



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 PM UTC

PDB ID : 2GK1 / pdb_00002gk1
Title : X-ray crystal structure of NGT-bound HexA
Authors : Lemieux, M.J.; Mark, B.L.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.;
James, M.N.
Deposited on : 2006-03-31
Resolution : 3.25 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

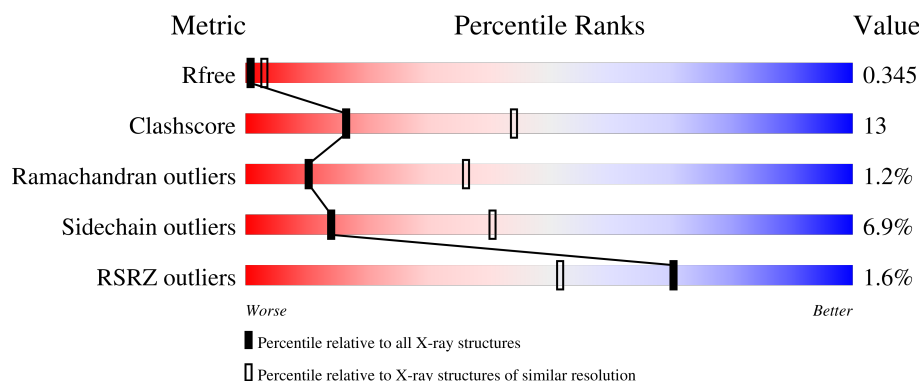
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



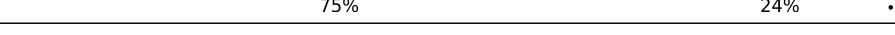
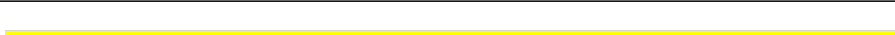
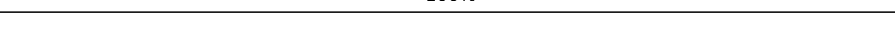
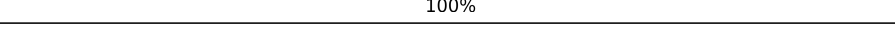
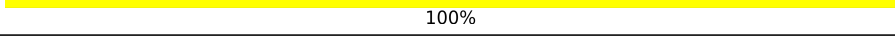
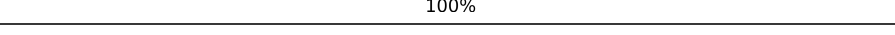
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	52	
1	C	52	
1	E	52	
1	G	52	
2	I	440	

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Mol	Chain	Length	Quality of chain
2	J	440	
2	K	440	
2	L	440	
3	B	58	
3	D	58	
3	F	58	
3	H	58	
4	M	190	
4	O	190	
4	Q	190	
4	S	190	
5	N	237	
5	P	237	
5	R	237	
5	T	237	
6	U	3	
6	V	3	
6	W	3	
6	Y	3	
6	d	3	
7	X	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	2	

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Mol	Chain	Length	Quality of chain
7	e	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	Y	1	-	-	X	-
6	NAG	Y	2	X	-	-	-
6	NAG	d	2	X	-	-	-
7	NAG	Z	1	X	-	-	-
7	NAG	Z	2	X	-	-	-
7	NAG	a	1	X	-	X	-
7	NAG	a	2	X	-	-	-
7	NAG	b	1	X	-	-	-
7	NAG	b	2	X	-	-	-
7	NAG	c	1	-	-	X	-
7	NAG	c	2	X	-	-	-
7	NAG	e	2	X	-	-	-
8	NGT	A	21	-	-	X	-
8	NGT	C	530	-	-	X	-
8	NGT	E	530	-	-	X	-
8	NGT	G	533	-	-	X	-
8	NGT	H	28	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 32011 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 Beta-hexosaminidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			
1	C	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			
1	E	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			
1	G	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			

- Molecule 2 is a protein called Beta-hexosaminidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			
2	J	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			
2	K	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			
2	L	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	436	VAL	ILE	variant	UNP P06865
J	436	VAL	ILE	variant	UNP P06865
K	436	VAL	ILE	variant	UNP P06865
L	436	VAL	ILE	variant	UNP P06865

- Molecule 3 is a protein called Beta-hexosaminidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			
3	D	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			
3	F	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			
3	H	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			

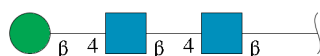
- Molecule 4 is a protein called Beta-hexosaminidase subunit beta chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			
4	O	189	Total	C	N	O	S	0	0	0
			1522	979	255	284	4			
4	Q	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			
4	S	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			

- Molecule 5 is a protein called Beta-hexosaminidase subunit beta chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			
5	P	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			
5	R	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			
5	T	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			

- Molecule 6 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
6	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

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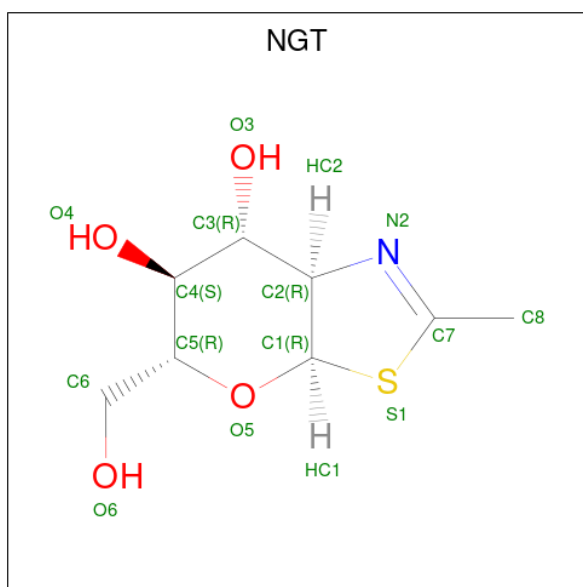
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	V	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	d	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 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
7	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TE TRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (CCD ID: NGT) (formula: C₈H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	B	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	C	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	D	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	E	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	F	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	G	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
8	H	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total	O	0	0
			5	5		
9	B	1	Total	O	0	0
			1	1		
9	C	2	Total	O	0	0
			2	2		
9	D	2	Total	O	0	0
			2	2		

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: Beta-hexosaminidase subunit alpha

Chain A: 



- Molecule 1: Beta-hexosaminidase subunit alpha

Chain C: 



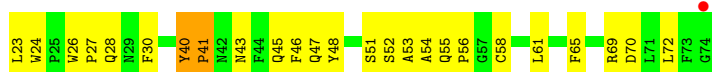
- Molecule 1: Beta-hexosaminidase subunit alpha

Chain E: 



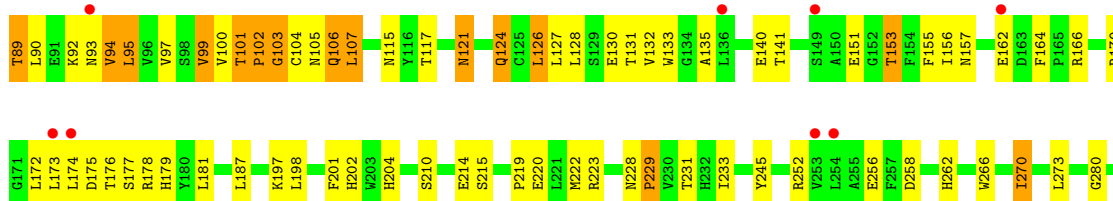
- Molecule 1: Beta-hexosaminidase subunit alpha

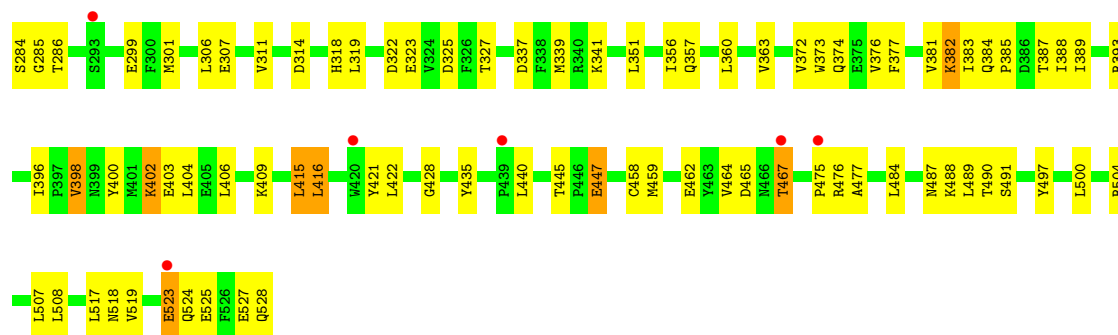
Chain G: 



- Molecule 2: Beta-hexosaminidase subunit alpha

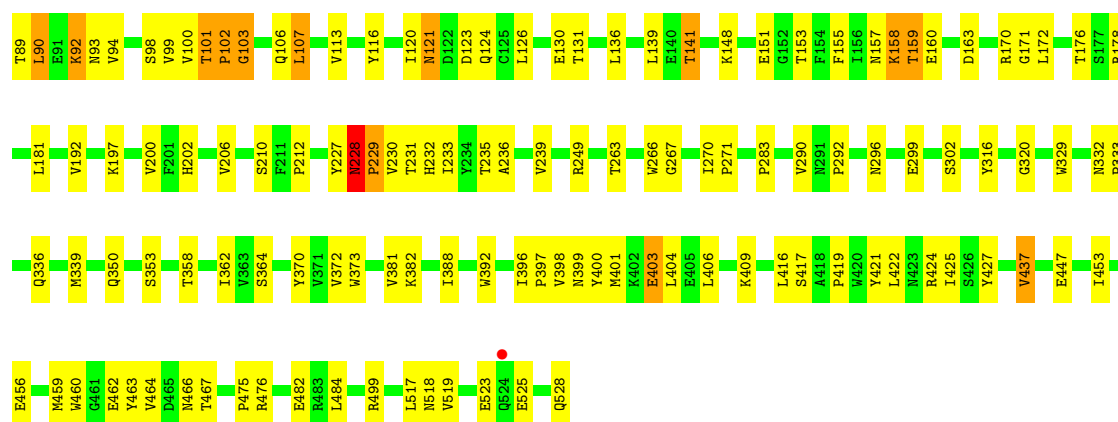
Chain I: 





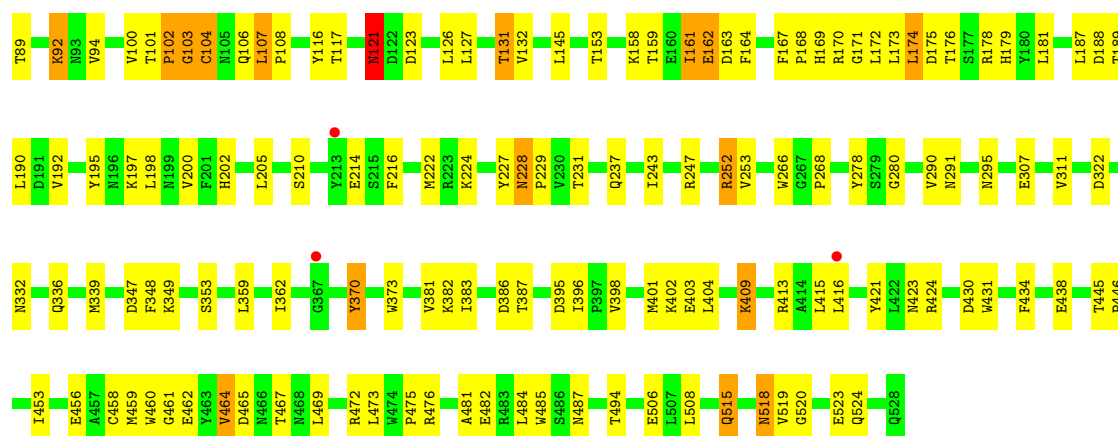
• Molecule 2: Beta-hexosaminidase subunit alpha

Chain J: 71% 26% .



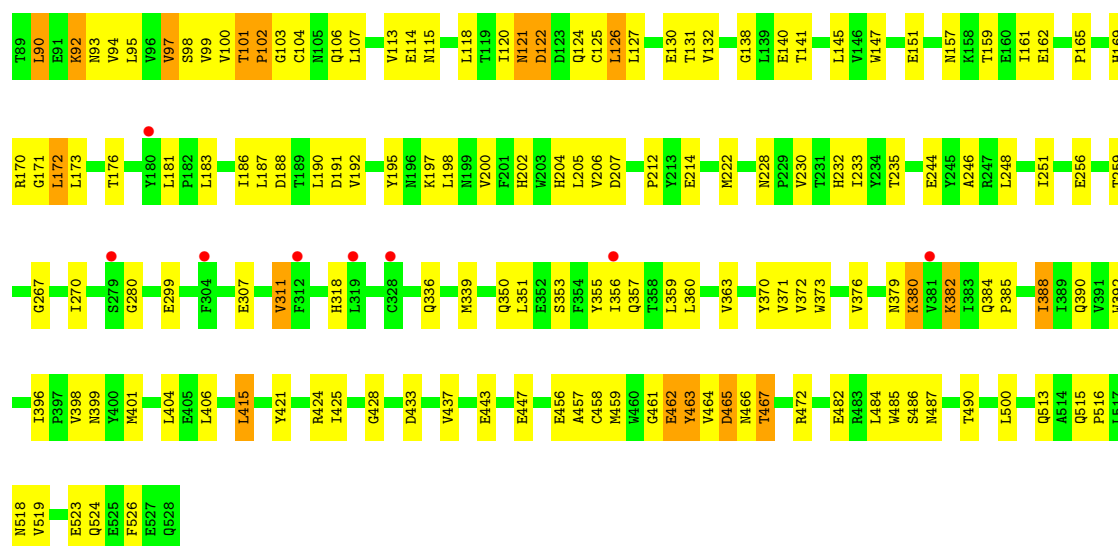
• Molecule 2: Beta-hexosaminidase subunit alpha

Chain K: 68% 28% .

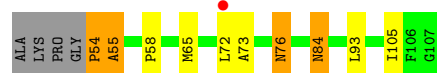
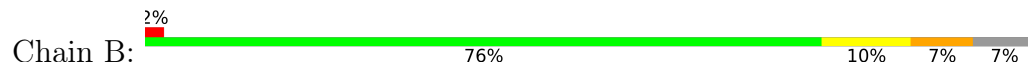


• Molecule 2: Beta-hexosaminidase subunit alpha

Chain L: 66% 30% .



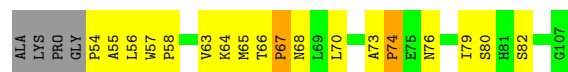
• Molecule 3: Beta-hexosaminidase subunit beta



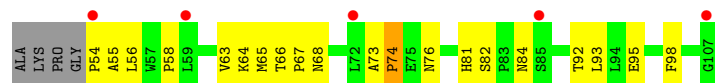
• Molecule 3: Beta-hexosaminidase subunit beta



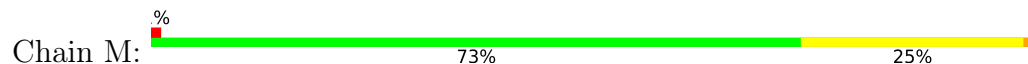
• Molecule 3: Beta-hexosaminidase subunit beta

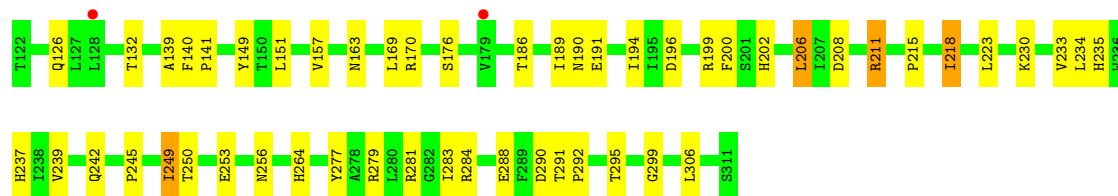


• Molecule 3: Beta-hexosaminidase subunit beta

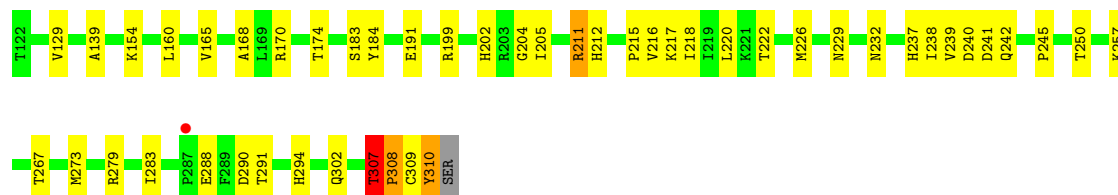
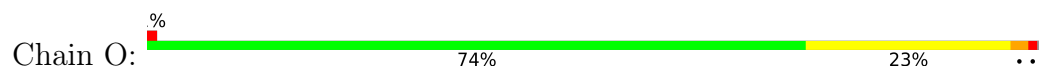


• Molecule 4: Beta-hexosaminidase subunit beta chain B

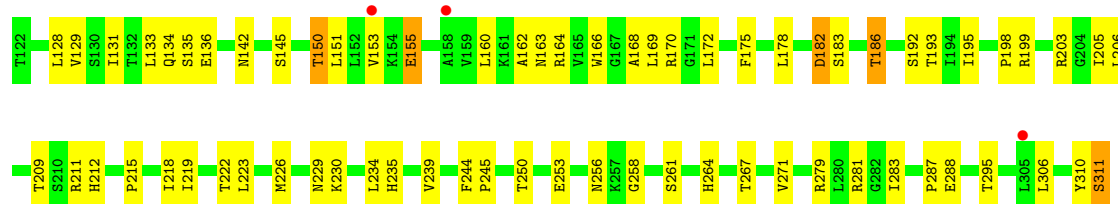




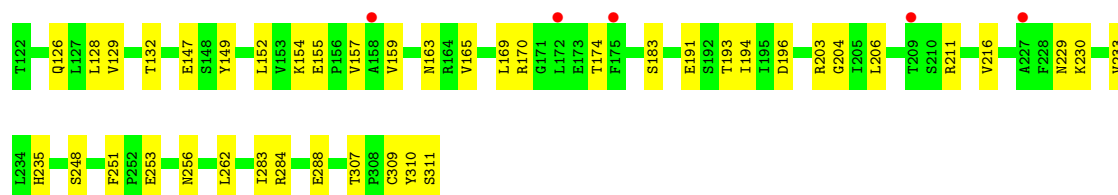
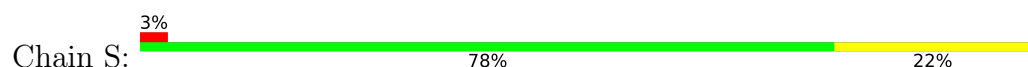
• Molecule 4: Beta-hexosaminidase subunit beta chain B



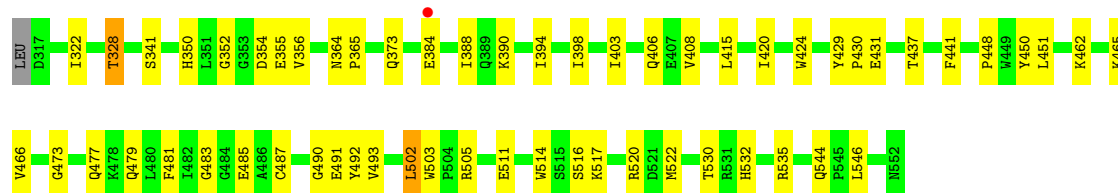
• Molecule 4: Beta-hexosaminidase subunit beta chain B



• Molecule 4: Beta-hexosaminidase subunit beta chain B

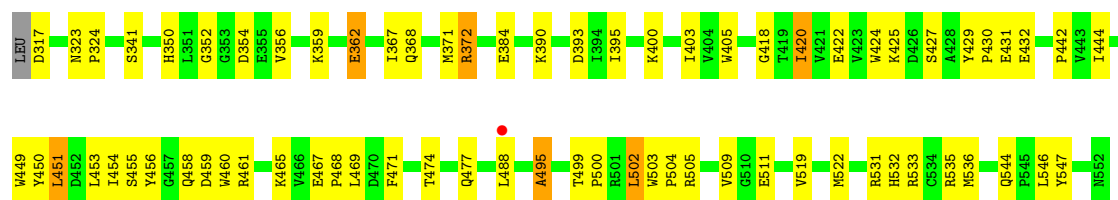


• Molecule 5: Beta-hexosaminidase subunit beta chain A



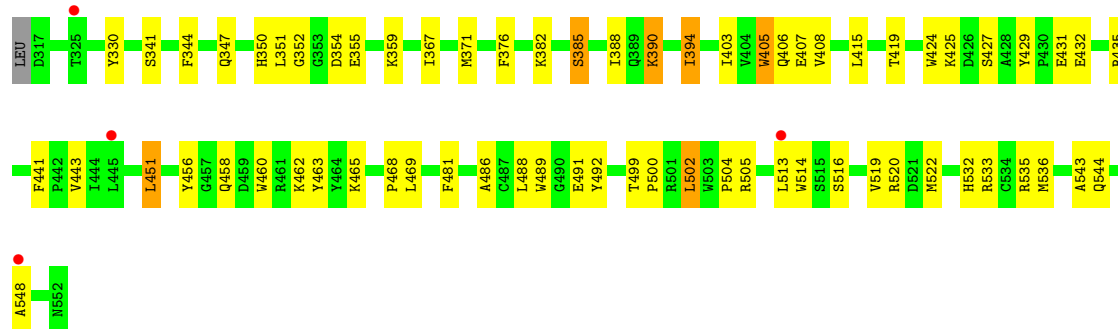
• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain P:  70% 27%



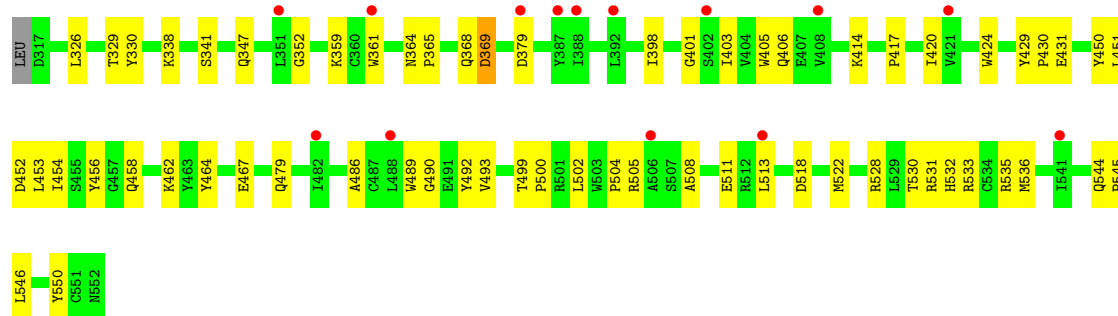
• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain R:  2% 71% 26%

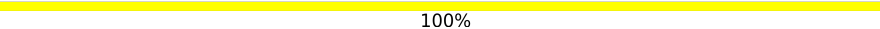


• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain T:  6% 73% 26%

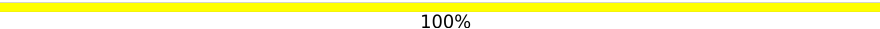


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%



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

Chain V:  100%

MAG1
MAG2
BMA3

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

Chain W:  100%

MAG1
MAG2
BMA3

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

Chain Y:  33% 67%

MAG1
MAG2
BMA3

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

Chain d:  67% 33%

MAG1
MAG2
BMA3

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

Chain X:  50% 50%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  50% 50%

MAG1
MAG2

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

Chain b:  50% 50%

MAG1
MAG2

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

Chain c:  50% 50%

MAG1
MAG2

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

Chain e:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	322.25Å 109.80Å 132.76Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	29.99 – 3.25 29.99 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.99-3.25) 97.6 (29.99-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.274 , 0.322 0.305 , 0.345	Depositor DCC
R_{free} test set	3599 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 8.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32011	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	0/457	0.89	0/624
1	C	0.47	0/457	0.83	0/624
1	E	0.46	0/457	0.79	2/624 (0.3%)
1	G	0.45	0/457	0.89	2/624 (0.3%)
2	I	0.48	0/3671	0.84	2/5004 (0.0%)
2	J	0.49	0/3671	0.84	2/5004 (0.0%)
2	K	0.50	0/3671	0.86	3/5004 (0.1%)
2	L	0.50	0/3671	0.86	1/5004 (0.0%)
3	B	2.83	3/445 (0.7%)	1.00	1/609 (0.2%)
3	D	0.40	0/445	0.87	2/609 (0.3%)
3	F	0.49	0/445	0.99	4/609 (0.7%)
3	H	0.47	0/445	0.86	0/609
4	M	0.46	0/1567	0.78	0/2134
4	O	0.50	1/1561 (0.1%)	0.94	5/2126 (0.2%)
4	Q	0.51	0/1567	0.85	1/2134 (0.0%)
4	S	0.45	0/1567	0.77	0/2134
5	N	0.48	0/1976	0.84	2/2680 (0.1%)
5	P	0.49	0/1976	0.87	0/2680
5	R	0.57	1/1976 (0.1%)	0.86	0/2680
5	T	0.47	0/1976	0.80	2/2680 (0.1%)
All	All	0.59	5/32458 (0.0%)	0.85	29/44196 (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
4	O	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	54	PRO	N-CA	47.73	2.18	1.47
3	B	54	PRO	N-CD	32.63	1.93	1.47
3	B	55	ALA	CA-CB	8.19	1.67	1.53
5	R	405	TRP	C-O	5.78	1.31	1.23
4	O	309	CYS	N-CA	5.73	1.53	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	309	CYS	N-CA-C	15.16	133.45	108.73
3	B	54	PRO	CA-N-CD	-12.69	94.23	112.00
2	I	104	CYS	N-CA-C	-8.26	101.21	112.03
4	O	307	THR	CA-C-N	7.34	129.02	119.84
4	O	307	THR	C-N-CA	7.34	129.02	119.84
3	F	66	THR	CA-C-N	7.22	128.86	119.84
3	F	66	THR	C-N-CA	7.22	128.86	119.84
1	G	40	TYR	CA-C-N	6.71	128.22	119.84
1	G	40	TYR	C-N-CA	6.71	128.22	119.84
2	J	228	ASN	CA-C-N	6.18	127.57	119.84
2	J	228	ASN	C-N-CA	6.18	127.57	119.84
2	I	124	GLN	N-CA-C	6.18	117.62	108.60
2	K	228	ASN	CA-C-N	6.16	127.54	119.84
2	K	228	ASN	C-N-CA	6.16	127.54	119.84
5	N	483	GLY	N-CA-C	6.04	118.30	110.45
5	N	328	THR	N-CA-C	-6.00	104.37	111.03
3	D	66	THR	CA-C-N	5.51	125.19	119.56
3	D	66	THR	C-N-CA	5.51	125.19	119.56
2	K	121	ASN	N-CA-C	5.50	115.38	108.45
1	E	40	TYR	CA-C-N	5.41	126.60	119.84
1	E	40	TYR	C-N-CA	5.41	126.60	119.84
4	Q	135	SER	N-CA-C	5.22	117.65	111.33
4	O	204	GLY	N-CA-C	5.21	118.72	110.96
2	L	104	CYS	N-CA-C	-5.20	105.23	112.30
4	O	308	PRO	N-CA-C	-5.14	101.88	112.47
5	T	467	GLU	CA-C-N	5.12	124.74	119.05
5	T	467	GLU	C-N-CA	5.12	124.74	119.05
3	F	73	ALA	CA-C-N	5.10	126.21	119.84
3	F	73	ALA	C-N-CA	5.10	126.21	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	O	308	PRO	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	441	0	397	31	0
1	C	441	0	397	22	0
1	E	441	0	397	31	0
1	G	441	0	397	26	0
2	I	3565	0	3442	126	0
2	J	3565	0	3441	105	0
2	K	3565	0	3441	105	0
2	L	3565	0	3438	110	1
3	B	428	0	416	11	0
3	D	428	0	416	8	0
3	F	428	0	416	9	0
3	H	428	0	416	20	0
4	M	1528	0	1511	39	0
4	O	1522	0	1504	37	0
4	Q	1528	0	1509	46	0
4	S	1528	0	1509	27	0
5	N	1921	0	1857	41	0
5	P	1921	0	1857	60	0
5	R	1921	0	1857	54	0
5	T	1921	0	1857	43	1
6	U	39	0	34	5	0
6	V	39	0	34	1	0
6	W	39	0	34	1	0
6	Y	39	0	33	7	0
6	d	39	0	34	1	0
7	X	28	0	25	1	0
7	Z	28	0	25	2	0
7	a	28	0	25	9	0
7	b	28	0	25	2	0
7	c	28	0	25	8	0
7	e	28	0	25	3	0
8	A	14	0	13	6	0
8	B	14	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	14	0	13	12	0
8	D	14	0	13	4	0
8	E	14	0	13	6	0
8	F	14	0	13	3	0
8	G	14	0	13	8	0
8	H	14	0	13	6	0
9	A	5	0	0	1	0
9	B	1	0	0	0	0
9	C	2	0	0	1	0
9	D	2	0	0	0	0
All	All	32011	0	30898	806	1

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 13.

All (806) 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)
2:J:157:ASN:HD21	6:Y:1:NAG:C1	1.16	1.58
2:I:115:ASN:HD21	6:U:1:NAG:C1	1.18	1.53
2:I:157:ASN:HD21	6:V:1:NAG:C1	1.34	1.40
3:B:54:PRO:N	3:B:54:PRO:CD	1.93	1.30
8:E:530:NGT:HC62	2:K:462:GLU:OE1	1.19	1.29
8:H:28:NGT:S1	5:T:450:TYR:HE2	1.61	1.23
1:A:66:GLN:HE21	1:A:66:GLN:HA	0.98	1.13
8:C:530:NGT:HC81	2:J:421:TYR:OH	1.47	1.12
2:I:100:VAL:HG12	2:I:102:PRO:HD2	1.33	1.10
2:K:170:ARG:HG2	2:K:484:LEU:HB3	1.35	1.09
3:B:54:PRO:N	3:B:54:PRO:CA	2.18	1.06
1:G:55:GLN:HG3	1:G:56:PRO:HD2	1.36	1.04
8:H:28:NGT:S1	5:T:450:TYR:CE2	2.52	1.03
8:C:530:NGT:HC81	2:J:421:TYR:HH	1.29	0.96
8:E:530:NGT:C6	2:K:462:GLU:OE1	2.13	0.96
5:N:532:HIS:HD2	5:N:535:ARG:HH21	1.10	0.95
1:A:66:GLN:HA	1:A:66:GLN:NE2	1.82	0.94
2:J:157:ASN:CG	6:Y:1:NAG:C1	2.43	0.92
8:H:28:NGT:HC62	5:T:452:ASP:OD2	1.68	0.92
2:L:130:GLU:HG2	7:c:1:NAG:H82	1.52	0.91
1:G:55:GLN:HG3	1:G:56:PRO:CD	1.99	0.91
5:N:532:HIS:CD2	5:N:535:ARG:HH21	1.88	0.90
2:K:178:ARG:HD2	2:K:462:GLU:OE2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLN:HE21	1:A:66:GLN:CA	1.81	0.89
2:J:427:TYR:CD1	5:P:453:LEU:HA	2.08	0.89
1:E:36:ARG:HB3	7:a:1:NAG:H82	1.54	0.88
8:E:530:NGT:HC62	2:K:462:GLU:CD	2.00	0.86
1:E:36:ARG:HB3	7:a:1:NAG:C8	2.06	0.86
2:L:130:GLU:HG2	7:c:1:NAG:C8	2.06	0.86
2:I:170:ARG:HG2	2:I:484:LEU:HB3	1.56	0.85
5:N:364:ASN:HD22	5:N:365:PRO:HD2	1.41	0.85
3:D:58:PRO:HB3	5:P:511:GLU:HA	1.58	0.85
2:I:100:VAL:CG1	2:I:102:PRO:HD2	2.07	0.85
1:G:30:PHE:HD2	2:L:161:ILE:HG12	1.42	0.84
8:F:26:NGT:HC2	5:R:355:GLU:OE1	1.78	0.84
3:F:67:PRO:O	7:b:1:NAG:H62	1.79	0.83
4:O:307:THR:HG21	5:P:367:ILE:HD11	1.60	0.83
8:G:533:NGT:C8	2:L:373:TRP:CE2	2.62	0.82
4:Q:142:ASN:HB2	5:R:347:GLN:OE1	1.79	0.82
2:K:465:ASP:OD2	2:K:467:THR:HG22	1.81	0.81
8:C:530:NGT:C8	2:J:421:TYR:OH	2.28	0.81
4:O:239:VAL:HG12	4:O:245:PRO:HD2	1.63	0.80
4:Q:205:ILE:HD13	5:R:486:ALA:HB3	1.62	0.80
5:R:350:HIS:HD2	5:R:352:GLY:H	1.30	0.79
5:P:420:ILE:HD13	5:P:442:PRO:HB2	1.63	0.79
2:L:90:LEU:HD13	2:L:92:LYS:HE3	1.64	0.79
1:C:53:ALA:HB1	2:J:101:THR:HA	1.65	0.79
5:N:406:GLN:NE2	5:N:424:TRP:H	1.80	0.79
1:E:55:GLN:HG3	1:E:56:PRO:HD2	1.63	0.79
2:L:459:MET:HE1	2:L:464:VAL:HG21	1.63	0.78
1:E:34:ASP:HA	7:a:1:NAG:HN2	1.51	0.76
2:I:115:ASN:CG	6:U:1:NAG:C1	2.58	0.76
2:I:467:THR:HG21	5:N:544:GLN:HA	1.67	0.76
8:D:24:NGT:S1	5:P:450:TYR:OH	2.43	0.75
5:P:532:HIS:HD2	5:P:535:ARG:HH21	1.32	0.75
8:A:21:NGT:N2	2:I:322:ASP:OD2	2.20	0.75
2:L:100:VAL:HG12	2:L:102:PRO:HD2	1.67	0.75
2:L:121:ASN:HD21	2:L:124:GLN:HG2	1.51	0.74
2:J:424:ARG:HA	5:P:456:TYR:CD1	2.22	0.74
2:K:467:THR:HG21	5:R:544:GLN:HA	1.69	0.74
5:R:432:GLU:HG2	5:R:435:ARG:HH21	1.51	0.74
2:I:131:THR:HG22	2:I:133:TRP:H	1.54	0.73
2:I:117:THR:HG22	2:I:162:GLU:HG3	1.69	0.73
5:P:532:HIS:CD2	5:P:535:ARG:HH21	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:100:VAL:HG12	2:J:102:PRO:HD2	1.68	0.73
5:R:504:PRO:HG3	5:R:533:ARG:HG3	1.70	0.73
2:I:170:ARG:NH2	2:I:197:LYS:O	2.22	0.73
8:B:22:NGT:O4	4:M:211:ARG:NH2	2.22	0.73
5:T:365:PRO:HA	5:T:368:GLN:HB2	1.71	0.72
5:N:451:LEU:O	5:N:505:ARG:NH2	2.22	0.72
2:I:229:PRO:HA	2:I:233:ILE:HD11	1.70	0.72
4:O:170:ARG:NH2	4:O:232:ASN:HB3	2.04	0.72
4:O:211:ARG:HD2	4:O:242:GLN:OE1	1.89	0.72
4:S:203:ARG:HG2	5:T:513:LEU:HB3	1.71	0.72
2:J:121:ASN:ND2	2:J:124:GLN:H	1.88	0.71
2:I:151:GLU:HG2	1:C:38:VAL:HG11	1.71	0.71
2:I:459:MET:HE1	2:I:464:VAL:HG11	1.72	0.71
9:A:534:HOH:O	2:I:421:TYR:HB2	1.90	0.70
2:J:398:VAL:HG12	2:J:403:GLU:HG2	1.73	0.70
1:E:35:GLN:C	7:a:1:NAG:H83	2.15	0.70
5:N:406:GLN:HE21	5:N:424:TRP:H	1.36	0.70
8:C:530:NGT:HC83	2:J:392:TRP:CD2	2.26	0.70
2:I:89:THR:HG22	2:I:90:LEU:H	1.56	0.70
5:R:451:LEU:O	5:R:505:ARG:NH2	2.25	0.70
2:J:427:TYR:HD1	5:P:453:LEU:HA	1.57	0.69
2:I:447:GLU:CD	2:I:447:GLU:H	2.00	0.69
2:K:107:LEU:HB2	2:K:108:PRO:HD2	1.74	0.69
4:M:141:PRO:O	4:M:284:ARG:HG2	1.92	0.69
4:M:295:THR:HG21	5:N:322:ILE:HD11	1.73	0.69
4:M:235:HIS:HB2	5:N:485:GLU:OE2	1.93	0.69
2:K:178:ARG:CD	2:K:462:GLU:OE2	2.42	0.68
2:K:100:VAL:HG12	2:K:102:PRO:HD2	1.73	0.68
1:E:43:ASN:HD22	2:K:92:LYS:HG2	1.59	0.68
1:E:45:GLN:HB3	4:S:262:LEU:HD23	1.76	0.68
4:S:229:ASN:OD1	5:T:532:HIS:HE1	1.77	0.67
2:K:192:VAL:HA	2:K:195:TYR:CD2	2.28	0.67
4:Q:229:ASN:OD1	5:R:532:HIS:HE1	1.78	0.67
1:A:55:GLN:HG3	1:A:56:PRO:HD2	1.76	0.67
2:I:377:PHE:HB2	2:I:389:ILE:HD12	1.75	0.67
8:C:530:NGT:O4	2:J:178:ARG:NH1	2.26	0.67
2:K:170:ARG:NH2	2:K:197:LYS:O	2.27	0.67
2:L:99:VAL:HG22	2:L:130:GLU:HA	1.76	0.67
4:O:307:THR:CG2	5:P:367:ILE:HD11	2.25	0.67
4:Q:183:SER:O	3:H:74:PRO:HD2	1.94	0.67
2:J:157:ASN:OD1	6:Y:1:NAG:C1	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:113:VAL:HG11	7:c:1:NAG:C8	2.25	0.66
2:L:228:ASN:HD22	2:L:230:VAL:H	1.42	0.66
2:K:101:THR:N	2:K:102:PRO:HD2	2.11	0.66
4:M:215:PRO:O	4:M:218:ILE:HG22	1.96	0.66
1:E:45:GLN:HB3	4:S:262:LEU:CD2	2.26	0.66
4:O:216:VAL:HG11	4:O:273:MET:HE3	1.78	0.66
5:R:390:LYS:O	5:R:394:ILE:HD12	1.96	0.65
2:K:214:GLU:HG3	2:K:222:MET:HE2	1.78	0.65
4:Q:136:GLU:OE2	4:Q:166:TRP:NE1	2.26	0.65
8:C:530:NGT:S1	2:J:421:TYR:HE1	2.20	0.65
4:O:307:THR:HG21	5:P:367:ILE:CD1	2.26	0.65
2:L:94:VAL:HA	2:L:125:CYS:SG	2.37	0.65
2:L:173:LEU:HA	2:L:202:HIS:HB3	1.78	0.65
2:I:121:ASN:HD21	2:I:124:GLN:HG2	1.60	0.65
1:G:30:PHE:CD2	2:L:161:ILE:HG12	2.30	0.64
2:L:371:VAL:HG22	2:L:388:ILE:HD12	1.79	0.64
2:I:115:ASN:ND2	6:U:1:NAG:C2	2.59	0.64
2:I:465:ASP:OD2	2:I:467:THR:HG22	1.97	0.64
5:P:451:LEU:O	5:P:505:ARG:NH2	2.30	0.64
1:E:36:ARG:CB	7:a:1:NAG:C8	2.76	0.64
8:G:533:NGT:HC82	2:L:373:TRP:CE2	2.33	0.64
1:A:49:ASP:OD1	1:A:51:SER:N	2.24	0.64
2:K:121:ASN:HD22	2:K:123:ASP:H	1.44	0.64
1:G:58:CYS:SG	1:G:61:LEU:HG	2.37	0.64
8:F:26:NGT:HO4	5:R:489:TRP:CG	2.16	0.64
2:I:459:MET:CE	2:I:464:VAL:HG11	2.28	0.64
4:Q:166:TRP:HA	4:Q:169:LEU:HD12	1.79	0.64
2:J:170:ARG:HG2	2:J:484:LEU:HB3	1.80	0.63
8:G:533:NGT:C8	2:L:373:TRP:CD2	2.82	0.63
2:J:89:THR:HG22	2:J:90:LEU:H	1.62	0.63
5:R:425:LYS:O	5:R:429:TYR:HB3	1.98	0.63
3:D:67:PRO:HA	7:Z:1:NAG:O5	1.98	0.63
4:S:310:TYR:HE1	5:T:364:ASN:ND2	1.96	0.63
3:H:58:PRO:HB3	5:T:511:GLU:HA	1.79	0.63
2:L:173:LEU:HB3	2:L:458:CYS:HA	1.81	0.62
5:R:415:LEU:HB2	5:R:441:PHE:CZ	2.33	0.62
2:J:206:VAL:HG12	2:J:212:PRO:HD2	1.82	0.62
5:R:533:ARG:HA	5:R:536:MET:CE	2.29	0.62
2:J:101:THR:O	2:J:102:PRO:C	2.42	0.62
5:R:499:THR:HB	5:R:500:PRO:HD3	1.81	0.61
2:J:102:PRO:O	2:J:103:GLY:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ALA:HB1	2:K:101:THR:HA	1.83	0.61
4:M:132:THR:HB	4:M:163:ASN:HA	1.83	0.61
8:H:28:NGT:HC5	5:T:489:TRP:CD1	2.34	0.61
3:B:58:PRO:HB3	5:N:511:GLU:HA	1.81	0.61
5:P:372:ARG:HH11	5:P:372:ARG:CG	2.14	0.61
8:A:21:NGT:O4	2:I:178:ARG:NH1	2.34	0.61
1:G:46:PHE:CD2	2:L:94:VAL:HG11	2.36	0.61
1:G:48:TYR:CZ	1:G:65:PHE:HE2	2.19	0.61
2:L:463:TYR:O	5:T:545:PRO:HG2	2.01	0.61
2:I:153:THR:HG23	2:J:151:GLU:HB3	1.83	0.60
3:D:67:PRO:HB3	7:Z:1:NAG:O6	2.01	0.60
1:G:43:ASN:HD22	2:L:92:LYS:HG2	1.66	0.60
2:I:101:THR:N	2:I:102:PRO:HD2	2.16	0.60
2:I:121:ASN:ND2	2:I:124:GLN:HG2	2.16	0.60
2:L:359:LEU:O	2:L:363:VAL:HG23	2.02	0.60
4:M:126:GLN:HB3	4:M:157:VAL:HG13	1.83	0.60
2:K:339:MET:HE1	2:K:348:PHE:HE1	1.67	0.60
1:G:52:SER:HA	2:L:97:VAL:HG23	1.83	0.60
2:I:151:GLU:HB3	2:J:153:THR:HG23	1.82	0.60
2:L:131:THR:HG22	2:L:132:VAL:H	1.66	0.60
2:L:339:MET:SD	2:L:351:LEU:HD22	2.41	0.60
4:M:239:VAL:HG12	4:M:245:PRO:HD2	1.84	0.60
5:T:424:TRP:HB2	5:T:450:TYR:OH	2.02	0.60
4:O:222:THR:O	4:O:226:MET:HG3	2.00	0.59
1:E:55:GLN:HG3	1:E:56:PRO:CD	2.32	0.59
4:Q:206:LEU:HA	4:Q:235:HIS:HB3	1.82	0.59
2:J:157:ASN:ND2	6:Y:1:NAG:C2	2.63	0.59
1:A:45:GLN:HG3	2:I:93:ASN:ND2	2.17	0.59
4:M:190:ASN:ND2	6:W:1:NAG:C1	2.66	0.59
5:P:372:ARG:NH1	5:P:372:ARG:HG3	2.16	0.59
2:J:467:THR:HG21	5:P:544:GLN:HA	1.84	0.59
5:P:372:ARG:HH11	5:P:372:ARG:HG3	1.66	0.59
5:N:465:LYS:O	5:N:520:ARG:NH2	2.36	0.59
2:J:417:SER:O	2:J:421:TYR:CE2	2.56	0.59
2:L:515:GLN:HB2	2:L:516:PRO:HD2	1.84	0.59
5:P:403:ILE:HG12	5:P:420:ILE:HB	1.84	0.58
5:N:490:GLY:HA2	5:N:493:VAL:HB	1.86	0.58
5:N:532:HIS:HD2	5:N:535:ARG:NH2	1.92	0.58
2:K:401:MET:HE1	2:K:438:GLU:O	2.03	0.58
5:N:473:GLY:HA2	5:N:477:GLN:NE2	2.19	0.58
3:H:67:PRO:HA	7:e:1:NAG:H2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ARG:N	7:a:1:NAG:H83	2.19	0.58
2:K:170:ARG:HG2	2:K:484:LEU:CB	2.22	0.58
2:J:121:ASN:HD21	2:J:124:GLN:H	1.50	0.58
2:K:169:HIS:NE2	2:K:200:VAL:HG11	2.19	0.58
4:Q:310:TYR:O	4:Q:311:SER:HB2	2.02	0.58
2:I:404:LEU:HD11	2:I:416:LEU:HG	1.84	0.57
5:N:403:ILE:HG23	5:N:420:ILE:HB	1.86	0.57
2:J:422:LEU:O	2:J:476:ARG:NH2	2.34	0.57
2:J:228:ASN:HD22	2:J:230:VAL:H	1.52	0.57
2:J:400:TYR:CE1	2:J:401:MET:HE2	2.40	0.57
5:N:415:LEU:HB2	5:N:441:PHE:CE1	2.40	0.57
2:K:108:PRO:HG2	2:K:252:ARG:HG2	1.86	0.57
4:Q:229:ASN:OD1	5:R:532:HIS:CE1	2.56	0.57
2:J:171:GLY:HA3	2:J:456:GLU:HG2	1.86	0.57
1:E:25:PRO:HD2	2:K:197:LYS:HD2	1.86	0.56
4:S:149:TYR:CZ	4:S:196:ASP:HB3	2.40	0.56
8:A:21:NGT:O3	2:I:262:HIS:CE1	2.58	0.56
2:K:145:LEU:HD11	2:K:161:ILE:HD11	1.88	0.56
8:A:21:NGT:HC82	2:I:373:TRP:CE2	2.41	0.56
8:E:530:NGT:O4	2:K:462:GLU:OE2	2.21	0.56
2:L:113:VAL:HG11	7:c:1:NAG:H82	1.87	0.56
5:P:488:LEU:HD22	5:P:502:LEU:HG	1.88	0.56
2:J:171:GLY:HA2	2:J:200:VAL:O	2.06	0.56
5:R:350:HIS:CD2	5:R:352:GLY:H	2.17	0.56
5:N:341:SER:OG	5:N:398:ILE:HD12	2.05	0.56
2:K:398:VAL:HG12	2:K:403:GLU:HG2	1.88	0.56
4:O:215:PRO:O	4:O:218:ILE:HG22	2.05	0.55
2:L:183:LEU:HA	2:L:186:ILE:HD12	1.87	0.55
4:S:132:THR:HB	4:S:163:ASN:HA	1.87	0.55
2:I:319:LEU:HD12	2:I:360:LEU:HD23	1.89	0.55
2:I:467:THR:CG2	5:N:544:GLN:HA	2.36	0.55
2:J:463:TYR:CE1	5:P:547:TYR:HD1	2.24	0.55
2:L:318:HIS:HE1	2:L:373:TRP:CD1	2.23	0.55
3:H:65:MET:HB2	7:e:1:NAG:H83	1.89	0.55
4:Q:129:VAL:HG22	4:Q:160:LEU:HD23	1.89	0.55
3:H:73:ALA:HB3	3:H:76:ASN:HB3	1.87	0.55
3:B:58:PRO:HD2	4:M:230:LYS:HD2	1.88	0.55
2:J:90:LEU:HD13	2:J:92:LYS:HE3	1.87	0.55
2:K:518:ASN:ND2	5:R:492:TYR:CE1	2.74	0.55
5:T:341:SER:OG	5:T:398:ILE:HD12	2.07	0.55
2:I:273:LEU:HD11	2:I:301:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:204:HIS:HE1	2:L:207:ASP:OD1	1.89	0.55
1:E:38:VAL:HG11	2:L:151:GLU:HG2	1.89	0.54
5:R:443:VAL:HG12	5:R:481:PHE:HA	1.88	0.54
4:M:170:ARG:HB3	4:M:230:LYS:HE3	1.88	0.54
2:K:176:THR:OG1	2:K:205:LEU:HA	2.07	0.54
1:G:52:SER:HB3	1:G:55:GLN:HE22	1.73	0.54
3:B:65:MET:HE3	4:M:190:ASN:HD22	1.73	0.54
2:L:357:GLN:CD	2:L:382:LYS:HB3	2.32	0.54
8:H:28:NGT:O6	5:T:450:TYR:HD2	1.90	0.54
8:C:530:NGT:HC83	2:J:392:TRP:CE3	2.42	0.54
2:J:170:ARG:NH2	2:J:197:LYS:O	2.40	0.54
2:K:100:VAL:HG12	2:K:102:PRO:CD	2.38	0.54
5:P:424:TRP:CZ2	5:P:425:LYS:HE2	2.43	0.54
8:D:24:NGT:S1	5:P:450:TYR:CZ	3.00	0.54
2:L:101:THR:N	2:L:102:PRO:HD2	2.23	0.54
2:I:170:ARG:HG2	2:I:484:LEU:CB	2.33	0.54
2:I:228:ASN:HD22	2:I:231:THR:H	1.56	0.54
1:A:38:VAL:HG22	2:I:155:PHE:HE1	1.72	0.53
2:J:136:LEU:HA	2:J:139:LEU:HD12	1.88	0.53
2:K:519:VAL:HG12	5:R:491:GLU:HA	1.90	0.53
6:Y:1:NAG:H61	6:Y:2:NAG:N2	2.24	0.53
1:A:23:LEU:HD21	2:I:141:THR:HG23	1.89	0.53
2:L:372:VAL:HG21	2:L:376:VAL:HG21	1.90	0.53
4:M:211:ARG:HD2	4:M:242:GLN:OE1	2.09	0.53
5:T:352:GLY:HA2	5:T:405:TRP:CD1	2.44	0.53
5:P:424:TRP:HB2	5:P:450:TYR:OH	2.09	0.53
2:L:467:THR:HG21	5:T:544:GLN:HA	1.91	0.53
3:H:81:HIS:HE1	3:H:95:GLU:OE2	1.91	0.53
1:A:45:GLN:HG3	2:I:93:ASN:HD21	1.74	0.53
8:C:530:NGT:C8	2:J:421:TYR:HH	2.10	0.53
1:G:23:LEU:HD11	2:L:141:THR:HG23	1.91	0.53
1:G:28:GLN:NE2	2:L:487:ASN:HD22	2.07	0.53
2:I:102:PRO:O	2:I:103:GLY:O	2.27	0.53
2:K:423:ASN:HB3	2:K:460:TRP:H	1.74	0.53
1:A:43:ASN:CG	1:A:43:ASN:O	2.52	0.52
2:L:114:GLU:CD	2:L:170:ARG:HH12	2.17	0.52
8:C:530:NGT:HO4	2:J:178:ARG:HH12	1.53	0.52
8:D:24:NGT:S1	5:P:450:TYR:CE2	3.03	0.52
2:L:228:ASN:ND2	2:L:230:VAL:H	2.07	0.52
2:J:99:VAL:HG22	2:J:130:GLU:HA	1.90	0.52
8:G:533:NGT:HC81	2:L:373:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:58:PRO:HD2	4:S:230:LYS:HD2	1.91	0.52
2:K:173:LEU:HA	2:K:202:HIS:HB3	1.91	0.52
2:L:170:ARG:HG2	2:L:484:LEU:HB3	1.91	0.52
5:N:390:LYS:O	5:N:394:ILE:HG13	2.09	0.52
8:C:530:NGT:HC83	2:J:392:TRP:CG	2.45	0.52
2:L:147:TRP:NE1	2:L:157:ASN:OD1	2.39	0.52
1:A:61:LEU:HD11	2:I:135:ALA:CB	2.40	0.52
2:I:525:GLU:OE1	4:M:264:HIS:HE1	1.93	0.52
2:J:417:SER:O	2:J:421:TYR:HE2	1.93	0.52
5:R:406:GLN:HE21	5:R:424:TRP:H	1.57	0.52
5:T:429:TYR:N	5:T:430:PRO:CD	2.72	0.52
6:d:1:NAG:H61	6:d:2:NAG:O7	2.09	0.52
5:R:415:LEU:HD22	5:R:419:THR:HG21	1.92	0.52
5:R:465:LYS:O	5:R:520:ARG:NH2	2.43	0.52
5:T:451:LEU:O	5:T:505:ARG:NH2	2.32	0.52
2:I:402:LYS:HD2	2:I:406:LEU:HD13	1.92	0.51
5:P:459:ASP:OD1	5:P:505:ARG:HD2	2.10	0.51
5:P:504:PRO:HG3	5:P:533:ARG:HG3	1.92	0.51
4:Q:267:THR:O	4:Q:271:VAL:HG23	2.09	0.51
2:J:210:SER:HB2	2:J:227:TYR:CE2	2.45	0.51
2:K:467:THR:CG2	5:R:544:GLN:HA	2.39	0.51
5:R:407:GLU:OE2	5:R:424:TRP:HZ2	1.92	0.51
4:S:310:TYR:CE1	5:T:364:ASN:ND2	2.77	0.51
2:I:101:THR:N	2:I:102:PRO:CD	2.73	0.51
4:Q:170:ARG:HD2	4:Q:230:LYS:HG2	1.92	0.51
2:L:518:ASN:ND2	2:L:519:VAL:H	2.09	0.51
8:C:530:NGT:S1	2:J:460:TRP:NE1	2.83	0.51
2:J:320:GLY:HA2	2:J:373:TRP:CD1	2.44	0.51
2:J:396:ILE:HG13	2:J:397:PRO:HA	1.92	0.51
2:J:459:MET:HE3	2:J:464:VAL:HG11	1.92	0.51
5:P:395:ILE:HG22	5:P:400:LYS:O	2.09	0.51
3:F:55:ALA:O	5:R:535:ARG:NH2	2.40	0.51
4:S:235:HIS:NE2	4:S:288:GLU:OE1	2.38	0.51
1:A:61:LEU:N	1:A:61:LEU:HD23	2.25	0.51
5:P:499:THR:HB	5:P:500:PRO:HD3	1.93	0.51
2:K:107:LEU:HB3	2:K:247:ARG:HG3	1.91	0.51
3:H:55:ALA:HB1	5:T:531:ARG:HG3	1.92	0.51
8:D:24:NGT:O3	4:O:294:HIS:CE1	2.64	0.51
4:Q:199:ARG:HH21	5:R:469:LEU:HD12	1.76	0.51
4:Q:203:ARG:HG2	5:R:513:LEU:HB3	1.92	0.51
4:Q:235:HIS:NE2	4:Q:288:GLU:OE1	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:64:LYS:HE3	4:S:193:THR:HB	1.93	0.51
2:I:97:VAL:HG12	2:I:126:LEU:HD21	1.93	0.51
2:I:524:GLN:O	2:I:524:GLN:HG2	2.10	0.51
4:M:299:GLY:HA3	4:M:306:LEU:HD12	1.93	0.51
2:J:113:VAL:HG21	7:X:1:NAG:H82	1.93	0.51
1:G:46:PHE:CD2	2:L:94:VAL:CG1	2.93	0.51
2:L:172:LEU:HD23	2:L:457:ALA:HB3	1.93	0.51
2:I:252:ARG:HB3	2:I:314:ASP:OD1	2.10	0.51
5:N:364:ASN:HD22	5:N:365:PRO:CD	2.19	0.51
7:e:1:NAG:H61	7:e:2:NAG:O7	2.11	0.51
4:M:151:LEU:HD23	4:M:194:ILE:HD13	1.94	0.50
4:M:202:HIS:CD2	4:M:233:VAL:HG21	2.46	0.50
5:P:362:GLU:O	5:P:368:GLN:NE2	2.44	0.50
5:R:533:ARG:HA	5:R:536:MET:HE2	1.93	0.50
5:T:504:PRO:HG3	5:T:533:ARG:HG3	1.92	0.50
5:T:530:THR:HG23	5:T:546:LEU:HD12	1.92	0.50
2:J:101:THR:N	2:J:102:PRO:HD2	2.26	0.50
2:J:202:HIS:ND1	2:J:456:GLU:OE1	2.44	0.50
2:K:424:ARG:HA	5:R:456:TYR:CD1	2.47	0.50
1:A:55:GLN:HG3	1:A:56:PRO:CD	2.42	0.50
2:I:99:VAL:CG2	2:I:100:VAL:N	2.74	0.50
2:J:350:GLN:HA	2:J:353:SER:HB2	1.94	0.50
2:J:475:PRO:HG2	2:J:517:LEU:CD1	2.41	0.50
4:O:302:GLN:HE21	4:O:302:GLN:HA	1.76	0.50
5:P:474:THR:H	5:P:477:GLN:NE2	2.09	0.50
4:S:126:GLN:HB3	4:S:157:VAL:HG13	1.94	0.50
5:T:326:LEU:O	5:T:329:THR:HG22	2.11	0.50
5:R:367:ILE:O	5:R:371:MET:HG2	2.12	0.50
1:C:23:LEU:HD11	2:J:141:THR:HG23	1.94	0.50
8:C:530:NGT:HC62	2:J:462:GLU:CD	2.37	0.50
5:P:430:PRO:O	5:P:471:PHE:HB2	2.12	0.50
4:M:249:ILE:HG12	1:C:57:GLY:HA2	1.93	0.50
1:E:30:PHE:CD2	2:K:161:ILE:HG12	2.47	0.50
2:K:353:SER:HA	2:K:381:VAL:HG13	1.93	0.50
2:L:214:GLU:HA	2:L:222:MET:HB2	1.94	0.50
2:I:459:MET:HE1	2:I:464:VAL:HG21	1.94	0.50
4:M:223:LEU:HD21	4:M:234:LEU:HD22	1.94	0.50
2:K:187:LEU:HA	2:K:190:LEU:HD12	1.93	0.50
2:K:228:ASN:HD22	2:K:231:THR:H	1.58	0.50
2:I:319:LEU:HD11	2:I:363:VAL:HG21	1.94	0.50
1:C:55:GLN:HG3	1:C:56:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:235:THR:O	2:J:239:VAL:HG23	2.12	0.50
1:E:30:PHE:HD2	2:K:161:ILE:HG12	1.75	0.50
1:A:39:LEU:HD11	2:I:156:ILE:HB	1.94	0.49
2:I:101:THR:O	2:I:102:PRO:C	2.54	0.49
1:E:46:PHE:CD2	2:K:94:VAL:CG1	2.94	0.49
1:G:53:ALA:HB1	2:L:101:THR:HG23	1.94	0.49
4:S:248:SER:HB3	4:S:251:PHE:O	2.12	0.49
5:T:533:ARG:HA	5:T:536:MET:HE3	1.93	0.49
5:R:388:ILE:HG21	5:R:408:VAL:HG13	1.94	0.49
2:I:428:GLY:HA2	5:N:492:TYR:CE2	2.47	0.49
5:P:461:ARG:O	5:P:465:LYS:HB2	2.13	0.49
2:K:198:LEU:HD11	2:K:481:ALA:HB2	1.94	0.49
2:L:307:GLU:O	2:L:311:VAL:HG23	2.11	0.49
2:L:113:VAL:HG11	7:c:1:NAG:H83	1.93	0.49
2:I:101:THR:O	2:I:103:GLY:N	2.46	0.49
2:I:220:GLU:HA	2:I:223:ARG:HB2	1.95	0.49
2:K:178:ARG:HD3	5:R:548:ALA:HB2	1.94	0.49
8:F:26:NGT:C2	5:R:355:GLU:OE1	2.56	0.49
5:R:533:ARG:HA	5:R:536:MET:HE3	1.93	0.49
1:G:55:GLN:CG	1:G:56:PRO:HD2	2.26	0.49
2:I:140:GLU:O	2:I:141:THR:C	2.55	0.49
2:I:325:ASP:OD2	2:I:327:THR:HB	2.13	0.49
1:C:25:PRO:HB3	2:J:482:GLU:HA	1.95	0.49
2:K:409:LYS:HZ2	2:K:409:LYS:HB2	1.77	0.49
2:K:421:TYR:HA	2:K:458:CYS:HB2	1.94	0.49
4:Q:253:GLU:HA	4:Q:256:ASN:HB2	1.94	0.49
5:T:329:THR:HG23	5:T:330:TYR:CD2	2.48	0.49
2:I:101:THR:H	2:I:102:PRO:HD2	1.77	0.49
2:L:176:THR:HG22	2:L:181:LEU:HB2	1.94	0.49
5:T:504:PRO:HD3	5:T:544:GLN:O	2.13	0.49
1:A:28:GLN:HE22	2:I:487:ASN:HD22	1.60	0.49
2:I:100:VAL:HG23	2:I:130:GLU:HG3	1.95	0.49
2:K:347:ASP:HB2	2:K:349:LYS:HE3	1.94	0.49
5:R:460:TRP:HA	5:R:463:TYR:HD2	1.77	0.49
2:L:169:HIS:HE1	2:L:456:GLU:OE2	1.96	0.49
2:I:151:GLU:CG	1:C:38:VAL:HG11	2.39	0.48
5:N:350:HIS:HD2	5:N:352:GLY:H	1.61	0.48
5:T:451:LEU:HD11	5:T:486:ALA:HB1	1.94	0.48
2:I:101:THR:H	2:I:102:PRO:CD	2.26	0.48
1:G:24:TRP:CZ3	2:L:500:LEU:HB2	2.48	0.48
1:G:48:TYR:HE2	1:G:61:LEU:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:131:THR:HG21	2:I:133:TRP:CD1	2.48	0.48
4:Q:175:PHE:O	4:Q:178:LEU:HB2	2.14	0.48
4:M:277:TYR:O	4:M:281:ARG:NH1	2.45	0.48
4:Q:142:ASN:CB	5:R:347:GLN:OE1	2.56	0.48
2:L:318:HIS:CE1	2:L:373:TRP:CD1	3.01	0.48
5:P:459:ASP:OD2	5:P:505:ARG:NH1	2.45	0.48
5:R:533:ARG:HG2	5:R:543:ALA:HB3	1.96	0.48
2:L:425:ILE:HB	5:T:454:ILE:HD12	1.96	0.48
2:I:422:LEU:O	2:I:476:ARG:NH2	2.46	0.48
9:C:7:HOH:O	2:J:421:TYR:HB2	2.13	0.48
2:J:107:LEU:HD22	2:J:107:LEU:H	1.78	0.48
4:O:170:ARG:HH21	4:O:232:ASN:HB3	1.77	0.48
1:E:43:ASN:ND2	2:K:92:LYS:HG2	2.28	0.48
2:I:204:HIS:CD2	2:I:256:GLU:OE1	2.66	0.48
2:J:419:PRO:HB2	2:J:437:VAL:HG21	1.95	0.48
2:K:117:THR:HG22	2:K:162:GLU:HG2	1.94	0.48
2:K:266:TRP:H	2:K:266:TRP:CD1	2.31	0.48
2:I:307:GLU:O	2:I:311:VAL:HG23	2.14	0.48
3:F:57:TRP:HA	3:F:58:PRO:C	2.38	0.48
2:I:518:ASN:ND2	2:I:519:VAL:H	2.12	0.48
4:O:310:TYR:N	4:O:310:TYR:CD1	2.81	0.48
4:M:139:ALA:O	4:M:279:ARG:HD2	2.14	0.47
5:N:530:THR:HG22	5:N:546:LEU:HD12	1.96	0.47
4:S:233:VAL:HG22	4:S:284:ARG:HD3	1.95	0.47
4:M:208:ASP:OD1	4:M:208:ASP:C	2.56	0.47
8:G:533:NGT:HC81	2:L:373:TRP:CE2	2.48	0.47
2:I:156:ILE:HG13	2:I:157:ASN:N	2.29	0.47
2:I:176:THR:HG22	2:I:181:LEU:HD12	1.97	0.47
1:C:36:ARG:HD3	6:Y:1:NAG:H62	1.96	0.47
2:L:222:MET:HG2	2:L:233:ILE:HD12	1.96	0.47
2:L:259:THR:HB	2:L:355:TYR:OH	2.13	0.47
2:I:115:ASN:ND2	6:U:1:NAG:N2	2.62	0.47
2:I:377:PHE:HB2	2:I:389:ILE:CD1	2.44	0.47
2:I:500:LEU:HG	2:I:517:LEU:HD11	1.96	0.47
4:O:232:ASN:HA	4:O:283:ILE:HG13	1.96	0.47
2:K:237:GLN:HB2	3:H:92:THR:CG2	2.45	0.47
5:T:406:GLN:HE21	5:T:424:TRP:H	1.62	0.47
1:A:52:SER:HB2	2:I:97:VAL:HA	1.97	0.47
2:J:157:ASN:O	2:J:159:THR:HG22	2.15	0.47
2:J:398:VAL:CG1	2:J:403:GLU:HG2	2.41	0.47
2:K:243:ILE:HA	2:K:253:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:82:SER:HA	4:Q:128:LEU:HD22	1.95	0.47
2:L:130:GLU:CG	7:c:1:NAG:H82	2.35	0.47
2:L:390:GLN:HG3	2:L:415:LEU:HB2	1.96	0.47
5:P:354:ASP:OD1	5:P:405:TRP:CD1	2.67	0.47
2:L:120:ILE:HB	2:L:159:THR:HG22	1.95	0.47
2:I:99:VAL:HG23	2:I:100:VAL:N	2.29	0.47
4:M:292:PRO:HA	5:N:322:ILE:HD12	1.96	0.47
2:J:116:TYR:CZ	2:J:163:ASP:HB3	2.50	0.47
4:O:216:VAL:O	4:O:220:LEU:HG	2.14	0.47
5:P:425:LYS:O	5:P:429:TYR:HB3	2.15	0.47
1:E:36:ARG:N	7:a:1:NAG:C8	2.78	0.47
1:E:46:PHE:HD2	2:K:94:VAL:CG1	2.28	0.47
2:K:107:LEU:H	2:K:107:LEU:HD13	1.79	0.47
2:K:459:MET:HE2	2:K:464:VAL:HG11	1.97	0.47
2:K:485:TRP:CD1	2:K:485:TRP:C	2.91	0.47
4:Q:142:ASN:HB2	5:R:347:GLN:CD	2.38	0.47
2:L:113:VAL:HG12	2:L:115:ASN:H	1.80	0.47
2:L:356:ILE:O	2:L:360:LEU:HG	2.14	0.47
2:J:364:SER:HB2	2:J:370:TYR:HE1	1.80	0.47
4:Q:222:THR:O	4:Q:226:MET:HG3	2.15	0.47
2:L:131:THR:HG22	2:L:132:VAL:N	2.29	0.47
2:L:244:GLU:O	2:L:248:LEU:HG	2.15	0.47
2:I:187:LEU:HD22	2:I:245:TYR:CG	2.50	0.47
2:L:424:ARG:HA	5:T:456:TYR:CD1	2.50	0.47
1:A:28:GLN:NE2	2:I:487:ASN:HD22	2.13	0.47
2:I:422:LEU:HD11	2:I:477:ALA:HB2	1.96	0.47
2:K:307:GLU:O	2:K:311:VAL:HG23	2.14	0.47
4:Q:279:ARG:C	4:Q:281:ARG:H	2.22	0.47
2:J:170:ARG:HG2	2:J:484:LEU:CB	2.45	0.46
5:R:388:ILE:HG12	5:R:408:VAL:HG11	1.96	0.46
2:L:379:ASN:O	2:L:380:LYS:C	2.58	0.46
5:T:490:GLY:HA2	5:T:493:VAL:HB	1.98	0.46
2:I:174:LEU:HB2	2:I:201:PHE:HE1	1.80	0.46
4:M:290:ASP:OD2	5:N:354:ASP:OD1	2.33	0.46
4:O:238:ILE:HG23	4:O:239:VAL:HG13	1.96	0.46
2:J:176:THR:HG22	2:J:181:LEU:HD12	1.97	0.46
2:J:302:SER:HA	2:J:362:ILE:HG21	1.96	0.46
5:P:372:ARG:CG	5:P:372:ARG:NH1	2.75	0.46
2:I:270:ILE:HG13	2:I:270:ILE:O	2.15	0.46
2:I:402:LYS:HD2	2:I:406:LEU:CD1	2.46	0.46
8:B:22:NGT:HC2	5:N:355:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:530:NGT:HC82	2:K:460:TRP:CH2	2.49	0.46
2:L:206:VAL:HG12	2:L:212:PRO:HD2	1.96	0.46
2:I:459:MET:HE1	2:I:464:VAL:CG1	2.43	0.46
2:J:290:VAL:O	2:J:292:PRO:HD3	2.15	0.46
4:S:152:LEU:HB2	4:S:159:VAL:HB	1.97	0.46
2:J:266:TRP:N	2:J:266:TRP:CD1	2.84	0.46
5:R:330:TYR:CG	5:R:390:LYS:HE2	2.50	0.46
3:H:56:LEU:O	5:T:528:ARG:NH1	2.46	0.46
2:I:398:VAL:HG12	2:I:403:GLU:HG2	1.98	0.46
2:J:235:THR:HG22	2:J:236:ALA:N	2.31	0.46
2:K:175:ASP:HB3	2:K:461:GLY:N	2.30	0.46
2:K:210:SER:HB2	2:K:227:TYR:CE2	2.51	0.46
2:K:224:LYS:HB3	2:K:268:PRO:HB2	1.98	0.46
1:G:28:GLN:HE22	2:L:487:ASN:HD22	1.61	0.46
8:G:533:NGT:HC82	2:L:373:TRP:CZ2	2.50	0.46
4:M:253:GLU:HA	4:M:256:ASN:HB2	1.97	0.46
2:K:404:LEU:HD11	2:K:416:LEU:HD13	1.97	0.46
2:K:424:ARG:HA	5:R:456:TYR:HD1	1.81	0.46
2:L:392:TRP:HB2	2:L:421:TYR:OH	2.15	0.46
3:H:54:PRO:HB2	3:H:56:LEU:HG	1.97	0.46
2:I:270:ILE:HG13	2:I:273:LEU:HB2	1.98	0.46
4:M:140:PHE:CE1	4:M:279:ARG:HD3	2.51	0.46
2:J:519:VAL:HA	4:O:212:HIS:CE1	2.51	0.46
4:Q:198:PRO:HB3	5:R:514:TRP:CE3	2.51	0.46
4:Q:261:SER:OG	4:Q:264:HIS:CD2	2.68	0.46
5:N:388:ILE:HG12	5:N:408:VAL:HG21	1.97	0.45
2:J:228:ASN:HD22	2:J:231:THR:H	1.65	0.45
2:J:232:HIS:O	2:J:233:ILE:HD13	2.16	0.45
2:K:216:PHE:CE2	2:K:307:GLU:HG3	2.51	0.45
4:Q:244:PHE:N	4:Q:258:GLY:O	2.42	0.45
8:G:533:NGT:C8	2:L:373:TRP:CZ2	2.97	0.45
2:J:100:VAL:HG12	2:J:102:PRO:CD	2.44	0.45
2:J:350:GLN:HA	2:J:353:SER:CB	2.46	0.45
2:J:400:TYR:HE1	2:J:401:MET:HE2	1.78	0.45
3:B:84:ASN:C	3:B:84:ASN:HD22	2.24	0.45
8:B:22:NGT:S1	5:N:450:TYR:OH	2.69	0.45
4:O:240:ASP:OD1	4:O:241:ASP:N	2.35	0.45
2:L:187:LEU:HA	2:L:190:LEU:HD12	1.97	0.45
4:S:307:THR:HG21	5:T:361:TRP:HD1	1.81	0.45
8:A:21:NGT:C8	2:I:373:TRP:CE2	3.00	0.45
2:I:173:LEU:HA	2:I:202:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLN:HE22	1:C:69:ARG:HD3	1.81	0.45
1:E:25:PRO:HB3	2:K:482:GLU:HA	1.97	0.45
4:O:288:GLU:HG3	5:P:350:HIS:CD2	2.52	0.45
2:L:101:THR:N	2:L:102:PRO:CD	2.79	0.45
2:L:170:ARG:NH2	2:L:197:LYS:O	2.50	0.45
2:L:465:ASP:C	2:L:467:THR:H	2.24	0.45
2:K:322:ASP:HB3	2:K:373:TRP:CD1	2.51	0.45
1:G:52:SER:OG	1:G:54:ALA:O	2.34	0.45
2:L:130:GLU:HG2	7:c:1:NAG:H81	1.92	0.45
2:I:100:VAL:CG1	2:I:102:PRO:CD	2.90	0.45
2:I:284:SER:C	2:I:286:THR:H	2.25	0.45
5:R:376:PHE:CD1	5:R:382:LYS:HD3	2.52	0.45
2:L:482:GLU:HG3	2:L:486:SER:OG	2.16	0.45
3:H:82:SER:HA	4:S:128:LEU:HD22	1.98	0.45
5:T:499:THR:HB	5:T:500:PRO:HD3	1.99	0.45
1:A:46:PHE:HD2	2:I:94:VAL:HG12	1.82	0.45
5:N:429:TYR:N	5:N:430:PRO:CD	2.80	0.45
2:K:171:GLY:HA2	2:K:200:VAL:O	2.17	0.45
2:K:188:ASP:O	2:K:192:VAL:HG23	2.17	0.45
2:I:475:PRO:HG3	2:I:504:ARG:HG3	1.98	0.45
3:B:65:MET:CE	4:M:190:ASN:HD22	2.30	0.45
2:K:116:TYR:CZ	2:K:163:ASP:HB3	2.52	0.45
2:K:179:HIS:CE1	5:R:548:ALA:HA	2.52	0.45
2:K:464:VAL:HG21	2:K:472:ARG:HD2	1.99	0.45
4:S:204:GLY:HA2	4:S:233:VAL:O	2.16	0.45
5:N:514:TRP:CD1	5:N:514:TRP:C	2.94	0.45
4:Q:175:PHE:HA	4:Q:178:LEU:HD12	1.98	0.45
2:L:246:ALA:HB1	2:L:251:ILE:HB	1.98	0.45
7:c:1:NAG:O7	7:c:1:NAG:O3	2.34	0.45
2:I:166:ARG:HH21	2:I:440:LEU:HD12	1.82	0.44
2:I:393:ARG:O	2:I:400:TYR:HB3	2.17	0.44
4:M:199:ARG:NH1	5:N:517:LYS:HA	2.32	0.44
2:J:467:THR:CG2	5:P:544:GLN:HA	2.46	0.44
2:K:202:HIS:HD1	2:K:456:GLU:CD	2.23	0.44
2:I:258:ASP:OD2	2:I:322:ASP:OD1	2.35	0.44
1:G:69:ARG:HG3	1:G:70:ASP:N	2.32	0.44
5:N:448:PRO:HB2	5:N:466:VAL:HG21	1.99	0.44
5:N:490:GLY:O	5:N:491:GLU:C	2.60	0.44
2:K:179:HIS:HB3	2:K:465:ASP:HB3	2.00	0.44
2:I:106:GLN:CD	2:I:106:GLN:H	2.23	0.44
2:J:404:LEU:HD11	2:J:416:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:TYR:C	3:D:103:GLY:N	2.75	0.44
2:K:523:GLU:CD	2:K:523:GLU:H	2.26	0.44
1:A:40:TYR:O	1:A:41:PRO:C	2.60	0.44
2:J:388:ILE:HG21	2:J:453:ILE:HD11	1.99	0.44
4:O:288:GLU:HB2	5:P:350:HIS:HB3	1.98	0.44
5:R:354:ASP:CG	5:R:405:TRP:CD1	2.95	0.44
2:L:188:ASP:O	2:L:192:VAL:HG23	2.18	0.44
4:Q:145:SER:HB3	4:Q:166:TRP:CD1	2.53	0.44
5:R:376:PHE:HD1	5:R:382:LYS:HD3	1.83	0.44
5:R:488:LEU:HD22	5:R:502:LEU:HG	1.99	0.44
1:G:40:TYR:HA	1:G:41:PRO:HD2	1.79	0.44
2:I:214:GLU:HA	2:I:222:MET:HB2	1.99	0.44
2:K:506:GLU:OE1	2:K:506:GLU:HA	2.18	0.44
8:H:28:NGT:O6	5:T:453:LEU:HG	2.18	0.44
5:T:403:ILE:HG12	5:T:420:ILE:HB	2.00	0.44
2:I:173:LEU:HB3	2:I:458:CYS:HA	2.00	0.44
1:C:36:ARG:HH11	6:Y:1:NAG:H62	1.83	0.44
4:O:215:PRO:HD2	5:P:495:ALA:HB2	1.99	0.44
2:K:168:PRO:HD2	2:K:453:ILE:O	2.18	0.44
2:K:178:ARG:NE	2:K:462:GLU:OE2	2.51	0.44
2:K:237:GLN:HB2	3:H:92:THR:HG21	1.99	0.44
4:Q:151:LEU:HD13	4:Q:160:LEU:HD13	1.99	0.44
4:M:200:PHE:CE1	5:N:481:PHE:CD1	3.06	0.44
5:N:502:LEU:HD13	5:N:503:TRP:CE2	2.52	0.44
1:C:41:PRO:HB3	1:C:73:PHE:HB3	1.99	0.44
5:P:429:TYR:O	5:P:432:GLU:HB2	2.17	0.44
2:K:445:THR:HB	2:K:446:PRO:HD2	2.00	0.44
2:L:118:LEU:HB3	2:L:161:ILE:HD12	1.99	0.44
5:T:464:TYR:HB2	5:T:508:ALA:HB1	2.00	0.44
2:I:131:THR:HG22	2:I:132:VAL:N	2.32	0.43
2:I:215:SER:O	2:I:219:PRO:HA	2.17	0.43
2:I:339:MET:SD	2:I:351:LEU:HD22	2.58	0.43
4:O:199:ARG:HH21	5:P:469:LEU:HD12	1.82	0.43
2:K:520:GLY:O	4:Q:212:HIS:HD2	2.00	0.43
2:L:120:ILE:HB	2:L:159:THR:CG2	2.48	0.43
2:I:435:TYR:HE2	2:I:491:SER:HA	1.82	0.43
2:J:392:TRP:HB2	2:J:421:TYR:OH	2.18	0.43
1:E:36:ARG:CB	7:a:1:NAG:H81	2.49	0.43
2:L:122:ASP:OD1	2:L:122:ASP:N	2.49	0.43
2:L:140:GLU:OE1	2:L:195:TYR:HD1	2.01	0.43
4:M:206:LEU:HB3	5:N:487:CYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:205:LEU:H	2:L:205:LEU:HD12	1.83	0.43
1:A:63:GLU:O	1:A:64:ALA:C	2.61	0.43
4:M:149:TYR:CZ	4:M:196:ASP:HB3	2.53	0.43
2:J:229:PRO:HA	2:J:233:ILE:HD11	2.00	0.43
4:O:302:GLN:HA	4:O:302:GLN:NE2	2.34	0.43
1:E:40:TYR:HA	1:E:41:PRO:HD2	1.79	0.43
1:E:58:CYS:C	2:K:104:CYS:SG	3.00	0.43
8:E:530:NGT:C8	2:K:460:TRP:CH2	3.01	0.43
2:J:463:TYR:HE1	5:P:547:TYR:HD1	1.64	0.43
1:E:52:SER:O	1:E:55:GLN:NE2	2.51	0.43
2:K:171:GLY:HA3	2:K:456:GLU:HG2	2.00	0.43
3:F:63:VAL:HG12	3:F:65:MET:HG2	2.01	0.43
1:G:55:GLN:HG3	1:G:56:PRO:HD3	1.95	0.43
8:G:533:NGT:HC81	2:L:373:TRP:CE3	2.54	0.43
2:L:513:GLN:HG3	2:L:526:PHE:CZ	2.54	0.43
2:I:357:GLN:OE1	2:I:382:LYS:HB3	2.18	0.43
3:B:105:ILE:HG12	4:M:176:SER:HA	2.01	0.43
1:C:59:SER:O	1:C:63:GLU:HG2	2.19	0.43
4:O:139:ALA:O	4:O:279:ARG:NH2	2.46	0.43
5:P:467:GLU:HA	5:P:468:PRO:HD2	1.88	0.43
2:L:97:VAL:HG12	2:L:126:LEU:HD21	2.01	0.43
2:L:99:VAL:CG2	2:L:130:GLU:HA	2.47	0.43
2:L:356:ILE:HD13	2:L:376:VAL:HG22	2.01	0.43
2:I:107:LEU:HD22	2:I:107:LEU:H	1.84	0.43
2:I:356:ILE:HD13	2:I:376:VAL:HG22	2.00	0.43
4:M:200:PHE:HE1	5:N:481:PHE:HD1	1.67	0.43
2:J:332:ASN:HA	2:J:333:PRO:HD3	1.80	0.43
4:O:202:HIS:CE1	5:P:444:ILE:HD13	2.54	0.43
2:K:100:VAL:C	2:K:102:PRO:HD2	2.43	0.43
4:Q:134:GLN:O	4:Q:164:ARG:NH1	2.41	0.43
4:Q:153:VAL:HB	4:Q:192:SER:H	1.84	0.43
5:R:516:SER:HB2	5:R:519:VAL:HG23	2.00	0.43
1:A:40:TYR:HA	1:A:41:PRO:HD2	1.88	0.43
2:I:95:LEU:HB2	2:I:126:LEU:HD23	2.00	0.43
2:I:177:SER:O	2:I:210:SER:HB3	2.18	0.43
4:M:200:PHE:CE1	5:N:481:PHE:HD1	2.36	0.43
2:J:235:THR:HG22	2:J:236:ALA:H	1.83	0.43
2:K:370:TYR:HD2	2:K:387:THR:HG23	1.84	0.43
3:F:54:PRO:HB2	3:F:56:LEU:HG	1.99	0.43
2:L:171:GLY:HA2	2:L:200:VAL:O	2.18	0.43
4:Q:215:PRO:O	4:Q:218:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:468:PRO:HB2	5:R:481:PHE:CZ	2.54	0.43
4:S:154:LYS:HD2	4:S:155:GLU:O	2.18	0.43
4:S:206:LEU:HA	4:S:235:HIS:O	2.19	0.43
2:I:384:GLN:HG3	2:I:385:PRO:HD2	2.00	0.43
4:O:237:HIS:CD2	4:O:288:GLU:OE1	2.72	0.43
5:P:503:TRP:HB3	5:P:536:MET:HE1	2.00	0.43
3:H:63:VAL:HA	4:S:194:ILE:HG13	2.01	0.43
2:I:387:THR:HG22	2:I:388:ILE:N	2.33	0.42
2:I:518:ASN:CG	2:I:519:VAL:H	2.26	0.42
2:J:447:GLU:H	2:J:447:GLU:CD	2.27	0.42
5:P:323:ASN:HA	5:P:324:PRO:HD3	1.94	0.42
2:K:101:THR:O	2:K:103:GLY:N	2.52	0.42
2:K:430:ASP:OD2	2:K:476:ARG:NH1	2.51	0.42
2:L:192:VAL:HA	2:L:195:TYR:CD2	2.54	0.42
2:J:316:TYR:CE2	2:J:388:ILE:HD11	2.53	0.42
2:K:469:LEU:HG	2:K:473:LEU:HD12	2.00	0.42
2:L:99:VAL:HG23	2:L:100:VAL:H	1.83	0.42
2:I:497:TYR:CD2	2:I:497:TYR:C	2.97	0.42
3:B:73:ALA:HB3	3:B:76:ASN:HB3	2.01	0.42
3:D:89:PRO:C	3:D:91:CYS:H	2.28	0.42
2:K:339:MET:HE1	2:K:348:PHE:CE1	2.52	0.42
4:Q:287:PRO:HB3	5:R:344:PHE:CZ	2.54	0.42
2:L:183:LEU:O	2:L:187:LEU:HG	2.19	0.42
3:H:55:ALA:CB	5:T:531:ARG:HG3	2.48	0.42
1:A:69:ARG:HB2	1:A:69:ARG:CZ	2.50	0.42
1:C:30:PHE:C	1:C:30:PHE:CD2	2.96	0.42
1:E:33:SER:HB3	2:K:158:LYS:O	2.19	0.42
3:F:74:PRO:HD2	4:S:183:SER:O	2.19	0.42
1:A:63:GLU:OE2	1:A:63:GLU:HA	2.20	0.42
3:B:72:LEU:HD11	4:M:189:ILE:HG22	2.02	0.42
4:O:211:ARG:HD3	4:O:211:ARG:N	2.34	0.42
4:O:237:HIS:CD2	4:O:288:GLU:CD	2.97	0.42
1:E:36:ARG:CG	7:a:1:NAG:H81	2.50	0.42
4:Q:182:ASP:OD1	4:Q:186:THR:N	2.52	0.42
1:G:69:ARG:CZ	1:G:69:ARG:HB2	2.48	0.42
2:I:388:ILE:CG2	2:I:415:LEU:HD22	2.49	0.42
2:J:353:SER:HA	2:J:381:VAL:HG13	2.00	0.42
5:P:422:GLU:HA	5:P:444:ILE:O	2.19	0.42
2:K:167:PHE:HA	2:K:168:PRO:HD3	1.94	0.42
4:Q:239:VAL:HG12	4:Q:245:PRO:HD2	2.02	0.42
2:L:169:HIS:CE1	2:L:456:GLU:OE2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:93:LEU:HD21	4:S:169:LEU:HD11	1.99	0.42
2:I:381:VAL:O	2:I:383:ILE:HG22	2.20	0.42
4:O:129:VAL:HG22	4:O:160:LEU:HD23	2.02	0.42
4:O:237:HIS:HD2	4:O:288:GLU:OE1	2.01	0.42
5:P:429:TYR:HA	5:P:432:GLU:HB2	2.02	0.42
1:E:30:PHE:HE2	2:K:159:THR:OG1	2.01	0.42
2:K:172:LEU:CD1	2:K:174:LEU:HD13	2.50	0.42
1:G:45:GLN:HG2	2:L:93:ASN:OD1	2.19	0.42
3:H:98:PHE:CE1	4:S:129:VAL:HG21	2.55	0.42
2:J:121:ASN:HD21	2:J:124:GLN:HG2	1.84	0.42
2:K:176:THR:HG22	2:K:181:LEU:HD12	2.00	0.42
4:Q:205:ILE:CD1	5:R:486:ALA:HB3	2.44	0.42
7:b:2:NAG:O7	7:b:2:NAG:H3	2.19	0.42
3:D:84:ASN:C	3:D:84:ASN:HD22	2.26	0.42
4:O:205:ILE:HG21	5:P:502:LEU:HD11	2.02	0.42
3:B:54:PRO:N	3:B:54:PRO:CG	2.81	0.42
1:C:26:TRP:HA	1:C:27:PRO:HD3	1.95	0.42
2:L:256:GLU:HB2	2:L:318:HIS:HB3	2.01	0.42
4:S:253:GLU:HA	4:S:256:ASN:HB2	2.02	0.42
1:C:33:SER:CB	2:J:158:LYS:HG2	2.49	0.41
1:C:40:TYR:HA	1:C:41:PRO:HD2	1.94	0.41
2:J:148:LYS:HA	2:J:153:THR:O	2.20	0.41
1:E:28:GLN:HE22	2:K:487:ASN:HD22	1.67	0.41
4:Q:168:ALA:O	4:Q:172:LEU:HG	2.20	0.41
2:L:165:PRO:HB3	2:L:485:TRP:CE3	2.55	0.41
2:L:188:ASP:O	2:L:191:ASP:HB2	2.20	0.41
4:M:126:GLN:HE21	4:M:126:GLN:HB2	1.71	0.41
2:J:121:ASN:HD22	2:J:123:ASP:H	1.67	0.41
1:E:28:GLN:HG3	2:K:164:PHE:O	2.19	0.41
2:K:101:THR:O	2:K:102:PRO:C	2.62	0.41
2:L:145:LEU:HD23	2:L:145:LEU:HA	1.95	0.41
2:L:384:GLN:HG3	2:L:385:PRO:HD2	2.01	0.41
3:H:68:ASN:HB3	4:S:191:GLU:HG2	2.02	0.41
5:T:452:ASP:OD2	5:T:489:TRP:HB2	2.20	0.41
8:A:21:NGT:HC2	2:I:323:GLU:OE1	2.19	0.41
5:N:424:TRP:HB2	5:N:450:TYR:OH	2.20	0.41
5:P:350:HIS:HD2	5:P:352:GLY:H	1.68	0.41
5:P:350:HIS:HA	5:P:403:ILE:O	2.20	0.41
2:K:131:THR:HG22	2:K:132:VAL:H	1.85	0.41
2:K:359:LEU:HA	2:K:362:ILE:HD12	2.02	0.41
2:K:386:ASP:O	2:K:413:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:350:GLN:HA	2:L:353:SER:HB3	2.02	0.41
3:H:66:THR:HA	3:H:67:PRO:HD3	1.95	0.41
2:I:175:ASP:C	2:I:175:ASP:OD1	2.63	0.41
2:I:202:HIS:CE1	2:I:318:HIS:CD2	3.09	0.41
2:I:337:ASP:O	2:I:341:LYS:HG2	2.20	0.41
1:C:38:VAL:HG22	2:J:155:PHE:CE1	2.55	0.41
2:J:160:GLU:OE2	2:J:160:GLU:HA	2.19	0.41
2:J:228:ASN:C	2:J:230:VAL:H	2.28	0.41
2:J:292:PRO:HG3	2:J:329:TRP:CZ2	2.55	0.41
5:P:449:TRP:CD1	5:P:509:VAL:HG22	2.55	0.41
1:G:55:GLN:CG	1:G:56:PRO:CD	2.84	0.41
2:L:433:ASP:O	2:L:437:VAL:HG23	2.20	0.41
2:L:524:GLN:HG2	2:L:524:GLN:O	2.20	0.41
1:A:66:GLN:HE22	1:A:69:ARG:HD3	1.84	0.41
2:I:99:VAL:HG22	2:I:130:GLU:HA	2.02	0.41
2:I:164:PHE:CD2	6:U:1:NAG:H62	2.55	0.41
2:I:383:ILE:HD11	2:I:387:THR:HG21	2.03	0.41
5:P:532:HIS:HD2	5:P:535:ARG:NH2	2.08	0.41
4:Q:131:ILE:HA	4:Q:162:ALA:O	2.20	0.41
4:Q:133:LEU:HD12	4:Q:163:ASN:HB3	2.02	0.41
1:A:52:SER:HA	2:I:97:VAL:HG23	2.02	0.41
1:A:59:SER:O	1:A:60:VAL:C	2.63	0.41
3:D:54:PRO:HB2	5:P:531:ARG:NH2	2.36	0.41
5:P:350:HIS:CD2	5:P:352:GLY:H	2.38	0.41
5:P:371:MET:H	5:P:371:MET:HG2	1.70	0.41
2:K:336:GLN:HA	2:K:339:MET:HE3	2.03	0.41
5:R:504:PRO:HD3	5:R:544:GLN:O	2.20	0.41
5:T:414:LYS:HD3	5:T:414:LYS:HA	1.97	0.41
1:A:26:TRP:HA	1:A:27:PRO:HD3	1.95	0.41
1:C:26:TRP:HB2	2:J:499:ARG:NH1	2.36	0.41
2:J:228:ASN:ND2	2:J:230:VAL:H	2.16	0.41
3:D:68:ASN:HB3	4:O:191:GLU:HG2	2.01	0.41
1:E:59:SER:O	1:E:63:GLU:HG2	2.21	0.41
2:K:278:TYR:CD1	2:K:332:ASN:HA	2.55	0.41
2:L:127:LEU:HD11	2:L:138:GLY:C	2.45	0.41
1:A:61:LEU:HD11	2:I:135:ALA:HB3	2.02	0.41
2:I:374:GLN:HA	2:I:389:ILE:HG23	2.03	0.41
2:J:425:ILE:HB	5:P:454:ILE:HD12	2.03	0.41
2:K:475:PRO:HD3	2:K:515:GLN:O	2.20	0.41
2:L:464:VAL:HG22	2:L:472:ARG:NH1	2.36	0.41
1:A:60:VAL:HG12	1:A:61:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:523:GLU:HG3	1:C:42:ASN:ND2	2.36	0.41
1:C:31:GLN:HB3	2:J:160:GLU:HB3	2.02	0.41
2:J:120:ILE:O	2:J:158:LYS:HA	2.20	0.41
2:J:518:ASN:CG	2:J:519:VAL:H	2.29	0.41
4:O:160:LEU:HD21	4:O:168:ALA:HA	2.02	0.41
2:K:290:VAL:HG12	2:K:291:ASN:N	2.36	0.41
2:K:431:TRP:HA	2:K:434:PHE:CD2	2.55	0.41
4:Q:223:LEU:HD21	4:Q:234:LEU:HD22	2.02	0.41
4:Q:295:THR:O	4:Q:306:LEU:HD21	2.21	0.41
1:A:42:ASN:ND2	1:A:42:ASN:H	2.17	0.41
4:O:237:HIS:HE1	4:O:240:ASP:OD2	2.04	0.41
4:O:290:ASP:HA	5:P:352:GLY:HA3	2.03	0.41
2:L:428:GLY:HA2	5:T:492:TYR:CZ	2.56	0.41
5:T:532:HIS:CD2	5:T:535:ARG:HH21	2.39	0.41
2:I:90:LEU:HD13	2:I:92:LYS:HD2	2.02	0.40
2:I:266:TRP:CD1	2:I:266:TRP:N	2.89	0.40
4:M:186:THR:HA	4:O:184:TYR:O	2.21	0.40
2:J:270:ILE:HA	2:J:271:PRO:HD2	1.99	0.40
2:L:232:HIS:NE2	5:T:550:TYR:HB2	2.36	0.40
2:L:401:MET:HA	2:L:404:LEU:HD12	2.02	0.40
2:L:461:GLY:O	2:L:462:GLU:C	2.64	0.40
1:A:46:PHE:CD2	2:I:94:VAL:HG12	2.55	0.40
4:O:229:ASN:OD1	5:P:532:HIS:HE1	2.03	0.40
4:Q:209:THR:O	4:Q:245:PRO:HG2	2.21	0.40
5:T:347:GLN:O	5:T:401:GLY:N	2.43	0.40
2:J:228:ASN:HA	2:J:229:PRO:HD3	1.77	0.40
2:K:423:ASN:OD1	2:K:460:TRP:HD1	2.05	0.40
3:F:70:LEU:HD21	4:Q:155:GLU:HB3	2.04	0.40
5:R:382:LYS:HA	5:R:385:SER:HB2	2.04	0.40
1:G:26:TRP:HA	1:G:27:PRO:HD3	1.85	0.40
2:I:179:HIS:HE1	2:I:462:GLU:O	2.05	0.40
5:N:437:THR:O	5:N:477:GLN:HG2	2.21	0.40
1:C:67:ARG:HD2	2:J:249:ARG:NH2	2.36	0.40
2:J:100:VAL:HG23	2:J:130:GLU:HG3	2.04	0.40
2:J:447:GLU:OE2	2:J:447:GLU:N	2.50	0.40
5:P:460:TRP:CD1	5:P:546:LEU:HD22	2.56	0.40
3:F:64:LYS:HE3	4:Q:193:THR:O	2.21	0.40
4:Q:150:THR:HG22	4:Q:195:ILE:HG12	2.02	0.40
2:L:447:GLU:H	2:L:447:GLU:CD	2.29	0.40
4:S:147:GLU:HB3	4:S:170:ARG:HG3	2.02	0.40
2:I:459:MET:HE1	2:I:464:VAL:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:235:HIS:NE2	4:M:288:GLU:OE1	2.42	0.40
4:M:291:THR:HG22	5:N:322:ILE:CD1	2.51	0.40
1:C:55:GLN:O	1:C:56:PRO:C	2.64	0.40
4:Q:219:ILE:O	4:Q:222:THR:HB	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:424:ARG:NH2	5:T:369:ASP:OD1[2_456]	1.93	0.27

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	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	6	26
1	C	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
1	E	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
1	G	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	6	26
2	I	438/440 (100%)	400 (91%)	30 (7%)	8 (2%)	6	29
2	J	438/440 (100%)	402 (92%)	29 (7%)	7 (2%)	7	30
2	K	438/440 (100%)	402 (92%)	31 (7%)	5 (1%)	11	38
2	L	438/440 (100%)	404 (92%)	25 (6%)	9 (2%)	5	25
3	B	52/58 (90%)	42 (81%)	8 (15%)	2 (4%)	2	15
3	D	52/58 (90%)	42 (81%)	10 (19%)	0	100	100
3	F	52/58 (90%)	45 (86%)	4 (8%)	3 (6%)	1	8
3	H	52/58 (90%)	45 (86%)	6 (12%)	1 (2%)	6	28
4	M	188/190 (99%)	177 (94%)	10 (5%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	187/190 (98%)	175 (94%)	12 (6%)	0	100	100
4	Q	188/190 (99%)	170 (90%)	17 (9%)	1 (0%)	24	55
4	S	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
5	N	234/237 (99%)	215 (92%)	19 (8%)	0	100	100
5	P	234/237 (99%)	213 (91%)	16 (7%)	5 (2%)	5	25
5	R	234/237 (99%)	210 (90%)	22 (9%)	2 (1%)	14	42
5	T	234/237 (99%)	217 (93%)	15 (6%)	2 (1%)	14	42
All	All	3847/3908 (98%)	3523 (92%)	276 (7%)	48 (1%)	10	36

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	103	GLY
3	B	55	ALA
2	J	102	PRO
2	J	103	GLY
2	K	102	PRO
5	R	458	GLN
2	L	102	PRO
2	L	380	LYS
2	L	462	GLU
2	J	466	ASN
5	P	427	SER
2	K	103	GLY
2	K	104	CYS
2	K	229	PRO
5	R	427	SER
2	I	488	LYS
4	M	237	HIS
5	P	458	GLN
5	P	495	ALA
3	F	76	ASN
2	I	102	PRO
2	I	280	GLY
1	G	41	PRO
2	L	490	THR
3	H	74	PRO
1	A	41	PRO
2	I	285	GLY
2	I	490	THR

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Mol	Chain	Res	Type
3	B	76	ASN
2	J	229	PRO
2	J	283	PRO
2	K	280	GLY
4	Q	182	ASP
2	L	267	GLY
2	L	466	ASN
5	T	417	PRO
5	T	458	GLN
2	J	437	VAL
5	P	519	VAL
3	F	67	PRO
2	L	103	GLY
2	L	465	ASP
5	P	418	GLY
3	F	74	PRO
2	L	280	GLY
2	I	229	PRO
2	I	101	THR
2	J	267	GLY

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	47/47 (100%)	38 (81%)	9 (19%)	1	6
1	C	47/47 (100%)	41 (87%)	6 (13%)	4	18
1	E	47/47 (100%)	41 (87%)	6 (13%)	4	18
1	G	47/47 (100%)	44 (94%)	3 (6%)	16	42
2	I	393/394 (100%)	359 (91%)	34 (9%)	9	31
2	J	393/394 (100%)	361 (92%)	32 (8%)	11	35
2	K	393/394 (100%)	364 (93%)	29 (7%)	13	38
2	L	393/394 (100%)	362 (92%)	31 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	47/49 (96%)	45 (96%)	2 (4%)	26	52
3	D	47/49 (96%)	45 (96%)	2 (4%)	26	52
3	F	47/49 (96%)	44 (94%)	3 (6%)	16	42
3	H	47/49 (96%)	46 (98%)	1 (2%)	47	66
4	M	174/174 (100%)	166 (95%)	8 (5%)	24	51
4	O	173/174 (99%)	161 (93%)	12 (7%)	14	41
4	Q	174/174 (100%)	167 (96%)	7 (4%)	28	54
4	S	174/174 (100%)	167 (96%)	7 (4%)	28	54
5	N	205/206 (100%)	195 (95%)	10 (5%)	22	50
5	P	205/206 (100%)	190 (93%)	15 (7%)	13	38
5	R	205/206 (100%)	193 (94%)	12 (6%)	18	45
5	T	205/206 (100%)	195 (95%)	10 (5%)	22	50
All	All	3463/3480 (100%)	3224 (93%)	239 (7%)	14	41

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	42	ASN
1	A	43	ASN
1	A	45	GLN
1	A	47	GLN
1	A	55	GLN
1	A	61	LEU
1	A	66	GLN
1	A	72	LEU
2	I	89	THR
2	I	94	VAL
2	I	95	LEU
2	I	99	VAL
2	I	105	ASN
2	I	106	GLN
2	I	107	LEU
2	I	121	ASN
2	I	126	LEU
2	I	127	LEU
2	I	128	LEU
2	I	153	THR

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Mol	Chain	Res	Type
2	I	172	LEU
2	I	198	LEU
2	I	270	ILE
2	I	299	GLU
2	I	306	LEU
2	I	372	VAL
2	I	382	LYS
2	I	396	ILE
2	I	398	VAL
2	I	402	LYS
2	I	409	LYS
2	I	415	LEU
2	I	416	LEU
2	I	445	THR
2	I	447	GLU
2	I	467	THR
2	I	489	LEU
2	I	507	LEU
2	I	508	LEU
2	I	523	GLU
2	I	527	GLU
2	I	528	GLN
3	B	84	ASN
3	B	93	LEU
4	M	169	LEU
4	M	191	GLU
4	M	206	LEU
4	M	211	ARG
4	M	218	ILE
4	M	249	ILE
4	M	250	THR
4	M	283	ILE
5	N	328	THR
5	N	356	VAL
5	N	373	GLN
5	N	384	GLU
5	N	431	GLU
5	N	462	LYS
5	N	479	GLN
5	N	502	LEU
5	N	516	SER
5	N	522	MET

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Mol	Chain	Res	Type
1	C	32	THR
1	C	35	GLN
1	C	55	GLN
1	C	71	LEU
1	C	72	LEU
1	C	73	PHE
2	J	90	LEU
2	J	92	LYS
2	J	93	ASN
2	J	94	VAL
2	J	98	SER
2	J	101	THR
2	J	106	GLN
2	J	107	LEU
2	J	121	ASN
2	J	126	LEU
2	J	131	THR
2	J	141	THR
2	J	158	LYS
2	J	159	THR
2	J	172	LEU
2	J	192	VAL
2	J	228	ASN
2	J	263	THR
2	J	296	ASN
2	J	299	GLU
2	J	336	GLN
2	J	339	MET
2	J	358	THR
2	J	372	VAL
2	J	382	LYS
2	J	399	ASN
2	J	403	GLU
2	J	406	LEU
2	J	409	LYS
2	J	523	GLU
2	J	525	GLU
2	J	528	GLN
3	D	66	THR
3	D	84	ASN
4	O	154	LYS
4	O	165	VAL

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Mol	Chain	Res	Type
4	O	174	THR
4	O	183	SER
4	O	211	ARG
4	O	217	LYS
4	O	250	THR
4	O	257	LYS
4	O	267	THR
4	O	291	THR
4	O	307	THR
4	O	310	TYR
5	P	317	ASP
5	P	341	SER
5	P	356	VAL
5	P	359	LYS
5	P	362	GLU
5	P	372	ARG
5	P	384	GLU
5	P	390	LYS
5	P	393	ASP
5	P	420	ILE
5	P	431	GLU
5	P	451	LEU
5	P	455	SER
5	P	502	LEU
5	P	522	MET
1	E	23	LEU
1	E	28	GLN
1	E	38	VAL
1	E	47	GLN
1	E	55	GLN
1	E	66	GLN
2	K	89	THR
2	K	92	LYS
2	K	106	GLN
2	K	107	LEU
2	K	121	ASN
2	K	126	LEU
2	K	127	LEU
2	K	131	THR
2	K	153	THR
2	K	161	ILE
2	K	162	GLU

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Mol	Chain	Res	Type
2	K	174	LEU
2	K	189	THR
2	K	252	ARG
2	K	295	ASN
2	K	370	TYR
2	K	382	LYS
2	K	383	ILE
2	K	395	ASP
2	K	396	ILE
2	K	402	LYS
2	K	409	LYS
2	K	415	LEU
2	K	464	VAL
2	K	494	THR
2	K	508	LEU
2	K	515	GLN
2	K	518	ASN
2	K	524	GLN
3	F	68	ASN
3	F	79	ILE
3	F	80	SER
4	Q	150	THR
4	Q	155	GLU
4	Q	186	THR
4	Q	211	ARG
4	Q	250	THR
4	Q	283	ILE
4	Q	311	SER
5	R	341	SER
5	R	351	LEU
5	R	359	LYS
5	R	385	SER
5	R	390	LYS
5	R	394	ILE
5	R	403	ILE
5	R	431	GLU
5	R	451	LEU
5	R	462	LYS
5	R	502	LEU
5	R	522	MET
1	G	47	GLN
1	G	51	SER

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Mol	Chain	Res	Type
1	G	72	LEU
2	L	90	LEU
2	L	92	LYS
2	L	95	LEU
2	L	97	VAL
2	L	98	SER
2	L	101	THR
2	L	106	GLN
2	L	107	LEU
2	L	121	ASN
2	L	122	ASP
2	L	126	LEU
2	L	162	GLU
2	L	172	LEU
2	L	198	LEU
2	L	235	THR
2	L	270	ILE
2	L	299	GLU
2	L	311	VAL
2	L	336	GLN
2	L	370	TYR
2	L	382	LYS
2	L	388	ILE
2	L	396	ILE
2	L	398	VAL
2	L	399	ASN
2	L	406	LEU
2	L	415	LEU
2	L	443	GLU
2	L	463	TYR
2	L	467	THR
2	L	523	GLU
3	H	84	ASN
4	S	165	VAL
4	S	174	THR
4	S	211	ARG
4	S	216	VAL
4	S	283	ILE
4	S	309	CYS
4	S	311	SER
5	T	338	LYS
5	T	359	LYS

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Mol	Chain	Res	Type
5	T	369	ASP
5	T	379	ASP
5	T	431	GLU
5	T	462	LYS
5	T	479	GLN
5	T	502	LEU
5	T	518	ASP
5	T	522	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	42	ASN
1	A	43	ASN
1	A	47	GLN
1	A	55	GLN
1	A	66	GLN
2	I	115	ASN
2	I	121	ASN
2	I	157	ASN
2	I	204	HIS
2	I	228	ASN
2	I	262	HIS
2	I	296	ASN
2	I	336	GLN
2	I	350	GLN
2	I	384	GLN
2	I	466	ASN
2	I	518	ASN
2	I	528	GLN
3	B	76	ASN
3	B	84	ASN
4	M	123	GLN
4	M	126	GLN
4	M	142	ASN
4	M	190	ASN
4	M	202	HIS
4	M	237	HIS
4	M	256	ASN
4	M	264	HIS
5	N	347	GLN

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Mol	Chain	Res	Type
5	N	364	ASN
5	N	373	GLN
5	N	406	GLN
5	N	477	GLN
5	N	532	HIS
1	C	28	GLN
1	C	45	GLN
1	C	55	GLN
1	C	66	GLN
2	J	106	GLN
2	J	121	ASN
2	J	124	GLN
2	J	204	HIS
2	J	228	ASN
2	J	336	GLN
2	J	350	GLN
2	J	466	ASN
2	J	518	ASN
3	D	76	ASN
3	D	81	HIS
3	D	84	ASN
3	D	102	HIS
4	O	123	GLN
4	O	126	GLN
4	O	202	HIS
4	O	237	HIS
4	O	302	GLN
5	P	350	HIS
5	P	373	GLN
5	P	406	GLN
5	P	458	GLN
5	P	477	GLN
5	P	532	HIS
1	E	28	GLN
1	E	43	ASN
1	E	47	GLN
1	E	55	GLN
1	E	66	GLN
2	K	106	GLN
2	K	121	ASN
2	K	204	HIS
2	K	228	ASN

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Mol	Chain	Res	Type
2	K	336	GLN
2	K	350	GLN
2	K	357	GLN
2	K	448	GLN
2	K	515	GLN
2	K	518	ASN
3	F	84	ASN
4	Q	123	GLN
4	Q	126	GLN
4	Q	134	GLN
4	Q	163	ASN
4	Q	202	HIS
4	Q	237	HIS
4	Q	264	HIS
5	R	350	HIS
5	R	406	GLN
5	R	477	GLN
5	R	532	HIS
1	G	28	GLN
1	G	43	ASN
1	G	47	GLN
1	G	55	GLN
2	L	93	ASN
2	L	105	ASN
2	L	121	ASN
2	L	169	HIS
2	L	204	HIS
2	L	228	ASN
2	L	296	ASN
2	L	336	GLN
2	L	350	GLN
2	L	384	GLN
2	L	466	ASN
2	L	518	ASN
3	H	76	ASN
3	H	84	ASN
4	S	123	GLN
4	S	126	GLN
4	S	134	GLN
4	S	237	HIS
4	S	264	HIS
5	T	364	ASN

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Mol	Chain	Res	Type
5	T	373	GLN
5	T	406	GLN
5	T	532	HIS

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 ⓘ

27 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	$\# Z > 2$
6	NAG	U	1	6,2	14,14,15	0.75	0	17,19,21	0.62	0
6	NAG	U	2	6	14,14,15	0.59	0	17,19,21	1.26	1 (5%)
6	BMA	U	3	6	11,11,12	0.62	0	15,15,17	1.33	2 (13%)
6	NAG	V	1	6,2	14,14,15	0.53	0	17,19,21	0.61	0
6	NAG	V	2	6	14,14,15	0.58	0	17,19,21	1.22	1 (5%)
6	BMA	V	3	6	11,11,12	0.76	0	15,15,17	2.17	3 (20%)
6	NAG	W	1	6	14,14,15	0.59	0	17,19,21	0.62	0
6	NAG	W	2	6	14,14,15	0.64	0	17,19,21	1.13	1 (5%)
6	BMA	W	3	6	11,11,12	2.26	2 (18%)	15,15,17	3.09	6 (40%)
7	NAG	X	1	2,7	14,14,15	0.65	0	17,19,21	0.89	1 (5%)
7	NAG	X	2	7	14,14,15	0.53	0	17,19,21	0.77	0
6	NAG	Y	1	6,2	14,14,15	1.02	2 (14%)	17,19,21	0.63	0
6	NAG	Y	2	6	14,14,15	1.14	2 (14%)	17,19,21	4.11	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	Y	3	6	11,11,12	0.61	0	15,15,17	1.79	2 (13%)
7	NAG	Z	1	4,7	14,14,15	0.48	0	17,19,21	0.62	0
7	NAG	Z	2	7	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
7	NAG	a	1	2,7	14,14,15	2.76	5 (35%)	17,19,21	0.77	1 (5%)
7	NAG	a	2	7	14,14,15	1.20	1 (7%)	17,19,21	1.93	3 (17%)
7	NAG	b	1	4,7	14,14,15	0.64	0	17,19,21	0.61	0
7	NAG	b	2	7	14,14,15	0.69	0	17,19,21	1.22	2 (11%)
7	NAG	c	1	2,7	14,14,15	2.01	3 (21%)	17,19,21	0.64	0
7	NAG	c	2	7	14,14,15	0.66	0	17,19,21	1.34	3 (17%)
6	NAG	d	1	6,2	14,14,15	0.58	0	17,19,21	0.61	0
6	NAG	d	2	6	14,14,15	0.63	0	17,19,21	1.23	2 (11%)
6	BMA	d	3	6	11,11,12	0.62	0	15,15,17	0.98	1 (6%)
7	NAG	e	1	4,7	14,14,15	1.07	1 (7%)	17,19,21	0.61	0
7	NAG	e	2	7	14,14,15	0.65	0	17,19,21	1.21	1 (5%)

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

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

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	3	BMA	O2-C2	6.61	1.57	1.43
7	a	1	NAG	O4-C4	-6.22	1.27	1.43
7	c	1	NAG	C2-N2	6.17	1.56	1.46
7	a	1	NAG	C1-C2	4.48	1.58	1.52
7	a	1	NAG	O5-C1	-4.37	1.36	1.43
7	a	1	NAG	C4-C5	-4.29	1.43	1.53
7	a	2	NAG	C1-C2	3.62	1.57	1.52
6	Y	2	NAG	O5-C1	-3.11	1.38	1.43
7	c	1	NAG	C1-C2	-2.73	1.48	1.52
6	W	3	BMA	C2-C3	2.60	1.56	1.52
7	e	1	NAG	C2-N2	2.54	1.50	1.46
7	a	1	NAG	C2-N2	-2.41	1.42	1.46
6	Y	1	NAG	C1-C2	2.29	1.55	1.52
6	Y	2	NAG	O5-C5	-2.28	1.39	1.43
6	Y	1	NAG	C2-N2	2.07	1.49	1.46
7	c	1	NAG	O5-C5	2.03	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	2	NAG	O5-C5-C6	10.51	128.11	107.66
6	Y	2	NAG	O5-C1-C2	10.45	127.45	111.29
6	W	3	BMA	C1-C2-C3	6.51	119.12	109.64
6	W	3	BMA	C1-O5-C5	-5.99	104.16	112.19
7	a	2	NAG	C1-O5-C5	5.93	120.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	3	BMA	C1-C2-C3	-5.71	101.33	109.64
6	Y	3	BMA	O5-C5-C6	5.00	117.40	107.66
6	V	3	BMA	C1-O5-C5	-4.74	105.84	112.19
6	W	3	BMA	O5-C5-C6	4.40	116.23	107.66
6	W	3	BMA	O2-C2-C1	4.26	118.98	109.22
6	W	3	BMA	O2-C2-C3	4.18	118.81	110.15
6	Y	2	NAG	C3-C4-C5	4.02	117.52	110.23
6	U	2	NAG	C2-N2-C7	3.79	127.98	122.90
6	Y	3	BMA	C1-O5-C5	-3.67	107.26	112.19
6	Y	2	NAG	C2-N2-C7	3.62	127.76	122.90
6	Y	2	NAG	O5-C5-C4	3.59	119.56	110.83
6	Y	2	NAG	C4-C3-C2	3.52	116.18	111.02
6	U	3	BMA	C1-O5-C5	3.49	116.87	112.19
7	e	2	NAG	C2-N2-C7	3.28	127.29	122.90
7	c	2	NAG	C4-C3-C2	3.11	115.57	111.02
7	a	2	NAG	C2-N2-C7	3.02	126.94	122.90
6	V	2	NAG	C4-C3-C2	2.73	115.02	111.02
6	d	2	NAG	C4-C3-C2	2.69	114.96	111.02
6	d	3	BMA	C1-O5-C5	-2.57	108.75	112.19
7	b	2	NAG	C4-C3-C2	2.56	114.77	111.02
6	W	2	NAG	C2-N2-C7	2.52	126.28	122.90
7	c	2	NAG	C2-N2-C7	2.45	126.18	122.90
6	U	3	BMA	C1-C2-C3	2.37	113.09	109.64
7	b	2	NAG	C2-N2-C7	2.34	126.04	122.90
7	c	2	NAG	C1-O5-C5	2.19	115.12	112.19
7	X	1	NAG	C1-O5-C5	2.15	115.06	112.19
7	a	2	NAG	O4-C4-C5	2.09	114.48	109.32
6	W	3	BMA	C2-C3-C4	-2.05	107.25	110.86
7	Z	2	NAG	C4-C3-C2	2.04	114.01	111.02
6	V	3	BMA	O5-C5-C6	2.03	111.61	107.66
6	d	2	NAG	C2-N2-C7	2.02	125.61	122.90
7	a	1	NAG	O7-C7-C8	-2.00	118.49	122.05

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	Y	2	NAG	C5
6	d	2	NAG	C1
7	Z	1	NAG	C1
7	Z	2	NAG	C1
7	a	1	NAG	C1
7	a	2	NAG	C1

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Mol	Chain	Res	Type	Atom
7	b	1	NAG	C1
7	b	2	NAG	C1
7	c	2	NAG	C1
7	e	2	NAG	C1

All (71) torsion outliers are listed below:

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

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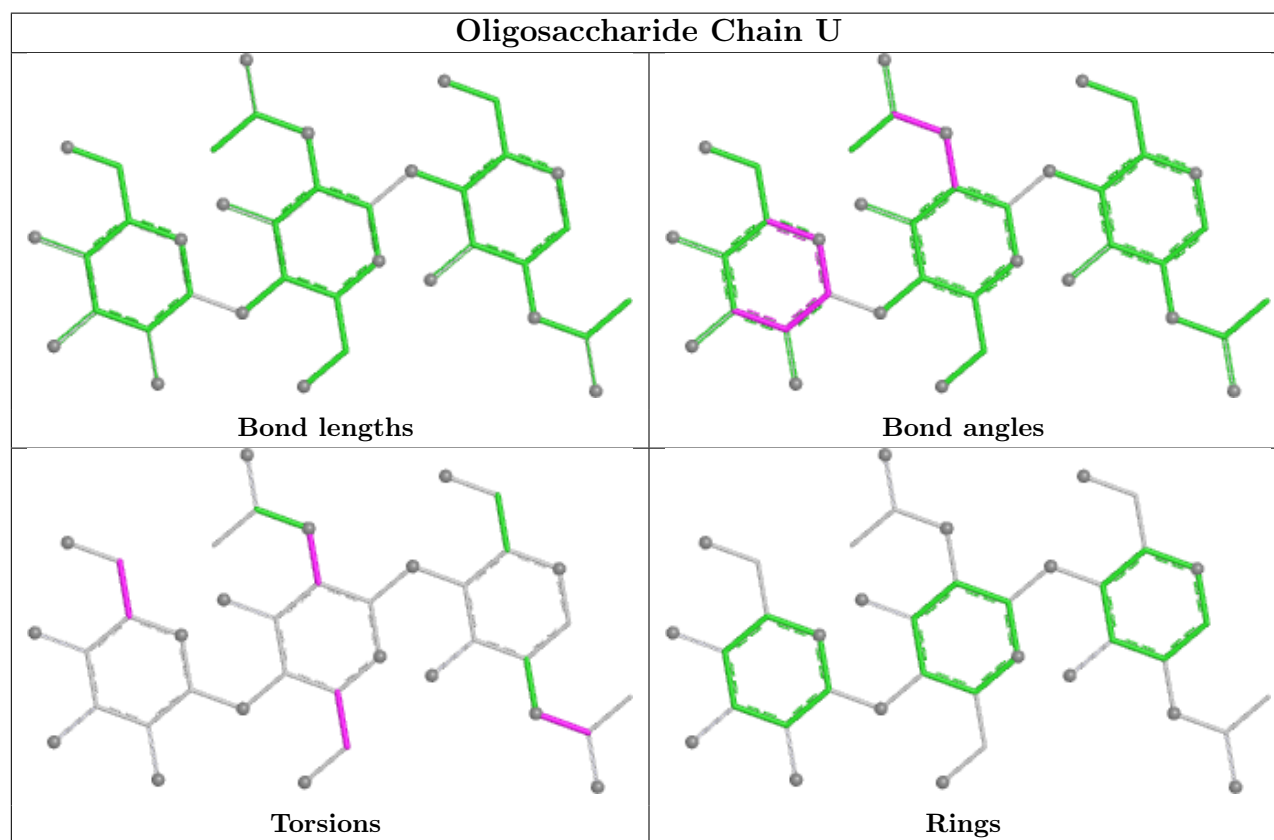
Mol	Chain	Res	Type	Atoms
7	Z	1	NAG	C8-C7-N2-C2
7	c	2	NAG	C8-C7-N2-C2
7	X	2	NAG	O7-C7-N2-C2
6	U	3	BMA	O5-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
6	U	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	c	2	NAG	O7-C7-N2-C2
6	W	1	NAG	C8-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	Y	2	NAG	C3-C2-N2-C7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

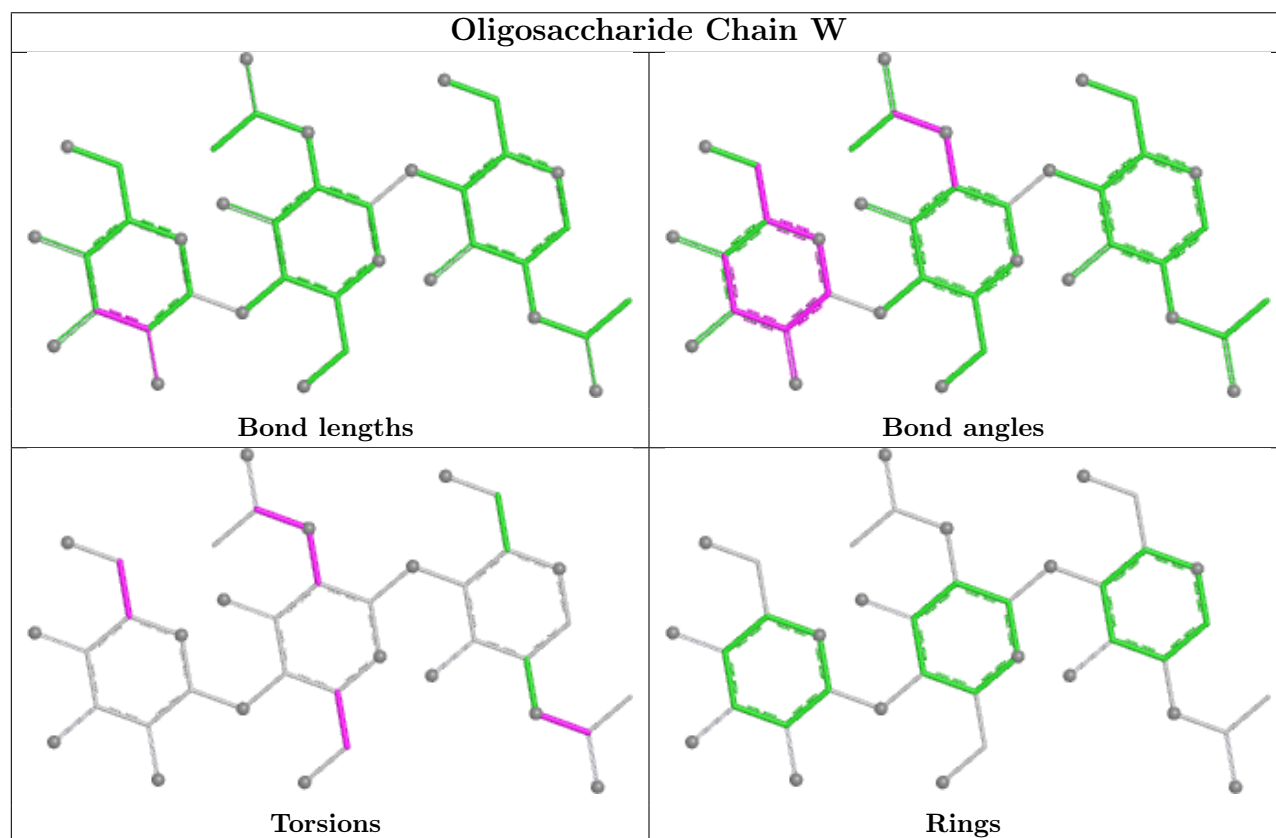
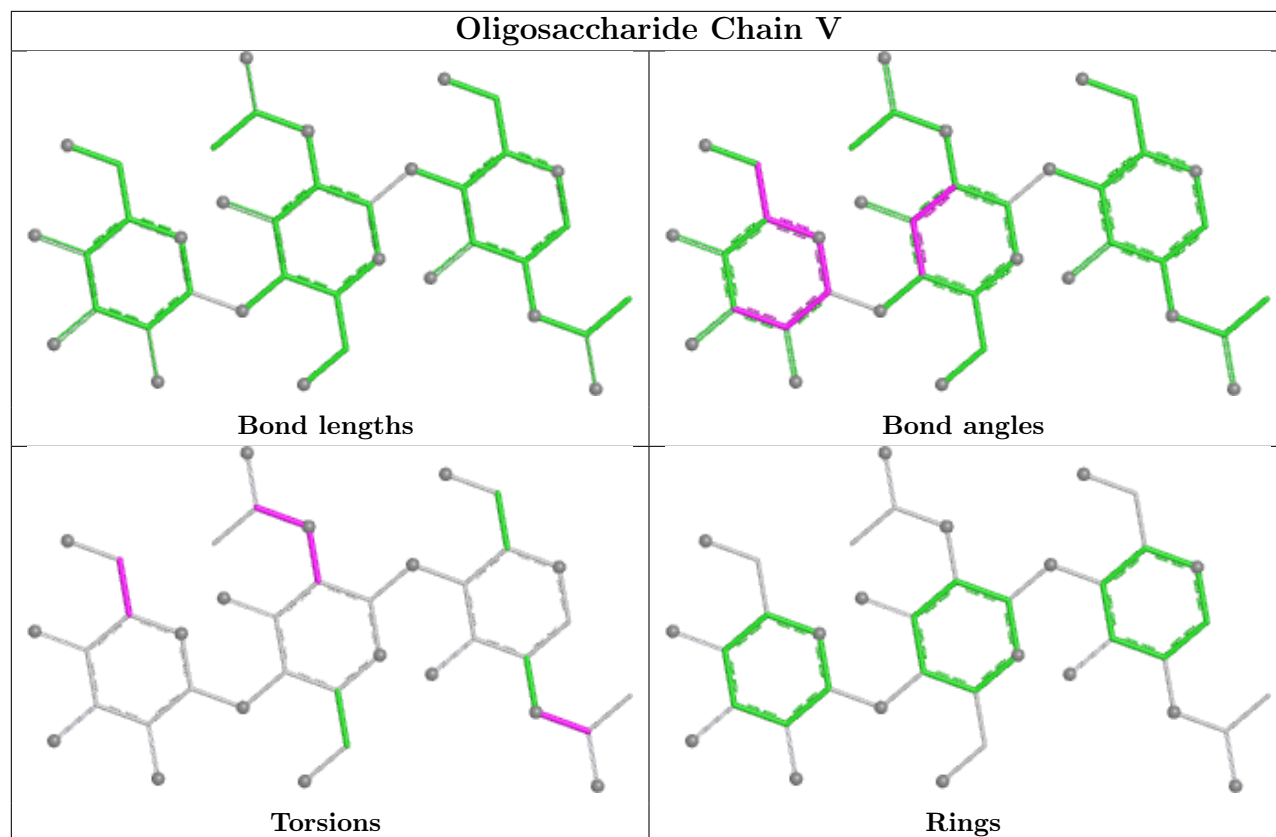
There are no ring outliers.

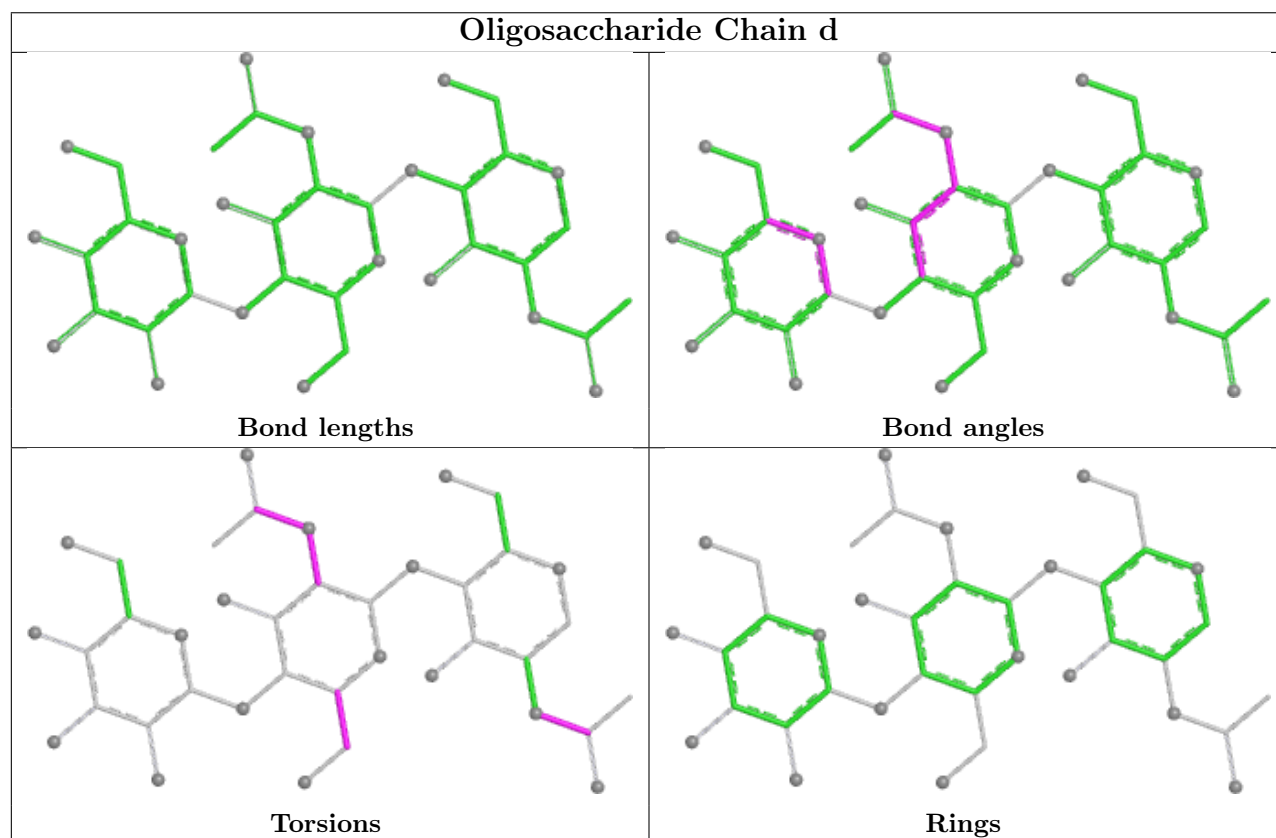
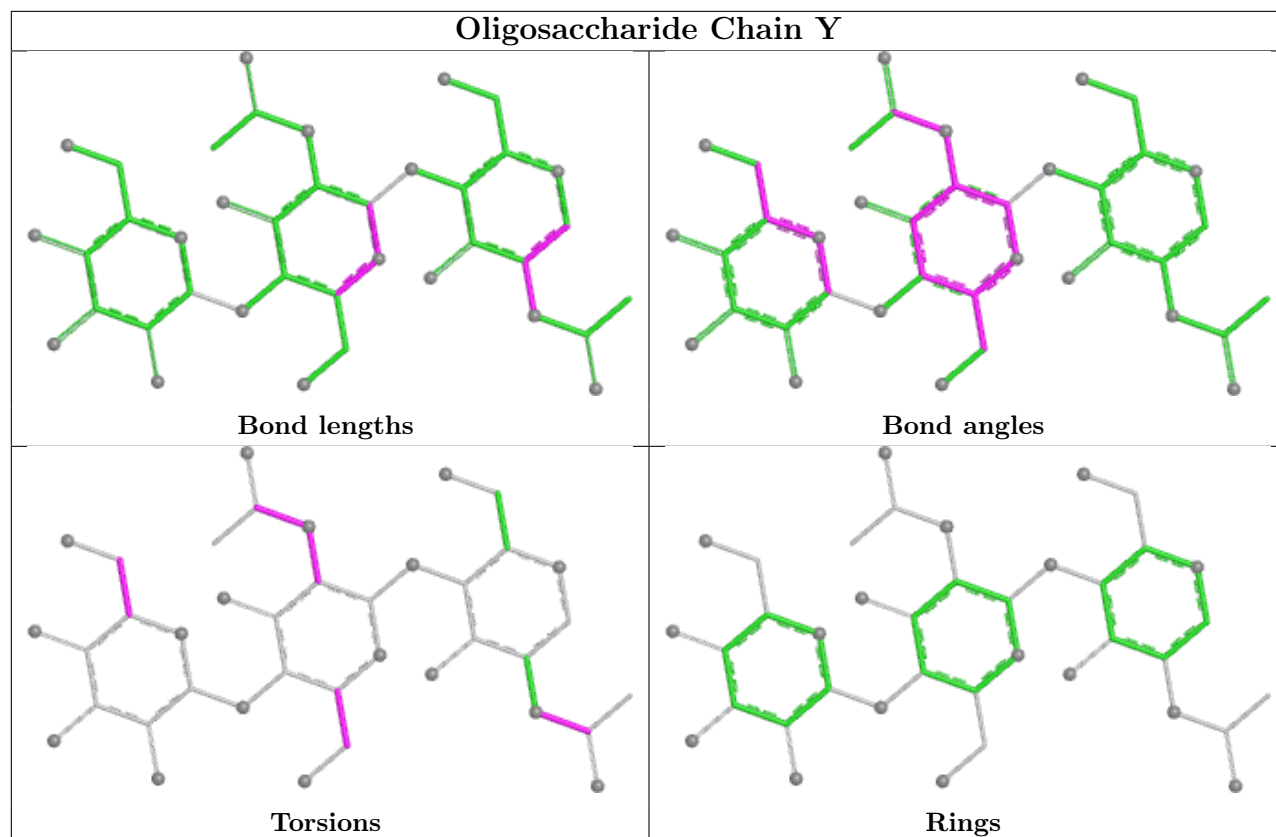
15 monomers are involved in 40 short contacts:

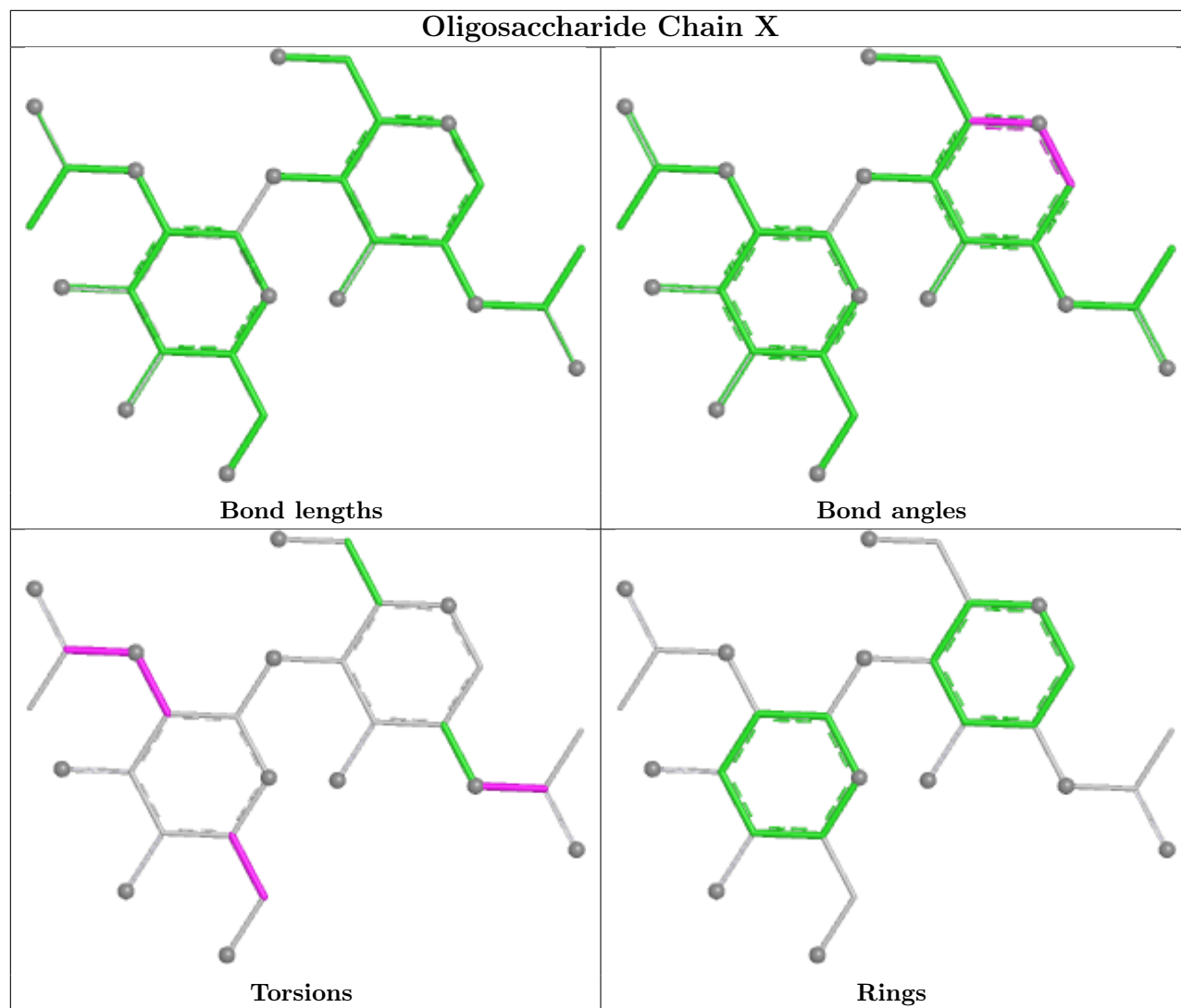
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Z	1	NAG	2	0
7	e	1	NAG	3	0
6	Y	1	NAG	7	0
7	X	1	NAG	1	0
7	b	2	NAG	1	0
6	U	1	NAG	5	0
6	V	1	NAG	1	0
7	a	1	NAG	9	0
6	d	1	NAG	1	0
7	b	1	NAG	1	0
6	Y	2	NAG	1	0
7	c	1	NAG	8	0
6	W	1	NAG	1	0
7	e	2	NAG	1	0
6	d	2	NAG	1	0

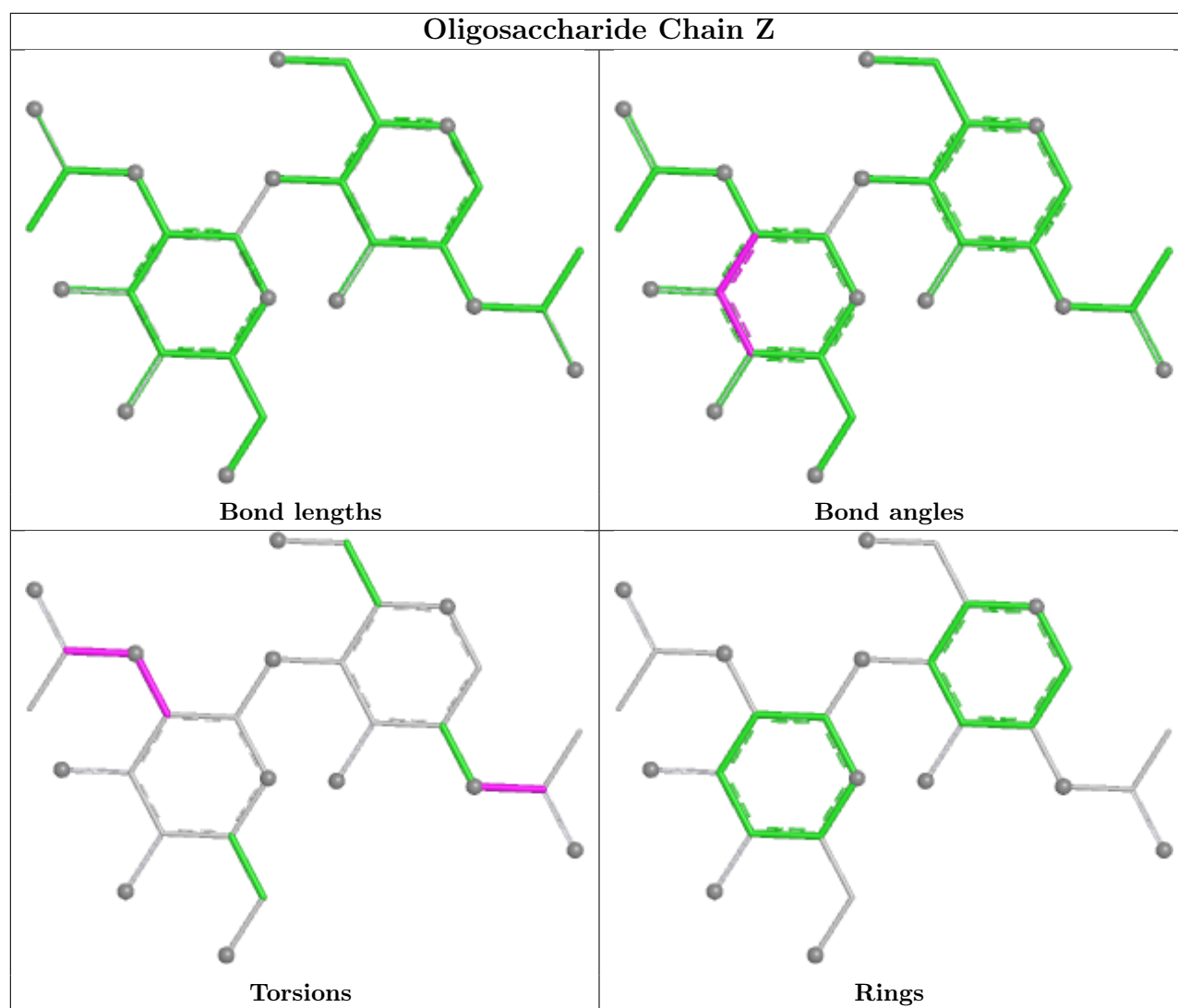
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

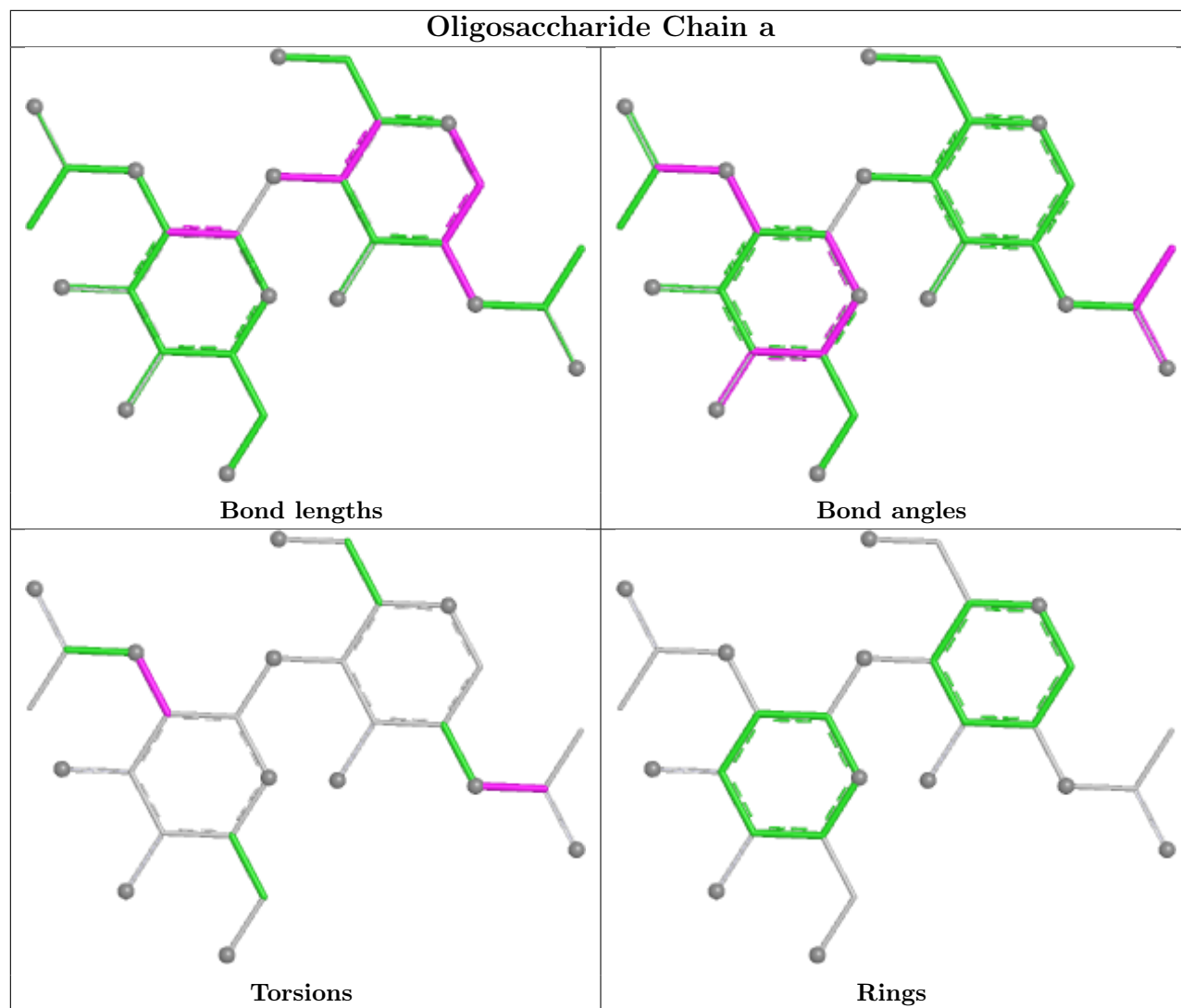


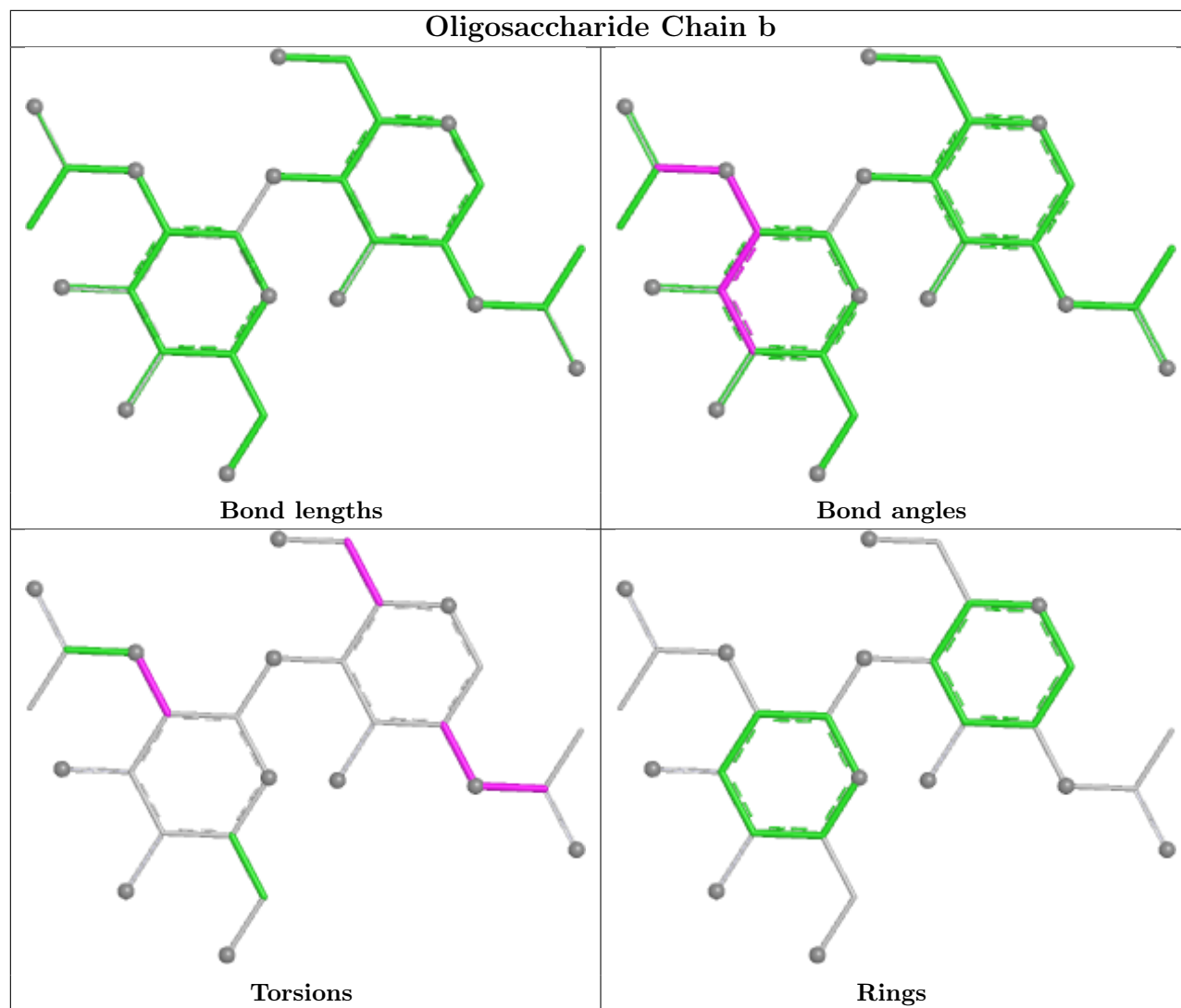


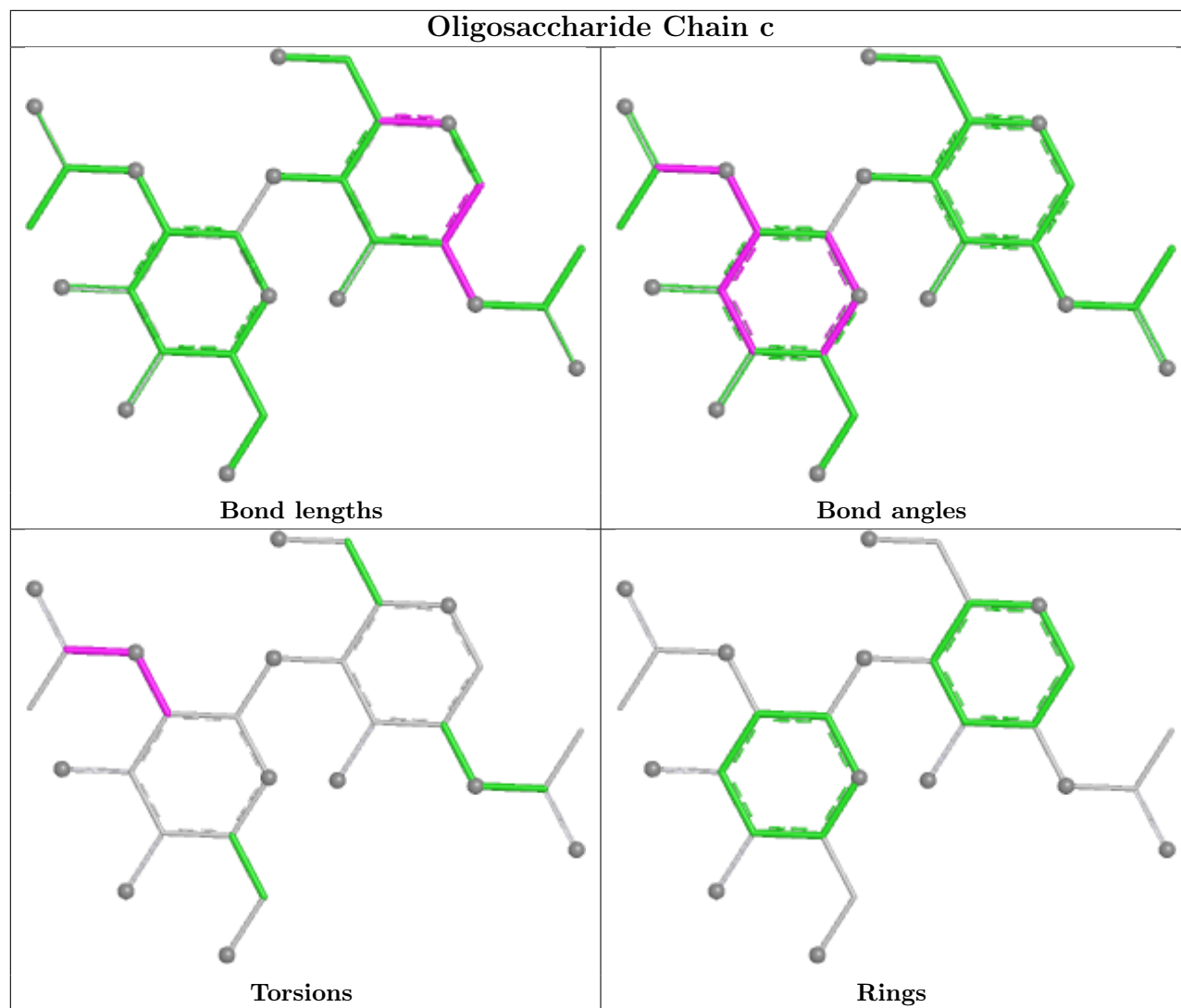


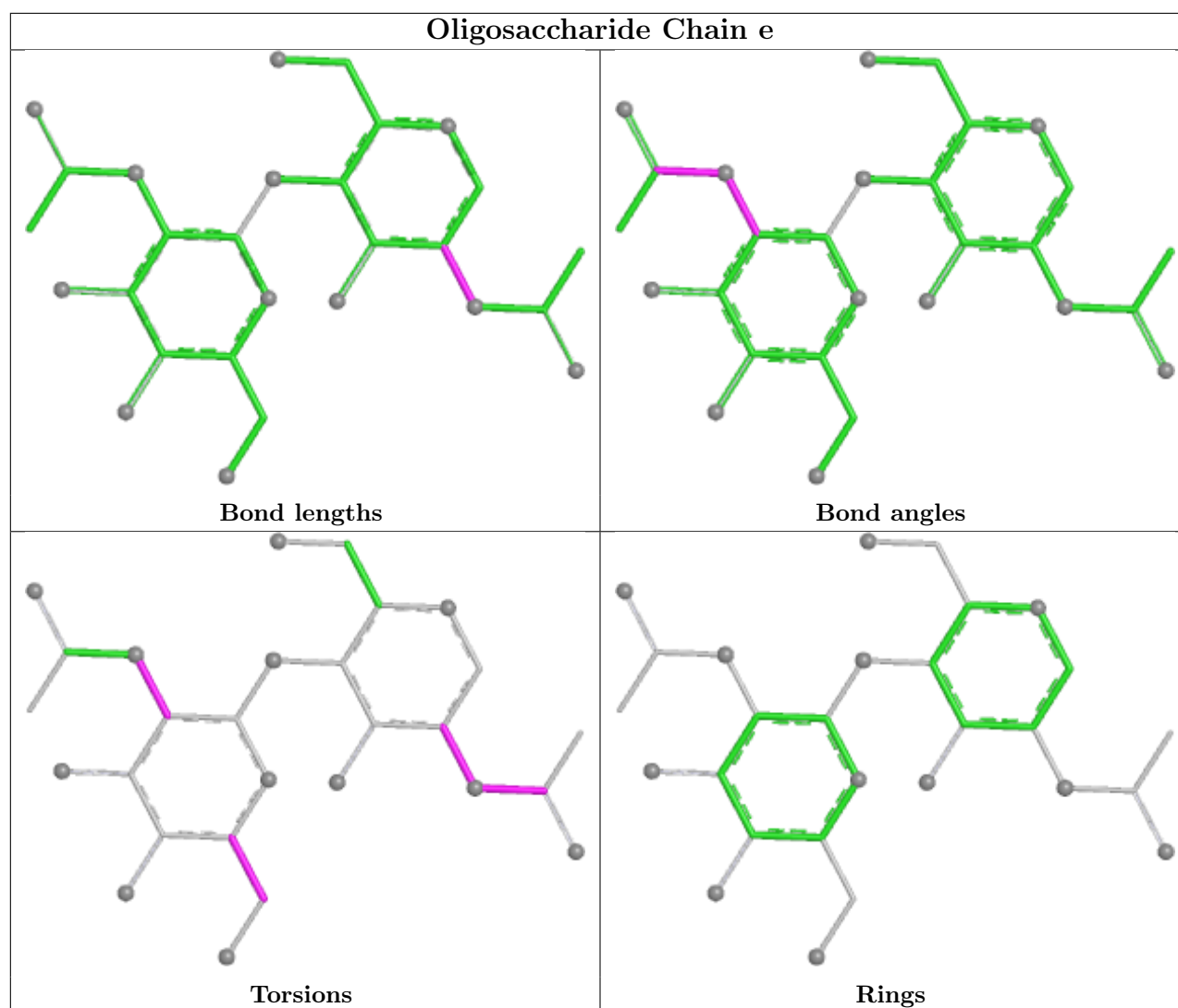












5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NGT	A	21	-	13,15,15	1.25	1 (7%)	14,22,22	0.88	1 (7%)
8	NGT	E	530	-	13,15,15	1.39	3 (23%)	14,22,22	0.88	1 (7%)
8	NGT	G	533	-	13,15,15	1.34	2 (15%)	14,22,22	0.87	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NGT	F	26	-	13,15,15	1.31	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	D	24	-	13,15,15	1.38	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	C	530	-	13,15,15	1.45	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	B	22	-	13,15,15	1.31	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	H	28	-	13,15,15	1.42	4 (30%)	14,22,22	0.88	1 (7%)

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
8	NGT	A	21	-	-	0/2/30/30	0/2/2/2
8	NGT	E	530	-	-	0/2/30/30	0/2/2/2
8	NGT	G	533	-	-	0/2/30/30	0/2/2/2
8	NGT	F	26	-	-	0/2/30/30	0/2/2/2
8	NGT	D	24	-	-	0/2/30/30	0/2/2/2
8	NGT	C	530	-	-	0/2/30/30	0/2/2/2
8	NGT	B	22	-	-	2/2/30/30	0/2/2/2
8	NGT	H	28	-	-	0/2/30/30	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	530	NGT	C3-C2	3.60	1.59	1.53
8	G	533	NGT	C3-C2	3.31	1.59	1.53
8	B	22	NGT	C3-C2	3.22	1.59	1.53
8	A	21	NGT	C3-C2	3.20	1.58	1.53
8	F	26	NGT	C3-C2	3.15	1.58	1.53
8	E	530	NGT	C3-C2	3.05	1.58	1.53
8	D	24	NGT	C3-C2	2.96	1.58	1.53
8	H	28	NGT	C3-C2	2.90	1.58	1.53
8	D	24	NGT	C2-N2	-2.70	1.45	1.47
8	F	26	NGT	C2-N2	-2.45	1.45	1.47
8	B	22	NGT	C2-N2	-2.41	1.45	1.47
8	C	530	NGT	C2-N2	-2.40	1.45	1.47
8	H	28	NGT	O5-C1	-2.39	1.38	1.42
8	E	530	NGT	C7-S1	2.20	1.78	1.77
8	H	28	NGT	C2-N2	-2.14	1.45	1.47
8	G	533	NGT	C2-N2	-2.13	1.45	1.47
8	E	530	NGT	C2-N2	-2.12	1.45	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	28	NGT	C7-S1	2.06	1.78	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	22	NGT	C1-O5-C5	2.36	116.80	112.56
8	C	530	NGT	C1-O5-C5	2.36	116.80	112.56
8	A	21	NGT	C1-O5-C5	2.36	116.79	112.56
8	E	530	NGT	C1-O5-C5	2.35	116.77	112.56
8	F	26	NGT	C1-O5-C5	2.35	116.77	112.56
8	H	28	NGT	C1-O5-C5	2.35	116.77	112.56
8	G	533	NGT	C1-O5-C5	2.34	116.76	112.56
8	D	24	NGT	C1-O5-C5	2.34	116.76	112.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	22	NGT	C4-C5-C6-O6
8	B	22	NGT	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	21	NGT	6	0
8	E	530	NGT	6	0
8	G	533	NGT	8	0
8	F	26	NGT	3	0
8	D	24	NGT	4	0
8	C	530	NGT	12	0
8	B	22	NGT	3	0
8	H	28	NGT	6	0

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	52/52 (100%)	0.35	0 100 100	31, 56, 60, 63	0
1	C	52/52 (100%)	-0.05	0 100 100	31, 55, 62, 62	0
1	E	52/52 (100%)	0.09	0 100 100	32, 54, 57, 59	0
1	G	52/52 (100%)	0.15	1 (1%) 66 48	31, 54, 59, 60	0
2	I	440/440 (100%)	0.50	14 (3%) 50 34	41, 53, 60, 66	0
2	J	440/440 (100%)	0.09	1 (0%) 91 85	42, 57, 62, 66	0
2	K	440/440 (100%)	0.14	3 (0%) 84 70	43, 57, 62, 64	0
2	L	440/440 (100%)	0.28	8 (1%) 67 48	42, 56, 60, 61	0
3	B	54/58 (93%)	0.03	1 (1%) 66 48	50, 58, 60, 60	0
3	D	54/58 (93%)	0.12	0 100 100	51, 57, 59, 60	0
3	F	54/58 (93%)	0.36	0 100 100	57, 60, 62, 63	0
3	H	54/58 (93%)	0.69	5 (9%) 14 11	56, 58, 60, 61	0
4	M	190/190 (100%)	0.23	2 (1%) 78 60	48, 55, 59, 63	0
4	O	189/190 (99%)	0.24	1 (0%) 87 76	28, 54, 57, 60	0
4	Q	190/190 (100%)	0.35	3 (1%) 70 52	54, 57, 61, 63	0
4	S	190/190 (100%)	0.45	5 (2%) 57 38	50, 56, 59, 61	0
5	N	236/237 (99%)	0.08	1 (0%) 88 78	21, 56, 60, 62	0
5	P	236/237 (99%)	0.21	1 (0%) 88 78	21, 57, 61, 62	0
5	R	236/237 (99%)	0.23	4 (1%) 69 50	21, 59, 63, 64	0
5	T	236/237 (99%)	0.69	14 (5%) 28 19	21, 57, 58, 59	0
All	All	3887/3908 (99%)	0.27	64 (1%) 70 52	21, 56, 61, 66	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S	175	PHE	5.1
2	L	279	SER	3.5
5	T	402	SER	3.4
2	L	312	PHE	3.3
2	I	93	ASN	3.2
2	L	356	ILE	3.2
1	G	74	GLY	3.1
4	Q	158	ALA	2.9
5	N	384	GLU	2.9
2	I	173	LEU	2.9
4	M	128	LEU	2.9
5	R	325	THR	2.8
5	T	392	LEU	2.8
4	Q	305	LEU	2.8
2	I	253	VAL	2.8
2	I	174	LEU	2.7
4	S	172	LEU	2.7
5	R	445	LEU	2.6
4	S	227	ALA	2.6
4	M	179	VAL	2.5
5	R	513	LEU	2.5
2	J	524	GLN	2.5
2	K	367	GLY	2.5
3	H	107	GLY	2.5
2	L	328	CYS	2.4
3	B	72	LEU	2.4
2	I	293	SER	2.4
2	L	381	VAL	2.4
5	T	421	VAL	2.4
5	T	388	ILE	2.4
2	K	213	TYR	2.3
5	R	548	ALA	2.3
2	I	439	PRO	2.3
2	I	467	THR	2.3
5	T	506	ALA	2.2
5	T	387	TYR	2.2
5	T	488	LEU	2.2
5	T	541	ILE	2.2
2	I	162	GLU	2.2
2	I	475	PRO	2.2
5	T	361	TRP	2.2
4	S	209	THR	2.1
2	I	149	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	54	PRO	2.1
5	T	379	ASP	2.1
2	I	254	LEU	2.1
3	H	85	SER	2.1
2	K	416	LEU	2.1
2	L	319	LEU	2.1
5	T	351	LEU	2.1
5	T	408	VAL	2.1
2	I	420	TRP	2.1
4	O	287	PRO	2.1
3	H	59	LEU	2.0
5	P	488	LEU	2.0
2	L	180	TYR	2.0
2	L	304	PHE	2.0
2	I	136	LEU	2.0
5	T	513	LEU	2.0
4	S	158	ALA	2.0
2	I	523	GLU	2.0
4	Q	153	VAL	2.0
3	H	72	LEU	2.0
5	T	482	ILE	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
6	NAG	Y	2	14/15	0.52	0.11	55,59,63,63	0
7	NAG	X	2	14/15	0.54	0.12	65,68,69,69	0
6	BMA	W	3	11/12	0.65	0.10	48,54,56,57	0
6	BMA	Y	3	11/12	0.66	0.10	46,49,51,51	0
6	BMA	V	3	11/12	0.67	0.09	52,53,55,56	0
6	BMA	U	3	11/12	0.71	0.07	50,52,54,55	0
6	NAG	W	2	14/15	0.72	0.10	61,66,68,68	0

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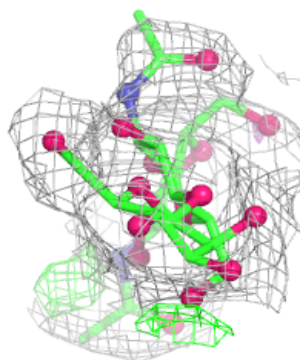
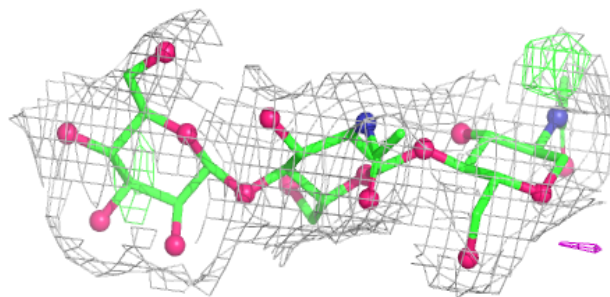
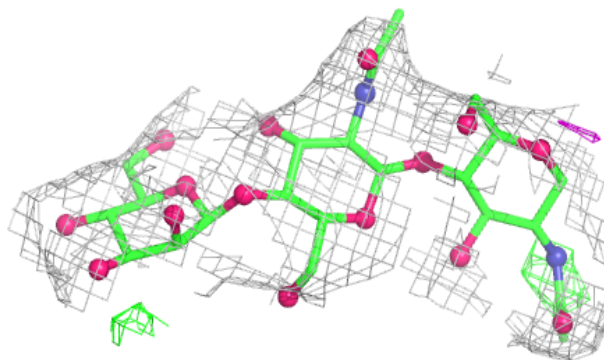
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	X	1	14/15	0.73	0.10	51,56,60,62	0
6	NAG	Y	1	14/15	0.73	0.11	45,47,48,51	0
7	NAG	Z	1	14/15	0.73	0.11	60,62,67,67	0
6	NAG	V	2	14/15	0.77	0.10	61,66,71,71	0
6	NAG	U	1	14/15	0.79	0.11	45,47,50,51	0
6	NAG	d	1	14/15	-	-	52,54,57,58	0
6	NAG	d	2	14/15	-	-	57,63,64,65	0
6	BMA	d	3	11/12	-	-	48,48,50,52	0
6	NAG	V	1	14/15	0.81	0.10	54,55,58,60	0
6	NAG	W	1	14/15	0.82	0.10	47,50,53,56	0
7	NAG	Z	2	14/15	0.83	0.06	74,76,78,78	0
6	NAG	U	2	14/15	0.84	0.09	58,61,63,63	0
7	NAG	a	1	14/15	-	-	58,59,62,64	0
7	NAG	a	2	14/15	-	-	73,76,78,79	0
7	NAG	b	1	14/15	-	-	61,62,62,66	0
7	NAG	b	2	14/15	-	-	73,76,77,77	0
7	NAG	c	1	14/15	-	-	59,60,63,65	0
7	NAG	c	2	14/15	-	-	72,75,76,76	0
7	NAG	e	1	14/15	-	-	61,62,63,66	0
7	NAG	e	2	14/15	-	-	73,76,76,76	0

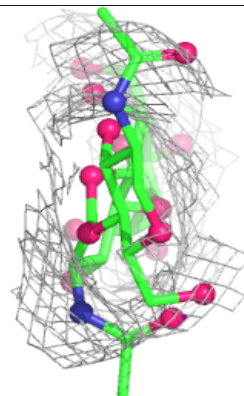
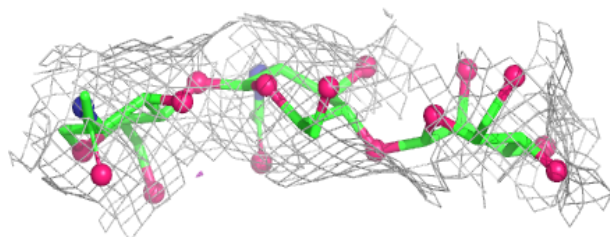
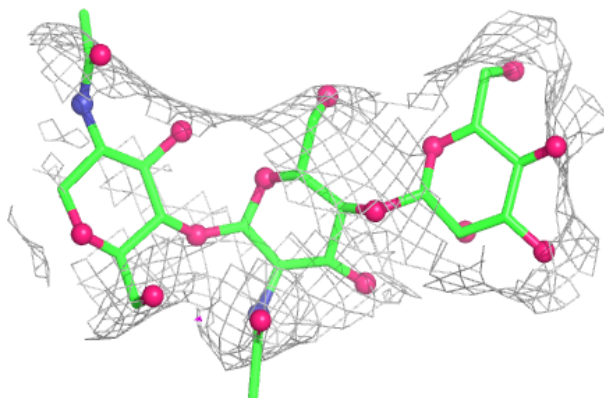
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

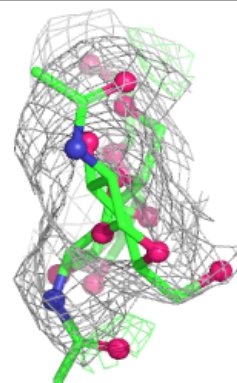
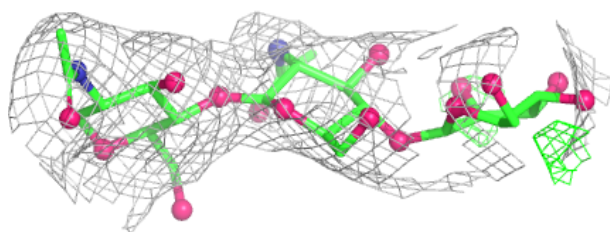
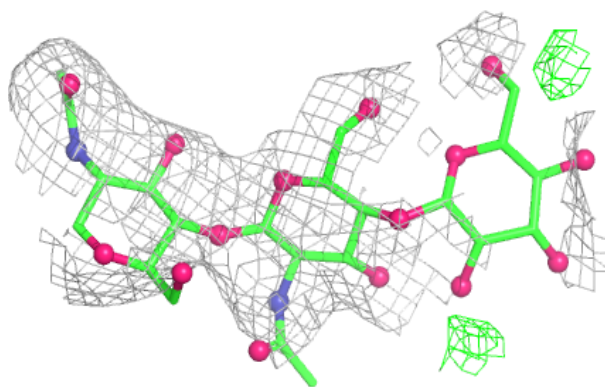
**Electron density around Chain V:**

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

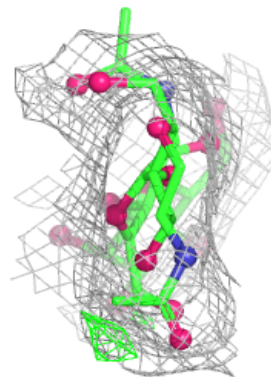
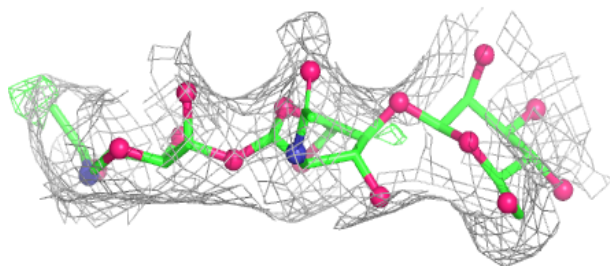
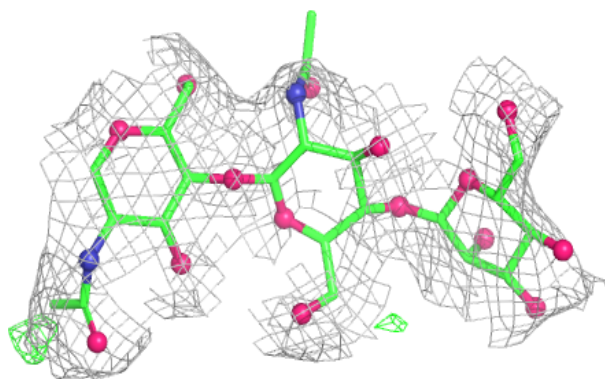


Electron density around Chain W:

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

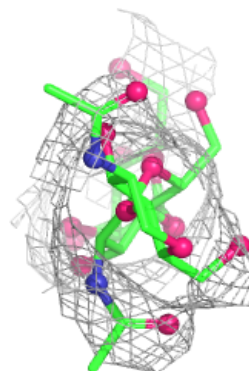
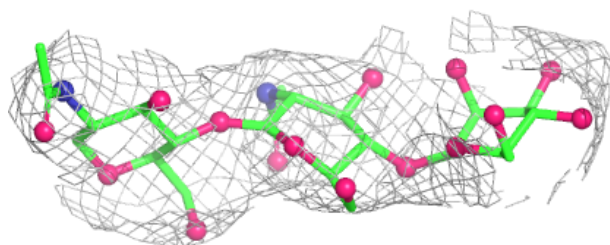
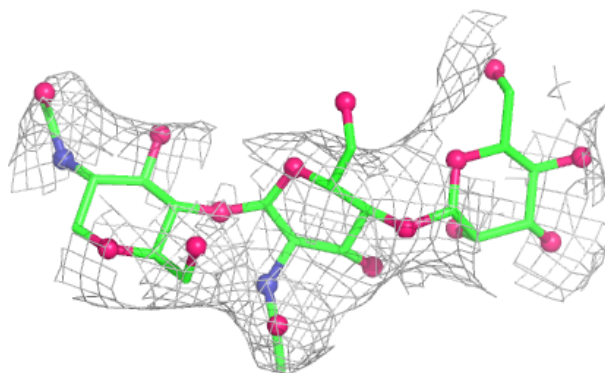
**Electron density around Chain Y:**

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

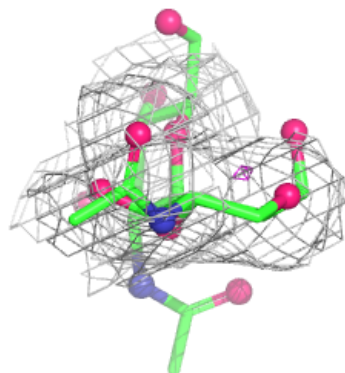
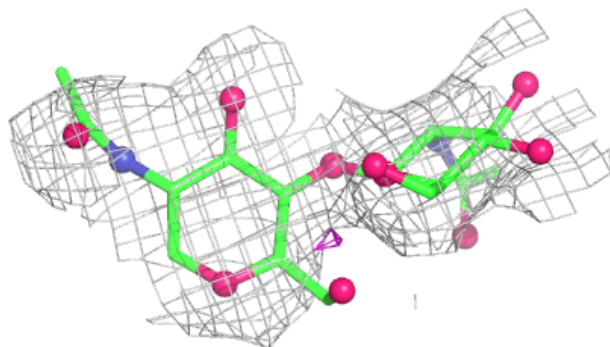
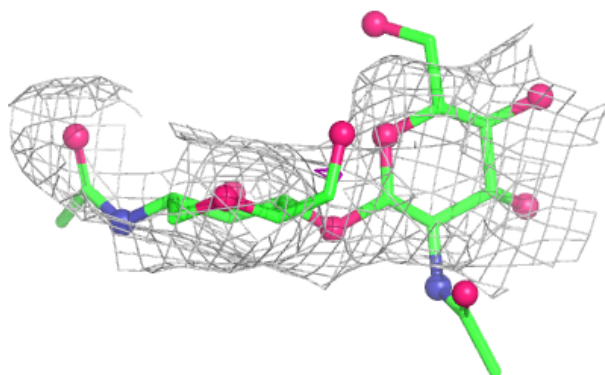


Electron density around Chain d:

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

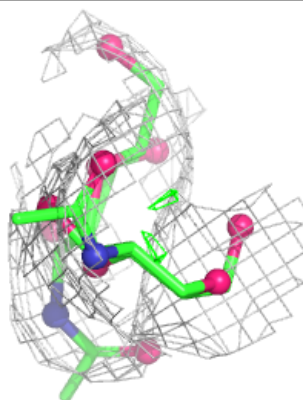
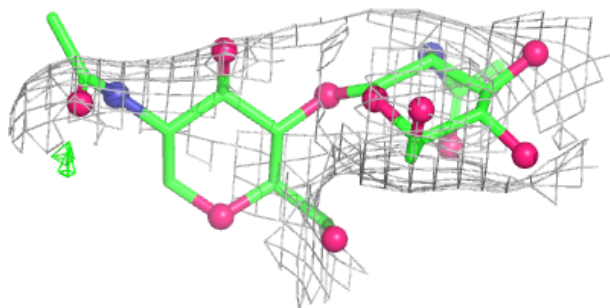
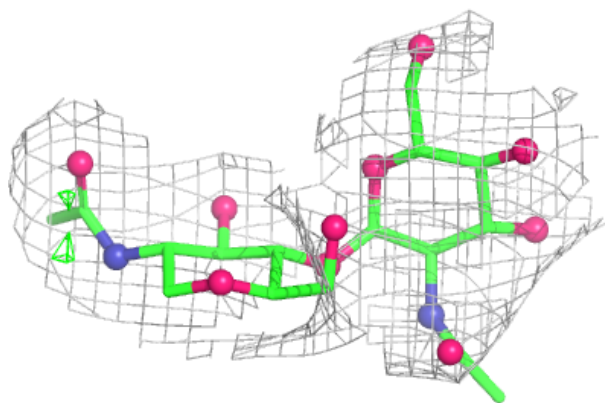
**Electron density around Chain X:**

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



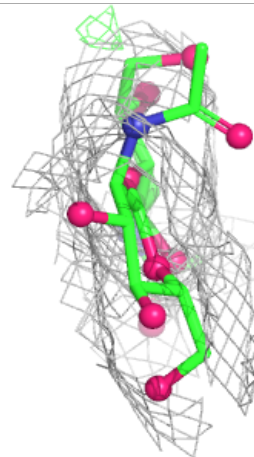
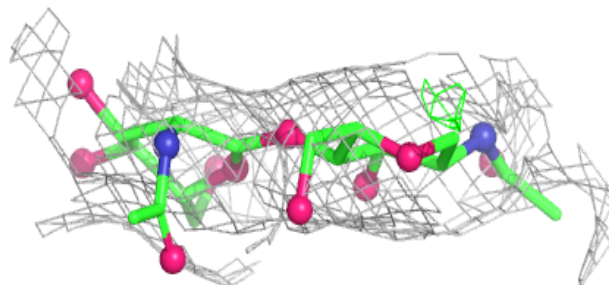
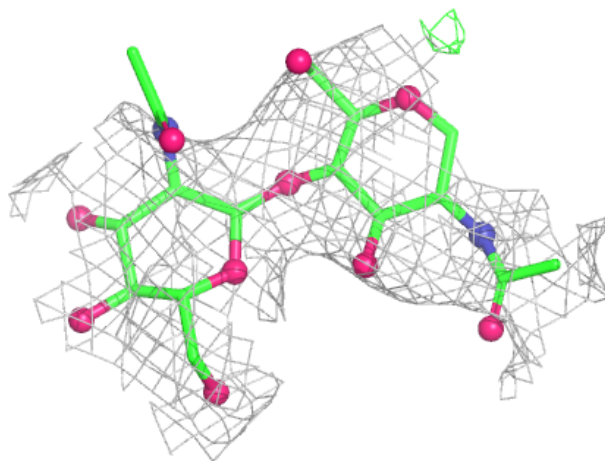
Electron density around Chain Z:

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



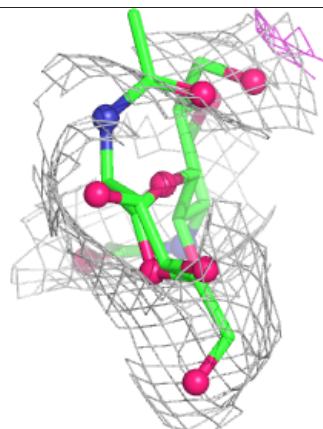
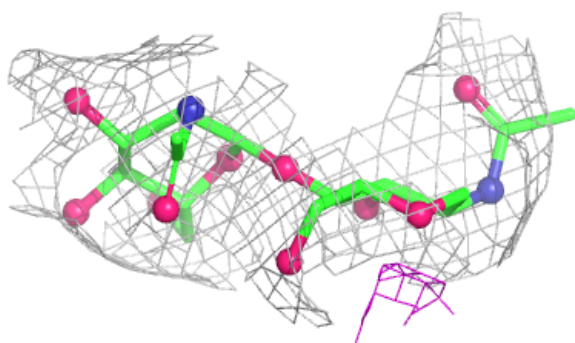
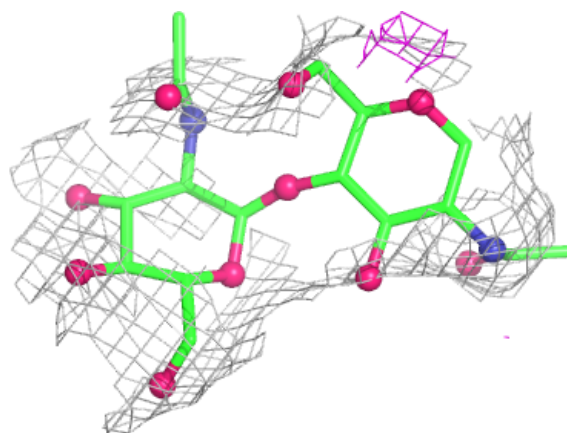
Electron density around Chain a:

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

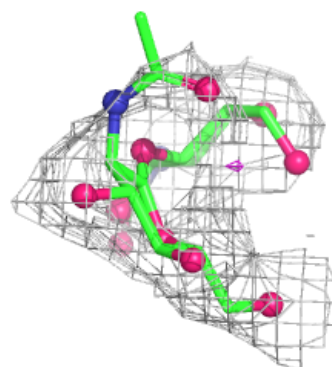
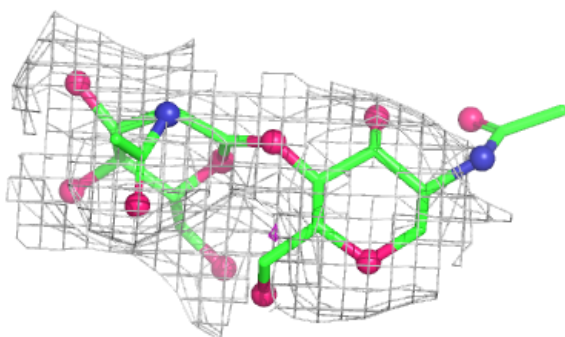


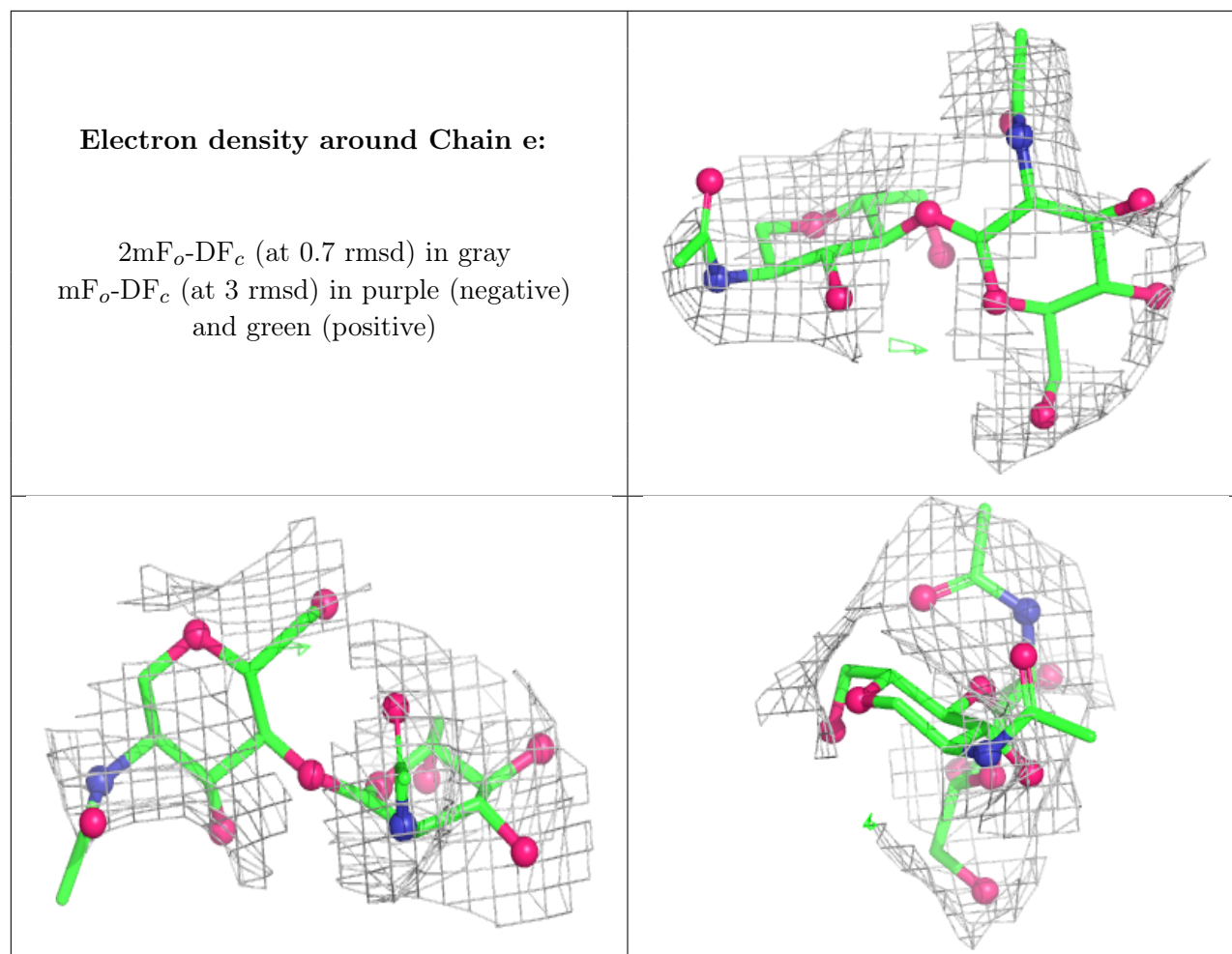
Electron density around Chain b:

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

**Electron density around Chain c:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NGT	H	28	14/14	0.61	0.15	48,50,53,54	0
8	NGT	E	530	14/14	0.63	0.12	47,49,52,53	0
8	NGT	G	533	14/14	0.65	0.15	47,47,49,50	0
8	NGT	C	530	14/14	0.73	0.12	44,46,49,50	0
8	NGT	F	26	14/14	0.86	0.10	40,41,42,43	0
8	NGT	A	21	14/14	0.89	0.09	33,35,37,37	0
8	NGT	B	22	14/14	0.90	0.09	38,39,41,44	0
8	NGT	D	24	14/14	0.91	0.09	39,41,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.