



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:38 PM UTC

PDB ID : 3FKU / pdb_00003fku
Title : Crystal structure of influenza hemagglutinin (H5) in complex with a broadly neutralizing antibody F10
Authors : Hwang, W.C.; Santelli, E.; Stec, B.; Wei, G.; Cadwell, G.; Bankston, L.A.; Sui, J.; Perez, S.; Aird, D.; Chen, L.M.; Ali, M.; Murakami, A.; Yammanuru, A.; Han, T.; Cox, N.; Donis, R.O.; Liddington, R.C.; Marasco, W.A.
Deposited on : 2008-12-17
Resolution : 3.20 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

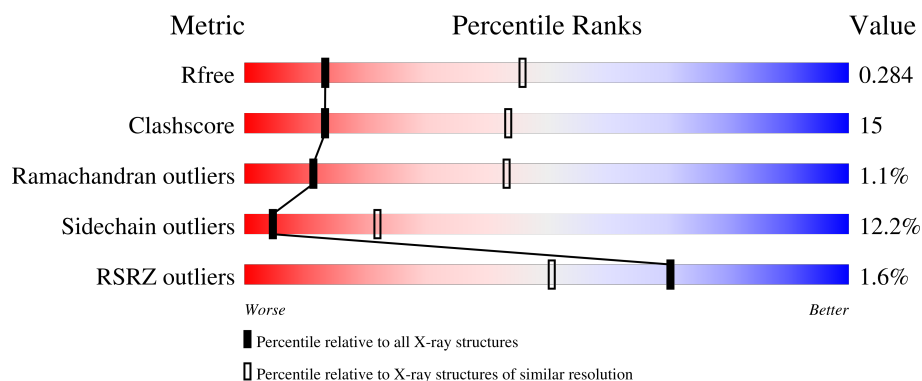
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



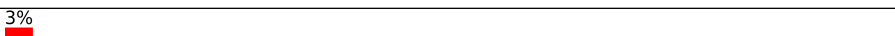
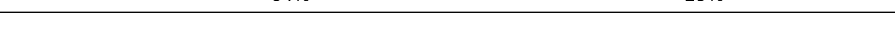
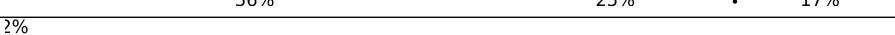
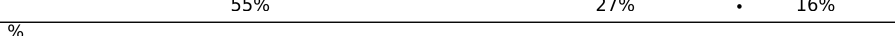
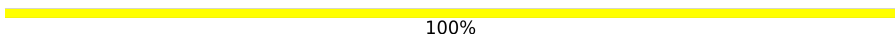
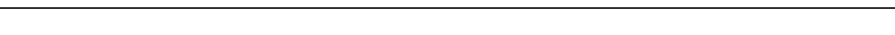
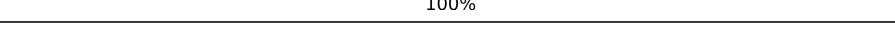
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	338	
1	C	338	
1	E	338	
1	G	338	

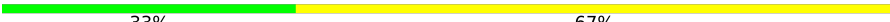
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Mol	Chain	Length	Quality of chain
1	I	338	
1	K	338	
2	B	182	
2	D	182	
2	F	182	
2	H	182	
2	J	182	
2	L	182	
3	S	280	
3	T	280	
3	U	280	
3	X	280	
3	Y	280	
3	Z	280	
4	M	2	
4	O	2	
4	Q	2	
4	V	2	
4	a	2	
4	c	2	
5	N	3	
5	P	3	
5	R	3	
5	W	3	
5	b	3	

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Mol	Chain	Length	Quality of chain
5	d	3	 33% 67%

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
5	NAG	W	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34975 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	C	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	E	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	G	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	I	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	K	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q5EP31
A	-2	ASP	-	expression tag	UNP Q5EP31
A	-1	PRO	-	expression tag	UNP Q5EP31
A	0	GLY	-	expression tag	UNP Q5EP31
A	1	TYR	-	expression tag	UNP Q5EP31
A	2	LEU	-	expression tag	UNP Q5EP31
A	3	LEU	-	expression tag	UNP Q5EP31
A	4	GLU	-	expression tag	UNP Q5EP31
C	-3	ALA	-	expression tag	UNP Q5EP31
C	-2	ASP	-	expression tag	UNP Q5EP31
C	-1	PRO	-	expression tag	UNP Q5EP31
C	0	GLY	-	expression tag	UNP Q5EP31
C	1	TYR	-	expression tag	UNP Q5EP31
C	2	LEU	-	expression tag	UNP Q5EP31
C	3	LEU	-	expression tag	UNP Q5EP31
C	4	GLU	-	expression tag	UNP Q5EP31
E	-3	ALA	-	expression tag	UNP Q5EP31

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ASP	-	expression tag	UNP Q5EP31
E	-1	PRO	-	expression tag	UNP Q5EP31
E	0	GLY	-	expression tag	UNP Q5EP31
E	1	TYR	-	expression tag	UNP Q5EP31
E	2	LEU	-	expression tag	UNP Q5EP31
E	3	LEU	-	expression tag	UNP Q5EP31
E	4	GLU	-	expression tag	UNP Q5EP31
G	-3	ALA	-	expression tag	UNP Q5EP31
G	-2	ASP	-	expression tag	UNP Q5EP31
G	-1	PRO	-	expression tag	UNP Q5EP31
G	0	GLY	-	expression tag	UNP Q5EP31
G	1	TYR	-	expression tag	UNP Q5EP31
G	2	LEU	-	expression tag	UNP Q5EP31
G	3	LEU	-	expression tag	UNP Q5EP31
G	4	GLU	-	expression tag	UNP Q5EP31
I	-3	ALA	-	expression tag	UNP Q5EP31
I	-2	ASP	-	expression tag	UNP Q5EP31
I	-1	PRO	-	expression tag	UNP Q5EP31
I	0	GLY	-	expression tag	UNP Q5EP31
I	1	TYR	-	expression tag	UNP Q5EP31
I	2	LEU	-	expression tag	UNP Q5EP31
I	3	LEU	-	expression tag	UNP Q5EP31
I	4	GLU	-	expression tag	UNP Q5EP31
K	-3	ALA	-	expression tag	UNP Q5EP31
K	-2	ASP	-	expression tag	UNP Q5EP31
K	-1	PRO	-	expression tag	UNP Q5EP31
K	0	GLY	-	expression tag	UNP Q5EP31
K	1	TYR	-	expression tag	UNP Q5EP31
K	2	LEU	-	expression tag	UNP Q5EP31
K	3	LEU	-	expression tag	UNP Q5EP31
K	4	GLU	-	expression tag	UNP Q5EP31

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	D	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	F	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	H	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	L	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP A8UDR4
B	178	SER	-	expression tag	UNP A8UDR4
B	179	LEU	-	expression tag	UNP A8UDR4
B	180	VAL	-	expression tag	UNP A8UDR4
B	181	PRO	-	expression tag	UNP A8UDR4
B	182	ARG	-	expression tag	UNP A8UDR4
D	177	ARG	-	expression tag	UNP A8UDR4
D	178	SER	-	expression tag	UNP A8UDR4
D	179	LEU	-	expression tag	UNP A8UDR4
D	180	VAL	-	expression tag	UNP A8UDR4
D	181	PRO	-	expression tag	UNP A8UDR4
D	182	ARG	-	expression tag	UNP A8UDR4
F	177	ARG	-	expression tag	UNP A8UDR4
F	178	SER	-	expression tag	UNP A8UDR4
F	179	LEU	-	expression tag	UNP A8UDR4
F	180	VAL	-	expression tag	UNP A8UDR4
F	181	PRO	-	expression tag	UNP A8UDR4
F	182	ARG	-	expression tag	UNP A8UDR4
H	177	ARG	-	expression tag	UNP A8UDR4
H	178	SER	-	expression tag	UNP A8UDR4
H	179	LEU	-	expression tag	UNP A8UDR4
H	180	VAL	-	expression tag	UNP A8UDR4
H	181	PRO	-	expression tag	UNP A8UDR4
H	182	ARG	-	expression tag	UNP A8UDR4
J	177	ARG	-	expression tag	UNP A8UDR4
J	178	SER	-	expression tag	UNP A8UDR4
J	179	LEU	-	expression tag	UNP A8UDR4
J	180	VAL	-	expression tag	UNP A8UDR4
J	181	PRO	-	expression tag	UNP A8UDR4
J	182	ARG	-	expression tag	UNP A8UDR4
L	177	ARG	-	expression tag	UNP A8UDR4
L	178	SER	-	expression tag	UNP A8UDR4
L	179	LEU	-	expression tag	UNP A8UDR4
L	180	VAL	-	expression tag	UNP A8UDR4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	181	PRO	-	expression tag	UNP A8UDR4
L	182	ARG	-	expression tag	UNP A8UDR4

- Molecule 3 is a protein called Neutralizing antibody F10.

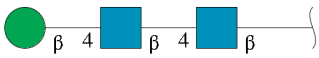
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	235	Total	C	N	O	S	0	0	0
			1765	1094	311	352	8			
3	Y	235	Total	C	N	O	S	0	0	0
			1765	1094	311	352	8			
3	Z	236	Total	C	N	O	S	0	0	0
			1769	1096	312	353	8			
3	S	233	Total	C	N	O	S	0	0	0
			1753	1088	309	348	8			
3	T	234	Total	C	N	O	S	0	0	0
			1759	1091	310	350	8			
3	U	234	Total	C	N	O	S	0	0	0
			1759	1091	310	350	8			

- Molecule 4 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
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	c	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.

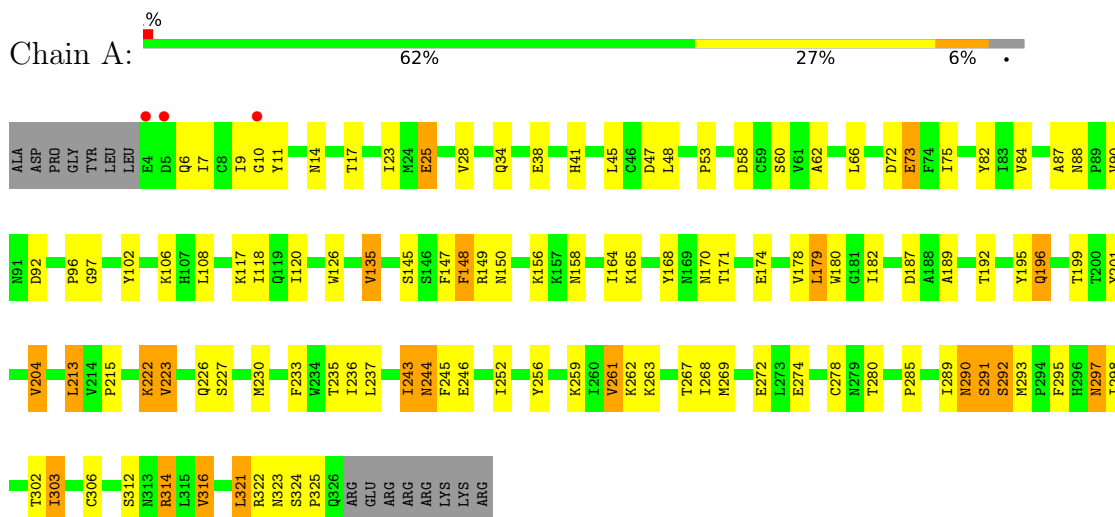


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	d	3	Total	C	N	O	0	0	0
			39	22	2	15			

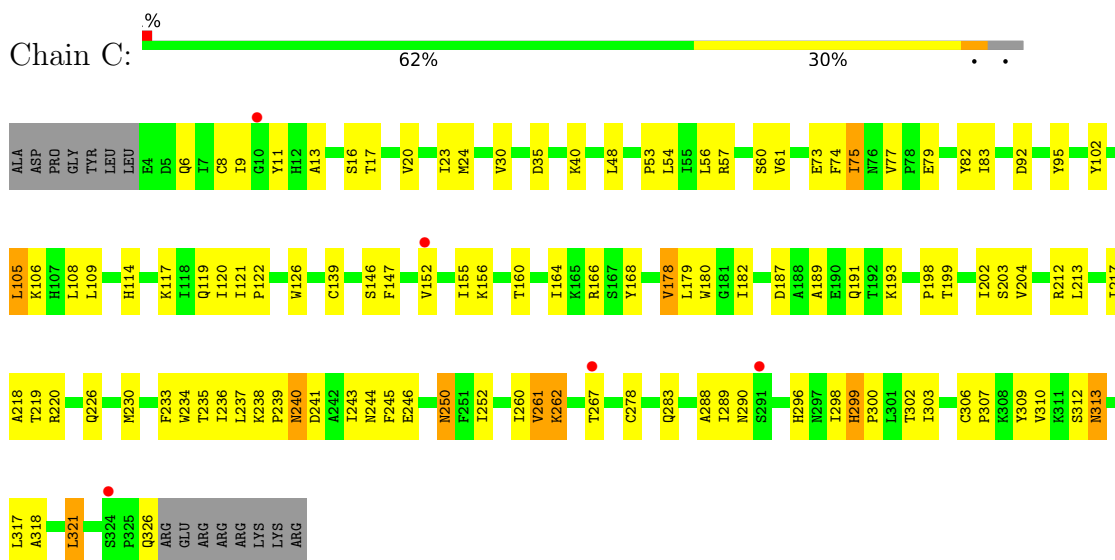
3 Residue-property plots [i](#)

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

• Molecule 1: Hemagglutinin

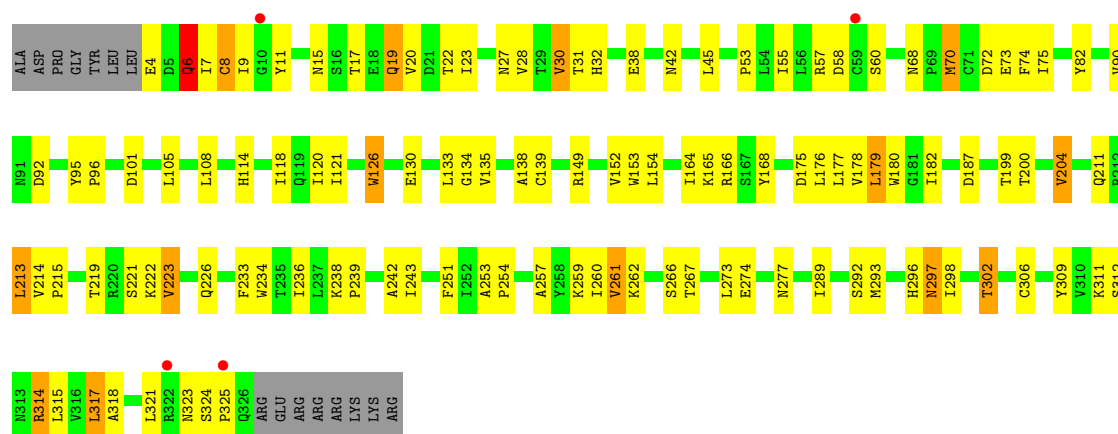


• Molecule 1: Hemagglutinin

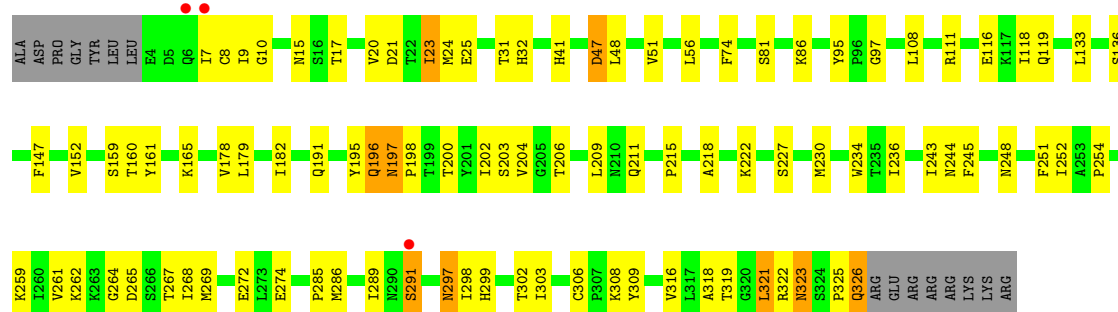


• Molecule 1: Hemagglutinin





• Molecule 1: Hemagglutinin

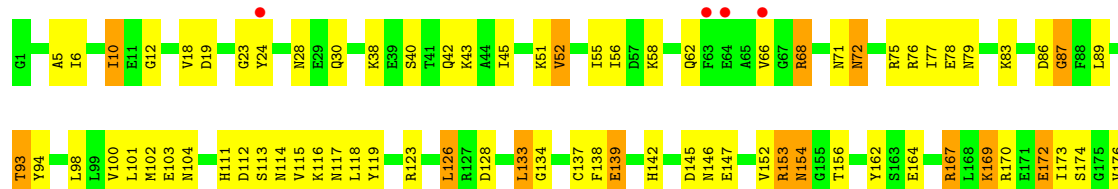


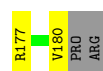
• Molecule 1: Hemagglutinin



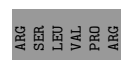
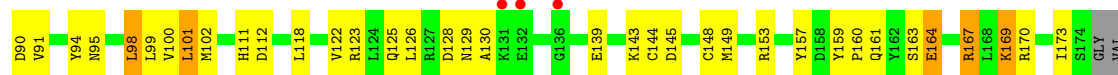
• Molecule 1: Hemagglutinin







• Molecule 2: Hemagglutinin HA2 chain



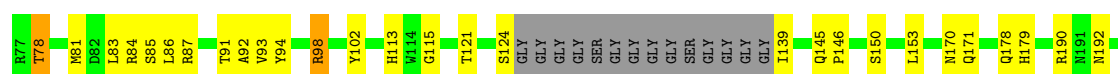
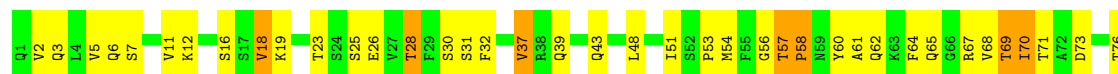
• Molecule 2: Hemagglutinin HA2 chain

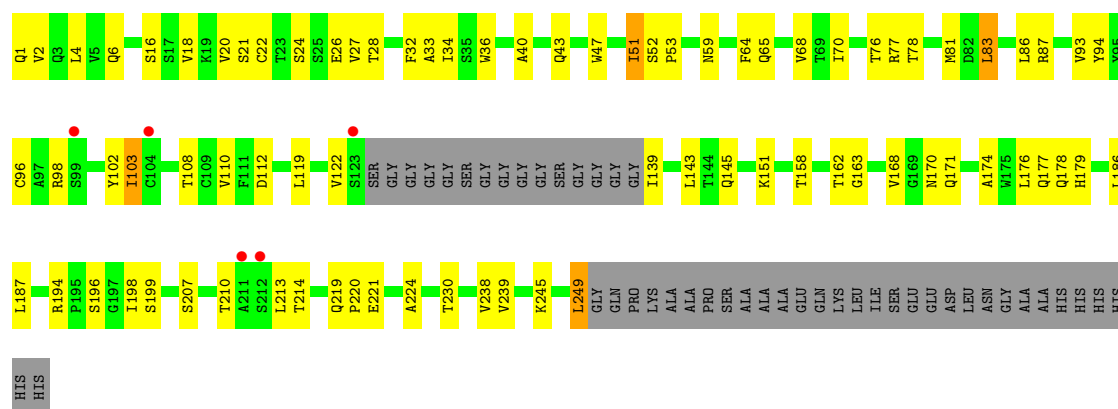


• Molecule 2: Hemagglutinin HA2 chain

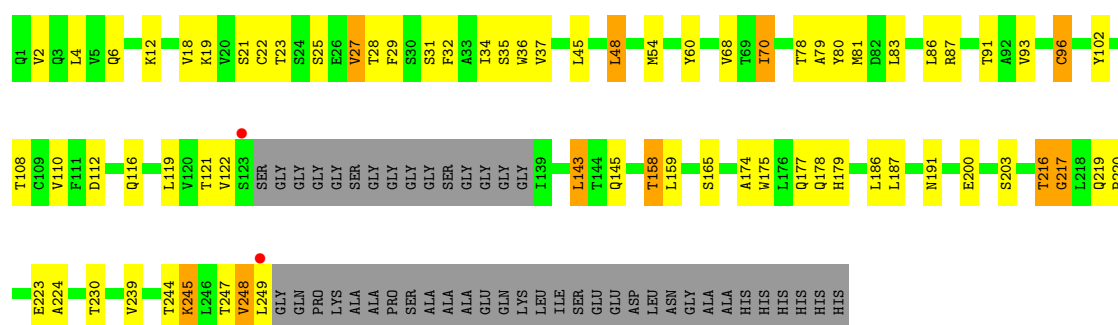


• Molecule 3: Neutralizing antibody F10





• Molecule 3: Neutralizing antibody F10



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



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



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



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

Chain V:  100%

MAG1
MAG2

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

Chain a:  50% 50%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain N:  33% 67%

MAG1
MAG2
BMA3

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

Chain P:  67% 33%

MAG1
MAG2
BMA3

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

Chain R:  100%

MAG1
MAG2
BMA3

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

Chain W:  67% 33%



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

Chain b:  100%



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

Chain d:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.30Å 118.50Å 338.90Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 (50.00-3.20) 85.0 (50.00-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.286 0.231 , 0.284	Depositor DCC
R_{free} test set	5677 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.116 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.107 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	34975	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/2629	0.88	2/3570 (0.1%)
1	C	0.65	0/2629	0.91	3/3570 (0.1%)
1	E	0.62	0/2629	0.86	2/3570 (0.1%)
1	G	0.63	0/2629	0.85	2/3570 (0.1%)
1	I	0.60	0/2629	0.87	5/3570 (0.1%)
1	K	0.62	0/2629	0.84	2/3570 (0.1%)
2	B	0.79	1/1482 (0.1%)	1.05	3/1992 (0.2%)
2	D	0.79	1/1482 (0.1%)	1.01	2/1992 (0.1%)
2	F	0.76	0/1482	1.02	2/1992 (0.1%)
2	H	0.61	0/1439	0.83	2/1934 (0.1%)
2	J	0.62	0/1439	0.84	0/1934
2	L	0.62	0/1439	0.84	1/1934 (0.1%)
3	S	0.56	0/1791	0.81	0/2436
3	T	0.53	0/1797	0.76	0/2444
3	U	0.58	0/1797	0.82	1/2444 (0.0%)
3	X	0.65	0/1803	0.89	1/2452 (0.0%)
3	Y	0.65	0/1803	0.92	4/2452 (0.2%)
3	Z	0.71	2/1807 (0.1%)	0.93	2/2457 (0.1%)
All	All	0.64	4/35335 (0.0%)	0.88	34/47883 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	3
1	G	0	1
1	I	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Y	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	127	ARG	CA-C	-6.12	1.50	1.53
3	Z	70	ILE	CA-CB	5.40	1.61	1.54
2	D	127	ARG	CA-C	-5.21	1.50	1.53
3	Z	167	ASN	CA-C	5.20	1.54	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	291	SER	N-CA-C	7.98	122.51	110.14
1	A	291	SER	N-CA-C	7.66	121.40	110.14
1	G	291	SER	N-CA-C	7.11	120.51	109.07
3	U	248	VAL	N-CA-C	6.84	117.44	111.56
2	B	127	ARG	N-CA-C	-6.60	102.42	108.75
1	A	14	ASN	N-CA-C	6.36	117.52	108.74
3	X	12	LYS	N-CA-C	6.22	118.41	109.14
2	F	176	VAL	N-CA-C	-6.20	104.70	110.53
1	C	299	HIS	CA-C-N	6.19	125.92	119.05
1	C	299	HIS	C-N-CA	6.19	125.92	119.05
2	F	23	GLY	N-CA-C	6.13	121.01	111.08
3	Y	76	THR	N-CA-C	-6.10	102.66	110.53
1	I	14	ASN	N-CA-C	5.96	116.46	108.23
3	Y	40	ALA	CA-C-N	5.71	126.97	119.84
3	Y	40	ALA	C-N-CA	5.71	126.97	119.84
2	D	126	LEU	CA-C-N	-5.64	116.95	123.04
2	D	126	LEU	C-N-CA	-5.64	116.95	123.04
1	K	77	VAL	N-CA-C	5.45	114.48	108.05
3	Y	148	SER	N-CA-C	5.38	116.20	107.32
1	G	23	ILE	N-CA-C	5.37	116.00	110.36
1	E	6	GLN	N-CA-C	5.35	116.41	108.60
2	L	115	VAL	CB-CA-C	-5.25	104.97	112.22
3	Z	196	SER	N-CA-C	5.23	116.67	110.97
1	I	284	THR	CA-C-N	5.19	124.91	119.82
1	I	284	THR	C-N-CA	5.19	124.91	119.82
1	C	6	GLN	N-CA-C	5.18	116.67	108.96
2	H	33	GLY	N-CA-C	5.17	120.70	110.83
3	Z	111	PHE	N-CA-C	5.14	117.04	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	291	SER	N-CA-C	5.10	118.53	109.96
2	H	60	ASN	N-CA-C	-5.09	107.20	113.41
1	I	6	GLN	N-CA-C	5.08	116.53	108.96
2	B	70	PHE	CA-C-N	5.03	128.21	120.82
2	B	70	PHE	C-N-CA	5.03	128.21	120.82
1	E	187	ASP	N-CA-C	5.02	115.66	108.74

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TRP	Peptide
1	A	290	ASN	Peptide
1	E	126	TRP	Peptide
1	E	323	ASN	Peptide
1	E	324	SER	Peptide
1	G	321	LEU	Peptide
1	I	290	ASN	Peptide
1	K	290	ASN	Peptide
3	Y	42	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2507	86	0
1	C	2567	0	2507	76	0
1	E	2567	0	2507	73	0
1	G	2567	0	2505	69	0
1	I	2567	0	2507	86	0
1	K	2567	0	2507	72	0
2	B	1455	0	1369	72	0
2	D	1455	0	1369	76	0
2	F	1455	0	1369	79	0
2	H	1412	0	1320	68	0
2	J	1412	0	1319	46	0
2	L	1412	0	1319	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	1753	0	1693	65	0
3	T	1759	0	1698	53	0
3	U	1759	0	1698	47	0
3	X	1765	0	1703	65	0
3	Y	1765	0	1703	45	0
3	Z	1769	0	1706	41	0
4	M	28	0	25	0	0
4	O	28	0	25	2	0
4	Q	28	0	25	1	0
4	V	28	0	23	0	0
4	a	28	0	25	0	0
4	c	28	0	25	1	0
5	N	39	0	34	0	0
5	P	39	0	34	0	0
5	R	39	0	34	0	0
5	W	39	0	34	2	0
5	b	39	0	34	0	0
5	d	39	0	34	0	0
All	All	34975	0	33658	1017	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1017) 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:C:302:THR:HG21	1:C:306:CYS:SG	1.63	1.36
2:H:98:LEU:CD2	2:H:102:MET:HE2	1.68	1.23
3:Y:158:THR:HG22	3:Y:214:THR:HG23	1.21	1.15
2:B:169:LYS:NZ	2:B:173:ILE:HG21	1.62	1.14
1:C:302:THR:CG2	1:C:306:CYS:SG	2.37	1.13
2:H:98:LEU:HD21	2:H:102:MET:HE2	1.14	1.06
1:A:108:LEU:HD21	1:A:236:ILE:HD11	1.37	1.04
1:I:204:VAL:HG23	1:I:209:LEU:HD23	1.42	1.00
2:H:98:LEU:HD21	2:H:102:MET:CE	1.93	0.98
1:A:187:ASP:OD1	1:A:189:ALA:HB3	1.64	0.97
2:B:169:LYS:HZ2	2:B:173:ILE:HG21	1.24	0.95
2:D:98:LEU:HD21	2:D:102:MET:HE2	1.49	0.93
2:F:98:LEU:CD2	2:F:102:MET:HE2	1.99	0.92
2:D:71:ASN:OD1	2:D:72:ASN:N	2.03	0.92
2:D:169:LYS:HZ2	2:D:173:ILE:HG21	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:LEU:HD21	2:F:102:MET:HE2	1.50	0.92
1:G:9:ILE:HD11	2:H:122:VAL:HG21	1.51	0.91
3:Y:162:THR:HG23	3:Y:210:THR:HB	1.53	0.91
3:S:178:GLN:O	3:S:224:ALA:HB1	1.71	0.90
2:D:169:LYS:NZ	2:D:173:ILE:HG21	1.86	0.89
1:G:302:THR:CG2	1:G:306:CYS:SG	2.62	0.87
1:G:302:THR:HG22	1:G:306:CYS:SG	2.15	0.87
3:Z:158:THR:OG1	3:Z:214:THR:HG22	1.73	0.86
1:I:172:ASN:N	1:I:172:ASN:HD22	1.72	0.86
3:X:68:VAL:HG22	3:X:83:LEU:HD13	1.57	0.84
3:Z:18:VAL:O	3:Z:82:ASP:HB2	1.77	0.84
1:A:230:MET:SD	1:A:252:ILE:HD11	2.19	0.83
1:I:108:LEU:HD13	1:I:236:ILE:HD11	1.61	0.82
2:B:123:ARG:O	2:B:126:LEU:O	1.98	0.81
2:B:102:MET:HE1	2:D:102:MET:HE1	1.62	0.81
1:I:100:ASN:HD22	1:I:101:ASP:N	1.77	0.81
2:B:169:LYS:HZ3	2:B:173:ILE:HG21	1.41	0.81
2:B:169:LYS:HZ2	2:B:173:ILE:CG2	1.92	0.81
1:K:20:VAL:HG21	1:K:318:ALA:HB2	1.61	0.81
1:A:156:LYS:NZ	1:A:192:THR:O	2.12	0.80
3:Z:87:ARG:O	3:Z:122:VAL:HG21	1.81	0.80
4:O:1:NAG:H4	4:O:2:NAG:N2	1.97	0.80
2:D:59:MET:HE2	2:F:94:TYR:CE1	2.17	0.79
2:H:52:VAL:CG2	3:U:28:THR:HG22	2.12	0.79
1:K:7:ILE:HD12	2:L:149:MET:HE1	1.64	0.79
1:I:204:VAL:HG23	1:I:209:LEU:CD2	2.13	0.78
1:A:297:ASN:C	1:A:297:ASN:HD22	1.91	0.78
2:F:173:ILE:HD12	2:F:173:ILE:C	2.09	0.78
3:Y:158:THR:CG2	3:Y:214:THR:HG23	2.10	0.78
1:A:9:ILE:HD11	2:B:122:VAL:HG21	1.66	0.78
1:C:191:GLN:HE21	1:C:250:ASN:HD21	1.30	0.78
2:F:42:GLN:HE22	3:X:102:TYR:H	1.32	0.77
1:E:213:LEU:HD12	1:E:233:PHE:CZ	2.19	0.77
1:K:230:MET:SD	1:K:252:ILE:HD11	2.24	0.77
1:A:213:LEU:HD11	1:A:233:PHE:CE1	2.20	0.77
1:C:121:ILE:O	1:C:121:ILE:HG22	1.84	0.77
1:C:9:ILE:HD11	2:D:122:VAL:HG21	1.65	0.77
3:Y:87:ARG:O	3:Y:122:VAL:HG21	1.84	0.77
1:A:7:ILE:HD12	2:B:149:MET:CE	2.16	0.76
1:C:48:LEU:HD22	1:C:303:ILE:CD1	2.15	0.76
3:Y:158:THR:HG22	3:Y:214:THR:CG2	2.11	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:248:VAL:HG23	3:U:249:LEU:HD12	1.67	0.76
1:I:20:VAL:HG11	1:I:318:ALA:HB2	1.66	0.76
3:U:4:LEU:HD22	3:U:22:CYS:SG	2.26	0.76
1:I:180:TRP:HZ3	1:I:235:THR:HG22	1.49	0.75
1:I:45:LEU:HD12	1:I:273:LEU:O	1.86	0.75
1:A:302:THR:CG2	1:A:306:CYS:SG	2.75	0.75
3:S:76:THR:OG1	3:S:78:THR:HG22	1.87	0.74
1:E:251:PHE:CE2	1:E:253:ALA:HB2	2.22	0.74
2:J:30:GLN:HE21	2:J:145:ASP:HB2	1.52	0.74
1:A:302:THR:HG21	1:A:306:CYS:SG	2.27	0.74
3:T:52:SER:HB2	3:T:103:ILE:HD12	1.69	0.74
1:G:147:PHE:CE1	1:G:230:MET:HE3	2.22	0.73
3:Z:68:VAL:HG22	3:Z:83:LEU:HB3	1.70	0.73
2:B:169:LYS:NZ	2:B:173:ILE:CG2	2.46	0.73
1:I:43:GLY:O	1:I:273:LEU:HD13	1.87	0.73
3:S:43:GLN:HG2	3:S:139:ILE:HG21	1.69	0.73
1:E:302:THR:HG23	1:E:306:CYS:SG	2.29	0.73
1:I:9:ILE:HD11	2:J:122:VAL:HG21	1.69	0.73
3:X:37:VAL:HG12	3:X:37:VAL:O	1.88	0.73
3:X:91:THR:HG23	3:X:121:THR:HA	1.69	0.73
3:X:76:THR:OG1	3:X:78:THR:HG23	1.89	0.73
1:E:108:LEU:HD13	1:E:236:ILE:HD11	1.70	0.72
3:T:177:GLN:HB2	3:T:187:LEU:HD11	1.71	0.72
2:L:169:LYS:HZ2	2:L:173:ILE:HG12	1.55	0.72
1:A:108:LEU:HD21	1:A:236:ILE:CD1	2.17	0.72
3:T:52:SER:CB	3:T:103:ILE:HD12	2.20	0.72
3:T:176:LEU:HD23	3:T:186:LEU:HA	1.71	0.72
2:D:98:LEU:HD23	2:D:98:LEU:C	2.15	0.71
2:H:51:LYS:HZ2	1:I:24:MET:HE2	1.55	0.71
2:D:169:LYS:HZ2	2:D:173:ILE:CG2	2.02	0.71
3:X:230:THR:HG22	3:X:231:TRP:N	2.06	0.71
1:K:284:THR:HG22	1:K:302:THR:OG1	1.89	0.71
1:A:289:ILE:HG12	1:A:298:ILE:HD12	1.71	0.71
2:B:129:ASN:ND2	2:B:157:TYR:OH	2.23	0.71
2:D:30:GLN:NE2	2:D:146:ASN:H	1.88	0.71
1:I:204:VAL:CG2	1:I:209:LEU:CD2	2.69	0.71
1:K:126:TRP:CD2	1:K:154:LEU:HD11	2.26	0.71
1:K:297:ASN:C	1:K:297:ASN:HD22	1.97	0.71
1:G:230:MET:SD	1:G:252:ILE:HD11	2.30	0.70
3:T:158:THR:HG22	3:T:214:THR:HG23	1.73	0.70
1:I:204:VAL:CG2	1:I:209:LEU:HD23	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TYR:CE1	2:B:6:ILE:HG23	2.26	0.70
1:K:7:ILE:CD1	2:L:149:MET:HE1	2.21	0.70
3:X:51:ILE:HB	3:X:70:ILE:HD11	1.74	0.70
1:G:51:VAL:HG12	1:G:81:SER:HB2	1.73	0.70
1:A:66:LEU:HD23	1:A:179:LEU:HD12	1.72	0.69
1:K:204:VAL:HG22	1:K:211:GLN:HB3	1.74	0.69
3:S:6:GLN:HE21	3:S:115:GLY:HA3	1.57	0.69
1:K:317:LEU:HD13	2:L:52:VAL:HG12	1.74	0.69
3:Z:146:PRO:O	3:Z:244:THR:HB	1.91	0.69
2:F:28:ASN:HD21	2:F:146:ASN:ND2	1.90	0.69
2:B:126:LEU:HD22	2:B:140:PHE:HE2	1.56	0.69
1:A:325:PRO:HB3	2:B:15:GLN:NE2	2.08	0.68
3:T:87:ARG:O	3:T:122:VAL:HG21	1.93	0.68
2:D:26:HIS:HB3	2:D:149:MET:HE2	1.74	0.68
2:H:98:LEU:HD23	2:H:102:MET:HE2	1.69	0.68
2:F:169:LYS:HZ2	2:F:173:ILE:CG2	2.05	0.68
2:D:179:LEU:HD12	2:D:179:LEU:N	2.09	0.68
2:H:80:LEU:CD2	2:J:80:LEU:HD21	2.24	0.68
3:S:159:LEU:HD23	3:S:244:THR:CG2	2.24	0.67
1:G:21:ASP:O	2:H:101:LEU:HD12	1.95	0.67
1:G:297:ASN:C	1:G:297:ASN:HD22	2.02	0.67
1:I:100:ASN:HD22	1:I:100:ASN:C	2.01	0.67
3:Y:177:GLN:HB2	3:Y:187:LEU:HD11	1.76	0.67
1:A:7:ILE:HD12	2:B:149:MET:HE3	1.76	0.67
1:E:176:LEU:HD11	1:E:257:ALA:HB3	1.77	0.67
1:K:7:ILE:CG1	2:L:149:MET:HE1	2.25	0.67
4:c:1:NAG:H4	4:c:2:NAG:N2	2.09	0.67
1:C:213:LEU:HD13	1:C:233:PHE:CE1	2.29	0.67
3:T:6:GLN:NE2	3:T:94:TYR:O	2.24	0.67
1:C:289:ILE:CD1	1:C:298:ILE:HD12	2.25	0.66
2:F:133:LEU:HB2	2:F:137:CYS:O	1.96	0.66
1:E:182:ILE:HD11	1:E:215:PRO:HG3	1.77	0.66
3:Y:201:ARG:HD2	3:Y:216:THR:O	1.95	0.66
3:Z:18:VAL:HG22	3:Z:86:LEU:HD22	1.77	0.66
1:C:75:ILE:HD12	1:C:75:ILE:O	1.96	0.66
3:U:78:THR:HG21	3:U:80:TYR:CZ	2.31	0.66
1:C:9:ILE:CD1	2:D:122:VAL:HG21	2.26	0.66
1:E:138:ALA:HB2	1:E:226:GLN:NE2	2.11	0.66
1:K:204:VAL:HG23	1:K:209:LEU:HD23	1.77	0.65
1:E:200:THR:O	1:E:214:VAL:HG13	1.96	0.65
3:X:6:GLN:HE21	3:X:115:GLY:HA3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:CB	2:B:149:MET:HE2	2.27	0.65
1:E:179:LEU:HD23	1:E:179:LEU:N	2.11	0.65
2:F:169:LYS:NZ	2:F:173:ILE:CG2	2.60	0.65
3:Z:172:GLY:O	3:Z:230:THR:HG21	1.97	0.65
1:A:204:VAL:HG12	1:A:245:PHE:CD2	2.32	0.64
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.79	0.64
1:G:302:THR:HG21	1:G:306:CYS:SG	2.36	0.64
3:X:60:TYR:HE2	3:X:70:ILE:HG23	1.62	0.64
3:X:64:PHE:HB3	3:X:68:VAL:HG23	1.80	0.64
2:F:173:ILE:HD12	2:F:174:SER:N	2.13	0.64
2:D:26:HIS:CB	2:D:149:MET:HE2	2.28	0.64
1:I:180:TRP:CZ3	1:I:235:THR:HG22	2.31	0.64
1:E:213:LEU:HD12	1:E:233:PHE:HZ	1.62	0.64
2:F:180:VAL:HG12	2:F:180:VAL:O	1.95	0.64
1:G:204:VAL:HG12	1:G:245:PHE:CD2	2.32	0.64
1:A:230:MET:SD	1:A:252:ILE:CD1	2.86	0.64
3:S:3:GLN:HB2	3:S:25:SER:HB2	1.80	0.63
1:A:58:ASP:HB3	1:A:90:VAL:HG22	1.79	0.63
1:C:119:GLN:NE2	1:C:122:PRO:HA	2.13	0.63
2:B:84:MET:HE1	2:D:84:MET:HA	1.80	0.63
1:E:302:THR:CG2	1:E:306:CYS:SG	2.86	0.63
1:A:120:ILE:HG22	1:A:168:TYR:CE1	2.34	0.63
1:A:120:ILE:HG22	1:A:168:TYR:CZ	2.33	0.63
2:H:130:ALA:HB1	2:H:139:GLU:O	1.98	0.63
2:D:42:GLN:HE22	3:Z:102:TYR:H	1.47	0.63
2:F:98:LEU:HD23	2:F:102:MET:HE2	1.80	0.63
3:U:87:ARG:O	3:U:122:VAL:HG21	1.98	0.63
1:C:289:ILE:HD11	1:C:298:ILE:HD12	1.81	0.63
2:B:84:MET:HE3	2:B:88:PHE:CE1	2.34	0.62
3:X:70:ILE:HD12	3:X:70:ILE:C	2.24	0.62
2:B:83:LYS:HE3	2:F:66:VAL:HG22	1.81	0.62
1:A:7:ILE:HG23	1:A:7:ILE:O	1.99	0.62
1:A:45:LEU:HD11	1:A:84:VAL:HG11	1.81	0.62
2:H:102:MET:HE1	2:L:102:MET:HE1	1.80	0.62
3:Y:30:SER:HA	3:Y:53:PRO:HB2	1.82	0.62
3:S:2:VAL:HG21	3:S:113:HIS:CG	2.35	0.62
1:A:7:ILE:HB	2:B:149:MET:HE1	1.81	0.62
2:B:49:THR:O	2:B:52:VAL:HG23	2.00	0.62
1:I:41:HIS:HB3	1:I:298:ILE:HD13	1.80	0.62
2:B:37:ASP:OD1	2:B:118:LEU:HD11	1.99	0.62
1:C:60:SER:OG	1:C:92:ASP:OD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:TYR:CE1	2:F:6:ILE:HG23	2.34	0.62
1:G:191:GLN:NE2	1:G:197:ASN:O	2.32	0.62
3:Y:60:TYR:HE2	3:Y:70:ILE:HG23	1.64	0.62
2:J:30:GLN:NE2	2:J:145:ASP:HB2	2.14	0.62
3:S:93:VAL:HG13	3:S:119:LEU:HD13	1.80	0.62
1:E:175:ASP:O	1:E:260:ILE:HD12	1.99	0.61
3:Y:70:ILE:HD12	3:Y:71:THR:N	2.15	0.61
3:U:110:VAL:HG11	3:U:174:ALA:HB2	1.81	0.61
1:C:17:THR:O	1:C:17:THR:HG22	2.00	0.61
2:B:5:ALA:HB1	2:B:115:VAL:HG12	1.82	0.61
3:U:18:VAL:HG13	3:U:86:LEU:HD22	1.81	0.61
1:G:204:VAL:HG22	1:G:211:GLN:HB3	1.82	0.61
1:I:7:ILE:HD12	2:J:149:MET:HE1	1.82	0.61
3:Y:20:VAL:HG12	3:Y:81:MET:HE2	1.80	0.61
2:B:80:LEU:C	2:B:80:LEU:HD23	2.26	0.61
1:K:70:MET:HE2	1:K:91:ASN:ND2	2.14	0.61
3:Y:30:SER:O	3:Y:54:MET:HB2	1.99	0.61
2:D:169:LYS:HZ2	2:D:173:ILE:HD13	1.65	0.61
2:F:52:VAL:HG21	3:X:28:THR:HG23	1.81	0.61
1:A:7:ILE:HD12	2:B:149:MET:HE1	1.83	0.61
2:L:26:HIS:HB3	2:L:149:MET:HE2	1.83	0.61
3:Y:143:LEU:HG	3:Y:239:VAL:HG13	1.83	0.61
1:A:261:VAL:HG12	1:A:262:LYS:N	2.15	0.61
2:D:176:VAL:O	2:D:179:LEU:HD13	2.00	0.61
3:T:110:VAL:CG1	3:T:174:ALA:HB2	2.31	0.61
1:C:120:ILE:HG22	1:C:168:TYR:CE1	2.36	0.60
1:C:302:THR:HG22	1:C:303:ILE:N	2.16	0.60
2:F:169:LYS:NZ	2:F:173:ILE:HG21	2.16	0.60
1:A:244:ASN:HB2	1:C:219:THR:HG23	1.84	0.60
1:G:20:VAL:HG21	1:G:318:ALA:HB2	1.82	0.60
1:C:204:VAL:HG22	1:C:245:PHE:CD2	2.36	0.60
3:U:158:THR:C	3:U:159:LEU:HD12	2.26	0.60
2:B:26:HIS:HB3	2:B:149:MET:HE2	1.83	0.60
2:D:66:VAL:HG22	2:F:83:LYS:HE3	1.83	0.60
1:G:147:PHE:HE1	1:G:230:MET:HE3	1.64	0.60
3:S:78:THR:HG23	3:S:80:TYR:CE2	2.37	0.60
3:U:143:LEU:HD22	3:U:239:VAL:HG23	1.83	0.60
2:H:51:LYS:NZ	1:I:24:MET:HE2	2.16	0.60
1:K:300:PRO:HB3	2:L:89:LEU:HD11	1.83	0.60
3:Y:6:GLN:NE2	3:Y:94:TYR:O	2.34	0.60
1:G:308:LYS:HZ2	2:H:62:GLN:HB3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:18:VAL:HG13	3:U:86:LEU:CD2	2.32	0.60
1:C:108:LEU:HD13	1:C:236:ILE:HD11	1.84	0.60
1:K:126:TRP:CE3	1:K:154:LEU:HD11	2.37	0.60
3:S:11:VAL:HG13	3:S:121:THR:O	2.02	0.60
3:Y:70:ILE:HD12	3:Y:70:ILE:C	2.27	0.60
3:X:153:LEU:HD13	3:X:248:VAL:HG11	1.83	0.59
3:S:68:VAL:HG22	3:S:83:LEU:HD13	1.83	0.59
1:G:24:MET:HE2	2:L:51:LYS:NZ	2.18	0.59
2:H:125:GLN:HE21	2:H:157:TYR:HB3	1.66	0.59
3:Y:20:VAL:HG21	3:Y:118:THR:HG21	1.85	0.59
2:B:52:VAL:HG21	3:Y:28:THR:HG22	1.85	0.59
1:K:70:MET:HE2	1:K:91:ASN:HD21	1.68	0.59
3:T:178:GLN:O	3:T:224:ALA:HB1	2.01	0.59
1:K:152:VAL:HG22	1:K:154:LEU:CD2	2.33	0.59
1:G:206:THR:HG22	1:G:243:ILE:HA	1.84	0.59
1:I:182:ILE:HG13	1:I:202:ILE:HD12	1.84	0.59
3:S:226:TYR:O	3:S:244:THR:HG22	2.03	0.59
3:Z:3:GLN:H	3:Z:25:SER:HB3	1.66	0.59
3:U:245:LYS:HE3	3:U:247:THR:HG23	1.84	0.59
2:H:129:ASN:ND2	2:H:157:TYR:OH	2.37	0.58
3:U:220:PRO:HA	3:U:248:VAL:HG21	1.85	0.58
3:U:223:GLU:OE2	3:U:247:THR:HG22	2.03	0.58
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.38	0.58
3:S:156:THR:HG22	3:S:216:THR:HA	1.85	0.58
3:T:207:SER:O	3:T:210:THR:HG22	2.04	0.58
2:B:113:SER:O	2:B:114:ASN:C	2.45	0.58
1:E:20:VAL:HG21	1:E:318:ALA:HB2	1.85	0.58
1:E:325:PRO:HG2	2:F:12:GLY:HA2	1.84	0.58
3:Z:36:TRP:CE2	3:Z:81:MET:HB2	2.38	0.58
1:E:297:ASN:C	1:E:297:ASN:HD22	2.11	0.58
1:C:204:VAL:HG22	1:C:245:PHE:HD2	1.68	0.58
2:H:52:VAL:CG2	3:U:28:THR:CG2	2.81	0.58
3:S:111:PHE:O	3:S:186:LEU:HD13	2.04	0.58
3:T:20:VAL:HG12	3:T:81:MET:HE2	1.84	0.58
1:E:114:HIS:HB3	1:E:262:LYS:HB2	1.85	0.58
3:X:171:GLN:O	3:X:190:ARG:HD2	2.04	0.58
2:F:123:ARG:O	2:F:126:LEU:O	2.20	0.57
1:A:195:TYR:O	1:A:196:GLN:HB3	2.04	0.57
1:G:8:CYS:HG	2:H:14:TRP:HZ2	1.51	0.57
1:A:222:LYS:HG3	1:A:227:SER:HB2	1.86	0.57
2:H:81:ASN:OD1	2:J:80:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:HB2	1:A:237:LEU:HD23	1.85	0.57
1:K:317:LEU:HD13	2:L:52:VAL:CG1	2.33	0.57
1:A:302:THR:HG22	1:A:303:ILE:N	2.18	0.57
3:X:230:THR:CG2	3:X:231:TRP:N	2.68	0.57
3:Z:145:GLN:NE2	3:Z:244:THR:HG22	2.20	0.57
2:B:5:ALA:HB1	2:B:115:VAL:CG1	2.34	0.57
1:C:230:MET:SD	1:C:252:ILE:HD11	2.45	0.57
1:E:309:TYR:CE2	2:F:89:LEU:HD13	2.40	0.57
2:J:169:LYS:NZ	2:J:173:ILE:HG21	2.18	0.57
3:T:2:VAL:HG13	3:T:26:GLU:HB3	1.87	0.57
2:H:79:ASN:HD22	2:L:68:ARG:HE	1.53	0.57
2:J:51:LYS:NZ	1:K:24:MET:HE2	2.20	0.57
3:S:47:TRP:CD2	3:S:238:VAL:HG23	2.39	0.57
3:S:179:HIS:CD2	3:S:224:ALA:HB2	2.40	0.57
2:D:167:ARG:HB3	2:D:170:ARG:CZ	2.34	0.57
2:F:30:GLN:HE21	2:F:146:ASN:H	1.51	0.57
1:K:169:ASN:O	1:K:171:THR:HG23	2.04	0.57
1:A:297:ASN:C	1:A:297:ASN:ND2	2.59	0.56
2:D:66:VAL:HG22	2:F:83:LYS:CE	2.35	0.56
2:H:56:ILE:HD11	3:U:27:VAL:HG12	1.87	0.56
2:H:26:HIS:HB3	2:H:149:MET:HE2	1.87	0.56
1:A:243:ILE:HG23	1:A:243:ILE:O	2.05	0.56
1:C:147:PHE:CZ	1:C:230:MET:HE1	2.40	0.56
1:K:9:ILE:HD11	2:L:24:TYR:CE2	2.39	0.56
2:H:169:LYS:HZ2	2:H:173:ILE:HG21	1.70	0.56
1:A:289:ILE:HG12	1:A:298:ILE:CD1	2.35	0.56
2:F:169:LYS:HZ2	2:F:173:ILE:HG22	1.70	0.56
1:G:108:LEU:HD13	1:G:236:ILE:HD11	1.88	0.56
2:L:42:GLN:HE21	3:T:102:TYR:HD1	1.51	0.56
1:A:302:THR:CG2	1:A:303:ILE:N	2.68	0.56
3:Z:32:PHE:CB	3:Z:98:ARG:HD2	2.35	0.56
1:C:313:ASN:C	1:C:313:ASN:HD22	2.14	0.56
2:H:61:THR:HG21	1:I:311:LYS:HD3	1.88	0.56
2:J:49:THR:HG21	3:S:32:PHE:CZ	2.40	0.56
1:K:66:LEU:HD23	1:K:179:LEU:HD12	1.88	0.56
1:A:47:ASP:O	1:A:280:THR:HG22	2.05	0.56
2:B:102:MET:HE1	2:D:102:MET:CE	2.32	0.56
1:E:96:PRO:HB3	1:E:223:VAL:HG23	1.88	0.56
1:I:230:MET:SD	1:I:252:ILE:HD11	2.46	0.56
3:Y:24:SER:O	3:Y:77:ARG:HD3	2.06	0.56
3:Z:28:THR:O	3:Z:28:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:178:GLN:O	3:U:224:ALA:HB1	2.06	0.56
1:A:38:GLU:OE1	1:A:291:SER:HB2	2.06	0.56
1:I:204:VAL:HG22	1:I:211:GLN:HB3	1.88	0.56
2:B:68:ARG:NE	2:D:79:ASN:HD22	2.04	0.55
2:D:169:LYS:NZ	2:D:173:ILE:HD13	2.21	0.55
3:X:70:ILE:HD12	3:X:71:THR:N	2.21	0.55
2:B:71:ASN:OD1	2:B:72:ASN:N	2.40	0.55
1:E:176:LEU:HD11	1:E:257:ALA:CB	2.35	0.55
1:G:309:TYR:CE2	2:H:89:LEU:HD13	2.42	0.55
3:S:93:VAL:CG1	3:S:119:LEU:HD13	2.36	0.55
2:J:72:ASN:O	2:J:72:ASN:ND2	2.39	0.55
2:L:72:ASN:HD22	2:L:72:ASN:C	2.15	0.55
1:E:45:LEU:HD12	1:E:273:LEU:HB2	1.89	0.55
1:E:72:ASP:O	1:E:74:PHE:N	2.38	0.55
2:H:52:VAL:HG23	3:U:28:THR:CG2	2.35	0.55
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.07	0.55
1:I:204:VAL:HA	1:I:244:ASN:O	2.07	0.55
1:A:314:ARG:HD3	1:A:316:VAL:HG23	1.89	0.55
2:B:167:ARG:HB3	2:B:170:ARG:NH2	2.22	0.55
1:C:180:TRP:HZ3	1:C:235:THR:HG22	1.71	0.55
3:S:57:THR:HG21	3:S:103:ILE:HD12	1.87	0.55
3:S:143:LEU:HD22	3:S:163:GLY:HA3	1.89	0.55
1:C:74:PHE:O	1:C:77:VAL:HG13	2.06	0.55
2:H:56:ILE:HD11	3:U:27:VAL:CG1	2.36	0.55
3:S:30:SER:HB3	3:S:54:MET:HE3	1.89	0.55
1:A:325:PRO:HB3	2:B:15:GLN:HE21	1.72	0.55
1:C:178:VAL:C	1:C:179:LEU:HD23	2.32	0.55
1:G:321:LEU:CD2	2:H:111:HIS:HB3	2.37	0.55
1:K:7:ILE:HD12	2:L:149:MET:CE	2.34	0.55
1:I:204:VAL:HG21	1:I:209:LEU:HD21	1.89	0.54
1:A:72:ASP:O	1:A:75:ILE:HG23	2.07	0.54
1:E:178:VAL:C	1:E:179:LEU:HD23	2.32	0.54
1:I:79:GLU:HB3	1:I:114:HIS:CG	2.42	0.54
1:I:311:LYS:H	2:J:93:THR:HG1	1.53	0.54
3:Z:153:LEU:HD21	3:Z:220:PRO:HD3	1.90	0.54
3:U:179:HIS:CD2	3:U:224:ALA:HB2	2.42	0.54
1:I:204:VAL:CG2	1:I:209:LEU:HD21	2.36	0.54
3:Y:32:PHE:CB	3:Y:98:ARG:HD2	2.38	0.54
2:H:51:LYS:HE3	1:I:24:MET:HE2	1.90	0.54
2:L:52:VAL:HG23	3:T:28:THR:HG22	1.89	0.54
3:S:43:GLN:CG	3:S:139:ILE:HG21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:99:LEU:HD12	2:L:99:LEU:O	2.07	0.54
3:Y:81:MET:HE3	3:Y:83:LEU:HB2	1.90	0.54
3:S:143:LEU:HD21	3:S:167:ASN:ND2	2.23	0.54
1:E:138:ALA:HB2	1:E:226:GLN:HE21	1.69	0.54
1:I:152:VAL:CG1	1:I:253:ALA:HB3	2.38	0.54
1:K:182:ILE:HD13	1:K:184:HIS:CE1	2.43	0.54
3:S:159:LEU:HD23	3:S:244:THR:HG23	1.88	0.54
1:C:61:VAL:HG11	1:C:109:LEU:HD22	1.90	0.54
1:K:302:THR:CG2	1:K:306:CYS:SG	2.96	0.53
3:U:70:ILE:HG22	3:U:81:MET:HG2	1.89	0.53
2:D:167:ARG:HB3	2:D:170:ARG:NH2	2.23	0.53
3:X:153:LEU:HA	3:X:248:VAL:HG13	1.90	0.53
1:A:195:TYR:O	1:A:196:GLN:CB	2.56	0.53
2:F:145:ASP:OD1	2:F:145:ASP:C	2.51	0.53
2:F:167:ARG:HB3	2:F:170:ARG:CZ	2.38	0.53
3:S:56:GLY:O	3:S:58:PRO:HD3	2.09	0.53
3:T:187:LEU:HD23	3:T:198:ILE:HD12	1.90	0.53
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.73	0.53
1:C:303:ILE:HD12	1:C:303:ILE:C	2.34	0.53
1:G:9:ILE:O	2:H:10:ILE:HD13	2.08	0.53
1:E:317:LEU:HD23	2:F:104:ASN:OD1	2.09	0.53
1:I:152:VAL:HG12	1:I:253:ALA:HB3	1.90	0.53
1:I:213:LEU:HD11	1:I:233:PHE:CZ	2.44	0.53
1:I:297:ASN:HD22	1:I:297:ASN:C	2.16	0.53
3:X:76:THR:O	3:X:78:THR:HG22	2.08	0.53
3:S:176:LEU:HD23	3:S:186:LEU:HA	1.91	0.53
3:T:6:GLN:HG2	3:T:22:CYS:HB3	1.91	0.53
3:U:177:GLN:HB2	3:U:187:LEU:HD21	1.90	0.53
2:B:126:LEU:HD22	2:B:140:PHE:CE2	2.43	0.53
2:F:51:LYS:HE2	2:F:103:GLU:OE1	2.09	0.53
2:D:80:LEU:O	2:D:80:LEU:HD23	2.08	0.53
1:K:151:VAL:HB	1:K:252:ILE:HG22	1.91	0.53
2:B:169:LYS:HZ2	2:B:173:ILE:HD13	1.74	0.53
2:D:145:ASP:OD1	2:D:145:ASP:C	2.52	0.53
1:I:172:ASN:N	1:I:172:ASN:ND2	2.44	0.53
1:E:126:TRP:CZ3	1:E:164:ILE:HD13	2.45	0.52
1:K:20:VAL:HG21	1:K:318:ALA:CB	2.35	0.52
3:T:143:LEU:HD11	3:T:230:THR:HG22	1.91	0.52
3:U:2:VAL:HG23	3:U:2:VAL:O	2.08	0.52
5:W:1:NAG:C6	5:W:2:NAG:H82	2.40	0.52
1:E:55:ILE:HG22	1:E:57:ARG:HG3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:3:GLN:HE21	3:S:3:GLN:HA	1.75	0.52
1:A:289:ILE:CD1	1:A:298:ILE:HD12	2.39	0.52
1:E:311:LYS:HG2	2:F:93:THR:HG21	1.92	0.52
1:G:285:PRO:HG2	1:G:299:HIS:CD2	2.43	0.52
1:K:20:VAL:HG22	1:K:30:VAL:HG11	1.90	0.52
1:K:267:THR:HB	1:K:303:ILE:HD13	1.91	0.52
1:K:317:LEU:CD1	2:L:52:VAL:HG12	2.38	0.52
3:S:92:ALA:HB3	3:S:94:TYR:CE1	2.44	0.52
3:T:143:LEU:HD21	3:T:168:VAL:HG23	1.92	0.52
2:F:24:TYR:CD1	2:F:153:ARG:HG3	2.45	0.52
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.44	0.52
1:E:126:TRP:CZ2	1:E:154:LEU:HD11	2.44	0.52
1:G:20:VAL:HG12	1:G:316:VAL:HG12	1.92	0.52
2:L:167:ARG:HA	2:L:170:ARG:HB2	1.90	0.52
3:S:32:PHE:HB3	3:S:98:ARG:HD3	1.92	0.52
3:T:151:LYS:O	3:T:249:LEU:HD23	2.10	0.52
2:J:91:VAL:HG12	2:J:92:TRP:N	2.23	0.52
1:K:178:VAL:C	1:K:179:LEU:HD23	2.35	0.52
2:D:176:VAL:O	2:D:179:LEU:CD1	2.57	0.52
1:E:289:ILE:CD1	1:E:298:ILE:HD12	2.40	0.52
2:J:48:VAL:O	2:J:49:THR:C	2.53	0.52
3:T:36:TRP:CE2	3:T:81:MET:HB2	2.45	0.52
3:U:68:VAL:HG22	3:U:83:LEU:HB3	1.91	0.52
2:F:154:ASN:C	2:F:154:ASN:HD22	2.18	0.52
1:K:182:ILE:HG22	1:K:231:GLU:HB3	1.91	0.52
1:A:25:GLU:HB3	1:A:28:VAL:HG23	1.92	0.52
1:G:7:ILE:HD12	2:H:149:MET:HE1	1.92	0.52
3:X:68:VAL:HG22	3:X:83:LEU:CD1	2.36	0.52
3:T:16:SER:O	3:T:86:LEU:HB2	2.10	0.52
2:H:52:VAL:HG23	3:U:28:THR:HG22	1.92	0.51
3:Y:193:ASP:OD2	3:Y:193:ASP:N	2.43	0.51
1:A:182:ILE:HD11	1:A:215:PRO:HG3	1.92	0.51
3:X:146:PRO:O	3:X:244:THR:HB	2.10	0.51
3:U:12:LYS:HG3	3:U:18:VAL:HG12	1.91	0.51
1:E:321:LEU:CD2	2:F:111:HIS:CG	2.93	0.51
1:G:95:TYR:CD2	1:G:230:MET:HG2	2.46	0.51
3:X:30:SER:HA	3:X:53:PRO:HB2	1.93	0.51
3:Z:177:GLN:O	3:Z:184:PRO:HA	2.10	0.51
2:J:98:LEU:CD2	2:J:102:MET:HE2	2.40	0.51
1:K:121:ILE:HD12	1:K:254:PRO:HD2	1.92	0.51
2:L:6:ILE:HD12	2:L:112:ASP:HA	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:50:GLY:C	3:Z:70:ILE:HD11	2.35	0.51
3:S:48:LEU:N	3:S:48:LEU:HD12	2.26	0.51
1:A:289:ILE:CG1	1:A:298:ILE:HD12	2.37	0.51
2:H:51:LYS:CE	1:I:24:MET:HE2	2.41	0.51
1:K:7:ILE:HG13	2:L:149:MET:HE1	1.91	0.51
3:T:47:TRP:CE3	3:T:238:VAL:HG23	2.45	0.51
3:T:110:VAL:HG11	3:T:174:ALA:HB2	1.91	0.51
1:I:20:VAL:HG12	1:I:316:VAL:HG12	1.91	0.51
1:I:303:ILE:C	1:I:303:ILE:HD12	2.35	0.51
1:K:302:THR:HG23	1:K:306:CYS:SG	2.50	0.51
3:T:158:THR:HG22	3:T:214:THR:CG2	2.40	0.51
2:B:174:SER:HB2	2:B:176:VAL:HG13	1.91	0.51
1:E:289:ILE:HD13	1:E:298:ILE:HD12	1.92	0.51
1:G:204:VAL:CG2	1:G:209:LEU:HD21	2.40	0.51
1:I:230:MET:SD	1:I:252:ILE:CD1	2.99	0.51
1:K:20:VAL:HG22	1:K:30:VAL:CG1	2.40	0.51
3:X:230:THR:HG22	3:X:231:TRP:O	2.11	0.51
2:H:49:THR:HG21	3:U:32:PHE:CZ	2.46	0.51
1:I:260:ILE:O	1:I:260:ILE:HG22	2.10	0.51
1:C:187:ASP:OD1	1:C:189:ALA:HB3	2.11	0.51
2:J:93:THR:HG22	2:J:94:TYR:N	2.25	0.51
1:K:297:ASN:C	1:K:297:ASN:ND2	2.64	0.51
3:Y:6:GLN:HE22	3:Y:95:TYR:HA	1.76	0.51
2:D:26:HIS:HB3	2:D:149:MET:CE	2.41	0.51
1:I:54:LEU:HD11	1:I:77:VAL:HG12	1.91	0.51
3:X:43:GLN:HG2	3:X:139:ILE:HG21	1.92	0.51
3:X:81:MET:HE3	3:X:83:LEU:HB2	1.92	0.51
3:Y:143:LEU:HG	3:Y:239:VAL:CG1	2.41	0.51
2:H:169:LYS:HZ2	2:H:173:ILE:CG2	2.24	0.50
1:K:202:ILE:HD11	1:K:251:PHE:HA	1.92	0.50
2:B:38:LYS:HD3	3:Y:103:ILE:HG21	1.92	0.50
2:F:98:LEU:HD21	2:F:102:MET:CE	2.33	0.50
1:K:102:TYR:CE2	1:K:106:LYS:HD2	2.46	0.50
2:L:48:VAL:O	2:L:52:VAL:HG22	2.11	0.50
3:Y:72:ALA:HA	3:Y:79:ALA:HA	1.93	0.50
3:Y:230:THR:HG23	3:Y:231:TRP:N	2.25	0.50
1:E:120:ILE:HG22	1:E:168:TYR:CE1	2.47	0.50
1:I:31:THR:HG22	1:I:323:ASN:OD1	2.11	0.50
1:I:302:THR:HG23	1:I:306:CYS:SG	2.52	0.50
3:S:12:LYS:HD2	3:S:18:VAL:HG12	1.94	0.50
3:S:159:LEU:HD23	3:S:244:THR:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:4:LEU:HD22	3:U:96:CYS:SG	2.52	0.50
1:A:11:TYR:HB2	1:A:321:LEU:HD13	1.93	0.50
2:D:44:ALA:O	2:D:48:VAL:HG23	2.12	0.50
2:H:169:LYS:NZ	2:H:173:ILE:HG21	2.27	0.50
1:C:114:HIS:HB2	1:C:262:LYS:HZ1	1.77	0.50
1:K:43:GLY:O	1:K:273:LEU:HD22	2.12	0.50
2:B:51:LYS:HE3	1:C:24:MET:HE3	1.93	0.50
1:G:108:LEU:CD1	1:G:236:ILE:HD11	2.41	0.50
1:K:34:GLN:HA	1:K:34:GLN:HE21	1.76	0.50
3:U:36:TRP:NE1	3:U:81:MET:HB2	2.27	0.50
1:A:84:VAL:O	1:A:84:VAL:HG12	2.11	0.50
1:A:302:THR:O	1:A:303:ILE:HG23	2.11	0.50
2:H:128:ASP:N	2:H:128:ASP:OD1	2.43	0.50
1:I:95:TYR:CG	1:I:230:MET:HE3	2.47	0.50
1:K:7:ILE:HG23	1:K:7:ILE:O	2.11	0.50
3:X:19:LYS:HA	3:X:81:MET:O	2.12	0.50
3:X:30:SER:CB	3:X:54:MET:HE3	2.41	0.50
3:S:3:GLN:HA	3:S:3:GLN:NE2	2.27	0.50
2:B:164:GLU:N	2:B:164:GLU:OE2	2.44	0.50
1:A:164:ILE:O	1:A:246:GLU:HA	2.12	0.50
1:G:147:PHE:CZ	1:G:230:MET:HE3	2.47	0.50
1:I:159:SER:O	1:I:160:THR:HG23	2.12	0.50
3:Y:213:LEU:HD22	3:Y:214:THR:N	2.27	0.50
1:A:179:LEU:N	1:A:179:LEU:HD23	2.27	0.49
3:T:18:VAL:CG1	3:T:86:LEU:HD11	2.42	0.49
2:B:30:GLN:NE2	2:B:146:ASN:H	2.10	0.49
2:B:79:ASN:HD22	2:F:68:ARG:NE	2.10	0.49
1:C:243:ILE:HG23	1:C:243:ILE:O	2.12	0.49
3:Y:60:TYR:CE2	3:Y:70:ILE:HG23	2.45	0.49
1:A:302:THR:HG23	1:A:306:CYS:SG	2.52	0.49
1:K:267:THR:CG2	1:K:268:ILE:N	2.75	0.49
3:S:219:GLN:HB3	3:S:220:PRO:HD2	1.94	0.49
3:T:179:HIS:CD2	3:T:224:ALA:HB2	2.47	0.49
1:C:156:LYS:HE2	1:C:193:LYS:O	2.12	0.49
2:D:172:GLU:C	2:D:174:SER:H	2.20	0.49
1:I:11:TYR:CZ	2:J:6:ILE:HG23	2.46	0.49
1:I:321:LEU:HD23	2:J:111:HIS:CG	2.48	0.49
3:Z:18:VAL:HG22	3:Z:86:LEU:CD2	2.42	0.49
3:Z:145:GLN:NE2	3:Z:244:THR:CG2	2.76	0.49
1:I:37:LEU:HD12	1:I:296:HIS:HA	1.93	0.49
3:X:30:SER:HB2	3:X:54:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:7:SER:HB3	3:Z:20:VAL:HG13	1.94	0.49
3:Z:29:PHE:C	3:Z:29:PHE:CD2	2.88	0.49
2:D:30:GLN:HE21	2:D:146:ASN:H	1.58	0.49
1:G:116:GLU:HB3	1:G:259:LYS:HB2	1.95	0.49
1:K:131:ALA:HB1	1:K:152:VAL:HG21	1.95	0.49
1:E:19:GLN:NE2	1:E:27:ASN:OD1	2.46	0.49
1:K:41:HIS:NE2	1:K:286:MET:HE2	2.28	0.49
3:T:112:ASP:HA	3:T:186:LEU:HD22	1.93	0.49
1:C:202:ILE:O	1:C:212:ARG:HA	2.13	0.49
2:F:173:ILE:C	2:F:173:ILE:CD1	2.79	0.49
1:G:289:ILE:HG22	1:G:291:SER:OG	2.13	0.49
1:I:121:ILE:HG21	1:I:126:TRP:CZ2	2.48	0.49
3:Y:51:ILE:HB	3:Y:70:ILE:HD11	1.94	0.49
1:A:171:THR:CB	1:G:118:ILE:HG22	2.42	0.49
1:A:321:LEU:HD23	2:B:111:HIS:CG	2.48	0.49
2:D:179:LEU:O	2:D:180:VAL:HG13	2.13	0.49
1:E:7:ILE:HG23	1:E:7:ILE:O	2.12	0.49
2:F:71:ASN:C	2:F:71:ASN:OD1	2.56	0.49
1:I:48:LEU:HD22	1:I:303:ILE:CD1	2.43	0.49
1:K:121:ILE:HG23	1:K:166:ARG:NH1	2.28	0.49
3:Z:158:THR:OG1	3:Z:214:THR:CG2	2.53	0.49
3:U:68:VAL:HG22	3:U:83:LEU:CB	2.42	0.49
2:B:4:GLY:N	2:B:112:ASP:OD2	2.46	0.49
2:F:30:GLN:NE2	2:F:146:ASN:H	2.11	0.49
3:Y:146:PRO:O	3:Y:244:THR:HG23	2.13	0.49
3:Y:187:LEU:HA	3:Y:198:ILE:HG13	1.94	0.49
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.95	0.48
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.48	0.48
1:C:317:LEU:HD13	2:D:52:VAL:HG22	1.95	0.48
3:X:51:ILE:HD11	3:X:56:GLY:O	2.13	0.48
3:Y:26:GLU:OE2	3:Y:98:ARG:NE	2.46	0.48
1:A:11:TYR:CZ	2:B:6:ILE:HG23	2.49	0.48
2:D:71:ASN:HB3	2:D:74:GLU:HG3	1.95	0.48
2:H:80:LEU:HD21	2:J:80:LEU:HD21	1.92	0.48
1:K:79:GLU:HB2	1:K:114:HIS:HB2	1.95	0.48
3:S:57:THR:CG2	3:S:103:ILE:HD12	2.43	0.48
3:S:210:THR:HG23	3:S:210:THR:O	2.13	0.48
1:G:41:HIS:HE2	1:G:286:MET:HE2	1.79	0.48
3:S:230:THR:HG22	3:S:231:TRP:N	2.29	0.48
3:T:64:PHE:O	3:T:65:GLN:C	2.56	0.48
5:W:1:NAG:H61	5:W:2:NAG:H82	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:VAL:HG11	2:D:108:LEU:HD21	1.95	0.48
1:E:95:TYR:N	1:E:139:CYS:SG	2.87	0.48
3:X:32:PHE:HB3	3:X:98:ARG:HD3	1.94	0.48
3:U:78:THR:HG22	3:U:79:ALA:N	2.28	0.48
3:U:6:GLN:H	3:U:116:GLN:HE22	1.61	0.48
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.28	0.48
2:H:164:GLU:HA	2:H:167:ARG:HD2	1.96	0.48
1:G:179:LEU:O	1:G:254:PRO:HB3	2.14	0.48
1:G:321:LEU:HD23	2:H:111:HIS:HB3	1.96	0.48
3:T:139:ILE:HG23	3:T:139:ILE:O	2.13	0.48
3:U:112:ASP:HA	3:U:186:LEU:HD22	1.96	0.48
1:C:53:PRO:HB3	1:C:82:TYR:CZ	2.49	0.48
1:E:9:ILE:HG13	2:F:119:TYR:HA	1.96	0.48
1:G:161:TYR:HB2	1:G:195:TYR:O	2.13	0.48
2:H:144:CYS:SG	2:H:145:ASP:N	2.87	0.48
3:X:170:ASN:HB2	3:X:171:GLN:OE1	2.14	0.48
3:Z:32:PHE:HB2	3:Z:98:ARG:HD2	1.95	0.48
1:C:237:LEU:CD1	1:C:241:ASP:HB3	2.44	0.48
1:C:313:ASN:C	1:C:313:ASN:ND2	2.72	0.48
2:D:98:LEU:CD2	2:D:102:MET:HE2	2.33	0.48
1:E:315:LEU:HG	2:F:100:VAL:HG21	1.95	0.48
2:J:152:VAL:HG22	2:J:157:TYR:CD1	2.49	0.48
3:Y:64:PHE:HB3	3:Y:68:VAL:HG13	1.96	0.48
1:A:135:VAL:HG23	1:A:145:SER:HB3	1.96	0.47
2:B:72:ASN:HD22	2:B:75:ARG:NH2	2.12	0.47
2:F:180:VAL:O	2:F:180:VAL:CG1	2.62	0.47
1:G:269:MET:HE2	1:G:285:PRO:HD3	1.96	0.47
2:B:169:LYS:NZ	2:B:173:ILE:HD13	2.29	0.47
2:F:24:TYR:CE1	2:F:153:ARG:HG3	2.49	0.47
1:I:100:ASN:C	1:I:100:ASN:ND2	2.72	0.47
3:Y:176:LEU:HD23	3:Y:186:LEU:HA	1.95	0.47
1:C:13:ALA:HB1	2:D:15:GLN:HE21	1.77	0.47
1:E:297:ASN:C	1:E:297:ASN:ND2	2.72	0.47
3:T:219:GLN:HB2	3:T:220:PRO:CD	2.44	0.47
3:U:37:VAL:CG1	3:U:45:LEU:HD12	2.44	0.47
2:D:38:LYS:NZ	3:Z:105:SER:OG	2.40	0.47
1:I:48:LEU:HD22	1:I:303:ILE:HD13	1.97	0.47
2:L:125:GLN:HE22	2:L:155:GLY:C	2.22	0.47
3:S:143:LEU:HD22	3:S:163:GLY:CA	2.45	0.47
1:A:9:ILE:HG13	2:B:119:TYR:HA	1.96	0.47
2:B:30:GLN:HE21	2:B:146:ASN:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:LYS:O	1:E:223:VAL:HG13	2.14	0.47
1:G:47:ASP:N	1:G:47:ASP:OD1	2.46	0.47
1:K:280:THR:HG21	1:K:288:ALA:HB1	1.95	0.47
1:C:261:VAL:HG22	1:C:262:LYS:N	2.28	0.47
1:C:310:VAL:C	1:C:312:SER:H	2.23	0.47
1:E:177:LEU:HD12	1:E:178:VAL:N	2.30	0.47
3:S:68:VAL:HG12	3:S:70:ILE:CG2	2.45	0.47
3:T:4:LEU:HD23	3:T:96:CYS:SG	2.55	0.47
3:T:219:GLN:HB2	3:T:220:PRO:HD2	1.96	0.47
3:U:48:LEU:HD22	3:U:81:MET:SD	2.54	0.47
1:A:87:ALA:HB2	1:A:272:GLU:OE2	2.14	0.47
2:B:51:LYS:HE3	1:C:24:MET:CE	2.44	0.47
1:G:202:ILE:HD11	1:G:251:PHE:HA	1.97	0.47
2:H:99:LEU:HD13	2:J:98:LEU:HD11	1.95	0.47
2:J:169:LYS:HZ2	2:J:173:ILE:HG12	1.80	0.47
1:K:109:LEU:HB3	1:K:268:ILE:HD11	1.97	0.47
1:K:152:VAL:HG22	1:K:154:LEU:HD23	1.95	0.47
2:L:28:ASN:ND2	2:L:145:ASP:HA	2.29	0.47
3:X:223:GLU:HB2	3:X:246:LEU:O	2.14	0.47
3:T:20:VAL:CG1	3:T:81:MET:HE2	2.45	0.47
3:U:219:GLN:O	3:U:248:VAL:HG11	2.13	0.47
2:B:177:ARG:C	2:B:179:LEU:H	2.22	0.47
1:G:41:HIS:NE2	1:G:286:MET:HE2	2.29	0.47
1:G:179:LEU:CD2	1:G:234:TRP:HB3	2.44	0.47
1:G:309:TYR:HE2	2:H:89:LEU:HD13	1.79	0.47
1:E:9:ILE:O	2:F:10:ILE:HD13	2.15	0.47
1:I:211:GLN:OE1	1:I:213:LEU:HD12	2.15	0.47
3:X:92:ALA:HB3	3:X:94:TYR:CE1	2.50	0.47
1:I:22:THR:HB	2:J:105:GLU:HB2	1.97	0.47
1:K:205:GLY:HA2	1:K:209:LEU:O	2.14	0.47
1:K:230:MET:SD	1:K:252:ILE:CD1	3.01	0.47
3:Z:178:GLN:O	3:Z:224:ALA:HB1	2.15	0.47
1:C:237:LEU:HD11	1:C:241:ASP:HB3	1.97	0.46
2:D:71:ASN:HB3	2:D:74:GLU:CG	2.45	0.46
2:J:44:ALA:HB2	2:J:114:ASN:HD22	1.80	0.46
3:Y:6:GLN:H	3:Y:116:GLN:HE22	1.63	0.46
3:Y:119:LEU:HD23	3:Y:120:VAL:N	2.30	0.46
2:B:98:LEU:CB	2:F:58:LYS:HZ3	2.27	0.46
1:C:95:TYR:N	1:C:139:CYS:SG	2.89	0.46
1:E:58:ASP:HB3	1:E:90:VAL:HG22	1.95	0.46
1:G:297:ASN:C	1:G:297:ASN:ND2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:LEU:HB3	1:I:81:SER:OG	2.16	0.46
1:K:9:ILE:HD12	2:L:118:LEU:HG	1.97	0.46
1:K:99:PHE:O	1:K:102:TYR:HB2	2.15	0.46
3:T:52:SER:HB3	3:T:103:ILE:HD12	1.97	0.46
2:F:126:LEU:HD21	2:F:152:VAL:CG2	2.46	0.46
2:L:93:THR:HG22	2:L:94:TYR:N	2.30	0.46
3:S:70:ILE:HG22	3:S:81:MET:HG2	1.96	0.46
1:A:97:GLY:HA3	1:A:230:MET:O	2.16	0.46
1:A:323:ASN:C	1:A:323:ASN:HD22	2.22	0.46
2:D:179:LEU:C	2:D:180:VAL:HG22	2.39	0.46
1:E:321:LEU:HD23	2:F:111:HIS:CG	2.50	0.46
1:G:25:GLU:OE2	1:G:322:ARG:NH2	2.47	0.46
1:G:297:ASN:HD22	1:G:298:ILE:N	2.13	0.46
1:K:120:ILE:HD13	1:K:257:ALA:HB2	1.97	0.46
3:X:64:PHE:O	3:X:65:GLN:C	2.58	0.46
2:D:6:ILE:HD11	2:D:111:HIS:HB3	1.97	0.46
2:D:169:LYS:HZ2	2:D:173:ILE:CD1	2.29	0.46
1:E:261:VAL:O	1:E:261:VAL:CG1	2.63	0.46
1:G:182:ILE:HD11	1:G:215:PRO:CA	2.46	0.46
2:J:128:ASP:OD1	2:J:128:ASP:N	2.48	0.46
1:K:13:ALA:HB1	1:K:323:ASN:ND2	2.30	0.46
3:S:226:TYR:HB2	3:S:244:THR:HG23	1.97	0.46
1:E:32:HIS:CD2	3:X:54:MET:HG3	2.50	0.46
1:C:239:PRO:O	1:C:240:ASN:HB2	2.16	0.46
1:K:206:THR:HG22	1:K:243:ILE:HA	1.98	0.46
3:Z:191:ASN:O	3:Z:192:ASN:HB2	2.14	0.46
3:S:70:ILE:HG22	3:S:81:MET:CG	2.45	0.46
3:T:47:TRP:CD2	3:T:238:VAL:HG23	2.51	0.46
3:U:60:TYR:HE2	3:U:70:ILE:HG23	1.81	0.46
1:C:120:ILE:HG22	1:C:168:TYR:CZ	2.51	0.46
1:E:243:ILE:HG23	1:E:243:ILE:O	2.16	0.46
1:I:300:PRO:HB3	2:J:89:LEU:HD11	1.96	0.46
3:X:178:GLN:O	3:X:224:ALA:HB1	2.16	0.46
3:T:143:LEU:HD12	3:T:239:VAL:HG12	1.97	0.46
2:F:169:LYS:HZ1	2:F:173:ILE:HG21	1.77	0.46
1:G:195:TYR:O	1:G:196:GLN:HB3	2.15	0.46
2:J:169:LYS:HZ2	2:J:173:ILE:HG21	1.80	0.46
2:L:113:SER:O	2:L:117:ASN:ND2	2.49	0.46
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.51	0.46
1:C:164:ILE:O	1:C:246:GLU:HA	2.16	0.46
2:F:72:ASN:HD22	2:F:75:ARG:NH2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.97	0.46
3:T:76:THR:O	3:T:78:THR:N	2.49	0.46
1:A:302:THR:HG21	1:A:306:CYS:CB	2.46	0.45
1:C:147:PHE:CE1	1:C:230:MET:HE1	2.51	0.45
1:C:218:ALA:HB3	1:C:220:ARG:NH1	2.31	0.45
1:I:190:GLU:O	1:I:194:LEU:HD13	2.17	0.45
1:I:200:THR:HG21	1:I:249:GLY:HA3	1.97	0.45
2:J:28:ASN:HD22	2:J:145:ASP:HA	1.80	0.45
3:X:3:GLN:H	3:X:25:SER:HB3	1.80	0.45
3:X:179:HIS:HA	3:X:224:ALA:HB1	1.98	0.45
3:T:93:VAL:CG1	3:T:119:LEU:HD12	2.46	0.45
3:X:225:ASP:OD1	3:X:245:LYS:HE3	2.16	0.45
3:S:93:VAL:HG13	3:S:119:LEU:CD1	2.46	0.45
3:S:179:HIS:NE2	3:S:224:ALA:HB2	2.31	0.45
3:U:175:TRP:HB3	3:U:187:LEU:HD12	1.98	0.45
1:A:23:ILE:CG2	2:F:51:LYS:HG3	2.46	0.45
1:C:11:TYR:HB2	1:C:321:LEU:CD1	2.47	0.45
2:J:167:ARG:HA	2:J:170:ARG:HB2	1.98	0.45
3:X:18:VAL:HG22	3:X:86:LEU:CD2	2.47	0.45
3:X:39:GLN:C	3:X:92:ALA:HB1	2.42	0.45
3:S:43:GLN:CB	3:S:139:ILE:HG21	2.47	0.45
2:D:169:LYS:NZ	2:D:173:ILE:CG2	2.67	0.45
1:E:238:LYS:HG3	1:E:239:PRO:HD2	1.99	0.45
1:G:325:PRO:O	1:G:326:GLN:C	2.58	0.45
2:H:45:ILE:CD1	3:U:54:MET:HE3	2.46	0.45
3:S:112:ASP:HA	3:S:186:LEU:HB2	1.98	0.45
3:U:216:THR:HG22	3:U:217:GLY:H	1.81	0.45
2:B:84:MET:HE3	2:B:88:PHE:HE1	1.78	0.45
1:I:100:ASN:ND2	1:I:101:ASP:N	2.55	0.45
1:C:191:GLN:NE2	1:C:250:ASN:HD21	2.05	0.45
2:D:38:LYS:O	2:D:39:GLU:C	2.59	0.45
1:I:174:GLU:OE1	1:I:174:GLU:N	2.49	0.45
2:L:169:LYS:NZ	2:L:173:ILE:HG21	2.32	0.45
3:Z:32:PHE:CD2	3:Z:98:ARG:NH1	2.85	0.45
3:T:51:ILE:HB	3:T:70:ILE:CD1	2.47	0.45
2:B:169:LYS:HZ2	2:B:173:ILE:CG1	2.30	0.45
2:D:70:PHE:CE2	2:D:77:ILE:HG13	2.52	0.45
2:F:45:ILE:HD13	3:X:102:TYR:HB2	1.99	0.45
1:G:8:CYS:SG	2:H:14:TRP:HZ2	2.39	0.45
1:C:213:LEU:CD1	1:C:233:PHE:CE1	2.98	0.45
1:I:6:GLN:HG2	2:J:27:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:43:GLN:HG2	3:S:139:ILE:CG2	2.42	0.45
2:B:45:ILE:HD13	3:Y:54:MET:HE3	1.99	0.45
1:I:95:TYR:CD2	1:I:230:MET:HE3	2.51	0.45
1:I:95:TYR:CD1	1:I:230:MET:HE3	2.51	0.45
1:K:102:TYR:CZ	1:K:106:LYS:HD2	2.52	0.45
1:K:300:PRO:HG2	1:K:301:LEU:HD13	1.98	0.45
3:Z:47:TRP:CG	3:Z:238:VAL:HB	2.51	0.45
3:S:10:GLU:O	3:S:120:VAL:HA	2.17	0.45
3:T:77:ARG:NH2	3:T:77:ARG:HB3	2.32	0.45
1:C:239:PRO:O	1:C:240:ASN:CB	2.65	0.45
1:E:6:GLN:HE21	2:F:139:GLU:HB2	1.82	0.45
1:G:289:ILE:HD11	1:G:298:ILE:HD12	1.97	0.45
1:I:186:ASN:HD21	1:I:227:SER:HB3	1.81	0.45
1:A:171:THR:HB	1:G:118:ILE:HG22	1.99	0.44
1:A:180:TRP:HZ3	1:A:235:THR:HG22	1.82	0.44
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.53	0.44
1:C:302:THR:CG2	1:C:303:ILE:N	2.79	0.44
2:D:61:THR:HG21	1:E:311:LYS:HE2	1.98	0.44
1:E:204:VAL:HG22	1:E:211:GLN:HB3	1.99	0.44
2:J:41:THR:CG2	3:S:102:TYR:CZ	3.00	0.44
2:J:98:LEU:HD21	2:J:102:MET:HE2	1.98	0.44
1:K:10:GLY:HA2	2:L:10:ILE:HD13	1.99	0.44
1:G:321:LEU:HD21	2:H:111:HIS:HB3	1.98	0.44
2:H:164:GLU:HA	2:H:167:ARG:CD	2.47	0.44
3:Z:64:PHE:O	3:Z:65:GLN:C	2.60	0.44
1:A:291:SER:OG	1:A:293:MET:N	2.49	0.44
2:B:26:HIS:ND1	2:B:26:HIS:C	2.75	0.44
2:D:164:GLU:N	2:D:164:GLU:OE2	2.51	0.44
1:E:60:SER:HB3	1:E:92:ASP:HA	1.98	0.44
2:F:154:ASN:ND2	2:F:156:THR:HG23	2.32	0.44
3:T:33:ALA:HA	3:T:53:PRO:HD3	1.98	0.44
1:E:6:GLN:HB2	2:F:138:PHE:O	2.18	0.44
2:L:28:ASN:O	2:L:29:GLU:C	2.60	0.44
1:A:201:TYR:HA	1:A:213:LEU:O	2.17	0.44
2:D:118:LEU:O	2:D:121:LYS:HB3	2.18	0.44
1:G:111:ARG:O	1:G:264:GLY:N	2.49	0.44
2:H:21:TRP:CZ3	2:H:45:ILE:HG13	2.52	0.44
1:K:13:ALA:HB1	1:K:323:ASN:HD21	1.83	0.44
2:B:140:PHE:HB3	2:B:142:HIS:O	2.18	0.44
1:C:237:LEU:HD22	1:C:243:ILE:HB	2.00	0.44
2:D:56:ILE:HD11	3:Z:27:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:CYS:SG	2:H:14:TRP:CZ2	3.10	0.44
3:X:6:GLN:NE2	3:X:115:GLY:HA3	2.30	0.44
1:A:7:ILE:O	1:A:7:ILE:CG2	2.66	0.44
1:A:180:TRP:CZ2	1:A:204:VAL:HG21	2.53	0.44
1:C:126:TRP:CE3	1:C:166:ARG:NH1	2.82	0.44
1:E:120:ILE:HG22	1:E:168:TYR:CZ	2.52	0.44
2:F:55:ILE:O	2:F:56:ILE:C	2.60	0.44
1:K:182:ILE:CG2	1:K:231:GLU:HB3	2.46	0.44
3:S:6:GLN:HE22	3:S:95:TYR:HA	1.82	0.44
1:E:105:LEU:HD13	1:E:234:TRP:CD2	2.52	0.44
2:J:86:ASP:O	2:J:90:ASP:OD2	2.34	0.44
1:K:176:LEU:HB3	1:K:237:LEU:HB3	2.00	0.44
3:Z:62:GLN:O	3:Z:63:LYS:C	2.60	0.44
1:A:291:SER:OG	1:A:292:SER:N	2.48	0.44
2:B:100:VAL:HG12	2:B:101:LEU:N	2.32	0.44
2:B:133:LEU:HB2	2:B:137:CYS:O	2.18	0.44
1:C:56:LEU:O	1:C:57:ARG:C	2.61	0.44
1:I:179:LEU:CD2	1:I:234:TRP:HB3	2.48	0.44
1:C:238:LYS:HG3	1:C:239:PRO:HD2	2.00	0.43
2:D:55:ILE:O	2:D:56:ILE:C	2.60	0.43
2:F:177:ARG:O	2:F:180:VAL:HG23	2.18	0.43
1:G:204:VAL:HG21	1:G:209:LEU:HD21	1.98	0.43
1:I:218:ALA:HB3	1:I:220:ARG:NH1	2.32	0.43
1:I:240:ASN:N	1:I:240:ASN:OD1	2.50	0.43
3:X:23:THR:HG23	3:X:78:THR:HB	1.99	0.43
3:X:51:ILE:CB	3:X:70:ILE:HD11	2.44	0.43
3:S:4:LEU:HD22	3:S:22:CYS:SG	2.58	0.43
3:T:68:VAL:HG12	3:T:83:LEU:HG	1.99	0.43
2:F:133:LEU:HD12	2:F:133:LEU:HA	1.81	0.43
1:I:56:LEU:HA	1:I:74:PHE:CZ	2.53	0.43
2:J:70:PHE:CD1	2:J:78:GLU:HA	2.53	0.43
2:L:94:TYR:HD2	2:L:95:ASN:HD22	1.66	0.43
3:Z:97:ALA:HB1	3:Z:111:PHE:HB3	2.00	0.43
3:T:18:VAL:HG12	3:T:86:LEU:HD11	1.99	0.43
2:B:30:GLN:NE2	2:B:145:ASP:HB2	2.34	0.43
2:B:163:SER:O	2:B:167:ARG:HG3	2.18	0.43
3:Z:19:LYS:HG2	3:Z:82:ASP:HB3	2.01	0.43
3:Z:39:GLN:OE1	3:Z:178:GLN:OE1	2.35	0.43
3:S:43:GLN:HB3	3:S:139:ILE:HG21	2.00	0.43
3:U:18:VAL:CG2	3:U:83:LEU:HD23	2.48	0.43
1:A:323:ASN:O	1:A:323:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:LEU:HD12	2:D:103:GLU:HG2	2.01	0.43
1:E:168:TYR:O	1:E:242:ALA:HA	2.17	0.43
2:F:126:LEU:HD21	2:F:152:VAL:HG22	2.00	0.43
1:K:20:VAL:CG2	1:K:30:VAL:HG11	2.48	0.43
3:X:32:PHE:CD1	3:X:32:PHE:N	2.86	0.43
3:Y:54:MET:HB2	3:Y:54:MET:HE2	1.92	0.43
3:T:170:ASN:N	3:T:170:ASN:HD22	2.15	0.43
1:A:269:MET:HE2	1:A:285:PRO:HD3	2.00	0.43
2:B:102:MET:HE1	2:D:102:MET:SD	2.59	0.43
2:D:124:LEU:HD13	2:F:134:GLY:HA2	2.00	0.43
2:D:142:HIS:CE1	2:D:157:TYR:OH	2.71	0.43
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.83	0.43
1:G:56:LEU:HA	1:G:74:PHE:CZ	2.53	0.43
1:I:9:ILE:HG23	2:J:118:LEU:HD23	2.00	0.43
1:I:75:ILE:HG13	1:I:76:ASN:N	2.34	0.43
2:L:172:GLU:OE2	2:L:173:ILE:N	2.51	0.43
3:U:93:VAL:HG22	3:U:119:LEU:HD13	2.00	0.43
1:A:106:LYS:HB3	1:A:268:ILE:HD12	2.00	0.43
1:A:117:LYS:NZ	1:A:150:ASN:HD21	2.17	0.43
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.83	0.43
2:D:66:VAL:HG22	2:F:83:LYS:NZ	2.34	0.43
2:D:68:ARG:NE	2:F:79:ASN:HD22	2.17	0.43
2:D:179:LEU:N	2:D:179:LEU:CD1	2.78	0.43
3:X:43:GLN:OE1	3:X:139:ILE:HG21	2.18	0.43
2:D:26:HIS:CB	2:D:149:MET:CE	2.97	0.43
1:E:38:GLU:O	1:E:296:HIS:HA	2.18	0.43
1:I:20:VAL:HG22	1:I:30:VAL:CG1	2.49	0.43
1:I:197:ASN:OD1	1:I:197:ASN:N	2.51	0.43
1:I:297:ASN:C	1:I:297:ASN:ND2	2.77	0.43
3:S:2:VAL:HG12	3:S:26:GLU:CD	2.43	0.43
2:F:154:ASN:C	2:F:154:ASN:ND2	2.76	0.43
1:I:64:TRP:HZ2	1:I:77:VAL:HG21	1.83	0.43
1:I:134:GLY:HA3	1:I:153:TRP:HB3	2.00	0.43
3:X:61:ALA:O	3:X:62:GLN:C	2.61	0.43
3:T:249:LEU:HD23	3:T:249:LEU:N	2.33	0.43
1:A:289:ILE:HG22	1:A:290:ASN:N	2.34	0.43
2:D:62:GLN:HG2	2:D:92:TRP:CD2	2.54	0.43
2:D:72:ASN:ND2	2:D:72:ASN:O	2.52	0.43
2:D:141:TYR:O	2:D:142:HIS:C	2.60	0.43
2:F:5:ALA:HB1	2:F:115:VAL:CG1	2.48	0.43
2:F:142:HIS:CD2	2:F:162:TYR:CD1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:ASN:C	1:G:323:ASN:HD22	2.27	0.43
2:H:48:VAL:O	2:H:49:THR:C	2.61	0.43
3:Y:7:SER:HB2	3:Y:20:VAL:HG23	2.00	0.43
3:S:36:TRP:CE2	3:S:81:MET:HB2	2.54	0.43
1:A:295:PHE:CZ	2:B:59:MET:HE3	2.54	0.43
1:C:299:HIS:HA	1:C:300:PRO:HD3	1.83	0.43
2:D:124:LEU:N	2:D:124:LEU:HD23	2.34	0.43
1:E:180:TRP:CZ2	1:E:204:VAL:HG21	2.54	0.43
1:G:97:GLY:HA3	1:G:230:MET:O	2.19	0.43
2:H:80:LEU:HD21	2:L:80:LEU:CD2	2.49	0.43
3:X:11:VAL:HG22	3:X:121:THR:HB	1.99	0.43
3:Z:36:TRP:CD2	3:Z:81:MET:HB2	2.54	0.43
3:U:91:THR:CG2	3:U:121:THR:HG23	2.49	0.43
2:B:98:LEU:HA	2:F:58:LYS:HZ3	1.85	0.42
1:C:20:VAL:HG21	1:C:318:ALA:HB2	2.01	0.42
1:E:11:TYR:CZ	2:F:6:ILE:HG23	2.54	0.42
1:G:7:ILE:HD12	2:H:149:MET:CE	2.49	0.42
1:G:10:GLY:HA3	2:H:14:TRP:CZ2	2.54	0.42
2:H:159:TYR:C	2:H:161:GLN:H	2.26	0.42
1:K:285:PRO:HD3	1:K:301:LEU:O	2.19	0.42
2:D:94:TYR:HD2	2:D:95:ASN:HD22	1.67	0.42
1:E:8:CYS:C	1:E:9:ILE:HD13	2.44	0.42
2:H:28:ASN:ND2	2:H:145:ASP:HA	2.33	0.42
2:H:118:LEU:O	2:H:122:VAL:HG23	2.19	0.42
1:C:17:THR:O	1:C:17:THR:CG2	2.67	0.42
2:D:68:ARG:CZ	2:F:79:ASN:HD22	2.32	0.42
2:F:71:ASN:OD1	2:F:72:ASN:N	2.52	0.42
2:H:80:LEU:HD23	2:J:80:LEU:HD21	1.98	0.42
2:H:167:ARG:HA	2:H:170:ARG:HB2	2.02	0.42
3:X:57:THR:HA	3:X:58:PRO:HD3	1.85	0.42
3:Z:47:TRP:CD2	3:Z:238:VAL:HB	2.54	0.42
3:T:143:LEU:HD23	3:T:163:GLY:HA3	2.00	0.42
3:U:244:THR:HG23	3:U:244:THR:O	2.18	0.42
2:D:169:LYS:HZ2	2:D:173:ILE:CG1	2.32	0.42
2:F:45:ILE:HD13	3:X:102:TYR:CB	2.49	0.42
2:F:86:ASP:O	2:F:87:GLY:C	2.62	0.42
2:J:94:TYR:C	2:J:94:TYR:CD2	2.97	0.42
3:Z:177:GLN:HB2	3:Z:187:LEU:HD11	2.01	0.42
1:A:60:SER:OG	1:A:92:ASP:OD2	2.24	0.42
1:I:204:VAL:HG12	1:I:245:PHE:CD2	2.55	0.42
1:K:146:SER:OG	1:K:147:PHE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:THR:HA	1:G:248:ASN:OD1	2.19	0.42
2:H:163:SER:O	2:H:167:ARG:HG3	2.19	0.42
2:J:42:GLN:HE22	3:S:102:TYR:N	2.18	0.42
3:U:37:VAL:HG11	3:U:45:LEU:HD12	2.01	0.42
1:A:147:PHE:CZ	1:A:148:PHE:HD1	2.38	0.42
2:D:164:GLU:O	2:D:165:GLU:C	2.61	0.42
1:E:309:TYR:HE2	2:F:89:LEU:HD13	1.84	0.42
1:G:323:ASN:HD22	1:G:325:PRO:HD3	1.83	0.42
2:H:73:LEU:HD22	1:K:101:ASP:OD2	2.19	0.42
2:H:94:TYR:O	2:H:95:ASN:C	2.62	0.42
1:I:108:LEU:CD1	1:I:236:ILE:HD11	2.41	0.42
1:I:120:ILE:HD13	1:I:257:ALA:HB2	2.02	0.42
3:X:203:SER:O	3:X:213:LEU:HD12	2.18	0.42
1:A:62:ALA:HB2	1:A:102:TYR:CE1	2.54	0.42
1:A:174:GLU:OE1	1:A:259:LYS:NZ	2.52	0.42
1:C:54:LEU:HD23	1:C:83:ILE:HG12	2.02	0.42
2:H:45:ILE:HD12	3:U:102:TYR:CG	2.54	0.42
2:J:169:LYS:HZ3	2:J:173:ILE:HG21	1.84	0.42
3:Z:93:VAL:HG22	3:Z:119:LEU:HD13	2.01	0.42
3:Z:156:THR:OG1	3:Z:216:THR:HG22	2.20	0.42
3:S:170:ASN:N	3:S:170:ASN:HD22	2.18	0.42
1:C:105:LEU:HD22	1:C:234:TRP:CD2	2.55	0.42
1:I:56:LEU:HD11	1:I:61:VAL:HG22	2.02	0.42
1:K:51:VAL:HG12	1:K:81:SER:HB2	2.02	0.42
2:L:5:ALA:HB2	2:L:116:LYS:HB2	2.02	0.42
3:X:145:GLN:O	3:X:146:PRO:C	2.62	0.42
3:X:196:SER:O	3:X:197:GLY:C	2.62	0.42
1:A:96:PRO:HB3	1:A:223:VAL:HG11	2.01	0.42
1:E:30:VAL:HG23	1:E:32:HIS:H	1.85	0.42
2:J:93:THR:HG23	2:J:97:GLU:OE1	2.20	0.42
2:L:71:ASN:HB2	2:L:74:GLU:OE1	2.19	0.42
3:X:73:ASP:OD2	3:X:76:THR:N	2.38	0.42
3:S:81:MET:HE2	3:S:81:MET:HB3	1.94	0.42
2:B:101:LEU:HD23	2:F:58:LYS:HE3	2.02	0.41
2:F:6:ILE:N	2:F:112:ASP:OD1	2.51	0.41
3:Y:20:VAL:CG2	3:Y:118:THR:HG21	2.48	0.41
3:T:27:VAL:HG13	3:T:77:ARG:NH1	2.35	0.41
1:A:118:ILE:HG21	1:A:259:LYS:HD2	2.02	0.41
1:C:300:PRO:HG3	1:C:309:TYR:CE2	2.55	0.41
1:G:267:THR:HG22	1:G:268:ILE:N	2.36	0.41
2:H:101:LEU:HD12	2:H:101:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:223:GLU:HB2	3:Z:248:VAL:HG23	2.02	0.41
3:S:18:VAL:HG11	3:S:120:VAL:CG1	2.50	0.41
1:C:187:ASP:HA	1:C:217:ILE:HG21	2.01	0.41
2:D:59:MET:HE2	2:F:94:TYR:HE1	1.77	0.41
2:D:89:LEU:HD23	2:D:89:LEU:HA	1.91	0.41
1:I:6:GLN:CG	2:J:27:SER:HB3	2.50	0.41
2:J:97:GLU:O	2:J:101:LEU:HD13	2.20	0.41
3:Y:119:LEU:HD23	3:Y:119:LEU:C	2.44	0.41
3:S:175:TRP:CG	3:S:213:LEU:HD22	2.56	0.41
3:U:110:VAL:CG1	3:U:174:ALA:HB2	2.50	0.41
1:C:180:TRP:CZ3	1:C:235:THR:HG22	2.52	0.41
2:F:113:SER:O	2:F:114:ASN:C	2.63	0.41
2:H:167:ARG:HB3	2:H:170:ARG:CZ	2.50	0.41
1:I:9:ILE:HD13	2:J:24:TYR:CD2	2.56	0.41
1:I:289:ILE:HG22	1:I:291:SER:H	1.85	0.41
1:I:321:LEU:HD23	2:J:111:HIS:ND1	2.34	0.41
1:K:267:THR:HG22	1:K:268:ILE:N	2.35	0.41
3:S:167:ASN:C	3:S:230:THR:HG21	2.44	0.41
3:T:187:LEU:CD2	3:T:198:ILE:HD12	2.51	0.41
1:A:10:GLY:HA2	2:B:10:ILE:HG21	2.02	0.41
1:C:283:GLN:OE1	1:C:288:ALA:HB2	2.19	0.41
1:G:48:LEU:HB3	1:G:81:SER:OG	2.20	0.41
3:Z:5:VAL:O	3:Z:22:CYS:HA	2.21	0.41
3:S:112:ASP:OD1	3:S:113:HIS:N	2.53	0.41
1:A:259:LYS:NZ	1:G:119:GLN:HE22	2.18	0.41
2:B:169:LYS:O	2:B:172:GLU:HG3	2.20	0.41
1:E:31:THR:HG23	1:E:321:LEU:O	2.21	0.41
2:H:49:THR:HG21	3:U:32:PHE:HZ	1.84	0.41
2:H:84:MET:HE2	2:H:85:GLU:HG3	2.02	0.41
2:H:123:ARG:O	2:H:126:LEU:O	2.37	0.41
3:X:76:THR:HG1	3:X:78:THR:HG23	1.85	0.41
2:H:6:ILE:HD12	2:H:112:ASP:HA	2.02	0.41
3:X:26:GLU:OE2	3:X:98:ARG:NH1	2.54	0.41
3:Y:32:PHE:CD2	3:Y:98:ARG:HD2	2.55	0.41
4:O:1:NAG:H61	4:O:2:NAG:O7	2.21	0.41
1:A:323:ASN:C	1:A:323:ASN:ND2	2.79	0.41
2:H:90:ASP:CG	2:L:61:THR:HG22	2.45	0.41
1:I:121:ILE:O	1:I:121:ILE:HG22	2.21	0.41
3:X:68:VAL:HG12	3:X:69:THR:N	2.36	0.41
3:Y:151:LYS:O	3:Y:248:VAL:HA	2.21	0.41
2:B:84:MET:HE1	2:D:84:MET:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:ALA:O	2:D:8:GLY:N	2.53	0.41
1:E:72:ASP:C	1:E:74:PHE:N	2.79	0.41
1:E:118:ILE:HG21	1:E:259:LYS:HD2	2.02	0.41
1:E:121:ILE:HD12	1:E:254:PRO:HG2	2.02	0.41
2:F:75:ARG:O	2:F:78:GLU:HB3	2.21	0.41
1:G:178:VAL:O	1:G:179:LEU:HD23	2.20	0.41
1:I:309:TYR:CD2	2:J:89:LEU:HD13	2.56	0.41
2:J:45:ILE:HD12	3:S:102:TYR:HB2	2.03	0.41
3:X:60:TYR:CE2	3:X:70:ILE:HG23	2.49	0.41
3:X:81:MET:HE3	3:X:83:LEU:CB	2.51	0.41
3:X:153:LEU:HD13	3:X:248:VAL:CG1	2.50	0.41
3:X:225:ASP:OD1	3:X:245:LYS:CE	2.69	0.41
3:Y:162:THR:HG23	3:Y:210:THR:CB	2.37	0.41
3:S:209:ASN:HD22	3:S:209:ASN:N	2.18	0.41
3:T:40:ALA:HB3	3:T:43:GLN:OE1	2.21	0.41
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.95	0.41
1:C:121:ILE:HG21	1:C:126:TRP:CZ2	2.56	0.41
1:E:130:GLU:HG2	1:E:133:LEU:HB2	2.02	0.41
1:G:195:TYR:O	1:G:196:GLN:CB	2.69	0.41
1:K:221:SER:O	1:K:229:ARG:NH2	2.53	0.41
3:X:16:SER:O	3:X:86:LEU:HG	2.21	0.41
3:X:145:GLN:HA	3:X:146:PRO:HD2	1.95	0.41
3:T:20:VAL:HG22	3:T:21:SER:N	2.36	0.41
2:B:72:ASN:ND2	2:B:72:ASN:O	2.55	0.40
1:E:314:ARG:CG	1:E:314:ARG:HH11	2.34	0.40
2:F:113:SER:OG	2:F:117:ASN:ND2	2.54	0.40
2:F:172:GLU:C	2:F:172:GLU:CD	2.89	0.40
1:I:172:ASN:HD22	1:I:172:ASN:H	1.64	0.40
3:X:67:ARG:NH1	3:X:84:ARG:O	2.54	0.40
3:Y:30:SER:O	3:Y:54:MET:HE2	2.21	0.40
3:T:32:PHE:CB	3:T:98:ARG:HD2	2.51	0.40
2:B:2:LEU:O	2:F:113:SER:OG	2.39	0.40
1:C:105:LEU:HD22	1:C:234:TRP:CG	2.56	0.40
1:C:296:HIS:HD2	1:C:307:PRO:HB2	1.86	0.40
2:F:145:ASP:OD1	2:F:147:GLU:N	2.52	0.40
1:I:53:PRO:HB3	1:I:82:TYR:CE2	2.57	0.40
1:K:168:TYR:O	1:K:242:ALA:HA	2.21	0.40
3:S:219:GLN:O	3:S:248:VAL:HG21	2.21	0.40
3:T:47:TRP:CD2	3:T:238:VAL:CG2	3.04	0.40
3:T:162:THR:CG2	3:T:163:GLY:N	2.85	0.40
2:D:169:LYS:HZ3	2:D:173:ILE:HG21	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:THR:OG1	1:G:32:HIS:ND1	2.49	0.40
3:X:2:VAL:HG21	3:X:113:HIS:CG	2.56	0.40
1:A:117:LYS:HG3	1:A:256:TYR:HB3	2.03	0.40
2:B:158:ASP:O	2:B:159:TYR:C	2.65	0.40
1:C:13:ALA:HB1	2:D:15:GLN:NE2	2.35	0.40
1:C:203:SER:HB3	1:C:212:ARG:HG3	2.04	0.40
2:D:30:GLN:HE21	2:D:145:ASP:HB2	1.87	0.40
1:E:42:ASN:OD1	1:E:42:ASN:C	2.63	0.40
1:E:68:ASN:OD1	1:E:70:MET:HG2	2.21	0.40
1:G:191:GLN:HE22	1:G:198:PRO:C	2.29	0.40
1:K:10:GLY:HA3	2:L:14:TRP:CZ2	2.56	0.40
3:Z:157:ALA:HB2	3:Z:218:LEU:HD11	2.02	0.40
1:E:152:VAL:CG1	1:E:253:ALA:HB3	2.51	0.40
2:F:128:ASP:OD1	2:F:128:ASP:C	2.65	0.40
1:K:202:ILE:HG22	1:K:203:SER:N	2.36	0.40
2:L:152:VAL:HG22	2:L:157:TYR:CD1	2.56	0.40
3:S:12:LYS:CD	3:S:18:VAL:HG12	2.51	0.40
4:Q:2:NAG:H83	4:Q:2:NAG:O3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/338 (95%)	278 (87%)	37 (12%)	6 (2%)	6	33
1	C	321/338 (95%)	282 (88%)	36 (11%)	3 (1%)	14	47
1	E	321/338 (95%)	271 (84%)	47 (15%)	3 (1%)	14	47
1	G	321/338 (95%)	280 (87%)	37 (12%)	4 (1%)	10	42
1	I	321/338 (95%)	282 (88%)	37 (12%)	2 (1%)	21	56
1	K	321/338 (95%)	287 (89%)	30 (9%)	4 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	178/182 (98%)	159 (89%)	16 (9%)	3 (2%)	7	35
2	D	178/182 (98%)	155 (87%)	20 (11%)	3 (2%)	7	35
2	F	178/182 (98%)	153 (86%)	24 (14%)	1 (1%)	21	56
2	H	172/182 (94%)	150 (87%)	19 (11%)	3 (2%)	7	35
2	J	172/182 (94%)	146 (85%)	23 (13%)	3 (2%)	7	35
2	L	172/182 (94%)	158 (92%)	13 (8%)	1 (1%)	21	56
3	S	229/280 (82%)	206 (90%)	21 (9%)	2 (1%)	14	47
3	T	230/280 (82%)	204 (89%)	25 (11%)	1 (0%)	30	62
3	U	230/280 (82%)	204 (89%)	25 (11%)	1 (0%)	30	62
3	X	231/280 (82%)	204 (88%)	25 (11%)	2 (1%)	14	47
3	Y	231/280 (82%)	203 (88%)	25 (11%)	3 (1%)	9	40
3	Z	232/280 (83%)	201 (87%)	29 (12%)	2 (1%)	14	47
All	All	4359/4800 (91%)	3823 (88%)	489 (11%)	47 (1%)	11	43

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	E	73	GLU
3	Y	43	GLN
2	B	128	ASP
2	B	178	SER
2	D	128	ASP
1	G	196	GLN
1	G	218	ALA
2	H	143	LYS
2	J	127	ARG
2	J	132	GLU
2	B	32	SER
2	J	29	GLU
3	Z	65	GLN
3	S	109	CYS
3	T	196	SER
1	A	158	ASN
1	C	240	ASN
1	E	15	ASN
1	E	277	ASN
2	F	87	GLY

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Mol	Chain	Res	Type
1	I	57	ARG
1	I	261	VAL
1	K	170	ASN
3	Y	123	SER
1	A	73	GLU
1	A	148	PHE
1	C	198	PRO
2	D	178	SER
1	G	15	ASN
2	H	32	SER
1	K	158	ASN
1	K	198	PRO
2	L	127	ARG
3	Z	180	GLN
1	A	34	GLN
1	K	261	VAL
3	U	217	GLY
1	G	261	VAL
1	A	261	VAL
2	D	173	ILE
2	H	160	PRO
3	X	58	PRO
3	Y	41	PRO
3	S	41	PRO
1	C	75	ILE
3	X	37	VAL

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	291/304 (96%)	259 (89%)	32 (11%)	6	26
1	C	291/304 (96%)	263 (90%)	28 (10%)	8	32
1	E	291/304 (96%)	257 (88%)	34 (12%)	5	23
1	G	291/304 (96%)	267 (92%)	24 (8%)	10	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	291/304 (96%)	260 (89%)	31 (11%)	6	27
1	K	291/304 (96%)	257 (88%)	34 (12%)	5	23
2	B	154/156 (99%)	121 (79%)	33 (21%)	1	6
2	D	154/156 (99%)	127 (82%)	27 (18%)	2	10
2	F	154/156 (99%)	129 (84%)	25 (16%)	2	12
2	H	149/156 (96%)	129 (87%)	20 (13%)	4	19
2	J	149/156 (96%)	127 (85%)	22 (15%)	3	15
2	L	149/156 (96%)	128 (86%)	21 (14%)	3	17
3	S	194/220 (88%)	180 (93%)	14 (7%)	13	44
3	T	195/220 (89%)	179 (92%)	16 (8%)	10	39
3	U	195/220 (89%)	172 (88%)	23 (12%)	5	23
3	X	196/220 (89%)	174 (89%)	22 (11%)	6	25
3	Y	196/220 (89%)	161 (82%)	35 (18%)	2	9
3	Z	196/220 (89%)	171 (87%)	25 (13%)	4	20
All	All	3827/4080 (94%)	3361 (88%)	466 (12%)	5	22

All (466) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	17	THR
1	A	25	GLU
1	A	48	LEU
1	A	73	GLU
1	A	88	ASN
1	A	135	VAL
1	A	149	ARG
1	A	165	LYS
1	A	178	VAL
1	A	179	LEU
1	A	199	THR
1	A	204	VAL
1	A	213	LEU
1	A	222	LYS
1	A	223	VAL
1	A	226	GLN
1	A	243	ILE

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Mol	Chain	Res	Type
1	A	244	ASN
1	A	263	LYS
1	A	267	THR
1	A	274	GLU
1	A	278	CYS
1	A	292	SER
1	A	297	ASN
1	A	303	ILE
1	A	312	SER
1	A	314	ARG
1	A	316	VAL
1	A	321	LEU
1	A	322	ARG
1	A	324	SER
2	B	10	ILE
2	B	18	VAL
2	B	19	ASP
2	B	26	HIS
2	B	29	GLU
2	B	41	THR
2	B	52	VAL
2	B	58	LYS
2	B	72	ASN
2	B	76	ARG
2	B	77	ILE
2	B	82	LYS
2	B	84	MET
2	B	93	THR
2	B	98	LEU
2	B	100	VAL
2	B	101	LEU
2	B	103	GLU
2	B	113	SER
2	B	116	LYS
2	B	118	LEU
2	B	121	LYS
2	B	127	ARG
2	B	133	LEU
2	B	147	GLU
2	B	151	SER
2	B	154	ASN
2	B	164	GLU

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Mol	Chain	Res	Type
2	B	167	ARG
2	B	169	LYS
2	B	172	GLU
2	B	176	VAL
2	B	180	VAL
1	C	8	CYS
1	C	16	SER
1	C	23	ILE
1	C	35	ASP
1	C	40	LYS
1	C	73	GLU
1	C	79	GLU
1	C	105	LEU
1	C	117	LYS
1	C	146	SER
1	C	152	VAL
1	C	155	ILE
1	C	160	THR
1	C	178	VAL
1	C	182	ILE
1	C	199	THR
1	C	226	GLN
1	C	244	ASN
1	C	250	ASN
1	C	260	ILE
1	C	261	VAL
1	C	262	LYS
1	C	267	THR
1	C	278	CYS
1	C	290	ASN
1	C	313	ASN
1	C	321	LEU
1	C	326	GLN
2	D	18	VAL
2	D	19	ASP
2	D	22	TYR
2	D	32	SER
2	D	43	LYS
2	D	54	SER
2	D	56	ILE
2	D	58	LYS
2	D	61	THR

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Mol	Chain	Res	Type
2	D	62	GLN
2	D	68	ARG
2	D	72	ASN
2	D	113	SER
2	D	118	LEU
2	D	124	LEU
2	D	128	ASP
2	D	148	CYS
2	D	150	GLU
2	D	153	ARG
2	D	154	ASN
2	D	164	GLU
2	D	167	ARG
2	D	168	LEU
2	D	169	LYS
2	D	172	GLU
2	D	179	LEU
2	D	180	VAL
1	E	4	GLU
1	E	6	GLN
1	E	8	CYS
1	E	17	THR
1	E	19	GLN
1	E	22	THR
1	E	23	ILE
1	E	28	VAL
1	E	30	VAL
1	E	70	MET
1	E	75	ILE
1	E	101	ASP
1	E	135	VAL
1	E	149	ARG
1	E	165	LYS
1	E	166	ARG
1	E	179	LEU
1	E	199	THR
1	E	204	VAL
1	E	213	LEU
1	E	219	THR
1	E	221	SER
1	E	223	VAL
1	E	261	VAL

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Mol	Chain	Res	Type
1	E	266	SER
1	E	267	THR
1	E	274	GLU
1	E	292	SER
1	E	293	MET
1	E	297	ASN
1	E	302	THR
1	E	312	SER
1	E	314	ARG
1	E	317	LEU
2	F	10	ILE
2	F	18	VAL
2	F	19	ASP
2	F	38	LYS
2	F	40	SER
2	F	43	LYS
2	F	52	VAL
2	F	62	GLN
2	F	68	ARG
2	F	72	ASN
2	F	76	ARG
2	F	77	ILE
2	F	93	THR
2	F	101	LEU
2	F	116	LYS
2	F	118	LEU
2	F	126	LEU
2	F	133	LEU
2	F	139	GLU
2	F	153	ARG
2	F	154	ASN
2	F	164	GLU
2	F	167	ARG
2	F	169	LYS
2	F	172	GLU
1	G	17	THR
1	G	23	ILE
1	G	47	ASP
1	G	86	LYS
1	G	133	LEU
1	G	136	SER
1	G	152	VAL

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Mol	Chain	Res	Type
1	G	159	SER
1	G	160	THR
1	G	165	LYS
1	G	197	ASN
1	G	203	SER
1	G	222	LYS
1	G	227	SER
1	G	244	ASN
1	G	262	LYS
1	G	265	ASP
1	G	272	GLU
1	G	274	GLU
1	G	297	ASN
1	G	303	ILE
1	G	319	THR
1	G	323	ASN
1	G	326	GLN
2	H	19	ASP
2	H	38	LYS
2	H	43	LYS
2	H	52	VAL
2	H	58	LYS
2	H	59	MET
2	H	64	GLU
2	H	69	GLU
2	H	73	LEU
2	H	75	ARG
2	H	80	LEU
2	H	91	VAL
2	H	98	LEU
2	H	100	VAL
2	H	101	LEU
2	H	148	CYS
2	H	153	ARG
2	H	164	GLU
2	H	167	ARG
2	H	169	LYS
1	I	8	CYS
1	I	73	GLU
1	I	77	VAL
1	I	100	ASN
1	I	117	LYS

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Mol	Chain	Res	Type
1	I	118	ILE
1	I	128	SER
1	I	135	VAL
1	I	149	ARG
1	I	165	LYS
1	I	172	ASN
1	I	178	VAL
1	I	182	ILE
1	I	197	ASN
1	I	199	THR
1	I	203	SER
1	I	204	VAL
1	I	219	THR
1	I	222	LYS
1	I	226	GLN
1	I	227	SER
1	I	240	ASN
1	I	273	LEU
1	I	274	GLU
1	I	297	ASN
1	I	302	THR
1	I	305	GLU
1	I	311	LYS
1	I	314	ARG
1	I	315	LEU
1	I	321	LEU
2	J	19	ASP
2	J	38	LYS
2	J	45	ILE
2	J	48	VAL
2	J	53	ASN
2	J	58	LYS
2	J	62	GLN
2	J	72	ASN
2	J	76	ARG
2	J	81	ASN
2	J	84	MET
2	J	93	THR
2	J	98	LEU
2	J	105	GLU
2	J	121	LYS
2	J	128	ASP

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Mol	Chain	Res	Type
2	J	137	CYS
2	J	139	GLU
2	J	150	GLU
2	J	154	ASN
2	J	164	GLU
2	J	167	ARG
1	K	8	CYS
1	K	22	THR
1	K	23	ILE
1	K	34	GLN
1	K	75	ILE
1	K	77	VAL
1	K	79	GLU
1	K	127	SER
1	K	136	SER
1	K	149	ARG
1	K	152	VAL
1	K	154	LEU
1	K	165	LYS
1	K	178	VAL
1	K	179	LEU
1	K	204	VAL
1	K	223	VAL
1	K	224	ASN
1	K	226	GLN
1	K	230	MET
1	K	236	ILE
1	K	259	LYS
1	K	265	ASP
1	K	267	THR
1	K	272	GLU
1	K	274	GLU
1	K	278	CYS
1	K	297	ASN
1	K	301	LEU
1	K	302	THR
1	K	314	ARG
1	K	315	LEU
1	K	317	LEU
1	K	321	LEU
2	L	19	ASP
2	L	22	TYR

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Mol	Chain	Res	Type
2	L	27	SER
2	L	29	GLU
2	L	38	LYS
2	L	41	THR
2	L	43	LYS
2	L	54	SER
2	L	58	LYS
2	L	76	ARG
2	L	93	THR
2	L	98	LEU
2	L	100	VAL
2	L	103	GLU
2	L	137	CYS
2	L	148	CYS
2	L	153	ARG
2	L	164	GLU
2	L	167	ARG
2	L	172	GLU
2	L	173	ILE
3	X	5	VAL
3	X	7	SER
3	X	18	VAL
3	X	28	THR
3	X	31	SER
3	X	48	LEU
3	X	57	THR
3	X	69	THR
3	X	70	ILE
3	X	78	THR
3	X	85	SER
3	X	87	ARG
3	X	93	VAL
3	X	98	ARG
3	X	124	SER
3	X	150	SER
3	X	192	ASN
3	X	201	ARG
3	X	207	SER
3	X	214	THR
3	X	245	LYS
3	X	246	LEU
3	Y	1	GLN

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Mol	Chain	Res	Type
3	Y	4	LEU
3	Y	5	VAL
3	Y	22	CYS
3	Y	25	SER
3	Y	29	PHE
3	Y	34	ILE
3	Y	57	THR
3	Y	68	VAL
3	Y	70	ILE
3	Y	83	LEU
3	Y	93	VAL
3	Y	103	ILE
3	Y	108	THR
3	Y	110	VAL
3	Y	121	THR
3	Y	145	GLN
3	Y	156	THR
3	Y	162	THR
3	Y	180	GLN
3	Y	190	ARG
3	Y	194	ARG
3	Y	205	SER
3	Y	213	LEU
3	Y	214	THR
3	Y	216	THR
3	Y	223	GLU
3	Y	233	SER
3	Y	234	SER
3	Y	238	VAL
3	Y	239	VAL
3	Y	244	THR
3	Y	245	LYS
3	Y	247	THR
3	Y	249	LEU
3	Z	5	VAL
3	Z	18	VAL
3	Z	19	LYS
3	Z	24	SER
3	Z	25	SER
3	Z	29	PHE
3	Z	30	SER
3	Z	48	LEU

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Mol	Chain	Res	Type
3	Z	62	GLN
3	Z	70	ILE
3	Z	82	ASP
3	Z	84	ARG
3	Z	103	ILE
3	Z	110	VAL
3	Z	122	VAL
3	Z	143	LEU
3	Z	178	GLN
3	Z	200	GLU
3	Z	205	SER
3	Z	215	ILE
3	Z	230	THR
3	Z	238	VAL
3	Z	244	THR
3	Z	245	LYS
3	Z	248	VAL
3	S	5	VAL
3	S	31	SER
3	S	34	ILE
3	S	54	MET
3	S	57	THR
3	S	70	ILE
3	S	81	MET
3	S	87	ARG
3	S	91	THR
3	S	170	ASN
3	S	192	ASN
3	S	201	ARG
3	S	238	VAL
3	S	249	LEU
3	T	1	GLN
3	T	24	SER
3	T	34	ILE
3	T	51	ILE
3	T	59	ASN
3	T	83	LEU
3	T	103	ILE
3	T	108	THR
3	T	145	GLN
3	T	171	GLN
3	T	194	ARG

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Mol	Chain	Res	Type
3	T	199	SER
3	T	213	LEU
3	T	221	GLU
3	T	245	LYS
3	T	249	LEU
3	U	19	LYS
3	U	21	SER
3	U	23	THR
3	U	25	SER
3	U	27	VAL
3	U	29	PHE
3	U	31	SER
3	U	34	ILE
3	U	35	SER
3	U	48	LEU
3	U	70	ILE
3	U	96	CYS
3	U	108	THR
3	U	143	LEU
3	U	145	GLN
3	U	158	THR
3	U	165	SER
3	U	191	ASN
3	U	200	GLU
3	U	203	SER
3	U	216	THR
3	U	230	THR
3	U	245	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	88	ASN
1	A	91	ASN
1	A	150	ASN
1	A	226	GLN
1	A	297	ASN
1	A	299	HIS
1	A	323	ASN
2	B	30	GLN
2	B	42	GLN

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Mol	Chain	Res	Type
2	B	53	ASN
2	B	60	ASN
2	B	72	ASN
2	B	79	ASN
2	B	95	ASN
2	B	129	ASN
2	B	146	ASN
2	B	154	ASN
1	C	41	HIS
1	C	91	ASN
1	C	142	GLN
1	C	186	ASN
1	C	191	GLN
1	C	197	ASN
1	C	240	ASN
1	C	299	HIS
1	C	313	ASN
2	D	15	GLN
2	D	25	HIS
2	D	30	GLN
2	D	42	GLN
2	D	53	ASN
2	D	60	ASN
2	D	62	GLN
2	D	72	ASN
2	D	79	ASN
2	D	95	ASN
2	D	125	GLN
2	D	142	HIS
2	D	146	ASN
1	E	6	GLN
1	E	19	GLN
1	E	88	ASN
1	E	150	ASN
1	E	186	ASN
1	E	191	GLN
1	E	226	GLN
1	E	296	HIS
1	E	297	ASN
2	F	30	GLN
2	F	42	GLN
2	F	72	ASN

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Mol	Chain	Res	Type
2	F	79	ASN
2	F	117	ASN
2	F	125	GLN
2	F	142	HIS
2	F	146	ASN
2	F	154	ASN
1	G	114	HIS
1	G	119	GLN
1	G	196	GLN
1	G	226	GLN
1	G	244	ASN
1	G	297	ASN
1	G	323	ASN
2	H	28	ASN
2	H	42	GLN
2	H	53	ASN
2	H	60	ASN
2	H	72	ASN
2	H	79	ASN
2	H	125	GLN
2	H	129	ASN
2	H	142	HIS
2	H	146	ASN
1	I	91	ASN
1	I	100	ASN
1	I	107	HIS
1	I	172	ASN
1	I	186	ASN
1	I	277	ASN
1	I	297	ASN
2	J	30	GLN
2	J	42	GLN
2	J	60	ASN
2	J	72	ASN
2	J	79	ASN
2	J	95	ASN
2	J	114	ASN
2	J	125	GLN
2	J	146	ASN
1	K	6	GLN
1	K	34	GLN
1	K	91	ASN

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Mol	Chain	Res	Type
1	K	114	HIS
1	K	184	HIS
1	K	224	ASN
1	K	226	GLN
1	K	283	GLN
1	K	297	ASN
1	K	299	HIS
1	K	323	ASN
2	L	28	ASN
2	L	30	GLN
2	L	42	GLN
2	L	60	ASN
2	L	71	ASN
2	L	95	ASN
2	L	117	ASN
2	L	125	GLN
2	L	142	HIS
2	L	146	ASN
3	X	170	ASN
3	X	192	ASN
3	X	219	GLN
3	Y	1	GLN
3	Y	43	GLN
3	Y	209	ASN
3	Y	219	GLN
3	Z	39	GLN
3	Z	43	GLN
3	Z	62	GLN
3	Z	113	HIS
3	Z	171	GLN
3	Z	191	ASN
3	S	3	GLN
3	S	6	GLN
3	S	39	GLN
3	S	43	GLN
3	S	170	ASN
3	S	171	GLN
3	S	178	GLN
3	T	1	GLN
3	T	39	GLN
3	T	62	GLN
3	T	170	ASN

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Mol	Chain	Res	Type
3	T	171	GLN
3	T	178	GLN
3	T	219	GLN
3	U	39	GLN
3	U	59	ASN
3	U	140	GLN
3	U	166	ASN
3	U	171	GLN
3	U	192	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

30 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	$\# Z > 2$
4	NAG	M	1	4,1	14,14,15	0.59	0	17,19,21	1.26	1 (5%)
4	NAG	M	2	4	14,14,15	0.57	0	17,19,21	1.40	1 (5%)
5	NAG	N	1	5,1	14,14,15	0.71	0	17,19,21	1.46	2 (11%)
5	NAG	N	2	5	14,14,15	0.41	0	17,19,21	0.73	0
5	BMA	N	3	5	11,11,12	0.52	0	15,15,17	1.27	2 (13%)
4	NAG	O	1	4,1	14,14,15	0.53	0	17,19,21	1.76	3 (17%)
4	NAG	O	2	4	14,14,15	0.71	1 (7%)	17,19,21	1.13	2 (11%)
5	NAG	P	1	5,1	14,14,15	0.55	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	P	2	5	14,14,15	0.51	0	17,19,21	0.91	1 (5%)
5	BMA	P	3	5	11,11,12	0.35	0	15,15,17	0.89	0
4	NAG	Q	1	4,1	14,14,15	0.58	0	17,19,21	1.84	5 (29%)
4	NAG	Q	2	4	14,14,15	0.83	0	17,19,21	1.27	2 (11%)
5	NAG	R	1	5,1	14,14,15	0.59	0	17,19,21	0.70	0
5	NAG	R	2	5	14,14,15	0.45	0	17,19,21	0.79	0
5	BMA	R	3	5	11,11,12	0.47	0	15,15,17	0.85	0
4	NAG	V	1	4,1	14,14,15	0.62	0	17,19,21	1.02	2 (11%)
4	NAG	V	2	4	14,14,15	0.68	0	17,19,21	1.32	1 (5%)
5	NAG	W	1	5,1	14,14,15	0.71	0	17,19,21	1.37	2 (11%)
5	NAG	W	2	5	14,14,15	0.68	0	17,19,21	1.10	0
5	BMA	W	3	5	11,11,12	0.69	0	15,15,17	1.52	3 (20%)
4	NAG	a	1	4,1	14,14,15	0.49	0	17,19,21	1.88	4 (23%)
4	NAG	a	2	4	14,14,15	0.81	0	17,19,21	1.14	0
5	NAG	b	1	5,1	14,14,15	0.61	0	17,19,21	1.19	2 (11%)
5	NAG	b	2	5	14,14,15	0.62	0	17,19,21	0.97	1 (5%)
5	BMA	b	3	5	11,11,12	0.63	0	15,15,17	1.17	1 (6%)
4	NAG	c	1	4,1	14,14,15	0.41	0	17,19,21	1.92	4 (23%)
4	NAG	c	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.43	2 (11%)
5	NAG	d	1	5,1	14,14,15	0.60	0	17,19,21	1.10	2 (11%)
5	NAG	d	2	5	14,14,15	0.66	0	17,19,21	1.09	1 (5%)
5	BMA	d	3	5	11,11,12	0.54	0	15,15,17	0.75	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
4	NAG	M	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	4/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	3/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	W	2	5	-	4/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
4	NAG	a	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	a	2	4	-	4/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	3/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
4	NAG	c	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	4/6/23/26	0/1/1/1
5	BMA	d	3	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	2	NAG	C1-C2	2.24	1.55	1.52
4	c	2	NAG	C1-C2	2.20	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	1	NAG	C1-O5-C5	4.89	118.74	112.19
4	M	2	NAG	C1-O5-C5	4.46	118.16	112.19
4	O	1	NAG	C4-C3-C2	-4.35	104.64	111.02
4	M	1	NAG	O5-C1-C2	-4.09	104.96	111.29
4	a	1	NAG	C4-C3-C2	-4.08	105.04	111.02
4	a	1	NAG	C1-O5-C5	4.02	117.57	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	1	NAG	C4-C3-C2	-3.79	105.46	111.02
4	Q	1	NAG	C1-C2-N2	3.65	116.18	110.43
4	V	2	NAG	C4-C3-C2	3.52	116.18	111.02
4	c	1	NAG	C4-C3-C2	-3.49	105.90	111.02
4	c	1	NAG	C1-C2-N2	3.48	115.92	110.43
5	N	1	NAG	C4-C3-C2	3.45	116.07	111.02
4	c	2	NAG	C1-O5-C5	3.44	116.80	112.19
4	Q	2	NAG	C4-C3-C2	3.37	115.95	111.02
4	O	1	NAG	C1-C2-N2	3.33	115.69	110.43
5	W	1	NAG	O5-C1-C2	-3.24	106.28	111.29
5	b	1	NAG	O5-C1-C2	-3.23	106.29	111.29
5	N	3	BMA	C1-C2-C3	3.19	114.28	109.64
4	O	2	NAG	C1-O5-C5	3.17	116.44	112.19
5	b	3	BMA	C1-C2-C3	3.15	114.23	109.64
5	W	3	BMA	C1-C2-C3	3.09	114.15	109.64
5	W	3	BMA	O5-C5-C6	3.08	113.66	107.66
5	d	2	NAG	C1-O5-C5	3.06	116.29	112.19
5	b	2	NAG	C4-C3-C2	2.96	115.35	111.02
5	b	1	NAG	C1-O5-C5	2.93	116.11	112.19
5	d	1	NAG	C1-C2-N2	-2.78	106.05	110.43
5	W	3	BMA	C1-O5-C5	2.75	115.88	112.19
4	Q	1	NAG	C1-O5-C5	2.72	115.84	112.19
4	a	1	NAG	C1-C2-N2	2.69	114.68	110.43
4	c	2	NAG	C4-C3-C2	2.66	114.91	111.02
5	N	1	NAG	O5-C1-C2	2.63	115.37	111.29
4	V	1	NAG	C2-N2-C7	2.57	126.35	122.90
4	O	1	NAG	O5-C1-C2	-2.55	107.34	111.29
5	W	1	NAG	C4-C3-C2	2.52	114.71	111.02
5	d	1	NAG	C1-O5-C5	2.49	115.52	112.19
4	Q	1	NAG	O4-C4-C3	2.49	116.24	110.38
4	a	1	NAG	O5-C1-C2	-2.47	107.47	111.29
4	Q	1	NAG	O5-C1-C2	-2.29	107.74	111.29
4	V	1	NAG	O5-C1-C2	-2.18	107.92	111.29
4	Q	2	NAG	C1-O5-C5	2.16	115.08	112.19
5	N	3	BMA	O5-C5-C4	-2.11	105.69	110.83
4	c	1	NAG	O5-C1-C2	-2.10	108.04	111.29
5	P	2	NAG	C4-C3-C2	2.07	114.05	111.02
4	O	2	NAG	C1-C2-N2	2.05	113.66	110.43

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
5	W	1	NAG	C1

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	C1-C2-N2-C7
4	Q	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C3-C2-N2-C7
4	V	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
4	a	1	NAG	C1-C2-N2-C7
4	a	1	NAG	O7-C7-N2-C2
4	c	1	NAG	C1-C2-N2-C7
4	c	1	NAG	O7-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
5	d	1	NAG	C8-C7-N2-C2
5	d	1	NAG	O7-C7-N2-C2
5	d	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C8-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	a	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	c	1	NAG	C8-C7-N2-C2
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	d	2	NAG	C8-C7-N2-C2
5	W	3	BMA	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
5	W	3	BMA	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
5	W	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
5	W	2	NAG	O7-C7-N2-C2
5	d	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
4	a	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C8-C7-N2-C2
4	c	1	NAG	O5-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
4	a	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C1-C2-N2-C7
4	c	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O7-C7-N2-C2
5	W	2	NAG	C4-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7
4	a	1	NAG	C3-C2-N2-C7

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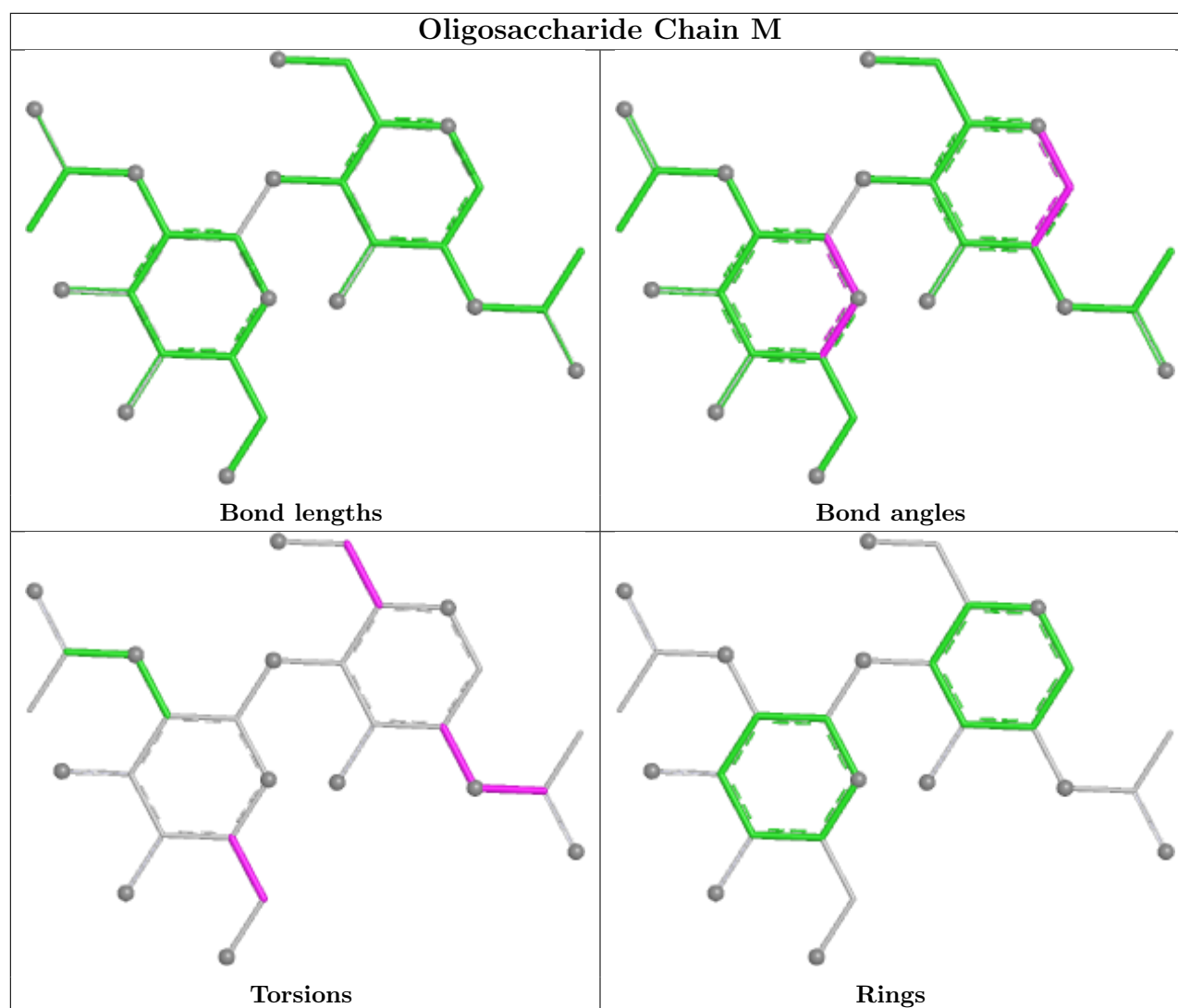
Mol	Chain	Res	Type	Atoms
5	b	2	NAG	O5-C5-C6-O6
5	N	1	NAG	C3-C2-N2-C7
5	R	1	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
5	R	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2

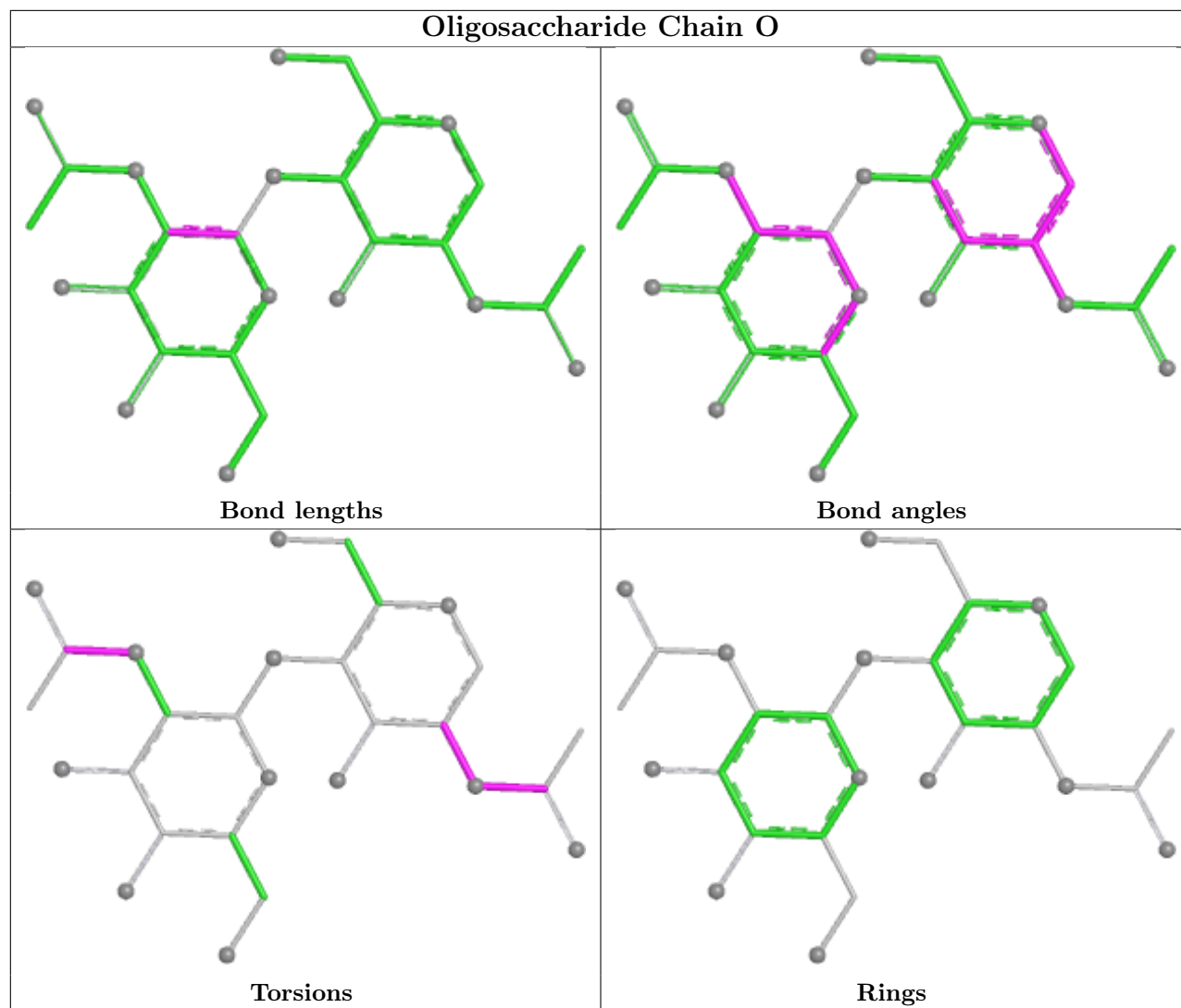
There are no ring outliers.

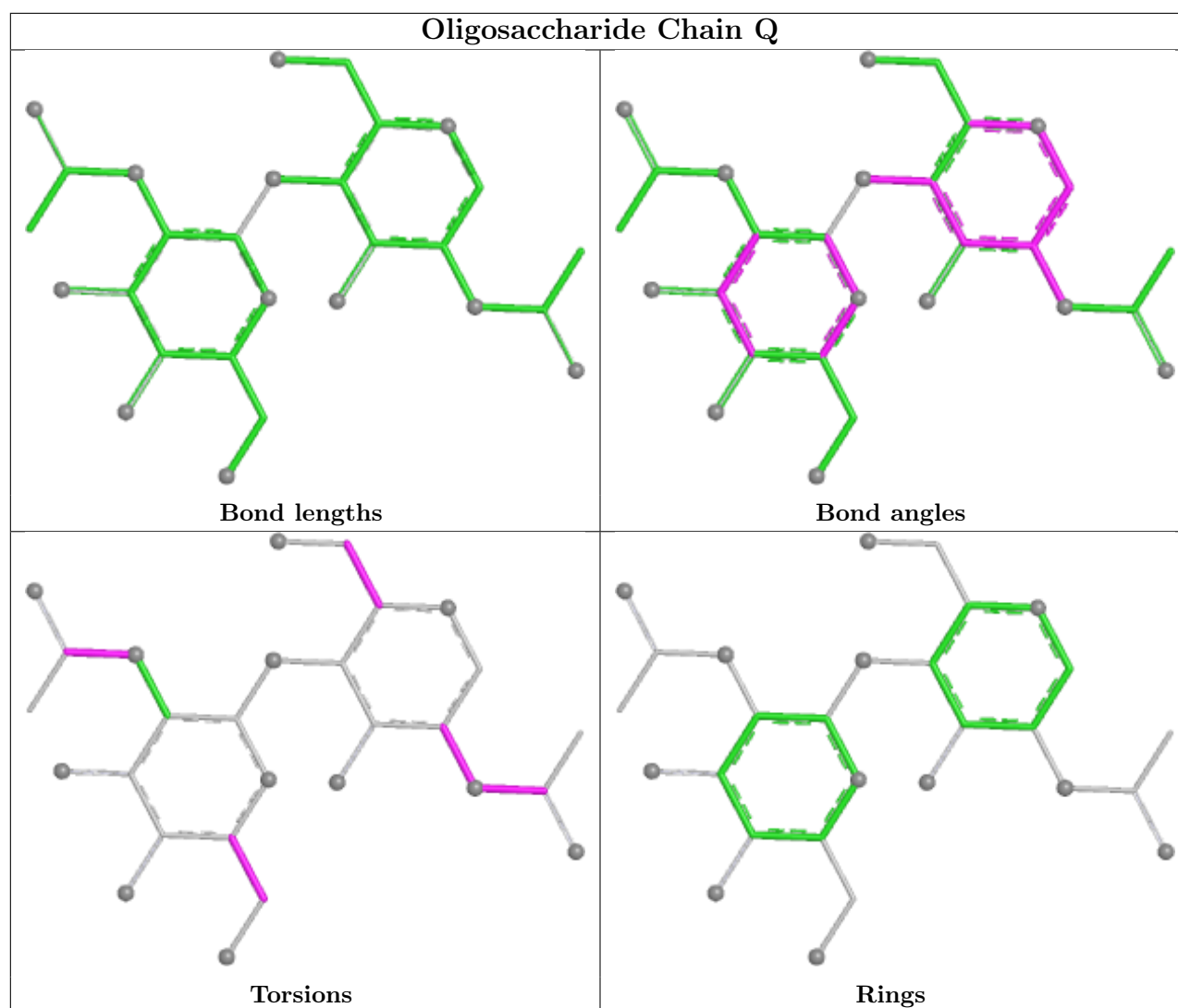
7 monomers are involved in 6 short contacts:

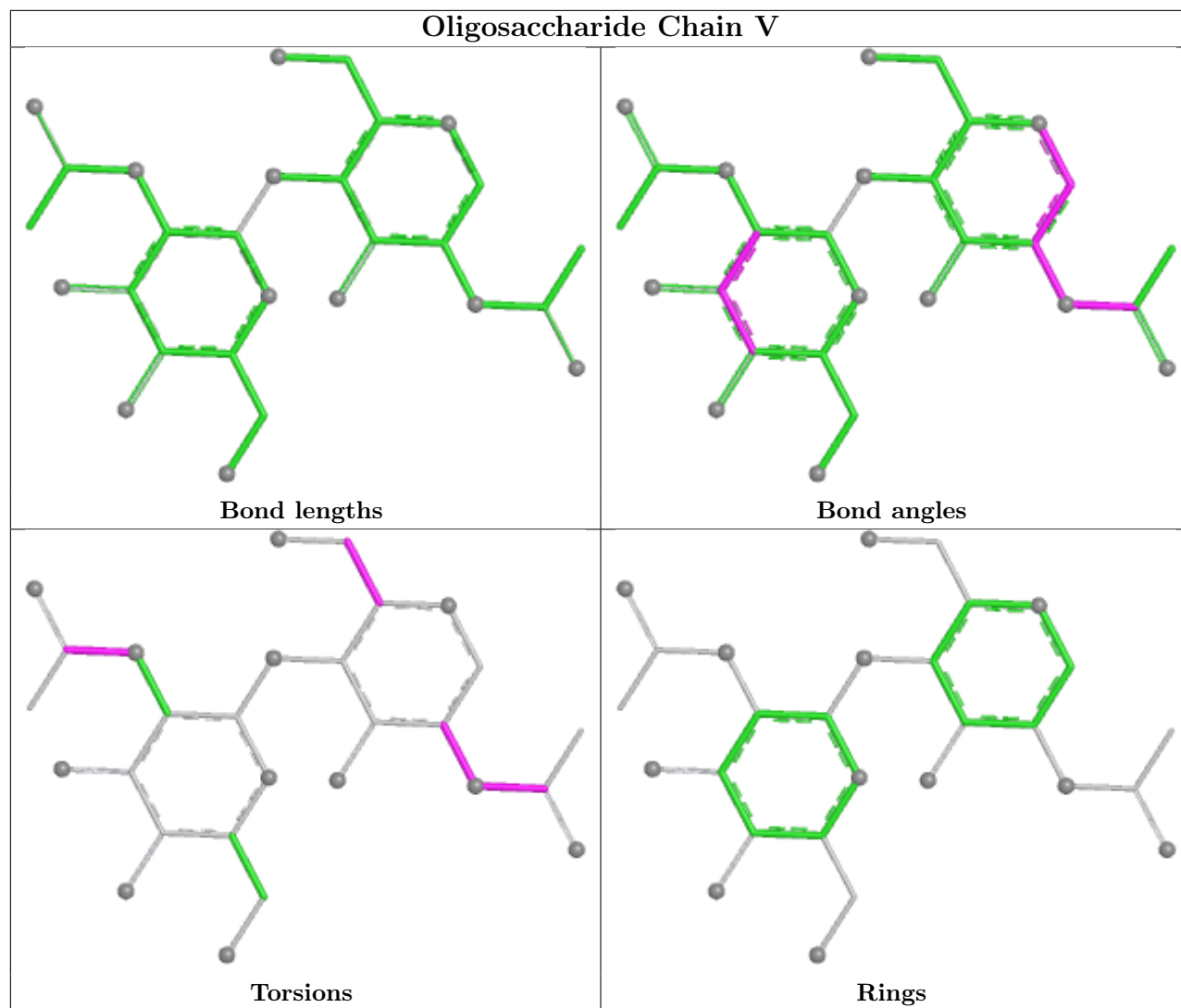
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	1	NAG	2	0
4	c	2	NAG	1	0
4	O	1	NAG	2	0
5	W	2	NAG	2	0
4	c	1	NAG	1	0
4	Q	2	NAG	1	0
4	O	2	NAG	2	0

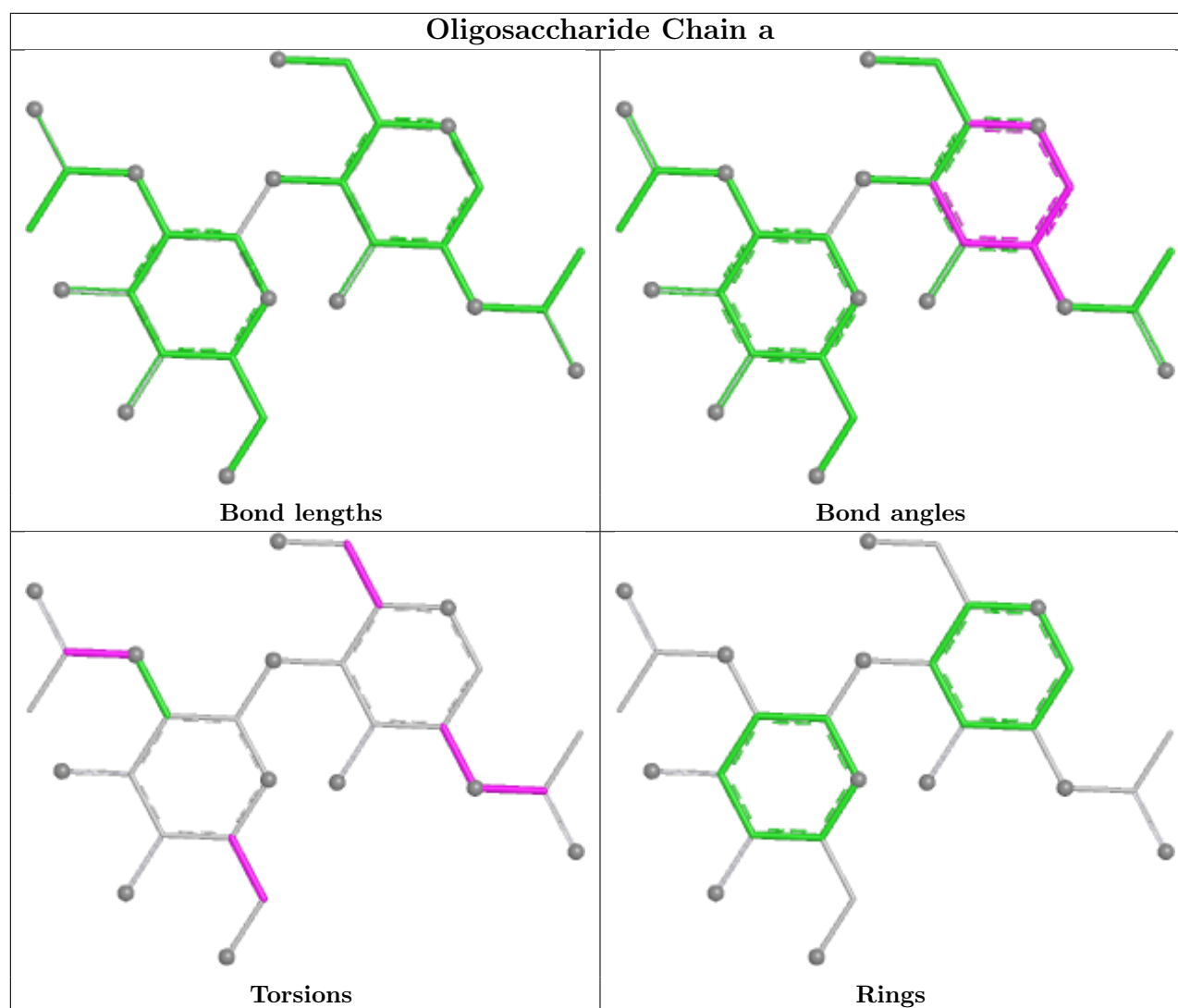
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

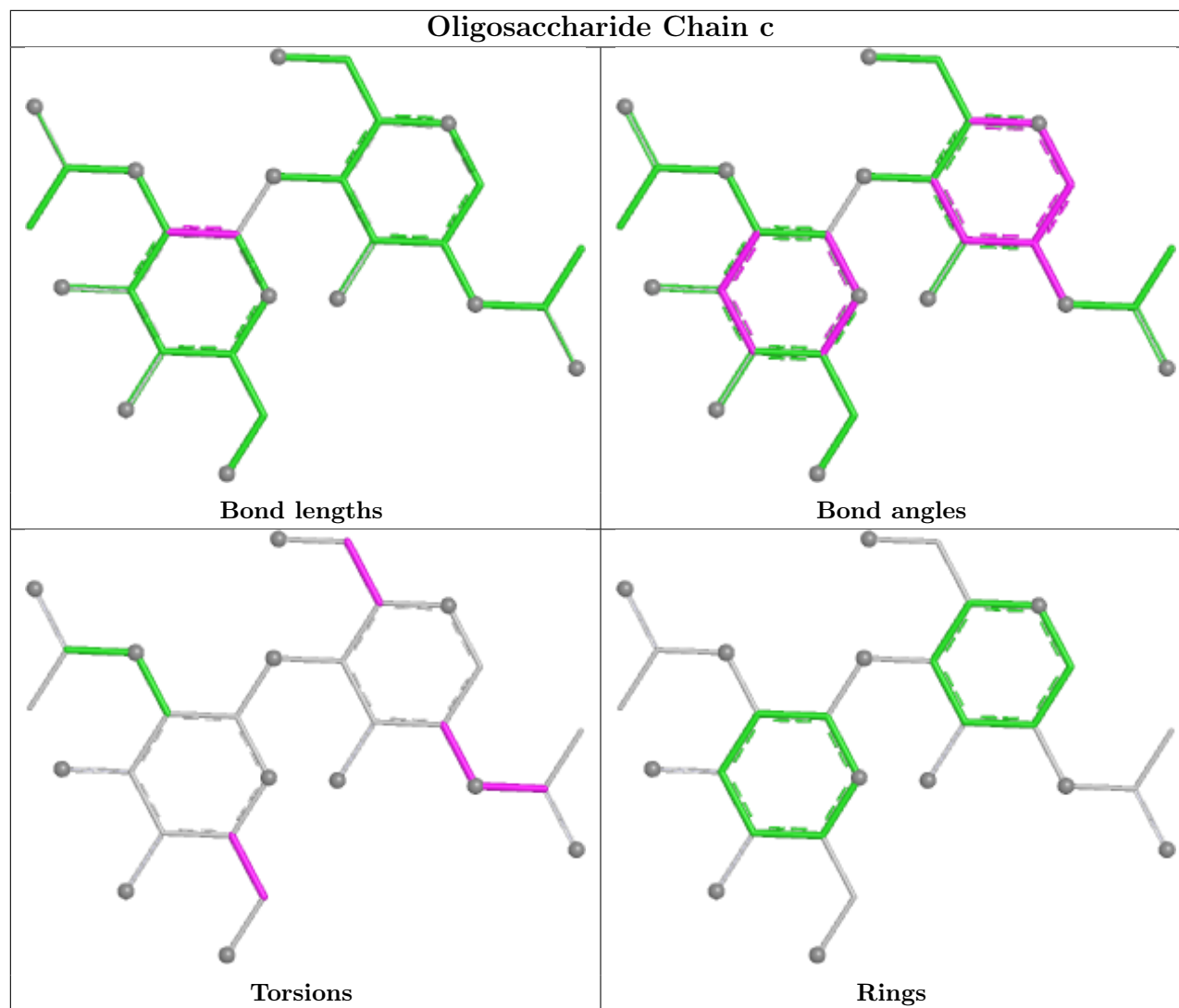


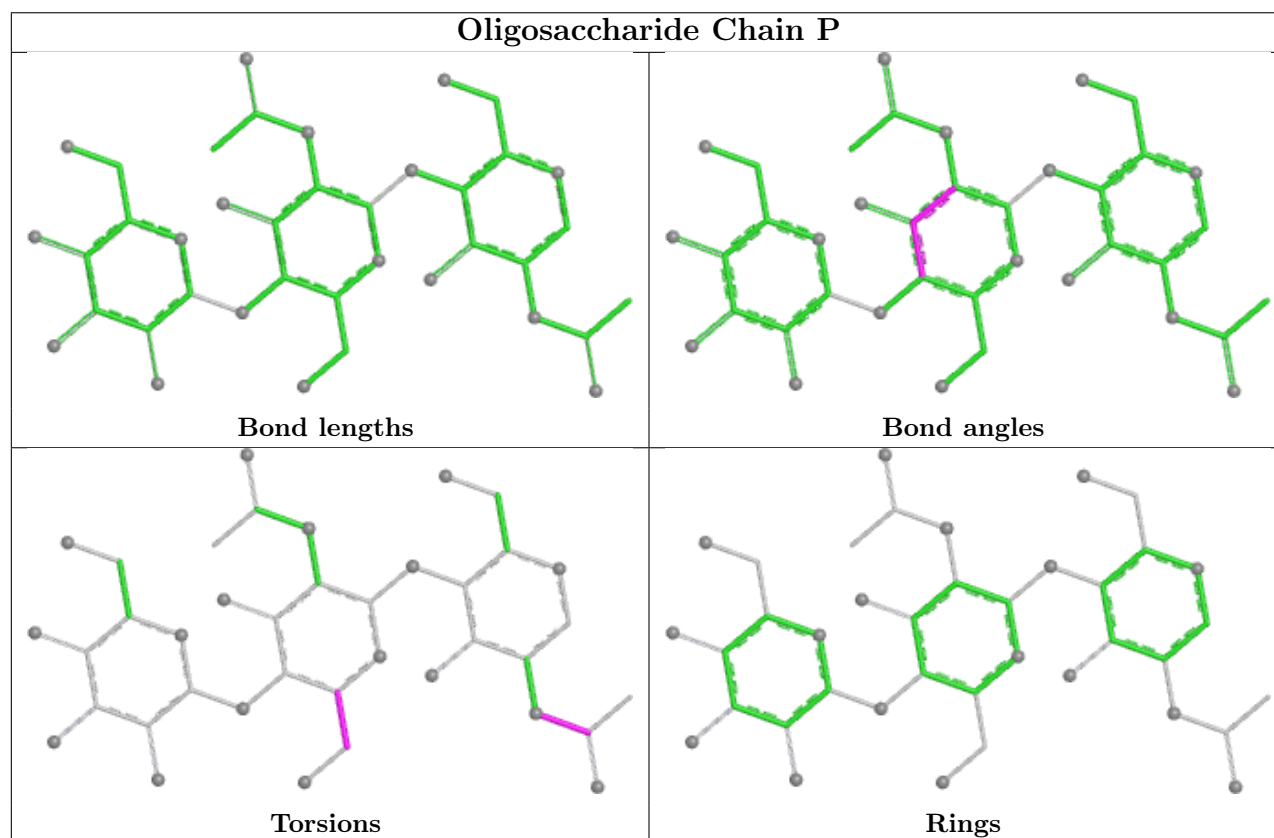
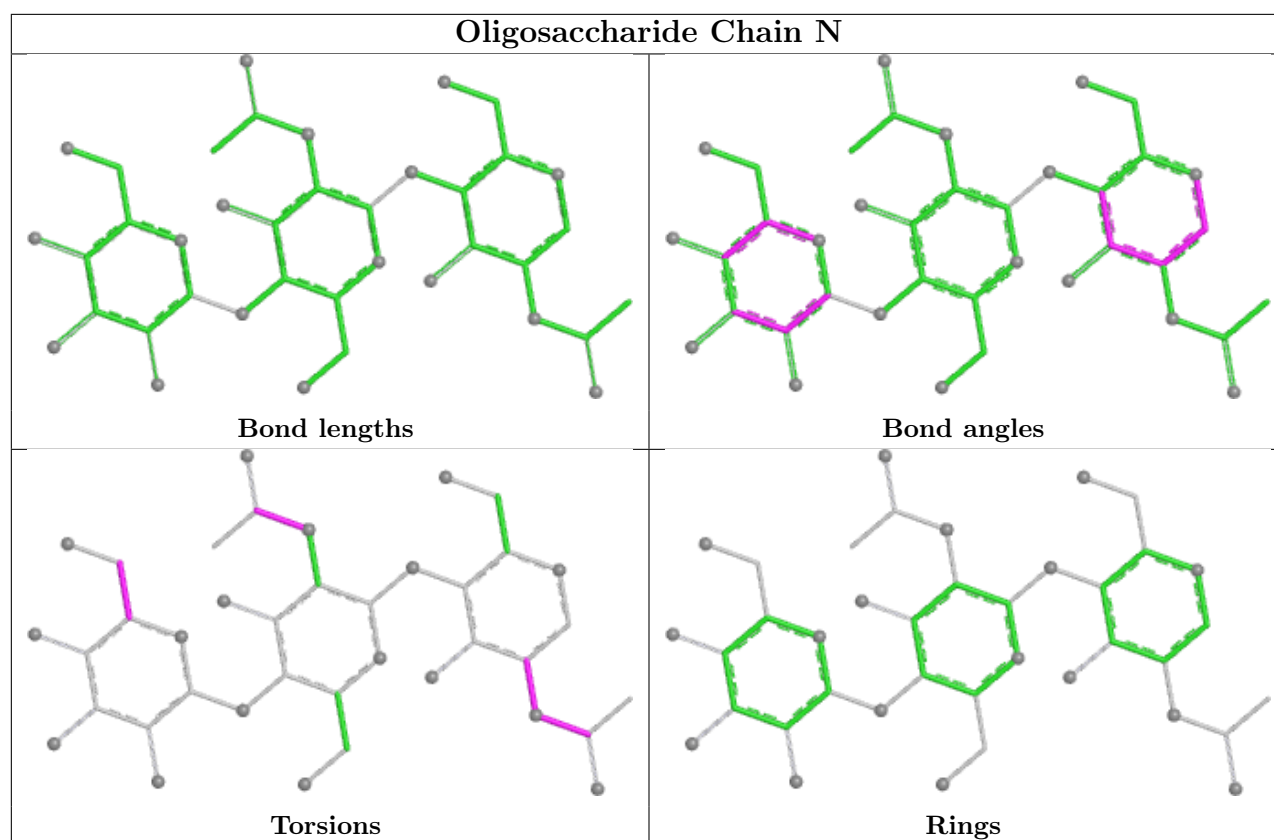


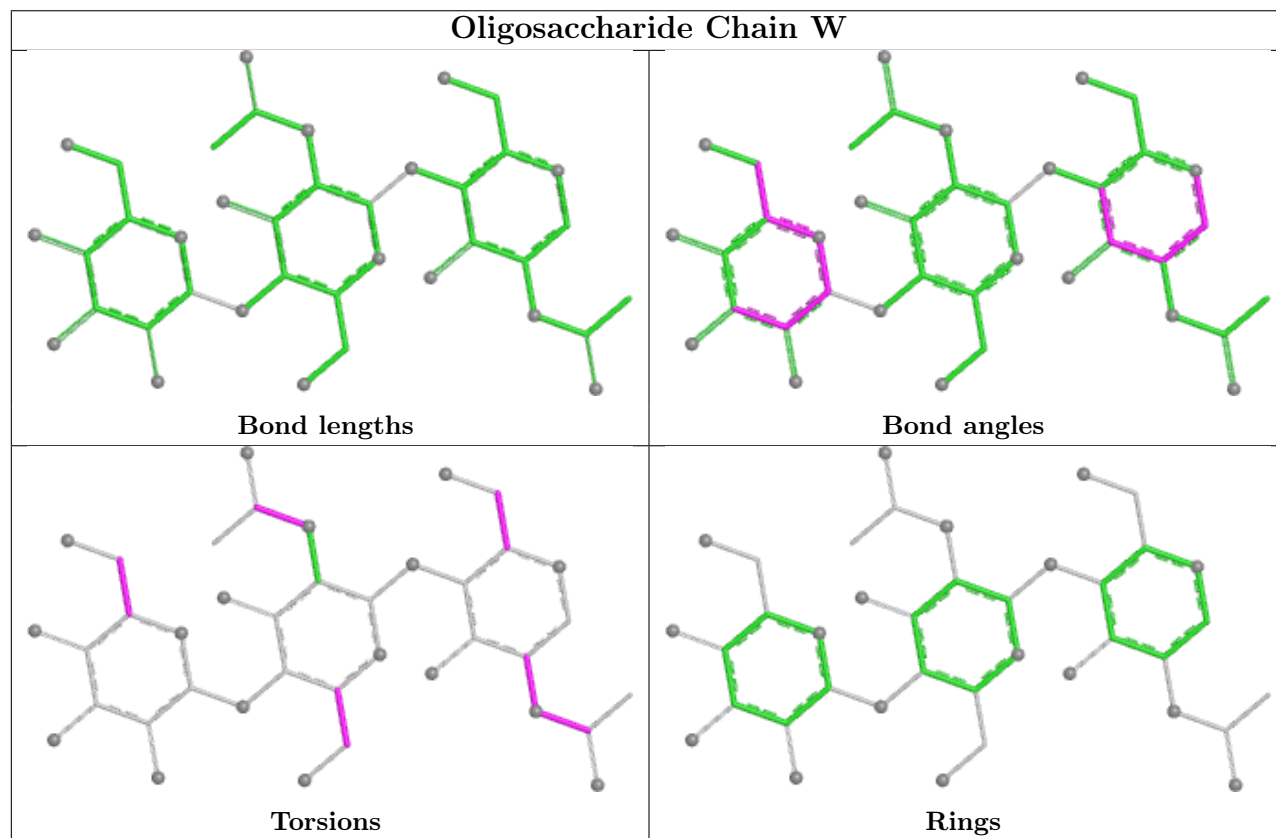
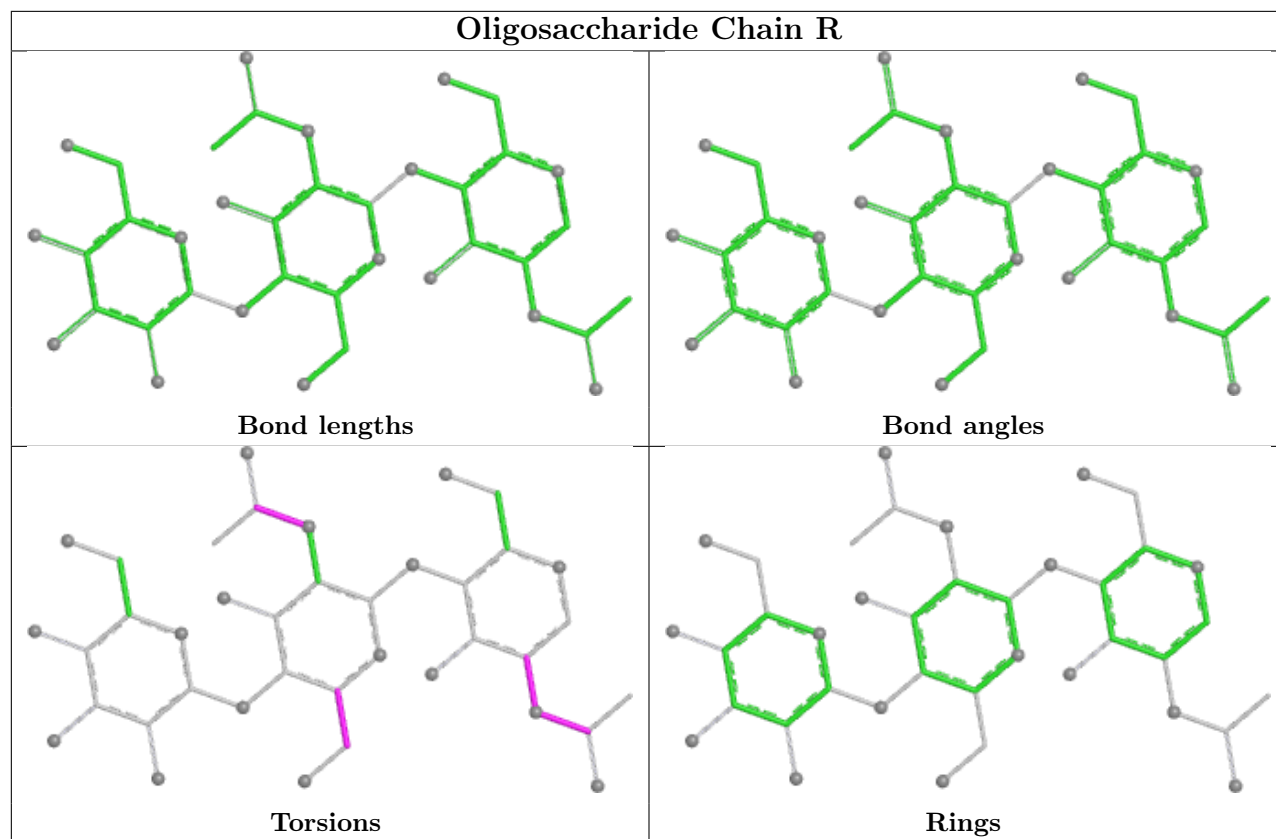


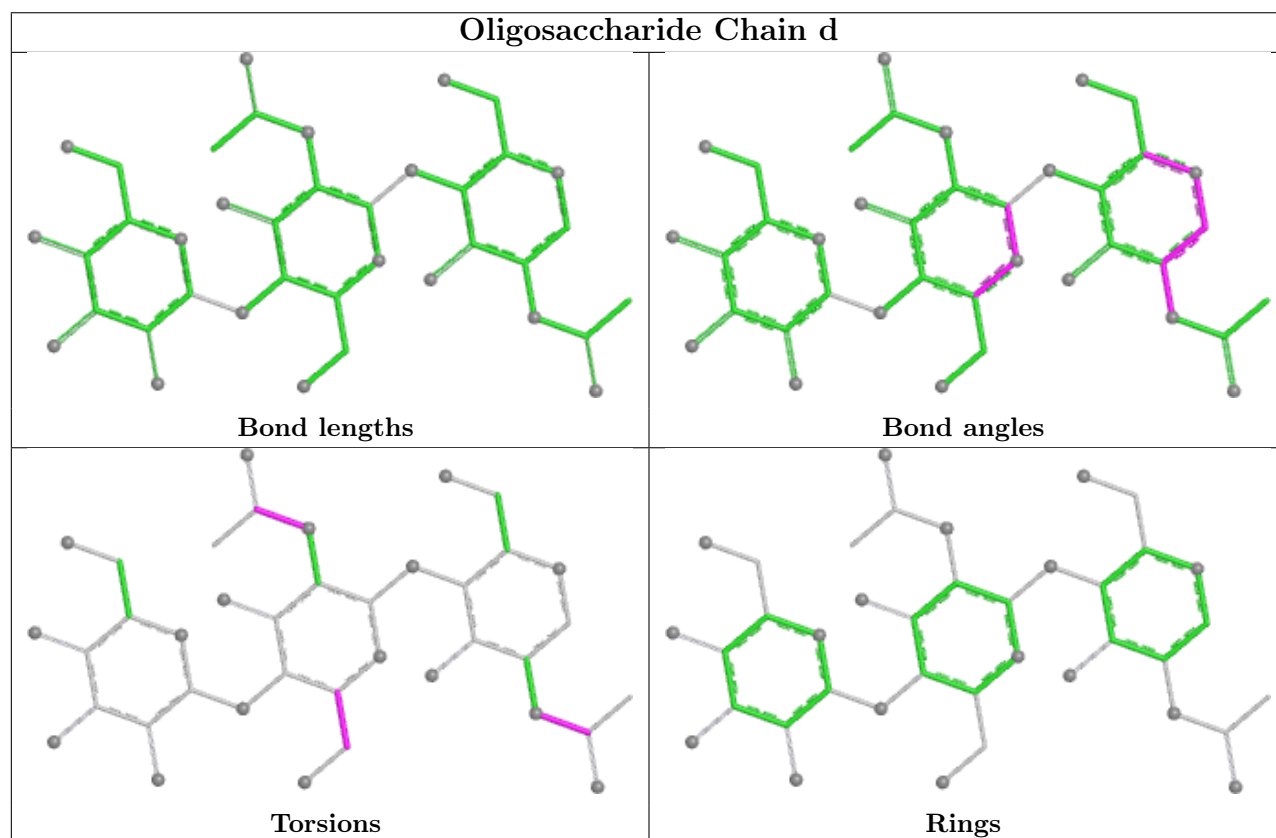
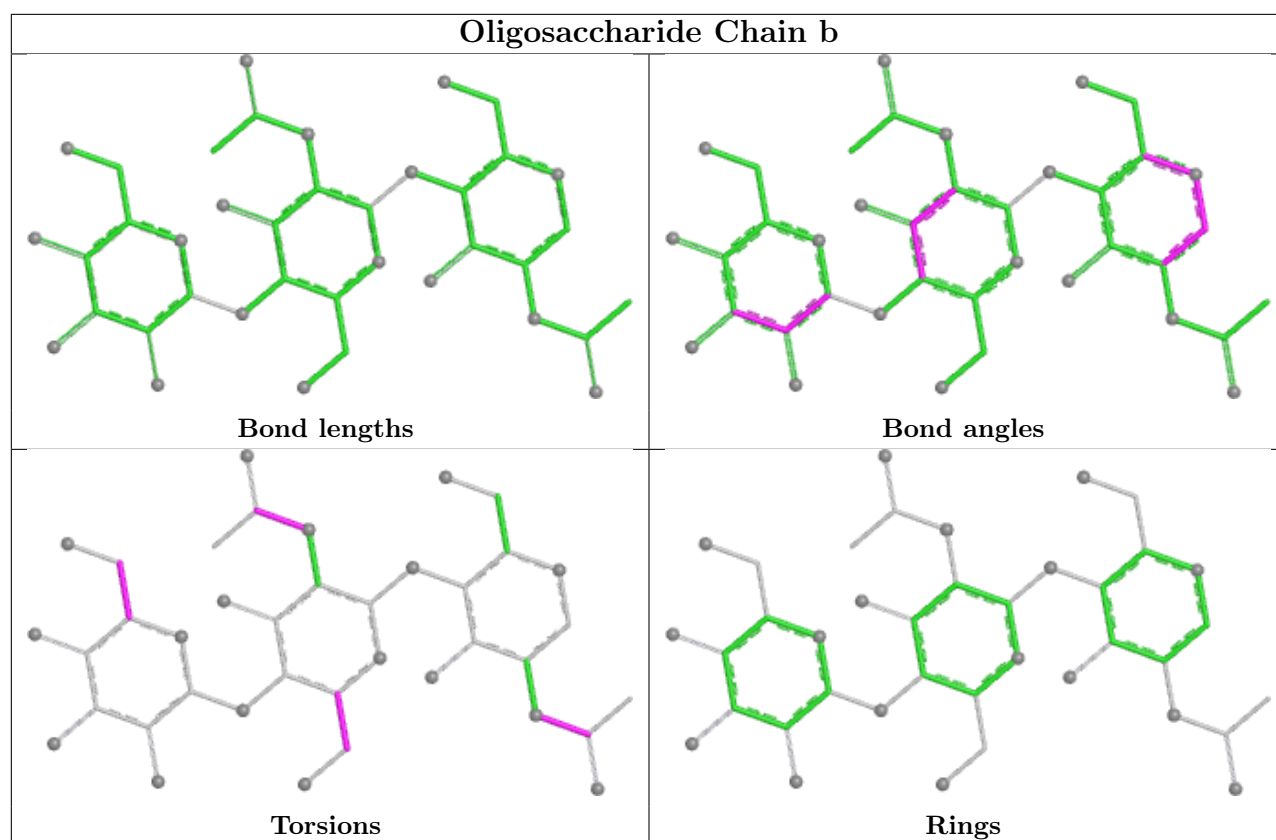












5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	323/338 (95%)	-0.00	3 (0%) 81 64	64, 86, 103, 127	0
1	C	323/338 (95%)	0.00	5 (1%) 72 52	60, 85, 101, 122	0
1	E	323/338 (95%)	0.07	4 (1%) 76 58	54, 86, 102, 135	0
1	G	323/338 (95%)	-0.14	3 (0%) 81 64	66, 86, 101, 106	0
1	I	323/338 (95%)	-0.11	1 (0%) 90 81	64, 84, 98, 113	0
1	K	323/338 (95%)	-0.06	4 (1%) 76 58	64, 85, 98, 120	0
2	B	180/182 (98%)	-0.04	6 (3%) 49 30	62, 82, 125, 138	0
2	D	180/182 (98%)	-0.10	3 (1%) 69 49	62, 82, 111, 141	0
2	F	180/182 (98%)	-0.01	4 (2%) 62 42	61, 81, 121, 141	0
2	H	174/182 (95%)	0.70	15 (8%) 16 11	61, 92, 118, 147	0
2	J	174/182 (95%)	0.43	8 (4%) 37 23	65, 89, 118, 130	0
2	L	174/182 (95%)	0.31	6 (3%) 48 30	64, 90, 117, 132	0
3	S	233/280 (83%)	0.13	1 (0%) 88 79	86, 117, 134, 143	0
3	T	234/280 (83%)	0.16	5 (2%) 63 43	82, 113, 136, 147	0
3	U	234/280 (83%)	0.20	2 (0%) 81 64	88, 117, 134, 142	0
3	X	235/280 (83%)	-0.40	0 100 100	45, 64, 87, 94	0
3	Y	235/280 (83%)	-0.37	0 100 100	42, 61, 84, 100	0
3	Z	236/280 (84%)	-0.35	2 (0%) 82 67	43, 62, 88, 115	0
All	All	4407/4800 (91%)	-0.00	72 (1%) 70 51	42, 86, 125, 147	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	66	VAL	5.7
2	J	66	VAL	5.3
2	L	66	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	H	66	VAL	4.8
2	B	66	VAL	4.7
2	D	66	VAL	4.6
2	H	65	ALA	3.8
2	H	1	GLY	3.7
3	U	249	LEU	3.6
2	H	67	GLY	3.5
3	U	123	SER	3.4
2	H	136	GLY	3.2
1	G	6	GLN	3.2
2	J	85	GLU	3.1
2	J	67	GLY	3.0
2	H	73	LEU	3.0
2	L	65	ALA	3.0
2	B	63	PHE	3.0
2	H	132	GLU	2.9
1	E	325	PRO	2.9
1	E	10	GLY	2.9
2	F	63	PHE	2.8
3	Z	249	LEU	2.8
2	H	69	GLU	2.8
2	H	63	PHE	2.8
2	H	68	ARG	2.8
1	A	5	ASP	2.8
1	C	324	SER	2.8
1	K	325	PRO	2.7
3	T	123	SER	2.7
2	H	64	GLU	2.6
2	H	131	LYS	2.6
2	B	8	GLY	2.6
2	L	83	LYS	2.5
1	K	321	LEU	2.5
2	J	2	LEU	2.5
2	L	2	LEU	2.5
1	A	10	GLY	2.5
2	J	1	GLY	2.4
3	T	211	ALA	2.4
3	T	99	SER	2.4
3	T	104	CYS	2.4
2	H	83	LYS	2.4
2	H	27	SER	2.4
2	J	65	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	7	ALA	2.3
3	S	9	ALA	2.3
3	T	212	SER	2.3
2	L	85	GLU	2.3
2	B	62	GLN	2.3
2	J	83	LYS	2.2
2	F	24	TYR	2.2
1	G	291	SER	2.2
1	C	152	VAL	2.2
1	E	59	CYS	2.2
2	F	64	GLU	2.2
3	Z	125	GLY	2.2
2	J	161	GLN	2.1
1	I	318	ALA	2.1
1	C	267	THR	2.1
1	C	10	GLY	2.1
2	D	67	GLY	2.1
1	C	291	SER	2.1
1	G	7	ILE	2.1
2	L	168	LEU	2.1
1	K	320	GLY	2.1
1	A	4	GLU	2.1
2	B	180	VAL	2.0
1	E	322	ARG	2.0
2	H	2	LEU	2.0
1	K	33	ALA	2.0
2	D	85	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	1	14/15	-	-	89,107,123,135	0

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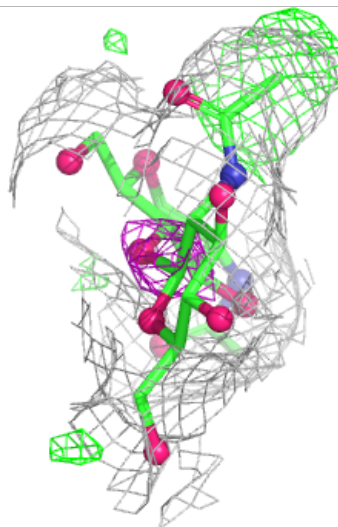
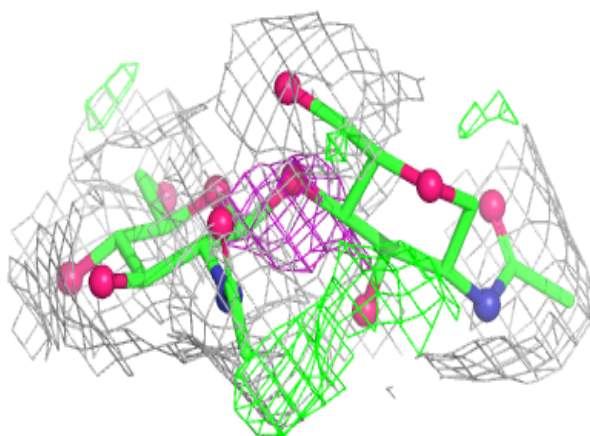
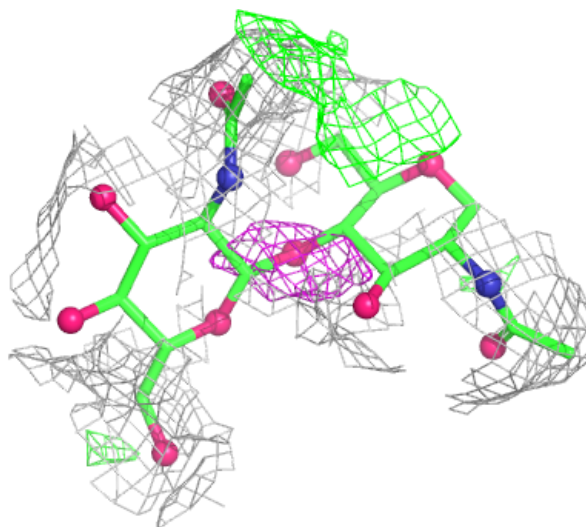
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	2	14/15	-	-	130,143,150,152	0
4	NAG	O	1	14/15	-	-	85,102,113,126	0
4	NAG	O	2	14/15	-	-	121,134,139,140	0
4	NAG	Q	1	14/15	-	-	93,112,126,138	0
4	NAG	Q	2	14/15	-	-	150,157,163,163	0
5	NAG	W	2	14/15	0.32	0.17	110,123,130,139	0
5	NAG	W	1	14/15	0.66	0.14	76,98,109,116	0
4	NAG	a	1	14/15	-	-	109,123,133,140	0
4	NAG	a	2	14/15	-	-	139,149,154,154	0
4	NAG	c	1	14/15	-	-	108,125,132,136	0
4	NAG	c	2	14/15	-	-	140,152,156,157	0
5	NAG	N	1	14/15	-	-	100,109,112,119	0
5	NAG	N	2	14/15	-	-	99,110,116,124	0
5	BMA	N	3	11/12	-	-	118,130,133,139	0
5	NAG	P	1	14/15	-	-	101,110,119,120	0
5	NAG	P	2	14/15	-	-	111,122,132,139	0
5	BMA	P	3	11/12	-	-	142,144,147,151	0
5	NAG	R	1	14/15	-	-	93,105,110,114	0
5	NAG	R	2	14/15	-	-	96,110,123,131	0
5	BMA	R	3	11/12	-	-	125,131,135,138	0
4	NAG	V	2	14/15	0.85	0.12	143,147,157,159	0
4	NAG	V	1	14/15	0.88	0.14	120,133,141,143	0
5	BMA	W	3	11/12	-	-	135,143,146,147	0
5	NAG	b	1	14/15	-	-	100,107,127,132	0
5	NAG	b	2	14/15	-	-	142,147,153,161	0
5	BMA	b	3	11/12	-	-	161,168,170,172	0
5	NAG	d	1	14/15	-	-	76,84,97,110	0
5	NAG	d	2	14/15	-	-	111,125,129,133	0
5	BMA	d	3	11/12	-	-	130,132,134,135	0

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

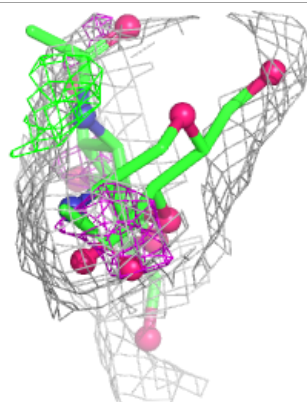
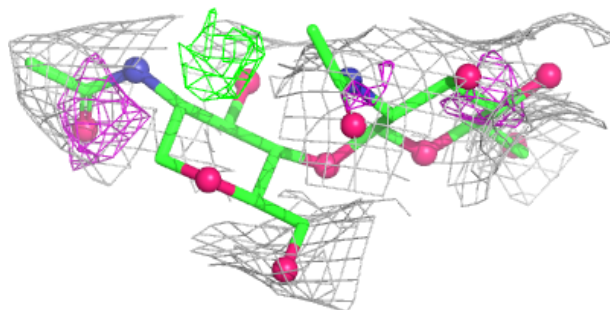
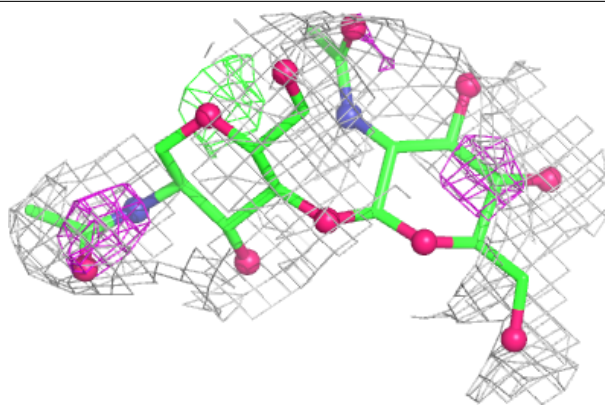
Electron density around Chain M:

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



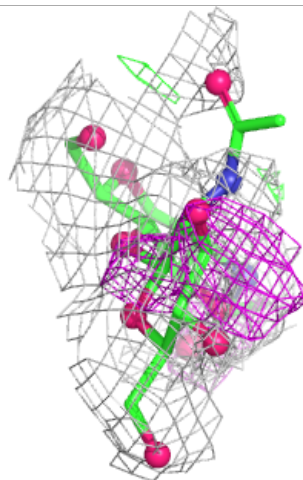
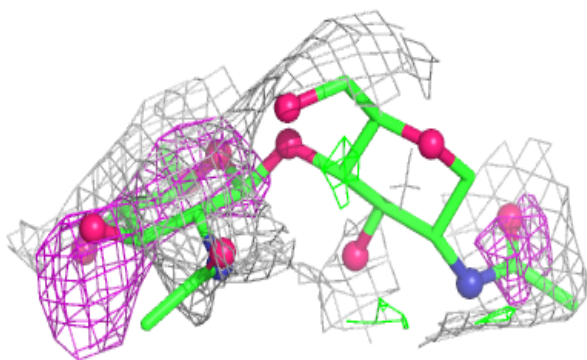
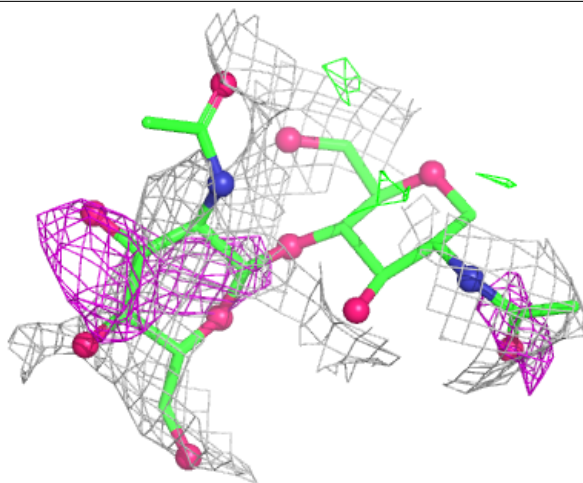
Electron density around Chain O:

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



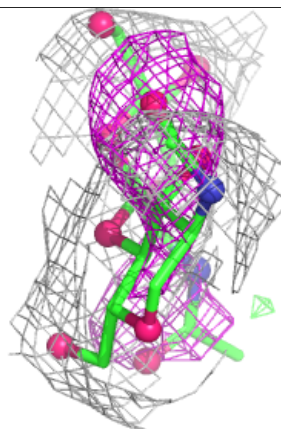
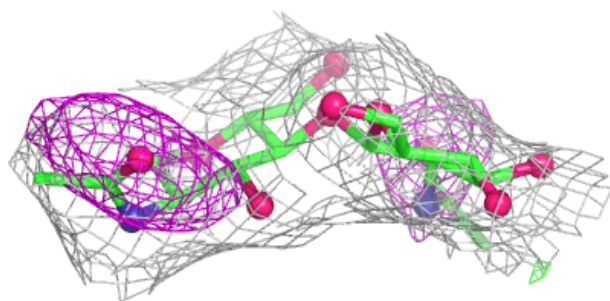
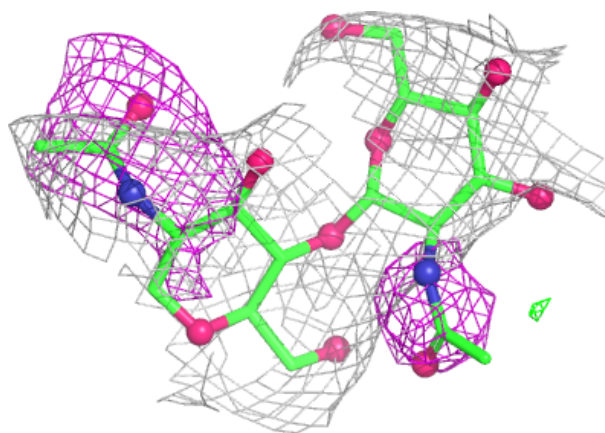
Electron density around Chain Q:

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



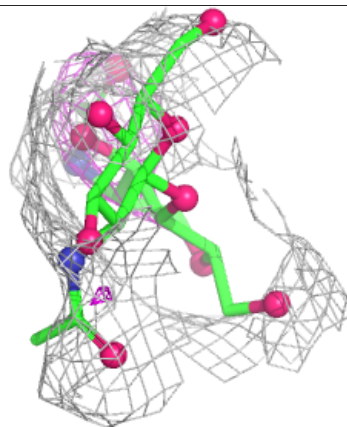
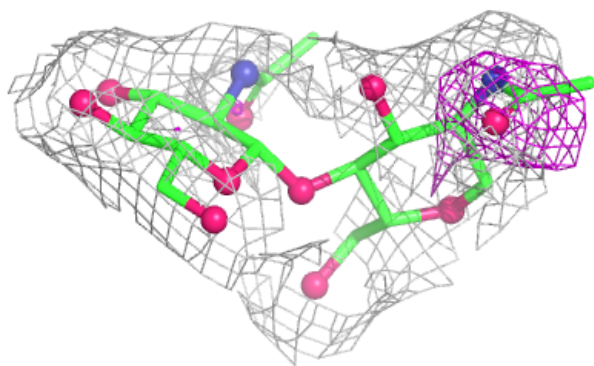
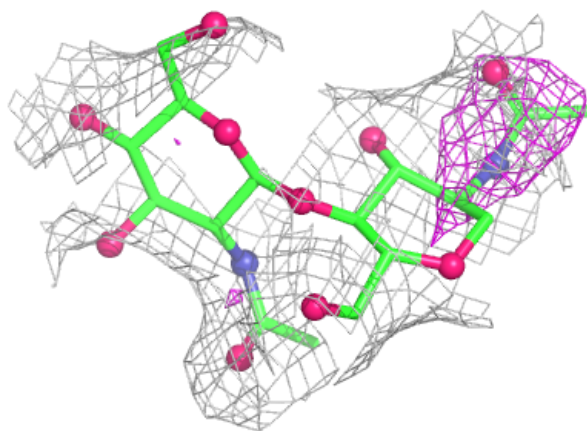
Electron density around Chain V:

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

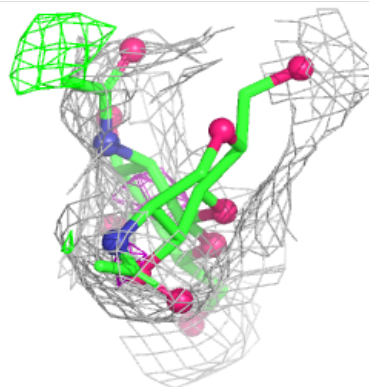
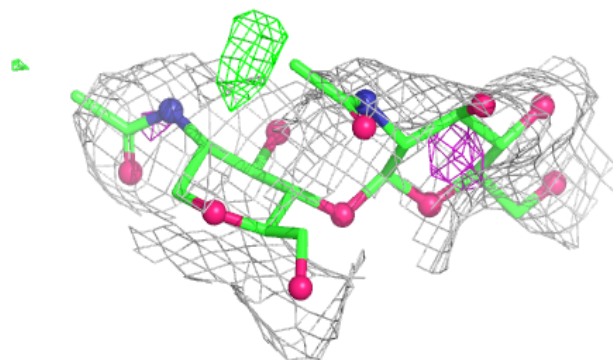
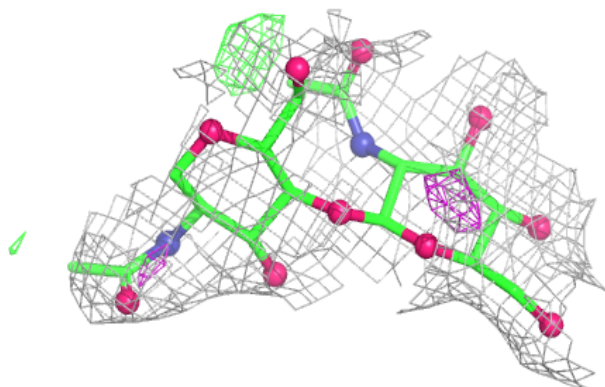


Electron density around Chain a:

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

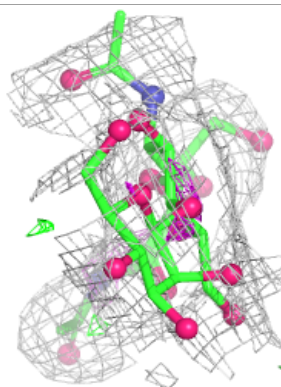
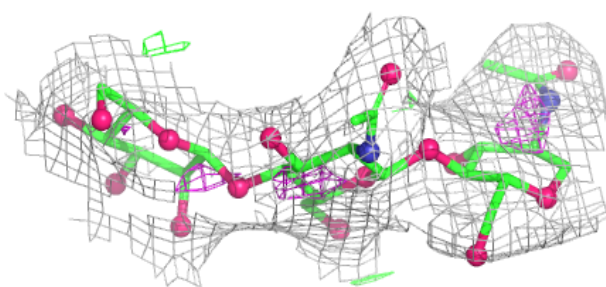
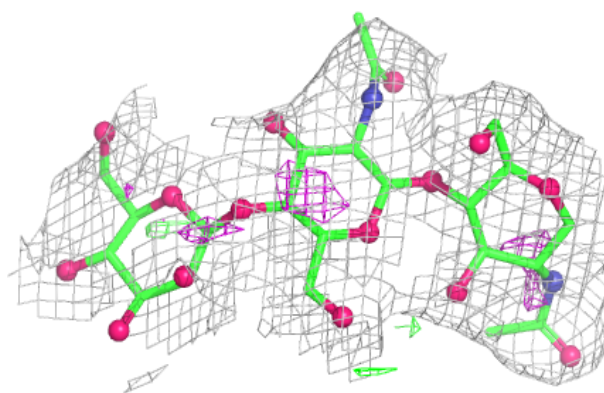
**Electron density around Chain c:**

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

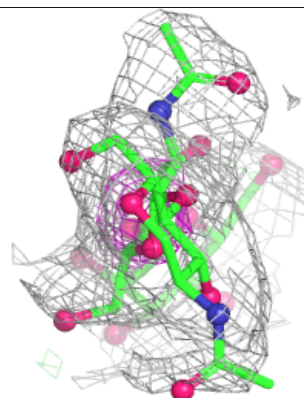
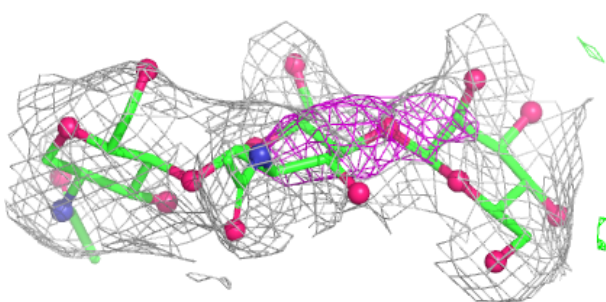
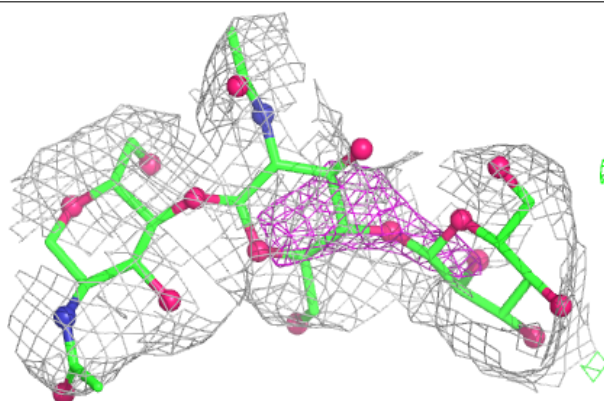


Electron density around Chain N:

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

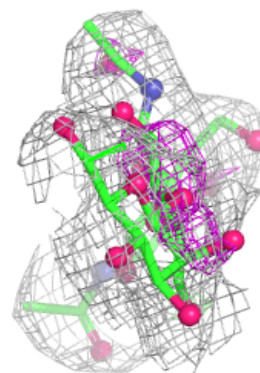
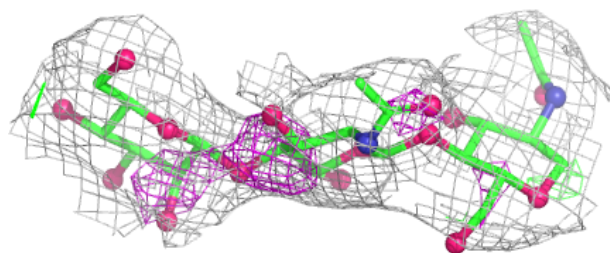
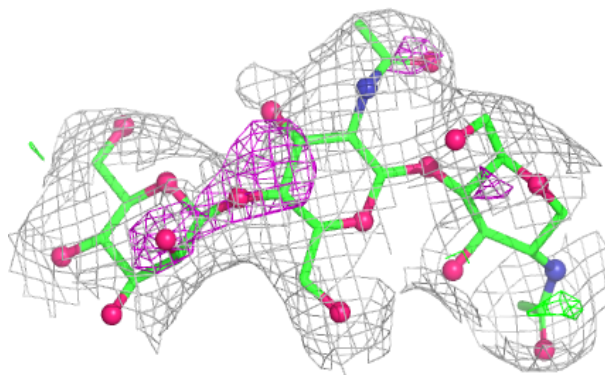
**Electron density around Chain P:**

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



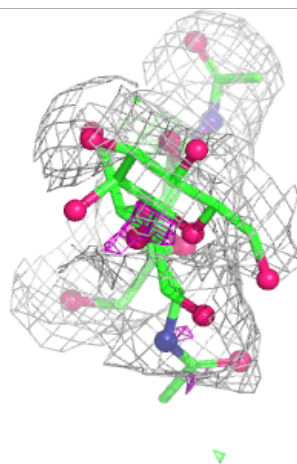
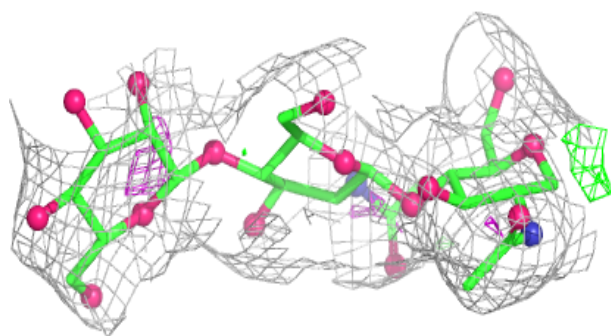
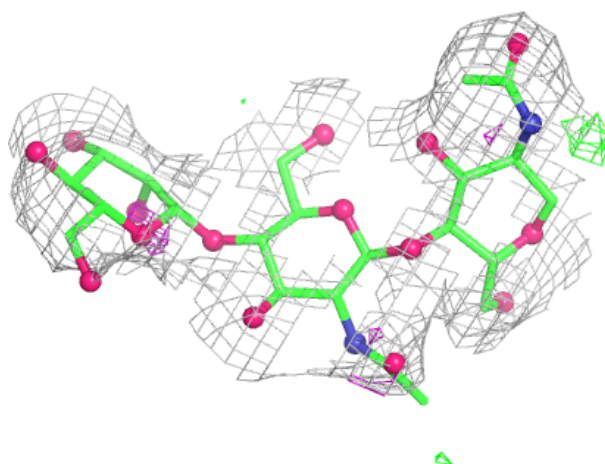
Electron density around Chain R:

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



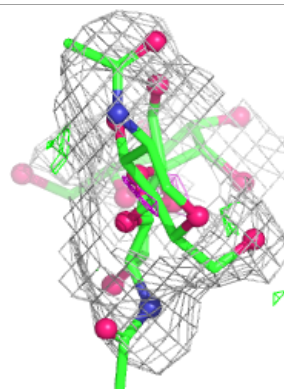
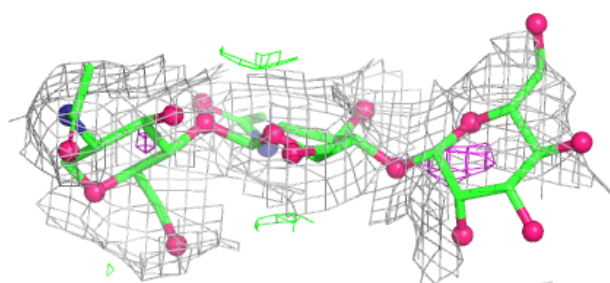
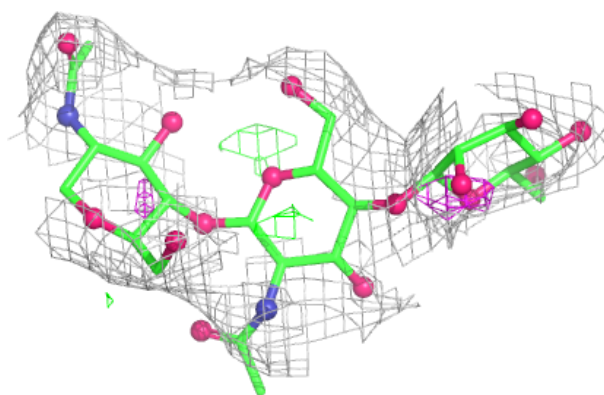
Electron density around Chain W:

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

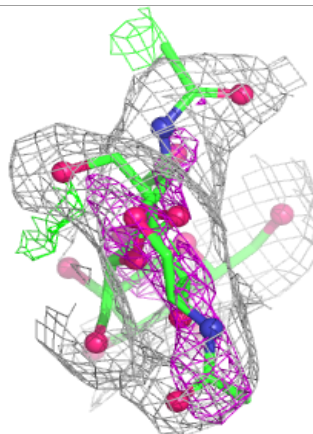
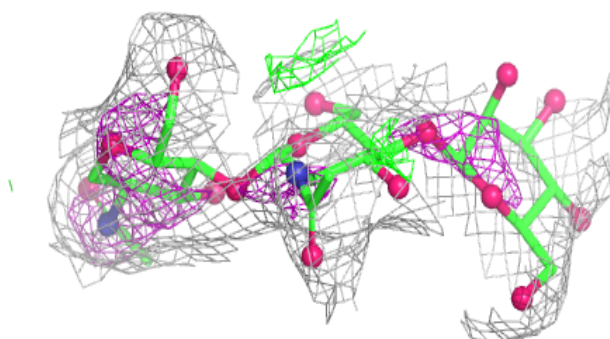
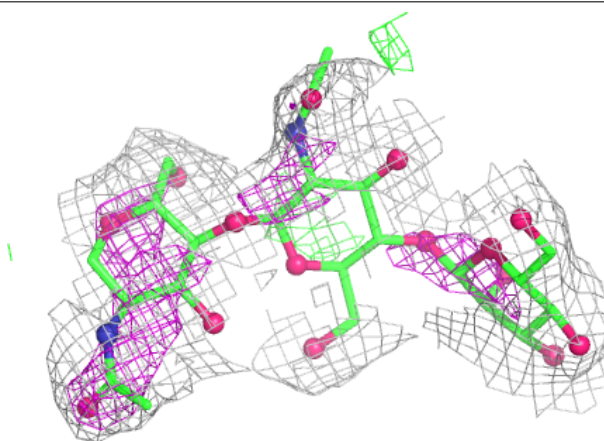


Electron density around Chain b:

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

**Electron density around Chain d:**

$2mF_o-DF_c$ (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.