TYR:C	2.92	0.48
1:D:354:ILE:HG12	1:D:355:SER:N	2.28	0.48
1:A:151:ILE:HD11	1:A:157:ILE:HG12	1.96	0.48
1:A:180:GLU:C	1:A:182:LYS:N	2.72	0.48
1:A:721:ILE:O	1:A:722:LEU:HD12	2.13	0.48
1:B:594:VAL:HG12	1:B:595:GLU:N	2.29	0.48
1:C:328:LEU:HD13	1:C:342:TYR:HE2	1.77	0.48
1:D:375:ASP:C	1:D:377:ARG:N	2.69	0.48
1:D:431:HIS:HB3	1:D:461:TYR:OH	2.13	0.48
2:G:1:NAG:O6	2:G:2:NAG:H2	2.14	0.48
1:A:132:THR:HG22	1:A:135:ASP:OD2	2.14	0.48
1:A:522:ASN:O	1:A:523:PHE:HB2	2.14	0.48
1:B:599:ILE:CD1	1:B:600:GLU:N	2.71	0.48
1:B:738:ALA:HB1	1:B:741:PRO:HB3	1.95	0.48
1:C:254:LEU:HD12	1:C:254:LEU:O	2.12	0.48
1:D:658:VAL:HG21	1:D:695:MET:HG2	1.96	0.48
1:A:130:LYS:HD3	1:A:652:SER:HA	1.96	0.48
1:A:159:ARG:O	1:A:160:GLU:O	2.31	0.48
1:B:159:ARG:O	1:B:160:GLU:C	2.56	0.48
1:B:286:ASN:ND2	1:B:286:ASN:N	2.62	0.48
1:B:362:ASN:N	1:B:362:ASN:OD1	2.47	0.48
1:D:176:THR:CG2	1:D:177:VAL:H	2.18	0.48
1:A:148:ALA:HB3	1:A:551:LEU:HD13	1.96	0.48
1:A:421:LYS:HE2	1:A:470:PRO:CD	2.40	0.48
1:B:183:LYS:HB2	1:B:183:LYS:HZ2	1.79	0.48
1:B:422:HIS:CE1	1:B:450:ARG:NH1	2.82	0.48
1:B:547:MET:O	1:B:567:THR:CB	2.61	0.48
1:C:249:PRO:HD3	1:C:306:TRP:CD2	2.48	0.48
1:D:238:SER:OG	1:D:239:ASN:N	2.45	0.48
1:D:249:PRO:HD3	1:D:306:TRP:CD2	2.48	0.48
1:D:363:GLY:O	1:D:365:THR:HG23	2.13	0.48
1:D:453:PRO:HA	1:D:459:LYS:HB3	1.95	0.48
1:D:762:LEU:HD21	7:X:4:MAN:O2	2.14	0.48
1:B:431:HIS:HB3	1:B:461:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ASP:C	1:C:377:ARG:N	2.70	0.47
1:C:828:SER:HB3	1:C:831:LEU:HB2	1.96	0.47
1:A:577:GLU:HG3	1:A:579:ASN:ND2	2.28	0.47
1:A:845:GLU:C	1:A:847:PHE:N	2.71	0.47
1:B:503:LEU:HD22	1:B:503:LEU:N	2.28	0.47
1:B:522:ASN:CB	1:B:524:ASN:OD1	2.62	0.47
1:B:538:TYR:CD2	1:B:640:LYS:HG3	2.49	0.47
1:B:544:SER:C	1:B:546:SER:H	2.22	0.47
1:C:537:THR:N	1:C:557:PRO:HD3	2.21	0.47
1:C:668:GLN:HB2	1:C:672:LEU:CD2	2.41	0.47
1:D:160:GLU:HG2	1:D:163:GLY:O	2.14	0.47
1:D:392:THR:HG23	1:D:393:LYS:HG3	1.95	0.47
1:D:599:ILE:CD1	1:D:600:GLU:N	2.72	0.47
1:D:668:GLN:HB2	1:D:672:LEU:CD2	2.43	0.47
1:A:208:GLU:O	1:A:216:THR:HG23	2.13	0.47
1:A:494:ASP:HB2	1:A:547:MET:HG3	1.96	0.47
1:B:213:HIS:C	1:B:215:TYR:H	2.23	0.47
1:B:765:ARG:O	1:B:765:ARG:CD	2.61	0.47
1:C:144:HIS:ND1	1:C:162:LYS:HD2	2.29	0.47
1:C:577:GLU:HG3	1:C:579:ASN:ND2	2.28	0.47
1:C:602:ASP:C	1:C:604:TYR:H	2.22	0.47
1:C:798:GLN:HG3	1:D:331:TYR:O	2.14	0.47
1:D:143:ILE:HD13	1:D:582:VAL:HG21	1.96	0.47
1:D:330:THR:HB	1:D:338:THR:O	2.14	0.47
1:D:522:ASN:CB	1:D:524:ASN:OD1	2.62	0.47
1:D:522:ASN:O	1:D:523:PHE:HB2	2.15	0.47
1:D:563:THR:CG2	1:D:572:LYS:HG3	2.44	0.47
1:A:160:GLU:HA	1:A:164:THR:O	2.15	0.47
1:A:395:ALA:HA	1:A:409:THR:O	2.14	0.47
1:A:431:HIS:HB3	1:A:461:TYR:OH	2.15	0.47
1:B:247:TRP:CZ3	1:B:254:LEU:HD23	2.49	0.47
1:C:494:ASP:HB2	1:C:547:MET:HG3	1.96	0.47
1:C:802:GLU:CD	1:D:332:THR:HG23	2.40	0.47
1:D:564:VAL:C	1:D:565:HIS:HD2	2.23	0.47
1:D:828:SER:HB3	1:D:831:LEU:HB2	1.97	0.47
1:C:685:GLU:HG3	1:C:686:LYS:N	2.30	0.47
1:D:180:GLU:C	1:D:182:LYS:N	2.73	0.47
1:D:503:LEU:HD22	1:D:503:LEU:N	2.28	0.47
1:D:533:VAL:HG23	1:D:533:VAL:O	2.14	0.47
1:D:765:ARG:O	1:D:765:ARG:CD	2.62	0.47
1:D:778:ALA:O	1:D:779:LEU:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:HG23	1:A:135:ASP:H	1.79	0.47
1:A:522:ASN:CB	1:A:524:ASN:OD1	2.62	0.47
1:A:537:THR:N	1:A:557:PRO:HD3	2.22	0.47
1:B:335:ILE:HG22	1:B:336:TYR:CD1	2.50	0.47
1:B:665:SER:HB2	8:B:36:HOH:O	2.15	0.47
1:B:818:ILE:HG23	1:B:820:PRO:HD3	1.96	0.47
1:C:528:LEU:H	1:C:528:LEU:CD1	2.27	0.47
1:C:563:THR:CG2	1:C:572:LYS:HG3	2.44	0.47
1:D:249:PRO:HD3	1:D:306:TRP:CE3	2.50	0.47
1:D:693:ARG:NH2	1:D:725:LYS:HD3	2.29	0.47
1:A:262:ILE:CB	1:A:276:VAL:HG12	2.42	0.47
1:A:668:GLN:HB2	1:A:672:LEU:CD2	2.42	0.47
1:B:159:ARG:O	1:B:160:GLU:O	2.32	0.47
1:B:192:TYR:C	1:B:192:TYR:CD1	2.92	0.47
1:B:255:ILE:HG23	1:B:306:TRP:CH2	2.49	0.47
1:B:565:HIS:O	1:B:573:MET:HE2	2.14	0.47
1:B:685:GLU:HG3	1:B:686:LYS:N	2.30	0.47
1:C:330:THR:HB	1:C:338:THR:O	2.15	0.47
1:C:448:PHE:HB3	1:C:450:ARG:NH2	2.30	0.47
1:C:522:ASN:O	1:C:523:PHE:HB2	2.15	0.47
1:C:538:TYR:O	1:C:554:CYS:O	2.33	0.47
1:C:564:VAL:C	1:C:565:HIS:HD2	2.23	0.47
1:C:778:ALA:O	1:C:779:LEU:C	2.58	0.47
1:D:130:LYS:HD3	1:D:652:SER:HA	1.97	0.47
1:D:254:LEU:C	1:D:254:LEU:CD1	2.88	0.47
1:D:375:ASP:O	1:D:377:ARG:N	2.47	0.47
1:D:448:PHE:HB3	1:D:450:ARG:NH2	2.29	0.47
1:D:528:LEU:H	1:D:528:LEU:CD1	2.28	0.47
2:E:2:NAG:H83	2:E:2:NAG:O3	2.15	0.47
1:A:375:ASP:C	1:A:377:ARG:N	2.72	0.47
1:A:422:HIS:CE1	1:A:450:ARG:NH1	2.83	0.47
1:A:548:ASP:O	1:A:567:THR:N	2.47	0.47
1:A:778:ALA:O	1:A:779:LEU:C	2.57	0.47
1:C:255:ILE:HG23	1:C:306:TRP:CH2	2.49	0.47
1:D:191:ARG:NH2	1:D:215:TYR:HB3	2.29	0.47
1:D:547:MET:O	1:D:567:THR:CB	2.62	0.47
1:D:685:GLU:HG3	1:D:686:LYS:N	2.30	0.47
1:A:564:VAL:C	1:A:565:HIS:HD2	2.22	0.47
1:B:254:LEU:C	1:B:254:LEU:CD1	2.87	0.47
1:B:375:ASP:O	1:B:377:ARG:N	2.48	0.47
1:B:395:ALA:HA	1:B:409:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:PHE:HB3	1:B:450:ARG:NH2	2.30	0.47
1:B:548:ASP:O	1:B:567:THR:N	2.48	0.47
1:C:247:TRP:CZ3	1:C:254:LEU:HD23	2.50	0.47
1:C:354:ILE:HG12	1:C:355:SER:N	2.30	0.47
1:D:132:THR:HG23	1:D:135:ASP:H	1.80	0.47
1:D:183:LYS:HB2	1:D:183:LYS:HZ2	1.79	0.47
1:A:192:TYR:CD1	1:A:192:TYR:C	2.93	0.47
1:A:286:ASN:ND2	1:A:286:ASN:N	2.63	0.47
1:A:528:LEU:H	1:A:528:LEU:CD1	2.28	0.47
1:A:533:VAL:O	1:A:533:VAL:HG23	2.14	0.47
1:A:544:SER:C	1:A:546:SER:H	2.23	0.47
1:A:594:VAL:HG12	1:A:595:GLU:N	2.30	0.47
1:B:624:LEU:CD2	1:B:656:VAL:HG23	2.42	0.47
1:C:132:THR:HG23	1:C:135:ASP:H	1.80	0.47
1:D:715:GLY:O	1:D:719:THR:CG2	2.58	0.47
1:A:563:THR:CG2	1:A:572:LYS:HG3	2.45	0.46
1:B:522:ASN:O	1:B:523:PHE:HB2	2.15	0.46
1:B:528:LEU:H	1:B:528:LEU:CD1	2.28	0.46
1:C:191:ARG:HH22	1:C:215:TYR:CB	2.26	0.46
1:C:215:TYR:CE1	1:C:301:HIS:CE1	3.03	0.46
1:C:802:GLU:OE1	1:D:332:THR:HG23	2.14	0.46
1:D:190:ILE:HD13	1:D:205:TYR:HA	1.97	0.46
1:D:262:ILE:CB	1:D:276:VAL:HG12	2.40	0.46
1:D:422:HIS:CE1	1:D:450:ARG:NH1	2.83	0.46
1:D:594:VAL:HG12	1:D:595:GLU:N	2.31	0.46
1:D:602:ASP:C	1:D:604:TYR:H	2.24	0.46
1:B:208:GLU:N	1:B:209:PRO:CD	2.76	0.46
1:B:354:ILE:HG12	1:B:355:SER:N	2.30	0.46
1:D:544:SER:C	1:D:546:SER:H	2.23	0.46
1:A:498:ASN:HB2	1:A:519:THR:H	1.81	0.46
1:A:554:CYS:O	1:A:555:GLU:CB	2.55	0.46
1:C:238:SER:OG	1:C:239:ASN:N	2.47	0.46
1:D:151:ILE:HD11	1:D:157:ILE:HG12	1.98	0.46
1:D:548:ASP:O	1:D:567:THR:N	2.48	0.46
1:A:535:ASN:OD1	2:I:1:NAG:N2	2.49	0.46
1:B:274:ARG:HE	1:B:277:SER:HB3	1.79	0.46
1:B:448:PHE:HZ	8:B:9:HOH:O	1.98	0.46
1:B:563:THR:CG2	1:B:572:LYS:HG3	2.45	0.46
1:C:563:THR:HG22	1:C:564:VAL:H	1.80	0.46
1:C:663:ARG:NH1	1:C:683:LEU:HD13	2.30	0.46
1:C:705:ARG:HD2	1:C:847:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:THR:HG22	1:D:564:VAL:H	1.80	0.46
1:D:577:GLU:HG3	1:D:579:ASN:ND2	2.30	0.46
2:V:1:NAG:O3	2:V:2:NAG:O5	2.25	0.46
1:A:254:LEU:C	1:A:254:LEU:CD1	2.88	0.46
1:B:130:LYS:HD3	1:B:652:SER:HA	1.98	0.46
1:B:646:GLU:O	1:B:650:VAL:HG23	2.16	0.46
1:C:274:ARG:HE	1:C:277:SER:HB3	1.81	0.46
1:C:427:GLU:HA	5:S:1:NAG:O7	2.16	0.46
1:D:153:ASP:HA	1:D:544:SER:HB2	1.97	0.46
1:D:160:GLU:HA	1:D:164:THR:O	2.16	0.46
1:D:274:ARG:HE	1:D:277:SER:HB3	1.81	0.46
1:D:522:ASN:HB3	1:D:524:ASN:OD1	2.15	0.46
1:A:194:ILE:H	1:A:194:ILE:CD1	2.13	0.46
1:A:274:ARG:HE	1:A:277:SER:HB3	1.80	0.46
1:A:522:ASN:HB3	1:A:524:ASN:OD1	2.15	0.46
1:A:685:GLU:HG3	1:A:686:LYS:N	2.30	0.46
1:A:715:GLY:O	1:A:719:THR:CG2	2.59	0.46
1:B:410:LEU:HA	1:B:410:LEU:HD23	1.83	0.46
1:C:422:HIS:CE1	1:C:450:ARG:NH1	2.84	0.46
1:D:395:ALA:HA	1:D:409:THR:O	2.15	0.46
1:D:421:LYS:HE2	1:D:470:PRO:CD	2.39	0.46
1:B:330:THR:HB	1:B:338:THR:O	2.15	0.46
1:B:602:ASP:C	1:B:604:TYR:H	2.24	0.46
1:C:196:PRO:C	1:C:198:ARG:H	2.24	0.46
1:C:400:ASN:ND2	1:C:405:VAL:HB	2.31	0.46
1:C:693:ARG:NH2	1:C:725:LYS:HD3	2.28	0.46
1:C:765:ARG:O	1:C:765:ARG:CD	2.63	0.46
1:D:375:ASP:C	1:D:377:ARG:H	2.24	0.46
1:A:148:ALA:CB	1:A:551:LEU:HD13	2.46	0.46
1:A:219:TYR:HB2	1:A:242:LEU:HD12	1.98	0.46
1:A:435:GLU:HG3	1:A:449:ILE:HG23	1.98	0.46
1:A:547:MET:O	1:A:567:THR:CB	2.61	0.46
1:A:566:ASN:CG	1:A:569:ASP:HB3	2.41	0.46
1:B:132:THR:HG23	1:B:135:ASP:H	1.81	0.46
1:B:214:SER:O	1:B:215:TYR:C	2.59	0.46
1:B:564:VAL:C	1:B:565:HIS:HD2	2.24	0.46
1:B:658:VAL:HG21	1:B:695:MET:HG2	1.98	0.46
1:B:778:ALA:O	1:B:779:LEU:C	2.58	0.46
1:C:159:ARG:O	1:C:160:GLU:O	2.33	0.46
1:A:144:HIS:ND1	1:A:162:LYS:HD2	2.31	0.46
1:B:190:ILE:CD1	1:B:205:TYR:HA	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:VAL:HG12	1:C:595:GLU:N	2.31	0.46
1:D:259:GLU:HA	1:D:281:GLU:OE1	2.15	0.46
1:D:705:ARG:HD2	1:D:847:PHE:O	2.16	0.46
2:K:1:NAG:O3	2:K:2:NAG:O5	2.30	0.46
1:A:569:ASP:OD2	5:J:1:NAG:C5	2.61	0.46
1:A:705:ARG:HD2	1:A:847:PHE:O	2.15	0.46
1:B:131:VAL:HG22	1:B:589:ARG:HG2	1.98	0.46
1:B:144:HIS:ND1	1:B:162:LYS:HD2	2.31	0.46
1:B:148:ALA:HB3	1:B:551:LEU:HD13	1.97	0.46
1:B:392:THR:HG23	1:B:393:LYS:HG3	1.97	0.46
1:B:807:LEU:HD13	1:B:814:TYR:HB3	1.97	0.46
1:C:197:ASP:OD2	1:C:197:ASP:C	2.59	0.46
1:A:131:VAL:HG22	1:A:589:ARG:HG2	1.97	0.45
1:A:491:LEU:HD11	1:A:503:LEU:HD21	1.98	0.45
1:A:563:THR:HG22	1:A:564:VAL:H	1.80	0.45
1:B:150:TRP:HA	1:B:156:PHE:HA	1.98	0.45
1:B:197:ASP:OD2	1:B:197:ASP:C	2.59	0.45
1:B:359:ILE:HD12	1:B:359:ILE:C	2.41	0.45
1:B:559:VAL:HA	1:B:560:PRO:HD3	1.82	0.45
1:B:796:HIS:C	1:B:798:GLN:N	2.74	0.45
1:C:148:ALA:HB3	1:C:551:LEU:HD13	1.98	0.45
1:C:191:ARG:HH11	1:C:191:ARG:HD3	1.37	0.45
1:C:761:GLY:C	1:C:763:ASP:N	2.74	0.45
1:D:286:ASN:ND2	1:D:286:ASN:N	2.63	0.45
1:D:650:VAL:O	1:D:654:GLY:HA2	2.16	0.45
1:A:143:ILE:HD13	1:A:582:VAL:HG21	1.98	0.45
1:A:196:PRO:C	1:A:198:ARG:H	2.24	0.45
1:A:326:MET:HE3	8:B:51:HOH:O	2.16	0.45
1:B:160:GLU:HA	1:B:164:THR:O	2.16	0.45
1:C:522:ASN:HB3	1:C:524:ASN:OD1	2.16	0.45
1:C:546:SER:C	1:C:548:ASP:H	2.24	0.45
2:Y:2:NAG:C3	2:Y:3:BMA:H2	2.46	0.45
1:A:798:GLN:HG3	1:B:331:TYR:O	2.17	0.45
1:B:563:THR:HG22	1:B:564:VAL:H	1.81	0.45
1:B:693:ARG:NH2	1:B:725:LYS:HD3	2.27	0.45
1:C:375:ASP:O	1:C:377:ARG:N	2.49	0.45
1:D:319:ASN:OD1	1:D:321:SER:CB	2.64	0.45
1:D:663:ARG:NH1	1:D:683:LEU:HD13	2.30	0.45
4:H:1:NAG:H62	4:H:2:NAG:O7	2.17	0.45
1:A:368:LEU:CD1	8:A:34:HOH:O	2.63	0.45
1:A:658:VAL:HG21	1:A:695:MET:HG2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLU:HA	1:C:164:THR:O	2.16	0.45
1:C:491:LEU:HD11	1:C:503:LEU:HD21	1.99	0.45
1:C:547:MET:O	1:C:567:THR:CB	2.61	0.45
1:D:498:ASN:HB3	1:D:519:THR:HG22	1.99	0.45
1:D:721:ILE:O	1:D:722:LEU:HD12	2.15	0.45
1:B:454:GLN:CD	1:B:483:GLY:H	2.24	0.45
1:B:537:THR:HG22	8:B:38:HOH:O	2.17	0.45
1:B:537:THR:N	1:B:557:PRO:HD3	2.21	0.45
1:B:761:GLY:C	1:B:763:ASP:N	2.74	0.45
1:C:143:ILE:HD13	1:C:582:VAL:HG21	1.99	0.45
1:C:721:ILE:O	1:C:722:LEU:HD12	2.15	0.45
1:D:491:LEU:HD11	1:D:503:LEU:HD21	1.98	0.45
1:D:559:VAL:HA	1:D:560:PRO:HD3	1.82	0.45
1:D:807:LEU:HD13	1:D:814:TYR:HB3	1.98	0.45
1:B:143:ILE:HD13	1:B:582:VAL:HG21	1.98	0.45
1:B:262:ILE:CB	1:B:276:VAL:HG12	2.41	0.45
1:C:658:VAL:HG21	1:C:695:MET:HG2	1.97	0.45
1:C:807:LEU:HD13	1:C:814:TYR:HB3	1.98	0.45
1:D:151:ILE:HD11	1:D:157:ILE:CD1	2.47	0.45
1:D:412:ASP:HB3	1:D:415:THR:HB	1.99	0.45
1:D:567:THR:CG2	1:D:568:THR:N	2.79	0.45
1:D:761:GLY:C	1:D:763:ASP:N	2.75	0.45
1:D:818:ILE:HG23	1:D:820:PRO:HD3	1.99	0.45
1:A:378:MET:HE3	1:A:378:MET:HB3	1.88	0.45
1:B:292:LEU:HD11	1:B:751:ALA:HB3	1.97	0.45
1:B:375:ASP:HB3	1:B:377:ARG:HH11	1.78	0.45
1:B:512:ARG:NH2	1:B:667:PHE:CE1	2.85	0.45
1:D:144:HIS:ND1	1:D:162:LYS:HD2	2.30	0.45
1:D:454:GLN:CD	1:D:483:GLY:H	2.25	0.45
1:A:134:GLU:CD	1:A:134:GLU:H	2.25	0.45
1:A:150:TRP:HA	1:A:156:PHE:HA	1.98	0.45
1:A:153:ASP:HA	1:A:544:SER:HB2	1.97	0.45
1:A:646:GLU:O	1:A:650:VAL:HG23	2.17	0.45
1:A:740:SER:OG	1:A:789:PRO:HD2	2.16	0.45
1:C:599:ILE:CD1	1:C:600:GLU:N	2.73	0.45
1:C:792:ASP:CG	1:C:824:HIS:HB2	2.42	0.45
1:D:148:ALA:HB3	1:D:551:LEU:HD13	1.99	0.45
1:D:197:ASP:OD2	1:D:197:ASP:C	2.59	0.45
1:D:210:ILE:HG22	1:D:211:TYR:CG	2.52	0.45
1:D:435:GLU:HG2	1:D:449:ILE:HG23	1.99	0.45
1:D:494:ASP:HB2	1:D:547:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:537:THR:N	1:D:557:PRO:HD3	2.21	0.45
1:A:292:LEU:HD11	1:A:751:ALA:HB3	1.98	0.45
1:A:422:HIS:CG	1:A:423:GLU:N	2.85	0.45
1:A:435:GLU:HG2	1:A:449:ILE:HG23	1.98	0.45
1:B:153:ASP:HA	1:B:544:SER:HB2	1.98	0.45
1:B:196:PRO:C	1:B:198:ARG:H	2.23	0.45
1:C:375:ASP:CG	1:C:377:ARG:HH12	2.25	0.45
1:C:498:ASN:HB2	1:C:519:THR:H	1.82	0.45
3:F:2:NDG:O3	3:F:3:MAN:C1	2.65	0.45
2:G:1:NAG:H2	2:G:2:NAG:H82	1.99	0.45
1:A:448:PHE:HB3	1:A:450:ARG:NH2	2.32	0.45
1:A:565:HIS:CD2	1:A:565:HIS:N	2.85	0.45
1:B:412:ASP:HB3	1:B:415:THR:HB	1.99	0.45
1:B:724:ALA:CB	1:B:731:GLN:N	2.80	0.45
1:C:254:LEU:C	1:C:254:LEU:CD1	2.88	0.45
1:C:332:THR:O	1:C:333:GLY:O	2.35	0.45
1:C:435:GLU:HG2	1:C:449:ILE:HG23	1.99	0.45
1:C:444:ARG:HG2	1:C:445:LYS:H	1.81	0.45
1:C:759:LEU:O	1:C:764:ASN:HB2	2.17	0.45
1:D:150:TRP:HA	1:D:156:PHE:HA	1.99	0.45
1:A:151:ILE:HD11	1:A:157:ILE:CD1	2.47	0.44
1:B:522:ASN:HB3	1:B:524:ASN:OD1	2.17	0.44
1:C:153:ASP:HA	1:C:544:SER:HB2	1.97	0.44
1:C:292:LEU:HD11	1:C:751:ALA:HB3	1.98	0.44
1:C:365:THR:O	1:C:365:THR:OG1	2.32	0.44
1:C:548:ASP:O	1:C:567:THR:N	2.49	0.44
1:C:566:ASN:CG	1:C:569:ASP:HB3	2.41	0.44
1:D:204:SER:HB3	1:D:219:TYR:CD2	2.51	0.44
6:W:1:NAG:HO6	6:W:2:NDG:C1	2.31	0.44
1:A:444:ARG:HG2	1:A:445:LYS:H	1.83	0.44
1:A:552:LEU:HD13	1:A:552:LEU:C	2.42	0.44
1:A:599:ILE:CB	1:A:608:MET:HE3	2.31	0.44
1:A:840:ILE:HG21	1:A:840:ILE:HD13	1.78	0.44
1:B:494:ASP:HB2	1:B:547:MET:HG3	1.99	0.44
1:B:543:PHE:CD2	1:B:550:PHE:HB3	2.52	0.44
1:B:567:THR:CG2	1:B:568:THR:N	2.79	0.44
1:B:580:GLU:O	1:B:581:HIS:C	2.61	0.44
1:C:454:GLN:CD	1:C:483:GLY:H	2.25	0.44
1:C:719:THR:HG22	1:C:738:ALA:HB2	1.98	0.44
1:D:543:PHE:CD2	1:D:550:PHE:HB3	2.52	0.44
5:S:1:NAG:H2	5:S:2:NAG:H82	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:NAG:H83	2:T:1:NAG:H3	1.99	0.44
1:A:663:ARG:NH1	1:A:683:LEU:HD13	2.32	0.44
1:A:808:ILE:HD13	1:B:819:TYR:CE1	2.52	0.44
1:B:299:LYS:HA	1:B:299:LYS:CE	2.47	0.44
1:B:491:LEU:HD11	1:B:503:LEU:HD21	1.99	0.44
1:B:546:SER:C	1:B:548:ASP:H	2.26	0.44
1:B:566:ASN:CG	1:B:569:ASP:HB3	2.42	0.44
1:C:565:HIS:CD2	1:C:565:HIS:N	2.86	0.44
1:C:567:THR:CG2	1:C:568:THR:N	2.79	0.44
1:D:131:VAL:HG22	1:D:589:ARG:HG2	1.99	0.44
1:D:302:ILE:C	1:D:302:ILE:CD1	2.81	0.44
1:A:197:ASP:OD2	1:A:197:ASP:C	2.61	0.44
1:A:543:PHE:CD2	1:A:550:PHE:HB3	2.53	0.44
1:A:567:THR:CG2	1:A:568:THR:N	2.80	0.44
1:A:580:GLU:O	1:A:581:HIS:C	2.61	0.44
1:B:599:ILE:HD13	1:B:600:GLU:N	2.31	0.44
1:B:650:VAL:O	1:B:654:GLY:HA2	2.17	0.44
1:C:422:HIS:CG	1:C:423:GLU:N	2.86	0.44
1:C:435:GLU:HG3	1:C:449:ILE:HG23	1.99	0.44
1:C:650:VAL:O	1:C:654:GLY:HA2	2.17	0.44
1:D:408:LEU:HD23	1:D:409:THR:H	1.82	0.44
1:D:546:SER:C	1:D:548:ASP:H	2.26	0.44
1:D:565:HIS:CD2	1:D:565:HIS:N	2.86	0.44
1:D:724:ALA:CB	1:D:731:GLN:N	2.81	0.44
5:S:1:NAG:H4	5:S:2:NAG:N2	2.32	0.44
1:A:210:ILE:HG22	1:A:211:TYR:CG	2.52	0.44
1:A:512:ARG:O	1:A:539:PHE:HB2	2.17	0.44
1:A:719:THR:HG22	1:A:738:ALA:HB2	1.99	0.44
1:B:492:ALA:CB	1:B:547:MET:HE1	2.47	0.44
1:B:705:ARG:HD2	1:B:847:PHE:O	2.18	0.44
1:C:150:TRP:HA	1:C:156:PHE:HA	1.99	0.44
1:C:185:GLU:HG2	1:C:186:SER:N	2.32	0.44
1:C:213:HIS:H	1:C:213:HIS:CD2	2.35	0.44
1:C:337:PRO:HD2	1:D:326:MET:HE1	2.00	0.44
1:C:580:GLU:O	1:C:581:HIS:C	2.60	0.44
1:C:811:LYS:NZ	1:D:837:ARG:HD2	2.33	0.44
1:D:134:GLU:CD	1:D:134:GLU:H	2.26	0.44
1:D:196:PRO:C	1:D:198:ARG:H	2.24	0.44
1:A:313:LEU:HB3	1:A:359:ILE:CD1	2.47	0.44
1:A:359:ILE:HD12	1:A:359:ILE:C	2.42	0.44
1:A:393:LYS:HB3	1:A:410:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:HIS:C	1:A:798:GLN:N	2.75	0.44
1:C:134:GLU:CD	1:C:134:GLU:H	2.26	0.44
1:C:359:ILE:HD12	1:C:359:ILE:C	2.42	0.44
1:C:796:HIS:C	1:C:798:GLN:N	2.75	0.44
1:D:512:ARG:NH2	1:D:667:PHE:CE1	2.86	0.44
1:D:740:SER:OG	1:D:789:PRO:HD2	2.17	0.44
1:D:759:LEU:O	1:D:764:ASN:HB2	2.18	0.44
1:A:788:HIS:ND1	1:A:800:THR:OG1	2.46	0.44
1:A:807:LEU:HD13	1:A:814:TYR:HB3	1.98	0.44
1:B:161:GLN:O	1:B:162:LYS:CG	2.65	0.44
1:B:438:VAL:HG21	1:B:490:ILE:CG2	2.45	0.44
1:B:528:LEU:N	1:B:528:LEU:CD1	2.81	0.44
1:C:599:ILE:HD13	1:C:600:GLU:N	2.33	0.44
1:C:724:ALA:CB	1:C:731:GLN:N	2.79	0.44
1:C:808:ILE:HD13	1:D:819:TYR:CE1	2.53	0.44
1:D:148:ALA:CB	1:D:551:LEU:HD13	2.48	0.44
1:D:161:GLN:OE1	1:D:164:THR:HG23	2.18	0.44
1:D:191:ARG:NH2	1:D:215:TYR:CD1	2.85	0.44
1:D:498:ASN:HB2	1:D:519:THR:H	1.82	0.44
1:D:675:GLU:OE1	1:D:675:GLU:HA	2.18	0.44
2:E:1:NAG:O3	2:E:2:NAG:O5	2.34	0.44
1:A:297:ILE:C	1:A:297:ILE:CD1	2.85	0.44
1:A:454:GLN:CD	1:A:483:GLY:H	2.25	0.44
1:A:684:GLU:HG3	1:A:717:LEU:CD2	2.48	0.44
1:B:161:GLN:OE1	1:B:164:THR:HG23	2.18	0.44
1:C:208:GLU:HA	1:C:209:PRO:HD3	1.80	0.44
1:C:297:ILE:C	1:C:297:ILE:CD1	2.85	0.44
1:C:362:ASN:OD1	1:C:362:ASN:N	2.50	0.44
1:D:601:ILE:O	1:D:602:ASP:HB2	2.18	0.44
1:D:693:ARG:HB2	1:D:693:ARG:HH11	1.83	0.44
1:A:346:LYS:H	1:B:336:TYR:HH	1.63	0.44
1:A:650:VAL:O	1:A:654:GLY:HA2	2.18	0.44
1:A:684:GLU:HG3	1:A:717:LEU:HD21	1.99	0.44
1:B:583:LYS:C	1:B:586:ILE:HG22	2.43	0.44
1:C:555:GLU:O	1:C:641:PHE:N	2.45	0.44
1:C:583:LYS:C	1:C:586:ILE:HG22	2.43	0.44
1:C:836:TYR:O	1:C:840:ILE:HG13	2.17	0.44
1:D:422:HIS:CG	1:D:423:GLU:N	2.85	0.44
1:A:185:GLU:HG2	1:A:186:SER:N	2.33	0.43
1:A:362:ASN:OD1	1:A:362:ASN:N	2.51	0.43
1:A:765:ARG:O	1:A:765:ARG:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:C	1:B:552:LEU:HD13	2.43	0.43
1:C:393:LYS:HB3	1:C:410:LEU:HD22	1.99	0.43
1:C:543:PHE:CD2	1:C:550:PHE:HB3	2.53	0.43
1:C:684:GLU:HG3	1:C:717:LEU:HD21	2.00	0.43
1:D:147:GLU:O	1:D:159:ARG:HD3	2.18	0.43
1:D:191:ARG:HB3	1:D:204:SER:OG	2.18	0.43
1:D:219:TYR:HD1	1:D:242:LEU:HB2	1.82	0.43
1:D:261:ASN:OD1	1:D:277:SER:HA	2.18	0.43
1:D:313:LEU:HB3	1:D:359:ILE:CD1	2.45	0.43
1:D:404:ASN:CA	1:D:430:LEU:HD23	2.48	0.43
1:D:492:ALA:CB	1:D:547:MET:HE1	2.48	0.43
1:D:528:LEU:N	1:D:528:LEU:CD1	2.81	0.43
1:D:580:GLU:O	1:D:581:HIS:C	2.60	0.43
1:A:165:VAL:HB	1:A:179:ILE:HB	1.99	0.43
1:A:238:SER:OG	1:A:239:ASN:N	2.46	0.43
1:A:332:THR:O	1:A:333:GLY:O	2.37	0.43
1:A:693:ARG:HH11	1:A:693:ARG:HB2	1.82	0.43
1:A:759:LEU:O	1:A:764:ASN:HB2	2.18	0.43
1:B:211:TYR:H	1:B:211:TYR:HD2	1.66	0.43
1:B:211:TYR:N	1:B:211:TYR:CD2	2.86	0.43
1:B:375:ASP:C	1:B:377:ARG:H	2.25	0.43
1:B:435:GLU:HG2	1:B:449:ILE:HG23	2.01	0.43
1:B:498:ASN:HB2	1:B:519:THR:H	1.82	0.43
1:B:565:HIS:CD2	1:B:565:HIS:N	2.86	0.43
1:C:262:ILE:CB	1:C:276:VAL:HG12	2.42	0.43
1:C:528:LEU:N	1:C:528:LEU:CD1	2.81	0.43
1:C:675:GLU:OE1	1:C:675:GLU:HA	2.18	0.43
1:D:187:LEU:O	1:D:188:ARG:C	2.61	0.43
1:D:218:TYR:CZ	1:D:241:LYS:HG3	2.53	0.43
1:D:438:VAL:HG21	1:D:490:ILE:CG2	2.45	0.43
1:D:566:ASN:CG	1:D:569:ASP:HB3	2.42	0.43
1:A:375:ASP:O	1:A:377:ARG:N	2.51	0.43
1:A:599:ILE:HD13	1:A:600:GLU:N	2.33	0.43
1:B:412:ASP:C	1:B:414:THR:N	2.77	0.43
1:B:759:LEU:O	1:B:764:ASN:HB2	2.18	0.43
1:C:187:LEU:O	1:C:188:ARG:C	2.61	0.43
1:C:286:ASN:ND2	1:C:286:ASN:N	2.63	0.43
1:C:408:LEU:HD23	1:C:409:THR:H	1.82	0.43
1:D:292:LEU:HD11	1:D:751:ALA:HB3	1.99	0.43
1:D:444:ARG:HG2	1:D:445:LYS:H	1.83	0.43
2:N:2:NAG:C3	2:N:3:BMA:H2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:HH22	1:A:215:TYR:HD2	1.64	0.43
1:A:454:GLN:NE2	1:A:483:GLY:N	2.66	0.43
1:A:512:ARG:NH2	1:A:667:PHE:CE1	2.86	0.43
1:A:567:THR:HG23	1:A:568:THR:H	1.83	0.43
1:B:148:ALA:CB	1:B:551:LEU:HD13	2.48	0.43
1:B:444:ARG:HG2	1:B:445:LYS:H	1.83	0.43
1:B:512:ARG:O	1:B:539:PHE:HB2	2.18	0.43
1:B:742:ILE:HD12	1:B:743:THR:N	2.34	0.43
1:C:375:ASP:OD1	1:C:377:ARG:NH1	2.51	0.43
1:C:412:ASP:HB3	1:C:415:THR:HB	1.99	0.43
1:C:438:VAL:HG21	1:C:490:ILE:CG2	2.45	0.43
1:C:512:ARG:NH2	1:C:667:PHE:CE1	2.86	0.43
1:D:359:ILE:HD12	1:D:359:ILE:C	2.43	0.43
1:D:362:ASN:OD1	1:D:362:ASN:N	2.50	0.43
1:D:489:LYS:HB3	1:D:503:LEU:HD23	2.01	0.43
1:D:535:ASN:OD1	2:Z:1:NAG:N2	2.52	0.43
1:D:588:ASP:N	1:D:588:ASP:OD2	2.52	0.43
1:D:684:GLU:HG3	1:D:717:LEU:HD21	2.00	0.43
1:A:583:LYS:C	1:A:586:ILE:HG22	2.43	0.43
1:B:319:ASN:OD1	1:B:321:SER:CB	2.65	0.43
1:B:403:GLN:OE1	1:B:755:ARG:HD3	2.18	0.43
1:B:422:HIS:CG	1:B:423:GLU:N	2.86	0.43
1:B:566:ASN:HD21	1:B:569:ASP:CB	2.32	0.43
1:B:663:ARG:NH1	1:B:683:LEU:HD13	2.32	0.43
1:B:719:THR:HG22	1:B:738:ALA:HB2	2.00	0.43
1:C:208:GLU:O	1:C:216:THR:HG23	2.19	0.43
1:C:492:ALA:CB	1:C:547:MET:HE1	2.47	0.43
1:D:245:ALA:O	1:D:255:ILE:O	2.36	0.43
1:D:719:THR:HG22	1:D:738:ALA:HB2	2.00	0.43
1:A:408:LEU:HD23	1:A:409:THR:H	1.83	0.43
1:A:412:ASP:HB3	1:A:415:THR:HB	1.99	0.43
1:B:138:SER:C	1:B:140:ASP:N	2.76	0.43
1:B:498:ASN:HB3	1:B:519:THR:HG22	1.99	0.43
1:C:148:ALA:CB	1:C:551:LEU:HD13	2.49	0.43
1:C:208:GLU:OE1	1:C:241:LYS:NZ	2.51	0.43
1:C:345:PRO:HA	1:D:336:TYR:OH	2.18	0.43
1:C:412:ASP:C	1:C:414:THR:N	2.77	0.43
1:D:135:ASP:CG	1:D:589:ARG:HH11	2.26	0.43
1:D:475:ASP:C	1:D:477:ILE:H	2.27	0.43
1:D:646:GLU:O	1:D:650:VAL:HG23	2.18	0.43
1:D:762:LEU:HD21	7:X:4:MAN:O3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:796:HIS:C	1:D:798:GLN:N	2.76	0.43
1:A:724:ALA:CB	1:A:731:GLN:N	2.80	0.43
1:A:792:ASP:CG	1:A:824:HIS:HB2	2.44	0.43
1:B:245:ALA:O	1:B:255:ILE:O	2.36	0.43
1:C:319:ASN:OD1	1:C:321:SER:CB	2.66	0.43
1:C:512:ARG:O	1:C:539:PHE:HB2	2.18	0.43
1:C:684:GLU:HG3	1:C:717:LEU:CD2	2.49	0.43
1:C:693:ARG:HH11	1:C:693:ARG:HB2	1.82	0.43
1:D:191:ARG:NE	1:D:215:TYR:HB3	2.33	0.43
6:W:2:NDG:O3	6:W:3:MAN:C1	2.66	0.43
1:A:135:ASP:CG	1:A:589:ARG:HH11	2.26	0.43
1:A:224:ILE:HG22	1:A:225:PRO:CD	2.41	0.43
1:A:498:ASN:HB3	1:A:519:THR:HG22	1.99	0.43
1:A:559:VAL:HA	1:A:560:PRO:HD3	1.81	0.43
1:A:675:GLU:OE1	1:A:675:GLU:HA	2.18	0.43
1:A:819:TYR:O	1:A:822:GLU:HB2	2.18	0.43
1:B:588:ASP:OD2	1:B:588:ASP:N	2.52	0.43
1:C:157:ILE:O	1:C:158:TYR:HB3	2.19	0.43
1:C:173:ASN:HB3	6:R:1:NAG:H83	2.00	0.43
1:C:299:LYS:HA	1:C:299:LYS:CE	2.49	0.43
1:A:138:SER:C	1:A:140:ASP:N	2.77	0.43
1:A:161:GLN:OE1	1:A:164:THR:HG23	2.19	0.43
1:A:187:LEU:O	1:A:188:ARG:C	2.62	0.43
1:A:797:PHE:HE1	1:A:818:ILE:HD11	1.82	0.43
1:B:158:TYR:CD2	1:B:166:ARG:CB	3.02	0.43
1:B:165:VAL:HB	1:B:179:ILE:HB	2.00	0.43
1:B:238:SER:OG	1:B:239:ASN:N	2.46	0.43
1:B:440:SER:O	1:B:442:ASP:N	2.52	0.43
1:B:475:ASP:C	1:B:477:ILE:H	2.27	0.43
1:C:402:ALA:HB3	1:C:404:ASN:OD1	2.19	0.43
1:C:538:TYR:HE2	1:C:638:ALA:HB1	1.84	0.43
1:D:599:ILE:HD13	1:D:600:GLU:N	2.33	0.43
1:D:684:GLU:HG3	1:D:717:LEU:CD2	2.49	0.43
1:A:329:PRO:HG3	1:B:331:TYR:CE2	2.52	0.43
1:A:375:ASP:CG	1:A:377:ARG:HH12	2.27	0.43
1:A:412:ASP:O	1:A:414:THR:N	2.52	0.43
1:A:467:SER:O	1:A:470:PRO:HD3	2.19	0.43
1:A:546:SER:C	1:A:548:ASP:H	2.27	0.43
1:A:555:GLU:O	1:A:641:PHE:N	2.46	0.43
1:B:151:ILE:HD11	1:B:157:ILE:HG12	2.01	0.43
1:B:408:LEU:HD23	1:B:409:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:GLN:NE2	1:C:483:GLY:N	2.67	0.43
1:D:224:ILE:HG22	1:D:225:PRO:CD	2.41	0.43
1:D:325:ILE:CD1	1:D:341:PRO:HB2	2.39	0.43
1:D:412:ASP:C	1:D:414:THR:N	2.77	0.43
1:A:161:GLN:O	1:A:162:LYS:CG	2.67	0.42
1:A:261:ASN:OD1	1:A:277:SER:HA	2.18	0.42
1:A:404:ASN:CA	1:A:430:LEU:HD23	2.49	0.42
1:A:438:VAL:HG21	1:A:490:ILE:CG2	2.45	0.42
1:A:663:ARG:HA	1:A:672:LEU:HD11	2.00	0.42
1:C:182:LYS:HD3	1:C:182:LYS:C	2.44	0.42
1:C:205:TYR:CZ	1:C:218:TYR:HB3	2.54	0.42
1:C:225:PRO:C	1:C:226:HIS:ND1	2.77	0.42
1:C:245:ALA:O	1:C:255:ILE:O	2.36	0.42
1:C:559:VAL:HA	1:C:560:PRO:HD3	1.81	0.42
1:C:740:SER:OG	1:C:789:PRO:HD2	2.18	0.42
1:A:210:ILE:H	1:A:214:SER:HB3	1.84	0.42
1:A:234:PRO:HB2	1:A:235:PRO:HD2	2.01	0.42
1:B:207:VAL:O	1:B:208:GLU:CB	2.67	0.42
1:C:151:ILE:HD11	1:C:157:ILE:HG12	2.01	0.42
1:C:375:ASP:CB	1:C:377:ARG:NH1	2.79	0.42
1:C:646:GLU:O	1:C:650:VAL:HG23	2.19	0.42
1:D:234:PRO:HB2	1:D:235:PRO:HD2	2.02	0.42
1:D:375:ASP:CB	1:D:377:ARG:NH1	2.80	0.42
2:G:1:NAG:C4	2:G:2:NAG:N2	2.82	0.42
1:A:319:ASN:OD1	1:A:321:SER:CB	2.66	0.42
1:A:492:ALA:CB	1:A:547:MET:HE1	2.49	0.42
1:A:798:GLN:HA	1:B:331:TYR:HB3	2.01	0.42
1:B:151:ILE:HD11	1:B:157:ILE:CD1	2.49	0.42
1:B:512:ARG:NH2	1:B:667:PHE:CZ	2.88	0.42
1:C:180:GLU:C	1:C:182:LYS:N	2.72	0.42
1:C:498:ASN:HB3	1:C:519:THR:HG22	2.00	0.42
1:D:378:MET:HE3	1:D:378:MET:HB3	1.89	0.42
1:D:454:GLN:NE2	1:D:483:GLY:N	2.65	0.42
1:D:583:LYS:C	1:D:586:ILE:HG22	2.44	0.42
1:D:663:ARG:HA	1:D:672:LEU:HD11	2.01	0.42
1:D:742:ILE:HD12	1:D:743:THR:N	2.35	0.42
1:A:663:ARG:HA	1:A:672:LEU:CD1	2.50	0.42
1:B:129:LYS:O	1:B:589:ARG:HG3	2.19	0.42
1:B:400:ASN:ND2	1:B:405:VAL:HB	2.35	0.42
1:B:566:ASN:ND2	1:B:569:ASP:HB2	2.35	0.42
1:B:797:PHE:HE1	1:B:818:ILE:HD11	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:O	1:C:589:ARG:HG3	2.19	0.42
1:C:297:ILE:HD11	1:C:298:LEU:HG	2.01	0.42
1:C:404:ASN:CA	1:C:430:LEU:HD23	2.49	0.42
1:C:429:TRP:HD1	1:C:430:LEU:O	2.03	0.42
1:C:440:SER:O	1:C:442:ASP:N	2.52	0.42
1:C:444:ARG:HG2	1:C:444:ARG:NH1	2.34	0.42
1:C:508:LEU:HD12	1:C:508:LEU:HA	1.90	0.42
1:C:552:LEU:HD13	1:C:552:LEU:C	2.45	0.42
1:C:601:ILE:O	1:C:602:ASP:HB2	2.19	0.42
1:C:649:MET:SD	1:C:840:ILE:HG22	2.59	0.42
1:C:792:ASP:OD1	1:C:824:HIS:HB2	2.18	0.42
1:D:138:SER:C	1:D:140:ASP:N	2.76	0.42
1:D:157:ILE:O	1:D:158:TYR:HB3	2.20	0.42
1:A:182:LYS:HD3	1:A:182:LYS:C	2.44	0.42
1:A:225:PRO:C	1:A:226:HIS:ND1	2.77	0.42
1:B:454:GLN:NE2	1:B:483:GLY:N	2.65	0.42
1:B:792:ASP:CG	1:B:824:HIS:HB2	2.45	0.42
1:C:131:VAL:HG22	1:C:589:ARG:HG2	2.01	0.42
1:C:375:ASP:C	1:C:377:ARG:H	2.25	0.42
1:D:129:LYS:O	1:D:589:ARG:HG3	2.19	0.42
1:D:161:GLN:O	1:D:162:LYS:CG	2.65	0.42
1:D:185:GLU:HG2	1:D:186:SER:N	2.34	0.42
1:D:552:LEU:HD13	1:D:552:LEU:C	2.44	0.42
2:Z:1:NAG:O3	2:Z:2:NAG:C1	2.67	0.42
1:A:245:ALA:O	1:A:255:ILE:O	2.37	0.42
1:B:313:LEU:HB3	1:B:359:ILE:CD1	2.48	0.42
1:B:365:THR:O	1:B:365:THR:OG1	2.34	0.42
1:B:444:ARG:HG2	1:B:444:ARG:NH1	2.33	0.42
1:C:378:MET:HE3	1:C:378:MET:HB3	1.89	0.42
1:C:412:ASP:O	1:C:414:THR:N	2.53	0.42
1:C:467:SER:O	1:C:470:PRO:HD3	2.19	0.42
1:D:225:PRO:C	1:D:226:HIS:ND1	2.78	0.42
6:L:1:NAG:O6	6:L:2:NDG:C1	2.67	0.42
1:A:145:ASP:HA	1:A:146:PRO:HD3	1.92	0.42
1:A:224:ILE:O	1:A:225:PRO:C	2.61	0.42
1:A:400:ASN:ND2	1:A:405:VAL:HB	2.34	0.42
1:A:501:TYR:CE1	1:A:547:MET:HE3	2.55	0.42
1:A:601:ILE:O	1:A:602:ASP:HB2	2.20	0.42
1:B:675:GLU:HA	1:B:675:GLU:OE1	2.18	0.42
1:C:135:ASP:CG	1:C:589:ARG:HH11	2.27	0.42
1:C:166:ARG:HG3	1:C:166:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASN:HB3	6:R:1:NAG:C8	2.50	0.42
1:C:324:PRO:HG2	1:C:349:SER:HB2	2.01	0.42
1:C:624:LEU:CD2	1:C:656:VAL:HG23	2.41	0.42
1:A:157:ILE:O	1:A:158:TYR:HB3	2.19	0.42
1:A:429:TRP:HD1	1:A:430:LEU:O	2.02	0.42
1:A:528:LEU:N	1:A:528:LEU:CD1	2.81	0.42
1:A:588:ASP:OD2	1:A:588:ASP:N	2.53	0.42
1:A:600:GLU:HB2	1:A:604:TYR:O	2.20	0.42
1:A:709:PHE:HB2	1:A:843:PHE:HZ	1.83	0.42
1:B:132:THR:O	1:B:135:ASP:HB2	2.19	0.42
1:B:225:PRO:C	1:B:226:HIS:ND1	2.78	0.42
1:B:535:ASN:OD1	5:O:1:NAG:N2	2.53	0.42
1:B:663:ARG:HA	1:B:672:LEU:HD11	2.02	0.42
1:B:840:ILE:HD13	1:B:840:ILE:HG21	1.80	0.42
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.82	0.42
1:C:421:LYS:HE2	1:C:470:PRO:CD	2.40	0.42
6:W:1:NAG:O6	6:W:2:NDG:O5	2.38	0.42
1:A:166:ARG:NH1	1:A:166:ARG:HG3	2.35	0.42
1:A:299:LYS:HA	1:A:299:LYS:CE	2.50	0.42
1:A:325:ILE:HD11	1:A:341:PRO:CB	2.39	0.42
1:A:462:HIS:HA	1:A:487:VAL:CG2	2.50	0.42
1:B:153:ASP:OD2	1:B:153:ASP:N	2.52	0.42
1:B:157:ILE:O	1:B:158:TYR:HB3	2.20	0.42
1:B:302:ILE:C	1:B:302:ILE:CD1	2.82	0.42
1:B:332:THR:O	1:B:333:GLY:O	2.37	0.42
1:B:529:SER:O	1:B:532:LEU:HB2	2.20	0.42
1:C:377:ARG:HH11	1:C:377:ARG:CG	2.33	0.42
1:C:512:ARG:NH2	1:C:667:PHE:CZ	2.88	0.42
1:D:211:TYR:HB2	1:D:294:GLU:OE1	2.18	0.42
1:D:375:ASP:OD1	1:D:377:ARG:NH1	2.52	0.42
1:D:375:ASP:CG	1:D:377:ARG:HH12	2.27	0.42
1:D:512:ARG:O	1:D:539:PHE:HB2	2.19	0.42
1:A:324:PRO:HG2	1:A:349:SER:HB2	2.00	0.42
1:B:134:GLU:H	1:B:134:GLU:CD	2.27	0.42
1:B:187:LEU:O	1:B:188:ARG:C	2.61	0.42
1:B:393:LYS:HB3	1:B:410:LEU:HD22	2.01	0.42
1:C:151:ILE:HD11	1:C:157:ILE:CD1	2.49	0.42
1:C:168:TRP:HH2	6:R:1:NAG:C1	2.33	0.42
1:C:224:ILE:HG22	1:C:225:PRO:CD	2.40	0.42
1:D:444:ARG:HG2	1:D:444:ARG:NH1	2.34	0.42
1:A:431:HIS:ND1	1:A:432:ARG:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ARG:NH2	1:A:667:PHE:CZ	2.88	0.41
1:B:489:LYS:HB3	1:B:503:LEU:HD23	2.02	0.41
1:B:601:ILE:O	1:B:602:ASP:HB2	2.20	0.41
1:B:693:ARG:HB2	1:B:693:ARG:HH11	1.84	0.41
1:C:138:SER:C	1:C:140:ASP:N	2.78	0.41
1:C:663:ARG:HA	1:C:672:LEU:HD11	2.01	0.41
1:D:435:GLU:HG3	1:D:449:ILE:HG23	1.98	0.41
1:D:709:PHE:HB2	1:D:843:PHE:HZ	1.83	0.41
1:A:235:PRO:HD2	1:A:263:TYR:CE2	2.55	0.41
1:B:170:VAL:HG11	1:B:573:MET:HE1	2.02	0.41
1:B:185:GLU:HG2	1:B:186:SER:N	2.35	0.41
1:B:224:ILE:HG22	1:B:225:PRO:CD	2.42	0.41
1:B:435:GLU:HG3	1:B:449:ILE:HG23	1.98	0.41
1:C:161:GLN:OE1	1:C:164:THR:HG23	2.19	0.41
1:C:600:GLU:HB2	1:C:604:TYR:O	2.20	0.41
1:D:165:VAL:HB	1:D:179:ILE:HB	2.01	0.41
1:D:182:LYS:HD3	1:D:182:LYS:C	2.45	0.41
1:D:558:GLY:O	1:D:559:VAL:C	2.63	0.41
1:A:529:SER:O	1:A:532:LEU:HB2	2.19	0.41
1:B:261:ASN:OD1	1:B:277:SER:HA	2.20	0.41
1:B:610:ILE:HD12	1:B:610:ILE:C	2.46	0.41
1:C:261:ASN:OD1	1:C:277:SER:HA	2.21	0.41
1:C:308:PRO:HD2	1:C:391:SER:HA	2.03	0.41
1:D:293:TYR:O	1:D:298:LEU:HB2	2.19	0.41
1:D:440:SER:O	1:D:442:ASP:N	2.53	0.41
1:D:793:GLU:OE1	1:D:793:GLU:N	2.37	0.41
6:L:1:NAG:O6	6:L:2:NDG:O5	2.37	0.41
6:L:2:NDG:O3	6:L:3:MAN:C1	2.69	0.41
1:A:138:SER:C	1:A:140:ASP:H	2.28	0.41
1:B:138:SER:C	1:B:140:ASP:H	2.27	0.41
1:B:147:GLU:O	1:B:159:ARG:HD3	2.20	0.41
1:B:235:PRO:HD2	1:B:263:TYR:CE2	2.56	0.41
1:B:467:SER:O	1:B:470:PRO:HD3	2.19	0.41
1:B:500:ILE:O	1:B:500:ILE:HG23	2.21	0.41
1:B:538:TYR:HE2	1:B:638:ALA:HB1	1.86	0.41
1:B:611:LEU:HD12	1:B:657:VAL:HG21	2.02	0.41
1:C:190:ILE:HB	1:C:207:VAL:CG2	2.50	0.41
1:C:235:PRO:HD2	1:C:263:TYR:CE2	2.54	0.41
1:D:299:LYS:HA	1:D:299:LYS:CE	2.50	0.41
6:L:1:NAG:O3	6:L:2:NDG:N2	2.54	0.41
1:A:440:SER:O	1:A:442:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ASP:O	1:B:414:THR:N	2.54	0.41
1:B:709:PHE:HB2	1:B:843:PHE:HZ	1.83	0.41
1:C:475:ASP:C	1:C:477:ILE:H	2.26	0.41
1:C:551:LEU:HD23	1:C:564:VAL:HG22	2.03	0.41
1:D:792:ASP:CG	1:D:824:HIS:HB2	2.46	0.41
6:R:1:NAG:O6	6:R:2:NDG:O5	2.39	0.41
2:V:1:NAG:HO3	2:V:2:NAG:C1	2.30	0.41
1:A:147:GLU:O	1:A:159:ARG:HD3	2.20	0.41
1:A:170:VAL:HG11	1:A:573:MET:HE1	2.03	0.41
1:A:308:PRO:HD2	1:A:391:SER:HA	2.03	0.41
1:A:345:PRO:HA	1:B:336:TYR:OH	2.20	0.41
1:A:475:ASP:C	1:A:477:ILE:H	2.27	0.41
1:B:234:PRO:HB2	1:B:235:PRO:HD2	2.03	0.41
1:B:558:GLY:O	1:B:559:VAL:C	2.63	0.41
1:C:165:VAL:HB	1:C:179:ILE:HB	2.02	0.41
1:C:431:HIS:ND1	1:C:432:ARG:HG3	2.36	0.41
1:C:489:LYS:HB3	1:C:503:LEU:HD23	2.03	0.41
1:D:138:SER:C	1:D:140:ASP:H	2.28	0.41
1:D:512:ARG:NH2	1:D:667:PHE:CZ	2.88	0.41
1:D:819:TYR:O	1:D:822:GLU:HB2	2.20	0.41
1:A:375:ASP:CB	1:A:377:ARG:NH1	2.79	0.41
1:B:182:LYS:HD3	1:B:182:LYS:C	2.45	0.41
1:C:189:ALA:HA	1:C:204:SER:O	2.21	0.41
1:C:588:ASP:OD2	1:C:588:ASP:N	2.52	0.41
1:D:132:THR:O	1:D:135:ASP:HB2	2.21	0.41
1:D:538:TYR:HE2	1:D:638:ALA:HB1	1.85	0.41
2:G:1:NAG:H4	2:G:2:NAG:C7	2.51	0.41
1:A:375:ASP:C	1:A:377:ARG:H	2.26	0.41
1:B:135:ASP:CG	1:B:589:ARG:HH11	2.28	0.41
1:B:204:SER:HB3	1:B:219:TYR:CD2	2.55	0.41
1:B:684:GLU:HG3	1:B:717:LEU:HD21	2.03	0.41
1:B:819:TYR:O	1:B:822:GLU:HB2	2.18	0.41
1:C:456:GLY:O	1:C:457:ARG:CB	2.68	0.41
1:C:811:LYS:HZ1	1:D:837:ARG:HD2	1.85	0.41
1:C:818:ILE:CG2	1:C:820:PRO:HD3	2.50	0.41
1:D:393:LYS:HB3	1:D:410:LEU:HD22	2.01	0.41
1:D:456:GLY:O	1:D:457:ARG:CB	2.69	0.41
1:D:467:SER:O	1:D:470:PRO:HD3	2.20	0.41
7:X:1:NAG:O6	7:X:2:NAG:H2	2.20	0.41
1:A:158:TYR:CD2	1:A:166:ARG:CB	3.02	0.41
1:A:444:ARG:HG2	1:A:444:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:HD23	1:A:564:VAL:HG22	2.03	0.41
1:A:834:HIS:HA	8:B:25:HOH:O	2.19	0.41
1:B:600:GLU:HB2	1:B:604:TYR:O	2.20	0.41
1:B:679:ARG:O	1:B:680:LEU:C	2.64	0.41
1:B:715:GLY:O	1:B:719:THR:CG2	2.59	0.41
1:C:147:GLU:O	1:C:159:ARG:HD3	2.21	0.41
1:C:170:VAL:HG11	1:C:573:MET:HE1	2.03	0.41
1:C:360:GLY:O	1:C:365:THR:HG22	2.20	0.41
1:C:608:MET:HE1	1:C:691:ALA:HA	2.02	0.41
1:C:611:LEU:HD12	1:C:657:VAL:HG21	2.02	0.41
1:C:663:ARG:HA	1:C:672:LEU:CD1	2.50	0.41
1:D:166:ARG:NH1	1:D:166:ARG:HG3	2.35	0.41
1:D:170:VAL:HG11	1:D:573:MET:HE1	2.03	0.41
1:D:308:PRO:HD2	1:D:391:SER:HA	2.03	0.41
1:D:522:ASN:O	1:D:523:PHE:CB	2.69	0.41
1:A:191:ARG:NH1	1:A:191:ARG:CG	2.75	0.41
1:A:297:ILE:HD11	1:A:298:LEU:HG	2.03	0.41
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.89	0.41
1:A:709:PHE:CE2	1:A:839:ILE:HD13	2.56	0.41
1:B:198:ARG:O	1:B:224:ILE:HG12	2.21	0.41
1:B:204:SER:HB3	1:B:219:TYR:CE2	2.56	0.41
1:B:567:THR:HG23	1:B:568:THR:H	1.82	0.41
1:B:740:SER:OG	1:B:789:PRO:HD2	2.21	0.41
1:B:841:ASN:ND2	4:H:1:NAG:H5	2.36	0.41
1:C:132:THR:O	1:C:135:ASP:HB2	2.21	0.41
1:C:153:ASP:CB	1:C:546:SER:HB2	2.51	0.41
1:D:610:ILE:HD12	1:D:610:ILE:C	2.46	0.41
1:D:792:ASP:OD1	1:D:824:HIS:HB2	2.21	0.41
1:D:840:ILE:HD13	1:D:840:ILE:HG21	1.80	0.41
1:A:459:LYS:H	1:A:459:LYS:HG2	1.81	0.40
1:B:262:ILE:H	1:B:276:VAL:HG13	1.86	0.40
1:B:456:GLY:O	1:B:457:ARG:CB	2.68	0.40
1:B:617:THR:CG2	1:B:618:ASP:N	2.58	0.40
1:C:161:GLN:O	1:C:162:LYS:CG	2.67	0.40
1:C:224:ILE:O	1:C:225:PRO:C	2.61	0.40
1:C:262:ILE:H	1:C:276:VAL:HG13	1.86	0.40
1:C:293:TYR:O	1:C:298:LEU:HB2	2.22	0.40
1:D:208:GLU:HA	1:D:209:PRO:HD3	1.71	0.40
1:D:429:TRP:HD1	1:D:430:LEU:O	2.04	0.40
1:D:453:PRO:O	1:D:458:GLY:O	2.40	0.40
2:N:1:NAG:H3	2:N:1:NAG:C8	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLY:O	1:A:365:THR:HG22	2.21	0.40
1:A:412:ASP:C	1:A:414:THR:N	2.76	0.40
1:B:158:TYR:CG	1:B:166:ARG:HB2	2.56	0.40
1:B:404:ASN:CA	1:B:430:LEU:HD23	2.51	0.40
1:B:528:LEU:O	1:B:570:LYS:HE3	2.21	0.40
1:B:684:GLU:HG3	1:B:717:LEU:CD2	2.51	0.40
1:B:765:ARG:O	1:B:765:ARG:CG	2.68	0.40
1:C:501:TYR:CE1	1:C:547:MET:HE3	2.56	0.40
1:C:840:ILE:HD13	1:C:840:ILE:HG21	1.57	0.40
1:D:500:ILE:O	1:D:500:ILE:HG23	2.20	0.40
1:D:529:SER:O	1:D:532:LEU:HB2	2.20	0.40
1:D:663:ARG:HA	1:D:672:LEU:CD1	2.51	0.40
1:A:132:THR:O	1:A:135:ASP:HB2	2.21	0.40
1:A:456:GLY:O	1:A:457:ARG:CB	2.68	0.40
1:A:538:TYR:HE2	1:A:638:ALA:HB1	1.86	0.40
1:A:792:ASP:OD1	1:A:824:HIS:HB2	2.21	0.40
1:B:308:PRO:HD2	1:B:391:SER:HA	2.03	0.40
1:B:324:PRO:HG2	1:B:349:SER:HB2	2.02	0.40
1:B:375:ASP:CG	1:B:377:ARG:HH12	2.29	0.40
1:C:313:LEU:HB3	1:C:359:ILE:CD1	2.47	0.40
1:C:331:TYR:CE2	1:D:329:PRO:HG3	2.56	0.40
1:C:500:ILE:O	1:C:500:ILE:HG23	2.21	0.40
1:C:797:PHE:HE1	1:C:818:ILE:HD11	1.84	0.40
1:D:324:PRO:HG2	1:D:349:SER:HB2	2.02	0.40
1:D:412:ASP:O	1:D:414:THR:N	2.55	0.40
1:A:293:TYR:O	1:A:298:LEU:HB2	2.21	0.40
1:A:365:THR:O	1:A:365:THR:OG1	2.32	0.40
1:A:375:ASP:OD1	1:A:377:ARG:NH1	2.53	0.40
1:A:522:ASN:O	1:A:523:PHE:CB	2.69	0.40
1:A:608:MET:HE1	1:A:691:ALA:HA	2.03	0.40
1:B:429:TRP:HD1	1:B:430:LEU:O	2.05	0.40
1:C:235:PRO:O	1:C:236:GLU:HB2	2.21	0.40
1:C:793:GLU:OE1	1:C:793:GLU:N	2.39	0.40
1:C:804:ILE:O	1:C:808:ILE:HG13	2.22	0.40
1:D:158:TYR:CG	1:D:166:ARG:HB2	2.56	0.40
1:D:262:ILE:H	1:D:276:VAL:HG13	1.84	0.40
1:D:608:MET:HE1	1:D:691:ALA:HA	2.02	0.40
1:D:804:ILE:O	1:D:808:ILE:HG13	2.22	0.40
1:A:402:ALA:HB3	1:A:404:ASN:OD1	2.21	0.40
1:A:528:LEU:O	1:A:570:LYS:HE3	2.21	0.40
1:B:166:ARG:HG3	1:B:166:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:LYS:H	1:C:459:LYS:HG2	1.81	0.40
1:C:529:SER:O	1:C:532:LEU:HB2	2.21	0.40
1:D:255:ILE:HG23	1:D:306:TRP:CZ2	2.56	0.40
1:D:297:ILE:HD11	1:D:298:LEU:HG	2.02	0.40
1:D:360:GLY:O	1:D:365:THR:HG22	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:SER:OG	1:D:362:ASN:OD1[2_546]	2.13	0.07
1:A:473:SER:OG	1:B:362:ASN:OD1[2_655]	2.17	0.03

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	721/723 (100%)	578 (80%)	97 (14%)	46 (6%)	1	6
1	B	721/723 (100%)	575 (80%)	98 (14%)	48 (7%)	1	5
1	C	721/723 (100%)	579 (80%)	95 (13%)	47 (6%)	1	5
1	D	721/723 (100%)	577 (80%)	94 (13%)	50 (7%)	1	5
All	All	2884/2892 (100%)	2309 (80%)	384 (13%)	191 (7%)	1	5

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	160	GLU
1	A	162	LYS
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	472	SER
1	A	473	SER
1	A	521	GLY
1	A	530	CYS
1	A	723	PRO
1	A	778	ALA
1	A	779	LEU
1	B	129	LYS
1	B	160	GLU
1	B	162	LYS
1	B	173	ASN
1	B	213	HIS
1	B	215	TYR
1	B	239	ASN
1	B	472	SER
1	B	473	SER
1	B	521	GLY
1	B	530	CYS
1	B	723	PRO
1	B	778	ALA
1	B	779	LEU
1	C	129	LYS
1	C	160	GLU
1	C	162	LYS
1	C	173	ASN
1	C	472	SER
1	C	473	SER
1	C	521	GLY
1	C	530	CYS
1	C	723	PRO
1	C	778	ALA
1	C	779	LEU
1	D	129	LYS
1	D	160	GLU
1	D	162	LYS
1	D	173	ASN
1	D	472	SER
1	D	473	SER
1	D	521	GLY
1	D	530	CYS
1	D	723	PRO
1	D	778	ALA

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Mol	Chain	Res	Type
1	D	779	LEU
1	A	215	TYR
1	A	239	ASN
1	A	333	GLY
1	A	373	PRO
1	A	413	ALA
1	A	441	LYS
1	A	444	ARG
1	A	453	PRO
1	A	457	ARG
1	A	478	GLN
1	A	533	VAL
1	A	554	CYS
1	A	567	THR
1	A	613	PRO
1	A	654	GLY
1	A	703	ARG
1	A	763	ASP
1	A	846	CYS
1	B	212	GLN
1	B	333	GLY
1	B	373	PRO
1	B	413	ALA
1	B	441	LYS
1	B	444	ARG
1	B	453	PRO
1	B	457	ARG
1	B	478	GLN
1	B	533	VAL
1	B	554	CYS
1	B	567	THR
1	B	613	PRO
1	B	654	GLY
1	B	763	ASP
1	B	846	CYS
1	C	239	ASN
1	C	333	GLY
1	C	373	PRO
1	C	413	ALA
1	C	441	LYS
1	C	444	ARG
1	C	453	PRO

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Mol	Chain	Res	Type
1	C	457	ARG
1	C	478	GLN
1	C	533	VAL
1	C	554	CYS
1	C	567	THR
1	C	613	PRO
1	C	654	GLY
1	C	703	ARG
1	C	763	ASP
1	C	846	CYS
1	D	206	ASN
1	D	212	GLN
1	D	239	ASN
1	D	246	GLY
1	D	333	GLY
1	D	373	PRO
1	D	413	ALA
1	D	441	LYS
1	D	444	ARG
1	D	453	PRO
1	D	457	ARG
1	D	478	GLN
1	D	533	VAL
1	D	554	CYS
1	D	567	THR
1	D	613	PRO
1	D	654	GLY
1	D	763	ASP
1	D	846	CYS
1	A	246	GLY
1	A	422	HIS
1	A	428	ALA
1	A	477	ILE
1	A	574	PHE
1	B	186	SER
1	B	246	GLY
1	B	422	HIS
1	B	428	ALA
1	B	477	ILE
1	B	574	PHE
1	B	703	ARG
1	C	186	SER

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Mol	Chain	Res	Type
1	C	246	GLY
1	C	422	HIS
1	C	428	ALA
1	C	477	ILE
1	C	574	PHE
1	D	186	SER
1	D	210	ILE
1	D	422	HIS
1	D	428	ALA
1	D	477	ILE
1	D	574	PHE
1	D	703	ARG
1	A	186	SER
1	A	225	PRO
1	A	364	PRO
1	A	603	ASP
1	B	225	PRO
1	B	364	PRO
1	B	545	HIS
1	B	603	ASP
1	C	225	PRO
1	C	364	PRO
1	C	545	HIS
1	C	603	ASP
1	D	225	PRO
1	D	364	PRO
1	D	545	HIS
1	D	603	ASP
1	A	167	LEU
1	A	507	ASP
1	A	545	HIS
1	A	572	LYS
1	A	761	GLY
1	B	167	LEU
1	B	507	ASP
1	B	572	LYS
1	B	761	GLY
1	C	167	LEU
1	C	210	ILE
1	C	445	LYS
1	C	507	ASP
1	C	572	LYS

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Mol	Chain	Res	Type
1	C	761	GLY
1	D	507	ASP
1	D	572	LYS
1	D	761	GLY
1	D	167	LEU
1	D	445	LYS
1	B	181	GLY
1	A	181	GLY
1	C	181	GLY
1	D	181	GLY
1	D	249	PRO
1	A	249	PRO
1	A	721	ILE
1	B	721	ILE
1	C	249	PRO
1	C	721	ILE
1	D	721	ILE
1	B	249	PRO
1	D	376	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	643/643 (100%)	574 (89%)	69 (11%)	6	26
1	B	643/643 (100%)	573 (89%)	70 (11%)	6	26
1	C	643/643 (100%)	574 (89%)	69 (11%)	6	26
1	D	643/643 (100%)	572 (89%)	71 (11%)	6	25
All	All	2572/2572 (100%)	2293 (89%)	279 (11%)	6	26

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	157	ILE

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Mol	Chain	Res	Type
1	A	164	THR
1	A	168	TRP
1	A	172	THR
1	A	182	LYS
1	A	183	LYS
1	A	194	ILE
1	A	202	LEU
1	A	213	HIS
1	A	215	TYR
1	A	216	THR
1	A	224	ILE
1	A	228	ASP
1	A	254	LEU
1	A	268	VAL
1	A	286	ASN
1	A	297	ILE
1	A	300	THR
1	A	302	ILE
1	A	325	ILE
1	A	328	LEU
1	A	364	PRO
1	A	386	VAL
1	A	401	ARG
1	A	408	LEU
1	A	409	THR
1	A	421	LYS
1	A	423	GLU
1	A	449	ILE
1	A	450	ARG
1	A	453	PRO
1	A	478	GLN
1	A	500	ILE
1	A	503	LEU
1	A	508	LEU
1	A	536	CYS
1	A	578	THR
1	A	588	ASP
1	A	589	ARG
1	A	599	ILE
1	A	610	ILE
1	A	624	LEU
1	A	626	LEU

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Mol	Chain	Res	Type
1	A	628	VAL
1	A	663	ARG
1	A	675	GLU
1	A	680	LEU
1	A	684	GLU
1	A	685	GLU
1	A	693	ARG
1	A	696	LEU
1	A	701	ILE
1	A	711	LYS
1	A	719	THR
1	A	723	PRO
1	A	731	GLN
1	A	742	ILE
1	A	768	GLU
1	A	781	GLU
1	A	790	THR
1	A	805	THR
1	A	816	LEU
1	A	818	ILE
1	A	823	SER
1	A	835	LEU
1	A	837	ARG
1	A	847	PHE
1	A	848	ARG
1	B	129	LYS
1	B	157	ILE
1	B	164	THR
1	B	168	TRP
1	B	172	THR
1	B	182	LYS
1	B	183	LYS
1	B	194	ILE
1	B	202	LEU
1	B	208	GLU
1	B	211	TYR
1	B	212	GLN
1	B	224	ILE
1	B	228	ASP
1	B	254	LEU
1	B	268	VAL
1	B	286	ASN

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Mol	Chain	Res	Type
1	B	297	ILE
1	B	300	THR
1	B	302	ILE
1	B	325	ILE
1	B	328	LEU
1	B	364	PRO
1	B	386	VAL
1	B	401	ARG
1	B	408	LEU
1	B	409	THR
1	B	421	LYS
1	B	423	GLU
1	B	449	ILE
1	B	450	ARG
1	B	453	PRO
1	B	478	GLN
1	B	500	ILE
1	B	503	LEU
1	B	508	LEU
1	B	532	LEU
1	B	536	CYS
1	B	578	THR
1	B	588	ASP
1	B	589	ARG
1	B	599	ILE
1	B	610	ILE
1	B	624	LEU
1	B	626	LEU
1	B	628	VAL
1	B	663	ARG
1	B	675	GLU
1	B	680	LEU
1	B	684	GLU
1	B	685	GLU
1	B	693	ARG
1	B	696	LEU
1	B	701	ILE
1	B	711	LYS
1	B	719	THR
1	B	723	PRO
1	B	731	GLN
1	B	742	ILE

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Mol	Chain	Res	Type
1	B	768	GLU
1	B	781	GLU
1	B	790	THR
1	B	805	THR
1	B	816	LEU
1	B	818	ILE
1	B	823	SER
1	B	835	LEU
1	B	837	ARG
1	B	847	PHE
1	B	848	ARG
1	C	129	LYS
1	C	157	ILE
1	C	164	THR
1	C	168	TRP
1	C	172	THR
1	C	182	LYS
1	C	183	LYS
1	C	194	ILE
1	C	213	HIS
1	C	220	VAL
1	C	224	ILE
1	C	228	ASP
1	C	254	LEU
1	C	268	VAL
1	C	286	ASN
1	C	297	ILE
1	C	300	THR
1	C	302	ILE
1	C	325	ILE
1	C	328	LEU
1	C	351	ASN
1	C	364	PRO
1	C	386	VAL
1	C	401	ARG
1	C	408	LEU
1	C	409	THR
1	C	421	LYS
1	C	423	GLU
1	C	449	ILE
1	C	450	ARG
1	C	453	PRO

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Mol	Chain	Res	Type
1	C	478	GLN
1	C	500	ILE
1	C	503	LEU
1	C	508	LEU
1	C	532	LEU
1	C	536	CYS
1	C	578	THR
1	C	588	ASP
1	C	589	ARG
1	C	599	ILE
1	C	610	ILE
1	C	624	LEU
1	C	626	LEU
1	C	628	VAL
1	C	663	ARG
1	C	675	GLU
1	C	680	LEU
1	C	684	GLU
1	C	685	GLU
1	C	693	ARG
1	C	696	LEU
1	C	701	ILE
1	C	711	LYS
1	C	719	THR
1	C	723	PRO
1	C	731	GLN
1	C	742	ILE
1	C	768	GLU
1	C	781	GLU
1	C	790	THR
1	C	816	LEU
1	C	818	ILE
1	C	823	SER
1	C	835	LEU
1	C	837	ARG
1	C	840	ILE
1	C	847	PHE
1	C	848	ARG
1	D	129	LYS
1	D	157	ILE
1	D	164	THR
1	D	168	TRP

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Mol	Chain	Res	Type
1	D	172	THR
1	D	182	LYS
1	D	183	LYS
1	D	194	ILE
1	D	202	LEU
1	D	208	GLU
1	D	213	HIS
1	D	215	TYR
1	D	224	ILE
1	D	228	ASP
1	D	254	LEU
1	D	268	VAL
1	D	286	ASN
1	D	297	ILE
1	D	300	THR
1	D	302	ILE
1	D	325	ILE
1	D	328	LEU
1	D	351	ASN
1	D	364	PRO
1	D	386	VAL
1	D	401	ARG
1	D	408	LEU
1	D	409	THR
1	D	421	LYS
1	D	423	GLU
1	D	449	ILE
1	D	450	ARG
1	D	453	PRO
1	D	478	GLN
1	D	500	ILE
1	D	503	LEU
1	D	508	LEU
1	D	532	LEU
1	D	536	CYS
1	D	578	THR
1	D	588	ASP
1	D	589	ARG
1	D	599	ILE
1	D	610	ILE
1	D	624	LEU
1	D	626	LEU

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Mol	Chain	Res	Type
1	D	628	VAL
1	D	663	ARG
1	D	675	GLU
1	D	680	LEU
1	D	684	GLU
1	D	685	GLU
1	D	693	ARG
1	D	696	LEU
1	D	701	ILE
1	D	711	LYS
1	D	719	THR
1	D	723	PRO
1	D	731	GLN
1	D	742	ILE
1	D	768	GLU
1	D	781	GLU
1	D	790	THR
1	D	805	THR
1	D	816	LEU
1	D	818	ILE
1	D	823	SER
1	D	835	LEU
1	D	837	ARG
1	D	847	PHE
1	D	848	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	422	HIS
1	A	478	GLN
1	A	609	GLN
1	A	668	GLN
1	B	239	ASN
1	B	422	HIS
1	B	478	GLN
1	B	609	GLN
1	B	668	GLN
1	C	422	HIS
1	C	478	GLN
1	C	609	GLN

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Mol	Chain	Res	Type
1	C	668	GLN
1	D	213	HIS
1	D	422	HIS
1	D	478	GLN
1	D	609	GLN
1	D	668	GLN

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 ⓘ

63 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.61	0	17,19,21	1.31	2 (11%)
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	0.79	1 (5%)
2	BMA	E	3	2	11,11,12	0.61	0	15,15,17	0.28	0
3	NAG	F	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	1.10	1 (5%)
3	NDG	F	2	3	14,14,15	0.84	0	17,19,21	1.17	2 (11%)
3	MAN	F	3	3	11,11,12	0.85	0	15,15,17	0.98	1 (6%)
3	BMA	F	4	3	11,11,12	0.71	0	15,15,17	1.10	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
2	NAG	G	2	2	14,14,15	0.88	0	17,19,21	1.47	4 (23%)
2	BMA	G	3	2	11,11,12	0.58	0	15,15,17	0.54	0
4	NAG	H	1	4,1	14,14,15	0.50	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	2	4	14,14,15	0.59	0	17,19,21	1.09	1 (5%)
4	BMA	H	3	4	11,11,12	1.17	1 (9%)	15,15,17	1.38	1 (6%)
4	MAN	H	4	4	11,11,12	0.84	1 (9%)	15,15,17	0.94	1 (6%)
2	NAG	I	1	2,1	14,14,15	0.89	1 (7%)	17,19,21	1.05	2 (11%)
2	NAG	I	2	2	14,14,15	0.57	0	17,19,21	0.67	0
2	BMA	I	3	2	11,11,12	0.46	0	15,15,17	0.27	0
5	NAG	J	1	5,1	14,14,15	1.57	3 (21%)	17,19,21	1.69	5 (29%)
5	NAG	J	2	5	14,14,15	1.98	3 (21%)	17,19,21	1.27	3 (17%)
2	NAG	K	1	2,1	14,14,15	0.87	1 (7%)	17,19,21	1.40	2 (11%)
2	NAG	K	2	2	14,14,15	0.71	0	17,19,21	0.69	0
2	BMA	K	3	2	11,11,12	0.54	0	15,15,17	0.28	0
6	NAG	L	1	6,1	14,14,15	0.86	1 (7%)	17,19,21	1.26	2 (11%)
6	NDG	L	2	6	14,14,15	0.68	0	17,19,21	1.44	3 (17%)
6	MAN	L	3	6	11,11,12	0.73	0	15,15,17	0.83	1 (6%)
5	NAG	M	1	5,1	14,14,15	0.61	0	17,19,21	1.33	2 (11%)
5	NAG	M	2	5	14,14,15	0.60	0	17,19,21	0.75	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.50	0	17,19,21	0.65	0
2	NAG	N	2	2	14,14,15	0.70	0	17,19,21	1.41	2 (11%)
2	BMA	N	3	2	11,11,12	0.55	0	15,15,17	0.54	0
5	NAG	O	1	5,1	14,14,15	0.96	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	O	2	5	14,14,15	0.67	0	17,19,21	0.71	0
5	NAG	P	1	5,1	14,14,15	1.18	1 (7%)	17,19,21	1.45	3 (17%)
5	NAG	P	2	5	14,14,15	0.71	0	17,19,21	0.71	1 (5%)
2	NAG	Q	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	1.33	2 (11%)
2	NAG	Q	2	2	14,14,15	0.95	1 (7%)	17,19,21	0.86	0
2	BMA	Q	3	2	11,11,12	0.60	0	15,15,17	0.39	0
6	NAG	R	1	6,1	14,14,15	0.72	0	17,19,21	1.48	4 (23%)
6	NDG	R	2	6	14,14,15	0.68	0	17,19,21	1.13	2 (11%)
6	MAN	R	3	6	11,11,12	0.66	0	15,15,17	0.79	0
5	NAG	S	1	5,1	14,14,15	0.60	0	17,19,21	0.94	1 (5%)
5	NAG	S	2	5	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
2	NAG	T	1	2,1	14,14,15	0.65	0	17,19,21	0.66	0
2	NAG	T	2	2	14,14,15	0.66	0	17,19,21	1.34	2 (11%)
2	BMA	T	3	2	11,11,12	0.54	0	15,15,17	0.31	0
5	NAG	U	1	5,1	14,14,15	0.93	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	U	2	5	14,14,15	0.58	0	17,19,21	0.69	0
2	NAG	V	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	1.73	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	V	2	2	14,14,15	0.66	0	17,19,21	0.78	1 (5%)
2	BMA	V	3	2	11,11,12	0.54	0	15,15,17	0.24	0
6	NAG	W	1	6,1	14,14,15	0.67	0	17,19,21	1.32	3 (17%)
6	NDG	W	2	6	14,14,15	0.77	0	17,19,21	1.61	3 (17%)
6	MAN	W	3	6	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
7	NAG	X	1	7,1	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
7	NAG	X	2	7	14,14,15	0.68	0	17,19,21	1.28	2 (11%)
7	MAN	X	3	7	11,11,12	0.93	0	15,15,17	2.26	5 (33%)
7	MAN	X	4	7	11,11,12	0.92	1 (9%)	15,15,17	1.74	3 (20%)
2	NAG	Y	1	2,1	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
2	NAG	Y	2	2	14,14,15	0.77	0	17,19,21	1.32	2 (11%)
2	BMA	Y	3	2	11,11,12	0.56	0	15,15,17	0.30	0
2	NAG	Z	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	1.14	3 (17%)
2	NAG	Z	2	2	14,14,15	0.73	0	17,19,21	0.69	0
2	BMA	Z	3	2	11,11,12	0.51	0	15,15,17	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	1/1/5/7	4/6/23/26	0/1/1/1
3	NDG	F	2	3	-	4/6/23/26	0/1/1/1
3	MAN	F	3	3	-	1/2/19/22	0/1/1/1
3	BMA	F	4	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	BMA	I	3	2	-	2/2/19/22	0/1/1/1
5	NAG	J	1	5,1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1
2	NAG	K	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	1/2/19/22	0/1/1/1
6	NAG	L	1	6,1	1/1/5/7	5/6/23/26	0/1/1/1
6	NDG	L	2	6	-	4/6/23/26	0/1/1/1
6	MAN	L	3	6	-	2/2/19/22	0/1/1/1
5	NAG	M	1	5,1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	N	2	2	-	4/6/23/26	0/1/1/1
2	BMA	N	3	2	-	2/2/19/22	0/1/1/1
5	NAG	O	1	5,1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	P	2	5	-	4/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NDG	R	2	6	-	4/6/23/26	0/1/1/1
6	MAN	R	3	6	-	2/2/19/22	0/1/1/1
5	NAG	S	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	4/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	T	2	2	-	4/6/23/26	0/1/1/1
2	BMA	T	3	2	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5,1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
2	NAG	V	1	2,1	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	V	2	2	-	4/6/23/26	0/1/1/1

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	NAG	C1-C2	6.05	1.60	1.52
5	J	1	NAG	O4-C4	3.70	1.52	1.43
5	P	1	NAG	C1-C2	3.33	1.56	1.52
5	J	1	NAG	C4-C5	3.11	1.59	1.53
5	J	2	NAG	O5-C5	2.94	1.49	1.43
2	K	1	NAG	C1-C2	2.86	1.56	1.52
2	I	1	NAG	C1-C2	2.84	1.56	1.52
5	U	1	NAG	C1-C2	2.83	1.56	1.52
5	O	1	NAG	C1-C2	2.74	1.56	1.52
2	Q	2	NAG	C1-C2	2.68	1.56	1.52
5	J	1	NAG	O5-C5	2.63	1.48	1.43
2	Z	1	NAG	C1-C2	2.54	1.55	1.52
4	H	3	BMA	C4-C5	2.48	1.58	1.53
7	X	4	MAN	C1-C2	2.45	1.58	1.52
2	V	1	NAG	C1-C2	2.44	1.55	1.52
3	F	1	NAG	C1-C2	2.43	1.55	1.52
6	L	1	NAG	C1-C2	2.41	1.55	1.52
2	Q	1	NAG	C1-C2	2.26	1.55	1.52
5	J	2	NAG	O5-C1	2.15	1.47	1.43
4	H	4	MAN	C2-C3	2.10	1.55	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	3	MAN	C1-C2-C3	6.18	118.64	109.64
4	H	3	BMA	C1-C2-C3	-4.64	102.89	109.64
7	X	4	MAN	C1-C2-C3	4.41	116.07	109.64
7	X	3	MAN	C1-O5-C5	4.40	118.09	112.19
6	W	2	NDG	C4-C3-C2	-4.05	105.09	111.02
2	N	2	NAG	C4-C3-C2	-3.96	105.22	111.02
2	V	1	NAG	O5-C1-C2	3.77	117.12	111.29
2	V	1	NAG	C3-C4-C5	-3.67	103.58	110.23
6	W	2	NDG	C2-N2-C7	-3.61	118.06	122.90
6	L	2	NDG	C4-C3-C2	-3.60	105.74	111.02
5	P	1	NAG	C3-C4-C5	-3.58	103.74	110.23
2	T	2	NAG	C4-C3-C2	-3.57	105.79	111.02
7	X	2	NAG	C4-C3-C2	3.53	116.19	111.02
5	J	1	NAG	C1-O5-C5	3.49	116.86	112.19
5	M	1	NAG	C2-N2-C7	-3.44	118.29	122.90
6	R	1	NAG	O5-C1-C2	3.39	116.53	111.29
2	Y	2	NAG	C4-C3-C2	-3.34	106.12	111.02
2	K	1	NAG	C3-C4-C5	-3.29	104.27	110.23
2	G	2	NAG	C4-C3-C2	3.26	115.80	111.02
6	L	2	NDG	C2-N2-C7	-3.17	118.65	122.90
2	G	2	NAG	C3-C4-C5	3.16	115.96	110.23
5	J	2	NAG	C1-O5-C5	3.15	116.41	112.19
4	H	2	NAG	C4-C3-C2	3.12	115.59	111.02
2	E	1	NAG	O5-C1-C2	3.10	116.09	111.29
2	Q	1	NAG	C3-C4-C5	-3.08	104.64	110.23
2	K	1	NAG	O5-C1-C2	3.08	116.06	111.29
2	Q	1	NAG	O5-C1-C2	3.03	115.97	111.29
7	X	4	MAN	C1-O5-C5	3.01	116.22	112.19
5	M	1	NAG	C4-C3-C2	-3.00	106.63	111.02
6	R	2	NDG	C2-N2-C7	-2.99	118.89	122.90
7	X	1	NAG	C4-C3-C2	-2.95	106.69	111.02
4	H	4	MAN	C1-C2-C3	2.93	113.91	109.64
2	T	2	NAG	C2-N2-C7	-2.93	118.97	122.90
2	Y	2	NAG	C2-N2-C7	-2.92	118.99	122.90
2	G	1	NAG	C2-N2-C7	-2.81	119.13	122.90
5	S	2	NAG	C2-N2-C7	-2.81	119.13	122.90
3	F	4	BMA	C1-C2-C3	2.81	113.74	109.64
2	E	1	NAG	C3-C4-C5	-2.80	105.16	110.23
7	X	4	MAN	O5-C1-C2	2.80	117.46	110.79
5	P	1	NAG	C4-C3-C2	2.76	115.07	111.02
5	S	1	NAG	C2-N2-C7	-2.72	119.26	122.90
2	V	1	NAG	C4-C3-C2	-2.68	107.08	111.02
6	R	1	NAG	C3-C4-C5	-2.68	105.37	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	1	NAG	C8-C7-N2	2.67	120.55	116.12
2	N	2	NAG	C2-N2-C7	-2.67	119.32	122.90
6	W	1	NAG	O5-C1-C2	2.61	115.33	111.29
3	F	2	NDG	C2-N2-C7	-2.61	119.40	122.90
3	F	1	NAG	O5-C1-C2	2.59	115.30	111.29
5	J	2	NAG	C2-N2-C7	-2.54	119.49	122.90
5	J	1	NAG	C4-C3-C2	2.52	114.71	111.02
7	X	3	MAN	O5-C1-C2	2.51	116.78	110.79
7	X	1	NAG	C2-N2-C7	-2.50	119.55	122.90
2	V	1	NAG	C1-O5-C5	2.48	115.51	112.19
6	L	1	NAG	C3-C4-C5	-2.48	105.74	110.23
5	J	1	NAG	C6-C5-C4	-2.43	107.04	113.02
6	L	3	MAN	C1-O5-C5	2.38	115.38	112.19
5	J	1	NAG	O4-C4-C5	2.36	115.13	109.32
6	R	2	NDG	C4-C3-C2	-2.34	107.59	111.02
6	L	1	NAG	O5-C1-C2	2.32	114.88	111.29
6	W	1	NAG	C2-N2-C7	-2.30	119.81	122.90
6	W	3	MAN	C1-O5-C5	2.30	115.27	112.19
3	F	2	NDG	C1-O5-C5	2.29	115.26	112.19
5	U	1	NAG	O5-C1-C2	2.29	114.83	111.29
5	M	2	NAG	C2-N2-C7	-2.25	119.89	122.90
5	J	2	NAG	O5-C1-C2	-2.23	107.84	111.29
6	W	1	NAG	C3-C4-C5	-2.22	106.20	110.23
7	X	3	MAN	O5-C5-C6	2.22	111.98	107.66
3	F	3	MAN	C1-O5-C5	2.21	115.15	112.19
6	L	2	NDG	C3-C4-C5	-2.21	106.22	110.23
2	E	2	NAG	C2-N2-C7	-2.18	119.97	122.90
2	I	1	NAG	O5-C1-C2	2.18	114.66	111.29
2	I	1	NAG	C3-C4-C5	-2.16	106.31	110.23
6	R	1	NAG	C1-O5-C5	2.13	115.04	112.19
5	P	1	NAG	C1-O5-C5	2.11	115.02	112.19
6	W	2	NDG	C1-O5-C5	2.11	115.01	112.19
2	Z	1	NAG	C2-N2-C7	-2.10	120.09	122.90
5	J	1	NAG	O5-C5-C6	-2.09	103.59	107.66
5	P	2	NAG	C2-N2-C7	-2.08	120.11	122.90
2	Z	1	NAG	O5-C1-C2	2.08	114.51	111.29
6	R	1	NAG	C2-N2-C7	-2.08	120.11	122.90
2	Z	1	NAG	C3-C4-C5	-2.07	106.48	110.23
2	G	2	NAG	C2-N2-C7	-2.07	120.13	122.90
7	X	3	MAN	C2-C3-C4	2.06	114.49	110.86
2	G	2	NAG	O5-C1-C2	-2.05	108.13	111.29
7	X	2	NAG	C3-C4-C5	2.03	113.91	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	2	NAG	C2-N2-C7	-2.03	120.18	122.90
6	W	3	MAN	C2-C3-C4	-2.02	107.30	110.86
5	O	1	NAG	C2-N2-C7	-2.02	120.19	122.90

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C1
2	G	1	NAG	C1
2	I	1	NAG	C1
2	K	1	NAG	C1
2	Q	1	NAG	C1
2	V	1	NAG	C1
2	Z	1	NAG	C1
3	F	1	NAG	C1
5	J	1	NAG	C1
5	M	1	NAG	C1
5	O	1	NAG	C1
5	S	1	NAG	C1
5	U	1	NAG	C1
6	L	1	NAG	C1
6	R	1	NAG	C1
6	W	1	NAG	C1
7	X	1	NAG	C1

All (198) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	I	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	N	1	NAG	C3-C2-N2-C7
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	Q	1	NAG	C3-C2-N2-C7
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	T	1	NAG	C3-C2-N2-C7
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
2	V	1	NAG	C3-C2-N2-C7
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	V	2	NAG	C8-C7-N2-C2
2	V	2	NAG	O7-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
2	Z	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C8-C7-N2-C2
2	Z	1	NAG	O7-C7-N2-C2
2	Z	2	NAG	C8-C7-N2-C2
2	Z	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	NDG	C8-C7-N2-C2
3	F	2	NDG	O7-C7-N2-C2
4	H	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C3-C2-N2-C7
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	O	1	NAG	C3-C2-N2-C7
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	P	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	U	1	NAG	C3-C2-N2-C7
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	R	2	NDG	C8-C7-N2-C2
6	R	2	NDG	O7-C7-N2-C2
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	X	2	NAG	C8-C7-N2-C2
7	X	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C4-C5-C6-O6
6	W	2	NDG	C8-C7-N2-C2
6	W	2	NDG	O7-C7-N2-C2
2	Y	2	NAG	O5-C5-C6-O6
6	L	2	NDG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	Z	3	BMA	O5-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
6	L	3	MAN	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	L	2	NDG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
3	F	2	NDG	O5-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
7	X	4	MAN	O5-C5-C6-O6
2	Z	3	BMA	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
3	F	4	BMA	C4-C5-C6-O6
6	L	2	NDG	C8-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
6	R	3	MAN	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
2	T	3	BMA	O5-C5-C6-O6
6	L	3	MAN	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	T	3	BMA	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	R	2	NDG	O5-C5-C6-O6
6	W	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	F	2	NDG	C4-C5-C6-O6
2	Y	1	NAG	C8-C7-N2-C2
2	Y	1	NAG	O7-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
6	L	2	NDG	O7-C7-N2-C2
4	H	3	BMA	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
2	V	3	BMA	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
6	R	3	MAN	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
7	X	4	MAN	C4-C5-C6-O6
7	X	3	MAN	O5-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
6	R	2	NDG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
2	Y	1	NAG	C1-C2-N2-C7
5	O	1	NAG	O5-C5-C6-O6
6	W	3	MAN	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Z	1	NAG	O5-C5-C6-O6
2	V	3	BMA	C4-C5-C6-O6
7	X	2	NAG	C3-C2-N2-C7
2	V	2	NAG	O5-C5-C6-O6
3	F	3	MAN	C4-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
6	W	3	MAN	O5-C5-C6-O6
2	Y	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C4-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

50 monomers are involved in 82 short contacts:

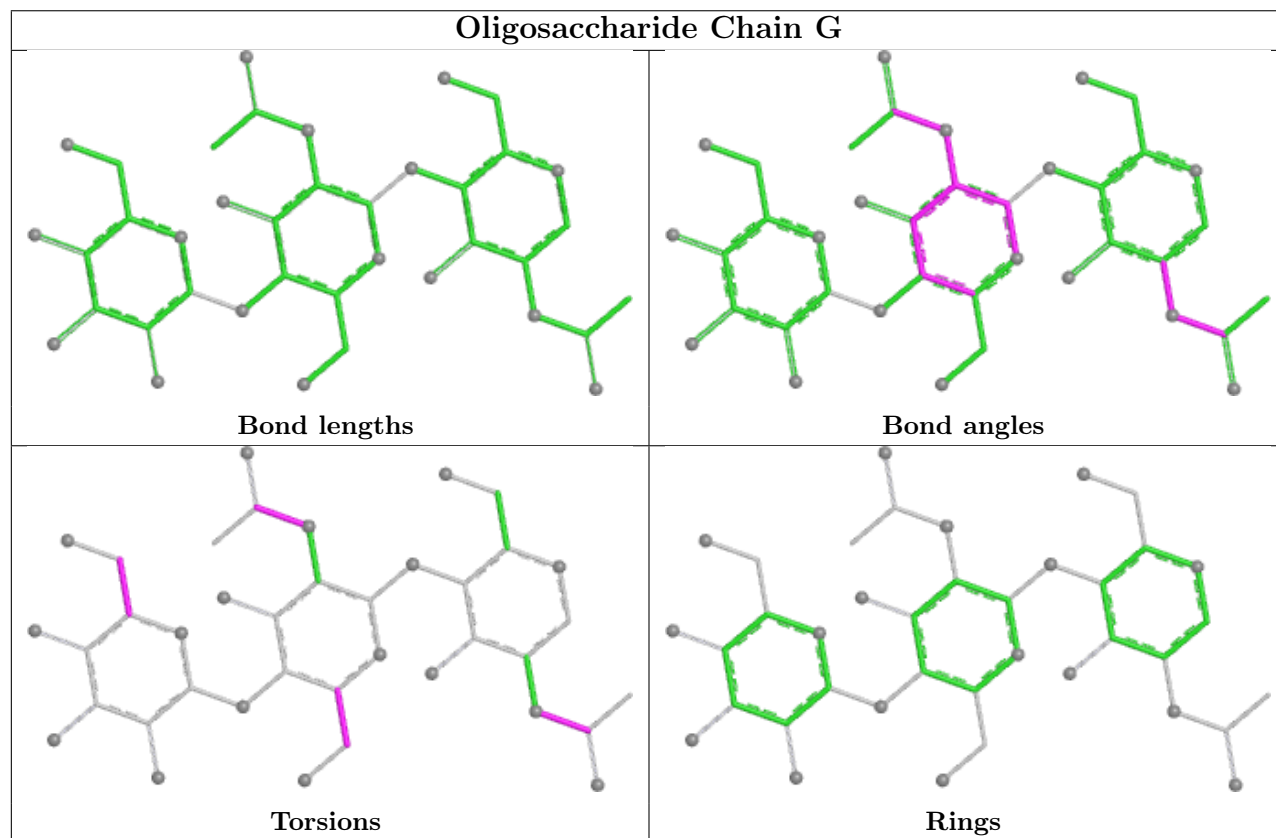
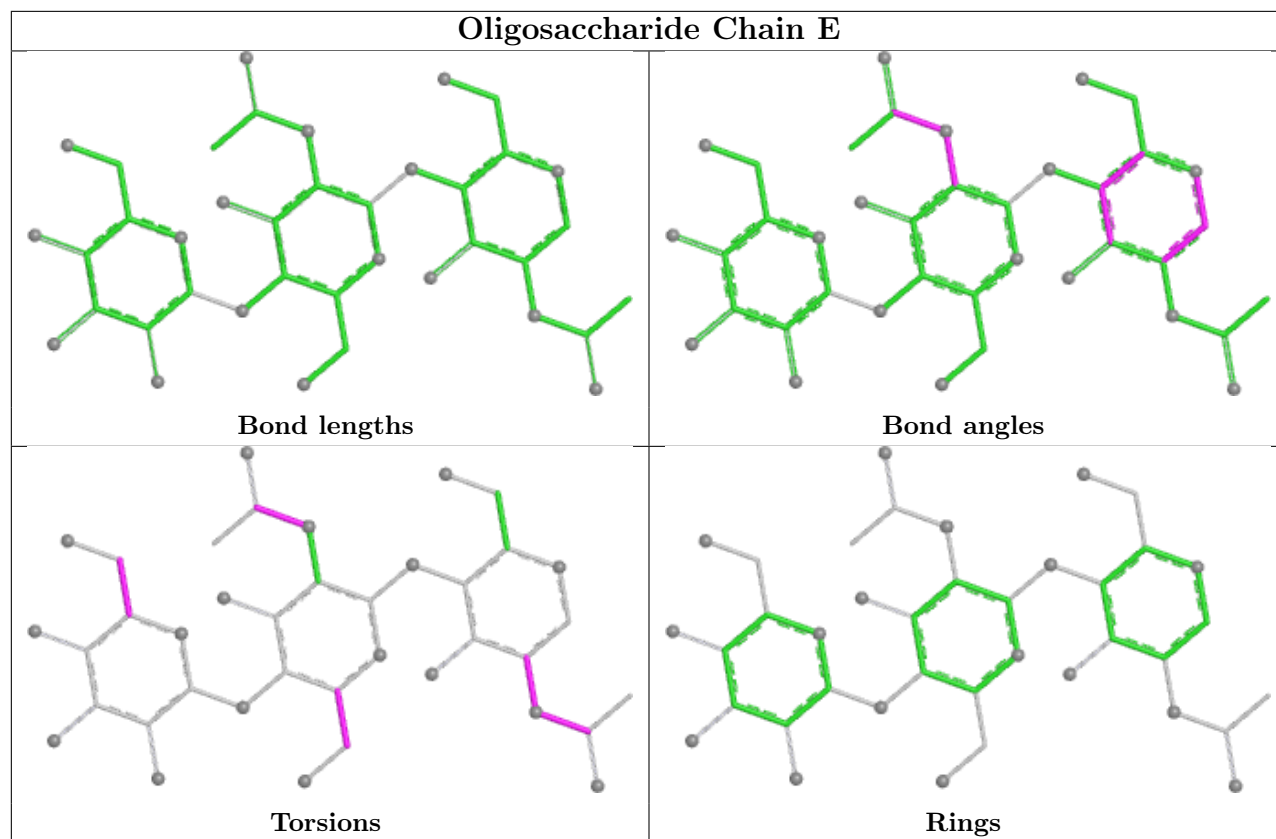
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1	NAG	1	0
7	X	2	NAG	3	0
2	Y	1	NAG	3	0
5	P	2	NAG	2	0
5	O	1	NAG	2	0
2	Q	2	NAG	1	0
2	E	1	NAG	1	0
4	H	3	BMA	6	0
2	K	1	NAG	1	0
5	O	2	NAG	1	0
2	T	3	BMA	2	0
2	Y	3	BMA	2	0
2	Y	2	NAG	2	0
4	H	4	MAN	2	0
6	W	3	MAN	1	0
3	F	3	MAN	1	0
7	X	4	MAN	6	0
2	Z	2	NAG	1	0
6	R	2	NDG	1	0
5	M	2	NAG	1	0
6	L	1	NAG	5	0

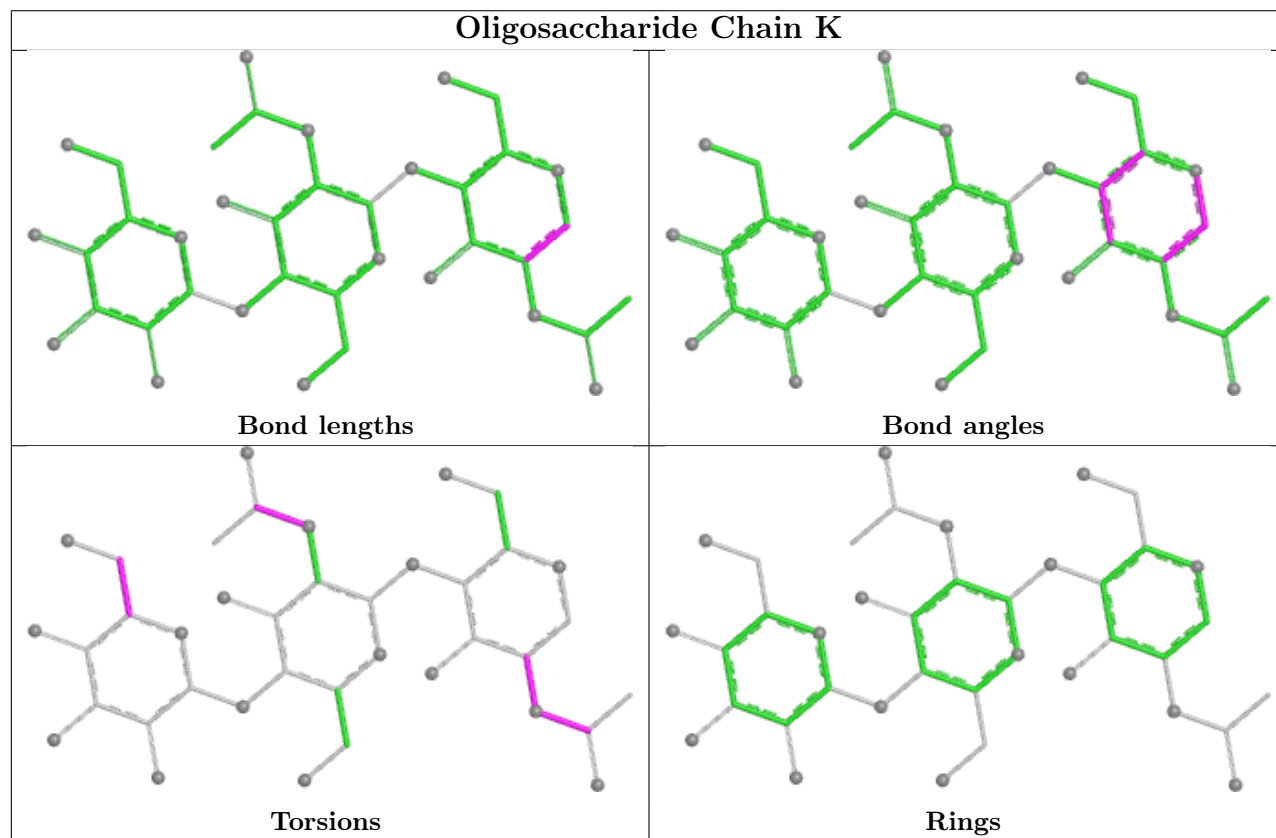
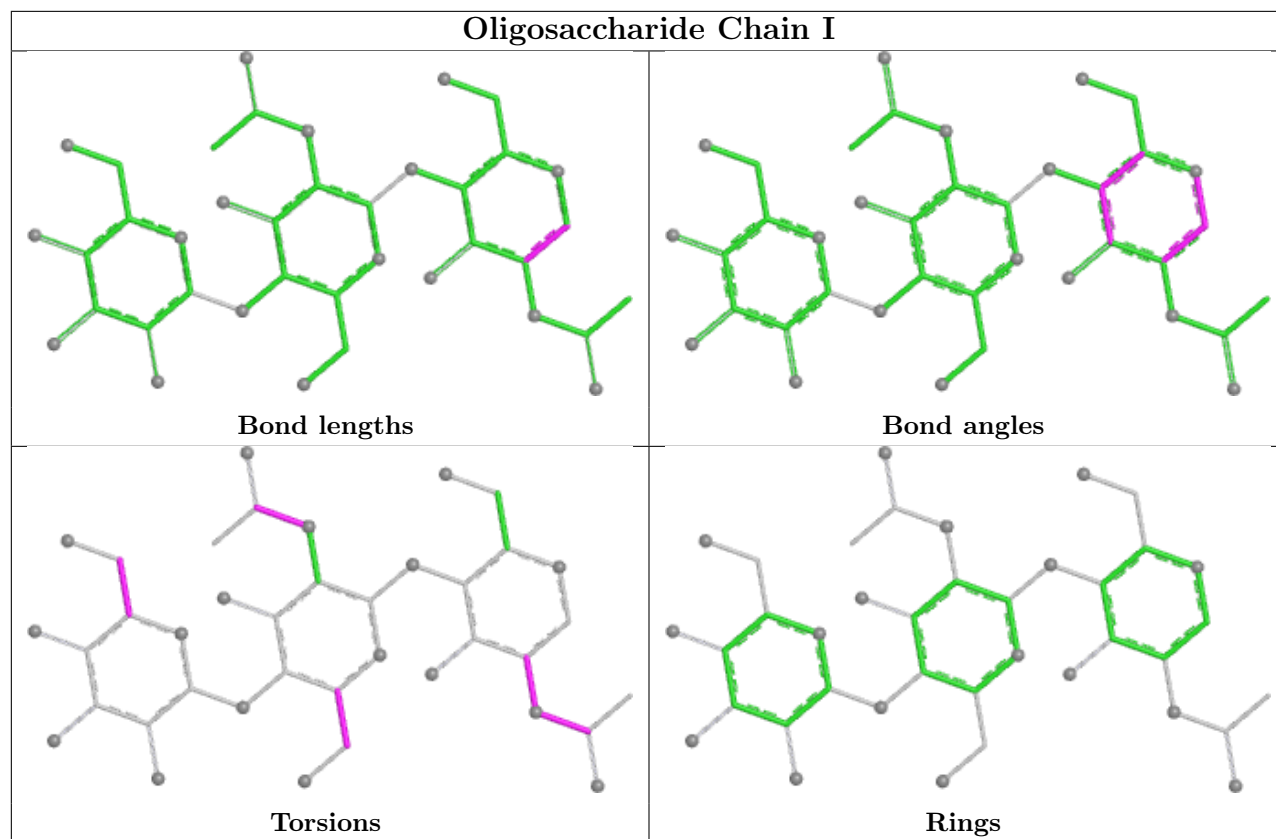
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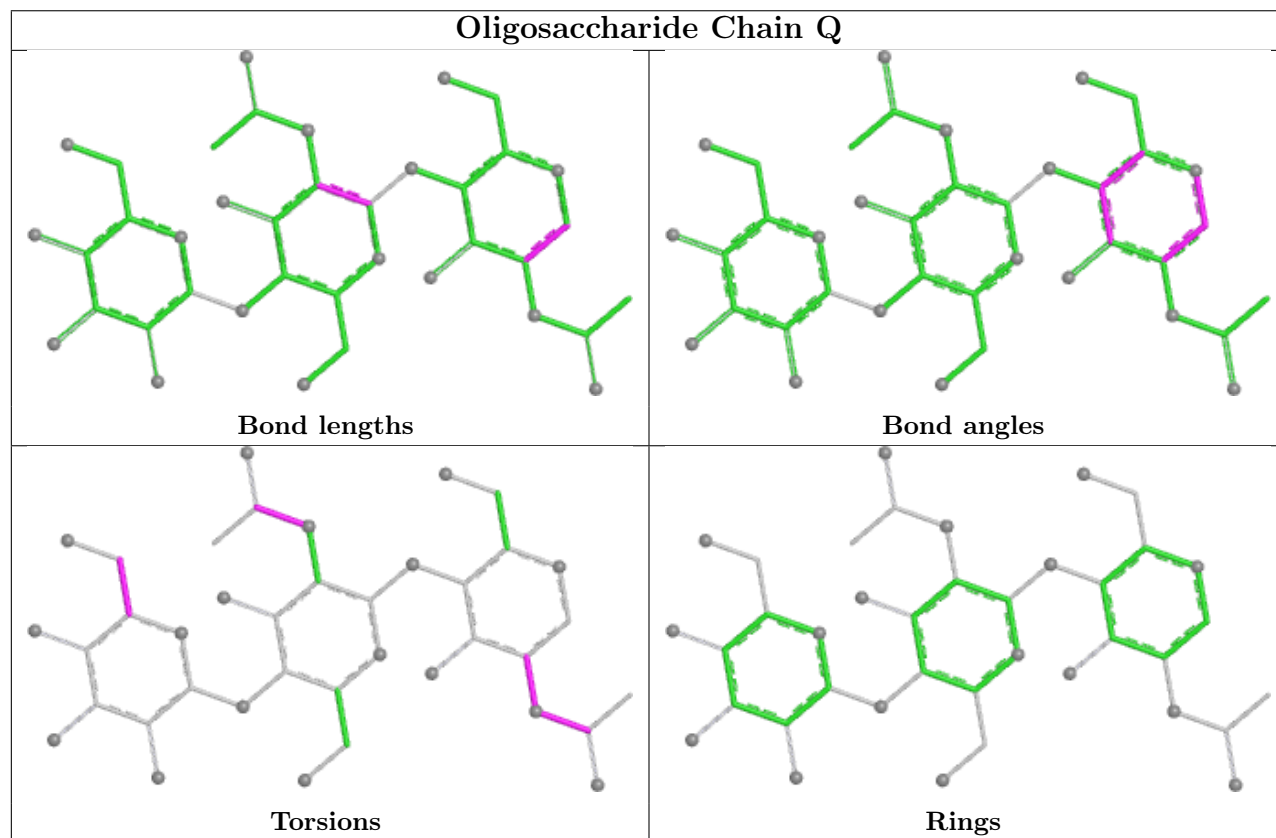
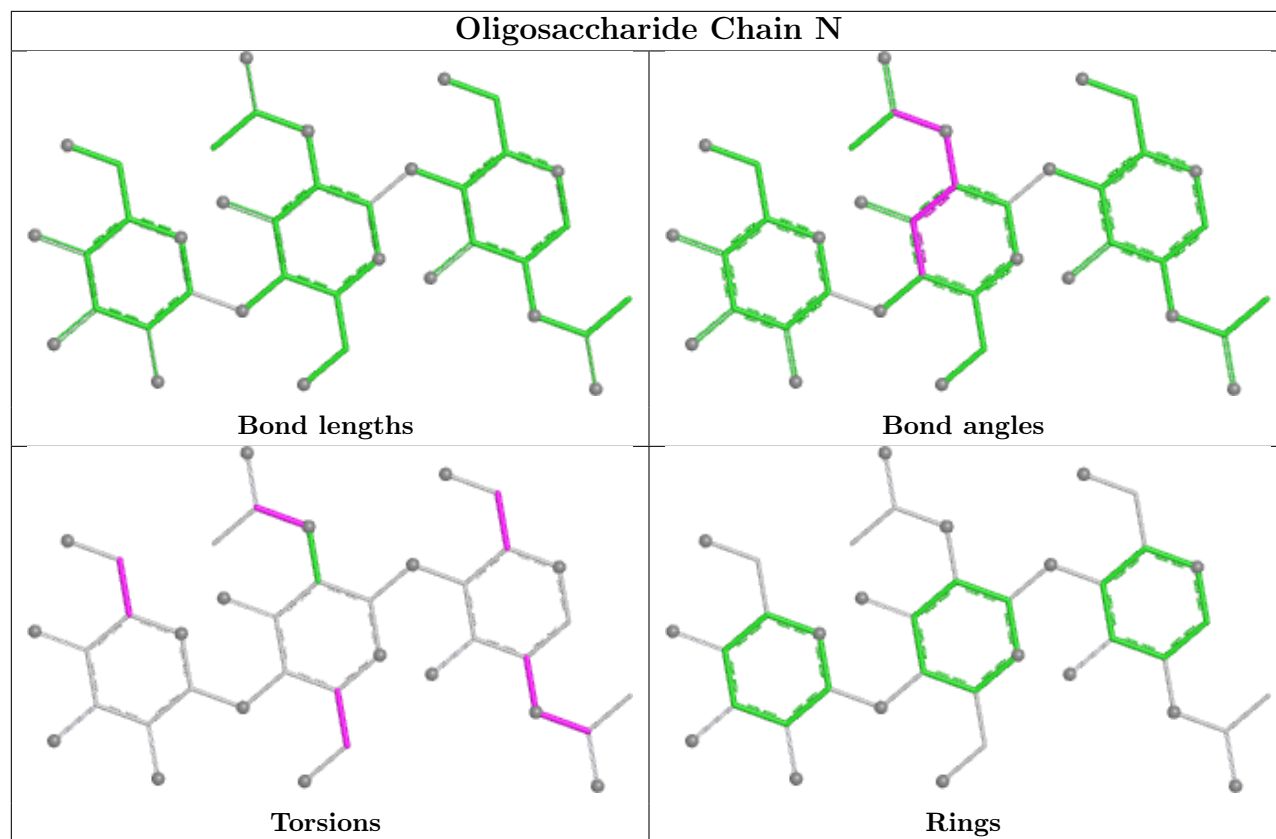
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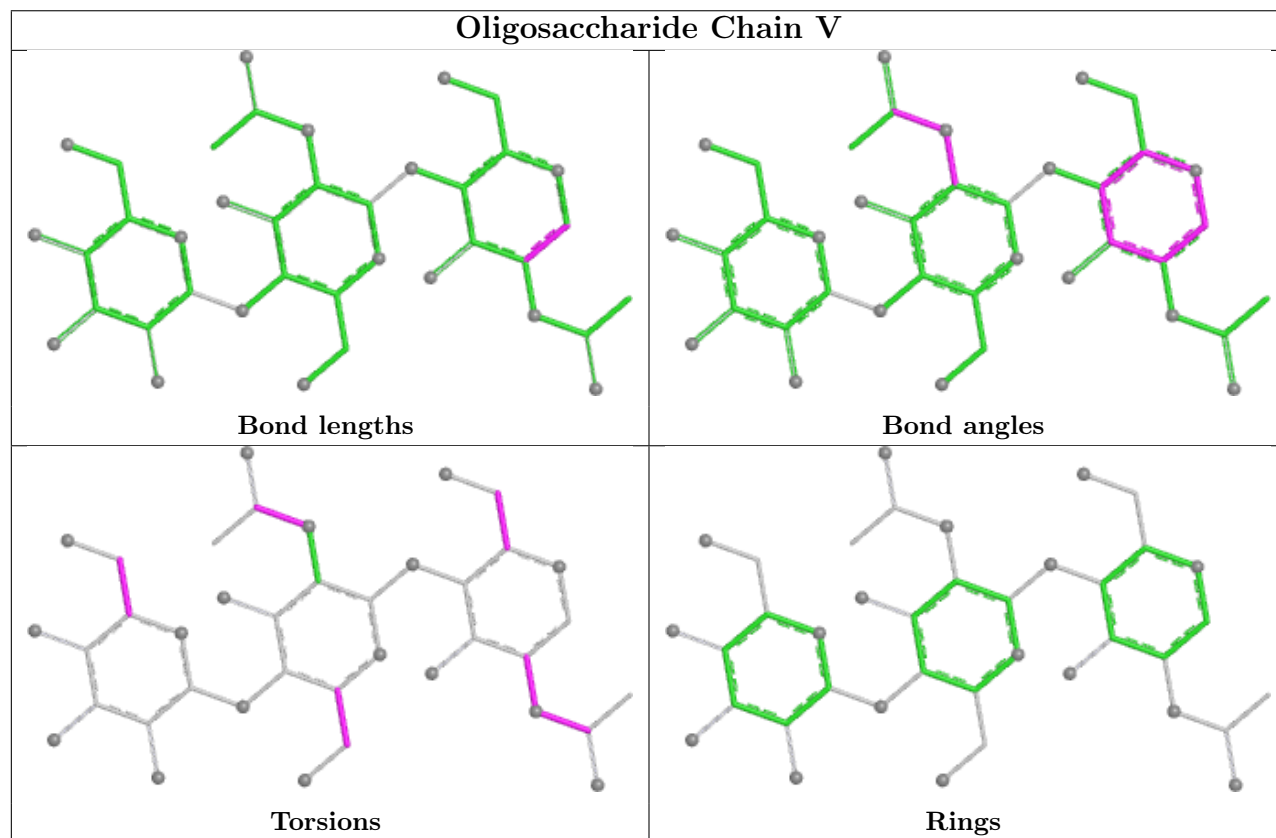
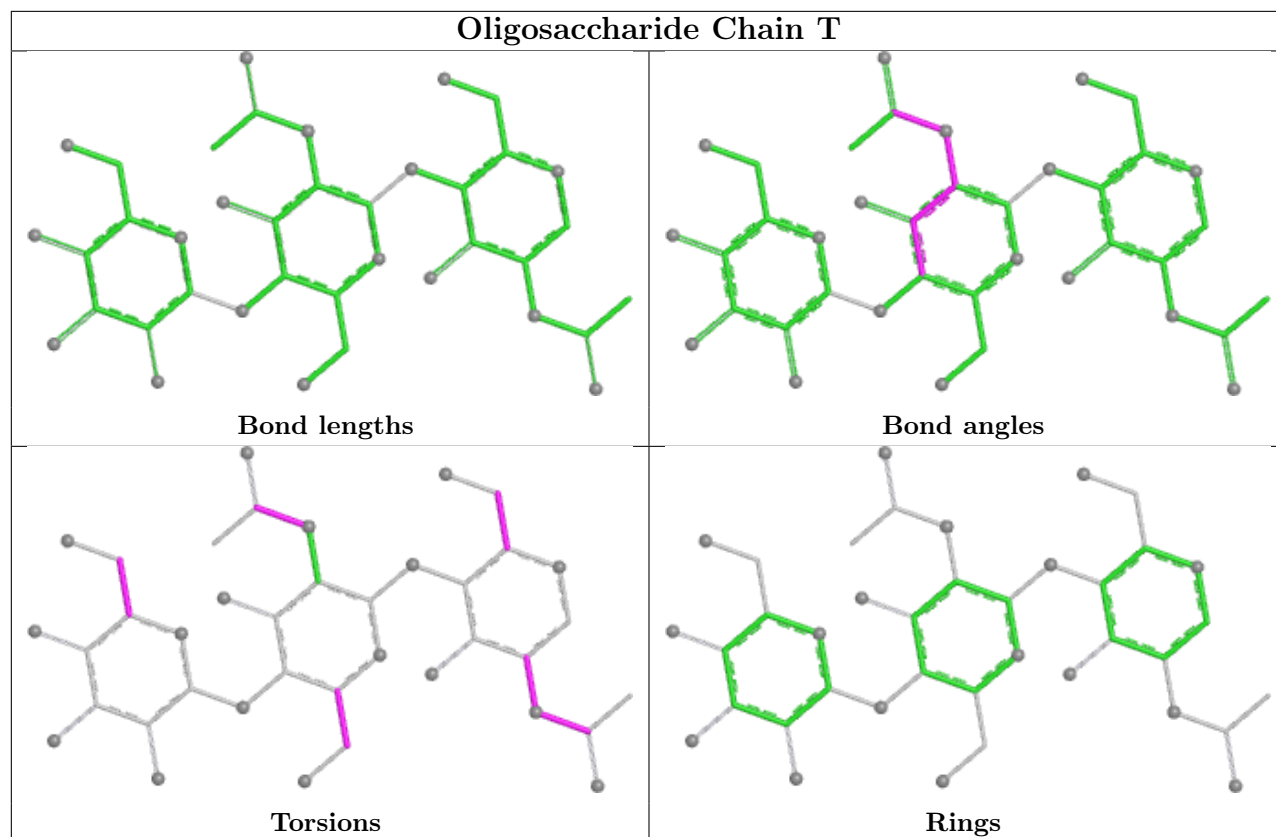
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	4	0
2	N	2	NAG	1	0
6	L	3	MAN	1	0
4	H	2	NAG	5	0
3	F	1	NAG	1	0
2	T	1	NAG	1	0
2	T	2	NAG	2	0
7	X	3	MAN	3	0
6	R	1	NAG	4	0
2	V	2	NAG	3	0
2	N	1	NAG	2	0
3	F	2	NDG	1	0
2	N	3	BMA	1	0
2	I	1	NAG	1	0
2	K	2	NAG	2	0
2	E	2	NAG	2	0
2	Z	1	NAG	2	0
4	H	1	NAG	3	0
5	S	1	NAG	4	0
7	X	1	NAG	4	0
6	W	2	NDG	3	0
2	G	1	NAG	10	0
2	G	2	NAG	8	0
6	W	1	NAG	3	0
6	L	2	NDG	5	0
2	V	1	NAG	2	0
5	S	2	NAG	3	0
5	P	1	NAG	2	0
2	V	3	BMA	1	0

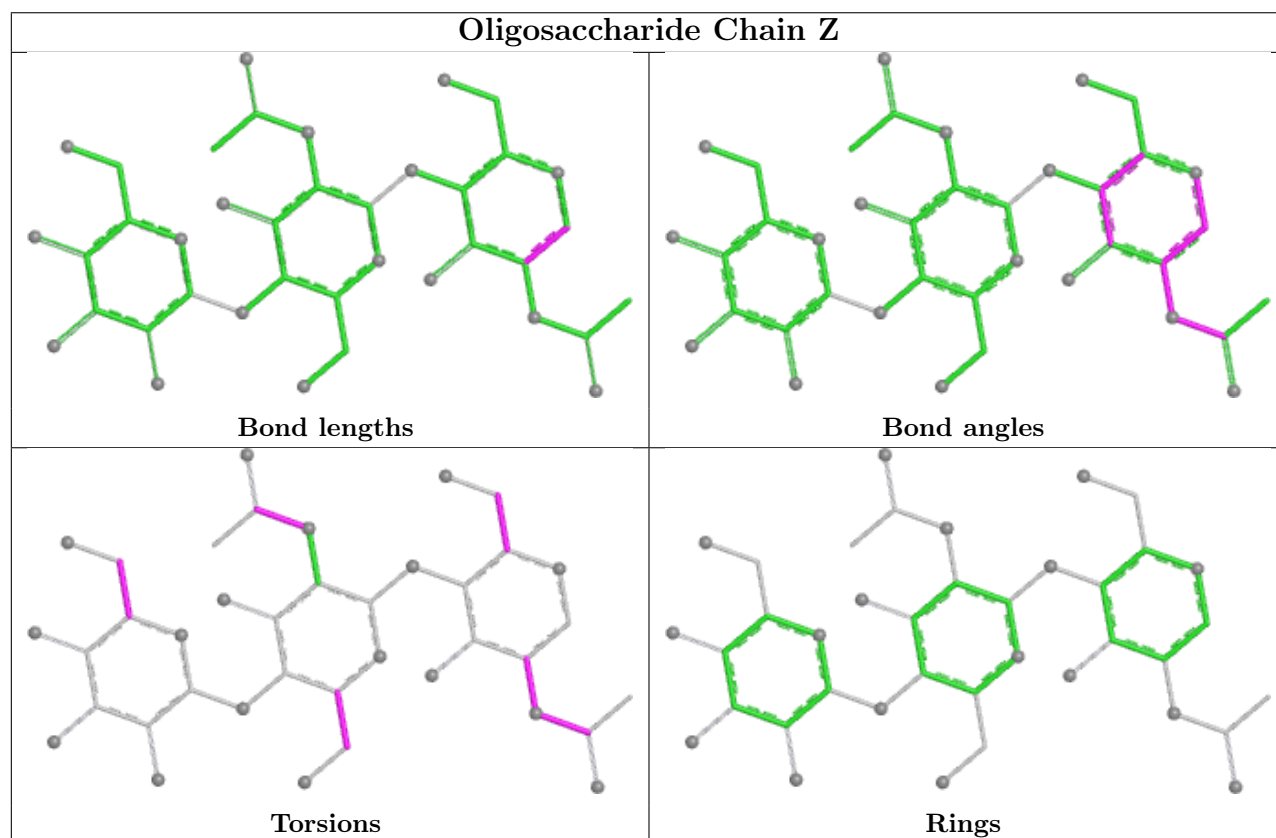
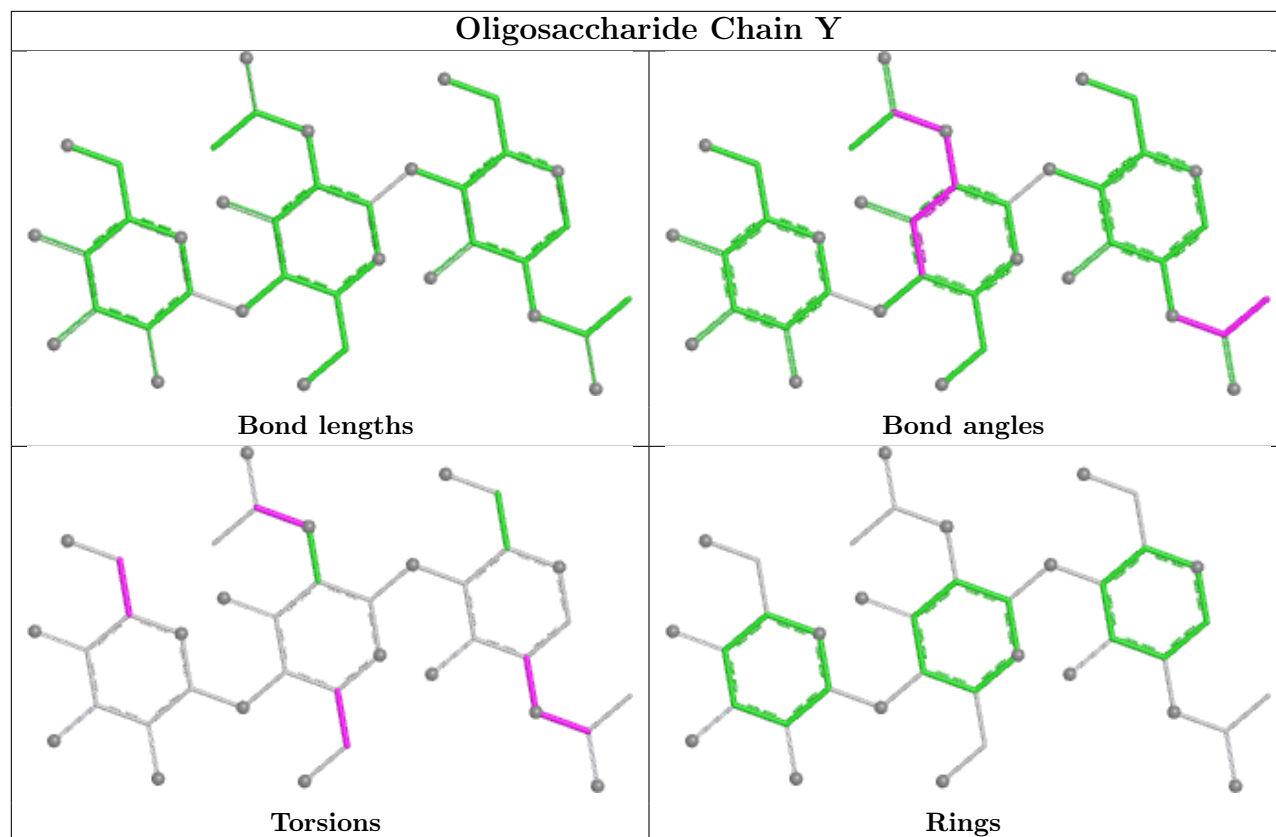
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



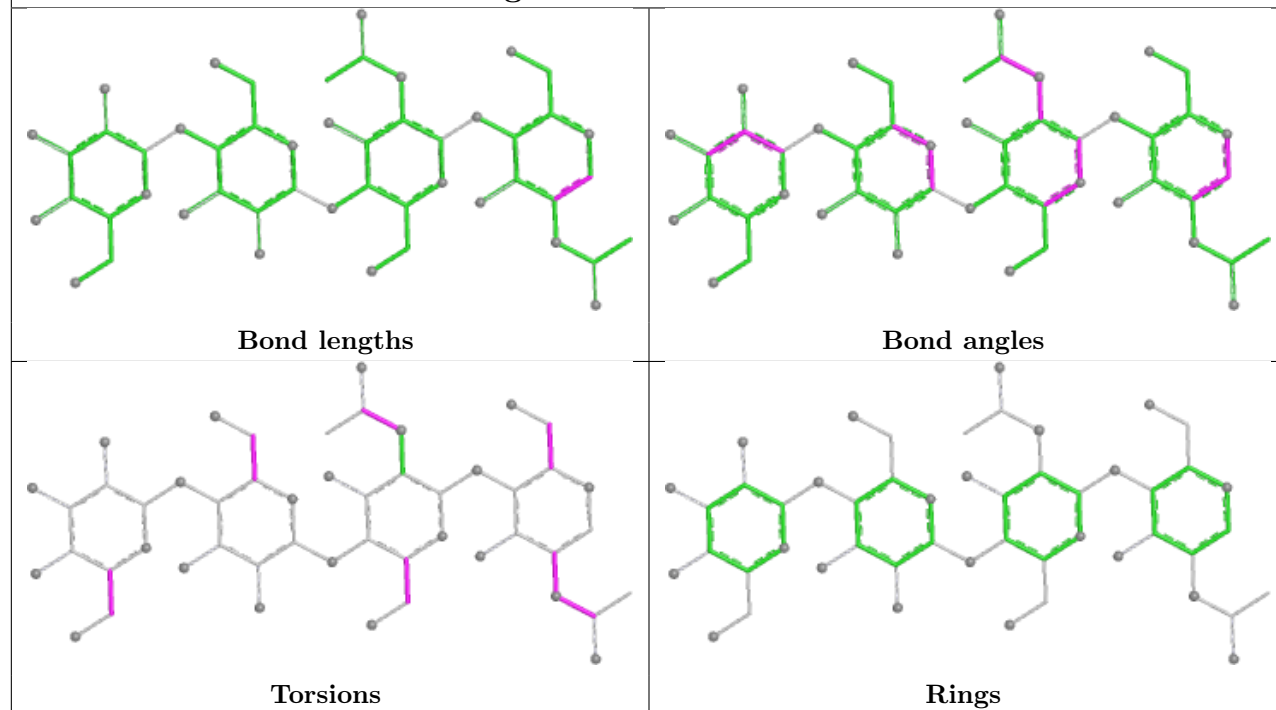




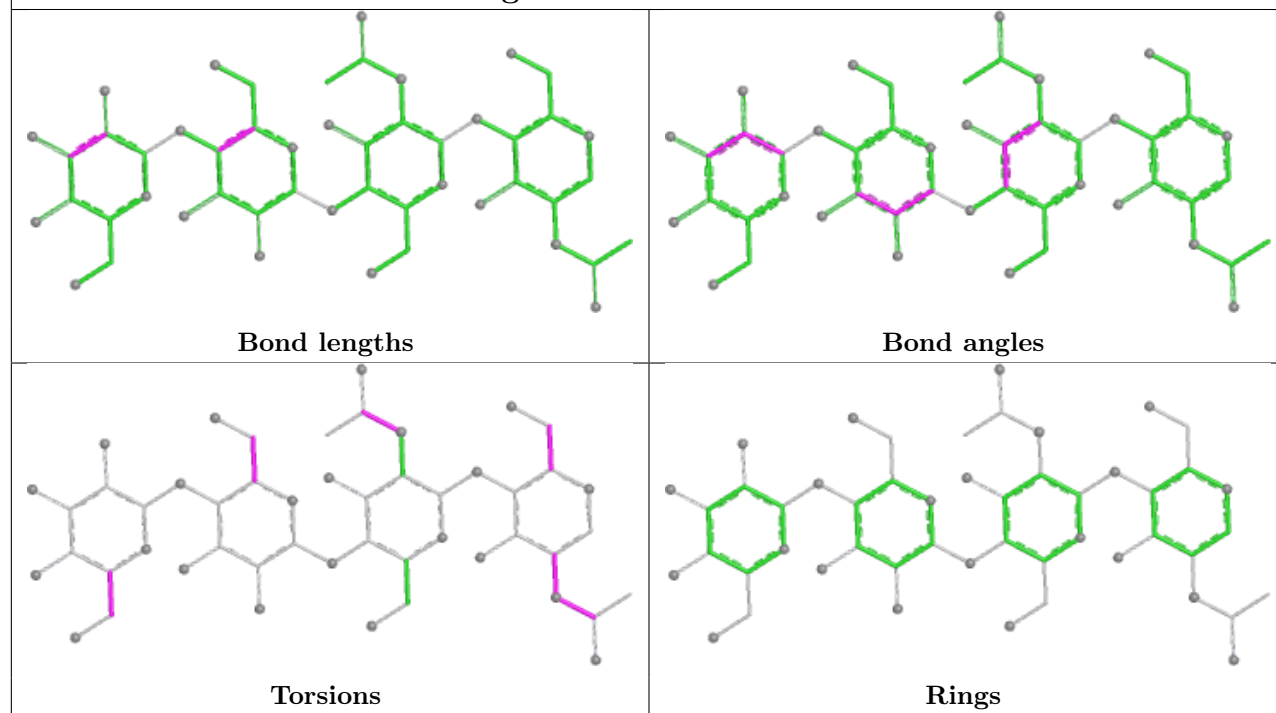


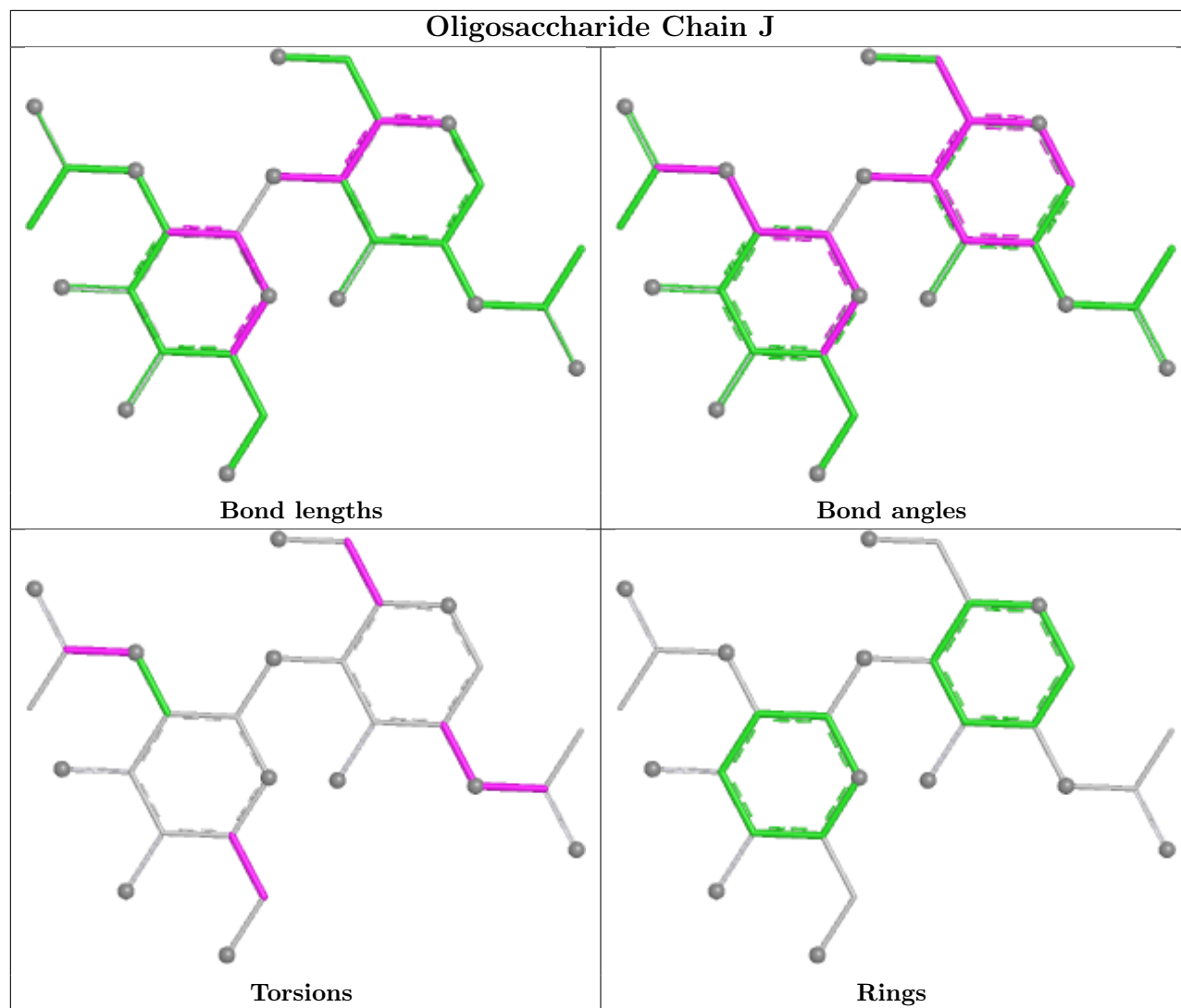


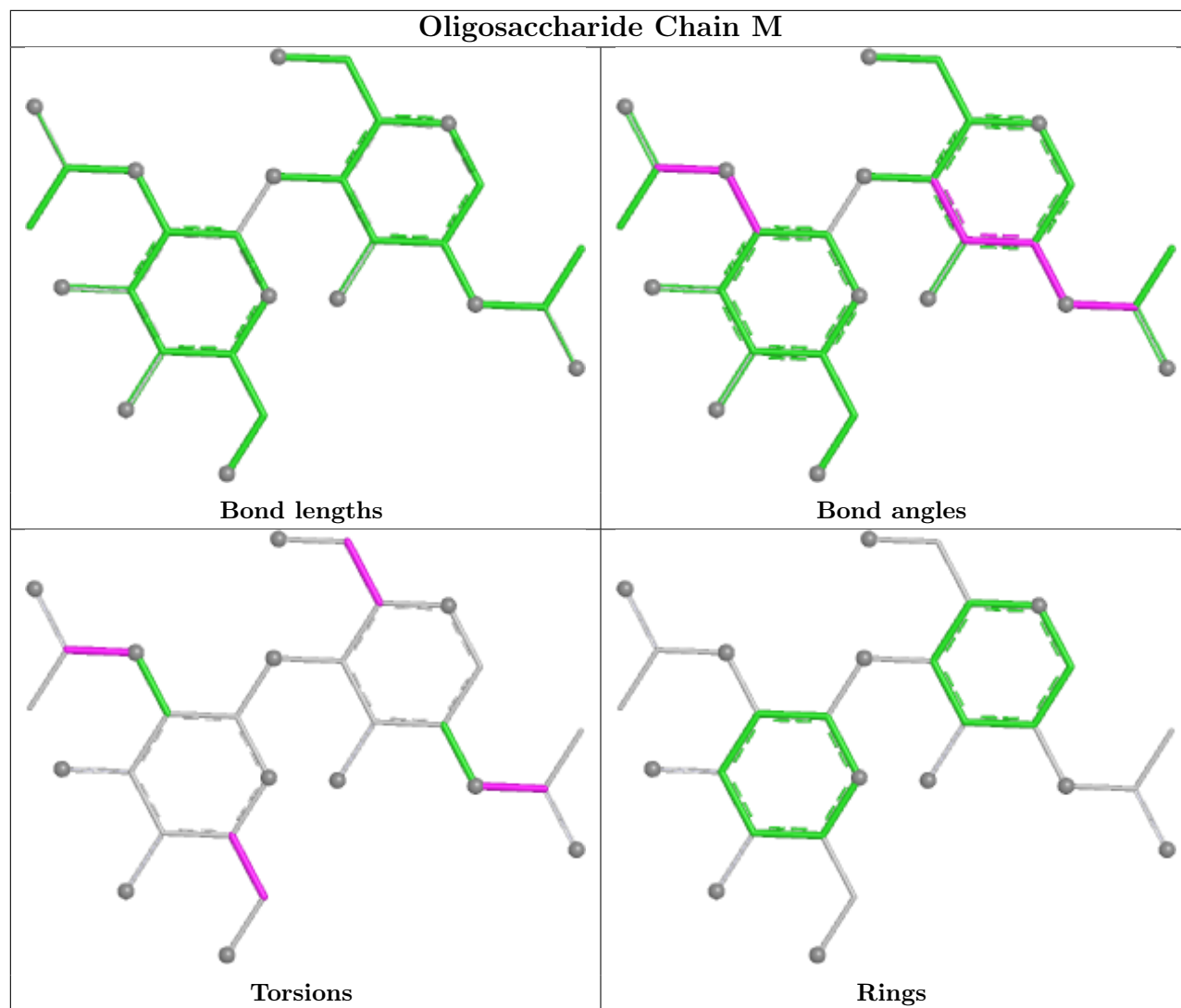
Oligosaccharide Chain F

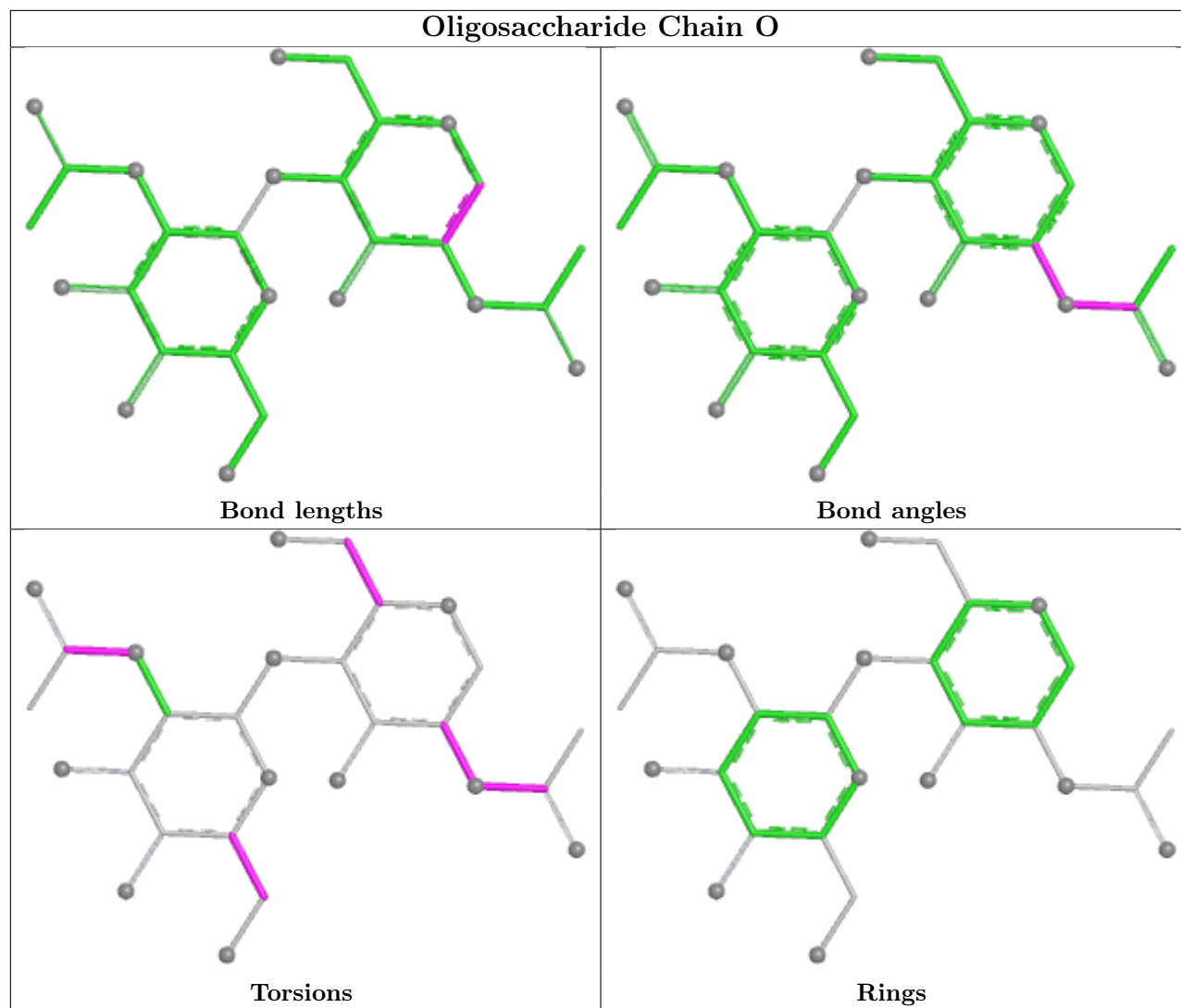


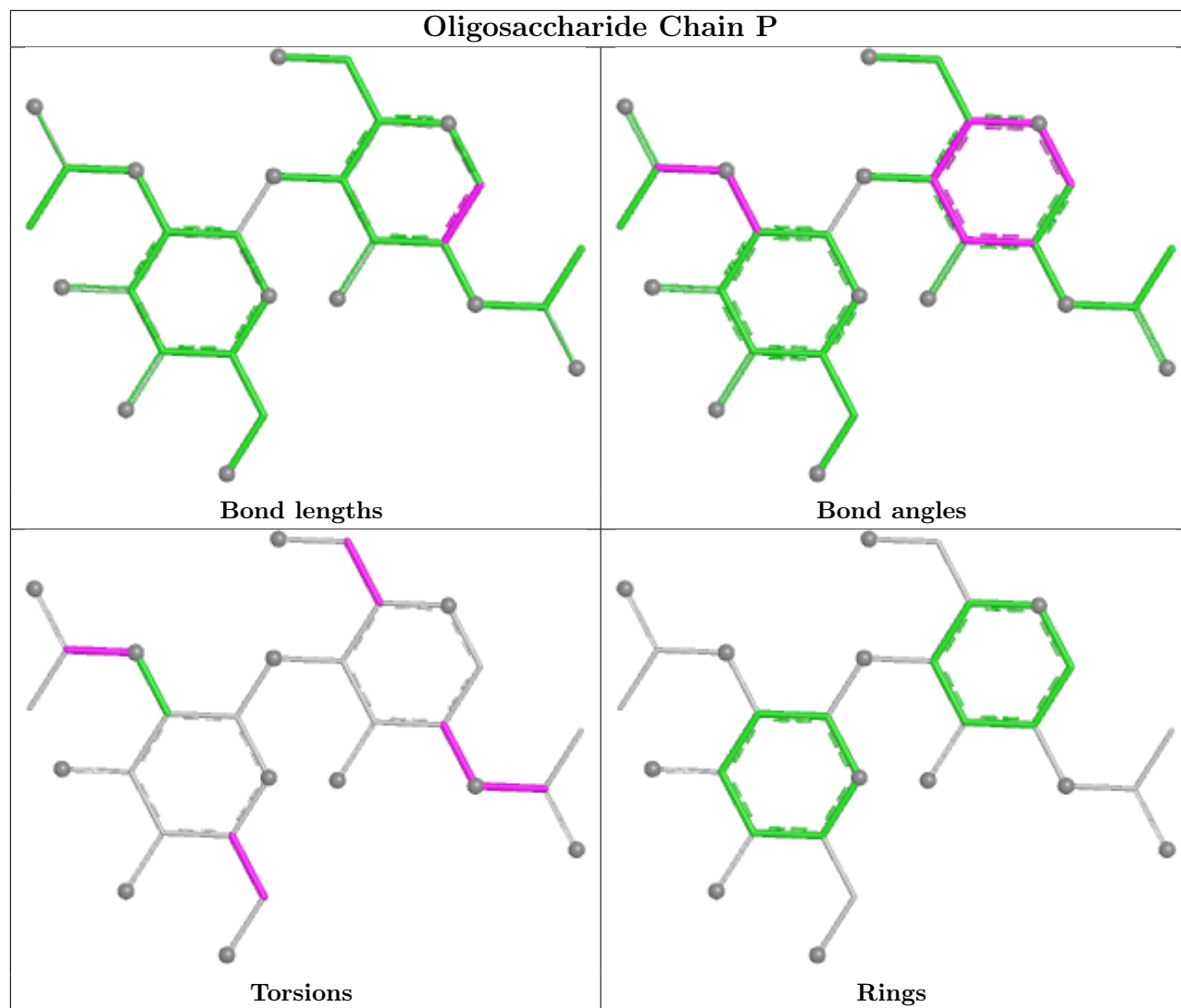
Oligosaccharide Chain H

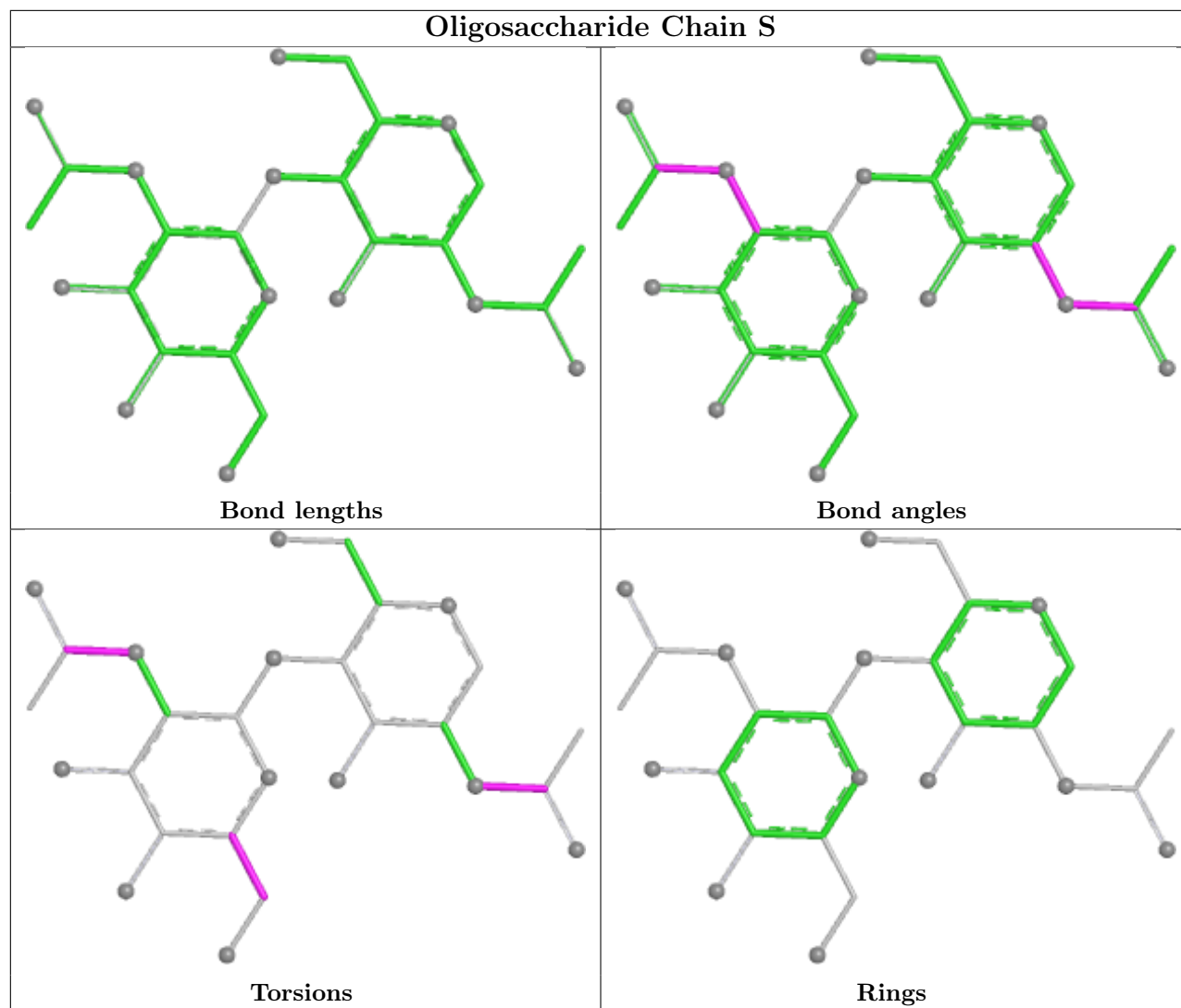


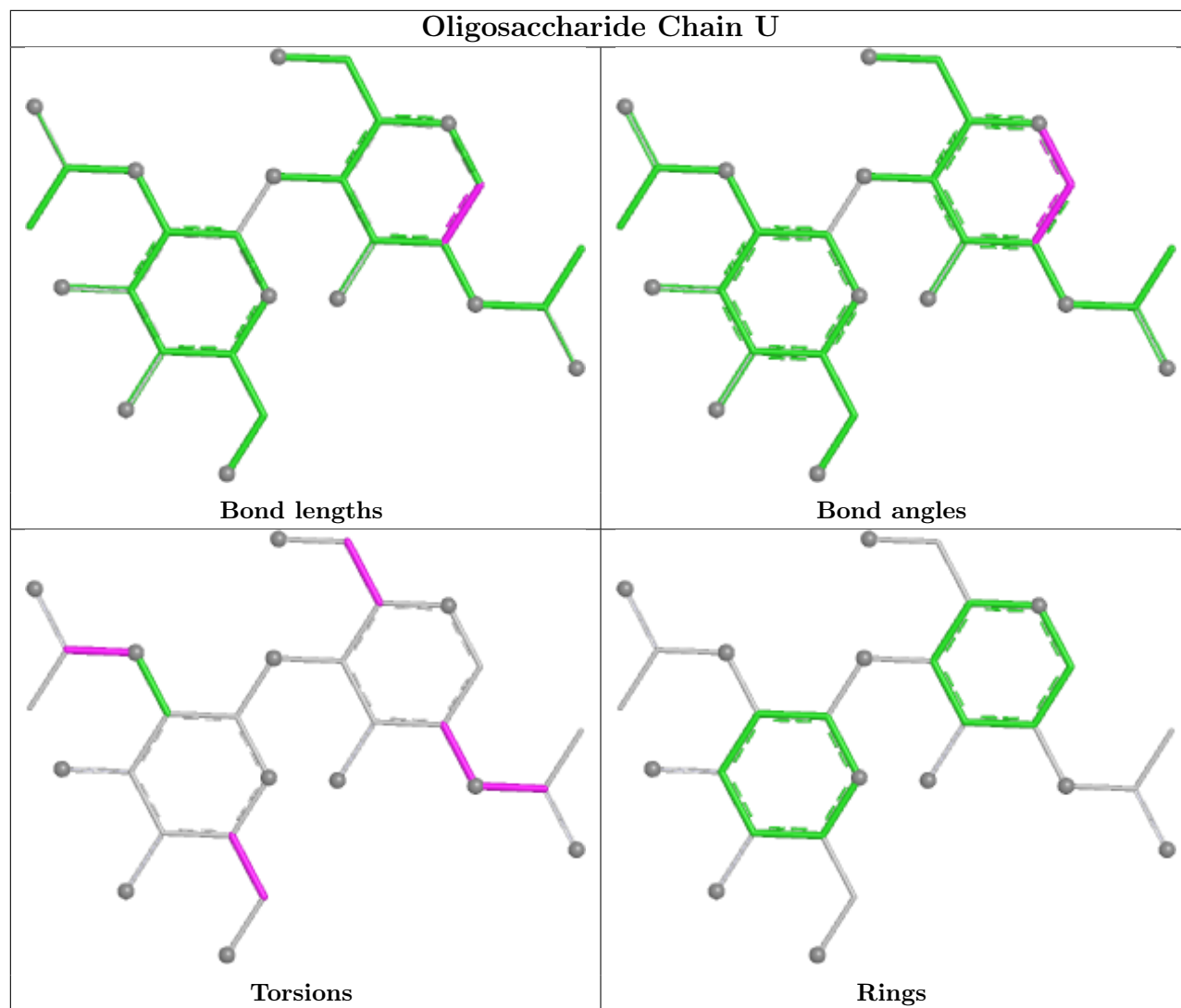


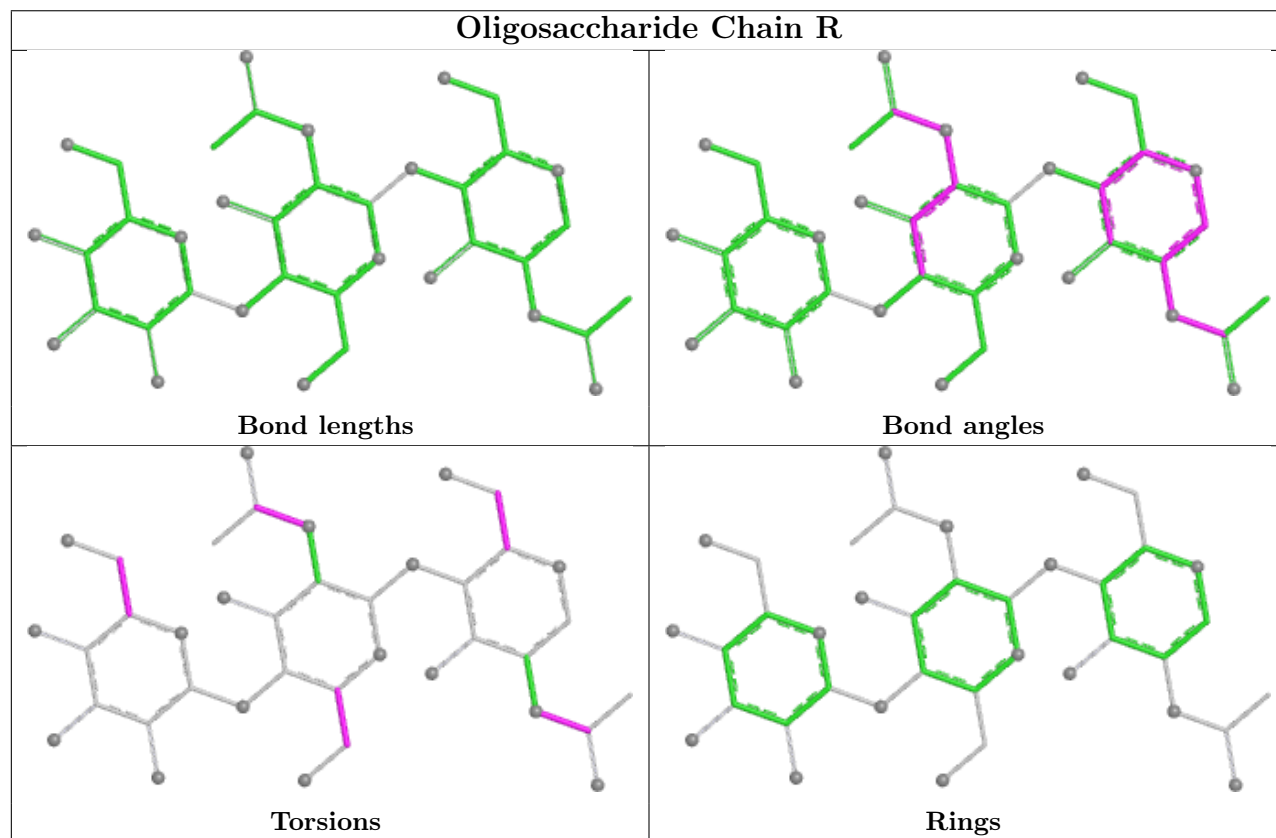
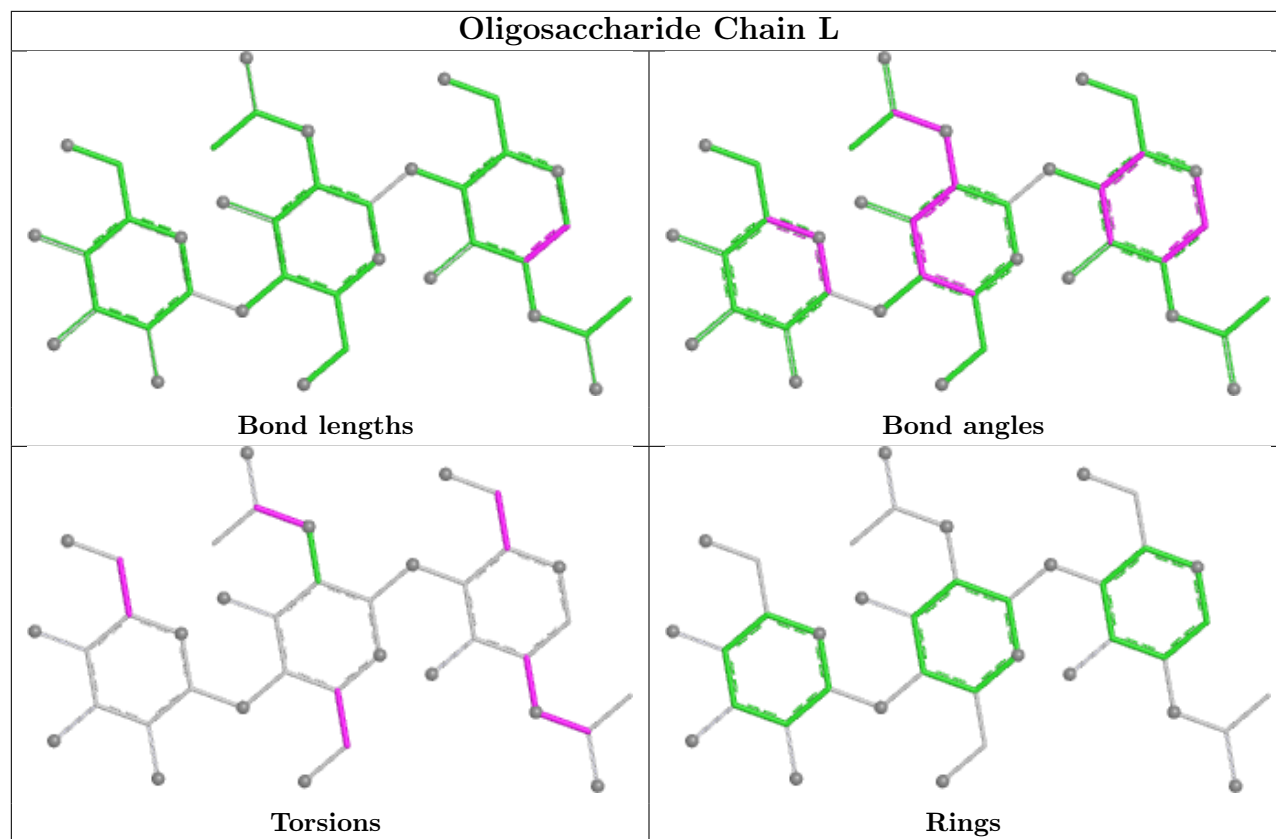


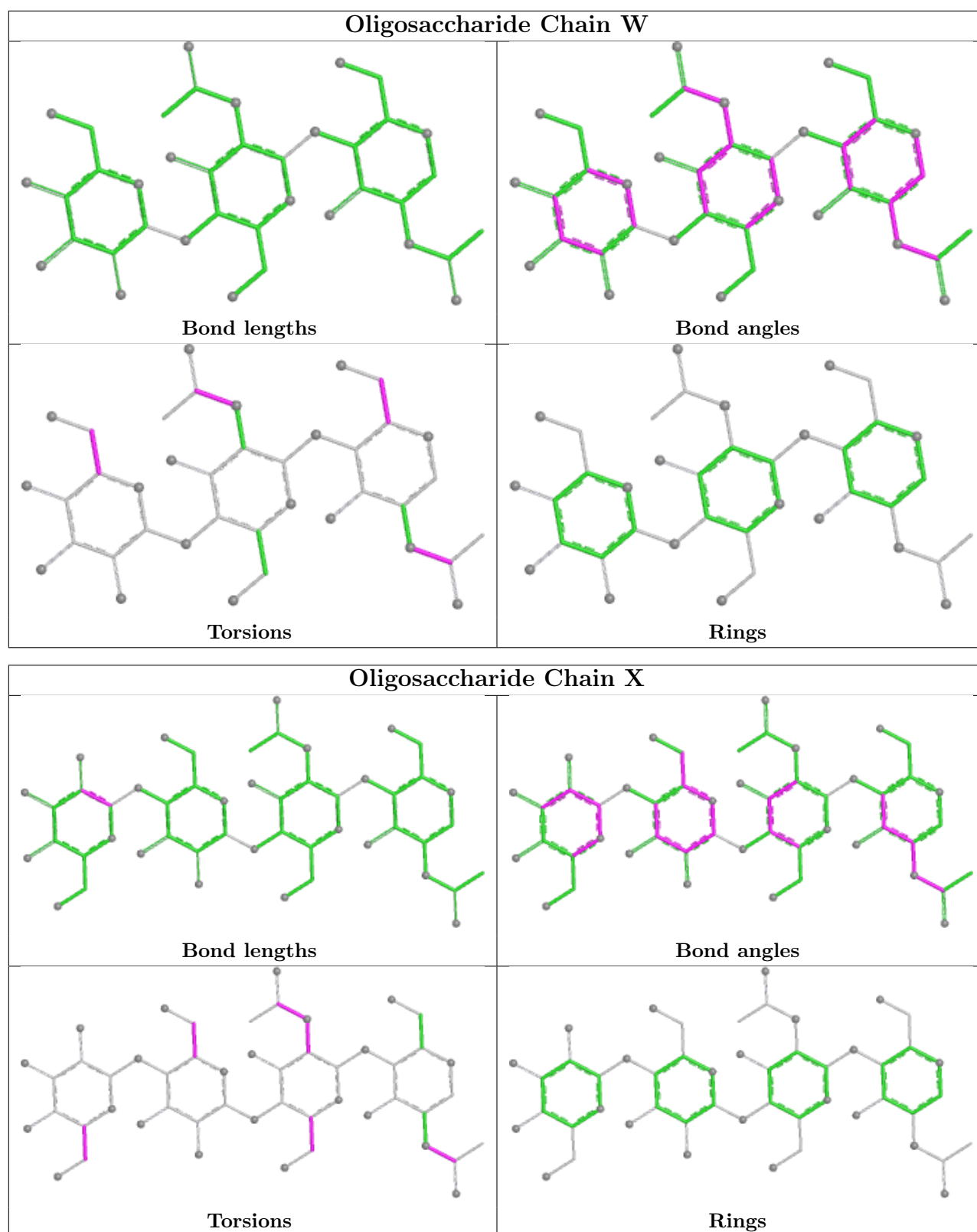












5.6 Ligand geometry ⓘ

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	723/723 (100%)	-1.42	0 100 100	35, 72, 106, 161	0
1	B	723/723 (100%)	-1.41	0 100 100	33, 72, 108, 161	0
1	C	723/723 (100%)	-1.41	0 100 100	32, 71, 106, 162	0
1	D	723/723 (100%)	-1.41	0 100 100	34, 71, 108, 162	0
All	All	2892/2892 (100%)	-1.41	0 100 100	32, 72, 108, 162	0

There are no RSRZ outliers to report.

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
2	BMA	I	3	11/12	0.88	0.09	150,152,153,153	0
2	BMA	E	3	11/12	0.89	0.09	131,135,137,137	0
4	MAN	H	4	11/12	0.90	0.06	146,148,150,150	0
7	MAN	X	4	11/12	0.92	0.06	163,165,166,167	0
3	BMA	F	4	11/12	0.93	0.05	113,116,118,119	0
2	BMA	Q	3	11/12	0.94	0.07	131,134,136,137	0
5	NAG	J	2	14/15	0.94	0.05	125,127,129,129	0
2	NAG	I	2	14/15	0.94	0.06	132,137,141,145	0
5	NAG	J	1	14/15	0.95	0.05	118,120,122,123	0

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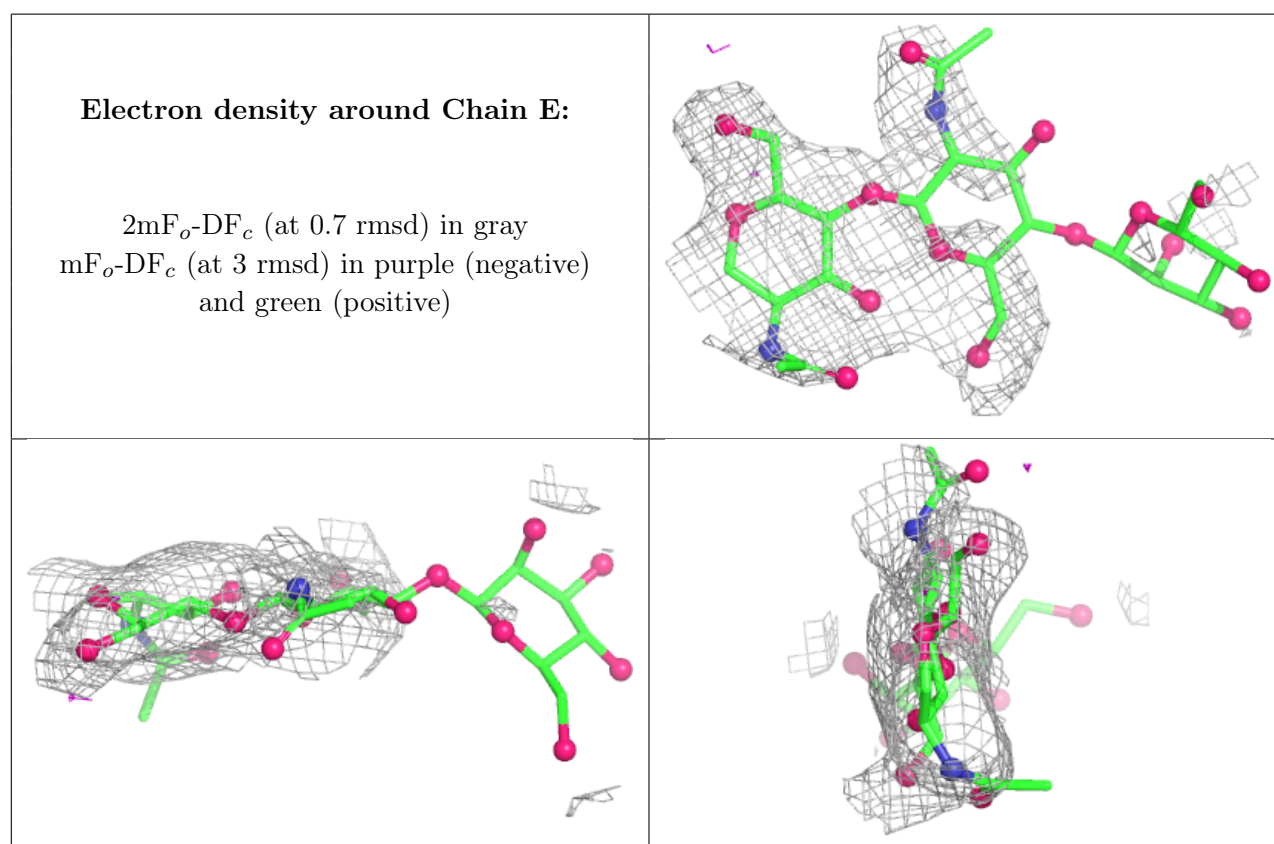
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	1	14/15	0.95	0.05	111,114,117,126	0
5	NAG	P	2	14/15	0.95	0.08	127,137,143,143	0
2	BMA	V	3	11/12	0.95	0.05	124,125,128,128	0
2	NAG	V	2	14/15	0.96	0.06	106,113,115,120	0
2	BMA	K	3	11/12	0.96	0.05	119,126,128,128	0
5	NAG	O	1	14/15	0.96	0.05	119,123,126,131	0
5	NAG	O	2	14/15	0.96	0.06	134,137,139,140	0
2	NAG	G	2	14/15	0.96	0.04	122,126,130,133	0
5	NAG	U	2	14/15	0.96	0.06	127,128,129,129	0
6	NDG	L	2	14/15	0.96	0.06	113,118,125,126	0
6	MAN	W	3	11/12	0.96	0.04	110,113,115,116	0
7	NAG	X	2	14/15	0.96	0.07	123,131,134,143	0
7	MAN	X	3	11/12	0.96	0.05	150,154,156,160	0
2	BMA	T	3	11/12	0.96	0.04	132,135,136,136	0
4	NAG	H	2	14/15	0.97	0.05	108,112,120,128	0
4	BMA	H	3	11/12	0.97	0.04	135,138,141,145	0
2	NAG	T	2	14/15	0.97	0.07	112,117,123,127	0
2	BMA	G	3	11/12	0.97	0.04	136,137,138,138	0
2	BMA	N	3	11/12	0.97	0.05	125,129,131,131	0
5	NAG	M	1	14/15	0.97	0.05	75,86,97,98	0
5	NAG	M	2	14/15	0.97	0.05	105,111,113,113	0
2	NAG	Q	2	14/15	0.97	0.05	103,113,117,124	0
2	NAG	Y	1	14/15	0.97	0.06	84,88,93,102	0
5	NAG	P	1	14/15	0.97	0.08	109,120,124,129	0
2	NAG	Y	2	14/15	0.97	0.04	109,118,122,130	0
5	NAG	S	2	14/15	0.97	0.05	108,111,115,117	0
5	NAG	U	1	14/15	0.97	0.05	109,118,121,123	0
2	BMA	Y	3	11/12	0.97	0.05	133,137,139,139	0
2	NAG	Z	1	14/15	0.97	0.05	113,118,122,129	0
6	MAN	L	3	11/12	0.97	0.05	129,132,133,134	0
6	MAN	R	3	11/12	0.97	0.04	125,127,128,130	0
6	NDG	W	2	14/15	0.97	0.06	104,109,110,112	0
2	NAG	Z	2	14/15	0.97	0.07	133,135,138,142	0
2	BMA	Z	3	11/12	0.97	0.04	144,146,148,148	0
3	MAN	F	3	11/12	0.97	0.04	103,108,110,111	0
2	NAG	E	2	14/15	0.97	0.05	104,111,118,126	0
2	NAG	E	1	14/15	0.98	0.06	52,71,76,91	0
3	NAG	F	1	14/15	0.98	0.06	86,91,98,99	0
3	NDG	F	2	14/15	0.98	0.03	86,94,99,103	0
6	NDG	R	2	14/15	0.98	0.05	102,110,118,119	0
2	NAG	K	2	14/15	0.98	0.04	107,115,119,123	0
6	NAG	W	1	14/15	0.98	0.05	93,96,100,101	0

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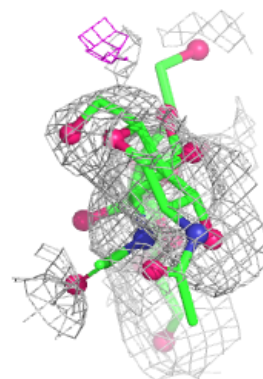
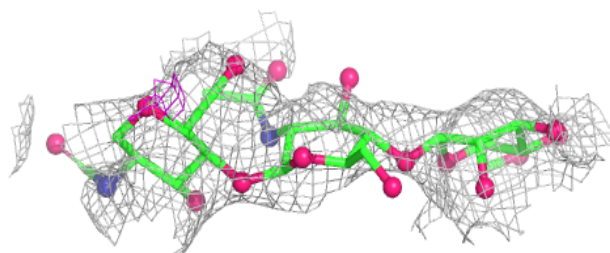
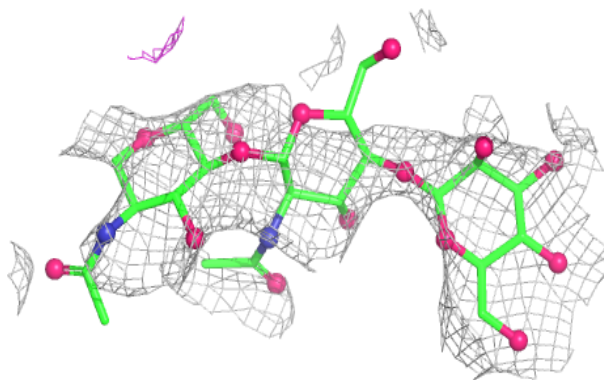
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	1	14/15	0.98	0.06	98,105,111,117	0
2	NAG	T	1	14/15	0.98	0.06	87,92,97,104	0
7	NAG	X	1	14/15	0.98	0.04	84,87,95,111	0
2	NAG	N	1	14/15	0.98	0.06	83,87,92,97	0
2	NAG	N	2	14/15	0.98	0.03	96,104,110,119	0
2	NAG	V	1	14/15	0.98	0.05	72,79,85,97	0
5	NAG	S	1	14/15	0.99	0.04	92,97,102,105	0
4	NAG	H	1	14/15	0.99	0.04	77,84,93,100	0
6	NAG	R	1	14/15	0.99	0.03	82,92,94,100	0
2	NAG	K	1	14/15	0.99	0.03	69,84,90,101	0
2	NAG	Q	1	14/15	0.99	0.06	69,77,81,95	0
6	NAG	L	1	14/15	0.99	0.04	98,101,104,109	0

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

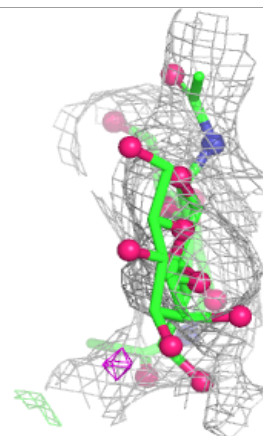
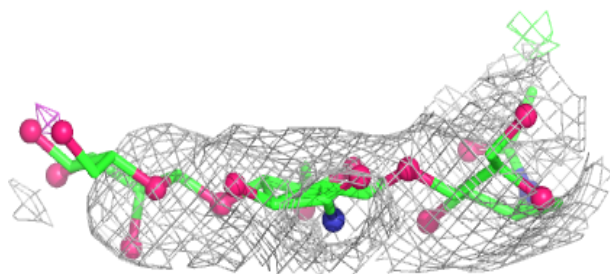
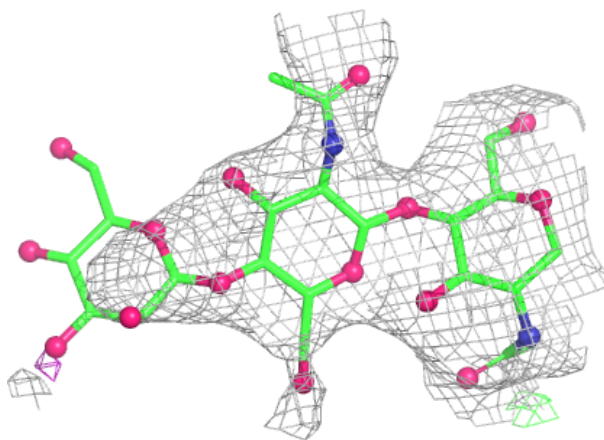


Electron density around Chain G:

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

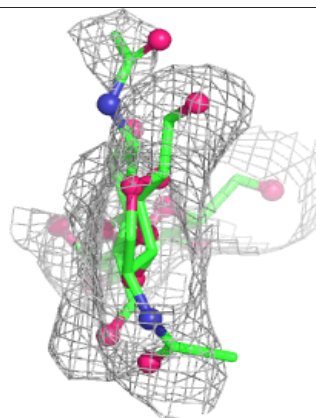
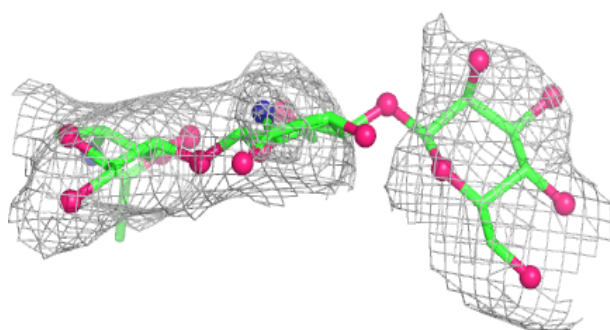
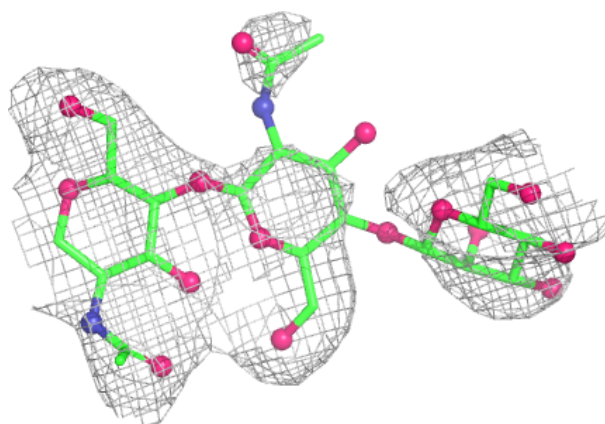
**Electron density around Chain I:**

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

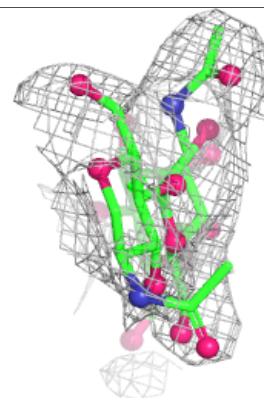
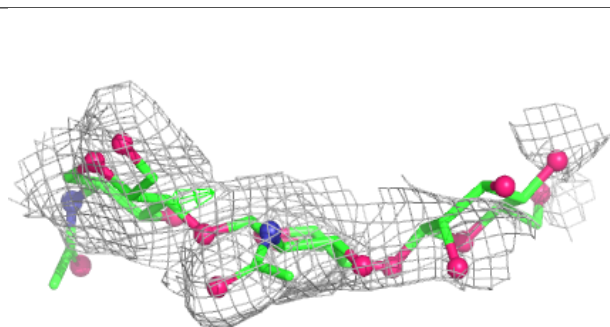
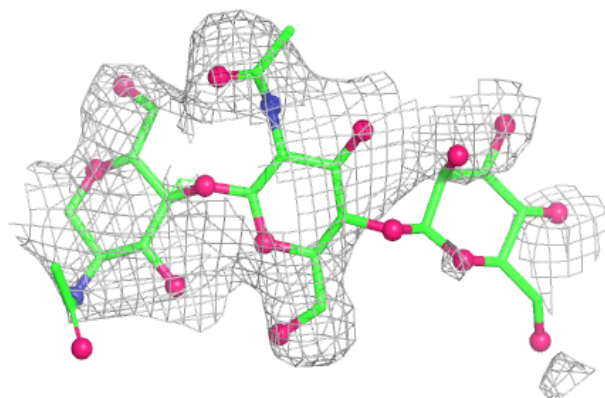


Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

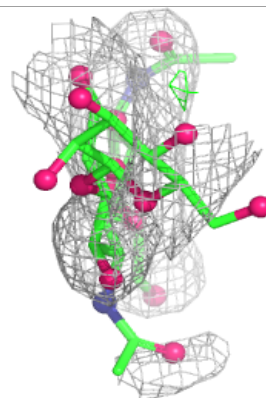
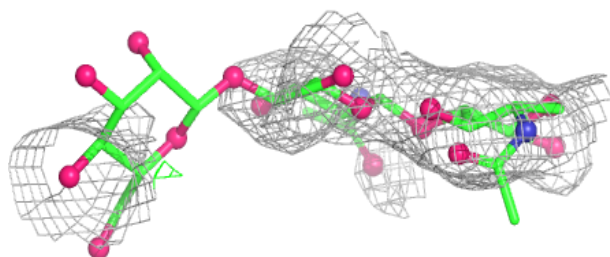
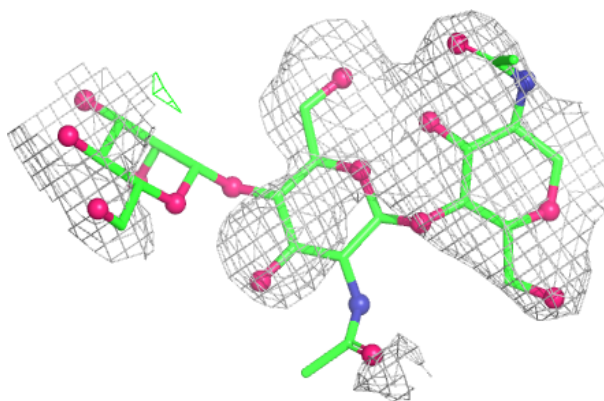
**Electron density around Chain N:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

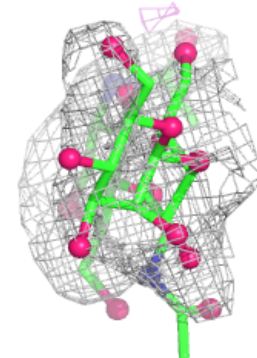
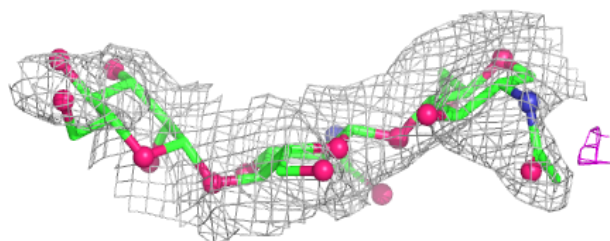
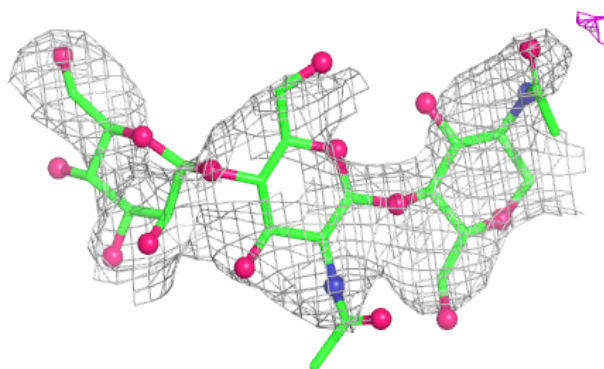


Electron density around Chain Q:

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

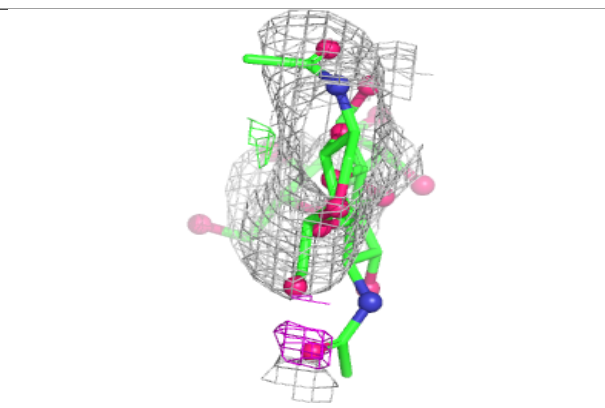
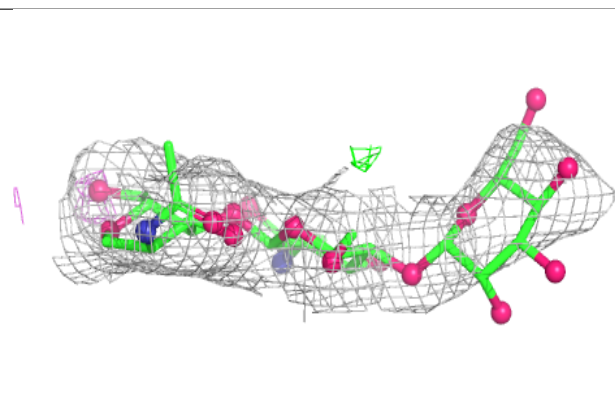
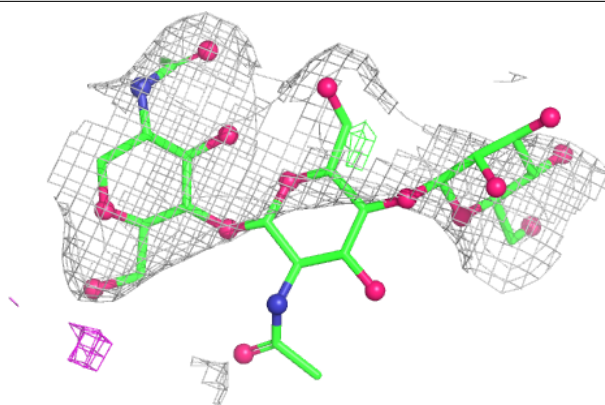
**Electron density around Chain T:**

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

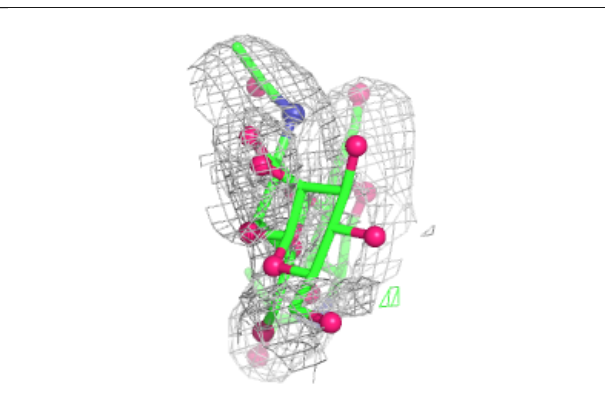
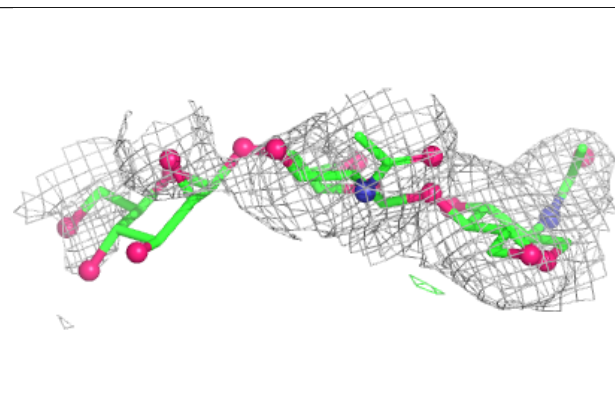
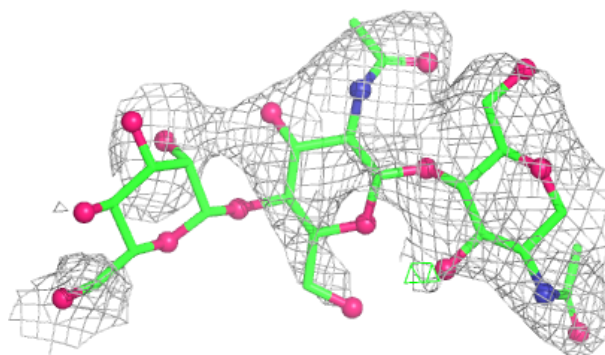


Electron density around Chain V:

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

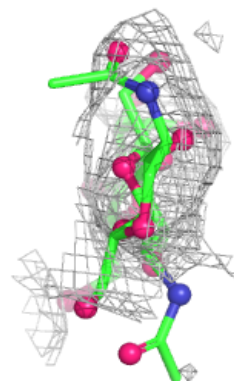
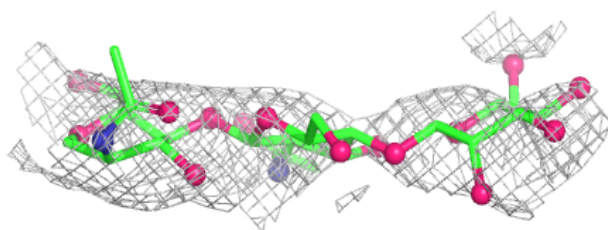
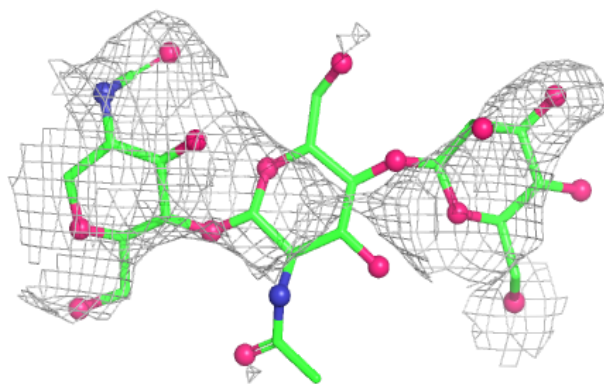
**Electron density around Chain Y:**

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

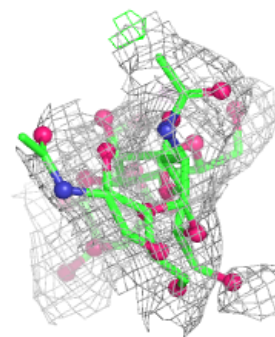
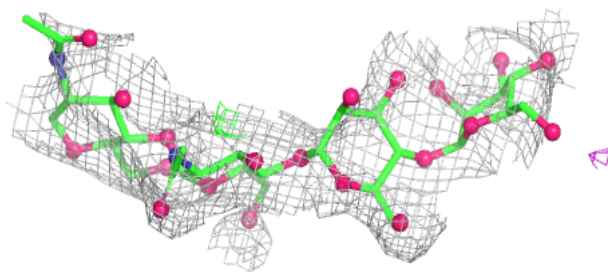
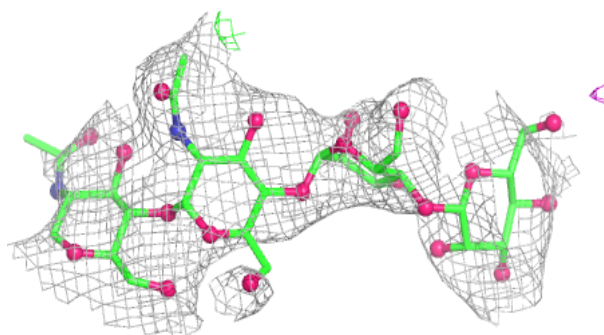


Electron density around Chain Z:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

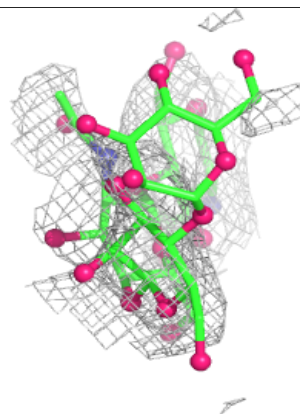
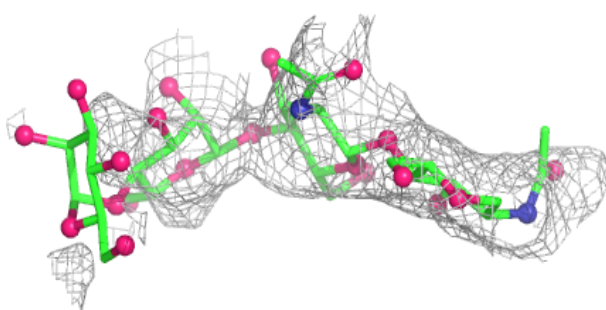
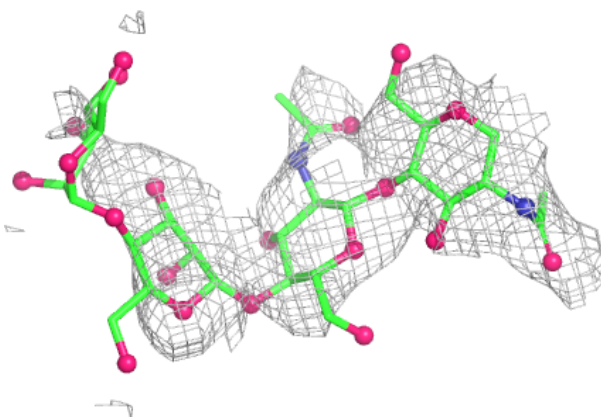
**Electron density around Chain F:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



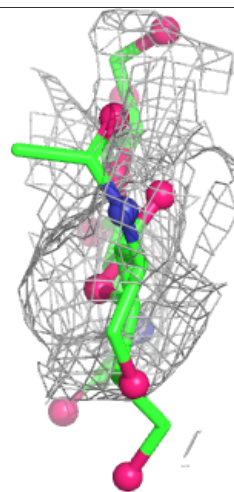
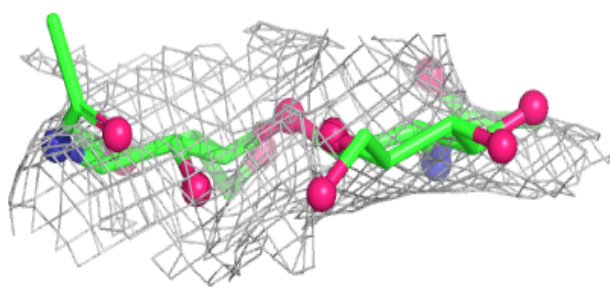
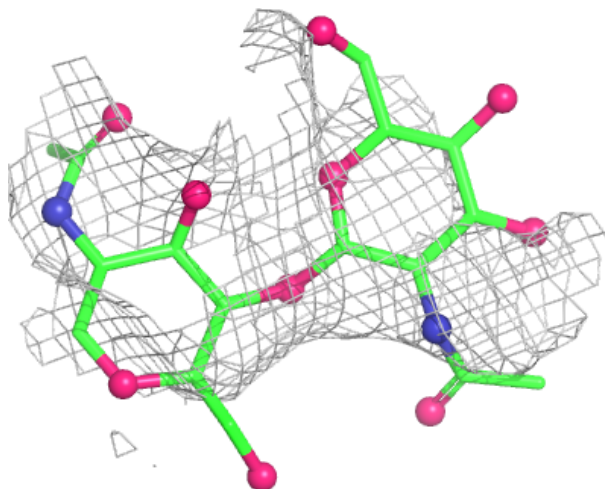
Electron density around Chain H:

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and green (positive)



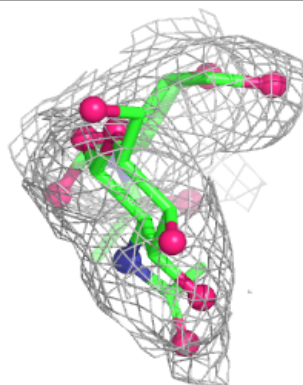
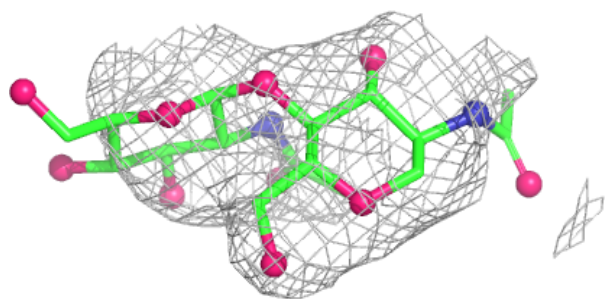
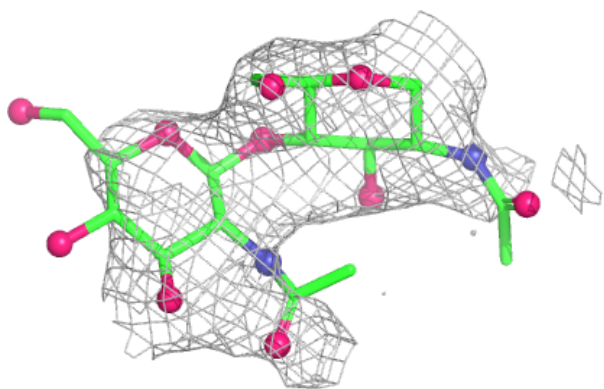
Electron density around Chain J:

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



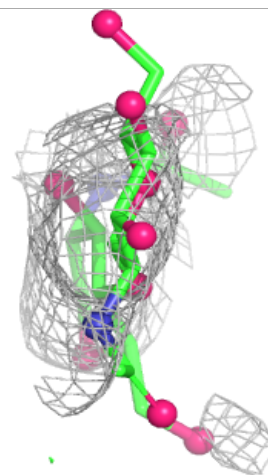
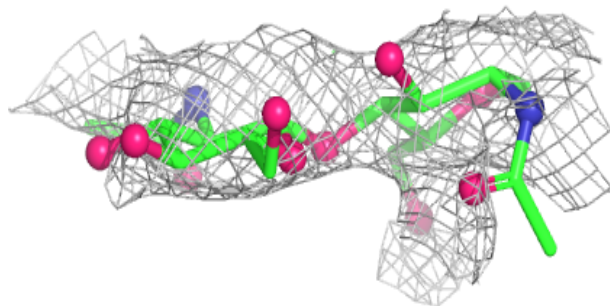
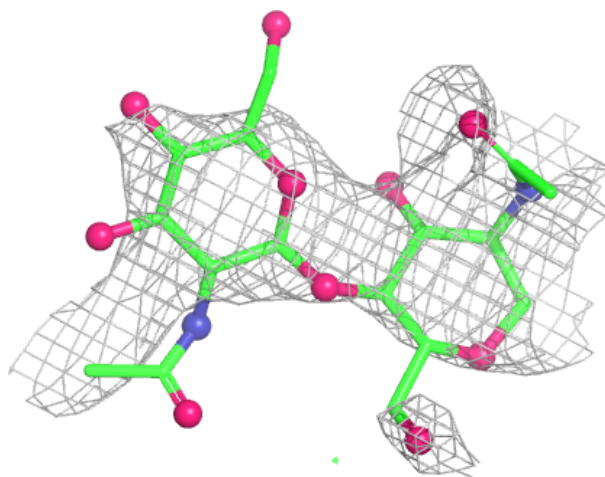
Electron density around Chain M:

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



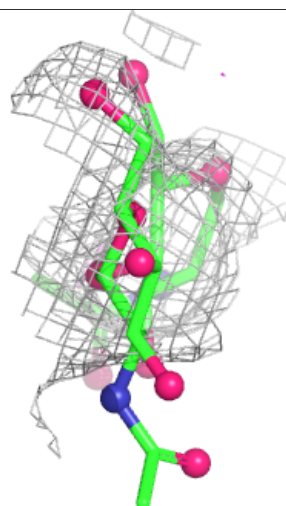
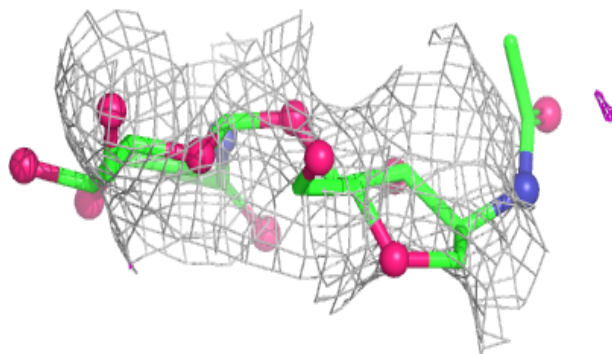
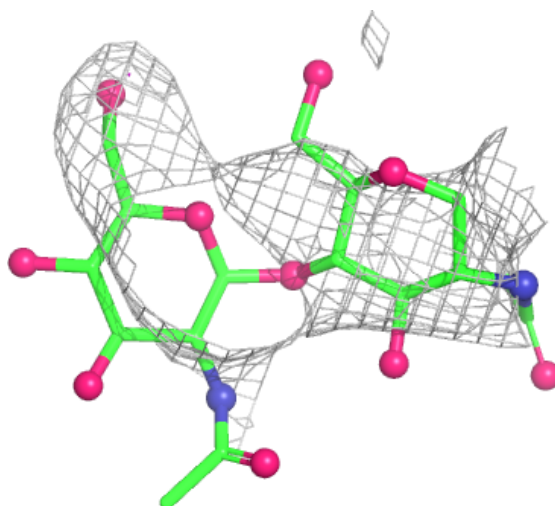
Electron density around Chain O:

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



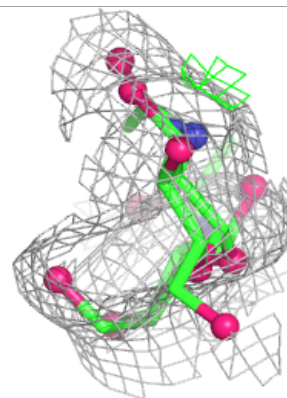
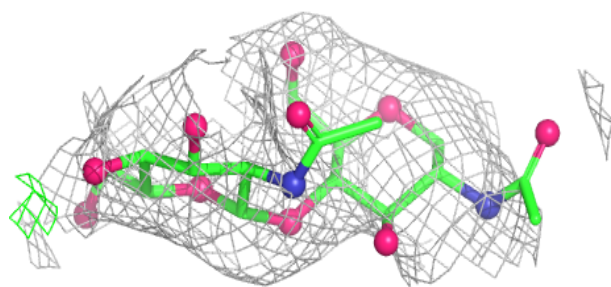
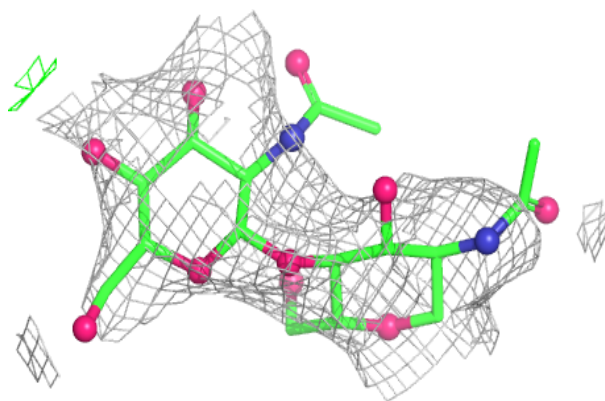
Electron density around Chain P:

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and green (positive)



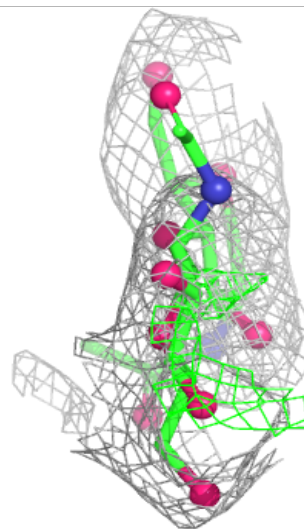
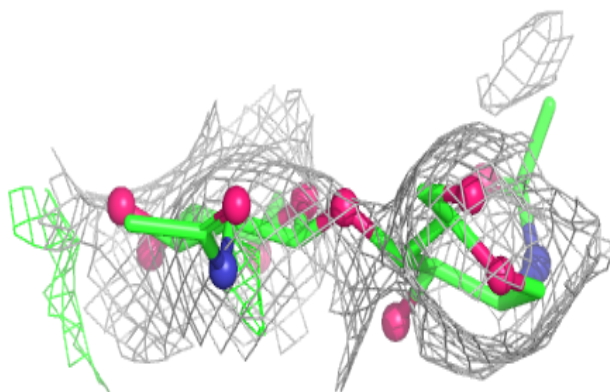
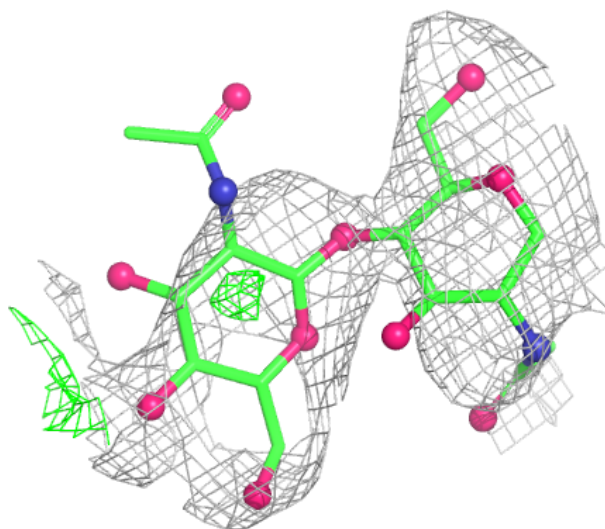
Electron density around Chain S:

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



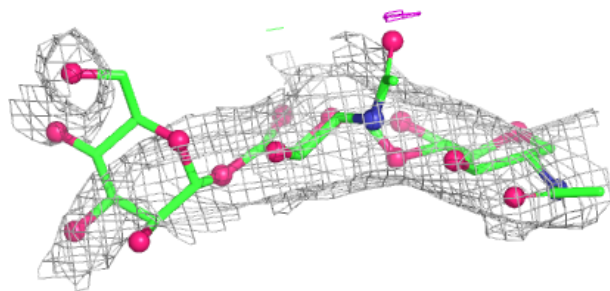
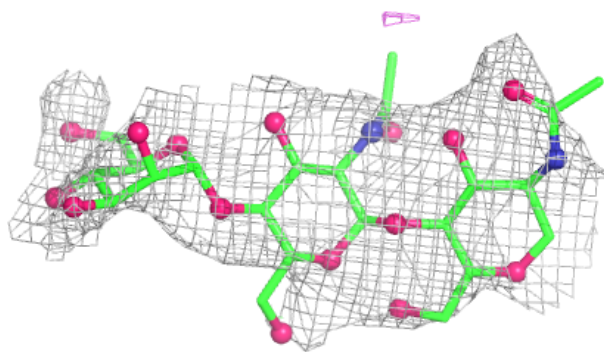
Electron density around Chain U:

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and green (positive)

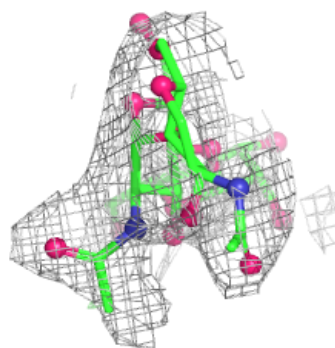
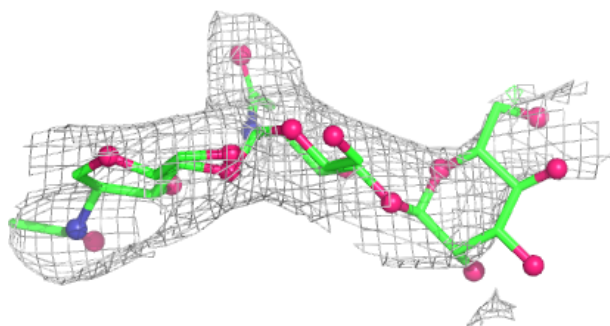
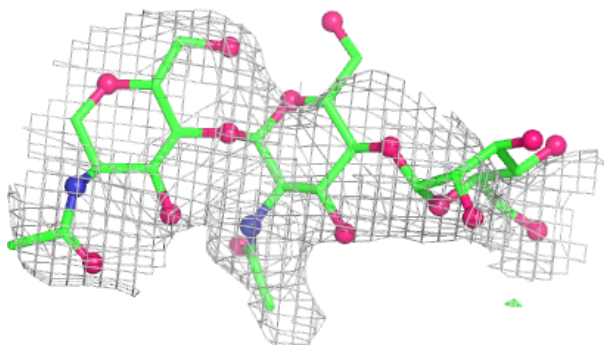


Electron density around Chain L:

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

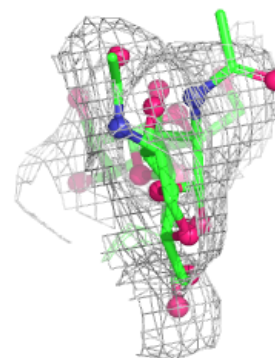
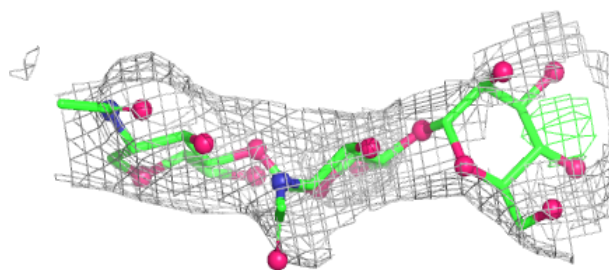
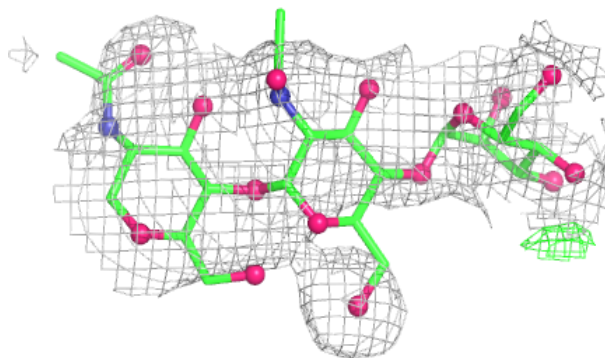
**Electron density around Chain R:**

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and green (positive)

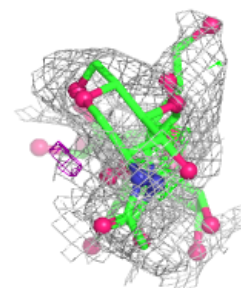
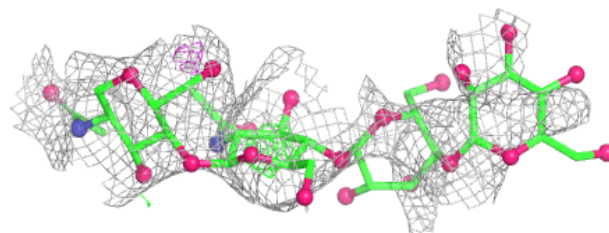
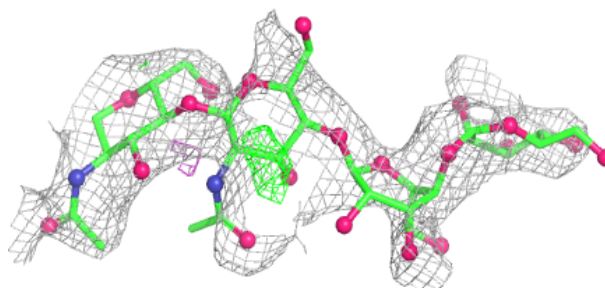


Electron density around Chain W:

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

**Electron density around Chain X:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.