



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:45 AM UTC

PDB ID : 3SLN / pdb_00003sln
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to H pentasaccharide
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.
Deposited on : 2011-06-24
Resolution : 2.84 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

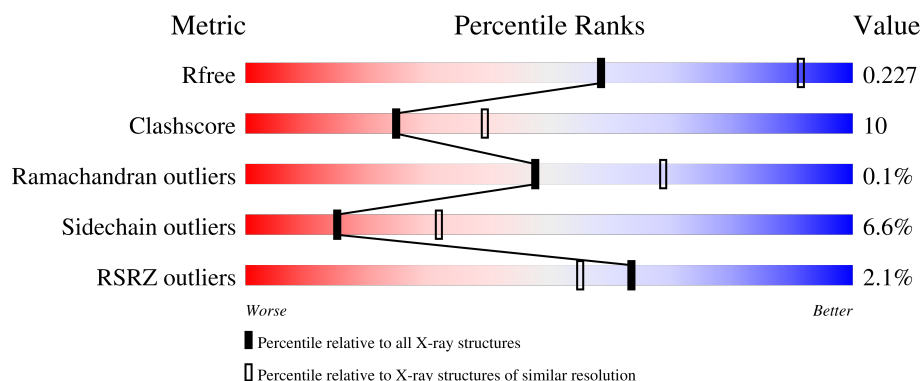
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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.



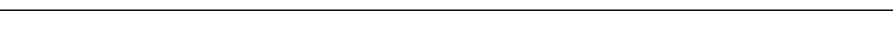
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	311	2% 83% 13% ..
1	B	311	% 78% 16% 5% .
1	C	311	78% 19% .
1	D	311	% 80% 15% ..
1	E	311	% 81% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	
2	K	5	
2	L	5	
2	M	5	
2	N	5	
2	O	5	
2	P	5	
2	Q	5	
2	R	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	K	1	-	-	X	-
2	GAL	K	2	-	-	X	-
2	BGC	N	1	-	-	X	-
2	GAL	N	2	-	-	X	-
2	FUC	O	5	-	-	X	-
2	GAL	P	2	-	-	X	-
2	BGC	R	1	-	-	X	-
2	GAL	R	2	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24066 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 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2404	1517	415	462	10			
1	B	308	Total	C	N	O	S	0	0	0
			2392	1510	411	461	10			
1	C	311	Total	C	N	O	S	0	0	0
			2403	1514	413	466	10			
1	D	307	Total	C	N	O	S	0	0	0
			2385	1507	410	458	10			
1	E	309	Total	C	N	O	S	0	0	0
			2406	1518	415	463	10			
1	F	308	Total	C	N	O	S	0	0	0
			2393	1511	411	461	10			
1	G	308	Total	C	N	O	S	0	0	0
			2383	1506	407	460	10			
1	H	292	Total	C	N	O	S	0	0	0
			2266	1441	385	431	9			
1	I	285	Total	C	N	O	S	0	0	0
			2184	1385	378	413	8			
1	J	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	10			

There are 30 discrepancies between the modelled and reference sequences:

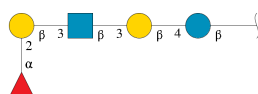
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
C	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
C	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
D	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
D	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
E	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
E	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
E	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
F	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
F	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
F	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
G	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
G	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
G	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
H	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
H	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
H	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
I	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
I	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
I	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
J	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
J	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
J	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	L	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	M	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	N	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	O	5	Total	C	N	O	0	0	0
			58	32	1	25			

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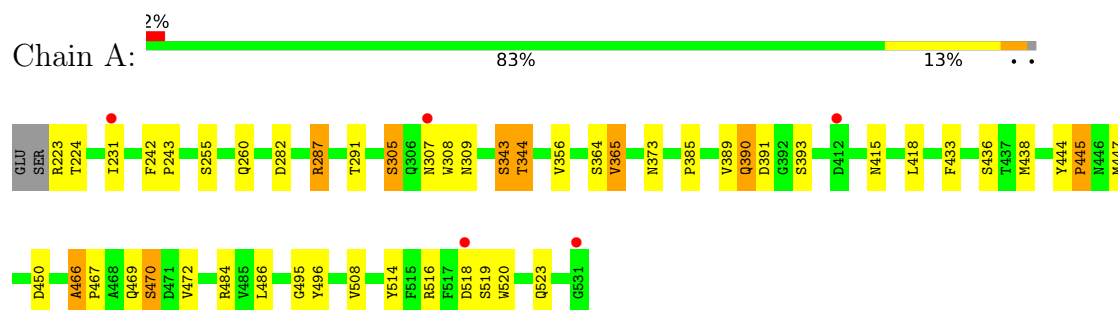
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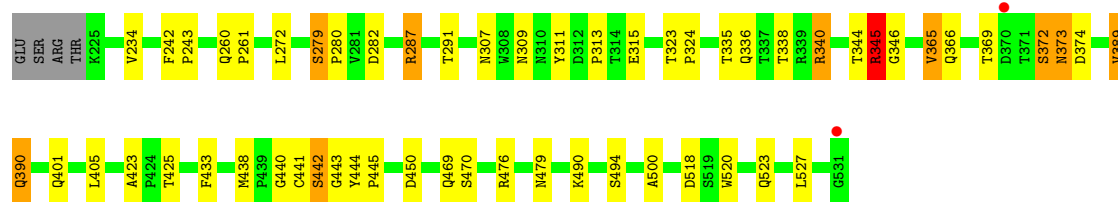
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	Q	5	Total	C	N	O	0	0	0
			58	32	1	25			
2	R	5	Total	C	N	O	0	0	0
			58	32	1	25			

3 Residue-property plots [i](#)

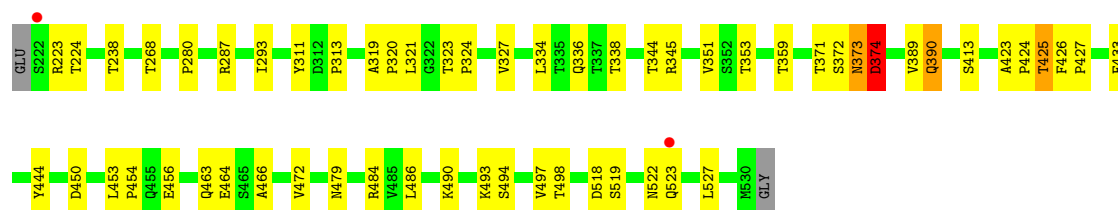
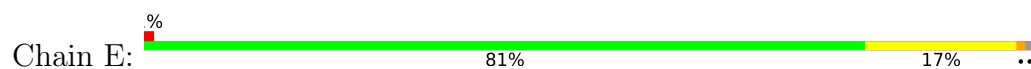
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Capsid

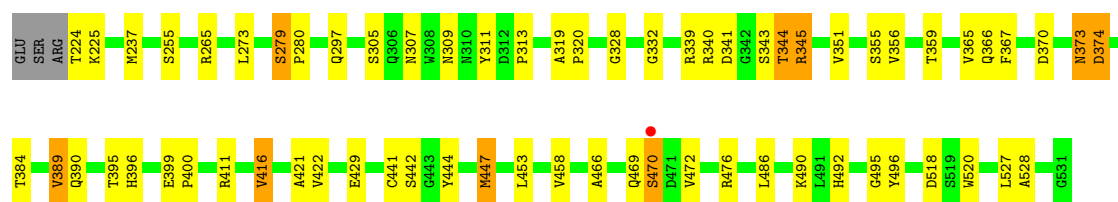
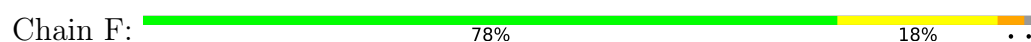




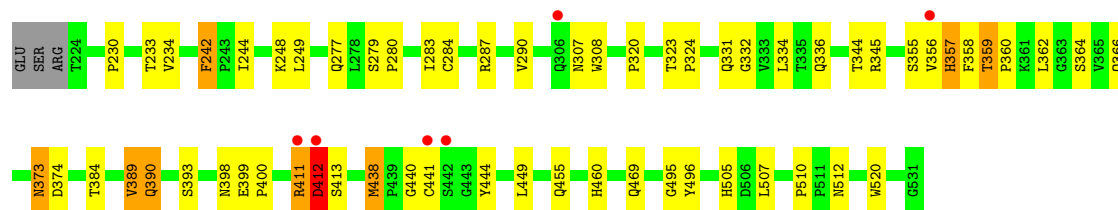
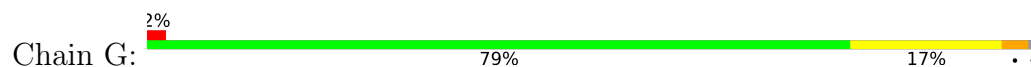
• Molecule 1: Capsid



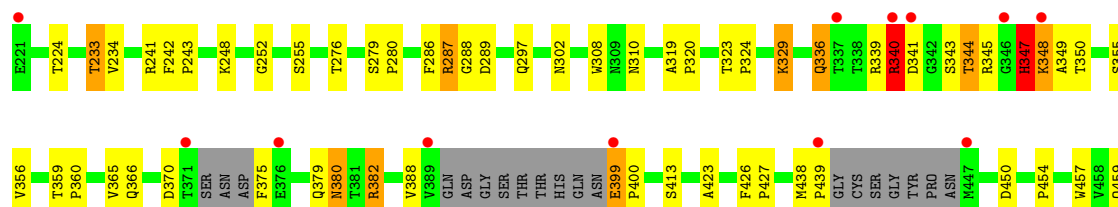
• Molecule 1: Capsid



• Molecule 1: Capsid

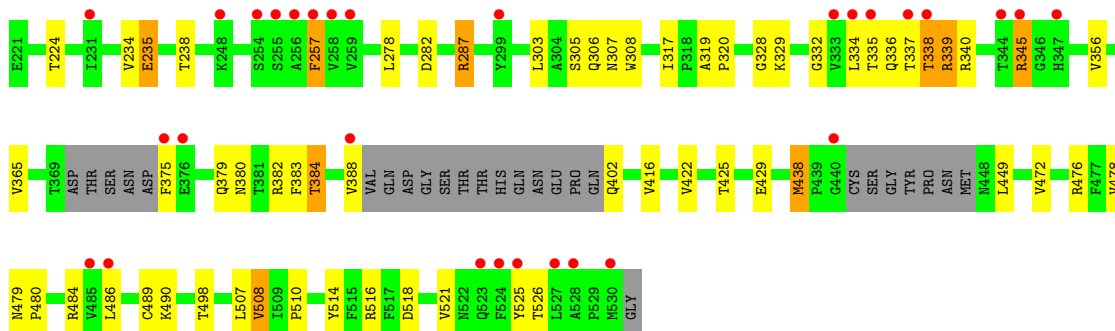
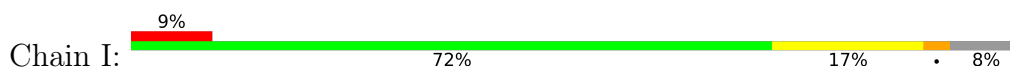


• Molecule 1: Capsid

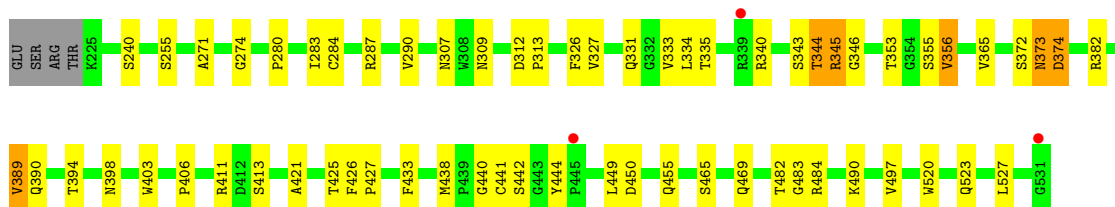
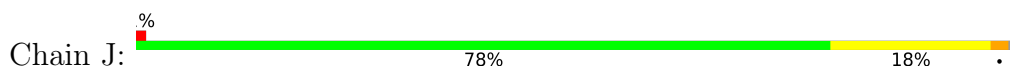




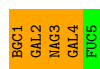
- Molecule 1: Capsid



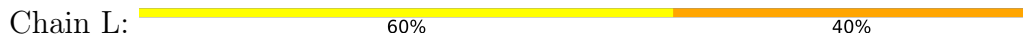
- Molecule 1: Capsid



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



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



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

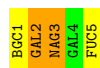
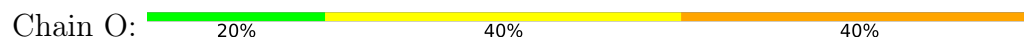




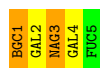
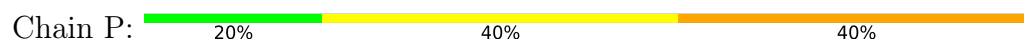
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	242.22Å 339.03Å 124.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 2.84 39.85 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.85-2.84) 99.1 (39.85-2.84)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.231 0.187 , 0.227	Depositor DCC
R_{free} test set	6014 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BGC, FUC, 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	1.27	4/2474 (0.2%)	1.25	11/3385 (0.3%)
1	B	1.20	1/2462 (0.0%)	1.22	6/3369 (0.2%)
1	C	1.18	5/2472 (0.2%)	1.22	9/3384 (0.3%)
1	D	1.17	4/2455 (0.2%)	1.20	12/3360 (0.4%)
1	E	1.18	3/2476 (0.1%)	1.16	2/3388 (0.1%)
1	F	1.06	2/2463 (0.1%)	1.28	21/3371 (0.6%)
1	G	1.05	3/2453 (0.1%)	1.19	9/3359 (0.3%)
1	H	1.12	5/2330 (0.2%)	1.15	8/3186 (0.3%)
1	I	1.08	3/2245 (0.1%)	1.06	4/3071 (0.1%)
1	J	1.04	3/2456 (0.1%)	1.15	6/3361 (0.2%)
All	All	1.14	33/24286 (0.1%)	1.19	88/33234 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	524	PHE	CA-CB	8.33	1.65	1.53
1	D	423	ALA	CA-CB	-8.28	1.41	1.54
1	H	340	ARG	CB-CG	-7.31	1.30	1.52
1	H	340	ARG	CZ-NH1	-7.30	1.22	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	508	VAL	CA-CB	6.63	1.61	1.54
1	H	344	THR	CA-CB	-6.22	1.43	1.53
1	F	421	ALA	CA-CB	-6.17	1.44	1.53
1	C	473	ALA	CA-CB	-5.98	1.44	1.53
1	D	401	GLN	C-O	5.88	1.30	1.23
1	A	436	SER	CA-C	-5.78	1.45	1.52
1	A	470	SER	C-O	-5.78	1.18	1.24
1	A	365	VAL	CA-CB	-5.72	1.46	1.55
1	I	525	TYR	CA-CB	5.67	1.66	1.53
1	C	407	ASP	CA-C	-5.51	1.45	1.53
1	G	242	PHE	CA-C	5.50	1.58	1.52
1	E	466	ALA	CA-CB	-5.42	1.43	1.53
1	E	425	THR	CA-CB	5.42	1.61	1.53
1	D	500	ALA	CA-CB	-5.41	1.45	1.52
1	F	396	HIS	CG-ND1	5.41	1.44	1.38
1	H	509	ILE	CA-CB	5.41	1.61	1.54
1	G	495	GLY	C-N	-5.34	1.25	1.33
1	I	257	PHE	CA-C	5.32	1.59	1.52
1	J	425	THR	CA-CB	5.18	1.60	1.53
1	I	508	VAL	CA-CB	5.16	1.59	1.53
1	J	271	ALA	CA-CB	-5.16	1.46	1.53
1	C	470	SER	C-O	-5.14	1.19	1.24
1	D	425	THR	C-O	-5.08	1.18	1.24
1	J	421	ALA	CA-CB	-5.07	1.44	1.53
1	H	423	ALA	CA-CB	-5.04	1.47	1.53
1	B	526	THR	CA-CB	5.03	1.60	1.53
1	C	257	PHE	C-O	5.02	1.30	1.23
1	E	359	THR	CA-CB	5.02	1.59	1.53
1	G	510	PRO	CA-C	5.00	1.56	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374	ASP	N-CA-C	13.76	126.28	111.28
1	G	374	ASP	N-CA-C	12.79	125.22	111.28
1	F	374	ASP	N-CA-C	11.16	123.53	111.36
1	F	344	THR	N-CA-C	10.31	126.45	109.24
1	J	374	ASP	N-CA-C	9.90	122.15	111.36
1	E	374	ASP	N-CA-C	9.65	121.56	111.14
1	C	496	TYR	N-CA-CB	-9.41	96.66	110.87
1	F	496	TYR	N-CA-CB	-8.71	97.99	111.05
1	A	496	TYR	N-CA-CB	-8.68	98.02	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	411	ARG	N-CA-C	-8.03	99.93	110.53
1	B	419	ALA	CA-C-N	7.55	127.54	119.76
1	B	419	ALA	C-N-CA	7.55	127.54	119.76
1	F	345	ARG	N-CA-CB	-7.50	98.08	110.68
1	G	496	TYR	N-CA-CB	-7.38	99.72	110.87
1	F	344	THR	CB-CA-C	-7.29	94.93	109.35
1	G	496	TYR	N-CA-C	6.98	119.75	109.69
1	F	528	ALA	CA-C-N	-6.91	112.64	119.90
1	F	528	ALA	C-N-CA	-6.91	112.64	119.90
1	C	463	GLN	CB-CA-C	-6.89	99.78	110.81
1	F	225	LYS	N-CA-C	6.83	118.26	109.65
1	A	496	TYR	N-CA-C	6.81	120.24	109.81
1	A	495	GLY	N-CA-C	6.76	124.49	114.95
1	F	496	TYR	N-CA-C	6.51	119.78	109.81
1	D	479	ASN	CA-C-N	-6.45	113.05	119.56
1	D	479	ASN	C-N-CA	-6.45	113.05	119.56
1	H	347	HIS	N-CA-C	6.44	120.79	109.96
1	B	461	PHE	N-CA-C	-6.44	104.18	111.14
1	A	282	ASP	N-CA-C	6.34	120.12	112.38
1	D	405	LEU	CA-C-N	6.34	126.31	120.03
1	D	405	LEU	C-N-CA	6.34	126.31	120.03
1	A	523	GLN	CB-CA-C	-6.31	100.32	110.79
1	F	395	THR	N-CA-CB	6.09	119.55	110.29
1	I	328	GLY	N-CA-C	6.09	118.21	110.96
1	F	359	THR	CA-C-N	-6.04	112.79	119.19
1	F	359	THR	C-N-CA	-6.04	112.79	119.19
1	H	233	THR	N-CA-C	-5.98	101.14	110.42
1	D	372	SER	N-CA-C	-5.93	105.87	114.12
1	E	464	GLU	N-CA-C	5.90	117.79	111.36
1	A	385	PRO	CA-C-N	-5.88	116.92	123.16
1	A	385	PRO	C-N-CA	-5.88	116.92	123.16
1	G	359	THR	CA-C-N	-5.88	112.62	119.32
1	G	359	THR	C-N-CA	-5.88	112.62	119.32
1	G	505	HIS	N-CA-C	5.81	117.86	107.80
1	C	496	TYR	N-CA-C	5.80	118.04	109.69
1	B	435	ARG	N-CA-C	5.73	118.73	109.40
1	B	465	SER	CB-CA-C	-5.70	103.40	111.95
1	H	279	SER	CA-C-N	-5.63	113.87	119.56
1	H	279	SER	C-N-CA	-5.63	113.87	119.56
1	J	497	VAL	N-CA-C	5.62	116.68	108.53
1	F	366	GLN	N-CA-C	5.62	118.25	108.76
1	J	483	GLY	N-CA-C	-5.60	107.53	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	496	TYR	CA-C-N	-5.54	115.42	123.06
1	F	496	TYR	C-N-CA	-5.54	115.42	123.06
1	F	458	VAL	N-CA-C	-5.52	105.12	110.42
1	F	416	VAL	N-CA-C	5.48	116.80	108.80
1	A	438	MET	CA-C-N	-5.44	114.18	119.78
1	A	438	MET	C-N-CA	-5.44	114.18	119.78
1	D	279	SER	CA-C-N	-5.43	114.22	119.87
1	D	279	SER	C-N-CA	-5.43	114.22	119.87
1	D	438	MET	CA-C-N	-5.41	114.39	119.85
1	D	438	MET	C-N-CA	-5.41	114.39	119.85
1	C	495	GLY	N-CA-C	5.41	125.99	113.18
1	C	510	PRO	O-C-N	5.37	123.67	121.15
1	C	509	ILE	CA-C-N	-5.32	115.83	119.66
1	C	509	ILE	C-N-CA	-5.32	115.83	119.66
1	I	422	VAL	N-CA-C	5.30	115.76	108.12
1	B	425	THR	N-CA-C	-5.30	104.61	111.71
1	F	466	ALA	CA-C-N	-5.28	114.51	119.85
1	F	466	ALA	C-N-CA	-5.28	114.51	119.85
1	D	425	THR	N-CA-C	-5.25	104.04	110.61
1	G	438	MET	CA-C-N	-5.24	113.91	120.51
1	G	438	MET	C-N-CA	-5.24	113.91	120.51
1	I	425	THR	N-CA-C	-5.23	106.66	112.57
1	C	369	THR	N-CA-C	5.23	115.19	108.34
1	H	349	ALA	N-CA-C	5.21	116.21	108.86
1	I	449	LEU	N-CA-C	5.21	117.21	107.99
1	H	329	LYS	N-CA-C	-5.16	99.38	108.20
1	D	369	THR	N-CA-C	5.09	115.01	108.34
1	J	331	GLN	CA-C-N	-5.09	118.24	122.16
1	J	331	GLN	C-N-CA	-5.09	118.24	122.16
1	H	252	GLY	CA-C-N	-5.06	115.02	120.03
1	H	252	GLY	C-N-CA	-5.06	115.02	120.03
1	F	237	MET	N-CA-C	5.05	117.57	110.14
1	C	358	PHE	N-CA-C	5.04	117.50	108.17
1	J	344	THR	CB-CA-C	5.04	119.26	109.33
1	A	466	ALA	CA-C-N	5.02	125.17	119.90
1	A	466	ALA	C-N-CA	5.02	125.17	119.90
1	F	396	HIS	N-CA-CB	-5.00	102.28	109.83

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	SER	Peptide
1	D	345	ARG	Sidechain
1	E	223	ARG	Sidechain
1	H	336	GLN	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	2404	0	2295	36	0
1	B	2392	0	2278	47	0
1	C	2403	0	2282	41	0
1	D	2385	0	2272	47	0
1	E	2406	0	2297	32	0
1	F	2393	0	2282	53	0
1	G	2383	0	2265	39	0
1	H	2266	0	2169	56	0
1	I	2184	0	2068	44	0
1	J	2386	0	2275	41	0
2	K	58	0	51	10	0
2	L	58	0	49	5	0
2	M	58	0	51	2	0
2	N	58	0	51	11	1
2	O	58	0	51	12	0
2	P	58	0	51	7	0
2	Q	58	0	51	5	0
2	R	58	0	51	15	0
All	All	24066	0	22889	461	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 10.

All (461) 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:G:411:ARG:O	1:G:412:ASP:HB3	1.45	1.17
2:Q:3:NAG:O3	2:Q:5:FUC:H5	1.44	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.01	1.15
1:H:382:ARG:HH11	1:H:382:ARG:CG	1.60	1.12
1:H:382:ARG:HG2	1:H:382:ARG:NH1	1.54	1.08
2:N:1:BGC:C6	2:N:2:GAL:C1	2.30	1.08
2:K:1:BGC:C6	2:K:2:GAL:C1	2.30	1.08
2:K:1:BGC:H6C2	2:K:2:GAL:C1	1.84	1.07
2:N:1:BGC:H6C2	2:N:2:GAL:C1	1.84	1.05
1:B:470:SER:HB2	1:B:520:TRP:HB3	1.39	1.04
1:H:339:ARG:HH11	1:H:345:ARG:CB	1.70	1.03
2:P:1:BGC:H6C1	2:P:2:GAL:C1	1.91	1.00
1:A:223:ARG:HG2	1:A:224:THR:H	1.26	1.00
1:D:443:GLY:HA2	2:O:5:FUC:C6	1.92	1.00
1:D:443:GLY:HA2	2:O:5:FUC:H61	1.44	0.99
2:M:2:GAL:H4	2:M:3:NAG:O5	1.61	0.98
1:G:438:MET:HE2	1:G:449:LEU:HB2	1.44	0.97
1:H:339:ARG:NH1	1:H:345:ARG:CB	2.28	0.96
2:P:2:GAL:H4	2:P:3:NAG:O5	1.64	0.96
1:F:390:GLN:HG2	1:F:444:TYR:C	1.91	0.93
1:D:443:GLY:CA	2:O:5:FUC:H63	1.99	0.92
1:H:347:HIS:N	1:H:347:HIS:CD2	2.34	0.92
1:F:373:ASN:HD22	1:F:373:ASN:H	0.99	0.92
1:B:470:SER:CB	1:B:520:TRP:HB3	2.00	0.90
1:F:373:ASN:H	1:F:373:ASN:ND2	1.70	0.90
2:P:1:BGC:C6	2:P:2:GAL:C1	2.50	0.90
1:B:339:ARG:HG3	1:B:339:ARG:NH1	1.81	0.88
1:I:336:GLN:HG2	1:I:337:THR:H	1.39	0.87
1:F:469:GLN:HB2	1:F:520:TRP:CG	2.11	0.85
1:H:382:ARG:HH11	1:H:382:ARG:HG2	0.71	0.85
1:D:443:GLY:CA	2:O:5:FUC:C6	2.55	0.83
2:P:1:BGC:H6C1	2:P:2:GAL:O5	1.78	0.83
1:F:373:ASN:HD22	1:F:373:ASN:N	1.69	0.82
1:I:336:GLN:CG	1:I:337:THR:H	1.93	0.80
2:L:1:BGC:C6	2:L:2:GAL:O2	2.30	0.80
1:I:339:ARG:HD2	1:I:345:ARG:NH1	1.97	0.80
1:H:347:HIS:N	1:H:347:HIS:HD2	1.77	0.80
2:P:2:GAL:C4	2:P:3:NAG:O5	2.30	0.80
1:H:347:HIS:CD2	1:H:347:HIS:H	1.95	0.79
1:C:481:ASP:CG	1:C:512:ASN:HD21	1.90	0.79
1:A:223:ARG:HG2	1:A:224:THR:N	1.98	0.78
1:B:412:ASP:OD2	1:J:394:THR:HG23	1.84	0.78
1:A:307:ASN:O	1:A:308:TRP:HB2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:ARG:CG	1:H:382:ARG:NH1	2.30	0.77
2:K:1:BGC:H6C2	2:K:2:GAL:H5	1.66	0.76
1:C:469:GLN:HG3	1:C:520:TRP:CD1	2.20	0.75
2:M:2:GAL:C4	2:M:3:NAG:O5	2.33	0.75
2:N:1:BGC:H6C2	2:N:2:GAL:H5	1.66	0.75
2:Q:3:NAG:O3	2:Q:5:FUC:C5	2.30	0.75
1:F:469:GLN:HB2	1:F:520:TRP:CD2	2.21	0.75
1:G:412:ASP:OD1	1:G:412:ASP:C	2.29	0.75
2:L:1:BGC:H6C2	2:L:2:GAL:O2	1.86	0.75
1:G:469:GLN:HB2	1:G:520:TRP:CD1	2.22	0.74
1:G:390:GLN:CG	1:G:444:TYR:H	2.01	0.74
1:D:390:GLN:HG2	1:D:444:TYR:C	2.11	0.74
1:H:297:GLN:NE2	1:H:370:ASP:O	2.20	0.74
1:H:438:MET:HG3	1:H:439:PRO:HD2	1.69	0.74
1:F:373:ASN:ND2	1:F:373:ASN:N	2.31	0.74
1:G:441:CYS:O	1:J:346:GLY:N	2.21	0.73
1:F:390:GLN:HE21	1:F:444:TYR:H	1.37	0.73
1:I:334:LEU:CD1	1:I:383:PHE:HB2	2.18	0.73
1:A:223:ARG:CG	1:A:224:THR:H	2.00	0.73
1:A:231:ILE:HG22	1:A:231:ILE:O	1.87	0.73
2:R:1:BGC:H6C2	2:R:2:GAL:O6	1.89	0.73
1:J:345:ARG:HD3	1:J:374:ASP:OD1	1.89	0.72
1:H:339:ARG:HB2	1:H:343:SER:O	1.88	0.72
1:A:343:SER:HB3	1:C:444:TYR:CE1	2.24	0.72
1:I:282:ASP:OD2	1:I:306:GLN:NE2	2.22	0.71
1:I:336:GLN:HB2	1:I:380:ASN:O	1.90	0.71
2:O:2:GAL:H4	2:O:3:NAG:O5	1.90	0.71
1:D:470:SER:OG	1:D:520:TRP:HB3	1.89	0.71
1:B:287:ARG:HH11	1:B:287:ARG:HB2	1.56	0.70
1:A:390:GLN:HG2	1:A:444:TYR:O	1.91	0.70
1:H:323:THR:HG22	1:H:324:PRO:HD2	1.74	0.69
1:C:453:LEU:HD21	1:C:495:GLY:O	1.92	0.69
1:I:336:GLN:CG	1:I:337:THR:N	2.54	0.69
1:D:390:GLN:HG3	1:D:444:TYR:H	1.57	0.69
1:E:338:THR:HG23	1:E:345:ARG:HH22	1.57	0.69
1:F:390:GLN:HG2	1:F:444:TYR:O	1.92	0.68
1:J:390:GLN:HG2	1:J:444:TYR:C	2.18	0.68
2:R:1:BGC:H6C2	2:R:2:GAL:O5	1.92	0.68
1:A:344:THR:HG22	1:C:442:SER:N	2.09	0.68
1:F:469:GLN:HB2	1:F:520:TRP:CD1	2.28	0.68
1:J:307:ASN:HD21	1:J:309:ASN:HB2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:480:PRO:HB3	1:I:514:TYR:HE2	1.58	0.68
1:C:253:PRO:HG3	2:L:1:BGC:H1	1.76	0.68
1:D:442:SER:HA	1:F:344:THR:O	1.94	0.68
1:C:311:TYR:O	1:C:313:PRO:HD3	1.94	0.68
1:G:469:GLN:HB2	1:G:520:TRP:CG	2.28	0.68
1:D:336:GLN:HB3	1:D:345:ARG:HH21	1.59	0.67
1:D:338:THR:OG1	1:D:345:ARG:NH1	2.24	0.67
1:F:472:VAL:HG11	1:F:490:LYS:HD3	1.75	0.67
1:G:390:GLN:HG2	1:G:444:TYR:C	2.19	0.67
1:B:390:GLN:HG2	1:B:444:TYR:C	2.20	0.66
1:I:476:ARG:HD3	1:I:518:ASP:OD2	1.95	0.66
2:R:1:BGC:C5	2:R:2:GAL:O5	2.42	0.66
1:B:343:SER:HB2	2:L:5:FUC:H63	1.78	0.65
1:H:336:GLN:HE21	1:H:379:GLN:HB2	1.61	0.65
1:J:373:ASN:OD1	1:J:373:ASN:N	2.29	0.65
1:H:336:GLN:OE1	1:H:375:PHE:HD1	1.80	0.65
1:E:373:ASN:N	1:E:373:ASN:OD1	2.29	0.65
2:K:1:BGC:H6C1	2:K:2:GAL:C1	2.26	0.65
1:H:286:PHE:CZ	1:H:323:THR:HG23	2.32	0.65
1:I:472:VAL:HG11	1:I:490:LYS:HD3	1.80	0.65
2:R:1:BGC:C6	2:R:2:GAL:O5	2.45	0.64
1:D:389:VAL:HG22	1:D:442:SER:HB3	1.78	0.64
1:D:373:ASN:OD1	1:D:373:ASN:N	2.30	0.64
2:L:1:BGC:H6C1	2:L:2:GAL:O2	1.97	0.64
1:A:287:ARG:HH11	1:A:287:ARG:HB2	1.62	0.64
1:G:373:ASN:OD1	1:G:373:ASN:N	2.30	0.64
1:A:344:THR:HG23	1:C:440:GLY:C	2.22	0.64
1:B:412:ASP:OD2	1:J:394:THR:CG2	2.46	0.64
1:C:469:GLN:CG	1:C:520:TRP:CD1	2.81	0.64
1:D:443:GLY:N	2:O:5:FUC:H63	2.13	0.64
1:H:344:THR:OG1	1:H:345:ARG:N	2.30	0.63
1:I:340:ARG:HD2	1:J:274:GLY:O	1.98	0.63
2:R:2:GAL:H4	2:R:3:NAG:O5	1.99	0.63
1:F:469:GLN:HA	1:F:469:GLN:OE1	1.98	0.63
1:H:286:PHE:CE1	1:H:323:THR:HG23	2.33	0.63
1:J:307:ASN:ND2	1:J:309:ASN:HB2	2.14	0.63
1:A:260:GLN:O	1:A:260:GLN:HG2	1.99	0.63
1:D:390:GLN:CG	1:D:444:TYR:H	2.12	0.62
2:N:1:BGC:H6C1	2:N:2:GAL:C1	2.26	0.62
1:H:476:ARG:HD3	1:H:518:ASP:OD2	1.99	0.62
1:G:390:GLN:HG3	1:G:444:TYR:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:BGC:C6	2:K:2:GAL:H5	2.31	0.61
1:G:390:GLN:HG2	1:G:444:TYR:H	1.64	0.61
1:D:390:GLN:HG2	1:D:445:PRO:N	2.15	0.61
1:B:472:VAL:HG11	1:B:490:LYS:HD3	1.83	0.61
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.81	0.61
1:J:394:THR:HG22	1:J:398:ASN:ND2	2.16	0.61
2:N:1:BGC:C6	2:N:2:GAL:H5	2.31	0.61
1:F:390:GLN:HG3	1:F:444:TYR:H	1.66	0.61
1:D:390:GLN:O	1:D:443:GLY:HA3	2.01	0.60
1:B:242:PHE:CD2	1:B:243:PRO:HD2	2.36	0.60
1:C:479:ASN:OD1	1:C:481:ASP:HB2	2.02	0.60
1:D:440:GLY:HA3	1:F:344:THR:HG21	1.83	0.60
1:D:390:GLN:HG3	1:D:444:TYR:N	2.17	0.60
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.36	0.60
1:D:307:ASN:OD1	1:D:309:ASN:HB2	2.01	0.59
1:J:490:LYS:HG3	1:J:527:LEU:HD11	1.85	0.59
1:G:412:ASP:OD1	1:G:413:SER:HB2	2.03	0.59
1:I:334:LEU:HA	1:I:382:ARG:O	2.03	0.58
2:O:2:GAL:C4	2:O:3:NAG:O5	2.49	0.58
1:C:223:ARG:NH2	1:H:276:THR:O	2.30	0.58
1:F:429:GLU:OE2	1:F:490:LYS:HE3	2.03	0.58
1:J:433:PHE:HB3	1:J:450:ASP:HB3	1.84	0.58
1:G:359:THR:O	1:G:360:PRO:C	2.44	0.58
1:B:471:ASP:HA	1:B:493:LYS:HD3	1.85	0.57
1:C:438:MET:HE2	1:C:449:LEU:HB2	1.85	0.57
1:D:443:GLY:C	2:O:5:FUC:H63	2.30	0.57
1:B:435:ARG:HB2	1:B:450:ASP:OD1	2.05	0.57
1:H:380:ASN:OD1	1:H:380:ASN:N	2.36	0.57
1:J:389:VAL:HG22	1:J:442:SER:HB3	1.86	0.56
1:F:469:GLN:CB	1:F:520:TRP:CD1	2.88	0.56
1:H:336:GLN:NE2	1:H:379:GLN:HB2	2.21	0.56
2:R:3:NAG:H2	2:R:5:FUC:H5	1.86	0.56
1:H:347:HIS:HD2	1:H:347:HIS:H	1.40	0.56
1:I:336:GLN:HG2	1:I:337:THR:N	2.16	0.56
1:C:268:THR:HG23	1:C:493:LYS:HA	1.88	0.56
1:F:389:VAL:HG22	1:F:442:SER:HB3	1.88	0.56
1:B:231:ILE:O	1:B:231:ILE:HG22	2.06	0.56
1:A:287:ARG:HB2	1:A:287:ARG:NH1	2.21	0.56
1:I:317:ILE:HD12	1:I:319:ALA:O	2.06	0.56
1:E:472:VAL:HG11	1:E:490:LYS:HD3	1.89	0.55
1:B:470:SER:OG	1:B:520:TRP:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:CD2	1:C:243:PRO:HD2	2.41	0.55
1:E:268:THR:HG23	1:E:493:LYS:HA	1.88	0.55
2:N:1:BGC:H6C2	2:N:2:GAL:C5	2.34	0.55
1:I:334:LEU:HD12	1:I:383:PHE:CA	2.38	0.54
1:J:327:VAL:HA	1:J:353:THR:OG1	2.08	0.54
1:H:438:MET:HG3	1:H:439:PRO:CD	2.37	0.54
1:H:365:VAL:CG1	1:H:366:GLN:N	2.70	0.54
1:H:528:ALA:O	1:H:529:PRO:C	2.50	0.54
2:Q:4:GAL:C1	2:Q:5:FUC:H5	2.35	0.54
1:F:390:GLN:HE21	1:F:444:TYR:N	2.03	0.54
1:J:389:VAL:HG23	1:J:441:CYS:HB2	1.90	0.54
1:J:438:MET:HE2	1:J:449:LEU:HB2	1.88	0.54
1:C:444:TYR:N	1:C:444:TYR:CD2	2.76	0.54
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.43	0.54
1:A:518:ASP:OD2	1:A:519:SER:OG	2.25	0.54
2:R:1:BGC:C6	2:R:2:GAL:O6	2.55	0.54
1:A:390:GLN:CG	1:A:444:TYR:O	2.56	0.53
1:A:444:TYR:N	1:A:444:TYR:CD2	2.76	0.53
1:H:399:GLU:HB2	1:H:400:PRO:HA	1.88	0.53
1:D:469:GLN:HG3	1:D:520:TRP:CD1	2.43	0.53
1:I:334:LEU:HD13	1:I:383:PHE:HD1	1.73	0.53
1:A:390:GLN:HG2	1:A:445:PRO:HA	1.91	0.53
1:J:343:SER:HB2	2:R:5:FUC:H63	1.91	0.53
1:D:287:ARG:HH11	1:D:287:ARG:HB2	1.73	0.53
1:G:280:PRO:HB3	1:G:455:GLN:HG2	1.90	0.53
2:K:1:BGC:H6C2	2:K:2:GAL:C5	2.34	0.53
1:B:389:VAL:HG23	1:B:441:CYS:HB2	1.90	0.53
1:D:443:GLY:N	2:O:5:FUC:C6	2.72	0.53
1:B:279:SER:HB3	1:B:282:ASP:HB2	1.91	0.52
1:E:371:THR:HG21	1:E:374:ASP:HB2	1.91	0.52
1:D:287:ARG:HB2	1:D:287:ARG:NH1	2.24	0.52
1:F:469:GLN:CG	1:F:520:TRP:CD1	2.92	0.52
1:F:470:SER:HB2	1:F:520:TRP:HB3	1.92	0.52
1:B:469:GLN:HB2	1:B:520:TRP:CG	2.44	0.52
1:D:336:GLN:O	1:D:344:THR:HA	2.09	0.52
1:F:390:GLN:CG	1:F:444:TYR:H	2.22	0.52
1:F:469:GLN:HB2	1:F:520:TRP:CE2	2.44	0.52
1:I:334:LEU:HD12	1:I:383:PHE:HA	1.91	0.52
1:A:344:THR:HB	1:C:443:GLY:O	2.10	0.51
1:B:232:LEU:HG	1:E:463:GLN:HE22	1.75	0.51
1:E:238:THR:N	1:E:456:GLU:OE1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:VAL:C	1:G:358:PHE:H	2.18	0.51
1:H:388:VAL:HG22	1:H:438:MET:HG2	1.92	0.51
1:F:328:GLY:HA3	1:F:400:PRO:HB3	1.91	0.51
1:E:327:VAL:HA	1:E:353:THR:OG1	2.11	0.51
1:H:323:THR:HG22	1:H:324:PRO:CD	2.40	0.51
1:J:394:THR:HG22	1:J:398:ASN:HD21	1.75	0.51
2:P:1:BGC:H6C1	2:P:2:GAL:C5	2.41	0.51
1:A:469:GLN:HB2	1:A:520:TRP:CG	2.47	0.50
1:H:348:LYS:HD3	1:H:370:ASP:OD2	2.11	0.50
1:F:265:ARG:HB3	1:F:273:LEU:HB2	1.93	0.50
1:F:374:ASP:OD1	1:F:374:ASP:O	2.30	0.50
1:F:469:GLN:HG3	1:F:520:TRP:CD1	2.46	0.50
1:I:489:CYS:HB2	1:I:498:THR:O	2.11	0.50
1:F:297:GLN:NE2	1:F:370:ASP:O	2.44	0.50
1:B:232:LEU:HG	1:E:463:GLN:NE2	2.27	0.50
1:H:242:PHE:CD2	1:H:243:PRO:HD2	2.47	0.50
1:J:356:VAL:HG23	1:J:411:ARG:HG3	1.94	0.50
1:A:391:ASP:C	1:A:391:ASP:OD1	2.55	0.49
1:E:351:VAL:O	1:E:351:VAL:HG13	2.12	0.49
1:B:390:GLN:CG	1:B:444:TYR:H	2.26	0.49
1:G:323:THR:HG23	1:G:324:PRO:HD2	1.93	0.49
1:A:344:THR:CG2	1:C:442:SER:N	2.73	0.49
1:A:445:PRO:O	1:A:447:MET:HG3	2.12	0.49
1:B:230:PRO:HD2	1:B:457:TRP:NE1	2.27	0.49
1:I:287:ARG:HH11	1:I:287:ARG:HB2	1.78	0.49
1:B:442:SER:HG	2:P:4:GAL:HO3	1.60	0.49
1:D:443:GLY:H	2:O:5:FUC:C6	2.25	0.49
2:R:2:GAL:C4	2:R:3:NAG:O5	2.61	0.49
1:B:336:GLN:HG3	1:B:381:THR:OG1	2.13	0.48
1:E:268:THR:CG2	1:E:493:LYS:HA	2.43	0.48
1:I:319:ALA:HB1	1:I:320:PRO:HD2	1.94	0.48
1:D:390:GLN:CG	1:D:444:TYR:N	2.74	0.48
1:F:490:LYS:HG3	1:F:527:LEU:HD11	1.95	0.48
1:G:412:ASP:OD1	1:G:412:ASP:O	2.30	0.48
1:A:223:ARG:HH11	1:A:223:ARG:HB2	1.78	0.48
1:B:339:ARG:HH11	1:B:339:ARG:CG	1.94	0.48
1:B:507:LEU:N	1:B:507:LEU:HD12	2.29	0.48
1:G:230:PRO:HG3	1:G:460:HIS:HB2	1.96	0.48
1:A:514:TYR:OH	1:A:516:ARG:NH2	2.47	0.48
1:E:338:THR:CG2	1:E:345:ARG:HH12	2.26	0.48
1:E:423:ALA:O	1:E:425:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:THR:HG21	1:H:512:ASN:HA	1.96	0.48
1:J:482:THR:OG1	1:J:484:ARG:HB2	2.14	0.48
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.49	0.48
1:J:283:ILE:O	1:J:284:CYS:HB2	2.14	0.48
1:A:242:PHE:CD2	1:A:243:PRO:HD2	2.48	0.47
1:C:307:ASN:OD1	1:C:309:ASN:HB2	2.14	0.47
1:I:338:THR:O	1:I:338:THR:OG1	2.30	0.47
1:C:389:VAL:HG22	1:C:442:SER:HB3	1.95	0.47
1:D:340:ARG:HE	1:D:340:ARG:HB3	1.47	0.47
1:E:433:PHE:HB3	1:E:450:ASP:HB3	1.96	0.47
1:F:453:LEU:HG	1:F:495:GLY:O	2.13	0.47
1:J:280:PRO:HB3	1:J:455:GLN:HG2	1.95	0.47
1:A:305:SER:HB2	1:A:309:ASN:O	2.13	0.47
1:C:320:PRO:HD2	1:C:360:PRO:HB2	1.96	0.47
1:I:438:MET:HE3	1:I:438:MET:HB3	1.66	0.47
1:A:307:ASN:O	1:A:308:TRP:CB	2.58	0.47
1:B:285:THR:HG22	1:B:385:PRO:CD	2.44	0.47
1:F:341:ASP:HB2	1:F:343:SER:H	1.79	0.47
1:C:453:LEU:CD2	1:C:495:GLY:O	2.62	0.47
1:B:280:PRO:HG2	1:E:280:PRO:HG2	1.97	0.47
1:C:323:THR:HG23	1:C:324:PRO:HD2	1.97	0.47
1:D:442:SER:CA	1:F:344:THR:O	2.60	0.47
1:E:390:GLN:HG3	1:E:444:TYR:H	1.80	0.47
1:F:469:GLN:CB	1:F:520:TRP:CG	2.90	0.47
1:C:242:PHE:CG	1:C:243:PRO:HD2	2.49	0.46
1:D:490:LYS:HG3	1:D:527:LEU:HD11	1.96	0.46
1:D:279:SER:HB3	1:D:282:ASP:HB2	1.97	0.46
1:D:346:GLY:N	1:F:441:CYS:O	2.47	0.46
1:H:319:ALA:HB1	1:H:320:PRO:HD2	1.97	0.46
1:E:323:THR:HG23	1:E:324:PRO:HD2	1.97	0.46
1:I:338:THR:O	1:I:339:ARG:C	2.56	0.46
2:K:1:BGC:C6	2:K:2:GAL:C5	2.92	0.46
1:F:311:TYR:O	1:F:313:PRO:HD3	2.15	0.46
1:I:306:GLN:C	1:I:308:TRP:H	2.24	0.46
1:A:223:ARG:HB2	1:A:223:ARG:NH1	2.29	0.46
1:G:332:GLY:HA3	1:G:384:THR:O	2.15	0.46
1:C:365:VAL:CG1	1:C:366:GLN:N	2.77	0.46
1:F:351:VAL:HB	1:F:367:PHE:CE1	2.51	0.46
1:J:403:TRP:CE3	1:J:403:TRP:HA	2.49	0.46
1:E:497:VAL:HG12	1:E:498:THR:N	2.31	0.46
1:I:334:LEU:HD12	1:I:383:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLN:NE2	1:F:444:TYR:H	2.08	0.46
1:I:429:GLU:OE2	1:I:490:LYS:HE3	2.16	0.46
1:I:319:ALA:HB1	1:I:320:PRO:CD	2.45	0.46
1:I:334:LEU:HD12	1:I:383:PHE:CB	2.47	0.45
1:D:311:TYR:O	1:D:313:PRO:HD3	2.17	0.45
2:N:1:BGC:C6	2:N:2:GAL:C5	2.92	0.45
2:N:1:BGC:H6C1	2:N:2:GAL:O5	2.17	0.45
1:G:242:PHE:O	1:G:244:ILE:N	2.49	0.45
1:D:242:PHE:CD2	1:D:243:PRO:HD2	2.51	0.45
1:E:311:TYR:O	1:E:313:PRO:HD3	2.17	0.45
1:A:344:THR:CG2	1:C:440:GLY:C	2.88	0.45
1:F:332:GLY:HA3	1:F:384:THR:O	2.16	0.45
1:B:440:GLY:HA3	1:E:344:THR:HG21	1.99	0.45
1:F:399:GLU:HB2	1:F:400:PRO:HA	1.99	0.45
1:H:280:PRO:HD3	1:H:459:GLN:HE22	1.82	0.45
1:H:339:ARG:NH1	1:H:345:ARG:O	2.50	0.45
1:J:326:PHE:O	1:J:406:PRO:HG3	2.17	0.45
2:R:1:BGC:C6	2:R:2:GAL:HO6	2.28	0.45
1:B:230:PRO:HD2	1:B:457:TRP:CD1	2.52	0.45
1:E:338:THR:CG2	1:E:345:ARG:HH22	2.27	0.45
1:J:345:ARG:HG3	2:R:5:FUC:O3	2.17	0.45
1:B:470:SER:HB2	1:B:520:TRP:CB	2.27	0.44
1:E:522:ASN:OD1	1:E:522:ASN:C	2.60	0.44
1:F:390:GLN:HG3	1:F:444:TYR:N	2.32	0.44
1:I:336:GLN:HG3	1:I:337:THR:HG23	1.98	0.44
2:K:1:BGC:H6C1	2:K:2:GAL:O5	2.17	0.44
1:G:389:VAL:HG23	1:G:441:CYS:HB2	1.99	0.44
1:H:339:ARG:C	1:H:341:ASP:N	2.73	0.44
1:D:389:VAL:HG23	1:D:441:CYS:HB2	2.00	0.44
1:F:307:ASN:HD21	1:F:309:ASN:HB2	1.81	0.44
1:H:323:THR:CG2	1:H:324:PRO:HD2	2.43	0.44
1:E:321:LEU:HD23	1:E:321:LEU:HA	1.64	0.44
1:F:399:GLU:HA	1:F:400:PRO:C	2.43	0.44
1:G:331:GLN:HB3	1:G:441:CYS:SG	2.58	0.44
1:H:287:ARG:HB3	1:H:308:TRP:CZ3	2.52	0.44
1:I:332:GLY:HA3	1:I:384:THR:O	2.18	0.44
1:J:240:SER:O	1:J:283:ILE:HD13	2.16	0.44
1:J:390:GLN:HG3	1:J:444:TYR:H	1.83	0.44
2:O:3:NAG:O3	2:O:5:FUC:H5	2.18	0.44
1:D:433:PHE:HB3	1:D:450:ASP:HB3	2.00	0.44
1:G:307:ASN:O	1:G:308:TRP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:PRO:HD3	1:H:459:GLN:NE2	2.33	0.44
2:Q:4:GAL:C2	2:Q:5:FUC:H5	2.46	0.44
1:D:323:THR:HG23	1:D:324:PRO:HD2	2.00	0.44
1:E:336:GLN:OE1	1:E:345:ARG:NH1	2.50	0.44
1:E:426:PHE:CD2	1:E:427:PRO:HD2	2.53	0.44
1:F:279:SER:HA	1:F:280:PRO:HD3	1.74	0.44
1:F:492:HIS:CD2	1:F:492:HIS:N	2.86	0.44
1:H:359:THR:N	1:H:360:PRO:CD	2.81	0.44
1:H:365:VAL:HG12	1:H:366:GLN:N	2.30	0.44
1:J:394:THR:CG2	1:J:398:ASN:HD21	2.31	0.44
1:J:469:GLN:HG3	1:J:520:TRP:CD1	2.52	0.44
1:D:389:VAL:HG22	1:D:442:SER:CB	2.45	0.44
1:G:277:GLN:OE1	1:G:279:SER:HB3	2.17	0.44
1:B:246:LEU:HD23	1:B:246:LEU:HA	1.81	0.44
1:E:484:ARG:HG3	1:E:484:ARG:HH11	1.83	0.44
1:E:518:ASP:O	1:E:519:SER:HB3	2.17	0.44
1:I:340:ARG:CD	1:J:274:GLY:O	2.65	0.44
1:J:390:GLN:HE21	1:J:444:TYR:H	1.66	0.44
1:A:415:ASN:HB3	1:A:418:LEU:HD21	1.99	0.43
1:I:235:GLU:H	1:I:235:GLU:HG2	1.41	0.43
1:F:390:GLN:CG	1:F:444:TYR:C	2.79	0.43
1:H:339:ARG:O	1:H:341:ASP:N	2.51	0.43
1:I:334:LEU:CD1	1:I:383:PHE:CB	2.94	0.43
1:C:332:GLY:HA3	1:C:384:THR:O	2.19	0.43
1:F:447:MET:HE2	1:F:447:MET:HB2	1.81	0.43
1:I:303:LEU:HD13	1:I:320:PRO:HG2	1.99	0.43
1:J:335:THR:HA	1:J:345:ARG:O	2.18	0.43
1:B:530:MET:O	1:B:531:GLY:C	2.61	0.43
1:D:280:PRO:HG3	1:F:280:PRO:HG2	2.00	0.43
1:D:476:ARG:HD2	1:D:476:ARG:N	2.31	0.43
2:R:3:NAG:N2	2:R:4:GAL:C1	2.82	0.43
1:B:332:GLY:HA3	1:B:384:THR:O	2.17	0.43
1:C:453:LEU:CG	1:C:495:GLY:O	2.66	0.43
1:D:365:VAL:CG1	1:D:366:GLN:N	2.81	0.43
1:J:482:THR:OG1	1:J:484:ARG:N	2.36	0.43
1:D:272:LEU:HB2	1:H:340:ARG:NH2	2.33	0.43
1:D:476:ARG:HD3	1:D:518:ASP:OD2	2.18	0.43
1:G:249:LEU:HB2	1:G:507:LEU:HB2	2.00	0.43
1:H:339:ARG:C	1:H:341:ASP:H	2.26	0.43
1:B:353:THR:HG22	1:B:358:PHE:CE1	2.54	0.43
1:C:279:SER:HB3	1:C:282:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ALA:HB1	1:C:320:PRO:HD2	2.01	0.43
1:G:344:THR:HG21	1:J:440:GLY:HA3	1.99	0.43
1:A:344:THR:HG23	1:C:440:GLY:O	2.18	0.43
1:D:335:THR:HA	1:D:345:ARG:O	2.19	0.42
1:G:336:GLN:O	1:G:344:THR:HA	2.19	0.42
1:J:312:ASP:HA	1:J:313:PRO:HD3	1.89	0.42
1:E:453:LEU:HA	1:E:454:PRO:HD3	1.92	0.42
1:I:478:VAL:HG21	1:I:516:ARG:NH1	2.34	0.42
1:A:343:SER:HB3	1:C:444:TYR:CZ	2.53	0.42
1:F:319:ALA:HB1	1:F:320:PRO:HD2	2.02	0.42
1:A:484:ARG:NH1	1:A:484:ARG:HG3	2.33	0.42
1:B:470:SER:O	1:B:520:TRP:CE3	2.73	0.42
1:H:469:GLN:OE1	1:H:469:GLN:HA	2.18	0.42
1:B:397:GLN:HB3	1:B:446:ASN:HB2	2.01	0.42
1:J:469:GLN:CG	1:J:520:TRP:CD1	3.02	0.42
1:G:390:GLN:HG2	1:G:444:TYR:N	2.32	0.42
1:H:297:GLN:HE21	1:H:370:ASP:C	2.22	0.42
2:N:1:BGC:C6	2:N:2:GAL:O5	2.67	0.42
2:R:1:BGC:H5	2:R:2:GAL:O5	2.05	0.42
2:R:3:NAG:O7	2:R:5:FUC:H3	2.19	0.42
1:A:466:ALA:HA	1:A:467:PRO:HD3	1.76	0.42
1:C:390:GLN:HG2	1:C:444:TYR:C	2.45	0.42
2:Q:1:BGC:H6C1	2:Q:2:GAL:O5	2.20	0.42
1:G:233:THR:HG21	1:G:512:ASN:HA	2.01	0.42
1:G:320:PRO:HD2	1:G:360:PRO:HB2	2.01	0.42
1:I:334:LEU:HD11	1:I:383:PHE:HB2	1.98	0.42
1:C:409:SER:HB2	1:C:413:SER:HB3	2.02	0.42
1:C:478:VAL:O	1:C:513:GLY:HA2	2.20	0.42
1:D:443:GLY:H	2:O:5:FUC:H63	1.84	0.42
1:E:490:LYS:HG3	1:E:527:LEU:HD21	2.02	0.42
2:K:3:NAG:N2	2:K:4:GAL:C1	2.83	0.42
1:A:433:PHE:HB3	1:A:450:ASP:HB3	2.02	0.41
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.84	0.41
1:B:438:MET:HE2	1:B:449:LEU:HB2	2.01	0.41
1:C:447:MET:HE3	1:C:447:MET:HB2	1.86	0.41
1:F:307:ASN:ND2	1:F:309:ASN:HB2	2.35	0.41
1:G:359:THR:HB	1:G:362:LEU:HB2	2.02	0.41
1:H:323:THR:CG2	1:H:324:PRO:CD	2.98	0.41
1:H:426:PHE:CD2	1:H:427:PRO:HD2	2.54	0.41
1:J:344:THR:O	2:R:5:FUC:H2	2.19	0.41
1:C:390:GLN:HB2	1:C:399:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:VAL:HG12	1:F:411:ARG:HG2	2.01	0.41
1:F:476:ARG:HD3	1:F:518:ASP:OD2	2.20	0.41
1:G:356:VAL:HG23	1:G:357:HIS:N	2.34	0.41
1:G:390:GLN:HE21	1:G:390:GLN:HB2	1.49	0.41
1:H:344:THR:H	1:H:344:THR:HG23	1.37	0.41
1:J:333:VAL:HG12	1:J:335:THR:HG22	2.00	0.41
1:B:419:ALA:HA	1:B:420:PRO:HD3	1.91	0.41
1:E:423:ALA:HB1	1:E:424:PRO:HD2	2.03	0.41
2:N:3:NAG:N2	2:N:4:GAL:C1	2.83	0.41
1:D:338:THR:HG1	1:D:345:ARG:HH12	1.61	0.41
1:G:230:PRO:HG3	1:G:460:HIS:CB	2.49	0.41
1:B:365:VAL:CG1	1:B:366:GLN:N	2.83	0.41
1:G:399:GLU:HB2	1:G:400:PRO:HA	2.02	0.41
1:H:454:PRO:HG2	1:H:457:TRP:CD1	2.56	0.41
1:I:307:ASN:O	1:I:308:TRP:HB2	2.21	0.41
1:C:277:GLN:OE1	1:C:279:SER:HB3	2.20	0.41
1:C:365:VAL:HG13	1:C:366:GLN:N	2.36	0.41
1:F:469:GLN:OE1	1:F:469:GLN:CA	2.68	0.41
1:I:479:ASN:HB2	1:I:510:PRO:HG3	2.02	0.41
1:B:461:PHE:O	1:B:462:TYR:C	2.64	0.41
1:G:283:ILE:O	1:G:284:CYS:HB2	2.21	0.41
1:G:356:VAL:C	1:G:358:PHE:N	2.79	0.41
1:H:336:GLN:OE1	1:H:375:PHE:CD1	2.68	0.41
2:K:2:GAL:H4	2:K:3:NAG:O5	2.21	0.41
1:B:390:GLN:O	1:B:390:GLN:HG3	2.18	0.41
1:G:323:THR:CG2	1:G:324:PRO:HD2	2.50	0.41
1:H:466:ALA:HA	1:H:467:PRO:HD3	1.95	0.41
1:I:388:VAL:HG11	1:I:438:MET:HE1	2.02	0.41
1:H:339:ARG:HD2	1:H:345:ARG:CB	2.51	0.41
1:I:336:GLN:OE1	1:I:375:PHE:HD1	2.03	0.41
2:N:2:GAL:H4	2:N:3:NAG:O5	2.21	0.41
1:I:282:ASP:CG	1:I:306:GLN:HE21	2.27	0.40
1:I:336:GLN:HG3	1:I:337:THR:N	2.35	0.40
1:J:390:GLN:CG	1:J:444:TYR:H	2.35	0.40
1:J:426:PHE:HA	1:J:427:PRO:HD3	1.96	0.40
1:H:241:ARG:HD3	1:H:450:ASP:O	2.21	0.40
1:H:288:GLY:HA3	1:H:302:ASN:O	2.21	0.40
1:A:344:THR:CG2	1:C:442:SER:H	2.34	0.40
1:B:390:GLN:HG2	1:B:444:TYR:N	2.36	0.40
1:E:319:ALA:HB1	1:E:320:PRO:CD	2.50	0.40
1:G:440:GLY:O	1:J:344:THR:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLN:N	1:D:261:PRO:CD	2.85	0.40
1:E:479:ASN:OD1	1:E:479:ASN:C	2.62	0.40
1:I:337:THR:O	1:I:345:ARG:HB3	2.21	0.40
1:B:390:GLN:HG2	1:B:445:PRO:N	2.36	0.40
1:C:453:LEU:HD11	1:C:495:GLY:O	2.21	0.40
1:F:319:ALA:O	1:F:320:PRO:C	2.65	0.40
1:H:224:THR:HG21	1:H:467:PRO:HG2	2.04	0.40
1:I:306:GLN:C	1:I:308:TRP:N	2.79	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:N:1:BGC:O2	2:N:2:GAL:O2[3_553]	1.29	0.91

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	307/311 (99%)	295 (96%)	11 (4%)	1 (0%)	36	55
1	B	306/311 (98%)	296 (97%)	10 (3%)	0	100	100
1	C	309/311 (99%)	296 (96%)	13 (4%)	0	100	100
1	D	305/311 (98%)	290 (95%)	15 (5%)	0	100	100
1	E	307/311 (99%)	296 (96%)	11 (4%)	0	100	100
1	F	306/311 (98%)	294 (96%)	12 (4%)	0	100	100
1	G	306/311 (98%)	286 (94%)	18 (6%)	2 (1%)	18	35
1	H	284/311 (91%)	270 (95%)	14 (5%)	0	100	100
1	I	277/311 (89%)	258 (93%)	19 (7%)	0	100	100
1	J	305/311 (98%)	292 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3012/3110 (97%)	2873 (95%)	136 (4%)	3 (0%)	48 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	357	HIS
1	G	412	ASP
1	A	445	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/272 (99%)	255 (94%)	15 (6%)	19 40
1	B	269/272 (99%)	250 (93%)	19 (7%)	13 29
1	C	269/272 (99%)	250 (93%)	19 (7%)	13 29
1	D	267/272 (98%)	253 (95%)	14 (5%)	21 43
1	E	271/272 (100%)	258 (95%)	13 (5%)	23 46
1	F	269/272 (99%)	253 (94%)	16 (6%)	18 37
1	G	267/272 (98%)	252 (94%)	15 (6%)	19 40
1	H	253/272 (93%)	232 (92%)	21 (8%)	10 23
1	I	238/272 (88%)	212 (89%)	26 (11%)	6 12
1	J	268/272 (98%)	252 (94%)	16 (6%)	17 36
All	All	2641/2720 (97%)	2467 (93%)	174 (7%)	15 32

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	287	ARG
1	A	291	THR
1	A	305	SER

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Mol	Chain	Res	Type
1	A	344	THR
1	A	356	VAL
1	A	364	SER
1	A	365	VAL
1	A	373	ASN
1	A	389	VAL
1	A	390	GLN
1	A	393	SER
1	A	470	SER
1	A	472	VAL
1	A	486	LEU
1	B	224	THR
1	B	231	ILE
1	B	279	SER
1	B	287	ARG
1	B	305	SER
1	B	339	ARG
1	B	364	SER
1	B	365	VAL
1	B	382	ARG
1	B	389	VAL
1	B	390	GLN
1	B	395	THR
1	B	412	ASP
1	B	413	SER
1	B	471	ASP
1	B	472	VAL
1	B	486	LEU
1	B	494	SER
1	B	522	ASN
1	C	221	GLU
1	C	244	ILE
1	C	248	LYS
1	C	287	ARG
1	C	291	THR
1	C	340	ARG
1	C	355	SER
1	C	364	SER
1	C	365	VAL
1	C	389	VAL
1	C	390	GLN
1	C	413	SER

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Mol	Chain	Res	Type
1	C	425	THR
1	C	444	TYR
1	C	447	MET
1	C	465	SER
1	C	469	GLN
1	C	486	LEU
1	C	493	LYS
1	D	234	VAL
1	D	287	ARG
1	D	291	THR
1	D	315	GLU
1	D	340	ARG
1	D	345	ARG
1	D	365	VAL
1	D	372	SER
1	D	373	ASN
1	D	389	VAL
1	D	390	GLN
1	D	442	SER
1	D	494	SER
1	D	523	GLN
1	E	224	THR
1	E	287	ARG
1	E	293	ILE
1	E	334	LEU
1	E	372	SER
1	E	373	ASN
1	E	374	ASP
1	E	389	VAL
1	E	390	GLN
1	E	413	SER
1	E	486	LEU
1	E	494	SER
1	E	523	GLN
1	F	224	THR
1	F	255	SER
1	F	279	SER
1	F	305	SER
1	F	339	ARG
1	F	340	ARG
1	F	345	ARG
1	F	355	SER

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Mol	Chain	Res	Type
1	F	365	VAL
1	F	373	ASN
1	F	389	VAL
1	F	416	VAL
1	F	422	VAL
1	F	447	MET
1	F	470	SER
1	F	486	LEU
1	G	234	VAL
1	G	248	LYS
1	G	287	ARG
1	G	290	VAL
1	G	334	LEU
1	G	345	ARG
1	G	355	SER
1	G	364	SER
1	G	366	GLN
1	G	373	ASN
1	G	389	VAL
1	G	390	GLN
1	G	393	SER
1	G	398	ASN
1	G	412	ASP
1	H	234	VAL
1	H	248	LYS
1	H	255	SER
1	H	287	ARG
1	H	289	ASP
1	H	310	ASN
1	H	329	LYS
1	H	340	ARG
1	H	347	HIS
1	H	348	LYS
1	H	350	THR
1	H	355	SER
1	H	356	VAL
1	H	380	ASN
1	H	382	ARG
1	H	399	GLU
1	H	413	SER
1	H	486	LEU
1	H	499	VAL

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Mol	Chain	Res	Type
1	H	509	ILE
1	H	523	GLN
1	I	224	THR
1	I	234	VAL
1	I	235	GLU
1	I	238	THR
1	I	257	PHE
1	I	278	LEU
1	I	287	ARG
1	I	305	SER
1	I	329	LYS
1	I	335	THR
1	I	338	THR
1	I	339	ARG
1	I	345	ARG
1	I	356	VAL
1	I	365	VAL
1	I	379	GLN
1	I	384	THR
1	I	402	GLN
1	I	416	VAL
1	I	438	MET
1	I	484	ARG
1	I	486	LEU
1	I	507	LEU
1	I	508	VAL
1	I	521	VAL
1	I	526	THR
1	J	255	SER
1	J	287	ARG
1	J	290	VAL
1	J	334	LEU
1	J	340	ARG
1	J	345	ARG
1	J	355	SER
1	J	356	VAL
1	J	365	VAL
1	J	372	SER
1	J	373	ASN
1	J	382	ARG
1	J	389	VAL
1	J	413	SER

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Mol	Chain	Res	Type
1	J	465	SER
1	J	523	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	A	366	GLN
1	B	357	HIS
1	B	463	GLN
1	B	469	GLN
1	B	523	GLN
1	C	469	GLN
1	C	501	HIS
1	C	505	HIS
1	C	512	ASN
1	D	310	ASN
1	D	366	GLN
1	D	390	GLN
1	D	417	HIS
1	D	505	HIS
1	E	309	ASN
1	E	331	GLN
1	E	397	GLN
1	E	417	HIS
1	E	505	HIS
1	E	523	GLN
1	F	297	GLN
1	F	366	GLN
1	F	373	ASN
1	F	390	GLN
1	F	523	GLN
1	G	263	ASN
1	G	347	HIS
1	G	366	GLN
1	G	390	GLN
1	G	398	ASN
1	G	492	HIS
1	H	336	GLN
1	H	347	HIS
1	H	366	GLN
1	H	463	GLN

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Mol	Chain	Res	Type
1	H	505	HIS
1	H	523	GLN
1	I	309	ASN
1	I	331	GLN
1	J	292	HIS
1	J	331	GLN
1	J	366	GLN
1	J	501	HIS
1	J	523	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

40 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	K	1	2	12,12,12	0.88	1 (8%)	17,17,17	1.87	3 (17%)
2	GAL	K	2	2	11,11,12	0.61	0	15,15,17	2.41	6 (40%)
2	NAG	K	3	2	14,14,15	1.55	2 (14%)	17,19,21	2.73	2 (11%)
2	GAL	K	4	2	11,11,12	1.47	2 (18%)	15,15,17	2.82	5 (33%)
2	FUC	K	5	2	10,10,11	0.40	0	14,14,16	0.85	0
2	BGC	L	1	2	12,12,12	0.59	0	17,17,17	1.76	4 (23%)
2	GAL	L	2	2	11,11,12	0.60	0	15,15,17	4.47	4 (26%)
2	NAG	L	3	2	14,14,15	1.77	1 (7%)	17,19,21	3.87	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	L	4	2	11,11,12	1.03	1 (9%)	15,15,17	2.06	5 (33%)
2	FUC	L	5	2	10,10,11	0.41	0	14,14,16	0.81	0
2	BGC	M	1	2	12,12,12	0.39	0	17,17,17	2.07	3 (17%)
2	GAL	M	2	2	11,11,12	0.43	0	15,15,17	2.29	4 (26%)
2	NAG	M	3	2	14,14,15	0.62	0	17,19,21	2.32	3 (17%)
2	GAL	M	4	2	11,11,12	0.81	0	15,15,17	2.19	4 (26%)
2	FUC	M	5	2	10,10,11	1.27	1 (10%)	14,14,16	2.69	3 (21%)
2	BGC	N	1	2	12,12,12	0.89	1 (8%)	17,17,17	1.87	3 (17%)
2	GAL	N	2	2	11,11,12	0.62	0	15,15,17	2.40	6 (40%)
2	NAG	N	3	2	14,14,15	1.56	2 (14%)	17,19,21	2.74	2 (11%)
2	GAL	N	4	2	11,11,12	1.47	2 (18%)	15,15,17	2.82	5 (33%)
2	FUC	N	5	2	10,10,11	0.40	0	14,14,16	0.84	0
2	BGC	O	1	2	12,12,12	0.49	0	17,17,17	0.76	1 (5%)
2	GAL	O	2	2	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
2	NAG	O	3	2	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
2	GAL	O	4	2	11,11,12	0.33	0	15,15,17	0.75	0
2	FUC	O	5	2	10,10,11	0.41	0	14,14,16	0.81	0
2	BGC	P	1	2	12,12,12	0.49	0	17,17,17	0.75	1 (5%)
2	GAL	P	2	2	11,11,12	0.37	0	15,15,17	0.81	0
2	NAG	P	3	2	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
2	GAL	P	4	2	11,11,12	0.33	0	15,15,17	0.75	0
2	FUC	P	5	2	10,10,11	0.41	0	14,14,16	0.81	0
2	BGC	Q	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	Q	2	2	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
2	NAG	Q	3	2	14,14,15	0.55	0	17,19,21	0.88	0
2	GAL	Q	4	2	11,11,12	0.33	0	15,15,17	0.76	1 (6%)
2	FUC	Q	5	2	10,10,11	0.42	0	14,14,16	0.81	0
2	BGC	R	1	2	12,12,12	0.49	0	17,17,17	0.76	1 (5%)
2	GAL	R	2	2	11,11,12	0.37	0	15,15,17	0.81	1 (6%)
2	NAG	R	3	2	14,14,15	0.55	0	17,19,21	1.00	0
2	GAL	R	4	2	11,11,12	0.33	0	15,15,17	0.75	0
2	FUC	R	5	2	10,10,11	0.41	0	14,14,16	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	-	2/2/19/22	0/1/1/1
2	NAG	K	3	2	-	0/6/23/26	0/1/1/1
2	GAL	K	4	2	-	2/2/19/22	0/1/1/1
2	FUC	K	5	2	-	-	0/1/1/1
2	BGC	L	1	2	-	2/2/22/22	0/1/1/1
2	GAL	L	2	2	-	1/2/19/22	0/1/1/1
2	NAG	L	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	4	2	-	2/2/19/22	0/1/1/1
2	FUC	L	5	2	-	-	0/1/1/1
2	BGC	M	1	2	-	2/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	NAG	M	3	2	-	0/6/23/26	0/1/1/1
2	GAL	M	4	2	-	1/2/19/22	0/1/1/1
2	FUC	M	5	2	-	-	0/1/1/1
2	BGC	N	1	2	-	2/2/22/22	0/1/1/1
2	GAL	N	2	2	-	2/2/19/22	0/1/1/1
2	NAG	N	3	2	-	0/6/23/26	0/1/1/1
2	GAL	N	4	2	-	2/2/19/22	0/1/1/1
2	FUC	N	5	2	-	-	0/1/1/1
2	BGC	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	0/2/19/22	0/1/1/1
2	NAG	O	3	2	-	1/6/23/26	0/1/1/1
2	GAL	O	4	2	-	2/2/19/22	0/1/1/1
2	FUC	O	5	2	-	-	0/1/1/1
2	BGC	P	1	2	-	1/2/22/22	0/1/1/1
2	GAL	P	2	2	-	2/2/19/22	0/1/1/1
2	NAG	P	3	2	-	1/6/23/26	0/1/1/1
2	GAL	P	4	2	-	0/2/19/22	0/1/1/1
2	FUC	P	5	2	-	-	0/1/1/1
2	BGC	Q	1	2	-	2/2/22/22	0/1/1/1
2	GAL	Q	2	2	-	2/2/19/22	0/1/1/1
2	NAG	Q	3	2	-	0/6/23/26	0/1/1/1
2	GAL	Q	4	2	-	2/2/19/22	0/1/1/1
2	FUC	Q	5	2	-	-	0/1/1/1
2	BGC	R	1	2	-	0/2/22/22	0/1/1/1
2	GAL	R	2	2	-	2/2/19/22	0/1/1/1
2	NAG	R	3	2	-	2/6/23/26	0/1/1/1
2	GAL	R	4	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	R	5	2	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	NAG	O3-C3	5.82	1.57	1.43
2	N	3	NAG	C1-C2	4.44	1.58	1.52
2	K	3	NAG	C1-C2	4.38	1.58	1.52
2	N	4	GAL	O5-C5	-3.30	1.37	1.43
2	K	4	GAL	O5-C5	-3.30	1.37	1.43
2	N	4	GAL	O5-C1	-3.28	1.38	1.43
2	K	4	GAL	O5-C1	-3.26	1.38	1.43
2	L	4	GAL	O5-C5	-2.79	1.38	1.43
2	N	1	BGC	C4-C5	-2.79	1.47	1.53
2	K	1	BGC	C4-C5	-2.77	1.47	1.53
2	M	5	FUC	O5-C5	-2.56	1.38	1.43
2	K	3	NAG	C3-C2	2.55	1.57	1.52
2	N	3	NAG	C3-C2	2.54	1.57	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GAL	O3-C3-C2	-12.73	84.07	110.05
2	L	2	GAL	O3-C3-C4	9.94	133.81	110.38
2	L	3	NAG	O3-C3-C4	-9.50	87.98	110.38
2	L	3	NAG	O3-C3-C2	9.14	128.38	109.40
2	M	5	FUC	C6-C5-C4	-9.10	96.44	113.08
2	N	3	NAG	C6-C5-C4	-8.97	91.00	113.02
2	K	3	NAG	C6-C5-C4	-8.95	91.04	113.02
2	M	3	NAG	C6-C5-C4	-7.37	94.92	113.02
2	N	4	GAL	C1-O5-C5	-7.14	102.62	112.19
2	K	4	GAL	C1-O5-C5	-7.13	102.63	112.19
2	K	2	GAL	O5-C5-C6	5.66	118.68	107.66
2	N	2	GAL	O5-C5-C6	5.65	118.67	107.66
2	M	1	BGC	O4-C4-C5	5.35	122.51	109.32
2	L	3	NAG	O5-C1-C2	-5.30	103.09	111.29
2	K	4	GAL	C1-C2-C3	5.15	117.15	109.64
2	N	4	GAL	C1-C2-C3	5.15	117.15	109.64
2	K	3	NAG	O5-C1-C2	-5.09	103.41	111.29
2	N	3	NAG	O5-C1-C2	-5.09	103.41	111.29
2	L	2	GAL	O5-C1-C2	-5.01	98.84	110.79
2	L	4	GAL	C1-C2-C3	4.92	116.81	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	4	GAL	C1-C2-C3	4.82	116.67	109.64
2	M	1	BGC	C3-C4-C5	-4.72	101.67	110.23
2	M	2	GAL	C1-O5-C5	-4.60	106.02	112.19
2	K	1	BGC	C6-C5-C4	-4.58	101.77	113.02
2	N	1	BGC	C6-C5-C4	-4.57	101.80	113.02
2	M	4	GAL	C6-C5-C4	-4.48	102.02	113.02
2	M	2	GAL	O5-C5-C4	-4.40	100.11	110.83
2	L	4	GAL	C1-O5-C5	-4.23	106.52	112.19
2	L	1	BGC	O5-C1-C2	-4.10	103.10	110.30
2	K	4	GAL	O5-C5-C4	-4.09	100.87	110.83
2	N	4	GAL	O5-C5-C4	-4.09	100.89	110.83
2	K	1	BGC	C3-C4-C5	-4.07	102.85	110.23
2	N	1	BGC	C3-C4-C5	-4.07	102.86	110.23
2	K	2	GAL	C1-O5-C5	-3.82	107.06	112.19
2	N	2	GAL	C1-O5-C5	-3.82	107.07	112.19
2	M	3	NAG	C4-C3-C2	-3.80	105.45	111.02
2	M	2	GAL	O5-C5-C6	3.74	114.94	107.66
2	N	2	GAL	O5-C5-C4	-3.65	101.94	110.83
2	K	2	GAL	O5-C5-C4	-3.65	101.94	110.83
2	M	4	GAL	O5-C1-C2	-3.56	102.29	110.79
2	L	1	BGC	O1-C1-C2	3.56	119.31	108.98
2	M	2	GAL	C2-C3-C4	-3.42	104.84	110.86
2	L	3	NAG	O5-C5-C6	2.90	113.31	107.66
2	K	1	BGC	O4-C4-C3	-2.89	103.56	110.38
2	L	3	NAG	O4-C4-C3	-2.89	103.56	110.38
2	N	1	BGC	O4-C4-C3	-2.89	103.57	110.38
2	M	1	BGC	O5-C5-C4	-2.84	104.59	109.70
2	M	4	GAL	O2-C2-C3	-2.77	104.42	110.15
2	K	2	GAL	C6-C5-C4	-2.76	106.23	113.02
2	N	2	GAL	C6-C5-C4	-2.76	106.24	113.02
2	L	3	NAG	C1-O5-C5	-2.64	108.65	112.19
2	K	2	GAL	C3-C4-C5	-2.63	105.47	110.23
2	L	2	GAL	C6-C5-C4	-2.62	106.59	113.02
2	N	2	GAL	C3-C4-C5	-2.61	105.50	110.23
2	L	3	NAG	C3-C4-C5	2.55	114.86	110.23
2	L	4	GAL	O5-C5-C4	-2.37	105.05	110.83
2	M	5	FUC	O5-C5-C4	2.37	113.82	109.55
2	M	3	NAG	C1-O5-C5	-2.31	109.09	112.19
2	L	3	NAG	O6-C6-C5	-2.29	103.53	111.33
2	N	4	GAL	C6-C5-C4	2.25	118.54	113.02
2	K	4	GAL	C6-C5-C4	2.24	118.52	113.02
2	L	3	NAG	O7-C7-N2	2.21	125.89	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	BGC	C1-C2-C3	-2.18	105.91	110.36
2	M	5	FUC	C1-C2-C3	-2.16	106.50	109.64
2	O	1	BGC	C1-O5-C5	-2.16	109.47	113.65
2	Q	1	BGC	C1-O5-C5	-2.16	109.47	113.65
2	R	1	BGC	C1-O5-C5	-2.15	109.49	113.65
2	P	1	BGC	C1-O5-C5	-2.13	109.54	113.65
2	L	4	GAL	O3-C3-C4	-2.11	105.40	110.38
2	N	4	GAL	O5-C5-C6	-2.10	103.57	107.66
2	K	4	GAL	O5-C5-C6	-2.09	103.59	107.66
2	L	3	NAG	C4-C3-C2	2.08	114.07	111.02
2	K	2	GAL	O3-C3-C4	-2.06	105.52	110.38
2	N	2	GAL	O3-C3-C4	-2.04	105.56	110.38
2	Q	4	GAL	C1-O5-C5	-2.04	109.45	112.19
2	R	2	GAL	C1-O5-C5	-2.03	109.47	112.19
2	O	3	NAG	C1-O5-C5	-2.02	109.47	112.19
2	P	3	NAG	C1-O5-C5	-2.01	109.49	112.19
2	Q	2	GAL	C1-O5-C5	-2.01	109.50	112.19
2	L	1	BGC	O5-C5-C4	2.01	113.31	109.70
2	L	4	GAL	O4-C4-C3	-2.00	105.65	110.38
2	O	2	GAL	C1-O5-C5	-2.00	109.50	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	2	GAL	O5-C5-C6-O6
2	Q	2	GAL	O5-C5-C6-O6
2	Q	1	BGC	C4-C5-C6-O6
2	R	2	GAL	C4-C5-C6-O6
2	M	1	BGC	O5-C5-C6-O6
2	L	1	BGC	O5-C5-C6-O6
2	M	1	BGC	C4-C5-C6-O6
2	L	3	NAG	O5-C5-C6-O6
2	O	4	GAL	O5-C5-C6-O6
2	L	3	NAG	C4-C5-C6-O6
2	O	4	GAL	C4-C5-C6-O6
2	Q	2	GAL	C4-C5-C6-O6
2	K	1	BGC	O5-C5-C6-O6
2	N	1	BGC	O5-C5-C6-O6
2	Q	4	GAL	O5-C5-C6-O6
2	Q	1	BGC	O5-C5-C6-O6
2	K	4	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	N	4	GAL	O5-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6
2	L	1	BGC	C4-C5-C6-O6
2	N	1	BGC	C4-C5-C6-O6
2	P	2	GAL	C4-C5-C6-O6
2	K	2	GAL	O5-C5-C6-O6
2	N	2	GAL	O5-C5-C6-O6
2	L	2	GAL	O5-C5-C6-O6
2	P	2	GAL	O5-C5-C6-O6
2	N	4	GAL	C4-C5-C6-O6
2	K	4	GAL	C4-C5-C6-O6
2	R	4	GAL	O5-C5-C6-O6
2	L	4	GAL	O5-C5-C6-O6
2	K	2	GAL	C4-C5-C6-O6
2	N	2	GAL	C4-C5-C6-O6
2	L	4	GAL	C4-C5-C6-O6
2	R	3	NAG	C4-C5-C6-O6
2	R	3	NAG	O5-C5-C6-O6
2	M	4	GAL	O5-C5-C6-O6
2	P	3	NAG	C4-C5-C6-O6
2	Q	4	GAL	C4-C5-C6-O6
2	O	3	NAG	C4-C5-C6-O6
2	P	1	BGC	O5-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 68 short contacts:

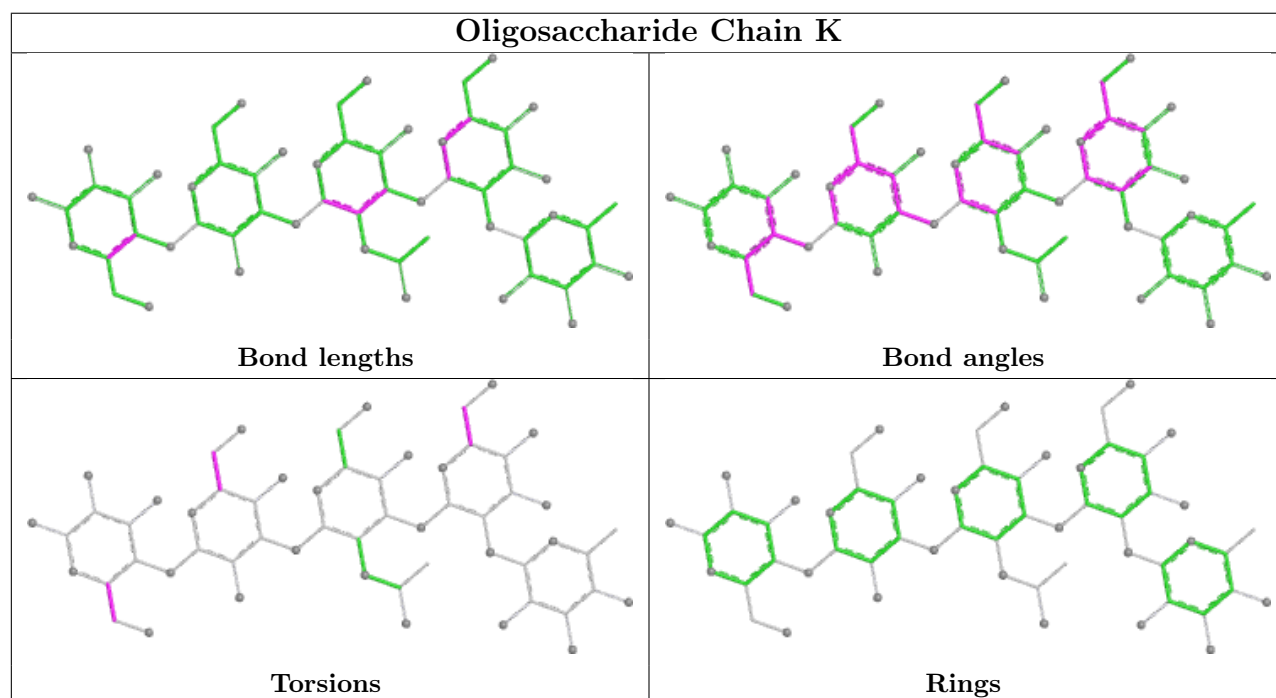
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	4	GAL	1	0
2	Q	4	GAL	2	0
2	R	4	GAL	1	0
2	N	1	BGC	9	1
2	K	1	BGC	8	0
2	O	2	GAL	2	0
2	P	3	NAG	2	0
2	Q	2	GAL	1	0
2	R	5	FUC	5	0
2	Q	1	BGC	1	0
2	M	3	NAG	2	0
2	R	3	NAG	5	0
2	Q	3	NAG	2	0
2	N	3	NAG	2	0

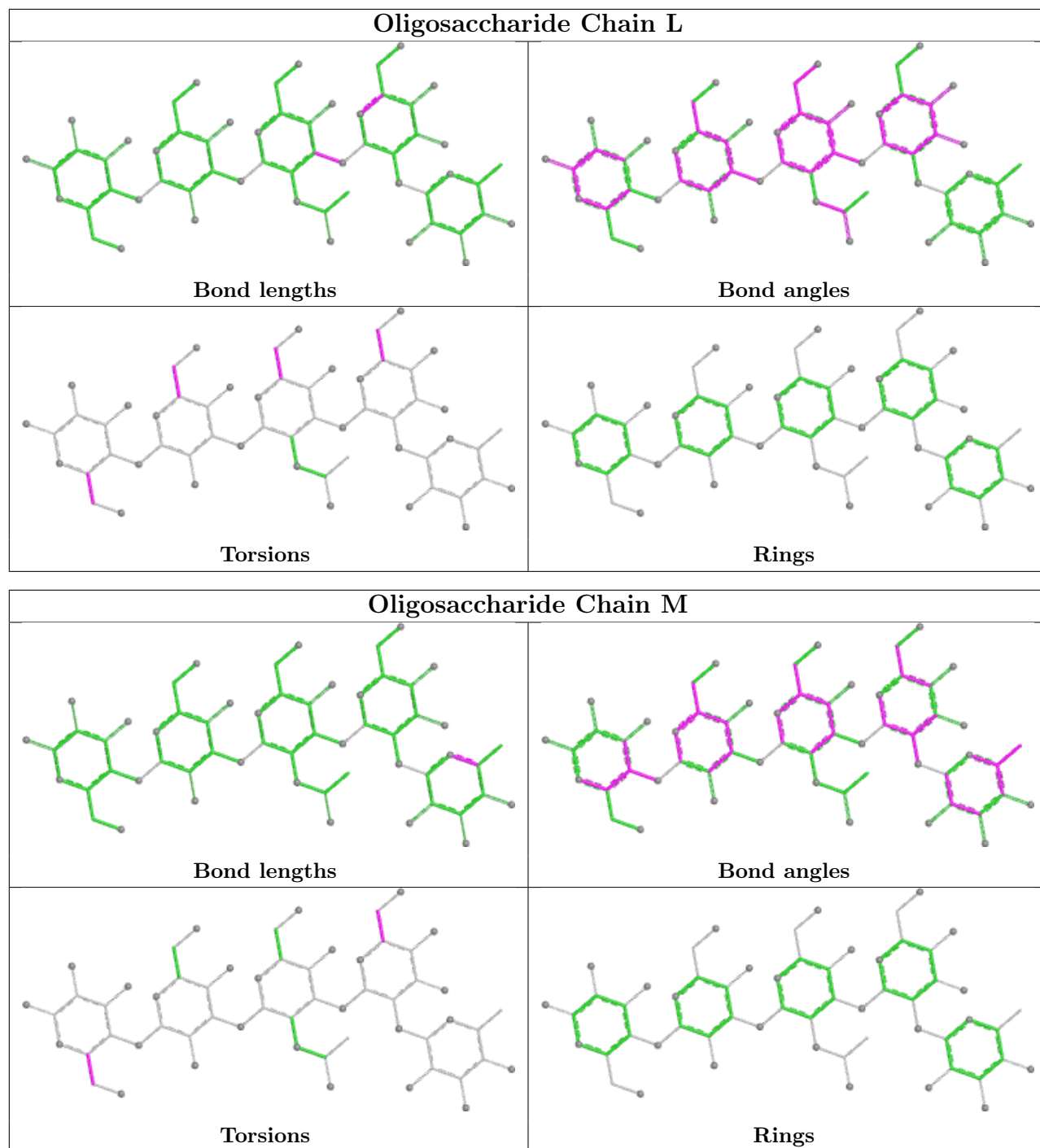
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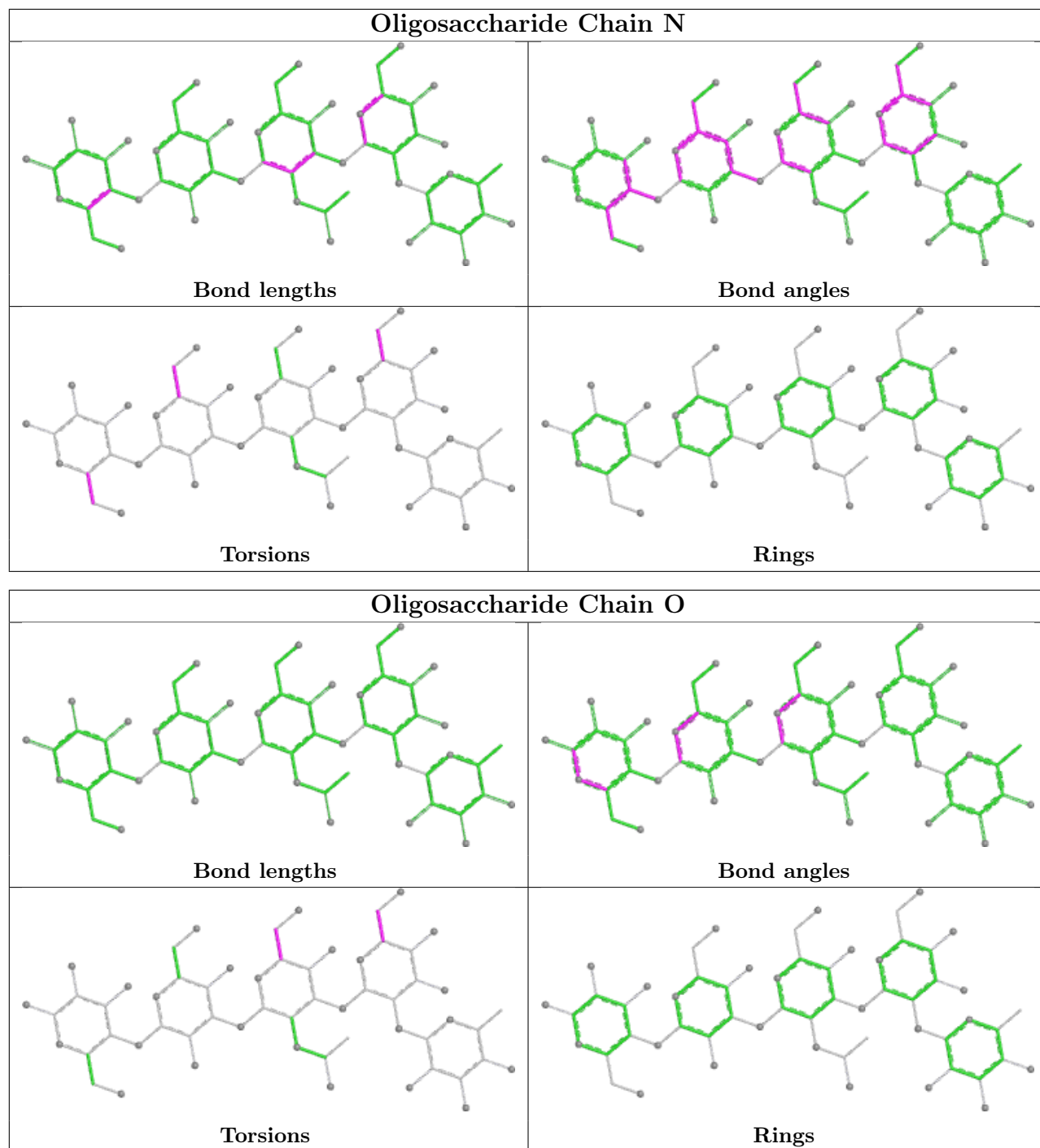
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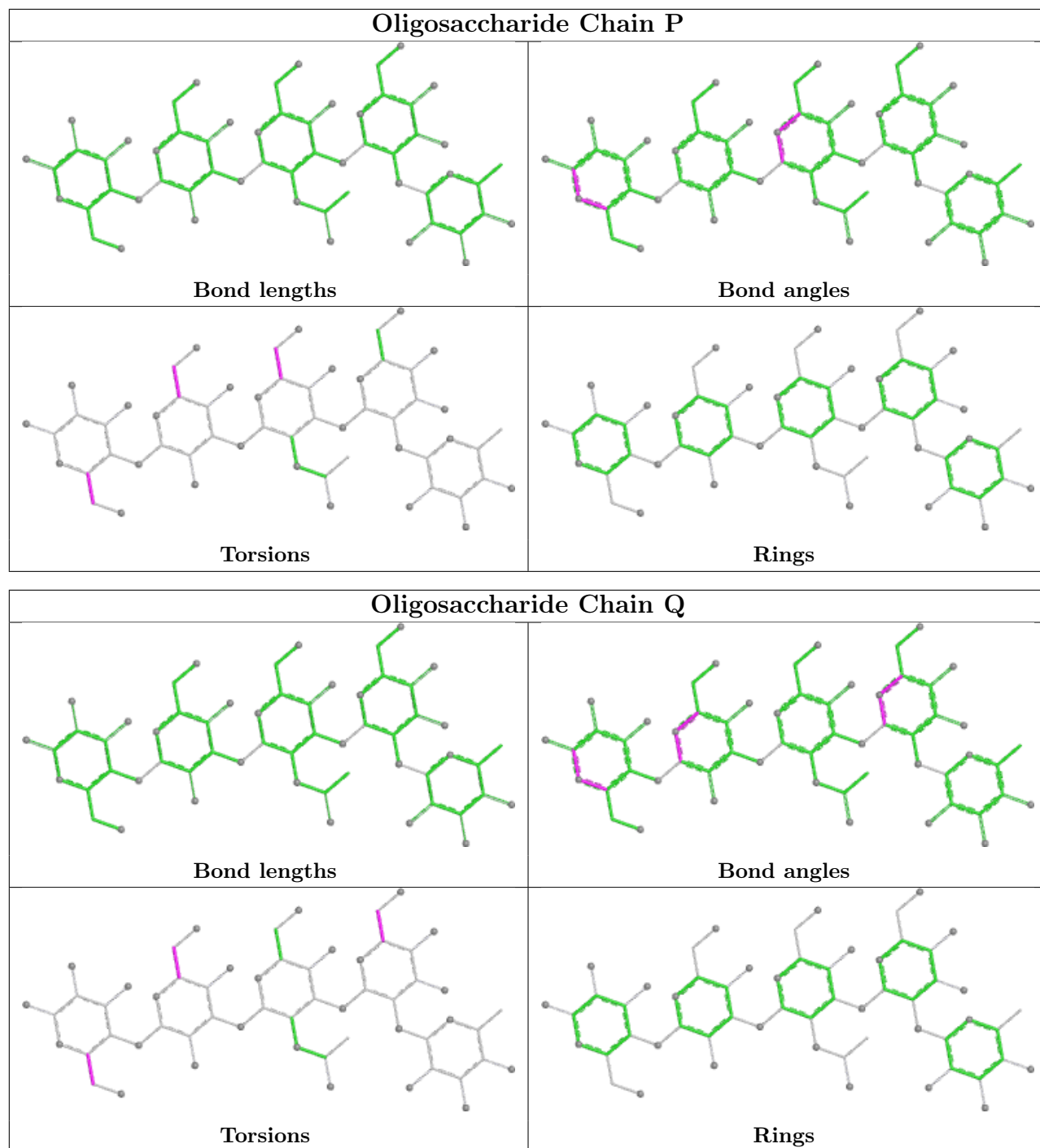
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	2	GAL	9	0
2	L	1	BGC	4	0
2	K	2	GAL	9	0
2	L	5	FUC	1	0
2	N	4	GAL	1	0
2	P	4	GAL	1	0
2	K	3	NAG	2	0
2	O	3	NAG	3	0
2	L	2	GAL	3	0
2	N	2	GAL	10	1
2	R	1	BGC	7	0
2	P	1	BGC	4	0
2	O	5	FUC	10	0
2	Q	5	FUC	4	0
2	P	2	GAL	6	0
2	M	2	GAL	2	0

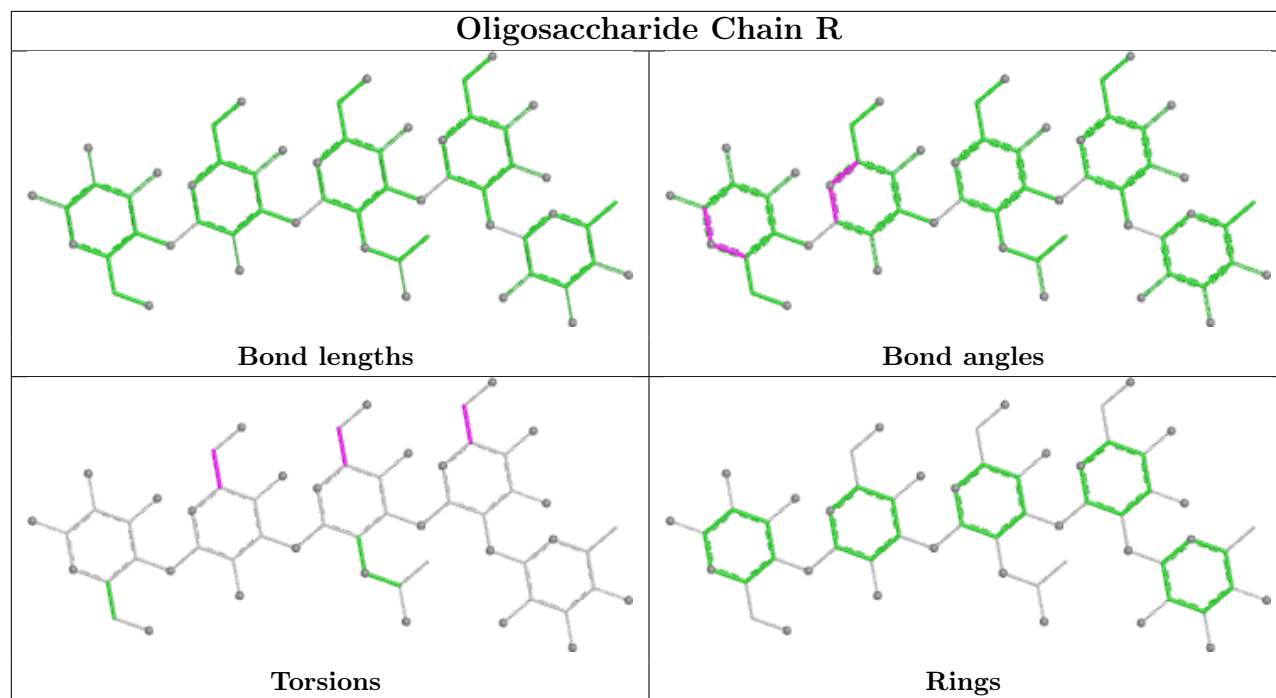
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [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	309/311 (99%)	-0.55	5 (1%) 70 64	29, 41, 66, 80	0
1	B	308/311 (99%)	-0.57	3 (0%) 79 75	32, 44, 67, 78	0
1	C	311/311 (100%)	-0.52	1 (0%) 90 89	30, 45, 68, 93	0
1	D	307/311 (98%)	-0.51	2 (0%) 84 80	29, 45, 77, 95	0
1	E	309/311 (99%)	-0.53	2 (0%) 85 83	32, 47, 76, 89	0
1	F	308/311 (99%)	-0.29	1 (0%) 90 89	38, 57, 87, 103	0
1	G	308/311 (99%)	-0.32	6 (1%) 66 59	41, 57, 82, 118	0
1	H	292/311 (93%)	-0.05	13 (4%) 38 30	34, 59, 93, 117	0
1	I	285/311 (91%)	0.63	29 (10%) 12 10	52, 83, 121, 146	0
1	J	307/311 (98%)	-0.35	3 (0%) 79 75	38, 53, 84, 105	0
All	All	3044/3110 (97%)	-0.31	65 (2%) 63 55	29, 52, 89, 146	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	SER	5.9
1	B	471	ASP	5.0
1	I	523	GLN	4.6
1	H	439	PRO	4.2
1	A	307	ASN	4.1
1	H	531	GLY	4.1
1	H	447	MET	4.1
1	I	257	PHE	4.1
1	I	388	VAL	4.0
1	I	337	THR	3.7
1	I	254	SER	3.5
1	I	524	PHE	3.5
1	I	256	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	440	GLY	3.5
1	I	376	GLU	3.5
1	H	371	THR	3.5
1	I	375	PHE	3.4
1	H	340	ARG	3.4
1	I	231	ILE	3.4
1	I	258	VAL	3.3
1	F	470	SER	3.2
1	G	442	SER	3.2
1	H	376	GLU	3.1
1	I	299	TYR	3.1
1	H	346	GLY	3.1
1	I	344	THR	3.1
1	E	222	SER	3.0
1	A	531	GLY	3.0
1	I	338	THR	3.0
1	J	531	GLY	2.9
1	J	445	PRO	2.9
1	H	341	ASP	2.8
1	H	399	GLU	2.7
1	G	356	VAL	2.7
1	G	412	ASP	2.7
1	A	412	ASP	2.7
1	G	411	ARG	2.7
1	I	248	LYS	2.6
1	I	527	LEU	2.6
1	G	441	CYS	2.6
1	A	518	ASP	2.6
1	I	486	LEU	2.5
1	I	530	MET	2.5
1	I	255	SER	2.4
1	I	259	VAL	2.4
1	G	306	GLN	2.4
1	I	525	TYR	2.4
1	I	335	THR	2.4
1	H	348	LYS	2.4
1	C	495	GLY	2.3
1	I	345	ARG	2.3
1	I	333	VAL	2.3
1	A	231	ILE	2.2
1	H	389	VAL	2.2
1	I	334	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	221	GLU	2.2
1	E	523	GLN	2.1
1	I	485	VAL	2.1
1	D	531	GLY	2.1
1	H	337	THR	2.1
1	J	339	ARG	2.1
1	I	528	ALA	2.0
1	I	347	HIS	2.0
1	B	310	ASN	2.0
1	D	370	ASP	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
2	BGC	M	1	12/12	-0.03	0.17	149,153,153,153	0
2	BGC	Q	1	12/12	0.17	0.18	145,149,150,150	0
2	BGC	O	1	12/12	0.19	0.17	145,146,147,147	0
2	NAG	L	3	14/15	0.26	0.28	155,162,164,166	0
2	BGC	P	1	12/12	0.35	0.13	162,163,164,164	0
2	GAL	M	2	11/12	0.35	0.17	147,151,153,153	0
2	GAL	L	4	11/12	0.36	0.19	137,144,147,148	0
2	GAL	R	2	11/12	0.36	0.18	151,152,154,154	0
2	BGC	K	1	12/12	0.37	0.13	139,141,141,141	0
2	BGC	N	1	12/12	0.38	0.17	139,141,141,141	0
2	GAL	N	2	11/12	0.38	0.18	132,135,137,137	0
2	GAL	Q	2	11/12	0.43	0.17	145,146,147,148	0
2	GAL	K	4	11/12	0.43	0.17	115,119,122,122	0
2	GAL	R	4	11/12	0.44	0.20	134,136,138,139	0
2	NAG	R	3	14/15	0.47	0.27	142,147,149,149	0
2	GAL	L	2	11/12	0.47	0.15	169,174,175,176	0
2	GAL	Q	4	11/12	0.48	0.16	129,132,135,135	0
2	GAL	P	2	11/12	0.48	0.14	158,161,163,163	0

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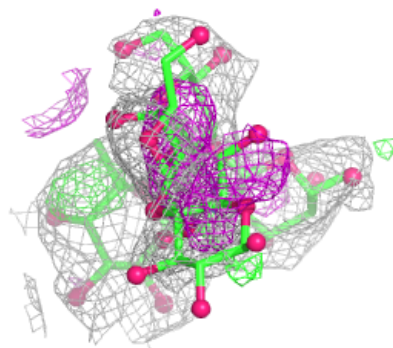
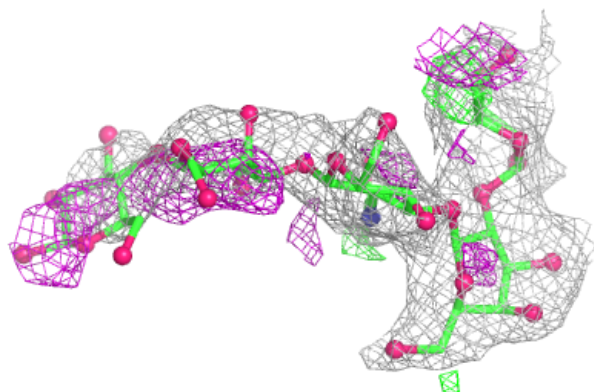
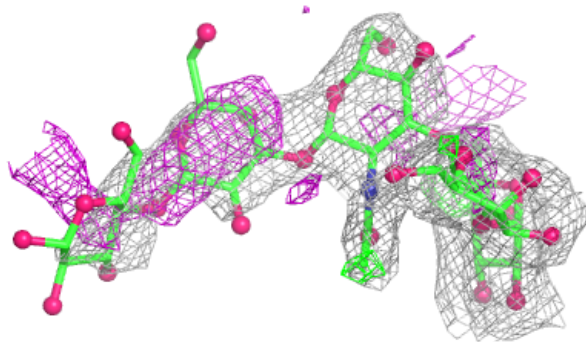
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	O	2	11/12	0.49	0.16	142,146,147,147	0
2	NAG	P	3	14/15	0.49	0.23	147,153,156,156	0
2	GAL	O	4	11/12	0.50	0.15	124,129,131,131	0
2	NAG	N	3	14/15	0.50	0.22	124,127,129,130	0
2	GAL	N	4	11/12	0.51	0.19	115,119,122,122	0
2	BGC	R	1	12/12	0.54	0.26	155,158,159,159	0
2	GAL	K	2	11/12	0.55	0.14	132,135,137,137	0
2	BGC	L	1	12/12	0.58	0.22	178,181,181,182	0
2	NAG	K	3	14/15	0.59	0.20	124,127,129,130	0
2	GAL	P	4	11/12	0.63	0.16	136,138,141,142	0
2	GAL	M	4	11/12	0.67	0.14	130,133,135,135	0
2	NAG	O	3	14/15	0.68	0.23	132,135,138,139	0
2	FUC	O	5	10/11	0.70	0.26	112,116,117,119	0
2	NAG	Q	3	14/15	0.75	0.22	138,142,143,143	0
2	FUC	N	5	10/11	0.75	0.21	101,104,107,109	0
2	NAG	M	3	14/15	0.75	0.18	137,140,142,144	0
2	FUC	Q	5	10/11	0.79	0.20	122,123,124,125	0
2	FUC	L	5	10/11	0.81	0.24	123,126,129,131	0
2	FUC	K	5	10/11	0.81	0.20	101,104,107,109	0
2	FUC	R	5	10/11	0.84	0.16	129,131,131,132	0
2	FUC	M	5	10/11	0.88	0.18	121,123,124,126	0
2	FUC	P	5	10/11	0.88	0.20	129,130,132,133	0

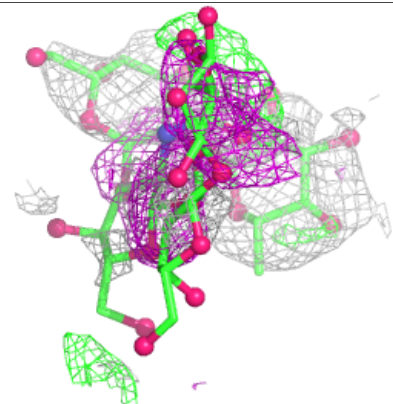
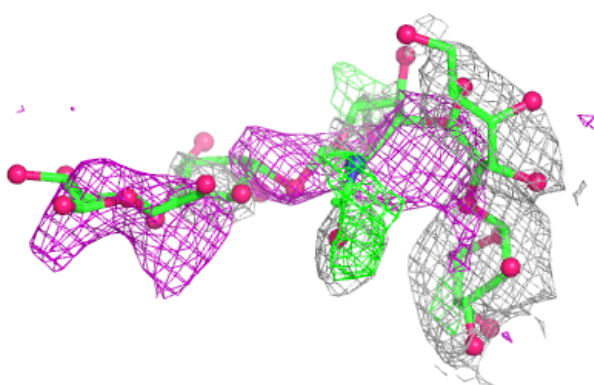
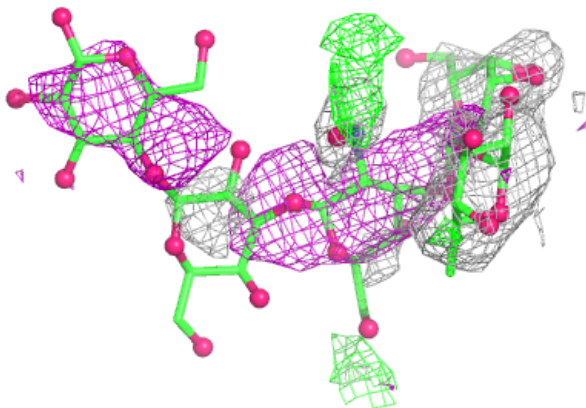
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

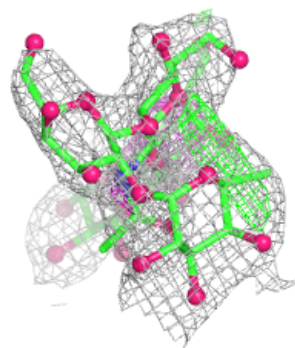
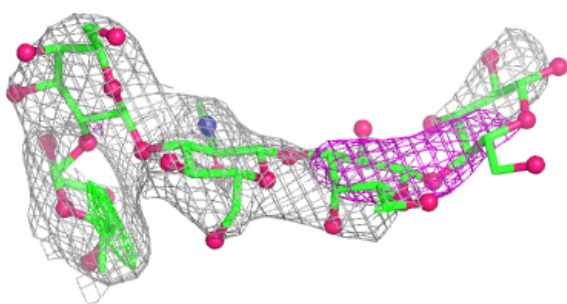
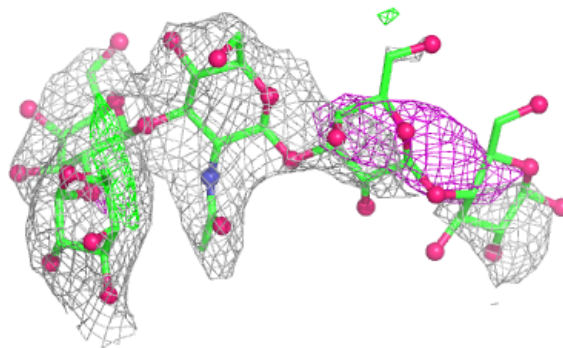
**Electron density around Chain L:**

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

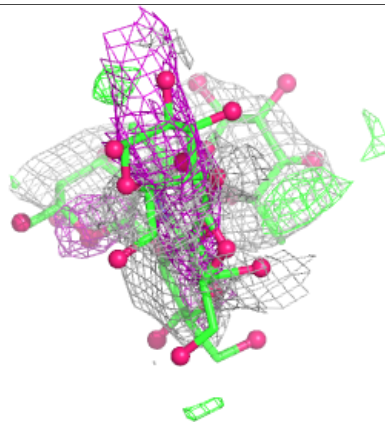
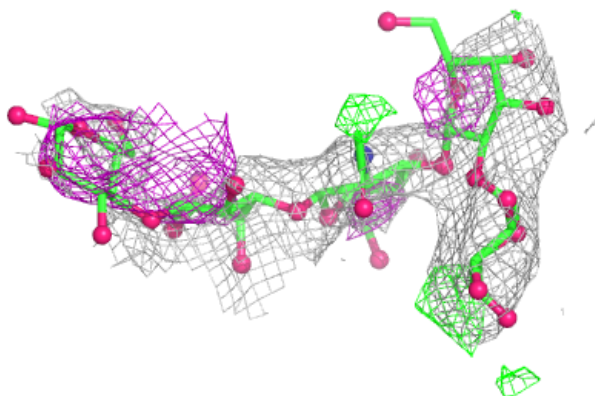
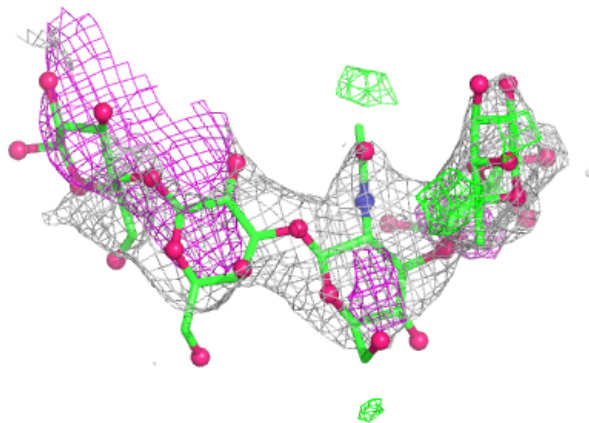


Electron density around Chain M:

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

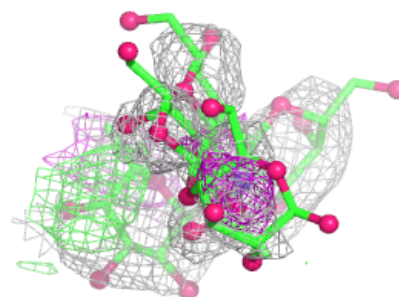
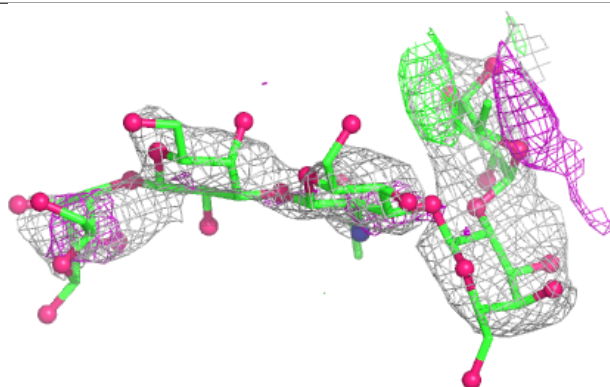
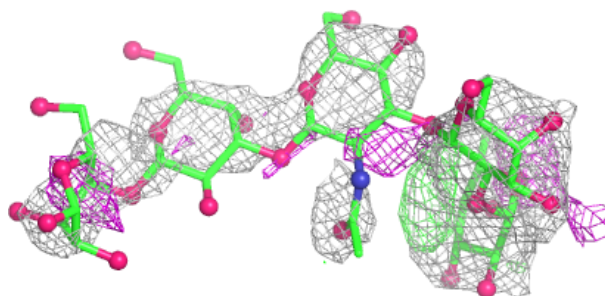
**Electron density around Chain N:**

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

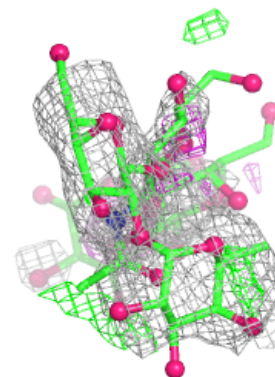
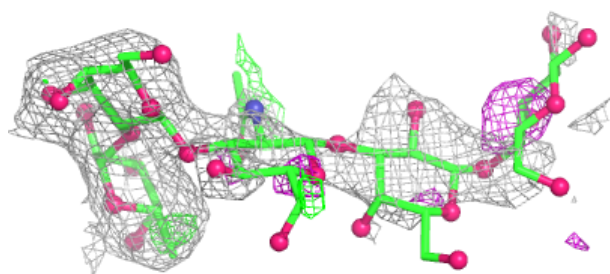
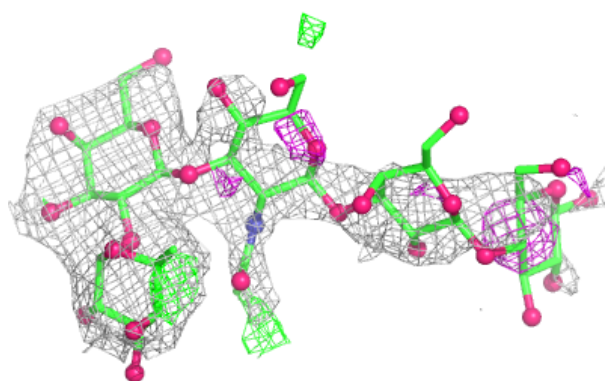


Electron density around Chain O:

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

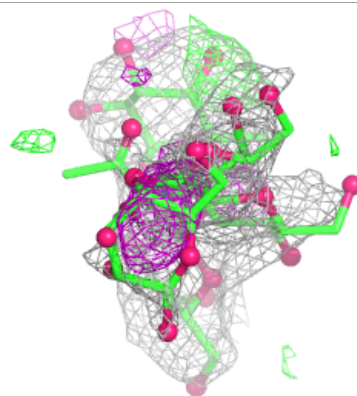
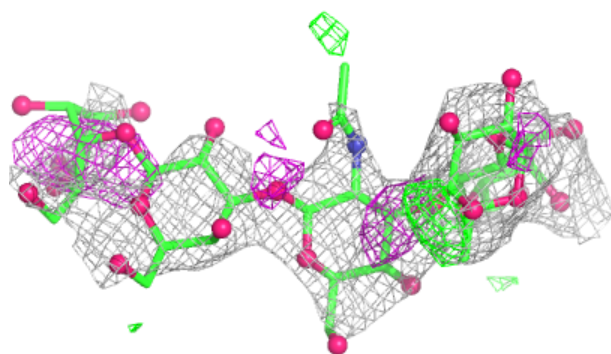
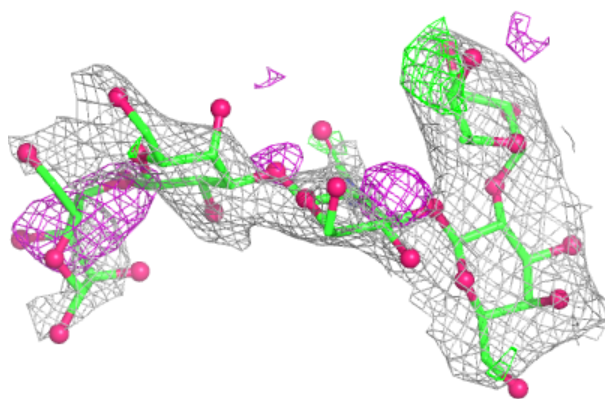
**Electron density around Chain P:**

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

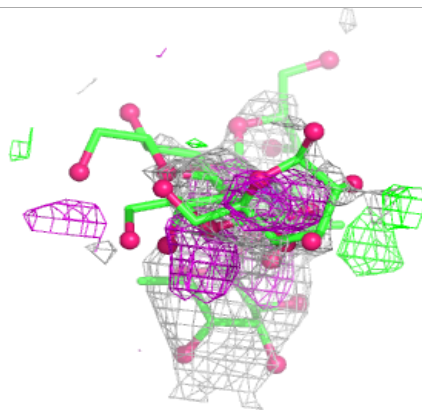
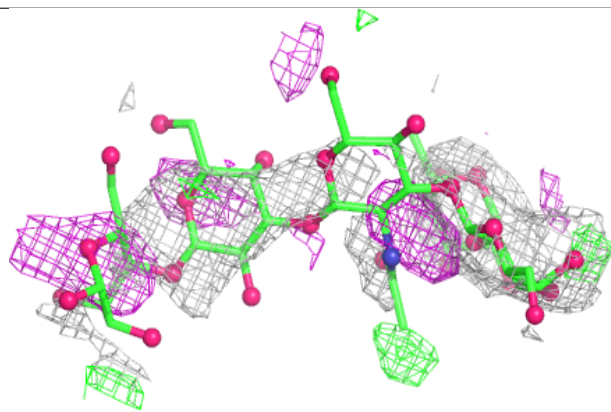
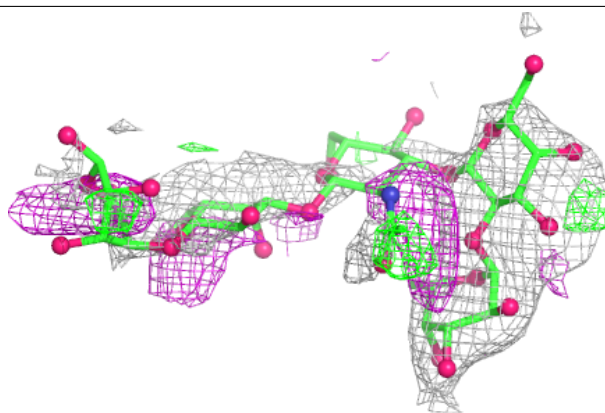


Electron density around Chain Q:

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

**Electron density around Chain R:**

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.