



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 PM UTC

PDB ID : 3WKN / pdb_00003wkn
Title : Crystal structure of the artificial protein AFFinger p17 (AF.p17) complexed with Fc fragment of human IgG
Authors : Watanabe, H.; Honda, S.
Deposited on : 2013-10-29
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

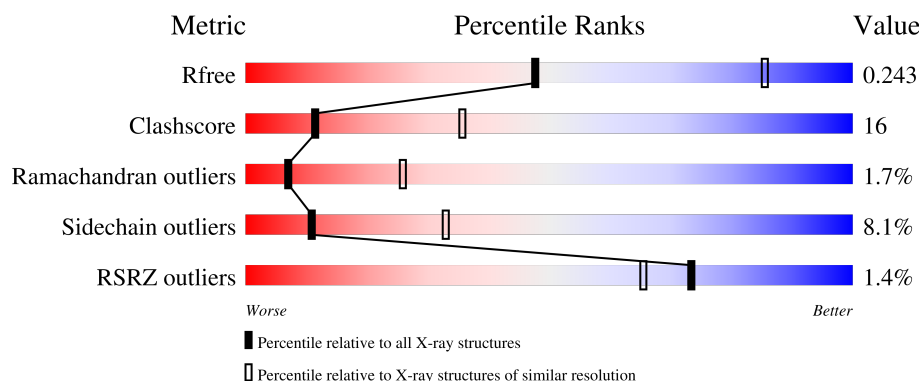
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	212	% 64% 30% 5% .
1	B	212	% 63% 31% 5% .
1	C	212	% 65% 29% 5% .
1	D	212	% 57% 39% . .
1	I	212	% 63% 29% 7% .

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Mol	Chain	Length	Quality of chain
1	J	212	
1	M	212	
1	N	212	
2	E	54	
2	F	54	
2	G	54	
2	H	54	
2	K	54	
2	L	54	
2	O	54	
2	P	54	
3	Q	9	
3	R	9	
3	S	9	
3	T	9	
3	U	9	
3	V	9	
3	W	9	
3	X	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17052 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	B	210	Total	C	N	O	S	0	0	0
			1675	1066	282	321	6			
1	A	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	D	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	I	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	J	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	M	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	N	210	Total	C	N	O	S	0	0	0
			1675	1066	282	321	6			

- Molecule 2 is a protein called AFFinger p17.

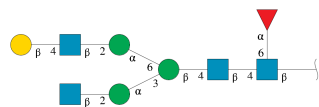
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	29	Total	C	N	O	S	0	0	0
			250	163	39	47	1			
2	F	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	G	47	Total	C	N	O	S	0	0	0
			392	256	61	74	1			
2	H	32	Total	C	N	O	S	0	0	0
			274	180	42	51	1			
2	K	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	L	47	Total	C	N	O	S	0	0	0
			392	256	61	74	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	P	43	Total	C	N	O	S	0	0	0
			363	236	57	69	1			

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

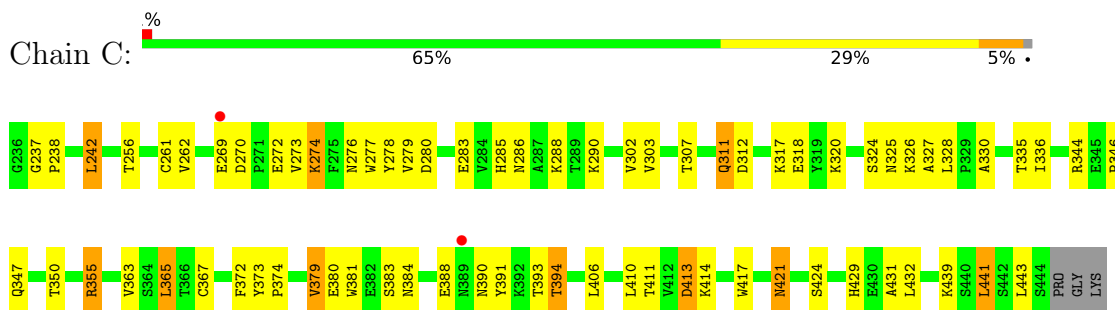


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	R	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	S	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	T	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	U	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	V	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	W	9	Total	C	N	O		0	0	0
			110	62	4	44				
3	X	9	Total	C	N	O		0	0	0
			110	62	4	44				

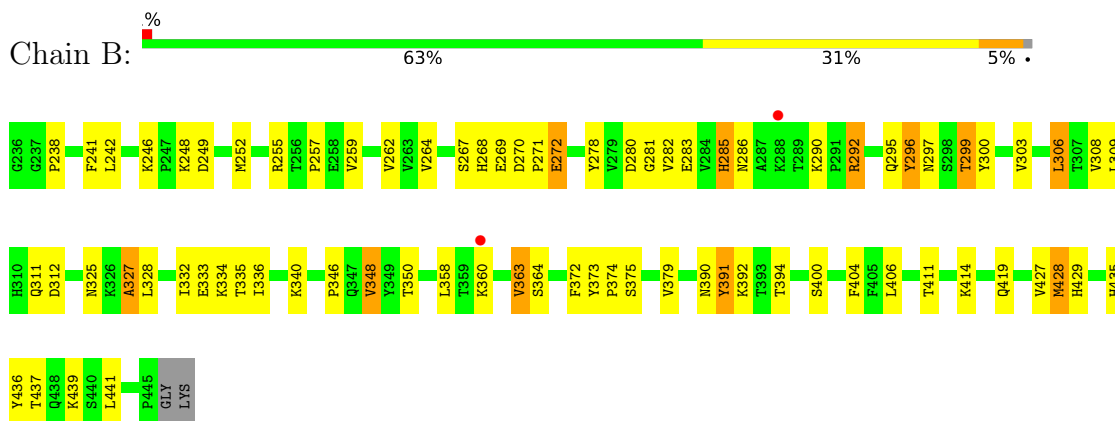
3 Residue-property plots

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

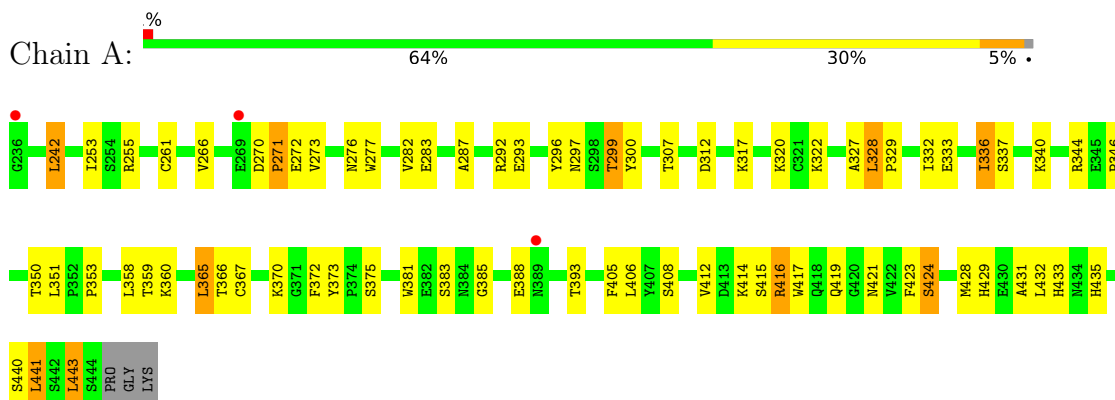
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region

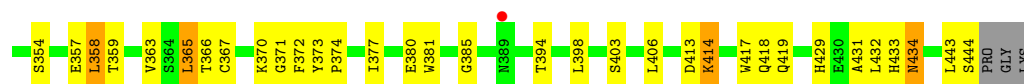


- Molecule 1: Ig gamma-1 chain C region

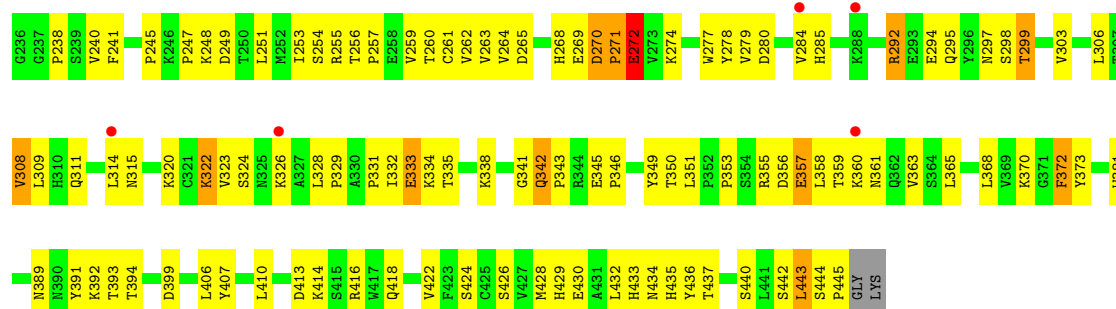


Chain D: 57% 39% 4%

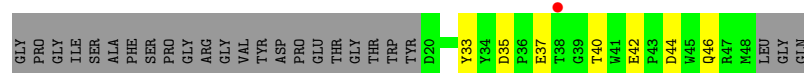




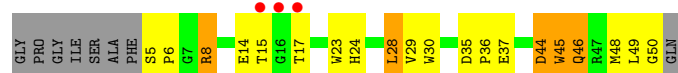
- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: AFFinger p17



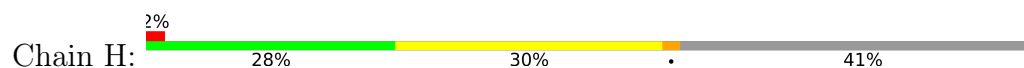
- Molecule 2: AFFinger p17



- Molecule 2: AFFinger p17



- Molecule 2: AFFinger p17

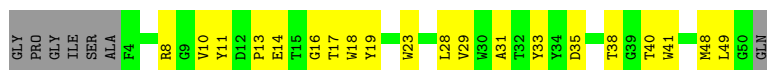


- Molecule 2: AFFinger p17





- Molecule 2: AFFfinger p17



- Molecule 2: AFFfinger p17



- Molecule 2: AFFfinger p17



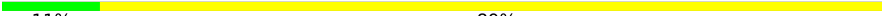
- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain S:  11% 89%



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

Chain T:  78% 22%



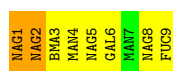
- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  78% 22%



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

Chain V:  11% 67% 22%

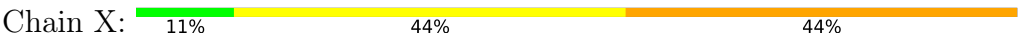


- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  44% 56%



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



MAG1
MAG2
BGL3
MAN4
MAG5
GAL6
MAN7
MAG8
FUC9

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.03Å 153.43Å 170.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 99.6 (20.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.242 0.200 , 0.243	Depositor DCC
R_{free} test set	3447 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17052	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.20	1/1714 (0.1%)	1.21	8/2335 (0.3%)
1	B	1.24	4/1722 (0.2%)	1.38	10/2347 (0.4%)
1	C	1.22	3/1714 (0.2%)	1.27	9/2335 (0.4%)
1	D	1.16	2/1714 (0.1%)	1.26	11/2335 (0.5%)
1	I	1.28	3/1714 (0.2%)	1.27	14/2335 (0.6%)
1	J	1.25	2/1714 (0.1%)	1.30	9/2335 (0.4%)
1	M	1.23	2/1714 (0.1%)	1.24	7/2335 (0.3%)
1	N	1.08	1/1722 (0.1%)	1.19	12/2347 (0.5%)
2	E	0.99	0/262	1.01	0/362
2	F	1.15	1/399 (0.3%)	1.02	1/551 (0.2%)
2	G	1.08	0/411	1.13	1/567 (0.2%)
2	H	0.99	0/287	0.92	0/396
2	K	1.08	0/399	1.19	2/551 (0.4%)
2	L	1.23	0/411	1.11	2/567 (0.4%)
2	O	1.04	0/399	1.01	1/551 (0.2%)
2	P	1.01	0/381	1.01	1/526 (0.2%)
All	All	1.19	19/16677 (0.1%)	1.23	88/22775 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	269	GLU	CD-OE1	14.49	1.52	1.25
1	M	269	GLU	CD-OE2	11.15	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	PRO	C-N	11.09	1.48	1.33
1	C	269	GLU	CD-OE1	9.75	1.43	1.25
1	D	360	LYS	CE-NZ	8.51	1.74	1.49
1	B	360	LYS	CE-NZ	7.71	1.72	1.49
1	I	348	VAL	CA-CB	-7.11	1.45	1.54
1	B	272	GLU	C-N	6.63	1.42	1.33
2	F	15	THR	CA-CB	6.03	1.63	1.53
1	J	443	LEU	CA-C	5.98	1.60	1.52
1	D	330	ALA	CA-CB	-5.95	1.46	1.53
1	B	428	MET	CA-C	-5.90	1.45	1.52
1	C	355	ARG	CZ-NH1	5.81	1.40	1.32
1	I	295	GLN	N-CA	5.79	1.53	1.46
1	J	244	PRO	CA-C	5.57	1.57	1.52
1	C	355	ARG	NE-CZ	5.29	1.38	1.33
1	I	321	CYS	N-CA	-5.06	1.40	1.46
1	N	372	PHE	N-CA	-5.06	1.39	1.46
1	A	336	ILE	CA-C	-5.01	1.46	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	PRO	CA-C-N	-21.26	92.80	122.77
1	B	271	PRO	C-N-CA	-21.26	92.80	122.77
1	N	357	GLU	N-CA-C	-10.53	101.48	114.75
1	I	394	THR	CA-C-N	-9.32	110.78	120.38
1	I	394	THR	C-N-CA	-9.32	110.78	120.38
1	D	357	GLU	N-CA-C	-7.84	103.69	113.18
1	B	394	THR	CA-C-N	-7.82	112.33	120.38
1	B	394	THR	C-N-CA	-7.82	112.33	120.38
1	J	310	HIS	N-CA-C	-7.81	102.73	111.71
1	C	256	THR	CA-C-N	7.77	128.38	119.99
1	C	256	THR	C-N-CA	7.77	128.38	119.99
1	J	389	ASN	N-CA-C	7.76	122.49	112.41
2	G	5	SER	N-CA-C	7.47	118.72	110.13
2	F	36	PRO	N-CA-C	-7.36	104.98	114.03
1	D	389	ASN	N-CA-C	7.21	121.01	112.93
1	I	295	GLN	N-CA-C	7.19	121.76	112.92
1	A	307	THR	N-CA-C	-6.67	101.55	110.55
1	J	386	GLN	CA-C-N	-6.67	113.12	119.85
1	J	386	GLN	C-N-CA	-6.67	113.12	119.85
1	B	268	HIS	N-CA-C	-6.59	104.50	112.54
1	I	297	ASN	N-CA-C	-6.59	105.11	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	351	LEU	CA-C-N	6.50	127.08	120.38
1	D	351	LEU	C-N-CA	6.50	127.08	120.38
1	J	282	VAL	N-CA-C	6.49	117.12	110.05
1	J	416	ARG	N-CA-C	-6.46	103.93	110.97
1	M	394	THR	CA-C-N	-6.45	113.74	120.38
1	M	394	THR	C-N-CA	-6.45	113.74	120.38
1	D	281	GLY	CA-C-N	-6.44	114.06	122.37
1	D	281	GLY	C-N-CA	-6.44	114.06	122.37
1	A	421	ASN	N-CA-C	6.44	118.61	110.24
1	I	357	GLU	N-CA-C	-6.37	104.99	112.89
2	K	5	SER	CA-C-N	6.33	125.75	118.85
2	K	5	SER	C-N-CA	6.33	125.75	118.85
1	D	370	LYS	N-CA-C	6.19	117.58	108.86
1	N	389	ASN	N-CA-C	6.17	120.42	113.01
1	A	328	LEU	CA-C-N	5.99	127.33	119.84
1	A	328	LEU	C-N-CA	5.99	127.33	119.84
1	J	361	ASN	N-CA-C	5.97	118.68	111.40
1	I	328	LEU	CA-C-N	5.93	127.25	119.84
1	I	328	LEU	C-N-CA	5.93	127.25	119.84
1	M	253	ILE	N-CA-C	5.76	117.19	110.62
1	M	345	GLU	CA-C-N	5.74	125.50	119.76
1	M	345	GLU	C-N-CA	5.74	125.50	119.76
1	C	363	VAL	N-CA-C	5.69	117.04	108.96
1	I	400	SER	N-CA-C	5.67	117.92	111.11
1	I	352	PRO	CA-C-N	5.56	125.54	120.03
1	I	352	PRO	C-N-CA	5.56	125.54	120.03
1	I	307	THR	N-CA-C	-5.55	102.67	110.50
1	N	370	LYS	N-CA-C	5.54	117.82	109.23
1	N	256	THR	CA-C-N	5.54	125.85	119.92
1	N	256	THR	C-N-CA	5.54	125.85	119.92
1	I	338	LYS	N-CA-C	-5.52	103.41	110.53
2	L	40	THR	N-CA-C	5.48	118.51	109.85
2	P	10	VAL	N-CA-C	5.47	117.98	108.95
1	N	345	GLU	CA-C-N	5.45	125.87	119.99
1	N	345	GLU	C-N-CA	5.45	125.87	119.99
1	D	338	LYS	N-CA-C	-5.42	102.98	110.35
1	D	369	VAL	CB-CA-C	-5.42	104.28	110.73
1	N	272	GLU	N-CA-C	5.40	118.24	109.06
2	L	8	ARG	N-CA-C	5.39	116.45	108.86
1	N	285	HIS	N-CA-C	-5.38	104.50	111.71
1	C	394	THR	CA-C-N	-5.38	114.84	120.38
1	C	394	THR	C-N-CA	-5.38	114.84	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	VAL	CB-CA-C	-5.35	104.19	111.15
1	B	272	GLU	O-C-N	-5.34	117.02	123.27
1	M	246	LYS	CA-C-N	5.34	126.52	119.84
1	M	246	LYS	C-N-CA	5.34	126.52	119.84
1	J	398	LEU	N-CA-C	5.26	117.33	109.59
2	O	45	TRP	N-CA-C	5.26	117.75	111.71
1	N	342	GLN	CA-C-N	5.20	126.34	119.84
1	N	342	GLN	C-N-CA	5.20	126.34	119.84
1	A	388	GLU	CA-C-N	-5.18	114.46	122.49
1	A	388	GLU	C-N-CA	-5.18	114.46	122.49
1	A	370	LYS	N-CA-C	5.17	117.53	109.52
1	D	394	THR	CA-C-N	-5.17	115.06	120.38
1	D	394	THR	C-N-CA	-5.17	115.06	120.38
1	C	237	GLY	CA-C-N	5.16	125.44	119.92
1	C	237	GLY	C-N-CA	5.16	125.44	119.92
1	N	399	ASP	N-CA-C	5.15	117.18	110.53
1	C	379	VAL	CB-CA-C	-5.11	102.62	110.50
1	B	348	VAL	N-CA-C	5.09	115.18	107.75
1	J	240	VAL	N-CA-C	5.08	115.28	108.17
1	B	272	GLU	CA-C-N	-5.04	115.44	122.75
1	B	272	GLU	C-N-CA	-5.04	115.44	122.75
1	I	356	ASP	N-CA-C	5.03	118.72	112.59
1	I	348	VAL	N-CA-C	5.02	115.14	108.11
1	B	391	TYR	N-CA-C	5.02	117.30	109.52
1	C	318	GLU	N-CA-C	5.00	116.89	108.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	296	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1668	0	1633	47	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1675	0	1640	60	0
1	C	1668	0	1633	51	1
1	D	1668	0	1633	56	0
1	I	1668	0	1633	48	0
1	J	1668	0	1633	58	0
1	M	1668	0	1633	48	0
1	N	1675	0	1639	92	0
2	E	250	0	211	4	0
2	F	381	0	327	11	0
2	G	392	0	336	12	0
2	H	274	0	234	11	0
2	K	381	0	327	8	0
2	L	392	0	336	15	0
2	O	381	0	327	15	0
2	P	363	0	309	16	0
3	Q	110	0	94	0	0
3	R	110	0	94	6	0
3	S	110	0	94	0	0
3	T	110	0	94	4	0
3	U	110	0	94	2	0
3	V	110	0	94	5	0
3	W	110	0	94	4	0
3	X	110	0	94	10	0
All	All	17052	0	16236	533	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 16.

All (533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:390:ASN:HD22	1:I:411:THR:HB	1.19	1.07
3:T:1:NAG:H61	3:T:2:NAG:H82	1.19	1.07
2:O:30:TRP:HA	2:O:48:MET:HE1	1.36	1.07
1:M:246:LYS:HD2	1:M:247:PRO:HD2	1.31	1.05
1:I:242:LEU:HD13	1:I:336:ILE:HG12	1.32	1.04
1:J:276:ASN:HB2	1:J:322:LYS:HB3	1.39	1.03
1:B:285:HIS:C	1:B:286:ASN:HD22	1.69	0.99
1:B:350:THR:HB	1:B:441:LEU:HD22	1.45	0.98
1:N:322:LYS:HB3	1:N:333:GLU:HB3	1.53	0.91
1:D:346:PRO:HD2	1:D:432:LEU:HD13	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:CE1	3:R:3:BMA:H2	2.11	0.86
1:I:390:ASN:ND2	1:I:411:THR:HB	1.90	0.85
1:J:279:VAL:HG23	1:J:280:ASP:H	1.42	0.85
1:I:242:LEU:CD1	1:I:336:ILE:HG12	2.06	0.84
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.62	0.82
1:C:312:ASP:HB3	1:C:317:LYS:HD2	1.61	0.82
2:O:30:TRP:HA	2:O:48:MET:CE	2.11	0.80
2:P:21:ALA:HB2	2:P:31:ALA:HB2	1.62	0.80
2:G:8:ARG:HH11	2:G:8:ARG:HA	1.47	0.79
1:C:311:GLN:HE21	1:C:311:GLN:HA	1.48	0.79
3:T:1:NAG:H61	3:T:2:NAG:C8	2.07	0.79
1:I:262:VAL:HG13	1:I:303:VAL:HG22	1.65	0.79
1:N:346:PRO:HB3	1:N:372:PHE:HB3	1.63	0.79
1:N:311:GLN:HE21	1:N:315:ASN:HD21	1.32	0.77
2:O:31:ALA:H	2:O:48:MET:HE3	1.51	0.76
1:A:320:LYS:HD2	1:A:333:GLU:HG3	1.68	0.75
1:I:240:VAL:HG21	1:I:323:VAL:HG21	1.67	0.75
1:N:253:ILE:HG12	2:P:48:MET:HB3	1.69	0.75
1:J:241:PHE:CZ	3:V:2:NAG:H61	2.21	0.75
1:J:292:ARG:CZ	1:J:292:ARG:HB3	2.16	0.75
1:J:246:LYS:HG3	1:J:247:PRO:HD2	1.67	0.75
1:C:242:LEU:HD13	1:C:336:ILE:HG12	1.70	0.74
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.68	0.74
3:X:2:NAG:H82	3:X:9:FUC:H4	1.69	0.74
1:N:353:PRO:HD3	1:N:365:LEU:HD23	1.69	0.73
1:A:429:HIS:CD2	1:A:431:ALA:H	2.06	0.73
2:P:21:ALA:HB2	2:P:31:ALA:CB	2.18	0.73
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.72	0.72
1:B:285:HIS:O	1:B:286:ASN:ND2	2.22	0.72
1:D:277:TRP:CE3	1:D:306:LEU:HD12	2.25	0.72
1:A:297:ASN:OD1	1:A:299:THR:OG1	2.08	0.72
1:J:398:LEU:HD12	1:J:399:ASP:N	2.05	0.72
1:N:272:GLU:HG2	1:N:292:ARG:HH22	1.55	0.71
1:M:274:LYS:HB3	1:M:324:SER:HB2	1.71	0.71
1:A:350:THR:O	1:A:351:LEU:HD23	1.91	0.70
1:N:279:VAL:O	1:N:280:ASP:HB2	1.90	0.70
1:N:428:MET:HG2	1:N:436:TYR:HD2	1.57	0.70
1:N:341:GLY:HA3	1:N:373:TYR:CE1	2.26	0.70
1:N:341:GLY:HA3	1:N:373:TYR:HE1	1.55	0.70
1:N:320:LYS:HG3	1:N:335:THR:HB	1.74	0.70
1:B:311:GLN:HG2	1:B:312:ASP:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:PRO:HB3	1:D:372:PHE:HB3	1.74	0.69
2:O:31:ALA:N	2:O:48:MET:HE3	2.07	0.69
1:C:346:PRO:HB3	1:C:372:PHE:HB3	1.73	0.69
1:C:312:ASP:CB	1:C:317:LYS:HD2	2.22	0.69
1:M:246:LYS:O	1:M:249:ASP:HB2	1.93	0.69
1:B:297:ASN:OD1	1:B:299:THR:HB	1.93	0.69
1:N:274:LYS:O	1:N:323:VAL:HG23	1.92	0.68
1:C:390:ASN:ND2	1:C:411:THR:HB	2.08	0.68
1:D:276:ASN:HB2	1:D:322:LYS:HB3	1.75	0.68
1:M:429:HIS:CD2	1:M:431:ALA:H	2.12	0.67
2:L:33:TYR:C	2:L:33:TYR:CD2	2.71	0.67
1:N:428:MET:HG2	1:N:436:TYR:CD2	2.29	0.67
1:A:350:THR:HB	1:A:441:LEU:HD13	1.76	0.67
1:N:324:SER:HB2	1:N:331:PRO:HB3	1.76	0.67
1:M:346:PRO:HB3	1:M:372:PHE:HB3	1.76	0.67
2:P:11:TYR:HB2	2:P:18:TRP:CE2	2.30	0.67
1:A:429:HIS:HD2	1:A:431:ALA:H	1.43	0.67
1:B:325:ASN:ND2	1:B:327:ALA:HB3	2.10	0.66
1:A:424:SER:HB3	1:A:440:SER:OG	1.95	0.66
1:I:265:ASP:OD1	3:U:1:NAG:N2	2.28	0.66
1:C:285:HIS:C	1:C:286:ASN:HD22	2.03	0.66
1:D:355:ARG:H	1:D:355:ARG:HD3	1.61	0.65
2:K:11:TYR:CE2	2:K:13:PRO:HA	2.32	0.65
1:C:325:ASN:ND2	1:C:327:ALA:H	1.95	0.65
1:D:383:SER:OG	1:D:422:VAL:O	2.10	0.65
2:P:38:THR:HB	2:P:40:THR:HG22	1.78	0.65
1:D:362:GLN:HA	1:D:413:ASP:HA	1.78	0.65
1:N:277:TRP:CE3	1:N:306:LEU:HD23	2.31	0.65
1:A:351:LEU:HB2	1:A:366:THR:HB	1.79	0.64
1:B:311:GLN:HG2	1:B:312:ASP:N	2.12	0.64
1:N:257:PRO:HB2	1:N:308:VAL:HG22	1.78	0.64
1:M:253:ILE:HG12	2:O:48:MET:HB3	1.78	0.64
2:O:31:ALA:H	2:O:48:MET:CE	2.10	0.64
1:I:325:ASN:ND2	1:I:327:ALA:HB3	2.13	0.63
1:N:334:LYS:HZ1	3:X:8:NAG:H81	1.63	0.63
1:D:301:ARG:NE	3:T:2:NAG:H81	2.13	0.63
1:A:417:TRP:O	1:A:443:LEU:HD12	1.99	0.63
1:B:292:ARG:HD2	1:B:300:TYR:CE1	2.34	0.63
1:I:429:HIS:CD2	1:I:431:ALA:H	2.17	0.63
2:L:23:TRP:CZ3	2:L:28:LEU:HB2	2.34	0.62
1:J:326:LYS:C	1:J:328:LEU:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:LYS:O	1:N:323:VAL:CG2	2.48	0.62
1:J:338:LYS:NZ	1:J:338:LYS:HA	2.15	0.62
1:B:259:VAL:HG12	1:B:336:ILE:HD11	1.82	0.62
1:I:311:GLN:HE21	2:K:45:TRP:HZ2	1.45	0.62
1:D:321:CYS:O	1:D:333:GLU:HA	2.00	0.62
1:N:269:GLU:O	1:N:271:PRO:HD3	2.00	0.62
2:L:11:TYR:HB2	2:L:18:TRP:CE2	2.34	0.62
1:M:429:HIS:HD2	1:M:431:ALA:H	1.47	0.61
1:J:318:GLU:HA	1:J:337:SER:OG	2.00	0.61
1:B:241:PHE:CD1	3:R:3:BMA:H2	2.35	0.61
1:D:406:LEU:C	1:D:406:LEU:HD12	2.25	0.61
1:J:436:TYR:HE1	1:J:438:GLN:HE21	1.47	0.61
1:N:254:SER:HB2	2:P:27:GLU:OE1	2.00	0.61
1:M:320:LYS:HG3	1:M:335:THR:HG22	1.83	0.61
1:N:264:VAL:HG11	3:X:1:NAG:O4	2.01	0.61
1:N:428:MET:HA	1:N:435:HIS:O	2.00	0.61
1:I:346:PRO:HB3	1:I:372:PHE:HB3	1.83	0.61
1:N:278:TYR:HD2	1:N:320:LYS:HD3	1.65	0.61
2:H:43:PRO:HB2	2:H:45:TRP:CE2	2.35	0.60
1:B:295:GLN:C	1:B:297:ASN:H	2.10	0.60
2:F:8:ARG:HD2	2:F:8:ARG:N	2.16	0.60
1:C:429:HIS:HD2	1:C:431:ALA:H	1.50	0.59
1:B:242:LEU:HD21	1:B:336:ILE:HG12	1.83	0.59
1:I:268:HIS:CE1	1:I:294:GLU:OE1	2.56	0.59
1:J:393:THR:HG23	1:J:408:SER:HB2	1.83	0.59
1:N:245:PRO:HD3	1:N:259:VAL:HG12	1.83	0.59
1:N:353:PRO:HD3	1:N:365:LEU:CD2	2.32	0.59
1:D:346:PRO:HD2	1:D:432:LEU:CD1	2.29	0.59
1:J:252:MET:HG2	2:L:29:VAL:HG13	1.84	0.59
1:I:240:VAL:CG2	1:I:323:VAL:HG21	2.32	0.58
1:D:238:PRO:HA	1:D:265:ASP:HB2	1.84	0.58
1:D:393:THR:HG23	1:D:408:SER:HB2	1.85	0.58
1:I:328:LEU:HD11	1:I:332:ILE:HD11	1.85	0.58
2:P:21:ALA:CB	2:P:31:ALA:HB2	2.33	0.58
1:A:242:LEU:HD13	1:A:336:ILE:HG12	1.84	0.58
1:D:248:LYS:HZ1	1:D:255:ARG:HH21	1.52	0.58
1:J:264:VAL:HG21	3:V:1:NAG:O4	2.04	0.58
1:D:253:ILE:HD12	1:D:310:HIS:ND1	2.19	0.58
2:F:8:ARG:HD2	2:F:8:ARG:H	1.69	0.58
1:C:238:PRO:HD2	1:C:328:LEU:HD13	1.84	0.58
1:N:391:TYR:CD1	1:N:391:TYR:C	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:406:LEU:C	1:N:406:LEU:HD12	2.29	0.57
1:C:429:HIS:CD2	1:C:431:ALA:H	2.23	0.57
1:B:292:ARG:NH1	1:B:292:ARG:HG2	2.19	0.57
1:A:312:ASP:OD1	1:A:317:LYS:HE3	2.04	0.57
1:D:301:ARG:HE	3:T:2:NAG:H81	1.68	0.57
3:X:2:NAG:H83	3:X:2:NAG:H3	1.85	0.57
1:J:241:PHE:N	1:J:241:PHE:CD2	2.72	0.57
1:M:242:LEU:HD13	1:M:336:ILE:HG12	1.86	0.57
1:N:294:GLU:HG2	1:N:295:GLN:H	1.69	0.57
1:C:261:CYS:HB2	1:C:277:TRP:CH2	2.40	0.57
1:D:400:SER:C	1:D:402:GLY:H	2.13	0.57
1:I:391:TYR:CD1	1:I:391:TYR:C	2.83	0.57
2:G:8:ARG:HA	2:G:8:ARG:NH1	2.17	0.57
1:B:249:ASP:OD1	1:B:255:ARG:HG2	2.05	0.57
1:D:368:LEU:HD13	1:D:407:TYR:CZ	2.40	0.57
1:J:401:ASP:OD1	1:J:401:ASP:C	2.46	0.57
1:C:421:ASN:N	1:C:421:ASN:HD22	2.02	0.57
2:G:35:ASP:CG	2:G:38:THR:HG22	2.29	0.57
1:I:365:LEU:HD11	1:I:417:TRP:CE3	2.39	0.57
1:B:295:GLN:O	1:B:297:ASN:N	2.38	0.56
2:K:11:TYR:HB2	2:K:18:TRP:CE2	2.39	0.56
1:J:284:VAL:HG11	1:J:306:LEU:HD11	1.87	0.56
1:I:365:LEU:HB2	1:I:410:LEU:HD23	1.88	0.56
1:M:351:LEU:HB2	1:M:366:THR:HB	1.87	0.56
1:I:271:PRO:O	1:I:272:GLU:C	2.49	0.56
1:N:278:TYR:HB2	1:N:320:LYS:HB3	1.87	0.56
1:J:290:LYS:HB2	1:J:290:LYS:NZ	2.21	0.56
1:M:322:LYS:NZ	1:M:333:GLU:OE2	2.35	0.56
1:M:334:LYS:HZ1	3:W:8:NAG:H83	1.71	0.56
1:I:365:LEU:HD12	1:I:441:LEU:HD21	1.88	0.56
1:M:349:TYR:CZ	1:N:357:GLU:HG3	2.41	0.56
2:K:11:TYR:OH	2:K:16:GLY:HA2	2.06	0.55
1:B:252:MET:HE3	2:F:29:VAL:HG22	1.87	0.55
1:I:399:ASP:OD2	1:I:400:SER:N	2.36	0.55
2:G:34:TYR:OH	2:G:39:GLY:HA2	2.06	0.55
1:B:390:ASN:ND2	1:B:411:THR:HB	2.21	0.55
1:N:264:VAL:HG12	1:N:265:ASP:N	2.22	0.55
1:I:246:LYS:HD3	3:U:6:GAL:O4	2.06	0.55
1:C:280:ASP:OD1	1:C:317:LYS:HG2	2.05	0.55
1:B:242:LEU:CD2	1:B:336:ILE:HG12	2.37	0.55
1:D:264:VAL:O	1:D:265:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:246:LYS:CD	1:M:247:PRO:HD2	2.21	0.55
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.72	0.55
1:N:295:GLN:HG2	3:X:1:NAG:H62	1.89	0.55
1:C:273:VAL:HG11	1:C:302:VAL:HG21	1.89	0.54
1:N:257:PRO:HB2	1:N:308:VAL:CG2	2.37	0.54
1:I:261:CYS:HB2	1:I:277:TRP:CZ2	2.42	0.54
1:M:365:LEU:HD11	1:M:417:TRP:CE3	2.42	0.54
1:A:358:LEU:O	1:A:414:LYS:NZ	2.38	0.54
1:J:398:LEU:HD12	1:J:398:LEU:C	2.32	0.54
1:N:264:VAL:HG12	1:N:265:ASP:H	1.73	0.54
1:N:270:ASP:OD2	1:N:326:LYS:HB2	2.08	0.54
1:D:263:VAL:HG21	1:D:323:VAL:HG11	1.90	0.54
2:H:34:TYR:CD2	2:H:35:ASP:N	2.76	0.54
2:L:35:ASP:HB3	2:L:38:THR:HG22	1.90	0.54
1:C:290:LYS:HD2	1:C:303:VAL:CG2	2.38	0.54
1:J:337:SER:O	1:J:338:LYS:O	2.26	0.54
1:N:356:ASP:OD1	1:N:356:ASP:N	2.41	0.54
1:C:270:ASP:CG	1:C:326:LYS:HD2	2.33	0.54
1:A:365:LEU:HD22	1:A:412:VAL:HG21	1.89	0.54
2:F:45:TRP:CD1	2:F:48:MET:HE3	2.43	0.53
1:N:358:LEU:HD23	1:N:363:VAL:HG11	1.88	0.53
1:D:312:ASP:O	1:D:317:LYS:HB2	2.07	0.53
2:L:17:THR:HB	2:L:19:TYR:CE2	2.43	0.53
1:B:379:VAL:HG22	1:B:427:VAL:HG22	1.89	0.53
3:R:3:BMA:O2	3:R:7:MAN:H5	2.09	0.53
3:X:2:NAG:C8	3:X:9:FUC:H4	2.38	0.53
1:A:320:LYS:HD2	1:A:333:GLU:CG	2.37	0.53
1:A:372:PHE:HE2	1:A:375:SER:HA	1.74	0.53
1:I:379:VAL:HG22	1:I:427:VAL:HG22	1.89	0.53
2:P:38:THR:CG2	2:P:40:THR:HG22	2.38	0.53
1:J:432:LEU:HD13	1:J:437:THR:HG22	1.90	0.53
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.90	0.53
1:D:432:LEU:HD21	1:D:437:THR:HG22	1.91	0.53
1:C:274:LYS:HB3	1:C:324:SER:OG	2.10	0.52
1:D:246:LYS:HB2	1:D:249:ASP:OD2	2.09	0.52
1:D:373:TYR:CG	1:D:374:PRO:HA	2.44	0.52
1:J:367:CYS:HB2	1:J:381:TRP:CZ2	2.44	0.52
1:J:279:VAL:HG13	1:J:284:VAL:HG22	1.92	0.52
1:J:433:HIS:HE2	2:L:41:TRP:CG	2.27	0.52
1:N:361:ASN:OD1	1:N:361:ASN:O	2.26	0.52
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:265:ASP:HB3	3:V:1:NAG:H82	1.91	0.52
1:J:406:LEU:C	1:J:406:LEU:HD12	2.35	0.52
2:F:44:ASP:OD2	2:F:44:ASP:C	2.52	0.52
1:D:328:LEU:HD13	1:D:332:ILE:HG13	1.92	0.52
1:A:428:MET:HA	1:A:435:HIS:O	2.10	0.52
1:N:334:LYS:NZ	3:X:8:NAG:H81	2.24	0.52
1:N:414:LYS:O	1:N:418:GLN:HG3	2.10	0.52
1:B:242:LEU:HD23	1:B:336:ILE:HG23	1.91	0.52
2:E:33:TYR:HD1	2:E:44:ASP:HB2	1.74	0.52
1:J:279:VAL:HG23	1:J:280:ASP:N	2.18	0.52
2:F:48:MET:C	2:F:50:GLY:H	2.18	0.51
1:A:271:PRO:O	1:A:273:VAL:HG23	2.09	0.51
1:J:264:VAL:HG13	1:J:265:ASP:OD1	2.10	0.51
1:M:373:TYR:CD1	1:M:374:PRO:HA	2.45	0.51
1:N:429:HIS:N	1:N:432:LEU:HD12	2.26	0.51
1:M:367:CYS:HB2	1:M:381:TRP:CZ2	2.45	0.51
1:B:246:LYS:HG3	3:R:6:GAL:O4	2.10	0.51
1:J:330:ALA:HB1	1:J:331:PRO:HD2	1.92	0.51
2:K:11:TYR:HB2	2:K:18:TRP:CZ2	2.46	0.51
1:B:290:LYS:HD2	1:B:303:VAL:CG2	2.41	0.51
1:I:240:VAL:HG21	1:I:323:VAL:CG2	2.40	0.51
1:J:323:VAL:O	1:J:332:ILE:HG22	2.11	0.51
1:B:295:GLN:C	1:B:297:ASN:N	2.67	0.51
1:C:262:VAL:HG13	1:C:303:VAL:HG12	1.92	0.50
1:I:345:GLU:HA	1:I:431:ALA:HB3	1.93	0.50
1:N:240:VAL:HG12	1:N:241:PHE:N	2.26	0.50
1:B:248:LYS:O	1:B:252:MET:HG3	2.11	0.50
1:A:350:THR:C	1:A:351:LEU:HD23	2.36	0.50
2:G:35:ASP:HB3	2:G:38:THR:HG22	1.94	0.50
1:C:421:ASN:N	1:C:421:ASN:ND2	2.60	0.50
2:F:23:TRP:CE2	2:F:28:LEU:HD23	2.46	0.50
1:D:365:LEU:HD21	1:D:412:VAL:CG1	2.42	0.50
1:B:325:ASN:HD22	1:B:327:ALA:HB3	1.77	0.50
1:J:417:TRP:CZ3	1:J:442:SER:HA	2.46	0.50
2:L:11:TYR:HB2	2:L:18:TRP:CD2	2.46	0.50
1:M:276:ASN:HB2	1:M:322:LYS:HB3	1.94	0.50
2:O:23:TRP:CH2	2:O:28:LEU:HD23	2.47	0.50
1:M:357:GLU:O	1:M:359:THR:N	2.45	0.49
1:N:311:GLN:HE21	1:N:315:ASN:ND2	2.06	0.49
1:A:293:GLU:HG3	2:K:23:TRP:CE2	2.48	0.49
2:L:48:MET:O	2:L:49:LEU:HD23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:422:VAL:HA	1:N:442:SER:HB3	1.93	0.49
1:C:390:ASN:HD21	1:C:411:THR:HB	1.73	0.49
2:E:35:ASP:OD2	1:A:360:LYS:HE2	2.12	0.49
1:J:290:LYS:HB2	1:J:290:LYS:HZ3	1.75	0.49
1:C:344:ARG:O	1:C:372:PHE:HA	2.12	0.49
1:B:375:SER:HB3	1:B:404:PHE:CE1	2.47	0.49
1:M:373:TYR:CD1	1:M:374:PRO:CA	2.95	0.49
1:C:272:GLU:H	1:C:272:GLU:CD	2.18	0.49
1:C:381:TRP:CE3	1:C:410:LEU:HD22	2.48	0.49
1:B:270:ASP:C	1:B:272:GLU:H	2.21	0.49
1:M:263:VAL:HG11	1:M:273:VAL:HG11	1.93	0.49
2:O:33:TYR:C	2:O:33:TYR:CD2	2.91	0.49
2:P:34:TYR:OH	2:P:39:GLY:HA2	2.13	0.49
1:B:267:SER:HB2	1:B:269:GLU:HG2	1.94	0.49
1:D:346:PRO:CD	1:D:432:LEU:HD13	2.32	0.49
1:N:368:LEU:HD13	1:N:407:TYR:CZ	2.47	0.49
1:B:270:ASP:C	1:B:272:GLU:N	2.71	0.49
1:A:293:GLU:HG3	2:K:23:TRP:CD2	2.48	0.49
1:A:393:THR:HG23	1:A:408:SER:HB2	1.95	0.49
1:I:388:GLU:HG3	1:I:410:LEU:HD11	1.94	0.49
2:P:38:THR:CB	2:P:40:THR:HG22	2.42	0.49
1:M:349:TYR:CE2	1:N:357:GLU:HG3	2.47	0.49
2:O:44:ASP:O	2:O:48:MET:HG3	2.12	0.49
1:D:320:LYS:HB2	1:D:335:THR:HG22	1.94	0.48
1:M:320:LYS:HG3	1:M:335:THR:CG2	2.43	0.48
1:B:348:VAL:HG12	1:B:439:LYS:HG3	1.95	0.48
1:I:328:LEU:HD21	1:I:332:ILE:HD12	1.95	0.48
1:I:374:PRO:O	1:I:429:HIS:HE1	1.95	0.48
1:B:428:MET:HA	1:B:435:HIS:O	2.13	0.48
1:I:309:LEU:HD12	1:I:309:LEU:H	1.78	0.48
1:J:265:ASP:HB3	3:V:1:NAG:C8	2.43	0.48
2:G:11:TYR:CE2	2:G:13:PRO:HA	2.48	0.48
1:D:379:VAL:HG22	1:D:427:VAL:HG22	1.95	0.48
1:J:279:VAL:O	1:J:318:GLU:O	2.32	0.48
1:J:346:PRO:HB3	1:J:372:PHE:HB3	1.96	0.48
2:H:19:TYR:CD1	2:H:33:TYR:HB3	2.49	0.48
2:O:15:THR:O	2:O:17:THR:HG23	2.14	0.48
1:B:246:LYS:HE2	3:R:6:GAL:O4	2.15	0.47
1:D:278:TYR:N	1:D:278:TYR:CD1	2.82	0.47
1:D:263:VAL:CG2	1:D:323:VAL:HG11	2.44	0.47
1:N:361:ASN:OD1	1:N:361:ASN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:LEU:C	1:C:330:ALA:H	2.23	0.47
1:D:344:ARG:O	1:D:372:PHE:HA	2.15	0.47
2:P:11:TYR:HE2	2:P:16:GLY:HA2	1.79	0.47
1:A:328:LEU:CD2	1:A:332:ILE:HG13	2.40	0.47
1:M:321:CYS:O	1:M:333:GLU:HA	2.14	0.47
1:M:354:SER:CB	1:N:349:TYR:HB3	2.45	0.47
1:N:255:ARG:HG2	1:N:255:ARG:HH11	1.80	0.47
1:C:393:THR:HG22	1:C:394:THR:N	2.29	0.47
1:J:297:ASN:OD1	1:J:299:THR:OG1	2.26	0.47
1:A:405:PHE:CZ	1:D:392:LYS:HB3	2.50	0.47
1:I:384:ASN:N	1:I:384:ASN:ND2	2.62	0.47
1:M:347:GLN:HB2	1:M:370:LYS:HG2	1.96	0.47
1:N:261:CYS:HB2	1:N:277:TRP:CZ2	2.49	0.47
1:B:373:TYR:CG	1:B:374:PRO:HA	2.49	0.46
1:I:265:ASP:HA	1:I:299:THR:HG21	1.95	0.46
1:N:277:TRP:CE3	1:N:306:LEU:CD2	2.98	0.46
1:B:257:PRO:HB2	1:B:308:VAL:HG22	1.97	0.46
1:I:268:HIS:HE1	1:I:294:GLU:OE1	1.97	0.46
1:J:417:TRP:CH2	1:J:442:SER:HA	2.50	0.46
2:P:21:ALA:HB1	2:P:30:TRP:O	2.15	0.46
1:M:371:GLY:HA2	1:M:403:SER:OG	2.15	0.46
1:N:240:VAL:HG22	1:N:263:VAL:HG22	1.98	0.46
1:C:373:TYR:CG	1:C:374:PRO:HA	2.51	0.46
2:E:33:TYR:CD1	2:E:44:ASP:HB2	2.50	0.46
2:H:23:TRP:CZ2	2:H:28:LEU:HD12	2.51	0.46
1:N:429:HIS:H	1:N:432:LEU:HD12	1.81	0.46
1:N:265:ASP:OD1	3:X:1:NAG:H82	2.15	0.46
1:N:294:GLU:HG2	1:N:295:GLN:N	2.29	0.46
1:M:377:ILE:HG21	1:M:406:LEU:HD21	1.98	0.46
2:P:42:GLU:HG3	2:P:43:PRO:HD2	1.98	0.46
1:B:278:TYR:CD2	1:B:283:GLU:HB2	2.51	0.46
2:L:11:TYR:CZ	2:L:16:GLY:HA2	2.50	0.46
1:N:323:VAL:HG22	1:N:324:SER:N	2.31	0.46
2:P:6:PRO:HG3	2:P:34:TYR:CD2	2.51	0.46
1:C:365:LEU:HD11	1:C:417:TRP:CE3	2.50	0.46
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.97	0.46
1:N:346:PRO:CB	1:N:372:PHE:HB3	2.39	0.46
1:C:391:TYR:CD1	1:C:391:TYR:C	2.93	0.46
1:N:443:LEU:HG	1:N:445:PRO:HD3	1.97	0.46
1:N:269:GLU:CD	1:N:269:GLU:H	2.23	0.45
2:H:44:ASP:OD2	2:H:46:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:325:ASN:HB3	1:I:328:LEU:HB2	1.98	0.45
1:N:413:ASP:HB2	1:N:416:ARG:HG3	1.98	0.45
1:A:253:ILE:HG12	2:G:48:MET:HB3	1.98	0.45
1:M:380:GLU:OE2	2:O:24:HIS:NE2	2.49	0.45
1:C:311:GLN:HA	1:C:311:GLN:NE2	2.25	0.45
2:H:34:TYR:HD2	2:H:35:ASP:H	1.62	0.45
1:N:346:PRO:HB3	1:N:372:PHE:CB	2.41	0.45
1:N:426:SER:HB3	1:N:436:TYR:OH	2.17	0.45
1:C:278:TYR:CD1	1:C:320:LYS:HD2	2.51	0.45
1:C:350:THR:CG2	1:C:439:LYS:HB3	2.46	0.45
1:D:382:GLU:HB2	1:D:386:GLN:O	2.17	0.45
1:C:381:TRP:HA	1:C:424:SER:O	2.17	0.45
1:D:377:ILE:HG13	1:D:428:MET:O	2.16	0.45
1:D:414:LYS:O	1:D:418:GLN:HG2	2.17	0.45
1:J:326:LYS:C	1:J:328:LEU:N	2.70	0.45
1:A:328:LEU:HA	1:A:329:PRO:HD2	1.72	0.45
1:A:415:SER:O	1:A:416:ARG:HB2	2.15	0.45
1:I:341:GLY:O	1:I:342:GLN:C	2.60	0.45
1:N:432:LEU:HD22	1:N:437:THR:HB	1.99	0.45
1:N:432:LEU:HD22	1:N:437:THR:CG2	2.47	0.45
1:B:296:TYR:CD2	1:J:274:LYS:HB2	2.52	0.45
1:A:353:PRO:HD3	1:A:365:LEU:HD12	1.99	0.45
1:D:258:GLU:HB3	1:D:305:VAL:HG23	1.98	0.45
1:M:238:PRO:HD2	1:M:328:LEU:HD13	1.98	0.45
1:N:435:HIS:N	1:N:435:HIS:CD2	2.84	0.45
1:D:382:GLU:O	1:D:424:SER:N	2.45	0.45
1:N:264:VAL:HG21	3:X:2:NAG:H2	1.98	0.45
1:M:414:LYS:HD3	1:M:418:GLN:CD	2.42	0.44
1:C:374:PRO:O	1:C:429:HIS:HE1	1.99	0.44
1:B:373:TYR:CD1	1:B:374:PRO:HA	2.52	0.44
1:I:365:LEU:HD11	1:I:417:TRP:CZ3	2.52	0.44
1:J:338:LYS:HA	1:J:338:LYS:HZ2	1.82	0.44
1:N:253:ILE:HG12	2:P:48:MET:CB	2.43	0.44
1:A:270:ASP:OD2	1:A:327:ALA:HB2	2.18	0.44
1:I:277:TRP:O	1:I:283:GLU:HG3	2.17	0.44
1:C:328:LEU:O	1:C:330:ALA:N	2.51	0.44
1:C:383:SER:HB3	1:C:388:GLU:OE2	2.18	0.44
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.62	0.44
1:A:365:LEU:HG	1:A:441:LEU:HD21	1.99	0.44
1:I:325:ASN:HD22	1:I:327:ALA:HB3	1.83	0.44
1:J:362:GLN:HB3	1:J:411:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:1:NAG:H62	3:W:9:FUC:H2	1.76	0.44
1:C:277:TRP:O	1:C:283:GLU:HA	2.17	0.44
1:A:433:HIS:HE2	2:G:41:TRP:CG	2.36	0.44
1:D:392:LYS:HD2	1:D:392:LYS:HA	1.75	0.44
1:J:311:GLN:HG2	1:J:315:ASN:HD21	1.81	0.44
1:J:391:TYR:HB3	1:J:410:LEU:HD12	1.98	0.44
3:W:5:NAG:H61	3:W:6:GAL:C1	2.48	0.44
1:B:436:TYR:CE2	2:F:24:HIS:HB2	2.52	0.44
1:M:277:TRP:CD1	1:M:287:ALA:CB	3.01	0.44
1:M:433:HIS:HE1	2:O:20:ASP:OD1	2.01	0.44
1:B:391:TYR:CD1	1:B:391:TYR:C	2.95	0.44
1:A:405:PHE:HZ	1:D:392:LYS:HB3	1.82	0.44
1:M:273:VAL:CG1	1:M:323:VAL:HG13	2.48	0.44
1:N:247:PRO:O	1:N:251:LEU:HG	2.18	0.44
1:B:238:PRO:HG2	1:B:328:LEU:HD21	1.99	0.44
2:H:41:TRP:N	2:H:41:TRP:CD1	2.85	0.44
1:J:261:CYS:HB2	1:J:277:TRP:CH2	2.52	0.44
1:J:338:LYS:O	1:J:339:ALA:HB3	2.17	0.44
1:J:415:SER:O	1:J:419:GLN:HG3	2.18	0.44
2:K:11:TYR:HE2	2:K:13:PRO:HA	1.77	0.44
1:M:432:LEU:O	1:M:433:HIS:C	2.61	0.44
2:O:38:THR:O	2:O:40:THR:HG23	2.17	0.44
1:I:429:HIS:HD2	1:I:431:ALA:H	1.63	0.44
1:J:237:GLY:HA2	1:J:327:ALA:O	2.18	0.44
1:M:373:TYR:CG	1:M:374:PRO:HA	2.53	0.43
1:C:328:LEU:C	1:C:330:ALA:N	2.76	0.43
1:A:383:SER:HB2	1:A:423:PHE:CD2	2.52	0.43
2:G:18:TRP:HB2	2:G:34:TYR:HB3	2.00	0.43
1:J:268:HIS:O	1:J:271:PRO:HD3	2.17	0.43
1:N:424:SER:HA	1:N:440:SER:HA	2.00	0.43
1:C:367:CYS:HB2	1:C:381:TRP:CZ2	2.53	0.43
1:B:292:ARG:HH11	1:B:292:ARG:CG	2.30	0.43
1:D:345:GLU:HG2	1:D:432:LEU:HD12	2.01	0.43
1:N:249:ASP:OD2	1:N:255:ARG:HD2	2.19	0.43
1:N:358:LEU:HD23	1:N:358:LEU:HA	1.92	0.43
2:O:43:PRO:HB2	2:O:45:TRP:NE1	2.33	0.43
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.53	0.43
1:C:288:LYS:HE2	1:C:288:LYS:HB3	1.88	0.43
1:B:257:PRO:HB2	1:B:308:VAL:CG2	2.48	0.43
1:B:348:VAL:CG1	1:B:439:LYS:HG3	2.49	0.43
1:A:416:ARG:HA	1:A:419:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:LYS:HD3	1:I:333:GLU:OE2	2.19	0.43
2:L:35:ASP:CG	2:L:38:THR:HG22	2.44	0.43
1:D:253:ILE:HA	1:D:310:HIS:CE1	2.53	0.43
1:I:245:PRO:HB2	1:I:250:THR:HG22	2.01	0.43
1:J:253:ILE:HG12	2:L:48:MET:HB3	2.01	0.43
1:N:434:ASN:O	1:N:435:HIS:HB2	2.19	0.43
1:C:274:LYS:HD2	1:C:276:ASN:ND2	2.34	0.43
2:F:29:VAL:O	2:F:30:TRP:HB2	2.18	0.43
1:N:328:LEU:HD21	1:N:332:ILE:HG12	2.00	0.43
1:M:271:PRO:HG2	1:M:272:GLU:OE2	2.18	0.43
1:N:381:TRP:CE2	1:N:410:LEU:HB2	2.54	0.43
1:N:393:THR:HG22	1:N:394:THR:O	2.19	0.43
2:P:40:THR:HG23	2:P:40:THR:O	2.19	0.43
1:C:326:LYS:O	1:C:326:LYS:HD3	2.19	0.42
1:C:346:PRO:HD2	1:C:432:LEU:HG	2.01	0.42
1:D:406:LEU:C	1:D:406:LEU:CD1	2.92	0.42
1:N:406:LEU:C	1:N:406:LEU:CD1	2.92	0.42
1:B:280:ASP:C	1:B:282:VAL:H	2.26	0.42
1:B:392:LYS:HA	1:B:392:LYS:HD3	1.85	0.42
2:E:42:GLU:OE1	1:A:359:THR:HB	2.20	0.42
1:D:342:GLN:HA	1:D:343:PRO:HD2	1.91	0.42
1:I:326:LYS:C	1:I:328:LEU:H	2.27	0.42
1:I:354:SER:O	1:I:355:ARG:C	2.61	0.42
1:J:241:PHE:HZ	3:V:2:NAG:H61	1.79	0.42
1:J:354:SER:O	1:J:355:ARG:C	2.62	0.42
1:M:443:LEU:HD12	1:M:444:SER:N	2.34	0.42
1:N:238:PRO:HB2	1:N:328:LEU:HD13	2.01	0.42
1:N:248:LYS:HG3	1:N:428:MET:HE1	2.00	0.42
1:C:312:ASP:CG	1:C:317:LYS:HD2	2.45	0.42
1:J:314:LEU:HD23	1:J:314:LEU:HA	1.87	0.42
1:N:259:VAL:HG13	1:N:308:VAL:HG11	2.01	0.42
1:N:360:LYS:O	1:N:414:LYS:HE2	2.18	0.42
1:N:433:HIS:O	1:N:434:ASN:HB2	2.19	0.42
2:L:13:PRO:O	2:L:14:GLU:C	2.62	0.42
1:C:413:ASP:O	1:C:414:LYS:C	2.62	0.42
1:I:261:CYS:HB2	1:I:277:TRP:CH2	2.55	0.42
1:C:350:THR:HB	1:C:441:LEU:HD22	2.01	0.42
1:B:285:HIS:C	1:B:286:ASN:ND2	2.55	0.42
1:N:406:LEU:HD12	1:N:406:LEU:O	2.19	0.42
1:B:262:VAL:HG22	1:B:303:VAL:HG12	2.02	0.42
1:I:265:ASP:HA	1:I:299:THR:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:384:ASN:N	1:I:384:ASN:HD22	2.18	0.42
1:J:329:PRO:HB2	1:J:330:ALA:H	1.61	0.42
1:M:263:VAL:CG1	1:M:302:VAL:HB	2.49	0.42
1:M:358:LEU:HD23	1:M:363:VAL:HG11	2.02	0.42
1:N:240:VAL:CG1	1:N:241:PHE:N	2.81	0.42
1:D:345:GLU:CG	1:D:432:LEU:HD12	2.50	0.42
1:D:355:ARG:H	1:D:355:ARG:CD	2.31	0.42
2:H:38:THR:C	2:H:40:THR:H	2.27	0.42
1:M:246:LYS:HD2	1:M:247:PRO:CD	2.23	0.42
2:O:12:ASP:HA	2:O:13:PRO:HD3	1.87	0.42
1:B:358:LEU:HD23	1:B:363:VAL:HG11	2.01	0.42
2:F:35:ASP:OD2	2:F:37:GLU:HB3	2.20	0.42
1:D:365:LEU:HD21	1:D:412:VAL:HG12	2.02	0.42
1:I:354:SER:HB2	1:J:349:TYR:HB3	2.00	0.42
1:C:379:VAL:O	1:C:380:GLU:HG3	2.21	0.41
1:D:277:TRP:CD2	1:D:306:LEU:HD12	2.54	0.41
1:D:368:LEU:HD13	1:D:407:TYR:CE1	2.55	0.41
1:D:413:ASP:OD1	1:D:416:ARG:HG3	2.20	0.41
2:H:23:TRP:CE3	2:H:26:GLY:O	2.73	0.41
1:M:272:GLU:O	1:M:325:ASN:ND2	2.53	0.41
1:C:290:LYS:HD2	1:C:303:VAL:HG21	2.01	0.41
1:I:328:LEU:HA	1:I:329:PRO:HD2	1.80	0.41
1:I:423:PHE:N	1:I:423:PHE:CD1	2.87	0.41
1:N:320:LYS:HE2	1:N:333:GLU:HB2	2.02	0.41
1:A:253:ILE:HG21	2:G:28:LEU:HD23	2.03	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.54	0.41
1:D:365:LEU:HD23	1:D:410:LEU:HD23	2.01	0.41
2:G:35:ASP:CB	2:G:38:THR:HG22	2.50	0.41
1:M:347:GLN:HB3	1:M:349:TYR:CZ	2.55	0.41
1:B:406:LEU:C	1:B:406:LEU:HD12	2.46	0.41
1:J:240:VAL:C	1:J:241:PHE:CD2	2.99	0.41
2:L:11:TYR:HB2	2:L:18:TRP:CZ2	2.55	0.41
1:N:260:THR:HG22	1:N:262:VAL:HG23	2.02	0.41
1:C:325:ASN:HB3	1:C:328:LEU:HB2	2.02	0.41
1:N:260:THR:HG21	3:X:5:NAG:H62	2.03	0.41
1:B:264:VAL:HG11	3:R:2:NAG:H2	2.03	0.41
1:B:292:ARG:HD2	1:B:300:TYR:CD1	2.54	0.41
1:A:358:LEU:HD21	1:A:417:TRP:HD1	1.86	0.41
1:C:421:ASN:ND2	1:C:421:ASN:H	2.17	0.41
1:J:346:PRO:HG2	1:J:432:LEU:HG	2.02	0.41
1:N:442:SER:O	1:N:444:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:CYS:HB2	1:D:277:TRP:CH2	2.56	0.41
1:D:365:LEU:HD21	1:D:412:VAL:HG11	2.02	0.41
2:H:23:TRP:CZ3	2:H:28:LEU:HB2	2.56	0.41
1:J:278:TYR:HA	1:J:282:VAL:O	2.20	0.41
2:L:31:ALA:O	2:L:48:MET:HE2	2.21	0.41
1:N:350:THR:C	1:N:351:LEU:HD23	2.45	0.41
1:C:278:TYR:CE2	1:C:283:GLU:HB2	2.55	0.41
1:B:311:GLN:CG	1:B:312:ASP:N	2.82	0.41
2:G:33:TYR:CD2	2:G:33:TYR:C	2.99	0.41
1:M:334:LYS:NZ	3:W:8:NAG:H83	2.34	0.41
1:M:373:TYR:CD1	1:M:374:PRO:N	2.89	0.41
1:N:414:LYS:O	1:N:414:LYS:HG2	2.20	0.41
1:A:406:LEU:HD12	1:A:406:LEU:C	2.46	0.40
1:D:248:LYS:NZ	1:D:255:ARG:HH21	2.17	0.40
1:B:259:VAL:CG1	1:B:336:ILE:HD11	2.50	0.40
1:B:332:ILE:HG22	1:B:333:GLU:N	2.36	0.40
1:B:429:HIS:O	1:B:435:HIS:HA	2.21	0.40
2:F:30:TRP:CE2	2:F:48:MET:HE1	2.56	0.40
1:D:297:ASN:O	1:D:298:SER:HB2	2.21	0.40
2:H:43:PRO:O	2:H:45:TRP:N	2.54	0.40
1:M:398:LEU:O	1:N:392:LYS:HE2	2.21	0.40
1:A:277:TRP:O	1:A:283:GLU:HG3	2.21	0.40
1:A:346:PRO:HG2	1:A:432:LEU:HD21	2.04	0.40
1:N:297:ASN:O	1:N:299:THR:N	2.54	0.40
1:B:414:LYS:HE2	1:B:414:LYS:HB3	1.85	0.40
1:A:344:ARG:HG3	1:A:373:TYR:HB3	2.03	0.40
1:J:345:GLU:HA	1:J:431:ALA:HB3	2.03	0.40
1:M:328:LEU:HD12	1:M:328:LEU:HA	1.99	0.40
1:M:434:ASN:HD22	1:M:434:ASN:HA	1.63	0.40
1:N:268:HIS:O	1:N:271:PRO:HG3	2.21	0.40
1:J:290:LYS:HD3	1:J:293:GLU:OE1	2.22	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)
1:C:355:ARG:NH2	1:A:287:ALA:O[2_454]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/212 (98%)	192 (93%)	12 (6%)	3 (1%)	9	30
1	B	208/212 (98%)	191 (92%)	14 (7%)	3 (1%)	9	30
1	C	207/212 (98%)	196 (95%)	10 (5%)	1 (0%)	24	54
1	D	207/212 (98%)	200 (97%)	7 (3%)	0	100	100
1	I	207/212 (98%)	191 (92%)	13 (6%)	3 (1%)	9	30
1	J	207/212 (98%)	181 (87%)	17 (8%)	9 (4%)	2	8
1	M	207/212 (98%)	196 (95%)	9 (4%)	2 (1%)	12	39
1	N	208/212 (98%)	181 (87%)	23 (11%)	4 (2%)	6	23
2	E	27/54 (50%)	25 (93%)	1 (4%)	1 (4%)	2	11
2	F	44/54 (82%)	34 (77%)	6 (14%)	4 (9%)	0	1
2	G	45/54 (83%)	42 (93%)	3 (7%)	0	100	100
2	H	30/54 (56%)	22 (73%)	7 (23%)	1 (3%)	3	13
2	K	44/54 (82%)	40 (91%)	3 (7%)	1 (2%)	5	19
2	L	45/54 (83%)	41 (91%)	4 (9%)	0	100	100
2	O	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
2	P	41/54 (76%)	33 (80%)	6 (15%)	2 (5%)	1	6
All	All	1978/2128 (93%)	1804 (91%)	140 (7%)	34 (2%)	7	26

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	ALA
2	E	37	GLU
1	J	279	VAL
1	J	329	PRO
1	J	338	LYS
2	K	37	GLU

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Mol	Chain	Res	Type
1	N	298	SER
1	N	299	THR
1	N	329	PRO
1	B	296	TYR
2	F	6	PRO
2	F	46	GLN
1	A	416	ARG
1	I	271	PRO
1	I	272	GLU
1	J	271	PRO
1	J	272	GLU
1	M	358	LEU
2	F	17	THR
2	F	49	LEU
1	A	385	GLY
1	J	339	ALA
2	H	49	LEU
1	J	401	ASP
1	M	385	GLY
1	N	271	PRO
1	C	443	LEU
1	A	271	PRO
2	P	13	PRO
2	P	16	GLY
1	I	329	PRO
1	J	281	GLY
1	J	237	GLY
1	B	281	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	194/196 (99%)	182 (94%)	12 (6%)	16	46
1	B	195/196 (100%)	182 (93%)	13 (7%)	15	43
1	C	194/196 (99%)	181 (93%)	13 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	194/196 (99%)	178 (92%)	16 (8%)	10	32
1	I	194/196 (99%)	172 (89%)	22 (11%)	5	19
1	J	194/196 (99%)	175 (90%)	19 (10%)	7	25
1	M	194/196 (99%)	181 (93%)	13 (7%)	15	43
1	N	195/196 (100%)	178 (91%)	17 (9%)	9	30
2	E	24/42 (57%)	22 (92%)	2 (8%)	10	32
2	F	37/42 (88%)	30 (81%)	7 (19%)	1	5
2	G	38/42 (90%)	35 (92%)	3 (8%)	11	34
2	H	26/42 (62%)	23 (88%)	3 (12%)	5	18
2	K	37/42 (88%)	34 (92%)	3 (8%)	11	33
2	L	38/42 (90%)	37 (97%)	1 (3%)	40	73
2	O	37/42 (88%)	36 (97%)	1 (3%)	39	73
2	P	35/42 (83%)	32 (91%)	3 (9%)	10	30
All	All	1826/1904 (96%)	1678 (92%)	148 (8%)	11	33

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	242	LEU
1	C	274	LYS
1	C	279	VAL
1	C	307	THR
1	C	311	GLN
1	C	335	THR
1	C	347	GLN
1	C	365	LEU
1	C	384	ASN
1	C	406	LEU
1	C	413	ASP
1	C	421	ASN
1	C	441	LEU
1	B	285	HIS
1	B	292	ARG
1	B	299	THR
1	B	306	LEU
1	B	309	LEU
1	B	334	LYS

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Mol	Chain	Res	Type
1	B	335	THR
1	B	340	LYS
1	B	363	VAL
1	B	364	SER
1	B	400	SER
1	B	419	GLN
1	B	437	THR
2	E	40	THR
2	E	46	GLN
2	F	5	SER
2	F	8	ARG
2	F	14	GLU
2	F	28	LEU
2	F	44	ASP
2	F	45	TRP
2	F	46	GLN
1	A	242	LEU
1	A	255	ARG
1	A	272	GLU
1	A	292	ARG
1	A	296	TYR
1	A	299	THR
1	A	337	SER
1	A	340	LYS
1	A	365	LEU
1	A	424	SER
1	A	441	LEU
1	A	443	LEU
1	D	273	VAL
1	D	282	VAL
1	D	292	ARG
1	D	305	VAL
1	D	306	LEU
1	D	336	ILE
1	D	347	GLN
1	D	360	LYS
1	D	361	ASN
1	D	365	LEU
1	D	389	ASN
1	D	409	LYS
1	D	411	THR
1	D	419	GLN

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Mol	Chain	Res	Type
1	D	432	LEU
1	D	444	SER
2	G	5	SER
2	G	40	THR
2	G	46	GLN
2	H	35	ASP
2	H	37	GLU
2	H	48	MET
1	I	239	SER
1	I	242	LEU
1	I	262	VAL
1	I	282	VAL
1	I	295	GLN
1	I	299	THR
1	I	306	LEU
1	I	307	THR
1	I	334	LYS
1	I	351	LEU
1	I	363	VAL
1	I	370	LYS
1	I	383	SER
1	I	384	ASN
1	I	391	TYR
1	I	410	LEU
1	I	412	VAL
1	I	415	SER
1	I	418	GLN
1	I	439	LYS
1	I	441	LEU
1	I	444	SER
1	J	241	PHE
1	J	264	VAL
1	J	268	HIS
1	J	272	GLU
1	J	273	VAL
1	J	285	HIS
1	J	290	LYS
1	J	292	ARG
1	J	332	ILE
1	J	337	SER
1	J	338	LYS
1	J	354	SER

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Mol	Chain	Res	Type
1	J	360	LYS
1	J	362	GLN
1	J	375	SER
1	J	398	LEU
1	J	400	SER
1	J	412	VAL
1	J	424	SER
2	K	28	LEU
2	K	38	THR
2	K	46	GLN
2	L	10	VAL
1	M	254	SER
1	M	259	VAL
1	M	264	VAL
1	M	292	ARG
1	M	307	THR
1	M	314	LEU
1	M	328	LEU
1	M	334	LYS
1	M	365	LEU
1	M	413	ASP
1	M	414	LYS
1	M	419	GLN
1	M	434	ASN
1	N	270	ASP
1	N	272	GLU
1	N	284	VAL
1	N	292	ARG
1	N	303	VAL
1	N	308	VAL
1	N	309	LEU
1	N	314	LEU
1	N	322	LYS
1	N	333	GLU
1	N	338	LYS
1	N	342	GLN
1	N	343	PRO
1	N	355	ARG
1	N	359	THR
1	N	430	GLU
1	N	443	LEU
2	O	28	LEU

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Mol	Chain	Res	Type
2	P	17	THR
2	P	47	ARG
2	P	48	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	ASN
1	C	286	ASN
1	C	311	GLN
1	C	315	ASN
1	C	325	ASN
1	C	347	GLN
1	C	362	GLN
1	C	384	ASN
1	C	386	GLN
1	C	390	ASN
1	C	419	GLN
1	C	421	ASN
1	C	429	HIS
1	C	434	ASN
1	B	276	ASN
1	B	286	ASN
1	B	295	GLN
1	B	325	ASN
1	B	390	ASN
1	B	421	ASN
1	B	435	HIS
2	E	46	GLN
2	F	24	HIS
2	F	46	GLN
1	A	268	HIS
1	A	286	ASN
1	A	295	GLN
1	A	311	GLN
1	A	315	ASN
1	A	384	ASN
1	A	429	HIS
1	A	438	GLN
1	D	268	HIS
1	D	276	ASN
1	D	295	GLN

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Mol	Chain	Res	Type
1	D	315	ASN
1	D	325	ASN
1	D	390	ASN
1	D	418	GLN
1	D	419	GLN
1	D	438	GLN
2	H	24	HIS
1	I	295	GLN
1	I	311	GLN
1	I	315	ASN
1	I	342	GLN
1	I	384	ASN
1	I	390	ASN
1	I	419	GLN
1	I	429	HIS
1	I	433	HIS
1	J	285	HIS
1	J	286	ASN
1	J	295	GLN
1	J	311	GLN
1	J	384	ASN
1	J	418	GLN
1	J	419	GLN
1	J	438	GLN
2	L	46	GLN
1	M	268	HIS
1	M	285	HIS
1	M	310	HIS
1	M	347	GLN
1	M	384	ASN
1	M	386	GLN
1	M	429	HIS
1	M	434	ASN
1	N	276	ASN
1	N	285	HIS
1	N	295	GLN
1	N	315	ASN
1	N	325	ASN
1	N	347	GLN
1	N	386	GLN
1	N	390	ASN
1	N	421	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

72 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	Q	1	1,3	14,14,15	0.67	0	17,19,21	1.45	3 (17%)
3	NAG	Q	2	3	14,14,15	0.64	0	17,19,21	1.34	2 (11%)
3	BMA	Q	3	3	11,11,12	0.72	0	15,15,17	0.97	0
3	MAN	Q	4	3	11,11,12	0.67	0	15,15,17	1.44	2 (13%)
3	NAG	Q	5	3	14,14,15	0.53	0	17,19,21	1.29	1 (5%)
3	GAL	Q	6	3	11,11,12	0.93	0	15,15,17	2.25	4 (26%)
3	MAN	Q	7	3	11,11,12	0.76	0	15,15,17	1.58	3 (20%)
3	NAG	Q	8	3	14,14,15	0.50	0	17,19,21	2.11	3 (17%)
3	FUC	Q	9	3	10,10,11	0.85	0	14,14,16	1.28	2 (14%)
3	NAG	R	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	1.51	5 (29%)
3	NAG	R	2	3	14,14,15	0.70	0	17,19,21	1.44	3 (17%)
3	BMA	R	3	3	11,11,12	0.85	0	15,15,17	1.57	3 (20%)
3	MAN	R	4	3	11,11,12	0.54	0	15,15,17	1.30	1 (6%)
3	NAG	R	5	3	14,14,15	0.59	0	17,19,21	1.74	3 (17%)
3	GAL	R	6	3	11,11,12	1.01	1 (9%)	15,15,17	1.59	3 (20%)
3	MAN	R	7	3	11,11,12	0.69	0	15,15,17	0.87	0
3	NAG	R	8	3	14,14,15	0.64	0	17,19,21	1.67	3 (17%)
3	FUC	R	9	3	10,10,11	0.93	0	14,14,16	1.22	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	S	1	1,3	14,14,15	0.82	0	17,19,21	1.45	1 (5%)
3	NAG	S	2	3	14,14,15	0.68	0	17,19,21	1.30	3 (17%)
3	BMA	S	3	3	11,11,12	0.47	0	15,15,17	1.66	2 (13%)
3	MAN	S	4	3	11,11,12	0.70	0	15,15,17	2.07	5 (33%)
3	NAG	S	5	3	14,14,15	0.96	0	17,19,21	1.60	3 (17%)
3	GAL	S	6	3	11,11,12	1.18	1 (9%)	15,15,17	1.86	5 (33%)
3	MAN	S	7	3	11,11,12	0.70	0	15,15,17	0.89	0
3	NAG	S	8	3	14,14,15	0.76	0	17,19,21	1.38	3 (17%)
3	FUC	S	9	3	10,10,11	1.03	0	14,14,16	1.54	2 (14%)
3	NAG	T	1	1,3	14,14,15	0.85	0	17,19,21	1.46	4 (23%)
3	NAG	T	2	3	14,14,15	0.74	0	17,19,21	1.83	3 (17%)
3	BMA	T	3	3	11,11,12	1.21	2 (18%)	15,15,17	1.41	3 (20%)
3	MAN	T	4	3	11,11,12	0.81	0	15,15,17	1.66	4 (26%)
3	NAG	T	5	3	14,14,15	0.73	0	17,19,21	1.48	4 (23%)
3	GAL	T	6	3	11,11,12	0.68	0	15,15,17	1.73	3 (20%)
3	MAN	T	7	3	11,11,12	0.70	0	15,15,17	1.04	1 (6%)
3	NAG	T	8	3	14,14,15	0.73	0	17,19,21	1.50	2 (11%)
3	FUC	T	9	3	10,10,11	0.87	0	14,14,16	1.04	1 (7%)
3	NAG	U	1	1,3	14,14,15	0.77	0	17,19,21	1.58	3 (17%)
3	NAG	U	2	3	14,14,15	0.81	0	17,19,21	1.62	3 (17%)
3	BMA	U	3	3	11,11,12	0.74	0	15,15,17	0.92	1 (6%)
3	MAN	U	4	3	11,11,12	0.70	0	15,15,17	1.42	1 (6%)
3	NAG	U	5	3	14,14,15	0.72	0	17,19,21	1.62	3 (17%)
3	GAL	U	6	3	11,11,12	0.97	0	15,15,17	1.58	3 (20%)
3	MAN	U	7	3	11,11,12	0.71	0	15,15,17	1.25	2 (13%)
3	NAG	U	8	3	14,14,15	0.60	0	17,19,21	1.06	1 (5%)
3	FUC	U	9	3	10,10,11	0.77	0	14,14,16	1.18	2 (14%)
3	NAG	V	1	1,3	14,14,15	0.84	0	17,19,21	1.48	3 (17%)
3	NAG	V	2	3	14,14,15	0.68	0	17,19,21	2.05	4 (23%)
3	BMA	V	3	3	11,11,12	0.57	0	15,15,17	1.05	1 (6%)
3	MAN	V	4	3	11,11,12	0.73	0	15,15,17	1.53	4 (26%)
3	NAG	V	5	3	14,14,15	0.66	0	17,19,21	1.70	3 (17%)
3	GAL	V	6	3	11,11,12	0.90	1 (9%)	15,15,17	1.41	2 (13%)
3	MAN	V	7	3	11,11,12	0.68	0	15,15,17	0.77	0
3	NAG	V	8	3	14,14,15	0.61	0	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	V	9	3	10,10,11	0.96	0	14,14,16	1.41	3 (21%)
3	NAG	W	1	1,3	14,14,15	0.53	0	17,19,21	1.28	3 (17%)
3	NAG	W	2	3	14,14,15	0.52	0	17,19,21	1.46	2 (11%)
3	BMA	W	3	3	11,11,12	0.68	0	15,15,17	1.40	1 (6%)
3	MAN	W	4	3	11,11,12	0.92	0	15,15,17	2.38	6 (40%)
3	NAG	W	5	3	14,14,15	0.93	0	17,19,21	1.48	2 (11%)
3	GAL	W	6	3	11,11,12	0.96	1 (9%)	15,15,17	1.46	2 (13%)
3	MAN	W	7	3	11,11,12	0.62	0	15,15,17	1.33	1 (6%)
3	NAG	W	8	3	14,14,15	0.83	0	17,19,21	1.96	3 (17%)
3	FUC	W	9	3	10,10,11	0.99	0	14,14,16	1.68	4 (28%)
3	NAG	X	1	1,3	14,14,15	0.56	0	17,19,21	1.38	2 (11%)
3	NAG	X	2	3	14,14,15	0.72	0	17,19,21	1.35	3 (17%)
3	BMA	X	3	3	11,11,12	0.67	0	15,15,17	0.69	0
3	MAN	X	4	3	11,11,12	0.70	0	15,15,17	1.39	2 (13%)
3	NAG	X	5	3	14,14,15	0.92	1 (7%)	17,19,21	1.28	2 (11%)
3	GAL	X	6	3	11,11,12	1.05	1 (9%)	15,15,17	1.53	4 (26%)
3	MAN	X	7	3	11,11,12	0.74	0	15,15,17	1.21	2 (13%)
3	NAG	X	8	3	14,14,15	0.50	0	17,19,21	0.90	0
3	FUC	X	9	3	10,10,11	0.76	0	14,14,16	0.99	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
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	5	3	-	4/6/23/26	0/1/1/1
3	GAL	Q	6	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	7	3	-	1/2/19/22	0/1/1/1
3	NAG	Q	8	3	-	4/6/23/26	0/1/1/1
3	FUC	Q	9	3	-	-	0/1/1/1
3	NAG	R	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	MAN	R	4	3	-	1/2/19/22	0/1/1/1
3	NAG	R	5	3	-	4/6/23/26	0/1/1/1
3	GAL	R	6	3	-	2/2/19/22	0/1/1/1
3	MAN	R	7	3	-	1/2/19/22	0/1/1/1
3	NAG	R	8	3	-	4/6/23/26	0/1/1/1
3	FUC	R	9	3	-	-	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
3	MAN	S	4	3	-	2/2/19/22	0/1/1/1
3	NAG	S	5	3	-	2/6/23/26	0/1/1/1
3	GAL	S	6	3	-	2/2/19/22	0/1/1/1
3	MAN	S	7	3	-	2/2/19/22	0/1/1/1
3	NAG	S	8	3	-	2/6/23/26	0/1/1/1
3	FUC	S	9	3	-	-	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	MAN	T	4	3	-	0/2/19/22	0/1/1/1
3	NAG	T	5	3	-	2/6/23/26	0/1/1/1
3	GAL	T	6	3	-	0/2/19/22	0/1/1/1
3	MAN	T	7	3	-	0/2/19/22	0/1/1/1
3	NAG	T	8	3	-	0/6/23/26	0/1/1/1
3	FUC	T	9	3	-	-	0/1/1/1
3	NAG	U	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1
3	MAN	U	4	3	-	2/2/19/22	0/1/1/1
3	NAG	U	5	3	-	2/6/23/26	0/1/1/1
3	GAL	U	6	3	-	2/2/19/22	0/1/1/1
3	MAN	U	7	3	-	2/2/19/22	0/1/1/1
3	NAG	U	8	3	-	4/6/23/26	0/1/1/1
3	FUC	U	9	3	-	-	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	V	4	3	-	1/2/19/22	0/1/1/1
3	NAG	V	5	3	-	3/6/23/26	0/1/1/1
3	GAL	V	6	3	-	0/2/19/22	0/1/1/1
3	MAN	V	7	3	-	2/2/19/22	0/1/1/1
3	NAG	V	8	3	-	3/6/23/26	0/1/1/1
3	FUC	V	9	3	-	-	0/1/1/1
3	NAG	W	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	MAN	W	4	3	-	1/2/19/22	0/1/1/1
3	NAG	W	5	3	-	0/6/23/26	0/1/1/1
3	GAL	W	6	3	-	2/2/19/22	0/1/1/1
3	MAN	W	7	3	-	0/2/19/22	0/1/1/1
3	NAG	W	8	3	-	4/6/23/26	0/1/1/1
3	FUC	W	9	3	-	-	0/1/1/1
3	NAG	X	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	X	2	3	-	5/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	MAN	X	4	3	-	2/2/19/22	0/1/1/1
3	NAG	X	5	3	-	4/6/23/26	0/1/1/1
3	GAL	X	6	3	-	2/2/19/22	0/1/1/1
3	MAN	X	7	3	-	2/2/19/22	0/1/1/1
3	NAG	X	8	3	-	2/6/23/26	0/1/1/1
3	FUC	X	9	3	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	C1-C2	2.50	1.55	1.52
3	S	6	GAL	C2-C3	2.46	1.56	1.52
3	T	3	BMA	C2-C3	-2.27	1.49	1.52
3	X	6	GAL	C4-C5	2.18	1.57	1.53
3	X	5	NAG	O5-C1	-2.16	1.40	1.43
3	W	6	GAL	C2-C3	2.15	1.55	1.52
3	V	6	GAL	C2-C3	2.13	1.55	1.52
3	R	6	GAL	C2-C3	2.07	1.55	1.52
3	T	3	BMA	O5-C5	-2.03	1.39	1.43

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	6	GAL	C1-O5-C5	6.56	120.98	112.19
3	W	8	NAG	C1-O5-C5	6.29	120.62	112.19
3	W	4	MAN	C1-O5-C5	-6.28	103.77	112.19
3	V	2	NAG	C2-N2-C7	-5.91	114.98	122.90
3	Q	8	NAG	C1-O5-C5	5.45	119.49	112.19
3	S	4	MAN	C1-O5-C5	5.15	119.09	112.19
3	V	5	NAG	C1-O5-C5	-5.08	105.38	112.19
3	S	3	BMA	C1-O5-C5	5.03	118.93	112.19
3	T	2	NAG	C1-O5-C5	4.79	118.60	112.19
3	U	2	NAG	C1-O5-C5	4.64	118.40	112.19
3	S	1	NAG	O5-C1-C2	-4.42	104.45	111.29
3	T	6	GAL	C1-O5-C5	4.29	117.94	112.19
3	U	1	NAG	C2-N2-C7	-4.26	117.20	122.90
3	T	4	MAN	C1-O5-C5	4.22	117.84	112.19
3	Q	5	NAG	C1-O5-C5	4.19	117.81	112.19
3	T	8	NAG	C2-N2-C7	-4.18	117.30	122.90
3	Q	7	MAN	C1-O5-C5	4.10	117.67	112.19
3	W	7	MAN	C1-O5-C5	4.07	117.64	112.19
3	W	2	NAG	C1-O5-C5	3.97	117.50	112.19
3	Q	8	NAG	C3-C4-C5	-3.97	103.04	110.23
3	R	5	NAG	C2-N2-C7	-3.96	117.59	122.90
3	R	5	NAG	C4-C3-C2	-3.94	105.24	111.02
3	W	4	MAN	C6-C5-C4	3.88	122.55	113.02
3	U	5	NAG	C1-O5-C5	3.88	117.39	112.19
3	R	3	BMA	C1-C2-C3	3.86	115.26	109.64
3	W	3	BMA	C1-O5-C5	3.67	117.11	112.19
3	Q	8	NAG	C4-C3-C2	-3.61	105.72	111.02
3	R	6	GAL	C1-O5-C5	3.56	116.96	112.19
3	S	5	NAG	C4-C3-C2	-3.55	105.82	111.02
3	U	6	GAL	O5-C5-C6	3.53	114.53	107.66
3	S	6	GAL	C1-C2-C3	3.51	114.75	109.64
3	X	1	NAG	C1-O5-C5	3.41	116.75	112.19
3	Q	1	NAG	C2-N2-C7	3.38	127.43	122.90
3	X	4	MAN	O3-C3-C2	-3.35	103.22	110.05
3	R	4	MAN	C1-O5-C5	3.34	116.67	112.19
3	R	8	NAG	C2-N2-C7	-3.33	118.44	122.90
3	T	2	NAG	C2-N2-C7	3.32	127.35	122.90
3	W	6	GAL	C1-C2-C3	3.32	114.48	109.64
3	S	5	NAG	C2-N2-C7	-3.32	118.45	122.90
3	X	2	NAG	C8-C7-N2	3.29	121.57	116.12
3	R	2	NAG	C4-C3-C2	-3.28	106.20	111.02
3	S	4	MAN	O4-C4-C5	3.27	117.38	109.32
3	Q	4	MAN	C3-C4-C5	-3.25	104.34	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	2	NAG	C1-O5-C5	3.25	116.54	112.19
3	R	8	NAG	C1-O5-C5	3.22	116.50	112.19
3	V	2	NAG	O5-C1-C2	-3.19	106.36	111.29
3	U	4	MAN	O4-C4-C5	3.15	117.09	109.32
3	R	8	NAG	C4-C3-C2	-3.15	106.40	111.02
3	V	6	GAL	C1-O5-C5	3.13	116.38	112.19
3	S	9	FUC	C6-C5-C4	3.08	118.72	113.08
3	W	9	FUC	C3-C4-C5	3.06	114.46	109.81
3	W	5	NAG	O5-C1-C2	-3.02	106.62	111.29
3	X	5	NAG	C2-N2-C7	-3.01	118.86	122.90
3	U	1	NAG	O5-C1-C2	-3.01	106.64	111.29
3	V	5	NAG	C2-N2-C7	-3.00	118.88	122.90
3	W	5	NAG	C2-N2-C7	-2.98	118.90	122.90
3	Q	2	NAG	O5-C5-C6	2.96	113.43	107.66
3	V	6	GAL	C1-C2-C3	2.96	113.95	109.64
3	R	5	NAG	O5-C1-C2	-2.95	106.73	111.29
3	R	1	NAG	C3-C4-C5	-2.91	104.95	110.23
3	T	5	NAG	C1-O5-C5	2.89	116.06	112.19
3	R	3	BMA	C2-C3-C4	2.86	115.89	110.86
3	Q	1	NAG	C3-C4-C5	-2.86	105.05	110.23
3	T	1	NAG	C1-O5-C5	2.85	116.01	112.19
3	U	9	FUC	O5-C5-C6	2.85	113.58	107.40
3	Q	2	NAG	C1-O5-C5	2.84	115.99	112.19
3	Q	6	GAL	O5-C1-C2	2.81	117.49	110.79
3	R	9	FUC	O5-C5-C6	2.80	113.47	107.40
3	S	8	NAG	C2-N2-C7	2.79	126.64	122.90
3	W	9	FUC	O5-C5-C6	2.75	113.38	107.40
3	V	4	MAN	O2-C2-C3	-2.75	104.46	110.15
3	V	8	NAG	C1-O5-C5	2.75	115.86	112.19
3	Q	7	MAN	O5-C1-C2	2.74	117.33	110.79
3	V	2	NAG	C1-O5-C5	2.73	115.85	112.19
3	X	6	GAL	C1-O5-C5	2.73	115.85	112.19
3	T	4	MAN	C3-C4-C5	-2.73	105.28	110.23
3	S	4	MAN	O3-C3-C4	-2.72	103.96	110.38
3	S	5	NAG	O4-C4-C5	2.70	115.97	109.32
3	T	5	NAG	O5-C1-C2	-2.69	107.13	111.29
3	V	9	FUC	O4-C4-C5	2.68	115.64	109.74
3	U	5	NAG	O5-C5-C6	2.68	112.87	107.66
3	U	2	NAG	C1-C2-N2	2.67	114.65	110.43
3	T	3	BMA	O2-C2-C3	-2.66	104.64	110.15
3	W	6	GAL	O5-C5-C6	2.65	112.81	107.66
3	V	1	NAG	O3-C3-C2	-2.63	103.93	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	4	MAN	C2-C3-C4	-2.63	106.23	110.86
3	S	8	NAG	C3-C4-C5	2.61	114.97	110.23
3	R	1	NAG	C1-C2-N2	2.60	114.53	110.43
3	U	9	FUC	C3-C4-C5	2.59	113.76	109.81
3	T	1	NAG	O5-C1-C2	-2.59	107.29	111.29
3	U	6	GAL	O5-C5-C4	-2.58	104.55	110.83
3	T	3	BMA	C1-O5-C5	2.57	115.63	112.19
3	S	4	MAN	O4-C4-C3	-2.56	104.34	110.38
3	R	6	GAL	O4-C4-C5	2.55	115.61	109.32
3	S	8	NAG	C4-C3-C2	2.55	114.75	111.02
3	Q	1	NAG	C1-C2-N2	-2.55	106.42	110.43
3	X	6	GAL	C3-C4-C5	2.54	114.84	110.23
3	Q	4	MAN	O3-C3-C2	-2.52	104.91	110.05
3	T	7	MAN	O6-C6-C5	-2.52	102.76	111.33
3	T	6	GAL	C3-C4-C5	2.50	114.76	110.23
3	W	1	NAG	C8-C7-N2	2.48	120.24	116.12
3	T	4	MAN	O3-C3-C2	2.48	115.11	110.05
3	W	1	NAG	O3-C3-C2	-2.47	104.27	109.40
3	X	2	NAG	O7-C7-N2	-2.47	117.62	121.98
3	V	4	MAN	O2-C2-C1	2.45	114.83	109.22
3	S	6	GAL	C3-C4-C5	2.45	114.67	110.23
3	Q	7	MAN	C1-C2-C3	2.44	113.20	109.64
3	V	3	BMA	C1-O5-C5	2.44	115.46	112.19
3	S	2	NAG	O5-C1-C2	-2.44	107.52	111.29
3	T	9	FUC	O5-C5-C6	2.44	112.69	107.40
3	S	6	GAL	O4-C4-C3	2.43	116.11	110.38
3	U	6	GAL	C1-C2-C3	2.43	113.18	109.64
3	W	9	FUC	C1-O5-C5	2.43	118.69	112.97
3	Q	6	GAL	C1-C2-C3	2.41	113.16	109.64
3	W	8	NAG	C2-N2-C7	2.41	126.13	122.90
3	V	4	MAN	O6-C6-C5	-2.39	103.19	111.33
3	U	1	NAG	C1-C2-N2	2.38	114.18	110.43
3	U	8	NAG	C4-C3-C2	-2.37	107.55	111.02
3	W	1	NAG	C3-C4-C5	-2.36	105.95	110.23
3	S	9	FUC	C2-C3-C4	-2.35	106.73	110.86
3	T	5	NAG	C2-N2-C7	-2.35	119.75	122.90
3	T	2	NAG	C4-C3-C2	-2.34	107.58	111.02
3	S	6	GAL	O3-C3-C2	2.34	114.83	110.05
3	Q	9	FUC	C3-C4-C5	2.34	113.36	109.81
3	S	2	NAG	O3-C3-C4	-2.33	104.89	110.38
3	V	5	NAG	O5-C5-C6	2.31	112.17	107.66
3	T	3	BMA	O3-C3-C2	-2.31	105.34	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	2	NAG	O5-C1-C2	-2.30	107.73	111.29
3	U	5	NAG	O7-C7-N2	-2.30	117.92	121.98
3	W	9	FUC	O5-C5-C4	2.28	113.66	109.55
3	R	1	NAG	C1-O5-C5	-2.26	109.16	112.19
3	W	4	MAN	O4-C4-C3	-2.25	105.07	110.38
3	T	6	GAL	C1-C2-C3	2.24	112.90	109.64
3	R	1	NAG	O5-C1-C2	-2.24	107.83	111.29
3	X	7	MAN	C1-O5-C5	-2.22	109.21	112.19
3	V	9	FUC	C1-O5-C5	2.21	118.19	112.97
3	V	2	NAG	C1-C2-N2	2.21	113.92	110.43
3	V	1	NAG	C8-C7-N2	2.21	119.78	116.12
3	X	9	FUC	O4-C4-C5	2.20	114.60	109.74
3	W	8	NAG	O7-C7-C8	-2.19	118.15	122.05
3	R	6	GAL	O4-C4-C3	-2.18	105.23	110.38
3	R	1	NAG	O5-C5-C6	2.18	111.90	107.66
3	V	1	NAG	O7-C7-N2	-2.17	118.14	121.98
3	W	4	MAN	C3-C4-C5	-2.17	106.30	110.23
3	R	9	FUC	C3-C4-C5	2.16	113.10	109.81
3	X	1	NAG	O5-C5-C6	2.16	111.87	107.66
3	R	2	NAG	O5-C1-C2	-2.16	107.95	111.29
3	S	3	BMA	C6-C5-C4	-2.16	107.72	113.02
3	X	7	MAN	O3-C3-C4	2.15	115.45	110.38
3	Q	9	FUC	C1-C2-C3	-2.15	106.51	109.64
3	U	3	BMA	O4-C4-C3	-2.15	105.31	110.38
3	T	4	MAN	C1-C2-C3	-2.15	106.52	109.64
3	W	4	MAN	O5-C1-C2	-2.14	105.68	110.79
3	X	6	GAL	C2-C3-C4	2.13	114.61	110.86
3	Q	6	GAL	C3-C4-C5	2.12	114.08	110.23
3	X	5	NAG	C6-C5-C4	-2.11	107.83	113.02
3	X	6	GAL	O4-C4-C5	2.11	114.51	109.32
3	R	3	BMA	O5-C5-C6	2.10	111.74	107.66
3	X	2	NAG	O5-C1-C2	-2.10	108.05	111.29
3	U	7	MAN	O5-C5-C6	2.10	111.74	107.66
3	T	5	NAG	O4-C4-C5	-2.08	104.19	109.32
3	U	2	NAG	O7-C7-C8	-2.04	118.41	122.05
3	U	7	MAN	C1-C2-C3	2.04	112.62	109.64
3	W	4	MAN	O6-C6-C5	-2.04	104.38	111.33
3	S	6	GAL	O5-C5-C6	2.04	111.63	107.66
3	S	4	MAN	O2-C2-C1	2.04	113.89	109.22
3	S	2	NAG	C1-O5-C5	2.03	114.91	112.19
3	T	8	NAG	C1-O5-C5	2.03	114.91	112.19
3	T	1	NAG	O7-C7-C8	-2.01	118.47	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	4	MAN	O3-C3-C4	2.01	115.12	110.38
3	T	1	NAG	O6-C6-C5	2.01	118.18	111.33
3	V	9	FUC	O5-C5-C4	2.00	113.16	109.55

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	5	NAG	C8-C7-N2-C2
3	Q	5	NAG	O7-C7-N2-C2
3	Q	8	NAG	C8-C7-N2-C2
3	Q	8	NAG	O7-C7-N2-C2
3	R	5	NAG	C8-C7-N2-C2
3	R	5	NAG	O7-C7-N2-C2
3	R	8	NAG	C8-C7-N2-C2
3	R	8	NAG	O7-C7-N2-C2
3	S	8	NAG	C8-C7-N2-C2
3	S	8	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	U	8	NAG	C8-C7-N2-C2
3	U	8	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	V	8	NAG	C8-C7-N2-C2
3	V	8	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	W	8	NAG	C8-C7-N2-C2
3	W	8	NAG	O7-C7-N2-C2
3	X	1	NAG	C8-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2
3	X	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	X	5	NAG	C8-C7-N2-C2
3	X	5	NAG	O7-C7-N2-C2
3	X	8	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	X	8	NAG	O7-C7-N2-C2
3	R	5	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	X	5	NAG	O5-C5-C6-O6
3	W	8	NAG	C4-C5-C6-O6
3	S	7	MAN	O5-C5-C6-O6
3	R	6	GAL	O5-C5-C6-O6
3	S	4	MAN	O5-C5-C6-O6
3	U	6	GAL	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	W	6	GAL	O5-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
3	X	6	GAL	C4-C5-C6-O6
3	R	5	NAG	C4-C5-C6-O6
3	S	7	MAN	C4-C5-C6-O6
3	X	5	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	Q	6	GAL	C4-C5-C6-O6
3	W	8	NAG	O5-C5-C6-O6
3	X	6	GAL	O5-C5-C6-O6
3	U	6	GAL	C4-C5-C6-O6
3	Q	4	MAN	O5-C5-C6-O6
3	W	6	GAL	C4-C5-C6-O6
3	R	2	NAG	C8-C7-N2-C2
3	R	6	GAL	C4-C5-C6-O6
3	S	4	MAN	C4-C5-C6-O6
3	S	6	GAL	O5-C5-C6-O6
3	X	4	MAN	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	R	8	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	Q	5	NAG	C4-C5-C6-O6
3	R	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C4-C5-C6-O6
3	Q	5	NAG	O5-C5-C6-O6
3	U	7	MAN	O5-C5-C6-O6
3	U	7	MAN	C4-C5-C6-O6
3	U	8	NAG	O5-C5-C6-O6
3	Q	6	GAL	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6

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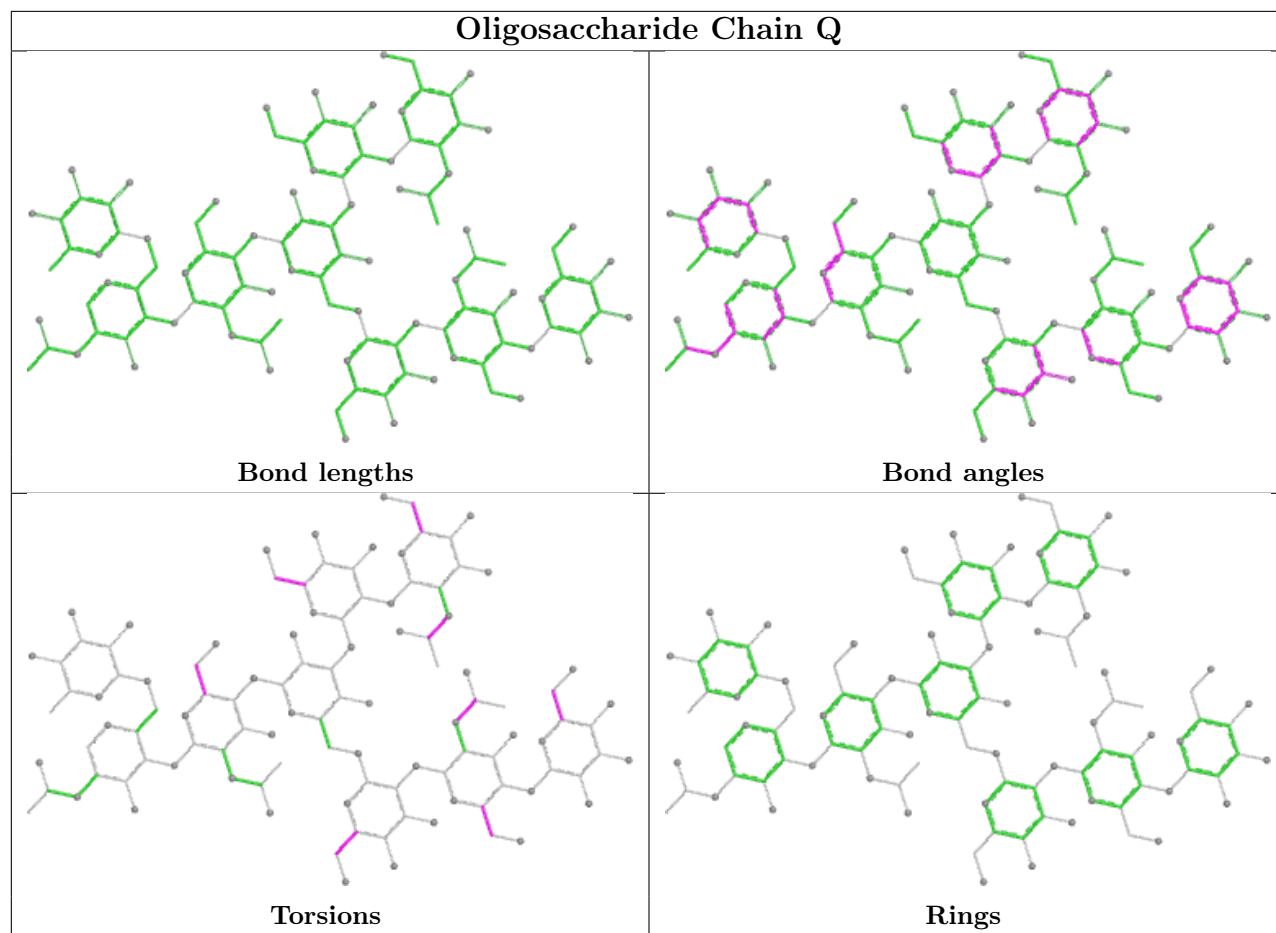
Mol	Chain	Res	Type	Atoms
3	T	2	NAG	C4-C5-C6-O6
3	S	6	GAL	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	U	5	NAG	O5-C5-C6-O6
3	U	4	MAN	O5-C5-C6-O6
3	Q	7	MAN	O5-C5-C6-O6
3	V	5	NAG	C8-C7-N2-C2
3	U	5	NAG	C4-C5-C6-O6
3	V	7	MAN	C4-C5-C6-O6
3	S	5	NAG	C4-C5-C6-O6
3	X	7	MAN	C4-C5-C6-O6
3	T	5	NAG	C8-C7-N2-C2
3	R	8	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	Q	8	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	S	5	NAG	O5-C5-C6-O6
3	X	4	MAN	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	V	3	BMA	C4-C5-C6-O6
3	Q	8	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	R	7	MAN	O5-C5-C6-O6
3	V	5	NAG	O7-C7-N2-C2
3	X	7	MAN	O5-C5-C6-O6
3	R	4	MAN	C4-C5-C6-O6
3	U	8	NAG	C4-C5-C6-O6
3	T	5	NAG	O7-C7-N2-C2
3	T	2	NAG	O5-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	V	5	NAG	C4-C5-C6-O6
3	U	4	MAN	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C1-C2-N2-C7
3	V	7	MAN	O5-C5-C6-O6
3	V	4	MAN	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	W	4	MAN	C4-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
3	V	8	NAG	O5-C5-C6-O6

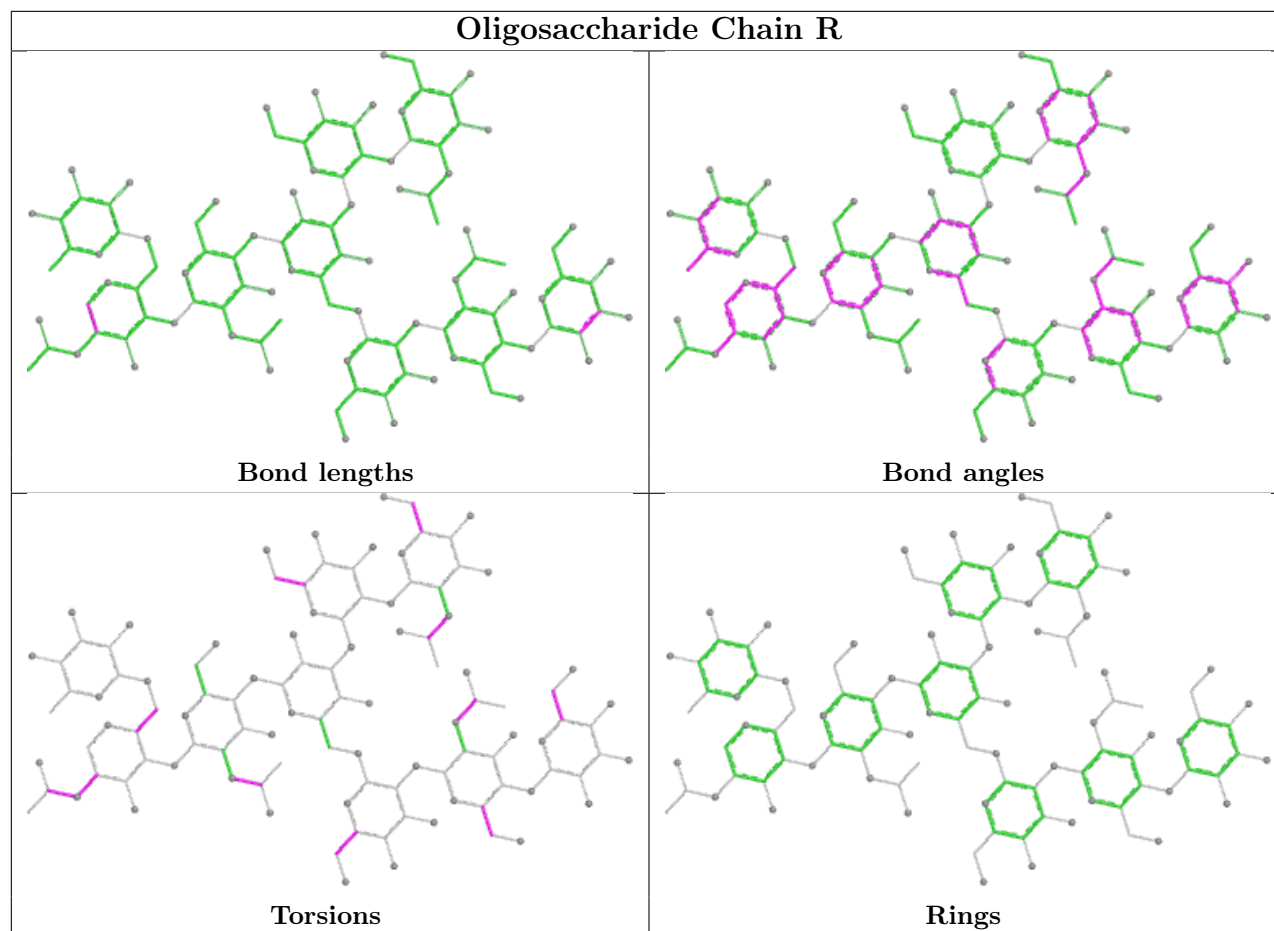
There are no ring outliers.

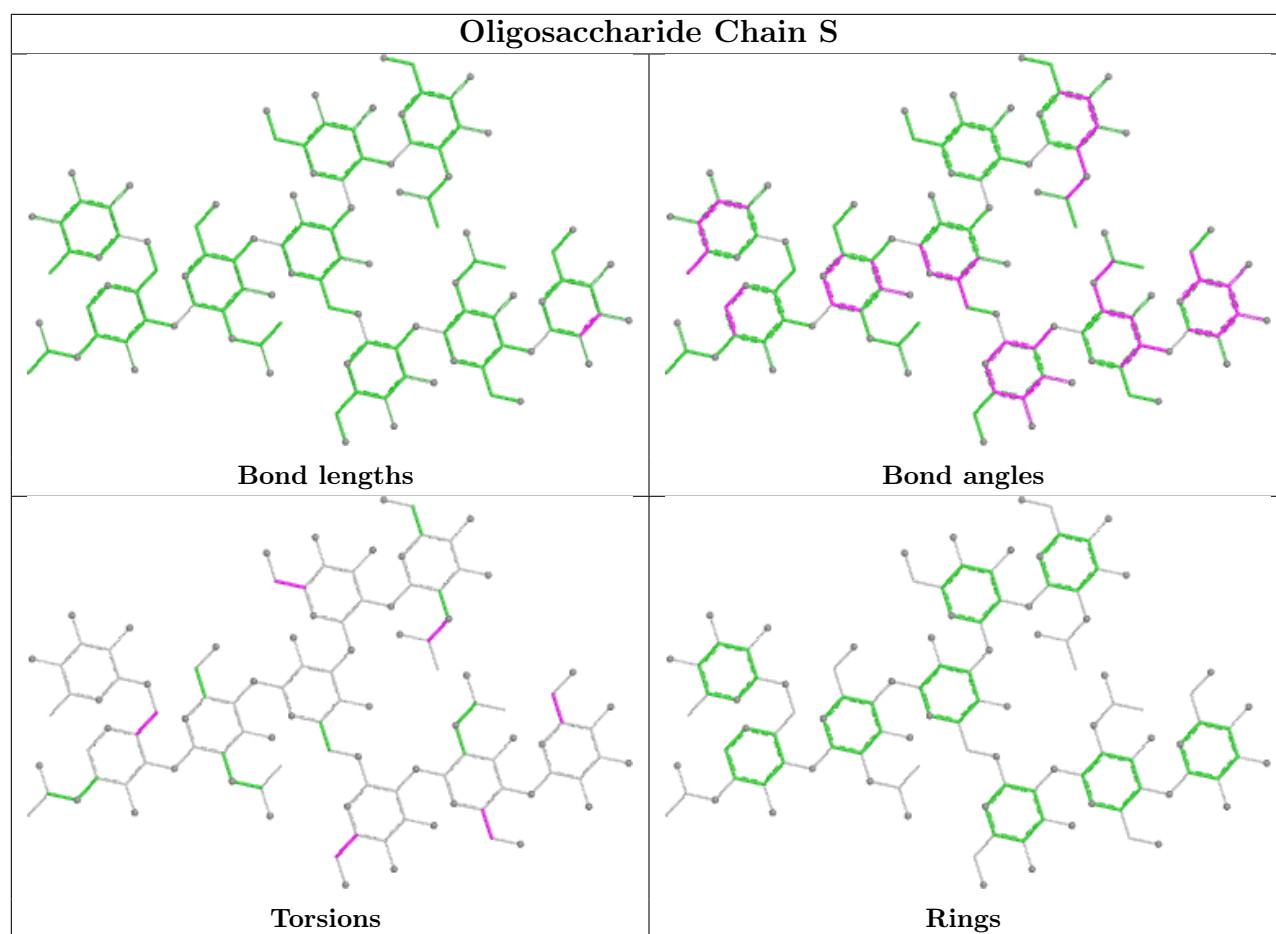
20 monomers are involved in 31 short contacts:

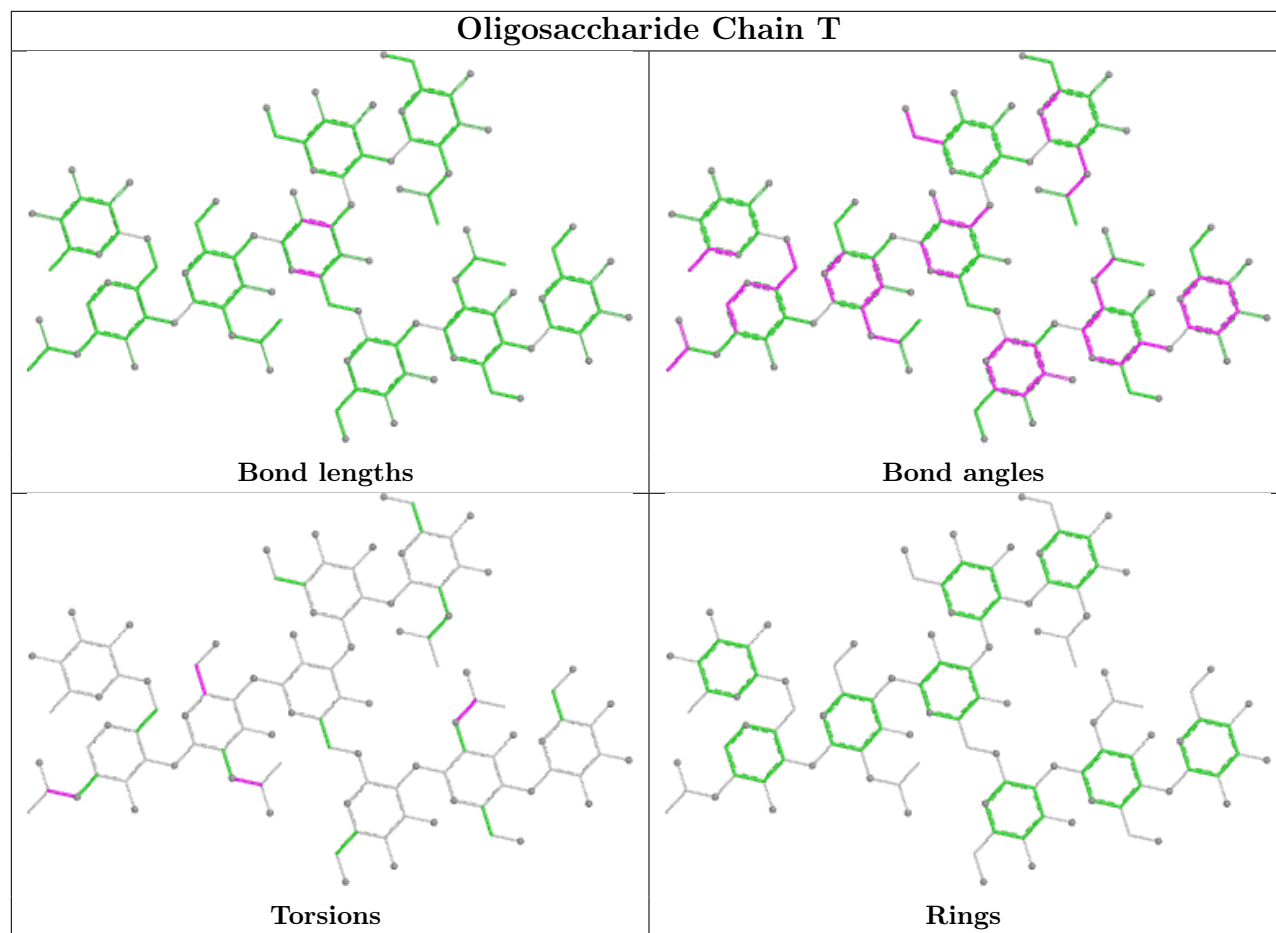
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	NAG	1	0
3	U	6	GAL	1	0
3	W	8	NAG	2	0
3	R	3	BMA	3	0
3	X	5	NAG	1	0
3	U	1	NAG	1	0
3	R	6	GAL	2	0
3	T	2	NAG	4	0
3	W	1	NAG	1	0
3	X	8	NAG	2	0
3	X	1	NAG	3	0
3	X	2	NAG	4	0
3	W	6	GAL	1	0
3	W	5	NAG	1	0
3	V	1	NAG	3	0
3	T	1	NAG	2	0
3	W	9	FUC	1	0
3	X	9	FUC	2	0
3	V	2	NAG	2	0
3	R	7	MAN	1	0

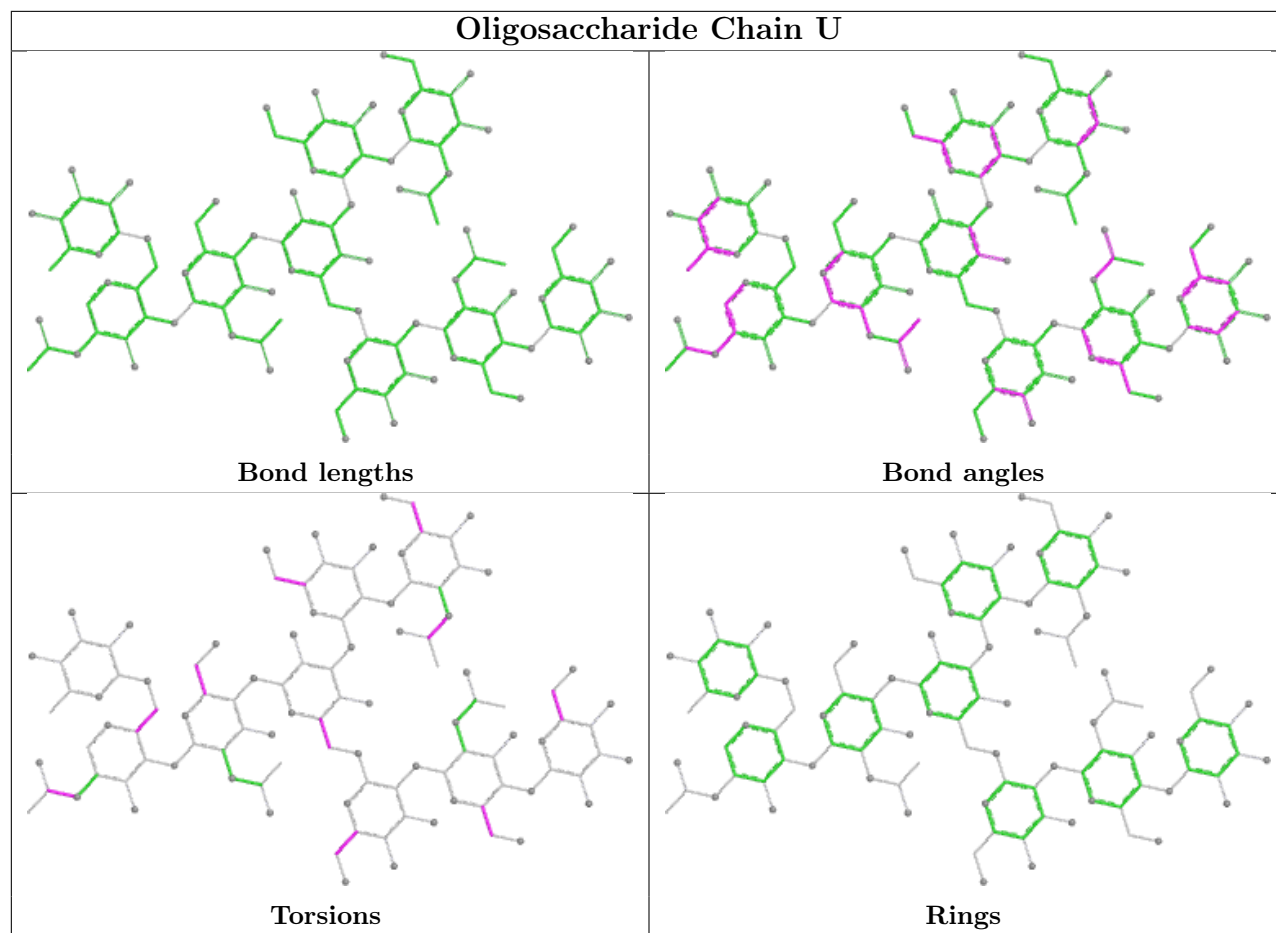
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

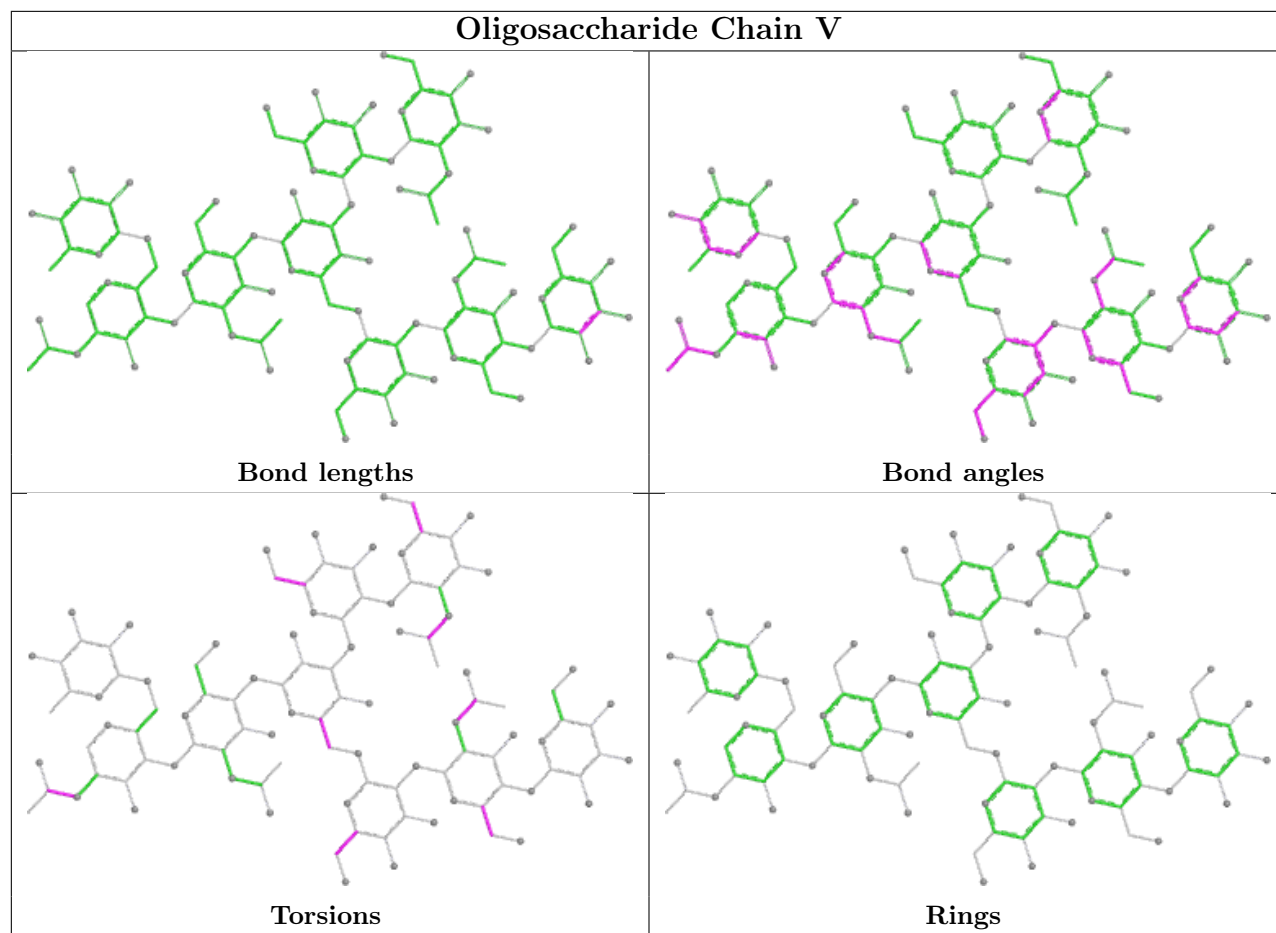


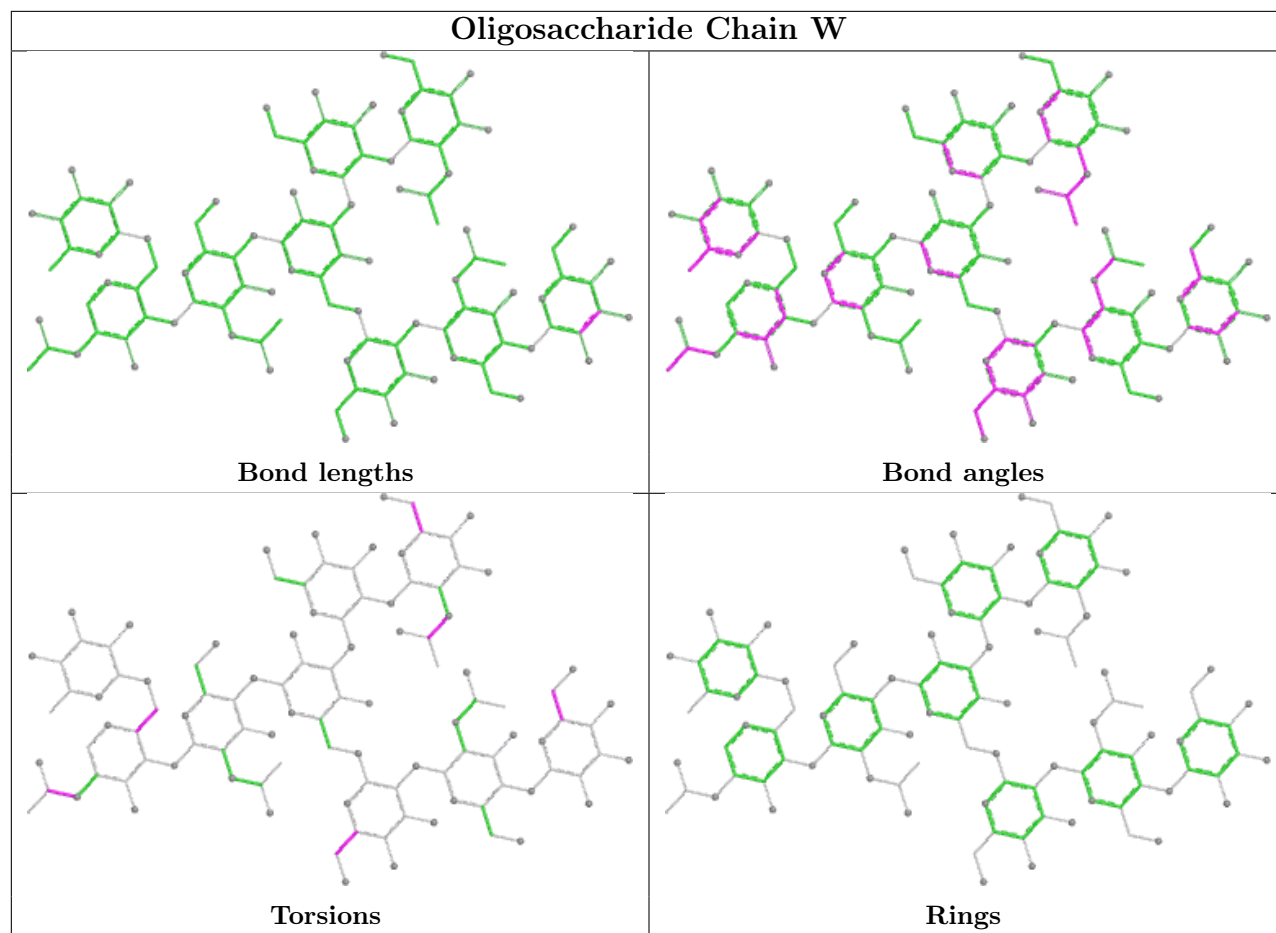


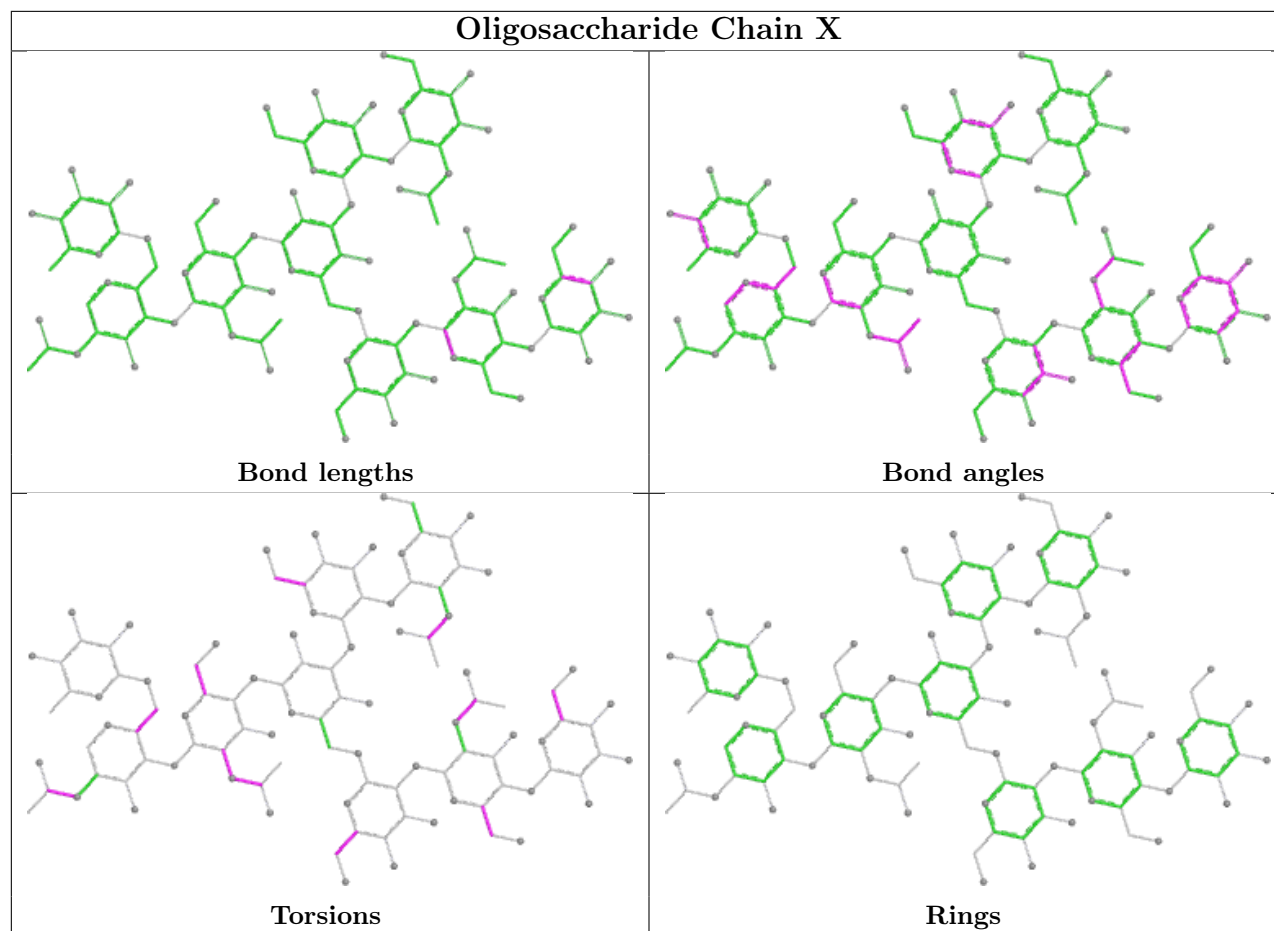












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/212 (98%)	-0.58	3 (1%) 73 65	20, 38, 61, 69	7 (3%)
1	B	210/212 (99%)	-0.54	2 (0%) 79 73	21, 40, 69, 77	7 (3%)
1	C	209/212 (98%)	-0.55	2 (0%) 79 73	16, 39, 66, 74	7 (3%)
1	D	209/212 (98%)	-0.53	3 (1%) 73 65	24, 43, 57, 67	7 (3%)
1	I	209/212 (98%)	-0.49	2 (0%) 79 73	20, 39, 66, 79	7 (3%)
1	J	209/212 (98%)	-0.21	2 (0%) 79 73	22, 45, 86, 94	4 (1%)
1	M	209/212 (98%)	-0.51	2 (0%) 79 73	21, 44, 59, 64	7 (3%)
1	N	210/212 (99%)	-0.04	5 (2%) 59 50	27, 58, 104, 108	7 (3%)
2	E	29/54 (53%)	0.06	1 (3%) 48 39	36, 64, 96, 101	0
2	F	46/54 (85%)	0.33	3 (6%) 25 20	36, 62, 98, 101	0
2	G	47/54 (87%)	-0.14	2 (4%) 40 31	28, 50, 88, 100	0
2	H	32/54 (59%)	0.30	1 (3%) 51 42	55, 82, 98, 102	0
2	K	46/54 (85%)	-0.30	0 100 100	25, 47, 80, 82	0
2	L	47/54 (87%)	-0.27	0 100 100	31, 47, 74, 87	0
2	O	46/54 (85%)	-0.33	0 100 100	44, 53, 74, 84	0
2	P	43/54 (79%)	0.23	0 100 100	43, 75, 108, 114	0
All	All	2010/2128 (94%)	-0.36	28 (1%) 73 65	16, 44, 88, 114	53 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	288	LYS	5.3
1	C	269	GLU	5.1
1	I	389	ASN	5.1
1	I	269	GLU	4.7
1	A	269	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	288	LYS	4.5
2	F	17	THR	4.3
1	A	389	ASN	4.2
1	C	389	ASN	3.3
1	N	284	VAL	3.2
1	N	326	LYS	3.1
2	F	16	GLY	3.1
1	M	269	GLU	3.1
1	N	360	LYS	3.0
1	M	389	ASN	2.8
2	F	15	THR	2.8
1	D	236	GLY	2.7
1	J	360	LYS	2.6
2	H	50	GLY	2.6
2	E	38	THR	2.5
1	B	360	LYS	2.5
2	G	4	PHE	2.3
1	N	314	LEU	2.2
1	D	288	LYS	2.1
1	A	236	GLY	2.1
2	G	9	GLY	2.1
1	J	280	ASP	2.1
1	D	360	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	R	8	14/15	0.54	0.14	103,108,110,111	0
3	NAG	W	8	14/15	0.58	0.13	102,106,108,108	0
3	NAG	X	8	14/15	0.59	0.12	106,108,109,110	0
3	FUC	S	9	10/11	0.62	0.16	82,87,89,89	0
3	NAG	S	8	14/15	0.69	0.10	78,89,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	R	9	10/11	0.70	0.17	94,97,99,102	0
3	NAG	Q	8	14/15	0.74	0.11	97,100,102,105	0
3	NAG	V	8	14/15	0.74	0.09	107,111,113,113	0
3	FUC	X	9	10/11	0.76	0.14	103,106,108,108	0
3	FUC	T	9	10/11	0.79	0.12	79,85,86,86	0
3	NAG	U	8	14/15	0.81	0.09	89,94,95,95	0
3	MAN	X	7	11/12	0.81	0.09	97,100,101,104	0
3	NAG	X	1	14/15	0.82	0.12	94,98,100,101	0
3	MAN	V	7	11/12	0.82	0.08	97,101,104,107	0
3	GAL	X	6	11/12	0.83	0.14	74,79,81,82	0
3	MAN	Q	4	11/12	0.83	0.11	74,77,84,86	0
3	GAL	R	6	11/12	0.83	0.16	80,86,88,88	0
3	MAN	Q	7	11/12	0.83	0.09	90,92,93,95	0
3	GAL	W	6	11/12	0.84	0.13	75,79,81,82	0
3	NAG	T	8	14/15	0.85	0.10	72,81,86,89	0
3	FUC	U	9	10/11	0.85	0.13	75,79,81,83	0
3	GAL	V	6	11/12	0.85	0.15	88,92,93,93	0
3	FUC	Q	9	10/11	0.85	0.12	80,84,88,90	0
3	FUC	V	9	10/11	0.86	0.12	86,89,91,92	0
3	GAL	S	6	11/12	0.86	0.14	53,58,62,63	0
3	BMA	V	3	11/12	0.87	0.07	72,82,85,92	0
3	NAG	X	2	14/15	0.87	0.10	83,89,91,92	0
3	MAN	R	4	11/12	0.88	0.09	80,82,85,88	0
3	GAL	T	6	11/12	0.88	0.11	66,70,72,75	0
3	NAG	V	1	14/15	0.88	0.09	66,69,72,77	0
3	MAN	U	7	11/12	0.88	0.07	71,74,77,83	0
3	NAG	Q	5	14/15	0.89	0.09	64,74,79,80	0
3	NAG	R	1	14/15	0.89	0.12	68,72,77,81	0
3	BMA	R	3	11/12	0.89	0.09	71,74,77,78	0
3	MAN	W	7	11/12	0.89	0.07	78,83,84,90	0
3	GAL	Q	6	11/12	0.89	0.11	66,69,72,72	0
3	FUC	W	9	10/11	0.89	0.09	77,79,82,82	0
3	GAL	U	6	11/12	0.90	0.12	50,57,59,61	0
3	BMA	X	3	11/12	0.90	0.07	79,86,89,93	0
3	MAN	R	7	11/12	0.91	0.08	84,86,88,95	0
3	NAG	V	2	14/15	0.91	0.08	62,70,74,74	0
3	NAG	S	1	14/15	0.91	0.08	54,58,68,69	0
3	BMA	W	3	11/12	0.91	0.08	53,57,59,62	0
3	NAG	R	5	14/15	0.91	0.10	78,81,91,94	0
3	BMA	Q	3	11/12	0.92	0.08	68,71,74,79	0
3	MAN	X	4	11/12	0.92	0.07	65,67,70,71	0
3	BMA	U	3	11/12	0.92	0.07	62,63,64,68	0

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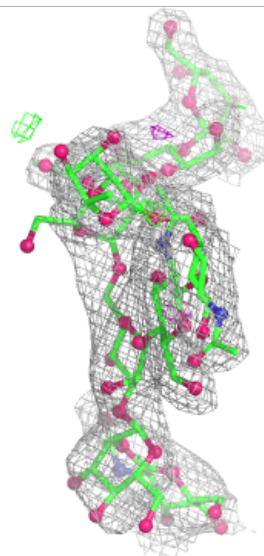
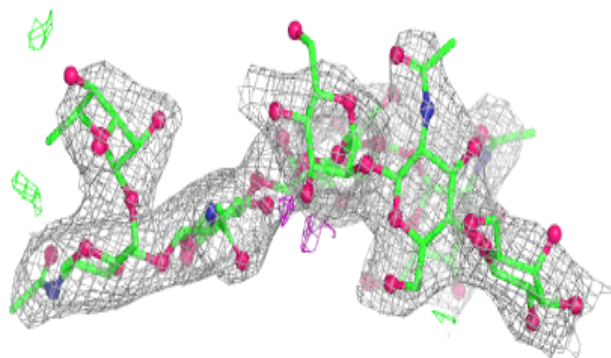
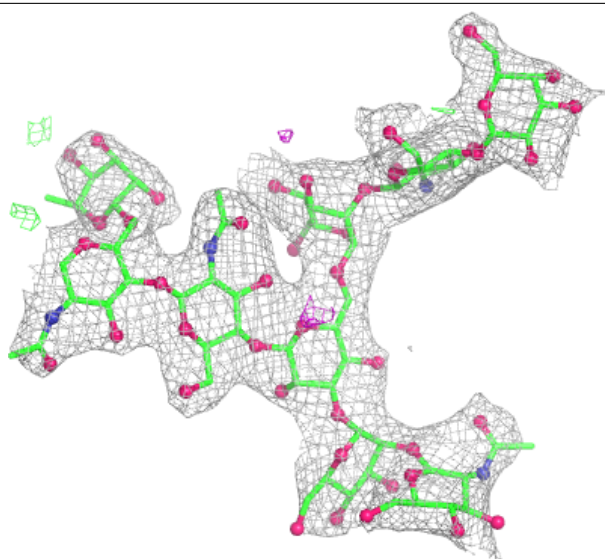
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	U	4	11/12	0.93	0.07	49,50,53,54	0
3	MAN	V	4	11/12	0.93	0.07	65,68,69,70	0
3	NAG	U	5	14/15	0.93	0.07	47,51,52,54	0
3	MAN	T	4	11/12	0.93	0.07	40,45,48,49	0
3	NAG	S	5	14/15	0.93	0.08	40,44,48,51	0
3	NAG	R	2	14/15	0.93	0.08	61,64,67,67	0
3	NAG	X	5	14/15	0.93	0.07	68,69,74,74	0
3	NAG	Q	1	14/15	0.93	0.08	62,64,67,74	0
3	MAN	W	4	11/12	0.93	0.08	54,56,62,63	0
3	NAG	U	1	14/15	0.93	0.08	64,66,70,70	0
3	NAG	Q	2	14/15	0.93	0.08	56,63,65,67	0
3	NAG	W	1	14/15	0.94	0.06	57,59,62,68	0
3	MAN	T	7	11/12	0.94	0.06	55,57,58,66	0
3	NAG	V	5	14/15	0.94	0.08	60,62,64,72	0
3	NAG	T	1	14/15	0.94	0.09	49,52,58,65	0
3	NAG	T	5	14/15	0.95	0.06	47,51,53,53	0
3	NAG	W	2	14/15	0.95	0.06	52,56,57,58	0
3	BMA	T	3	11/12	0.95	0.06	45,46,48,52	0
3	MAN	S	7	11/12	0.95	0.05	63,64,66,72	0
3	NAG	W	5	14/15	0.95	0.07	42,53,57,61	0
3	NAG	U	2	14/15	0.95	0.08	52,60,62,62	0
3	BMA	S	3	11/12	0.96	0.05	50,53,53,58	0
3	MAN	S	4	11/12	0.96	0.07	48,54,55,56	0
3	NAG	S	2	14/15	0.96	0.06	47,51,53,54	0
3	NAG	T	2	14/15	0.97	0.06	42,46,51,54	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.

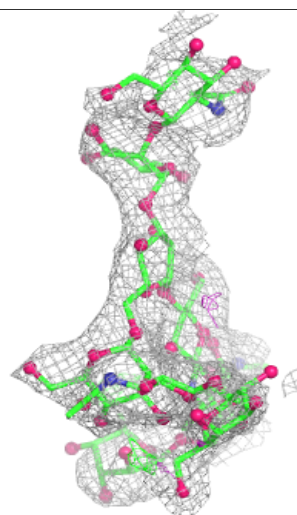
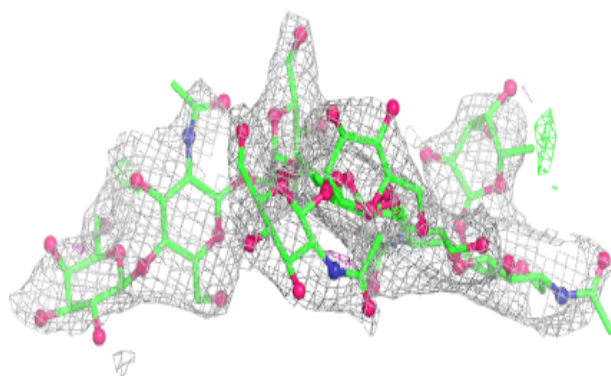
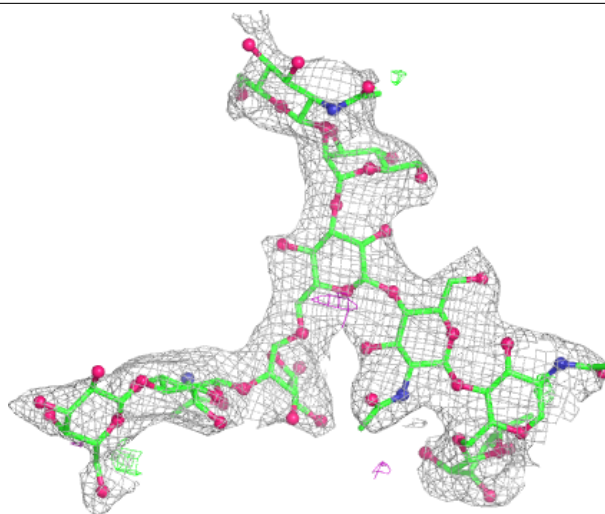
Electron density around Chain Q:

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



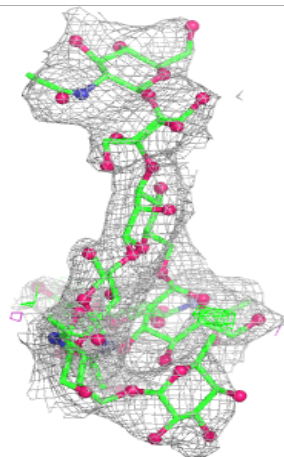
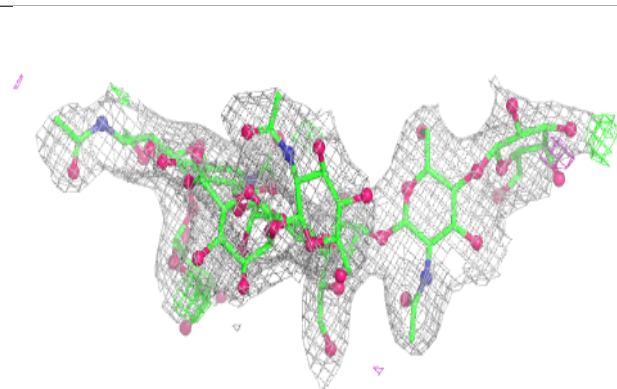
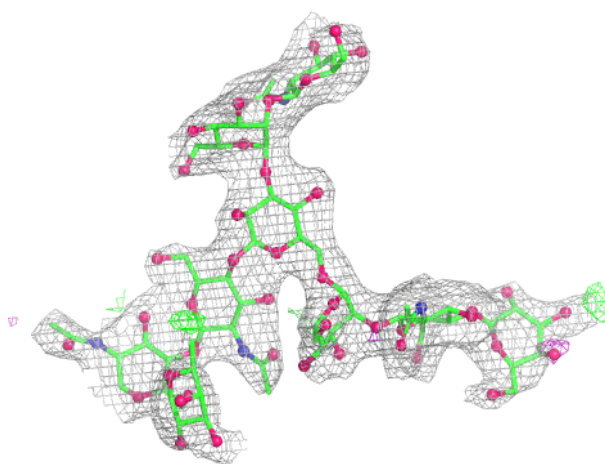
Electron density around Chain R:

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



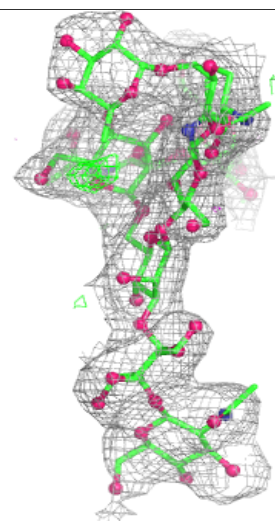
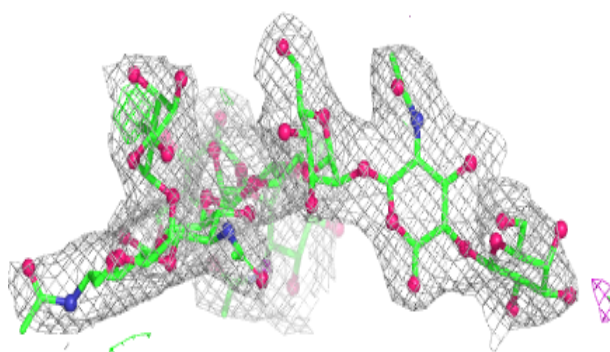
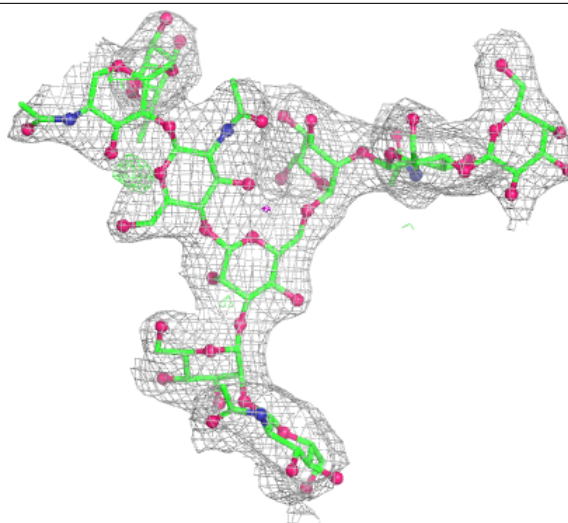
Electron density around Chain S:

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



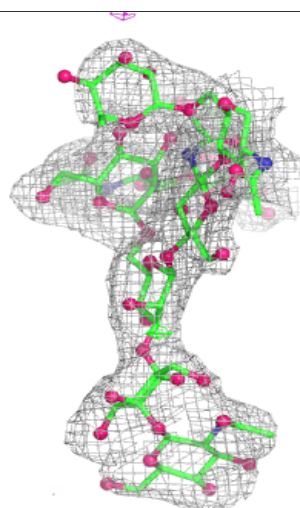
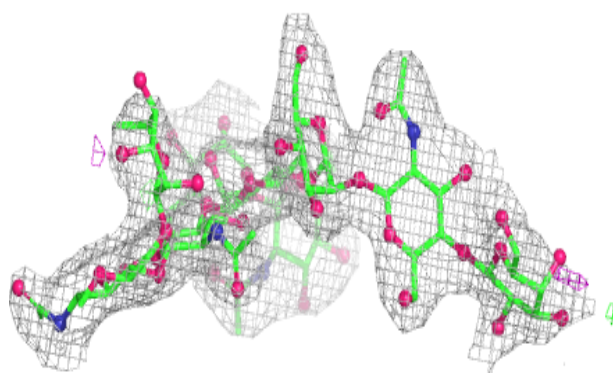
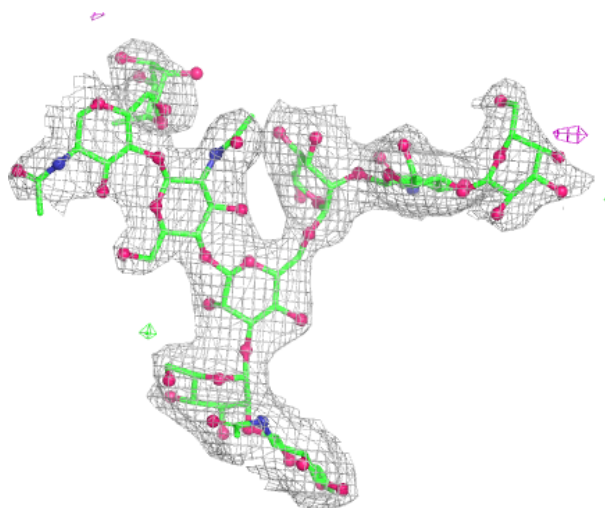
Electron density around Chain T:

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



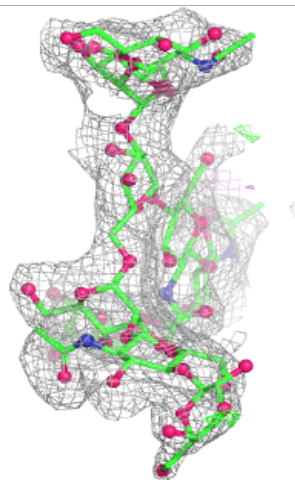
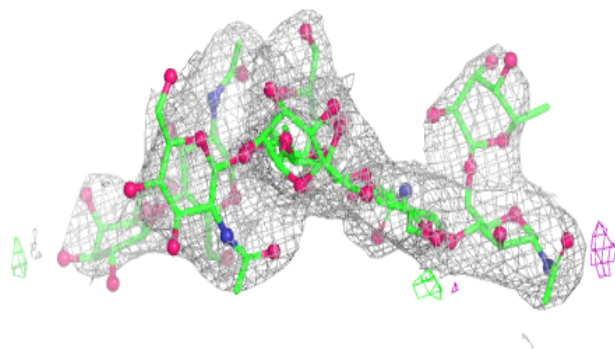
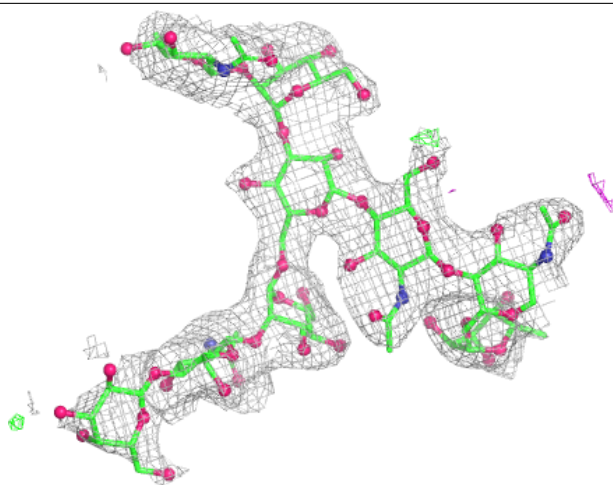
Electron density around Chain U:

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



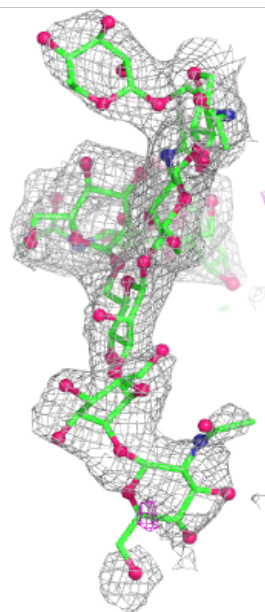
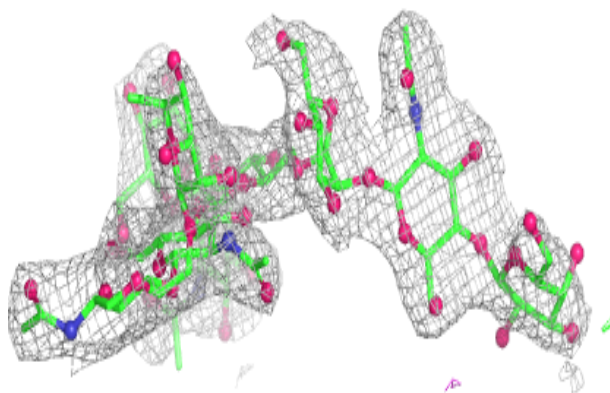
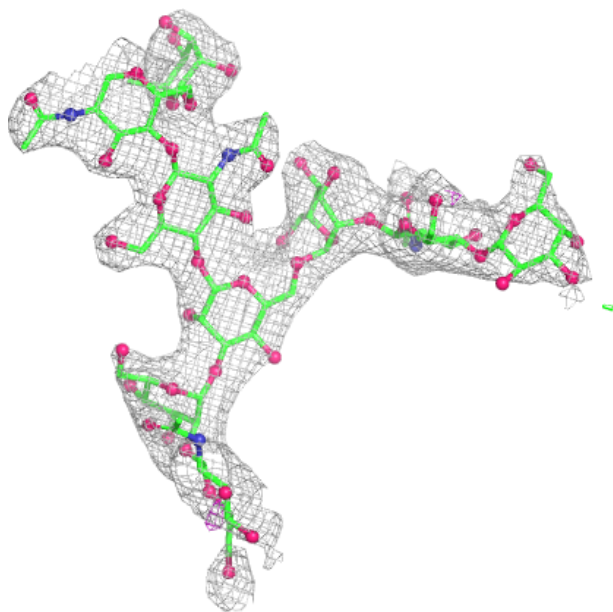
Electron density around Chain V:

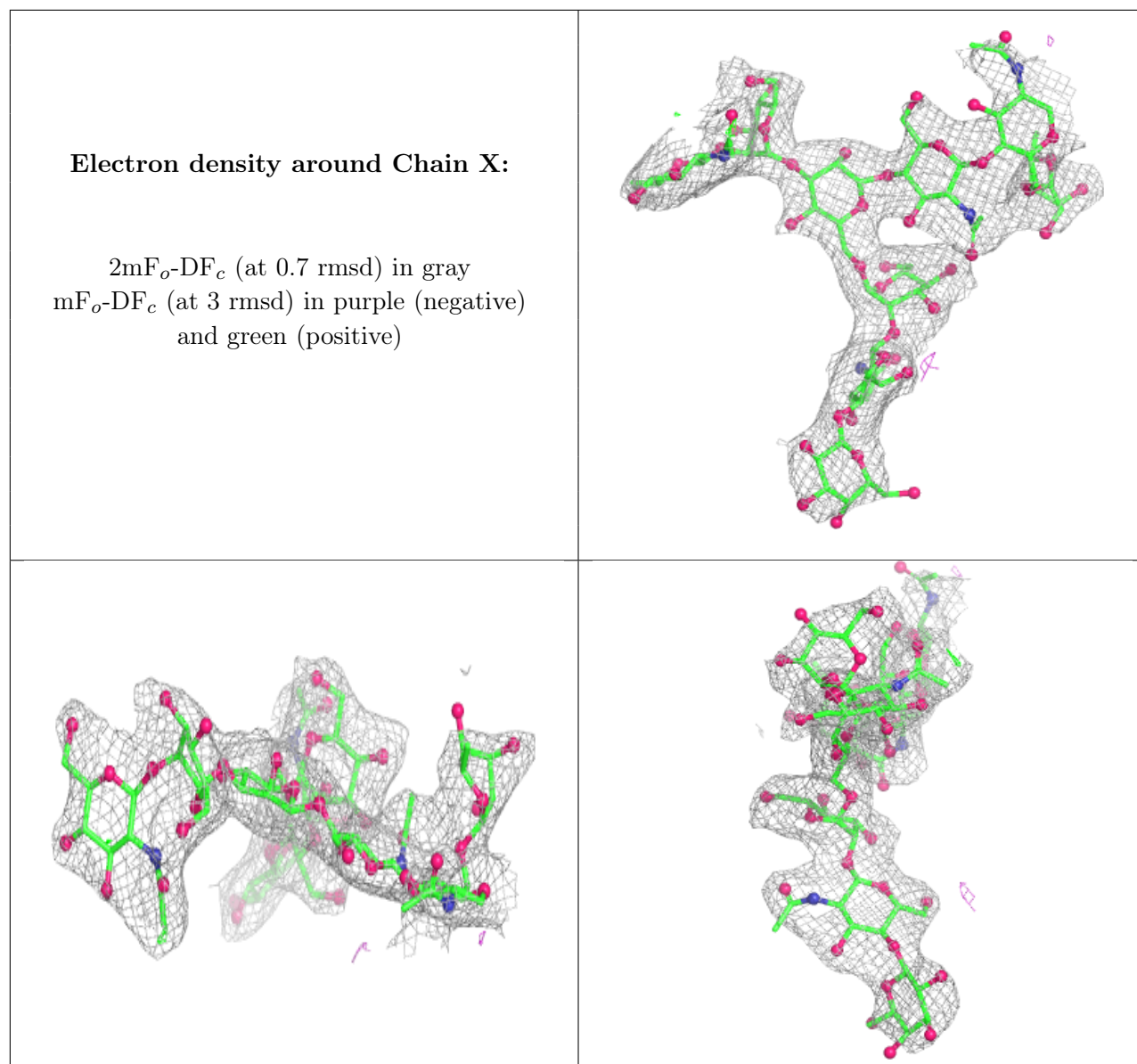
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.