



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:08 AM UTC

PDB ID : 3SEJ / pdb_00003sej
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to Secretor Lewis HBGA (LeB)
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.
Deposited on : 2011-06-10
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

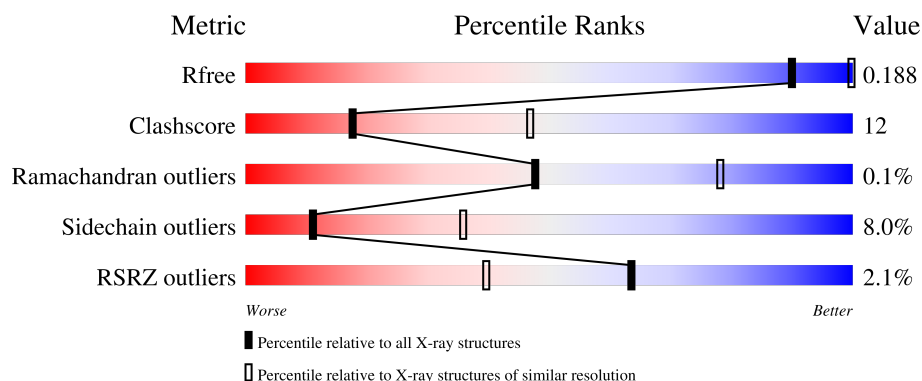
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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.



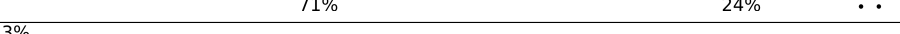
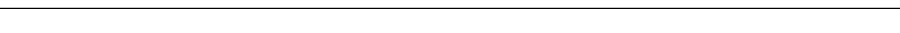
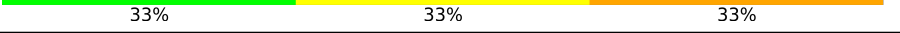
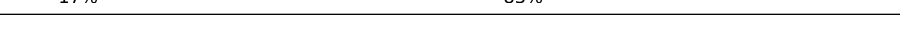
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	311	% 76% 21% ..
1	B	311	76% 21% ..
1	C	311	79% 19% .
1	D	311	% 75% 20% ..
1	E	311	74% 22% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	
2	K	6	
2	L	6	
2	M	6	
2	N	6	
2	O	6	
2	P	6	
2	Q	6	
2	R	6	

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	FUC	M	5	-	-	X	-
2	FUC	M	6	-	-	X	-
2	FUC	N	5	-	-	X	-
2	FUC	N	6	-	-	X	-
2	FUC	Q	5	-	-	X	-
2	BGC	R	1	-	-	X	-
2	GAL	R	2	-	-	X	-
2	FUC	R	6	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24569 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
			2403	1517	415	461	10			
1	B	307	Total	C	N	O	S	0	0	0
			2382	1505	407	460	10			
1	C	311	Total	C	N	O	S	0	0	0
			2416	1524	417	465	10			
1	D	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	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
			2380	1505	407	458	10			
1	H	300	Total	C	N	O	S	0	0	0
			2291	1456	393	432	10			
1	I	284	Total	C	N	O	S	0	0	0
			2128	1347	371	402	8			
1	J	307	Total	C	N	O	S	0	0	0
			2383	1506	410	457	10			

There are 30 discrepancies between the modelled and reference sequences:

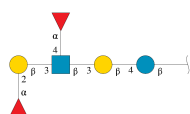
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER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

Continued on next page...

Continued from previous page...

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)-[alpha-L-fucopyranose-(1-4)]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	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	L	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	M	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	N	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	O	6	Total	C	N	O	0	0	0
			68	38	1	29			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	Q	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	R	6	Total	C	N	O	0	0	0
			68	38	1	29			

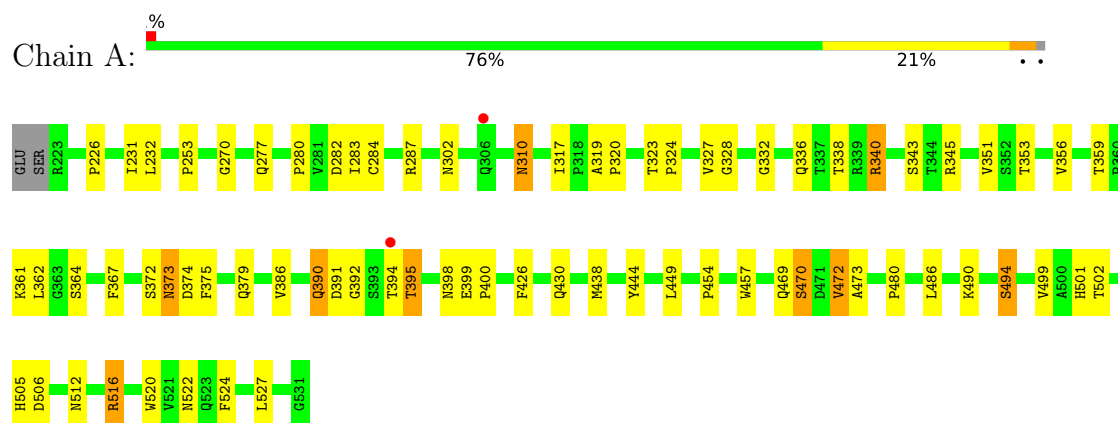
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	54	Total	O	0	0
			54	54		
3	C	53	Total	O	0	0
			53	53		
3	D	57	Total	O	0	0
			57	57		
3	E	46	Total	O	0	0
			46	46		
3	F	45	Total	O	0	0
			45	45		
3	G	41	Total	O	0	0
			41	41		
3	H	36	Total	O	0	0
			36	36		
3	I	18	Total	O	0	0
			18	18		
3	J	39	Total	O	0	0
			39	39		

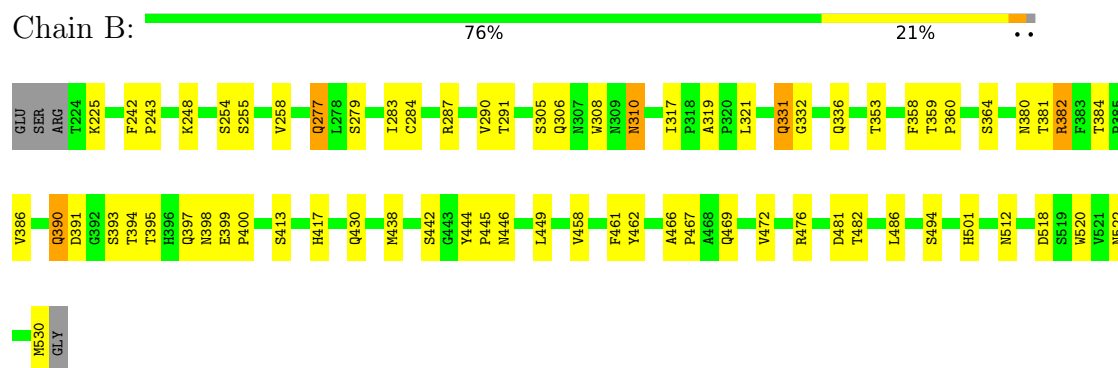
3 Residue-property plots

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.

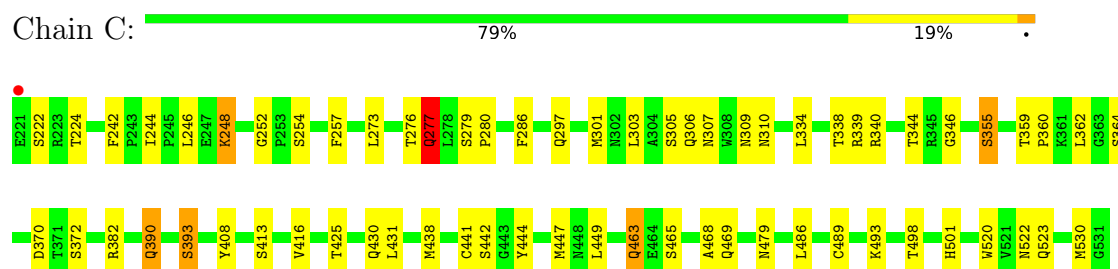
• Molecule 1: Capsid



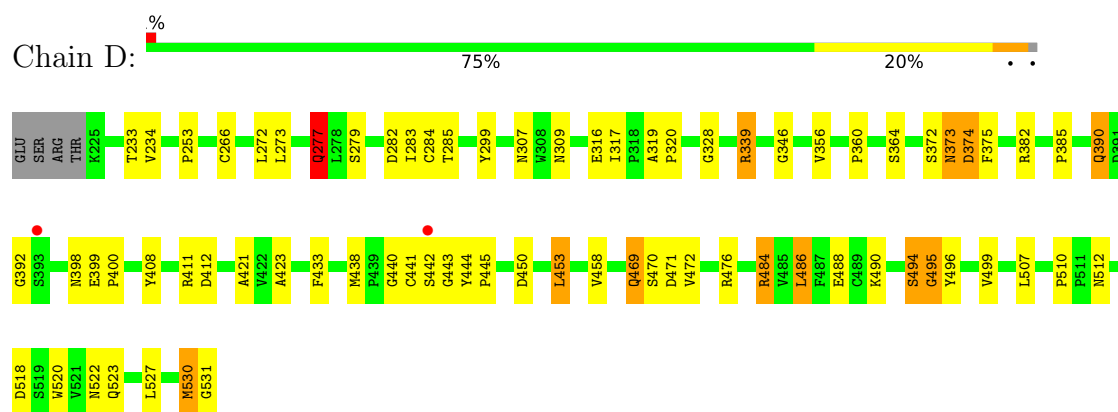
• Molecule 1: Capsid



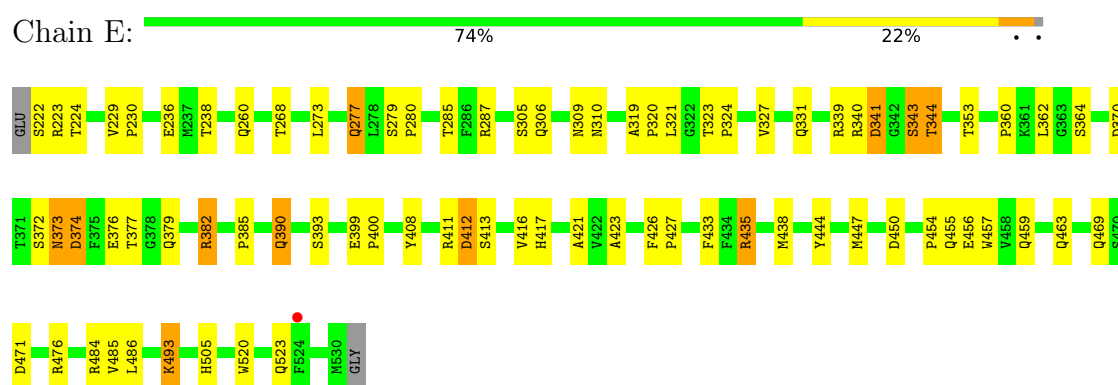
• Molecule 1: Capsid



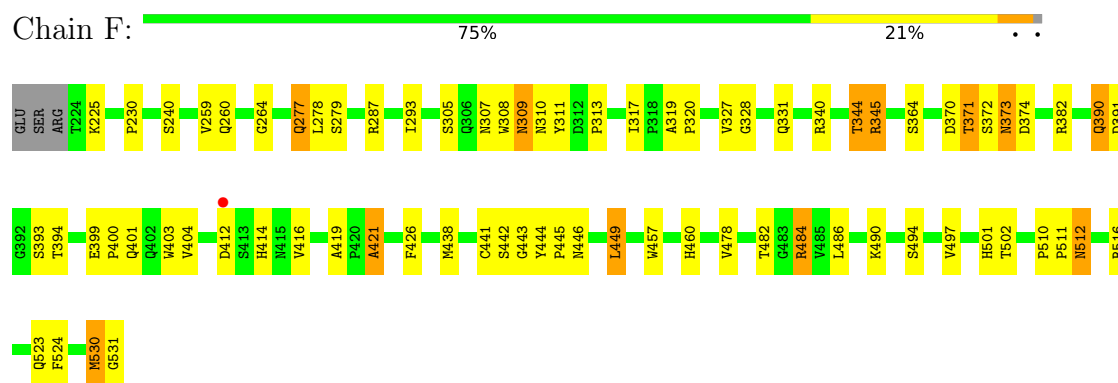
• Molecule 1: Capsid



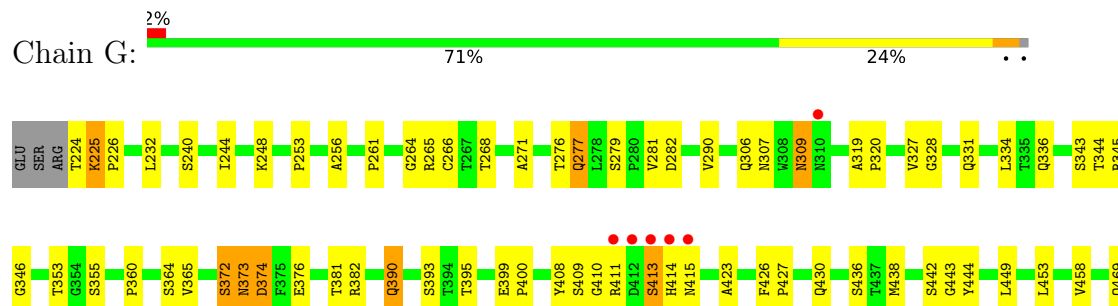
• Molecule 1: Capsid

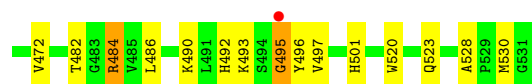


• Molecule 1: Capsid

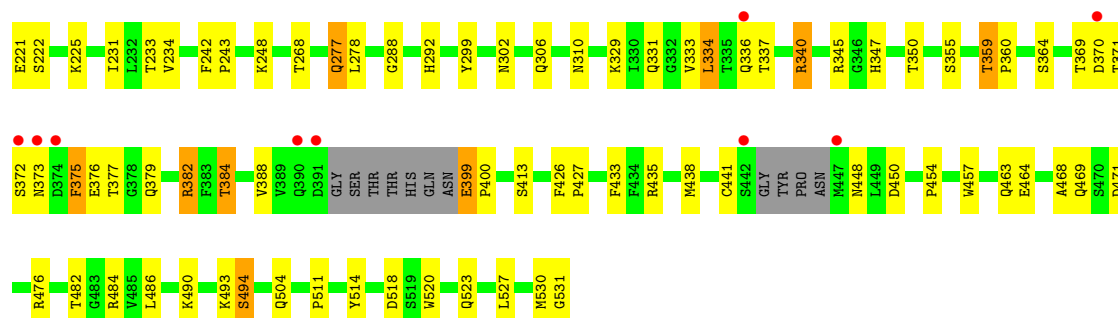


• Molecule 1: Capsid

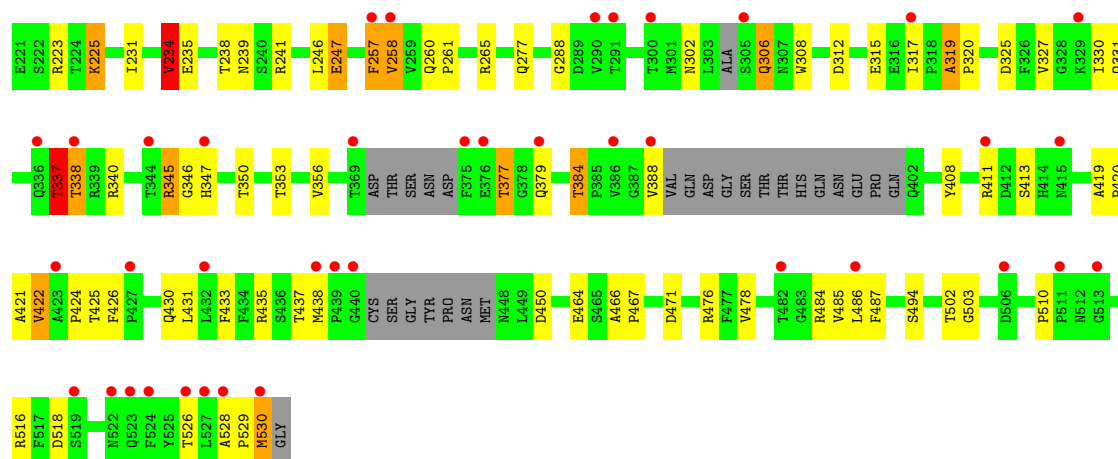




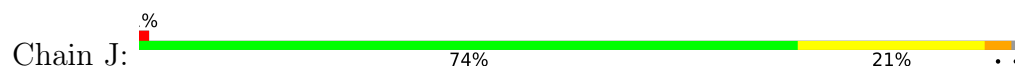
• Molecule 1: Capsid



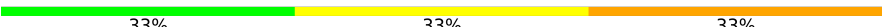
• Molecule 1: Capsid

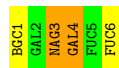


• Molecule 1: Capsid



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

Chain K:  33% 33% 33%



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

Chain L:  17% 83%



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

Chain M:  33% 67%



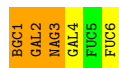
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N:  33% 67%



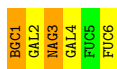
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain O:  17% 33% 50%

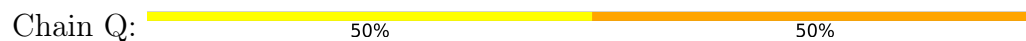


- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain P:  17% 50% 33%



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]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)-[alpha-L-fucopyranose-(1-4)]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	242.74Å 339.78Å 125.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.04 49.38 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.38-3.04) 99.7 (49.38-3.04)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.223 (Not available) , 0.188	Depositor DCC
R_{free} test set	4924 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24569	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: FUC, BGC, NAG, 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	1.12	2/2473 (0.1%)	1.18	4/3384 (0.1%)
1	B	1.05	0/2452	1.13	4/3357 (0.1%)
1	C	1.04	2/2486 (0.1%)	1.12	2/3401 (0.1%)
1	D	1.04	4/2456 (0.2%)	1.15	7/3361 (0.2%)
1	E	1.03	1/2476 (0.0%)	1.17	5/3388 (0.1%)
1	F	0.97	2/2463 (0.1%)	1.16	8/3371 (0.2%)
1	G	0.99	0/2450	1.14	12/3355 (0.4%)
1	H	1.02	0/2356	1.14	8/3225 (0.2%)
1	I	1.15	4/2188 (0.2%)	1.12	15/2993 (0.5%)
1	J	1.05	1/2453 (0.0%)	1.12	6/3357 (0.2%)
All	All	1.05	16/24253 (0.1%)	1.14	71/33192 (0.2%)

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	E	0	1
1	J	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	317	ILE	C-O	-8.61	1.18	1.24
1	D	423	ALA	CA-CB	-7.28	1.44	1.54
1	F	317	ILE	C-O	-6.44	1.19	1.24
1	C	277	GLN	CA-C	5.99	1.59	1.52
1	I	510	PRO	CA-C	5.89	1.56	1.52
1	A	473	ALA	CA-CB	-5.71	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	421	ALA	CA-CB	-5.48	1.44	1.53
1	F	421	ALA	CA-CB	-5.42	1.44	1.53
1	E	376	GLU	CA-C	-5.38	1.46	1.52
1	C	359	THR	CA-CB	5.24	1.59	1.53
1	I	327	VAL	CA-CB	5.21	1.60	1.53
1	I	234	VAL	CA-CB	5.21	1.60	1.54
1	D	476	ARG	CA-C	-5.21	1.46	1.52
1	D	277	GLN	CA-C	5.19	1.59	1.52
1	I	258	VAL	CA-CB	5.15	1.59	1.53
1	A	516	ARG	C-O	-5.15	1.18	1.23

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	374	ASP	N-CA-C	13.66	126.25	111.36
1	E	374	ASP	N-CA-C	12.53	124.67	111.14
1	F	374	ASP	N-CA-C	11.75	124.17	111.36
1	A	374	ASP	N-CA-C	11.38	123.76	111.36
1	G	495	GLY	N-CA-C	11.06	130.54	114.95
1	I	247	GLU	N-CA-C	10.60	122.92	111.36
1	J	495	GLY	N-CA-C	9.48	129.75	115.63
1	I	346	GLY	N-CA-C	9.41	135.48	113.18
1	J	374	ASP	N-CA-C	9.25	121.36	111.28
1	D	374	ASP	N-CA-C	9.23	121.34	111.28
1	H	373	ASN	CB-CA-C	-8.86	106.36	116.63
1	F	225	LYS	N-CA-C	7.90	119.29	109.57
1	G	496	TYR	N-CA-CB	-7.90	98.94	110.87
1	D	496	TYR	N-CA-C	7.71	121.05	109.95
1	F	344	THR	N-CA-C	7.57	121.56	108.76
1	I	347	HIS	N-CA-C	7.17	121.16	109.76
1	D	453	LEU	CA-C-N	-7.11	112.67	119.85
1	D	453	LEU	C-N-CA	-7.11	112.67	119.85
1	J	496	TYR	N-CA-CB	-6.81	100.55	110.70
1	F	419	ALA	CA-C-N	6.74	126.77	119.89
1	F	419	ALA	C-N-CA	6.74	126.77	119.89
1	C	463	GLN	CB-CA-C	-6.66	100.37	110.90
1	J	481	ASP	N-CA-C	6.56	118.22	111.14
1	E	435	ARG	N-CA-C	6.46	120.00	109.59
1	G	423	ALA	N-CA-C	6.39	113.97	108.22
1	D	496	TYR	N-CA-CB	-6.37	100.91	110.60
1	I	422	VAL	N-CA-C	6.35	117.27	108.12
1	H	448	ASN	N-CA-C	6.30	119.50	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	278	LEU	N-CA-C	6.26	120.11	112.23
1	I	345	ARG	N-CA-C	6.23	118.86	111.33
1	A	399	GLU	N-CA-C	6.20	113.80	108.22
1	H	384	THR	CA-C-N	6.02	125.93	119.85
1	H	384	THR	C-N-CA	6.02	125.93	119.85
1	F	373	ASN	N-CA-C	5.89	121.43	112.54
1	J	518	ASP	N-CA-C	5.88	120.75	112.93
1	G	497	VAL	N-CA-C	5.87	116.33	108.11
1	D	339	ARG	N-CA-C	5.85	119.52	112.38
1	H	233	THR	N-CA-C	-5.84	101.37	110.42
1	E	223	ARG	N-CA-C	5.82	118.76	107.71
1	J	278	LEU	N-CA-C	5.78	118.80	111.69
1	G	256	ALA	N-CA-C	5.73	118.30	111.71
1	B	225	LYS	N-CA-C	5.70	117.80	109.71
1	B	258	VAL	CA-C-N	-5.54	115.85	122.22
1	B	258	VAL	C-N-CA	-5.54	115.85	122.22
1	H	435	ARG	N-CA-C	5.45	118.36	109.59
1	G	528	ALA	CA-C-N	-5.36	114.04	119.83
1	G	528	ALA	C-N-CA	-5.36	114.04	119.83
1	E	423	ALA	N-CA-C	5.34	113.03	108.22
1	H	359	THR	CA-C-N	5.30	125.36	119.32
1	H	359	THR	C-N-CA	5.30	125.36	119.32
1	C	257	PHE	N-CA-C	5.29	116.83	108.96
1	I	306	GLN	N-CA-C	5.27	116.88	111.03
1	D	495	GLY	N-CA-C	5.22	123.41	115.63
1	I	319	ALA	CA-C-N	-5.21	114.43	119.90
1	I	319	ALA	C-N-CA	-5.21	114.43	119.90
1	I	435	ARG	N-CA-C	5.19	117.95	109.59
1	I	528	ALA	N-CA-C	-5.18	102.63	109.84
1	F	449	LEU	N-CA-C	5.16	117.20	108.02
1	B	458	VAL	CB-CA-C	-5.15	105.29	111.88
1	I	408	TYR	N-CA-C	5.12	116.67	111.14
1	G	458	VAL	N-CA-C	-5.12	105.51	110.42
1	G	225	LYS	CA-C-N	5.11	125.02	119.76
1	G	225	LYS	C-N-CA	5.11	125.02	119.76
1	E	459	GLN	N-CA-C	-5.09	105.62	111.07
1	I	257	PHE	N-CA-C	5.09	117.89	109.85
1	A	270	GLY	CA-C-N	-5.06	115.86	122.99
1	A	270	GLY	C-N-CA	-5.06	115.86	122.99
1	I	337	THR	CA-C-N	5.05	130.79	121.70
1	I	337	THR	C-N-CA	5.05	130.79	121.70
1	I	234	VAL	N-CA-C	5.02	115.74	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	355	SER	N-CA-C	5.02	116.76	110.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	344	THR	Peptide
1	J	345	ARG	Sidechain

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	2403	0	2292	60	0
1	B	2382	0	2264	39	0
1	C	2416	0	2304	46	0
1	D	2386	0	2275	49	0
1	E	2406	0	2297	49	0
1	F	2393	0	2282	58	0
1	G	2380	0	2263	67	0
1	H	2291	0	2167	55	0
1	I	2128	0	1939	50	0
1	J	2383	0	2273	58	0
2	K	68	0	60	2	0
2	L	68	0	60	8	0
2	M	68	0	60	15	0
2	N	68	0	60	18	0
2	O	68	0	60	6	0
2	P	68	0	60	6	0
2	Q	68	0	60	21	0
2	R	68	0	60	21	0
3	A	68	0	0	9	0
3	B	54	0	0	12	0
3	C	53	0	0	13	0
3	D	57	0	0	10	0
3	E	46	0	0	13	0
3	F	45	0	0	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	41	0	0	8	0
3	H	36	0	0	16	0
3	I	18	0	0	10	0
3	J	39	0	0	6	0
All	All	24569	0	22836	583	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (583) 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:J:345:ARG:HD3	2:Q:5:FUC:O3	1.40	1.20
1:J:345:ARG:HG2	1:J:345:ARG:HH21	1.07	1.18
1:H:231:ILE:HB	3:H:545:HOH:O	1.40	1.18
1:B:481:ASP:HB2	3:B:181:HOH:O	1.43	1.16
1:F:512:ASN:HB3	3:F:544:HOH:O	1.50	1.12
1:H:376:GLU:HA	3:H:149:HOH:O	1.48	1.12
1:J:394:THR:HB	1:J:398:ASN:HD21	1.04	1.09
2:Q:1:BGC:H6C1	2:Q:2:GAL:C1	1.82	1.08
2:N:5:FUC:H61	2:N:6:FUC:H61	1.37	1.07
1:J:226:PRO:HD2	3:J:541:HOH:O	1.52	1.06
2:M:5:FUC:H61	2:M:6:FUC:H61	1.37	1.06
2:L:3:NAG:O3	2:L:5:FUC:H5	1.57	1.05
1:G:409:SER:HB2	1:G:413:SER:CB	1.87	1.04
1:E:417:HIS:HD2	3:E:148:HOH:O	1.37	1.04
2:R:5:FUC:H61	2:R:6:FUC:H61	1.08	1.03
2:R:1:BGC:H3	2:R:2:GAL:O5	1.59	1.02
1:E:310:ASN:HB2	3:E:155:HOH:O	1.59	1.02
2:M:3:NAG:O3	2:M:5:FUC:H5	1.61	1.01
1:H:345:ARG:HA	3:H:542:HOH:O	1.59	1.00
2:L:3:NAG:H61	2:L:6:FUC:C1	1.92	1.00
1:G:409:SER:HB2	1:G:413:SER:HB3	1.40	1.00
1:J:394:THR:HB	1:J:398:ASN:ND2	1.75	0.99
2:R:5:FUC:C6	2:R:6:FUC:H61	1.92	0.99
1:F:370:ASP:HB2	3:F:119:HOH:O	1.62	0.99
2:P:3:NAG:O3	2:P:6:FUC:H5	1.65	0.97
1:A:336:GLN:OE1	1:A:375:PHE:HD1	1.50	0.93
1:F:523:GLN:HB2	3:F:187:HOH:O	1.69	0.93
1:D:307:ASN:HA	3:D:553:HOH:O	1.67	0.93
1:J:345:ARG:HH21	1:J:345:ARG:CG	1.82	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:HE21	1:A:379:GLN:HB2	1.33	0.92
1:C:370:ASP:HB2	3:C:547:HOH:O	1.69	0.91
2:N:5:FUC:C6	2:N:6:FUC:H61	2.00	0.91
1:I:337:THR:HG21	3:J:539:HOH:O	1.69	0.91
1:J:345:ARG:HG2	1:J:345:ARG:NH2	1.84	0.89
3:F:533:HOH:O	2:P:1:BGC:H6C1	1.72	0.88
2:M:3:NAG:H61	2:M:6:FUC:C1	2.03	0.88
1:A:390:GLN:OE1	1:A:391:ASP:O	1.91	0.87
1:F:494:SER:HB2	3:F:551:HOH:O	1.74	0.87
1:E:370:ASP:HB2	3:E:44:HOH:O	1.74	0.86
2:R:3:NAG:O3	2:R:6:FUC:H5	1.74	0.86
2:R:5:FUC:H61	2:R:6:FUC:C6	2.00	0.86
1:H:531:GLY:HA2	3:H:544:HOH:O	1.75	0.85
1:F:390:GLN:HG2	1:F:444:TYR:C	2.01	0.85
1:B:291:THR:HG21	3:B:563:HOH:O	1.75	0.85
2:N:3:NAG:H61	2:N:6:FUC:C1	2.07	0.83
1:J:345:ARG:CD	2:Q:5:FUC:O3	2.25	0.83
1:G:453:LEU:HD21	1:G:495:GLY:O	1.78	0.83
1:D:442:SER:HA	1:F:344:THR:O	1.79	0.83
1:D:518:ASP:HB3	3:D:558:HOH:O	1.80	0.82
1:A:394:THR:HB	1:A:398:ASN:HD21	1.43	0.82
1:E:484:ARG:HB3	3:E:556:HOH:O	1.78	0.82
1:B:310:ASN:HB2	3:B:48:HOH:O	1.80	0.81
1:A:391:ASP:OD2	1:A:394:THR:HG23	1.82	0.79
1:G:373:ASN:N	1:G:373:ASN:ND2	2.30	0.79
2:M:1:BGC:O6	2:M:2:GAL:C1	2.31	0.79
1:E:523:GLN:HB2	3:E:553:HOH:O	1.82	0.79
1:I:337:THR:CG2	1:I:338:THR:OG1	2.30	0.79
1:J:338:THR:CG2	1:J:345:ARG:NH1	2.46	0.79
1:F:382:ARG:HD2	3:F:175:HOH:O	1.83	0.78
2:O:3:NAG:H61	2:O:6:FUC:C1	2.13	0.78
2:R:1:BGC:H5	2:R:2:GAL:O5	1.83	0.78
1:C:469:GLN:HG3	1:C:520:TRP:CD1	2.19	0.78
1:D:453:LEU:HD21	1:D:495:GLY:O	1.83	0.78
1:G:382:ARG:HD2	3:G:189:HOH:O	1.84	0.77
1:D:317:ILE:HG22	1:H:340:ARG:HD3	1.64	0.77
1:F:530:MET:HA	3:F:130:HOH:O	1.83	0.76
1:D:307:ASN:OD1	1:D:309:ASN:HB2	1.84	0.76
2:O:1:BGC:C6	2:O:1:BGC:O1	2.30	0.76
1:J:338:THR:HG22	1:J:345:ARG:NH1	2.01	0.75
1:I:356:VAL:CG1	1:I:411:ARG:HD2	2.15	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:OE1	1:A:375:PHE:CD1	2.39	0.75
1:J:307:ASN:ND2	1:J:309:ASN:HB2	2.02	0.75
2:Q:4:GAL:O5	2:Q:6:FUC:H5	1.87	0.75
1:G:438:MET:HE2	1:G:449:LEU:HB2	1.69	0.75
1:I:356:VAL:HG12	1:I:411:ARG:HD2	1.67	0.75
1:I:337:THR:HG23	1:I:338:THR:OG1	1.87	0.74
1:F:310:ASN:HA	3:F:546:HOH:O	1.86	0.74
1:A:494:SER:HB2	3:A:58:HOH:O	1.85	0.74
1:B:476:ARG:HD3	1:B:518:ASP:OD2	1.88	0.74
2:N:3:NAG:C6	2:N:6:FUC:C1	2.65	0.74
1:C:430:GLN:HG3	1:C:501:HIS:O	1.88	0.73
2:N:5:FUC:H61	2:N:6:FUC:C6	2.17	0.73
1:C:425:THR:HA	3:C:551:HOH:O	1.87	0.73
1:C:393:SER:OG	2:L:6:FUC:H2	1.88	0.73
1:B:390:GLN:HG2	1:B:444:TYR:C	2.14	0.73
1:B:469:GLN:HB2	1:B:520:TRP:CG	2.23	0.73
2:M:4:GAL:O5	2:M:6:FUC:H5	1.88	0.73
1:I:485:VAL:HG23	3:I:541:HOH:O	1.89	0.72
2:N:4:GAL:O5	2:N:6:FUC:H5	1.88	0.72
1:C:438:MET:HE2	1:C:449:LEU:HB2	1.71	0.72
1:J:391:ASP:HB3	1:J:394:THR:OG1	1.89	0.72
1:J:390:GLN:HG2	1:J:444:TYR:C	2.14	0.72
1:H:379:GLN:HB3	3:H:185:HOH:O	1.90	0.71
1:G:409:SER:HB2	1:G:413:SER:HB2	1.72	0.71
1:J:394:THR:CB	1:J:398:ASN:HD21	1.93	0.71
1:J:453:LEU:HD21	1:J:495:GLY:O	1.91	0.71
1:J:469:GLN:HG3	1:J:520:TRP:CD1	2.25	0.71
1:G:390:GLN:HG3	1:G:444:TYR:H	1.56	0.70
1:H:268:THR:HG23	1:H:493:LYS:HA	1.71	0.70
2:M:4:GAL:C2	2:M:5:FUC:H5	2.20	0.70
1:D:494:SER:HB2	3:D:136:HOH:O	1.91	0.70
1:I:476:ARG:HD3	1:I:518:ASP:OD2	1.91	0.70
1:C:277:GLN:HG3	1:C:306:GLN:HE22	1.56	0.70
1:D:440:GLY:HA3	1:F:344:THR:HG21	1.74	0.70
2:K:3:NAG:O6	2:K:6:FUC:C1	2.40	0.69
1:I:430:GLN:HE22	1:I:503:GLY:H	1.39	0.69
1:I:337:THR:HG22	1:I:338:THR:CB	2.22	0.69
1:J:310:ASN:HA	3:J:534:HOH:O	1.92	0.69
1:B:310:ASN:HB3	3:B:213:HOH:O	1.92	0.68
1:H:347:HIS:HD2	1:H:372:SER:CB	2.07	0.68
1:J:307:ASN:HD21	1:J:309:ASN:HB2	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASP:HB3	1:A:394:THR:HG23	1.76	0.68
1:G:443:GLY:HA2	2:Q:5:FUC:H61	1.77	0.67
1:E:360:PRO:HD2	1:E:408:TYR:O	1.94	0.67
1:I:239:ASN:N	1:I:246:LEU:HG	2.09	0.67
1:A:340:ARG:HG2	3:B:45:HOH:O	1.93	0.67
1:E:236:GLU:HA	3:E:533:HOH:O	1.93	0.67
1:A:231:ILE:HG22	1:A:231:ILE:O	1.94	0.67
1:A:336:GLN:NE2	1:A:379:GLN:HB2	2.09	0.67
1:A:394:THR:CB	1:A:398:ASN:HD21	2.08	0.67
1:J:277:GLN:OE1	1:J:279:SER:HB3	1.95	0.67
1:H:336:GLN:HE21	1:H:375:PHE:HD1	1.43	0.66
2:M:4:GAL:C1	2:M:5:FUC:H5	2.25	0.66
1:G:409:SER:CB	1:G:413:SER:CB	2.71	0.66
1:G:482:THR:OG1	1:G:484:ARG:HG2	1.94	0.66
2:R:4:GAL:C1	2:R:6:FUC:H5	2.26	0.66
1:A:356:VAL:HG13	3:A:22:HOH:O	1.95	0.66
1:B:331:GLN:HG3	3:B:560:HOH:O	1.96	0.66
1:J:345:ARG:HD3	2:Q:5:FUC:HO3	1.56	0.66
1:G:443:GLY:H	2:Q:5:FUC:C6	2.09	0.65
2:L:1:BGC:O6	2:L:2:GAL:C1	2.44	0.65
1:A:470:SER:HB3	1:A:520:TRP:HB3	1.77	0.65
1:J:345:ARG:HD2	1:J:374:ASP:OD1	1.97	0.65
2:N:5:FUC:C5	2:N:6:FUC:H61	2.27	0.65
1:A:373:ASN:N	1:A:373:ASN:OD1	2.30	0.65
1:I:238:THR:O	1:I:246:LEU:HD11	1.97	0.65
1:A:390:GLN:HG2	1:A:444:TYR:C	2.22	0.64
1:A:302:ASN:HB3	3:A:536:HOH:O	1.97	0.64
1:I:345:ARG:CB	3:I:542:HOH:O	2.46	0.64
2:Q:3:NAG:O3	2:Q:6:FUC:H5	1.96	0.64
1:B:242:PHE:CD2	1:B:243:PRO:HD2	2.32	0.64
1:D:373:ASN:OD1	1:D:373:ASN:N	2.29	0.64
1:G:469:GLN:HG3	1:G:520:TRP:CD1	2.33	0.64
2:R:1:BGC:H6C1	2:R:2:GAL:H2	1.80	0.64
1:H:399:GLU:HB2	1:H:400:PRO:HA	1.79	0.64
1:I:337:THR:HG22	1:I:338:THR:HB	1.79	0.64
1:I:319:ALA:HB1	1:I:320:PRO:HD2	1.78	0.64
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.33	0.64
1:E:390:GLN:HG3	1:E:444:TYR:H	1.63	0.64
1:G:277:GLN:OE1	1:G:279:SER:HB3	1.97	0.64
1:G:453:LEU:CD2	1:G:495:GLY:O	2.46	0.64
1:J:476:ARG:HD3	1:J:518:ASP:OD2	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ASN:N	1:E:373:ASN:OD1	2.30	0.63
1:A:391:ASP:HB3	1:A:394:THR:CG2	2.28	0.63
1:H:221:GLU:N	1:H:469:GLN:NE2	2.46	0.63
1:I:225:LYS:NZ	1:I:464:GLU:O	2.24	0.63
1:F:482:THR:OG1	1:F:484:ARG:HG2	1.99	0.63
1:G:469:GLN:HB2	1:G:520:TRP:CG	2.33	0.63
1:G:443:GLY:HA2	2:Q:5:FUC:C6	2.29	0.63
1:H:426:PHE:CD2	1:H:427:PRO:HD2	2.33	0.63
2:K:4:GAL:O5	2:K:6:FUC:H5	1.97	0.63
1:F:287:ARG:HD3	3:F:532:HOH:O	1.98	0.62
3:B:68:HOH:O	1:E:382:ARG:HD2	1.99	0.62
1:J:373:ASN:OD1	1:J:373:ASN:N	2.30	0.62
2:M:5:FUC:H61	2:M:6:FUC:C6	2.22	0.62
2:R:1:BGC:C3	2:R:2:GAL:O5	2.30	0.62
1:D:392:GLY:HA3	2:N:6:FUC:O5	2.00	0.62
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.81	0.62
1:F:531:GLY:HA2	3:F:141:HOH:O	1.98	0.62
1:I:317:ILE:HD12	1:I:319:ALA:O	2.00	0.62
1:H:463:GLN:HG2	3:H:547:HOH:O	1.98	0.62
1:F:345:ARG:HG3	2:N:5:FUC:O3	2.00	0.61
1:H:388:VAL:HG21	1:H:438:MET:HE3	1.81	0.61
2:Q:4:GAL:C1	2:Q:6:FUC:H5	2.30	0.61
1:D:531:GLY:HA3	3:D:113:HOH:O	1.99	0.61
1:B:382:ARG:HD2	3:B:178:HOH:O	2.00	0.61
2:M:3:NAG:C6	2:M:6:FUC:C1	2.78	0.61
2:N:5:FUC:O5	2:N:6:FUC:H61	2.00	0.61
1:I:234:VAL:HG13	3:I:536:HOH:O	2.00	0.61
2:O:3:NAG:O3	2:O:6:FUC:H5	2.00	0.61
1:A:469:GLN:HB2	1:A:520:TRP:CG	2.35	0.61
1:H:399:GLU:CB	1:H:400:PRO:HA	2.31	0.61
1:I:247:GLU:CB	3:I:538:HOH:O	2.49	0.61
1:I:337:THR:HG22	1:I:338:THR:OG1	2.00	0.60
1:H:268:THR:CG2	1:H:493:LYS:HA	2.31	0.60
1:H:494:SER:HB2	3:H:535:HOH:O	2.01	0.60
1:E:426:PHE:CD2	1:E:427:PRO:HD2	2.36	0.60
1:J:345:ARG:CG	1:J:345:ARG:NH2	2.46	0.60
1:F:373:ASN:OD1	1:F:373:ASN:N	2.30	0.60
1:E:280:PRO:HA	3:E:543:HOH:O	2.01	0.59
1:G:390:GLN:HG2	1:G:444:TYR:C	2.27	0.59
1:I:487:PHE:HA	3:I:537:HOH:O	2.03	0.59
1:F:390:GLN:CG	1:F:444:TYR:H	2.15	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:NAG:O3	2:P:6:FUC:C5	2.46	0.59
1:E:277:GLN:OE1	1:E:279:SER:HB3	2.03	0.59
1:E:341:ASP:HB3	1:E:343:SER:H	1.67	0.59
1:I:238:THR:HG22	1:I:239:ASN:O	2.03	0.58
2:M:1:BGC:H6	2:M:2:GAL:C1	2.16	0.58
1:B:353:THR:HG22	1:B:358:PHE:CE1	2.38	0.58
1:A:343:SER:HB3	1:C:444:TYR:CE1	2.38	0.58
1:D:453:LEU:CD2	1:D:495:GLY:O	2.50	0.58
1:A:472:VAL:HG13	1:A:490:LYS:HB3	1.85	0.58
1:F:328:GLY:HA3	1:F:400:PRO:HB3	1.85	0.58
1:A:390:GLN:HG3	1:A:444:TYR:H	1.68	0.58
1:F:260:GLN:HG3	1:F:421:ALA:HA	1.86	0.58
1:I:235:GLU:HG3	3:I:536:HOH:O	2.03	0.58
1:F:371:THR:O	1:F:371:THR:CG2	2.51	0.57
1:J:392:GLY:HA3	2:R:6:FUC:C1	2.34	0.57
1:E:277:GLN:HG3	1:E:306:GLN:HE22	1.67	0.57
1:C:222:SER:HB2	3:C:538:HOH:O	2.04	0.57
1:G:443:GLY:N	2:Q:5:FUC:H63	2.20	0.57
2:L:3:NAG:O3	2:L:5:FUC:C5	2.43	0.57
1:G:319:ALA:HB1	1:G:320:PRO:HD2	1.86	0.57
1:J:356:VAL:HG23	1:J:411:ARG:HG3	1.87	0.57
1:H:288:GLY:HA3	1:H:302:ASN:O	2.04	0.57
1:B:277:GLN:OE1	1:B:279:SER:HB3	2.05	0.57
1:D:233:THR:HG21	1:D:512:ASN:HA	1.86	0.57
1:H:490:LYS:HG3	1:H:527:LEU:HD21	1.87	0.56
1:G:443:GLY:H	2:Q:5:FUC:H63	1.69	0.56
1:C:360:PRO:HD2	1:C:408:TYR:O	2.05	0.56
1:C:390:GLN:HG3	1:C:444:TYR:H	1.70	0.56
1:E:463:GLN:HG2	3:E:541:HOH:O	2.05	0.56
1:F:310:ASN:HB2	3:F:557:HOH:O	2.04	0.56
1:G:453:LEU:CG	1:G:495:GLY:O	2.53	0.56
2:P:4:GAL:C1	2:P:6:FUC:H5	2.35	0.56
1:B:391:ASP:OD2	1:B:394:THR:HG23	2.05	0.56
1:A:232:LEU:HD21	1:C:463:GLN:NE2	2.20	0.56
1:G:523:GLN:HB2	3:G:546:HOH:O	2.05	0.56
1:H:493:LYS:HD2	3:H:533:HOH:O	2.05	0.56
2:L:3:NAG:C6	2:L:6:FUC:C1	2.72	0.56
1:E:229:VAL:HB	1:E:230:PRO:HD2	1.88	0.56
1:C:390:GLN:HG2	1:C:444:TYR:C	2.31	0.56
1:F:390:GLN:HG3	1:F:444:TYR:H	1.71	0.56
2:R:1:BGC:H1	2:R:2:GAL:O6	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:GLY:HA3	2:N:6:FUC:C1	2.35	0.56
2:N:4:GAL:H2	2:N:6:FUC:H62	1.87	0.56
1:D:399:GLU:HB2	1:D:400:PRO:HA	1.89	0.55
3:D:111:HOH:O	1:F:279:SER:HB2	2.05	0.55
2:N:1:BGC:O6	2:N:2:GAL:C1	2.54	0.55
1:B:438:MET:HE2	1:B:449:LEU:HB2	1.88	0.55
1:B:287:ARG:NE	3:B:537:HOH:O	2.39	0.55
1:H:382:ARG:HH11	1:H:382:ARG:HB2	1.72	0.55
1:I:258:VAL:HG23	1:I:258:VAL:O	2.06	0.55
1:B:358:PHE:C	1:B:360:PRO:HD3	2.31	0.55
1:G:372:SER:C	1:G:373:ASN:HD22	2.15	0.55
1:I:238:THR:C	1:I:246:LEU:CD1	2.80	0.55
1:F:443:GLY:O	1:F:445:PRO:HD3	2.07	0.55
1:D:507:LEU:HG	1:D:530:MET:HE3	1.87	0.55
1:H:523:GLN:CB	3:H:537:HOH:O	2.54	0.55
1:F:371:THR:O	1:F:371:THR:HG23	2.06	0.54
1:H:399:GLU:N	3:H:91:HOH:O	2.40	0.54
1:H:231:ILE:CG2	3:H:545:HOH:O	2.54	0.54
1:H:376:GLU:CA	3:H:149:HOH:O	2.24	0.54
1:H:242:PHE:CD2	1:H:243:PRO:HD2	2.42	0.54
1:G:248:LYS:HE2	3:G:542:HOH:O	2.07	0.54
1:B:332:GLY:HA2	1:B:386:VAL:HG23	1.89	0.54
1:C:286:PHE:CD1	3:C:165:HOH:O	2.53	0.54
1:E:260:GLN:HG3	1:E:421:ALA:HA	1.90	0.54
1:H:388:VAL:CG2	1:H:438:MET:HE3	2.37	0.54
1:E:260:GLN:HG3	1:E:421:ALA:CA	2.38	0.54
1:H:277:GLN:HG2	1:H:278:LEU:H	1.73	0.54
1:E:390:GLN:HG2	1:E:444:TYR:C	2.32	0.54
1:J:438:MET:HE2	1:J:449:LEU:HB2	1.89	0.54
1:A:253:PRO:HD2	3:A:124:HOH:O	2.08	0.54
1:G:443:GLY:CA	2:Q:5:FUC:C6	2.86	0.54
1:F:443:GLY:C	1:F:445:PRO:HD3	2.33	0.53
1:F:230:PRO:HG2	1:F:457:TRP:CD1	2.43	0.53
1:A:390:GLN:CD	1:A:391:ASP:O	2.51	0.53
1:B:317:ILE:HD12	1:B:319:ALA:O	2.08	0.53
1:D:319:ALA:HB1	1:D:320:PRO:HD2	1.89	0.53
1:B:417:HIS:HE1	3:B:49:HOH:O	1.91	0.53
1:I:424:PRO:C	1:I:426:PHE:H	2.17	0.53
2:N:3:NAG:O3	2:N:5:FUC:H5	2.09	0.53
2:R:4:GAL:O5	2:R:6:FUC:H5	2.08	0.53
1:A:392:GLY:HA3	2:M:6:FUC:O5	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:GLN:NE2	3:C:557:HOH:O	2.42	0.53
1:E:433:PHE:HB3	1:E:450:ASP:HB3	1.90	0.53
1:G:232:LEU:HD21	1:J:463:GLN:NE2	2.24	0.53
1:J:277:GLN:OE1	1:J:279:SER:N	2.41	0.53
1:G:244:ILE:HD12	1:G:436:SER:HB3	1.91	0.53
1:F:307:ASN:HD21	1:F:309:ASN:HB2	1.74	0.52
1:G:276:THR:HA	3:G:541:HOH:O	2.07	0.52
3:G:532:HOH:O	1:J:279:SER:HB2	2.09	0.52
1:A:226:PRO:HD2	3:A:533:HOH:O	2.10	0.52
1:C:523:GLN:HB3	3:C:183:HOH:O	2.09	0.52
1:I:430:GLN:NE2	1:I:503:GLY:H	2.06	0.52
1:J:285:THR:HG22	1:J:385:PRO:HD3	1.90	0.52
2:N:4:GAL:H2	2:N:6:FUC:C6	2.40	0.52
1:I:377:THR:HG21	3:I:533:HOH:O	2.10	0.52
1:J:443:GLY:HA2	2:R:6:FUC:H63	1.91	0.52
1:A:283:ILE:O	1:A:284:CYS:HB2	2.08	0.52
1:D:283:ILE:O	1:D:284:CYS:HB2	2.10	0.52
1:H:222:SER:H	1:H:469:GLN:HE22	1.58	0.52
2:M:5:FUC:C6	2:M:6:FUC:H61	2.25	0.52
1:H:530:MET:HA	3:H:546:HOH:O	2.10	0.52
1:I:485:VAL:HG12	3:I:544:HOH:O	2.09	0.51
1:A:328:GLY:HA3	1:A:400:PRO:HB3	1.91	0.51
1:H:376:GLU:CB	3:H:149:HOH:O	2.57	0.51
1:B:277:GLN:HB2	1:B:321:LEU:HB3	1.93	0.51
1:F:390:GLN:CG	1:F:444:TYR:N	2.74	0.51
1:G:472:VAL:CG1	1:G:490:LYS:HB3	2.40	0.51
2:O:1:BGC:O1	2:O:1:BGC:H6C1	2.09	0.51
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.75	0.51
1:D:272:LEU:O	1:D:273:LEU:HD23	2.11	0.51
1:E:390:GLN:HG3	1:E:444:TYR:N	2.24	0.51
1:G:372:SER:C	1:G:373:ASN:ND2	2.69	0.51
1:I:238:THR:O	1:I:246:LEU:CD1	2.59	0.51
1:I:239:ASN:HA	1:I:246:LEU:HD21	1.92	0.51
1:A:506:ASP:HB3	3:A:19:HOH:O	2.09	0.51
1:H:231:ILE:CB	3:H:545:HOH:O	2.21	0.51
1:G:530:MET:HA	3:G:43:HOH:O	2.09	0.51
1:A:394:THR:O	1:A:395:THR:C	2.51	0.51
1:A:472:VAL:CG1	1:A:490:LYS:HB3	2.41	0.51
1:H:292:HIS:HB2	1:H:299:TYR:CE1	2.46	0.51
1:G:443:GLY:CA	2:Q:5:FUC:H63	2.42	0.51
2:N:4:GAL:C1	2:N:6:FUC:H5	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HE2	3:C:540:HOH:O	2.12	0.50
1:C:522:ASN:C	1:C:522:ASN:OD1	2.53	0.50
1:H:340:ARG:HH11	1:H:340:ARG:CG	2.25	0.50
1:D:253:PRO:HD2	3:D:182:HOH:O	2.11	0.50
1:H:340:ARG:HH11	1:H:340:ARG:HG2	1.77	0.50
1:I:529:PRO:O	1:I:530:MET:O	2.30	0.50
1:D:453:LEU:CG	1:D:495:GLY:O	2.60	0.50
1:E:287:ARG:HD3	3:E:110:HOH:O	2.11	0.50
1:F:240:SER:OG	1:F:264:GLY:HA3	2.12	0.50
1:H:221:GLU:N	1:H:469:GLN:HE21	2.08	0.50
1:H:382:ARG:HH11	1:H:382:ARG:CG	2.25	0.50
2:O:1:BGC:O1	2:O:1:BGC:H6C2	2.10	0.50
1:E:222:SER:HB3	3:E:93:HOH:O	2.11	0.50
1:F:230:PRO:HD3	1:F:460:HIS:CD2	2.47	0.50
1:I:384:THR:HG23	3:I:203:HOH:O	2.12	0.50
1:F:400:PRO:HD2	1:F:446:ASN:O	2.11	0.50
1:A:232:LEU:HD21	1:C:463:GLN:HE22	1.77	0.49
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.94	0.49
1:D:486:LEU:HD11	1:D:510:PRO:HD3	1.94	0.49
1:H:482:THR:OG1	1:H:484:ARG:HG2	2.12	0.49
1:I:315:GLU:HB3	1:I:317:ILE:HG12	1.93	0.49
1:A:280:PRO:HG3	1:C:280:PRO:HG2	1.93	0.49
1:A:351:VAL:HB	1:A:367:PHE:CE1	2.47	0.49
1:B:481:ASP:OD2	1:B:512:ASN:ND2	2.44	0.49
1:E:268:THR:HG23	1:E:493:LYS:HA	1.92	0.49
1:F:399:GLU:HB2	1:F:400:PRO:HA	1.94	0.49
1:F:426:PHE:CE1	1:F:524:PHE:HA	2.47	0.49
1:G:344:THR:O	1:J:442:SER:HA	2.12	0.49
1:J:360:PRO:HD2	1:J:408:TYR:O	2.13	0.49
1:G:373:ASN:N	1:G:373:ASN:HD22	2.09	0.49
1:C:468:ALA:HA	1:C:520:TRP:CZ2	2.47	0.49
1:J:392:GLY:HA3	2:R:6:FUC:O5	2.13	0.49
1:A:327:VAL:HA	1:A:353:THR:OG1	2.13	0.49
1:D:356:VAL:HG12	1:D:411:ARG:HG3	1.94	0.49
1:G:443:GLY:N	2:Q:5:FUC:C6	2.74	0.49
1:A:505:HIS:HE1	3:A:152:HOH:O	1.96	0.49
1:C:277:GLN:HG3	1:C:306:GLN:NE2	2.25	0.49
1:J:453:LEU:CD2	1:J:495:GLY:O	2.61	0.49
1:F:311:TYR:O	1:F:313:PRO:HD3	2.13	0.48
1:D:339:ARG:HG3	3:D:568:HOH:O	2.12	0.48
1:C:425:THR:C	3:C:551:HOH:O	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:PRO:HD2	1:D:408:TYR:O	2.14	0.48
1:E:438:MET:O	1:E:447:MET:HB3	2.13	0.48
1:G:334:LEU:O	1:G:346:GLY:HA2	2.14	0.48
1:F:390:GLN:HG3	1:F:444:TYR:N	2.29	0.48
1:F:438:MET:HE2	1:F:449:LEU:HB2	1.96	0.48
1:A:391:ASP:CB	1:A:394:THR:HG23	2.41	0.48
1:C:301:MET:HG2	1:C:303:LEU:HD23	1.95	0.48
1:D:523:GLN:HG2	3:D:532:HOH:O	2.13	0.48
1:G:345:ARG:HB3	2:R:5:FUC:H2	1.96	0.48
1:H:370:ASP:O	1:H:371:THR:C	2.56	0.48
1:H:476:ARG:HD3	1:H:518:ASP:OD2	2.13	0.48
1:D:472:VAL:HG11	1:D:490:LYS:HG2	1.95	0.47
1:F:490:LYS:O	1:F:497:VAL:HA	2.14	0.47
1:G:268:THR:HG23	1:G:493:LYS:HA	1.95	0.47
1:B:390:GLN:CG	1:B:444:TYR:H	2.27	0.47
1:D:328:GLY:HA3	1:D:400:PRO:HB3	1.96	0.47
1:E:277:GLN:HG3	1:E:306:GLN:NE2	2.30	0.47
1:E:399:GLU:HB2	1:E:400:PRO:HA	1.96	0.47
1:H:511:PRO:HA	3:H:548:HOH:O	2.14	0.47
1:E:390:GLN:CG	1:E:444:TYR:H	2.27	0.47
1:F:277:GLN:OE1	1:F:279:SER:HB3	2.13	0.47
1:G:399:GLU:HB2	1:G:400:PRO:HA	1.96	0.47
1:I:288:GLY:HA3	1:I:302:ASN:O	2.14	0.47
1:I:379:GLN:CB	3:I:205:HOH:O	2.62	0.47
2:Q:5:FUC:H61	2:Q:6:FUC:H61	1.96	0.47
1:A:359:THR:HB	1:A:362:LEU:HD12	1.96	0.47
1:C:425:THR:CA	3:C:551:HOH:O	2.55	0.47
1:C:489:CYS:HB2	1:C:498:THR:O	2.14	0.47
1:G:426:PHE:CD2	1:G:427:PRO:HD2	2.49	0.47
1:H:369:THR:C	1:H:371:THR:H	2.22	0.47
2:R:3:NAG:O3	2:R:6:FUC:C5	2.56	0.47
1:F:414:HIS:ND1	2:Q:2:GAL:H62	2.30	0.47
1:H:333:VAL:HG12	1:H:334:LEU:N	2.30	0.47
1:I:306:GLN:C	1:I:308:TRP:H	2.21	0.47
1:J:338:THR:HG21	1:J:345:ARG:NH1	2.27	0.47
1:J:488:GLU:HG3	1:J:527:LEU:HD22	1.96	0.47
1:D:484:ARG:HG2	3:D:552:HOH:O	2.14	0.47
1:F:260:GLN:HG3	1:F:421:ALA:CA	2.44	0.47
1:A:317:ILE:HD12	1:A:319:ALA:O	2.14	0.46
1:C:393:SER:HG	2:L:6:FUC:H2	1.78	0.46
1:F:307:ASN:ND2	1:F:309:ASN:HB2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:4:GAL:H2	2:Q:6:FUC:H62	1.97	0.46
3:B:564:HOH:O	1:J:412:ASP:HA	2.15	0.46
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.49	0.46
1:A:490:LYS:HG3	1:A:527:LEU:HD11	1.95	0.46
1:J:390:GLN:HG2	1:J:445:PRO:N	2.30	0.46
1:H:382:ARG:HH11	1:H:382:ARG:CB	2.28	0.46
2:R:4:GAL:H2	2:R:6:FUC:H62	1.98	0.46
1:A:394:THR:HB	1:A:398:ASN:ND2	2.20	0.46
1:D:469:GLN:HG3	1:D:520:TRP:CD1	2.50	0.46
2:R:5:FUC:C5	2:R:6:FUC:H61	2.43	0.46
1:C:355:SER:HA	3:C:558:HOH:O	2.15	0.46
1:D:390:GLN:HG2	1:D:445:PRO:HA	1.97	0.46
2:N:3:NAG:O6	2:N:6:FUC:C1	2.64	0.46
1:C:334:LEU:O	1:C:346:GLY:HA2	2.16	0.46
1:H:382:ARG:CG	1:H:382:ARG:NH1	2.78	0.46
1:J:392:GLY:H	2:R:6:FUC:H2	1.81	0.46
1:A:502:THR:HG23	3:A:559:HOH:O	2.16	0.45
1:G:414:HIS:O	1:G:415:ASN:C	2.57	0.45
1:B:394:THR:OG1	1:B:398:ASN:ND2	2.46	0.45
1:B:461:PHE:O	1:B:462:TYR:C	2.59	0.45
1:I:422:VAL:HG23	1:I:431:LEU:HD11	1.97	0.45
1:B:390:GLN:HG2	1:B:445:PRO:N	2.30	0.45
1:F:287:ARG:CD	3:F:532:HOH:O	2.62	0.45
1:G:261:PRO:O	1:G:265:ARG:NH1	2.49	0.45
1:I:330:ILE:HD12	1:I:353:THR:CG2	2.46	0.45
1:A:430:GLN:HG3	1:A:501:HIS:O	2.17	0.45
1:B:336:GLN:HG3	1:B:381:THR:OG1	2.16	0.45
1:D:277:GLN:OE1	1:D:279:SER:HB3	2.16	0.45
1:J:390:GLN:HE21	1:J:390:GLN:HB2	1.56	0.45
1:A:336:GLN:HE21	1:A:379:GLN:CB	2.17	0.45
1:H:468:ALA:HA	1:H:520:TRP:CZ2	2.52	0.45
1:J:248:LYS:HE2	3:J:542:HOH:O	2.17	0.45
1:B:332:GLY:HA3	1:B:384:THR:O	2.16	0.45
1:F:259:VAL:HG13	1:F:403:TRP:CZ3	2.52	0.45
1:G:327:VAL:HA	1:G:353:THR:OG1	2.17	0.45
1:A:390:GLN:HG3	1:A:444:TYR:N	2.32	0.45
1:C:344:THR:O	2:M:5:FUC:H2	2.16	0.45
1:C:523:GLN:CB	3:C:183:HOH:O	2.63	0.45
1:E:417:HIS:CD2	3:E:148:HOH:O	2.29	0.45
1:H:454:PRO:HG2	1:H:457:TRP:CD1	2.52	0.45
1:E:323:THR:HG22	1:E:324:PRO:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HG3	1:A:512:ASN:O	2.18	0.45
1:B:287:ARG:NH1	1:B:306:GLN:HA	2.32	0.45
1:G:343:SER:HB3	1:J:444:TYR:CE1	2.52	0.45
1:H:359:THR:N	1:H:360:PRO:HD3	2.31	0.45
1:B:397:GLN:HB3	1:B:446:ASN:HB2	1.99	0.44
1:C:273:LEU:O	1:C:276:THR:HB	2.17	0.44
1:I:466:ALA:HA	1:I:467:PRO:HD3	1.87	0.44
1:D:390:GLN:HG3	1:D:444:TYR:H	1.82	0.44
1:E:319:ALA:HB1	1:E:320:PRO:HD2	1.99	0.44
1:E:435:ARG:HB2	1:E:450:ASP:OD1	2.16	0.44
1:F:319:ALA:HB1	1:F:320:PRO:HD2	1.98	0.44
1:G:279:SER:HB2	3:J:39:HOH:O	2.18	0.44
2:M:4:GAL:C2	2:M:5:FUC:C5	2.90	0.44
1:B:399:GLU:HB2	1:B:400:PRO:HA	1.98	0.44
1:I:433:PHE:HB3	1:I:450:ASP:HB3	1.98	0.44
1:F:478:VAL:HG21	1:F:516:ARG:NH1	2.32	0.44
1:F:516:ARG:HA	3:F:540:HOH:O	2.18	0.44
1:B:442:SER:HA	1:E:344:THR:O	2.18	0.44
1:C:338:THR:O	1:C:339:ARG:C	2.61	0.44
1:E:238:THR:N	1:E:456:GLU:OE1	2.47	0.44
1:F:501:HIS:CD2	1:F:502:THR:N	2.86	0.44
1:I:261:PRO:HG2	1:I:265:ARG:HD3	1.98	0.44
2:M:4:GAL:H62	2:M:6:FUC:H3	2.00	0.44
1:A:391:ASP:CG	1:A:394:THR:HG23	2.42	0.44
1:C:276:THR:HA	3:C:550:HOH:O	2.18	0.44
1:E:476:ARG:HG3	1:E:485:VAL:HG11	2.00	0.44
1:G:225:LYS:HA	1:G:226:PRO:HD3	1.92	0.44
1:J:328:GLY:HA3	1:J:400:PRO:HB3	2.00	0.44
1:A:310:ASN:HA	3:A:549:HOH:O	2.18	0.44
1:D:346:GLY:N	1:F:441:CYS:O	2.51	0.44
1:I:340:ARG:HG3	1:J:317:ILE:HG22	2.00	0.44
1:B:308:TRP:CH2	1:B:380:ASN:HB3	2.53	0.43
1:D:486:LEU:CD1	1:D:510:PRO:HD3	2.48	0.43
1:F:307:ASN:O	1:F:308:TRP:HB2	2.17	0.43
1:H:277:GLN:HG3	1:H:306:GLN:NE2	2.33	0.43
1:A:319:ALA:O	1:A:320:PRO:C	2.61	0.43
1:E:230:PRO:HG2	1:E:457:TRP:CD1	2.53	0.43
1:G:430:GLN:HG3	1:G:501:HIS:O	2.18	0.43
1:B:287:ARG:CD	3:B:537:HOH:O	2.65	0.43
1:D:470:SER:OG	1:D:520:TRP:HB3	2.18	0.43
1:E:321:LEU:N	1:E:321:LEU:HD23	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:510:PRO:HA	1:F:511:PRO:HD3	1.81	0.43
1:D:441:CYS:O	1:F:345:ARG:C	2.61	0.43
1:G:472:VAL:HG11	1:G:490:LYS:HB3	1.99	0.43
1:D:442:SER:OG	2:N:5:FUC:C1	2.66	0.43
1:I:260:GLN:HG3	1:I:421:ALA:HA	2.00	0.43
1:G:281:VAL:HG12	1:J:281:VAL:HG12	2.00	0.43
1:G:492:HIS:O	1:G:495:GLY:N	2.49	0.43
1:H:225:LYS:NZ	1:H:464:GLU:O	2.43	0.43
1:H:382:ARG:NH1	1:H:382:ARG:HG3	2.33	0.43
1:I:478:VAL:HG21	1:I:516:ARG:HD3	2.00	0.43
2:R:1:BGC:C6	2:R:2:GAL:H2	2.48	0.43
1:A:232:LEU:CD2	1:C:463:GLN:HE22	2.31	0.43
1:F:401:GLN:HA	3:F:199:HOH:O	2.19	0.43
1:C:307:ASN:OD1	1:C:309:ASN:HB2	2.19	0.43
1:D:390:GLN:O	1:D:443:GLY:HA3	2.19	0.43
1:E:377:THR:O	1:E:379:GLN:HG2	2.19	0.43
2:P:4:GAL:O4	2:P:4:GAL:O6	2.31	0.43
1:A:361:LYS:O	1:A:361:LYS:HG3	2.19	0.42
1:C:277:GLN:CG	1:C:306:GLN:HE22	2.28	0.42
1:G:344:THR:HG21	1:J:440:GLY:HA3	2.01	0.42
1:H:514:TYR:N	1:H:514:TYR:CD2	2.86	0.42
1:I:419:ALA:HA	1:I:420:PRO:HD3	1.90	0.42
1:J:312:ASP:HA	1:J:313:PRO:HD3	1.90	0.42
1:E:438:MET:HE3	1:E:438:MET:HB2	1.95	0.42
1:I:478:VAL:HG21	1:I:516:ARG:NH1	2.34	0.42
1:J:233:THR:HG21	1:J:512:ASN:HA	2.02	0.42
1:E:471:ASP:HB2	3:E:553:HOH:O	2.17	0.42
1:G:336:GLN:OE1	1:G:345:ARG:HD2	2.20	0.42
1:C:431:LEU:HA	1:C:431:LEU:HD23	1.81	0.42
1:F:512:ASN:OD1	1:F:512:ASN:N	2.51	0.42
2:O:1:BGC:C3	2:O:2:GAL:O5	2.65	0.42
1:C:523:GLN:CA	3:C:183:HOH:O	2.67	0.42
1:E:268:THR:CG2	1:E:493:LYS:HA	2.49	0.42
1:G:453:LEU:HG	1:G:495:GLY:O	2.19	0.42
1:E:411:ARG:O	1:E:412:ASP:C	2.61	0.42
1:J:405:LEU:HA	1:J:405:LEU:HD23	1.69	0.42
2:L:1:BGC:O6	2:L:1:BGC:O4	2.30	0.42
1:A:438:MET:HE2	1:A:449:LEU:HB2	2.01	0.42
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.54	0.42
1:J:528:ALA:O	1:J:529:PRO:C	2.62	0.42
1:E:469:GLN:HG3	1:E:520:TRP:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:PRO:HD2	1:G:408:TYR:O	2.20	0.42
1:I:238:THR:C	1:I:246:LEU:HD11	2.44	0.42
1:I:258:VAL:O	1:I:258:VAL:CG2	2.66	0.42
1:I:260:GLN:HG3	1:I:421:ALA:CA	2.50	0.42
1:D:299:TYR:CE1	1:D:375:PHE:HB2	2.54	0.42
1:H:530:MET:HG2	1:H:531:GLY:N	2.33	0.42
1:G:409:SER:CB	1:G:413:SER:HB2	2.43	0.42
1:I:241:ARG:NE	1:I:325:ASP:OD2	2.42	0.42
1:B:283:ILE:O	1:B:284:CYS:HB2	2.20	0.41
1:F:230:PRO:HD3	1:F:460:HIS:CG	2.54	0.41
1:G:240:SER:OG	1:G:264:GLY:HA3	2.20	0.41
1:G:328:GLY:HA3	1:G:400:PRO:HB3	2.01	0.41
1:B:466:ALA:HA	1:B:467:PRO:HD2	1.92	0.41
1:D:488:GLU:HG3	1:D:527:LEU:HD22	2.02	0.41
1:F:287:ARG:NE	3:F:532:HOH:O	2.53	0.41
1:A:332:GLY:HA2	1:A:386:VAL:HG23	2.01	0.41
1:A:454:PRO:HD2	1:A:457:TRP:CG	2.55	0.41
1:E:454:PRO:O	1:E:455:GLN:C	2.59	0.41
1:H:433:PHE:HB3	1:H:450:ASP:HB3	2.03	0.41
1:B:430:GLN:HG3	1:B:501:HIS:O	2.20	0.41
1:F:391:ASP:HB3	1:F:394:THR:HG23	2.02	0.41
1:G:266:CYS:HA	1:G:271:ALA:O	2.21	0.41
1:E:323:THR:HG23	1:E:324:PRO:HD2	2.01	0.41
1:G:253:PRO:HA	3:G:552:HOH:O	2.21	0.41
1:B:359:THR:N	1:B:360:PRO:HD3	2.36	0.41
1:D:285:THR:HG22	1:D:385:PRO:HD2	2.01	0.41
1:G:232:LEU:HD21	1:J:463:GLN:HE21	1.86	0.41
1:G:307:ASN:OD1	1:G:309:ASN:HB2	2.21	0.41
1:A:338:THR:OG1	1:A:345:ARG:NH2	2.47	0.41
1:C:252:GLY:HA2	1:C:430:GLN:HE22	1.86	0.41
1:C:479:ASN:OD1	1:C:479:ASN:C	2.63	0.41
1:D:390:GLN:NE2	1:D:398:ASN:OD1	2.53	0.41
1:C:246:LEU:HD23	1:C:246:LEU:HA	1.76	0.41
1:C:438:MET:HE3	1:C:438:MET:HB2	1.91	0.41
1:F:327:VAL:HG23	1:F:404:VAL:O	2.20	0.41
1:G:469:GLN:CG	1:G:520:TRP:CD1	3.03	0.41
1:H:468:ALA:HA	1:H:520:TRP:CH2	2.55	0.41
1:J:433:PHE:HB3	1:J:450:ASP:HB3	2.03	0.41
1:E:285:THR:HG22	1:E:385:PRO:CD	2.51	0.41
1:G:410:GLY:C	1:G:411:ARG:O	2.61	0.41
1:G:472:VAL:HG11	1:G:490:LYS:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:443:GLY:CA	2:R:6:FUC:H63	2.50	0.41
2:P:4:GAL:H2	2:P:6:FUC:H62	2.02	0.41
2:Q:1:BGC:C6	2:Q:2:GAL:C1	2.67	0.41
1:C:242:PHE:O	1:C:244:ILE:N	2.53	0.40
1:D:266:CYS:HB2	1:D:458:VAL:HG13	2.02	0.40
1:G:306:GLN:CB	3:G:89:HOH:O	2.68	0.40
1:J:417:HIS:HE1	3:J:549:HOH:O	2.04	0.40
2:Q:2:GAL:O3	2:Q:3:NAG:O7	2.39	0.40
1:D:438:MET:HE3	1:D:438:MET:HB2	1.95	0.40
1:D:453:LEU:HD11	1:D:495:GLY:O	2.21	0.40
1:D:522:ASN:HB2	3:D:77:HOH:O	2.21	0.40
1:F:319:ALA:HB1	1:F:320:PRO:CD	2.51	0.40
1:J:327:VAL:HG23	1:J:404:VAL:O	2.21	0.40
1:C:279:SER:HA	1:C:280:PRO:HD3	1.93	0.40
1:J:316:GLU:C	1:J:317:ILE:HG23	2.46	0.40
1:D:319:ALA:HB1	1:D:320:PRO:CD	2.50	0.40
1:A:426:PHE:CE1	1:A:524:PHE:HA	2.56	0.40
1:C:447:MET:HE3	1:C:447:MET:HB2	1.94	0.40
1:E:327:VAL:HA	1:E:353:THR:OG1	2.22	0.40
1:E:505:HIS:HE1	3:E:12:HOH:O	2.04	0.40
1:G:443:GLY:CA	2:Q:5:FUC:H61	2.48	0.40

There are no symmetry-related clashes.

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%)	293 (95%)	14 (5%)	0	100	100
1	B	305/311 (98%)	294 (96%)	11 (4%)	0	100	100
1	C	309/311 (99%)	294 (95%)	15 (5%)	0	100	100
1	D	305/311 (98%)	297 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	307/311 (99%)	290 (94%)	17 (6%)	0	100	100
1	F	306/311 (98%)	290 (95%)	16 (5%)	0	100	100
1	G	306/311 (98%)	295 (96%)	11 (4%)	0	100	100
1	H	294/311 (94%)	278 (95%)	16 (5%)	0	100	100
1	I	274/311 (88%)	252 (92%)	20 (7%)	2 (1%)	18	49
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3018/3110 (97%)	2878 (95%)	138 (5%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	425	THR
1	I	231	ILE

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	269/272 (99%)	253 (94%)	16 (6%)	18	47
1	B	268/272 (98%)	248 (92%)	20 (8%)	12	38
1	C	271/272 (100%)	248 (92%)	23 (8%)	10	34
1	D	268/272 (98%)	250 (93%)	18 (7%)	15	43
1	E	271/272 (100%)	248 (92%)	23 (8%)	10	34
1	F	269/272 (99%)	250 (93%)	19 (7%)	13	40
1	G	266/272 (98%)	246 (92%)	20 (8%)	12	38
1	H	249/272 (92%)	226 (91%)	23 (9%)	8	30
1	I	219/272 (80%)	196 (90%)	23 (10%)	6	25
1	J	267/272 (98%)	243 (91%)	24 (9%)	9	31
All	All	2617/2720 (96%)	2408 (92%)	209 (8%)	11	36

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	282	ASP
1	A	310	ASN
1	A	340	ARG
1	A	364	SER
1	A	372	SER
1	A	373	ASN
1	A	390	GLN
1	A	395	THR
1	A	470	SER
1	A	472	VAL
1	A	486	LEU
1	A	494	SER
1	A	499	VAL
1	A	516	ARG
1	A	522	ASN
1	B	248	LYS
1	B	254	SER
1	B	255	SER
1	B	277	GLN
1	B	290	VAL
1	B	305	SER
1	B	310	ASN
1	B	331	GLN
1	B	364	SER
1	B	382	ARG
1	B	390	GLN
1	B	393	SER
1	B	395	THR
1	B	413	SER
1	B	472	VAL
1	B	482	THR
1	B	486	LEU
1	B	494	SER
1	B	522	ASN
1	B	530	MET
1	C	224	THR
1	C	248	LYS
1	C	254	SER
1	C	277	GLN
1	C	297	GLN
1	C	305	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	310	ASN
1	C	340	ARG
1	C	355	SER
1	C	362	LEU
1	C	364	SER
1	C	372	SER
1	C	382	ARG
1	C	390	GLN
1	C	393	SER
1	C	413	SER
1	C	416	VAL
1	C	441	CYS
1	C	442	SER
1	C	465	SER
1	C	486	LEU
1	C	493	LYS
1	C	530	MET
1	D	234	VAL
1	D	277	GLN
1	D	282	ASP
1	D	316	GLU
1	D	364	SER
1	D	372	SER
1	D	373	ASN
1	D	374	ASP
1	D	382	ARG
1	D	390	GLN
1	D	412	ASP
1	D	469	GLN
1	D	471	ASP
1	D	484	ARG
1	D	486	LEU
1	D	494	SER
1	D	499	VAL
1	D	530	MET
1	E	224	THR
1	E	273	LEU
1	E	277	GLN
1	E	305	SER
1	E	309	ASN
1	E	331	GLN
1	E	339	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	340	ARG
1	E	341	ASP
1	E	343	SER
1	E	362	LEU
1	E	364	SER
1	E	372	SER
1	E	373	ASN
1	E	374	ASP
1	E	382	ARG
1	E	390	GLN
1	E	393	SER
1	E	412	ASP
1	E	413	SER
1	E	416	VAL
1	E	486	LEU
1	E	493	LYS
1	F	277	GLN
1	F	293	ILE
1	F	305	SER
1	F	309	ASN
1	F	331	GLN
1	F	340	ARG
1	F	345	ARG
1	F	364	SER
1	F	371	THR
1	F	372	SER
1	F	390	GLN
1	F	393	SER
1	F	412	ASP
1	F	416	VAL
1	F	442	SER
1	F	484	ARG
1	F	486	LEU
1	F	512	ASN
1	F	530	MET
1	G	224	THR
1	G	277	GLN
1	G	282	ASP
1	G	290	VAL
1	G	309	ASN
1	G	331	GLN
1	G	364	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	365	VAL
1	G	372	SER
1	G	373	ASN
1	G	374	ASP
1	G	376	GLU
1	G	381	THR
1	G	390	GLN
1	G	393	SER
1	G	395	THR
1	G	413	SER
1	G	442	SER
1	G	484	ARG
1	G	486	LEU
1	H	234	VAL
1	H	248	LYS
1	H	277	GLN
1	H	310	ASN
1	H	329	LYS
1	H	331	GLN
1	H	334	LEU
1	H	337	THR
1	H	340	ARG
1	H	350	THR
1	H	355	SER
1	H	364	SER
1	H	375	PHE
1	H	377	THR
1	H	382	ARG
1	H	384	THR
1	H	399	GLU
1	H	413	SER
1	H	441	CYS
1	H	471	ASP
1	H	486	LEU
1	H	494	SER
1	H	504	GLN
1	I	223	ARG
1	I	225	LYS
1	I	234	VAL
1	I	257	PHE
1	I	277	GLN
1	I	312	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	331	GLN
1	I	337	THR
1	I	338	THR
1	I	350	THR
1	I	377	THR
1	I	384	THR
1	I	388	VAL
1	I	413	SER
1	I	437	THR
1	I	438	MET
1	I	471	ASP
1	I	484	ARG
1	I	486	LEU
1	I	494	SER
1	I	502	THR
1	I	526	THR
1	I	530	MET
1	J	225	LYS
1	J	273	LEU
1	J	277	GLN
1	J	282	ASP
1	J	287	ARG
1	J	290	VAL
1	J	305	SER
1	J	309	ASN
1	J	338	THR
1	J	343	SER
1	J	345	ARG
1	J	364	SER
1	J	373	ASN
1	J	376	GLU
1	J	382	ARG
1	J	390	GLN
1	J	393	SER
1	J	413	SER
1	J	416	VAL
1	J	447	MET
1	J	481	ASP
1	J	484	ARG
1	J	486	LEU
1	J	494	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	331	GLN
1	A	336	GLN
1	A	366	GLN
1	A	390	GLN
1	A	396	HIS
1	A	398	ASN
1	A	505	HIS
1	A	522	ASN
1	B	306	GLN
1	B	331	GLN
1	B	366	GLN
1	B	390	GLN
1	B	417	HIS
1	C	306	GLN
1	C	347	HIS
1	C	430	GLN
1	C	463	GLN
1	C	505	HIS
1	C	523	GLN
1	D	306	GLN
1	D	310	ASN
1	D	357	HIS
1	D	417	HIS
1	D	505	HIS
1	E	306	GLN
1	E	331	GLN
1	E	347	HIS
1	E	357	HIS
1	E	366	GLN
1	E	397	GLN
1	E	414	HIS
1	E	417	HIS
1	E	505	HIS
1	F	309	ASN
1	F	347	HIS
1	F	366	GLN
1	F	390	GLN
1	F	397	GLN
1	F	501	HIS
1	G	263	ASN
1	G	366	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	373	ASN
1	G	390	GLN
1	H	306	GLN
1	H	331	GLN
1	H	347	HIS
1	H	366	GLN
1	H	379	GLN
1	H	463	GLN
1	H	469	GLN
1	H	479	ASN
1	H	505	HIS
1	I	306	GLN
1	I	366	GLN
1	I	430	GLN
1	I	463	GLN
1	I	469	GLN
1	I	504	GLN
1	J	306	GLN
1	J	390	GLN
1	J	398	ASN
1	J	417	HIS
1	J	501	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

48 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	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	K	2	2	11,11,12	0.37	0	15,15,17	0.81	0
2	NAG	K	3	2	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
2	GAL	K	4	2	11,11,12	0.32	0	15,15,17	0.75	1 (6%)
2	FUC	K	5	2	10,10,11	0.42	0	14,14,16	0.81	0
2	FUC	K	6	2	10,10,11	0.42	0	14,14,16	0.81	0
2	BGC	L	1	2	12,12,12	0.53	0	17,17,17	1.52	4 (23%)
2	GAL	L	2	2	11,11,12	0.54	0	15,15,17	1.23	2 (13%)
2	NAG	L	3	2	14,14,15	0.98	1 (7%)	17,19,21	2.08	5 (29%)
2	GAL	L	4	2	11,11,12	1.97	3 (27%)	15,15,17	2.41	5 (33%)
2	FUC	L	5	2	10,10,11	1.89	3 (30%)	14,14,16	3.64	5 (35%)
2	FUC	L	6	2	10,10,11	1.66	3 (30%)	14,14,16	2.60	6 (42%)
2	BGC	M	1	2	12,12,12	0.48	0	17,17,17	0.94	1 (5%)
2	GAL	M	2	2	11,11,12	0.33	0	15,15,17	0.79	0
2	NAG	M	3	2	14,14,15	0.97	1 (7%)	17,19,21	2.28	3 (17%)
2	GAL	M	4	2	11,11,12	1.58	2 (18%)	15,15,17	2.41	3 (20%)
2	FUC	M	5	2	10,10,11	1.40	1 (10%)	14,14,16	2.78	4 (28%)
2	FUC	M	6	2	10,10,11	0.41	0	14,14,16	0.82	0
2	BGC	N	1	2	12,12,12	0.84	0	17,17,17	2.15	6 (35%)
2	GAL	N	2	2	11,11,12	0.68	0	15,15,17	1.75	3 (20%)
2	NAG	N	3	2	14,14,15	0.90	1 (7%)	17,19,21	2.40	2 (11%)
2	GAL	N	4	2	11,11,12	1.74	3 (27%)	15,15,17	2.76	6 (40%)
2	FUC	N	5	2	10,10,11	0.44	0	14,14,16	0.75	0
2	FUC	N	6	2	10,10,11	0.45	0	14,14,16	0.91	0
2	BGC	O	1	2	12,12,12	1.15	1 (8%)	17,17,17	2.12	5 (29%)
2	GAL	O	2	2	11,11,12	1.04	1 (9%)	15,15,17	2.15	7 (46%)
2	NAG	O	3	2	14,14,15	0.99	1 (7%)	17,19,21	1.73	4 (23%)
2	GAL	O	4	2	11,11,12	2.02	2 (18%)	15,15,17	2.30	6 (40%)
2	FUC	O	5	2	10,10,11	0.63	0	14,14,16	0.95	0
2	FUC	O	6	2	10,10,11	0.40	0	14,14,16	0.81	0
2	BGC	P	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	P	2	2	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
2	NAG	P	3	2	14,14,15	0.55	0	17,19,21	0.89	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	0.42	0	14,14,16	0.81	0
2	FUC	P	6	2	10,10,11	0.43	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.56	0	17,19,21	0.88	1 (5%)
2	GAL	Q	4	2	11,11,12	0.33	0	15,15,17	0.75	0
2	FUC	Q	5	2	10,10,11	0.41	0	14,14,16	0.81	0
2	FUC	Q	6	2	10,10,11	0.41	0	14,14,16	0.81	0
2	BGC	R	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	R	2	2	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
2	NAG	R	3	2	14,14,15	0.55	0	17,19,21	0.88	0
2	GAL	R	4	2	11,11,12	0.32	0	15,15,17	0.75	0
2	FUC	R	5	2	10,10,11	0.42	0	14,14,16	0.81	0
2	FUC	R	6	2	10,10,11	0.42	0	14,14,16	0.81	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	-	0/2/19/22	0/1/1/1
2	NAG	K	3	2	-	2/6/23/26	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	FUC	K	6	2	-	-	0/1/1/1
2	BGC	L	1	2	-	2/2/22/22	0/1/1/1
2	GAL	L	2	2	-	2/2/19/22	0/1/1/1
2	NAG	L	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	4	2	-	1/2/19/22	0/1/1/1
2	FUC	L	5	2	-	-	0/1/1/1
2	FUC	L	6	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	-	2/2/19/22	0/1/1/1
2	FUC	M	5	2	-	-	0/1/1/1
2	FUC	M	6	2	-	-	0/1/1/1
2	BGC	N	1	2	-	2/2/22/22	0/1/1/1
2	GAL	N	2	2	-	1/2/19/22	0/1/1/1
2	NAG	N	3	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	4	GAL	O5-C1	-4.58	1.36	1.43
2	O	4	GAL	O5-C5	-4.20	1.35	1.43
2	L	5	FUC	O5-C5	-4.03	1.35	1.43
2	M	4	GAL	O5-C1	-3.97	1.37	1.43
2	M	5	FUC	O5-C1	-3.93	1.37	1.43
2	L	4	GAL	O5-C1	-3.87	1.37	1.43
2	L	4	GAL	O5-C5	-3.85	1.36	1.43
2	N	4	GAL	O5-C1	-3.47	1.37	1.43
2	O	1	BGC	C4-C5	3.46	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	GAL	C2-C3	-2.81	1.48	1.52
2	O	2	GAL	O5-C1	-2.79	1.39	1.43
2	M	4	GAL	O5-C5	-2.79	1.38	1.43
2	L	6	FUC	O5-C5	-2.73	1.38	1.43
2	L	3	NAG	C4-C5	-2.68	1.47	1.53
2	N	4	GAL	O5-C5	-2.66	1.38	1.43
2	L	6	FUC	O5-C1	-2.60	1.39	1.43
2	L	5	FUC	C4-C5	-2.38	1.47	1.52
2	N	4	GAL	C4-C5	-2.22	1.48	1.53
2	O	3	NAG	C4-C5	-2.16	1.48	1.53
2	N	3	NAG	C4-C3	-2.13	1.46	1.52
2	L	5	FUC	O4-C4	-2.07	1.37	1.43
2	M	3	NAG	C4-C5	-2.05	1.48	1.53
2	L	6	FUC	C1-C2	-2.04	1.47	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	5	FUC	C6-C5-C4	-9.93	94.92	113.08
2	N	3	NAG	C6-C5-C4	-8.70	91.65	113.02
2	M	3	NAG	C6-C5-C4	-7.56	94.45	113.02
2	L	5	FUC	O5-C5-C4	-7.06	96.85	109.55
2	N	4	GAL	C1-O5-C5	-6.91	102.93	112.19
2	M	5	FUC	O5-C1-C2	-6.84	94.48	110.79
2	L	6	FUC	C6-C5-C4	-6.66	100.90	113.08
2	M	4	GAL	C1-O5-C5	-6.37	103.65	112.19
2	L	4	GAL	C1-O5-C5	-6.37	103.66	112.19
2	L	3	NAG	C6-C5-C4	-5.59	99.29	113.02
2	N	4	GAL	C6-C5-C4	-5.17	100.33	113.02
2	M	5	FUC	O5-C5-C4	-4.86	100.81	109.55
2	O	2	GAL	C1-O5-C5	-4.80	105.75	112.19
2	N	1	BGC	C1-O5-C5	-4.68	104.60	113.65
2	N	1	BGC	C6-C5-C4	-4.64	101.63	113.02
2	N	2	GAL	C6-C5-C4	-4.57	101.81	113.02
2	O	1	BGC	O5-C5-C4	4.51	117.82	109.70
2	O	3	NAG	C6-C5-C4	-4.46	102.08	113.02
2	M	4	GAL	C6-C5-C4	-4.43	102.14	113.02
2	L	5	FUC	O5-C1-C2	-4.38	100.34	110.79
2	O	4	GAL	O2-C2-C3	4.33	119.13	110.15
2	O	1	BGC	C3-C4-C5	4.25	117.94	110.23
2	O	4	GAL	C1-O5-C5	-4.24	106.50	112.19
2	L	6	FUC	O5-C1-C2	-4.12	100.97	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	5	FUC	C2-C3-C4	4.01	117.92	110.86
2	L	3	NAG	C2-N2-C7	-3.91	117.67	122.90
2	L	4	GAL	O5-C5-C4	-3.59	102.10	110.83
2	O	4	GAL	O3-C3-C4	-3.56	101.99	110.38
2	M	3	NAG	O5-C5-C6	-3.43	100.99	107.66
2	L	4	GAL	O2-C2-C3	3.32	117.02	110.15
2	N	4	GAL	O5-C1-C2	-3.29	102.95	110.79
2	M	5	FUC	O2-C2-C3	-3.29	103.34	110.15
2	L	4	GAL	O3-C3-C2	-3.24	103.44	110.05
2	O	4	GAL	O5-C5-C4	-3.19	103.07	110.83
2	M	3	NAG	O5-C1-C2	-3.18	106.37	111.29
2	L	2	GAL	C6-C5-C4	-3.09	105.42	113.02
2	N	1	BGC	O1-C1-C2	-3.04	100.15	108.98
2	M	4	GAL	O3-C3-C2	-3.01	103.91	110.05
2	L	6	FUC	O3-C3-C4	-3.01	103.29	110.38
2	O	3	NAG	O5-C1-C2	-3.00	106.65	111.29
2	O	1	BGC	O5-C5-C6	-2.98	99.05	106.44
2	O	2	GAL	C6-C5-C4	-2.93	105.82	113.02
2	N	2	GAL	C1-O5-C5	-2.90	108.29	112.19
2	O	1	BGC	C1-O5-C5	-2.84	108.17	113.65
2	L	3	NAG	C1-O5-C5	2.83	115.97	112.19
2	O	1	BGC	O3-C3-C4	-2.77	103.84	110.38
2	N	1	BGC	O5-C5-C4	-2.72	104.80	109.70
2	N	1	BGC	C3-C4-C5	-2.71	105.32	110.23
2	L	1	BGC	O5-C5-C4	-2.68	104.87	109.70
2	L	5	FUC	O4-C4-C5	-2.63	103.94	109.74
2	N	4	GAL	O3-C3-C4	-2.61	104.21	110.38
2	N	4	GAL	C1-C2-C3	2.57	113.39	109.64
2	L	6	FUC	O2-C2-C1	-2.56	103.36	109.22
2	L	2	GAL	O5-C1-C2	-2.54	104.74	110.79
2	O	2	GAL	O2-C2-C3	-2.52	104.92	110.15
2	N	1	BGC	O2-C2-C1	-2.52	103.42	109.25
2	O	2	GAL	O5-C5-C6	2.52	112.57	107.66
2	O	3	NAG	O4-C4-C5	2.51	115.50	109.32
2	N	4	GAL	O5-C5-C4	-2.46	104.85	110.83
2	O	2	GAL	C2-C3-C4	2.43	115.14	110.86
2	M	1	BGC	C1-O5-C5	-2.42	108.97	113.65
2	L	1	BGC	O5-C1-C2	2.42	114.55	110.30
2	L	3	NAG	C3-C4-C5	2.40	114.59	110.23
2	L	3	NAG	O5-C5-C6	-2.39	103.00	107.66
2	O	4	GAL	O4-C4-C3	-2.29	104.97	110.38
2	N	3	NAG	O5-C5-C6	2.28	112.09	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	GAL	O5-C1-C2	-2.27	105.37	110.79
2	O	2	GAL	C1-C2-C3	2.27	112.94	109.64
2	L	1	BGC	C1-O5-C5	-2.24	109.31	113.65
2	Q	1	BGC	C1-O5-C5	-2.15	109.50	113.65
2	O	4	GAL	C6-C5-C4	-2.14	107.75	113.02
2	R	1	BGC	C1-O5-C5	-2.14	109.51	113.65
2	K	1	BGC	C1-O5-C5	-2.14	109.51	113.65
2	L	5	FUC	O2-C2-C3	-2.12	105.76	110.15
2	N	2	GAL	O5-C1-C2	-2.10	105.78	110.79
2	P	1	BGC	C1-O5-C5	-2.08	109.62	113.65
2	L	6	FUC	O4-C4-C3	-2.07	105.51	110.38
2	K	3	NAG	C1-O5-C5	-2.05	109.44	112.19
2	Q	2	GAL	C1-O5-C5	-2.04	109.45	112.19
2	L	1	BGC	O5-C5-C6	2.04	111.49	106.44
2	L	6	FUC	C3-C4-C5	2.04	112.91	109.81
2	R	2	GAL	C1-O5-C5	-2.04	109.45	112.19
2	Q	3	NAG	C1-O5-C5	-2.03	109.47	112.19
2	L	4	GAL	O4-C4-C3	-2.01	105.63	110.38
2	P	3	NAG	C1-O5-C5	-2.01	109.49	112.19
2	O	3	NAG	C4-C3-C2	2.01	113.97	111.02
2	K	4	GAL	C1-O5-C5	-2.01	109.49	112.19
2	P	2	GAL	C1-O5-C5	-2.01	109.49	112.19

There are no chirality outliers.

All (42) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

40 monomers are involved in 97 short contacts:

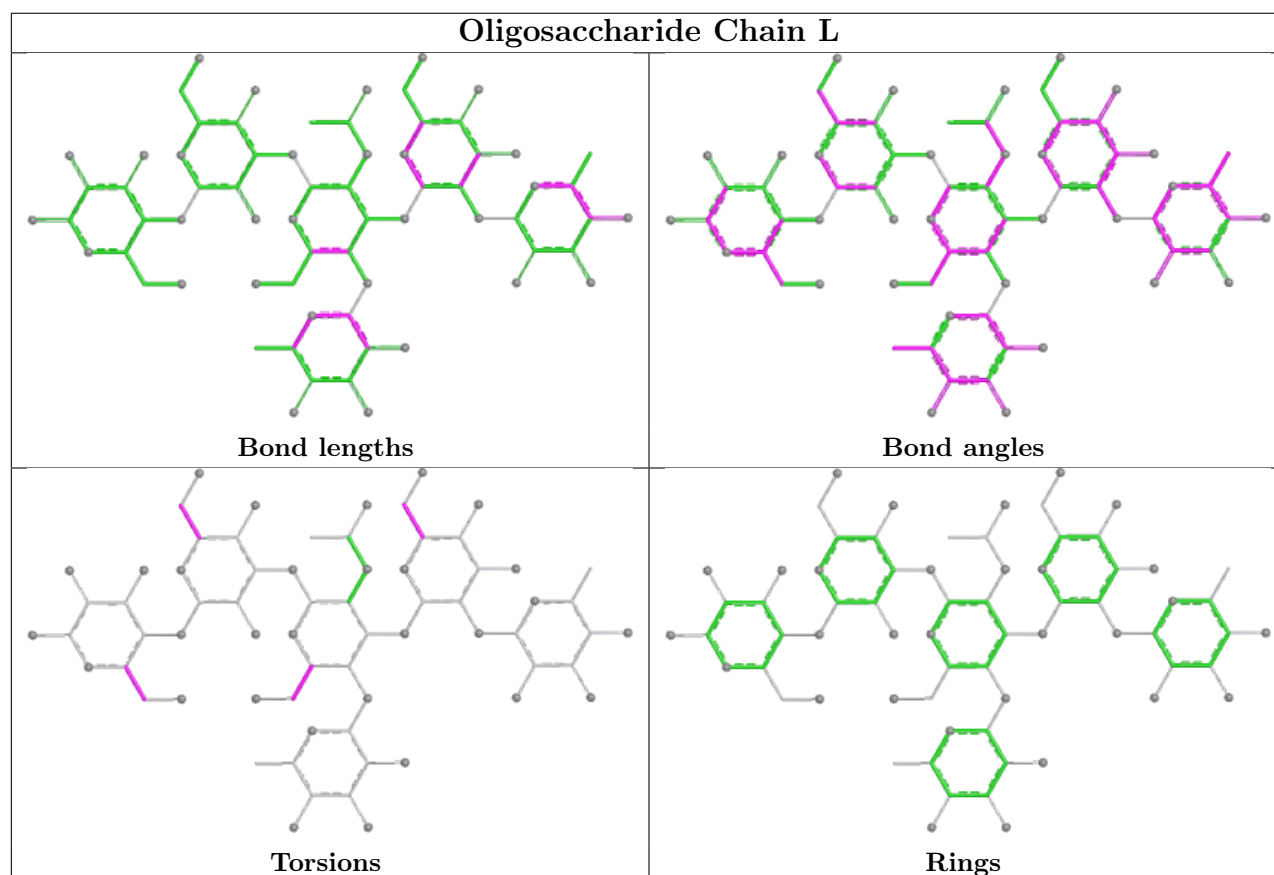
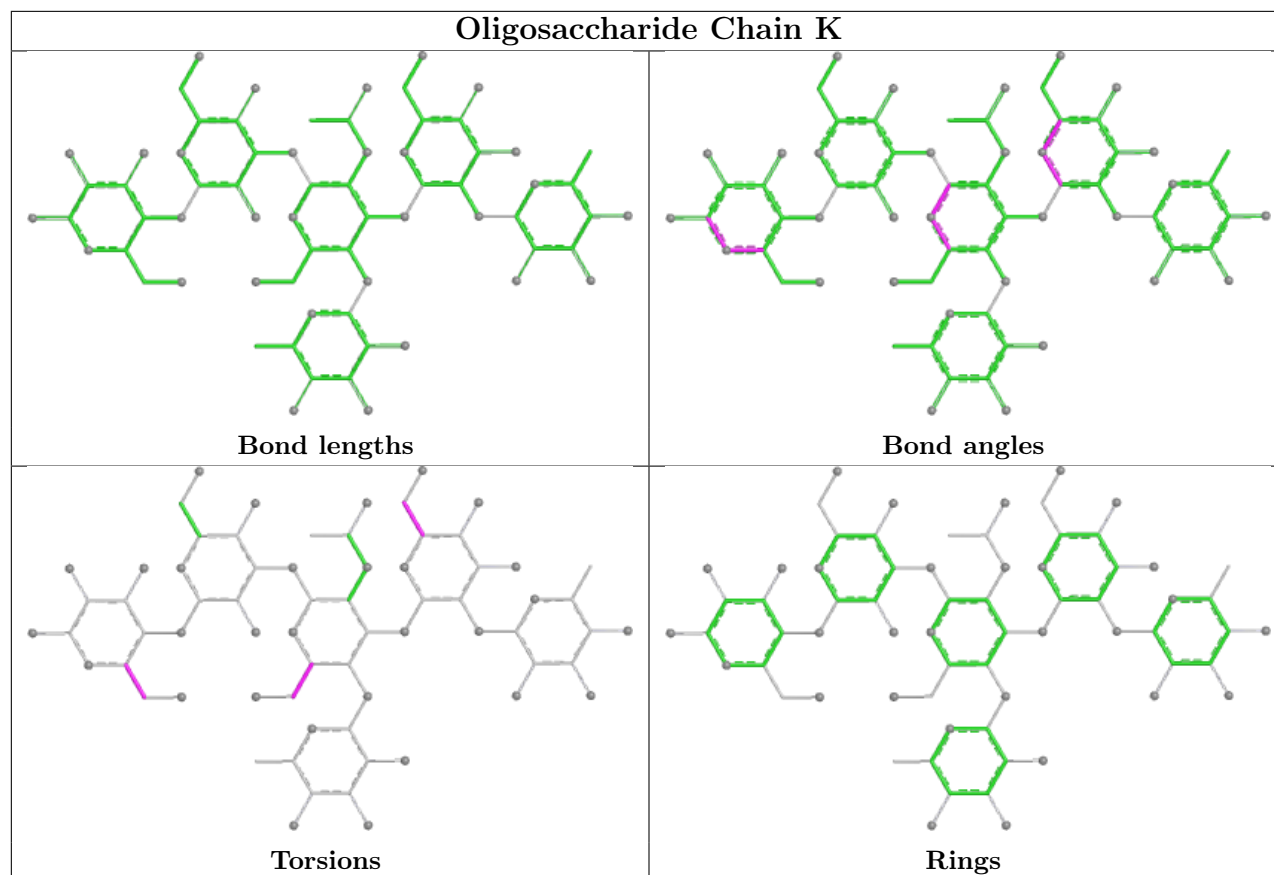
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	BGC	2	0
2	O	3	NAG	2	0
2	P	3	NAG	2	0
2	K	3	NAG	1	0
2	N	2	GAL	1	0
2	R	6	FUC	14	0
2	N	6	FUC	14	0
2	K	6	FUC	2	0
2	M	4	GAL	5	0
2	Q	5	FUC	13	0

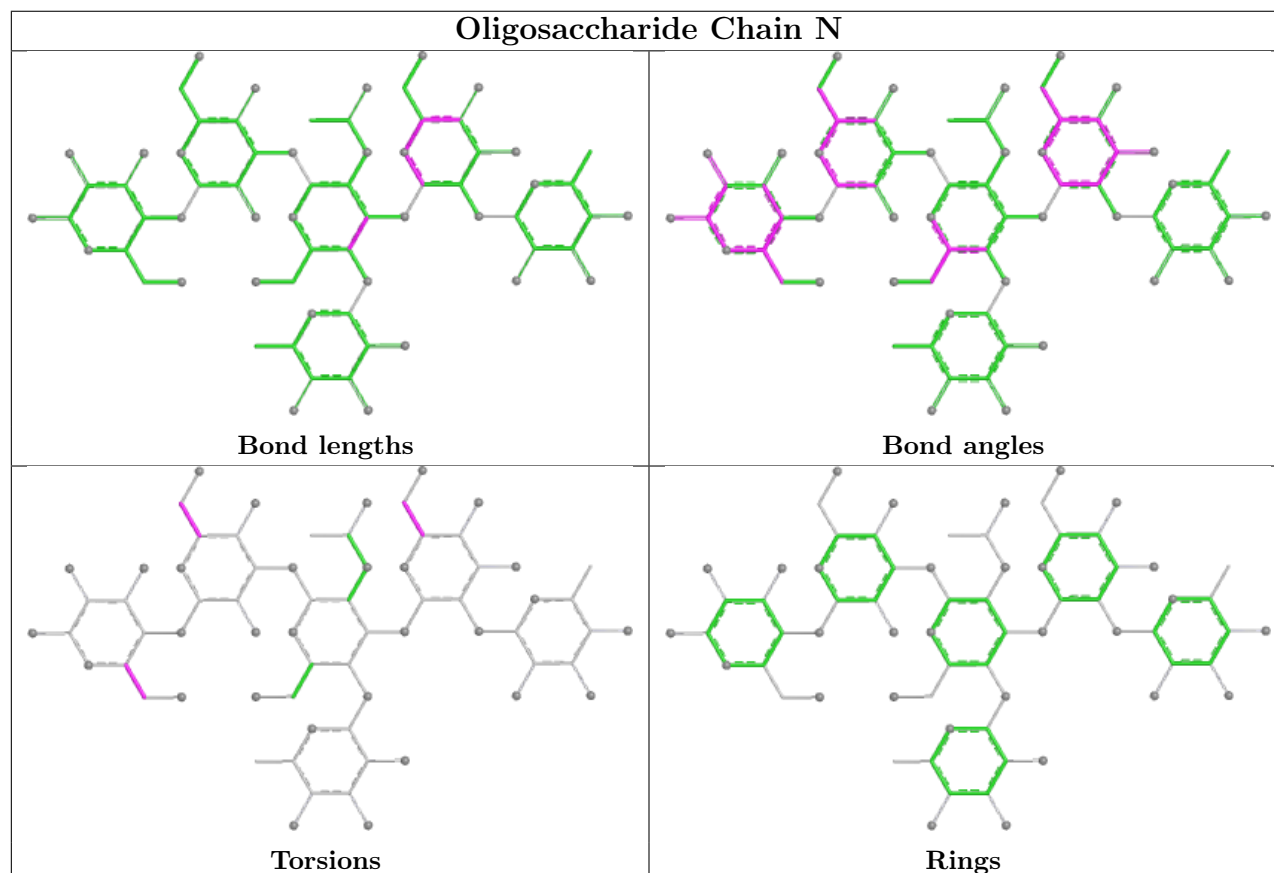
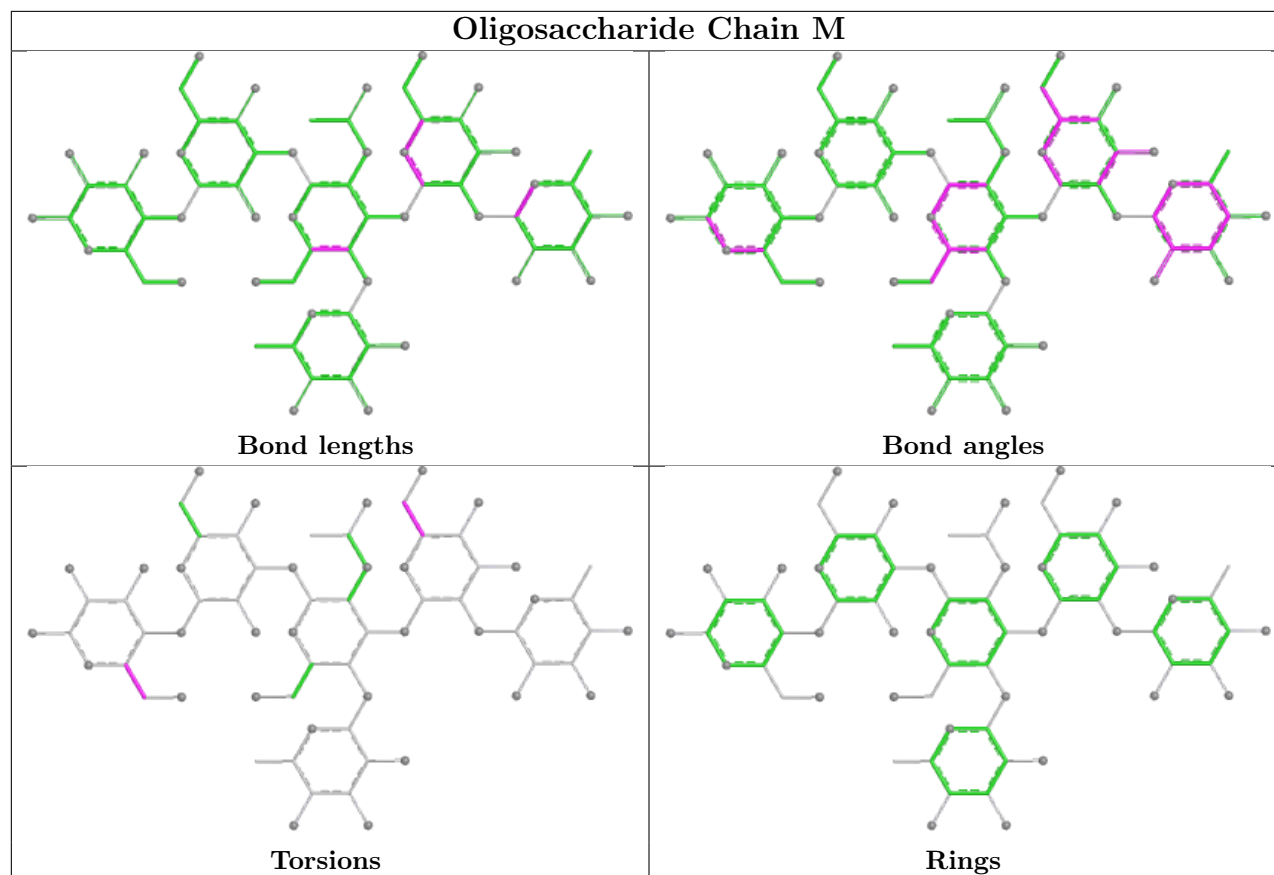
Continued on next page...

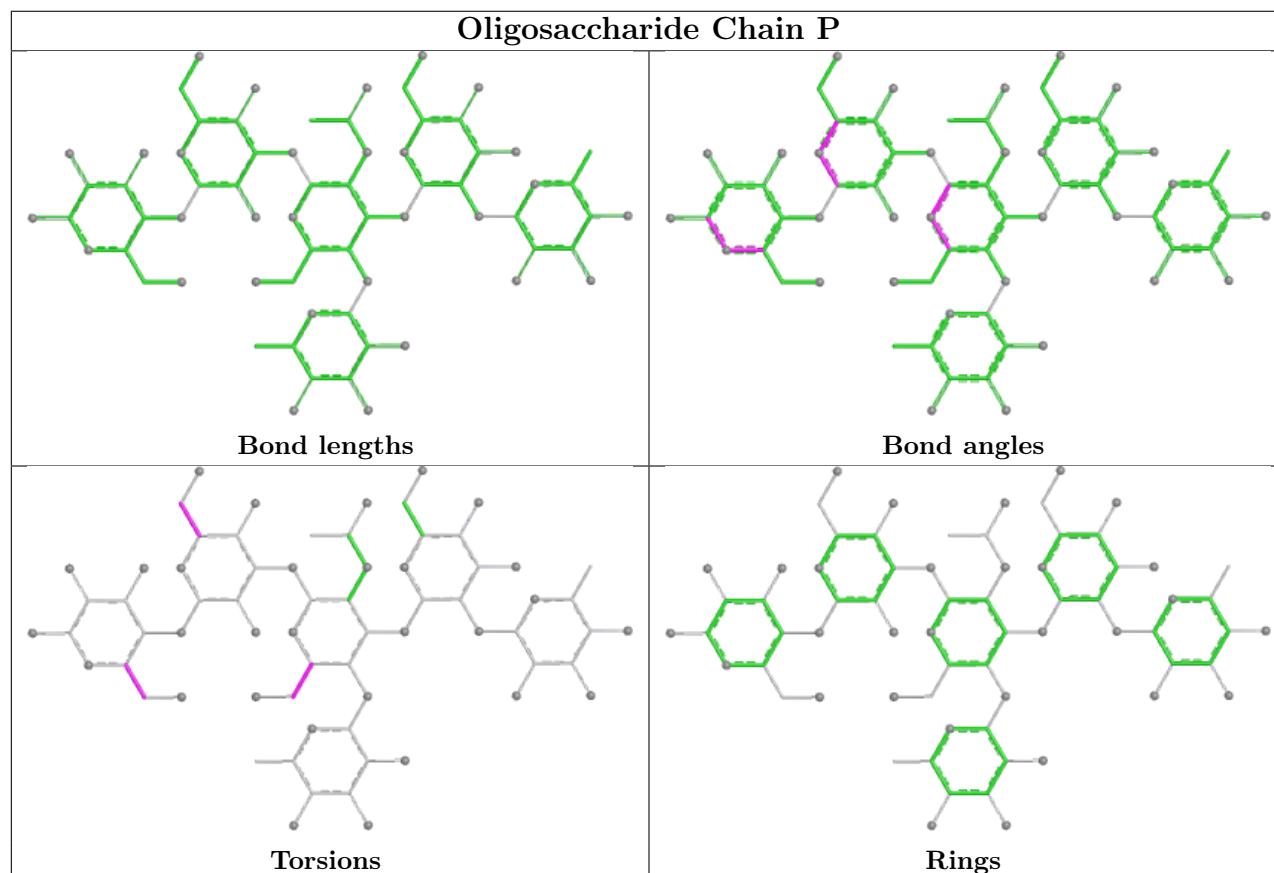
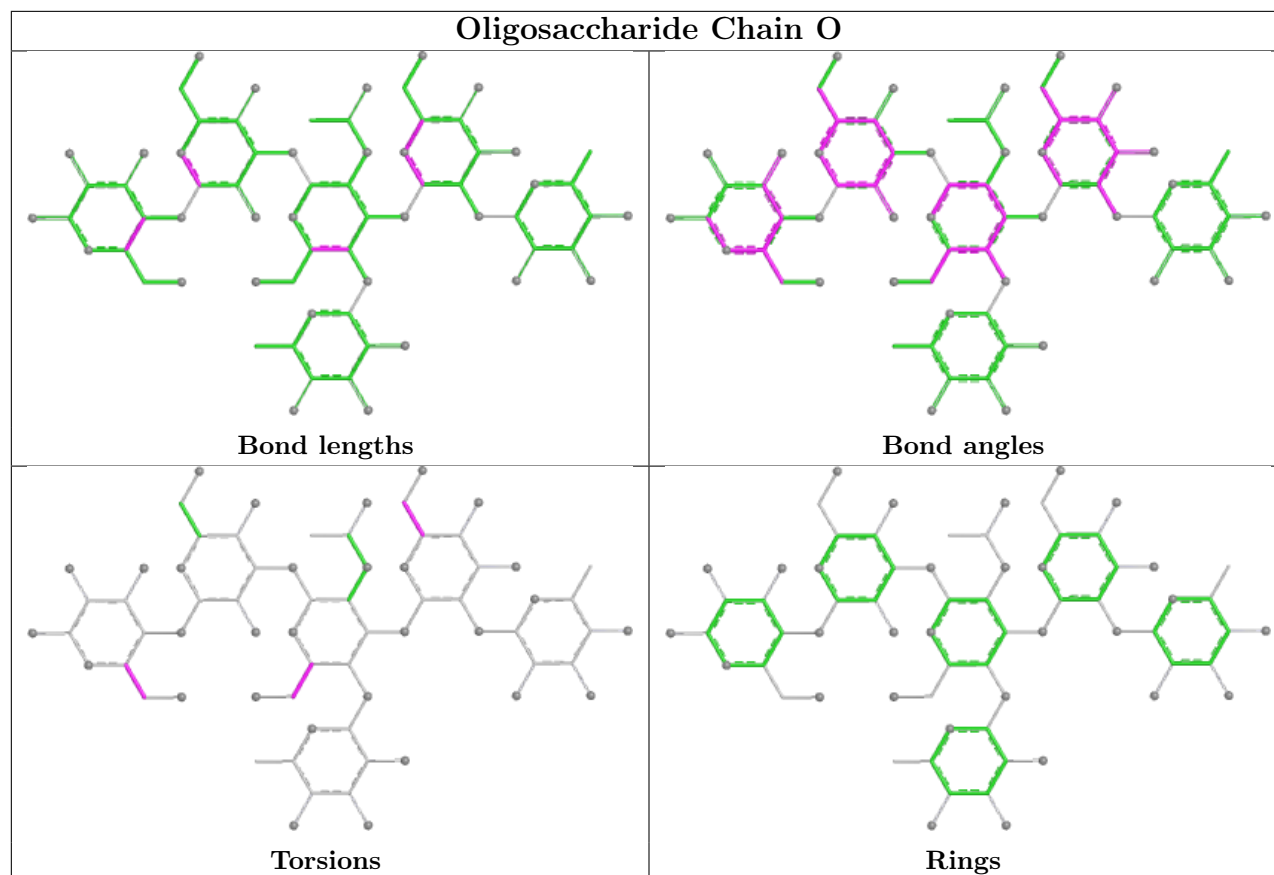
Continued from previous page...

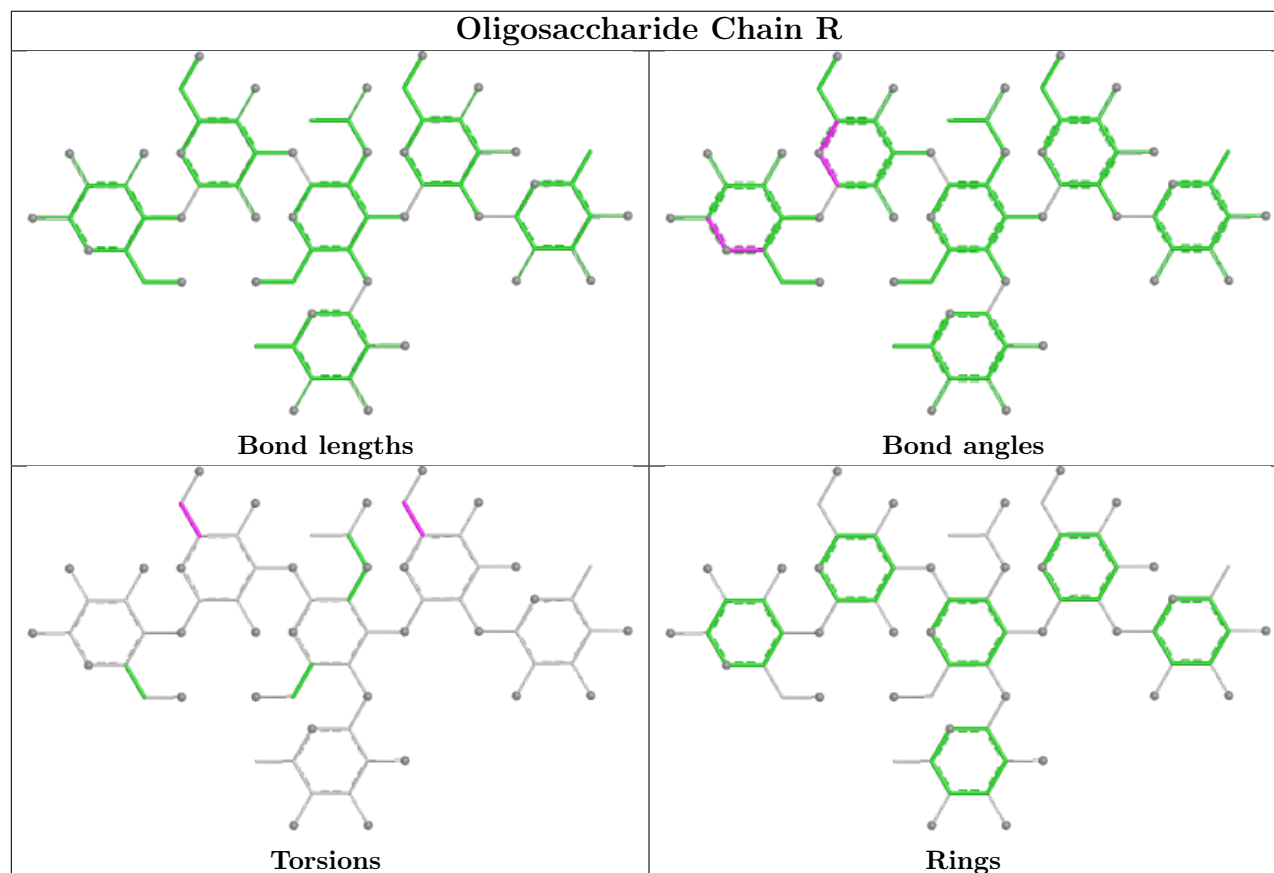
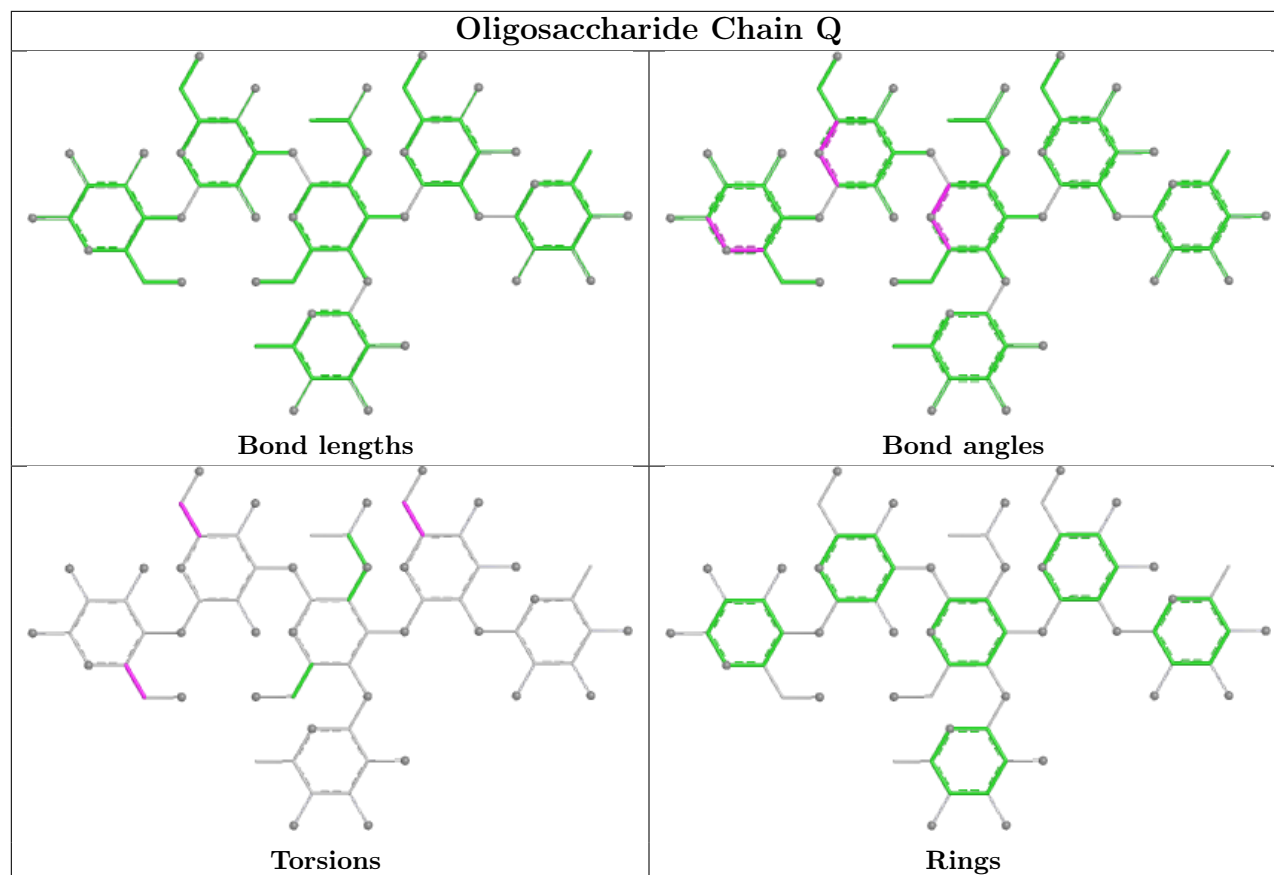
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	BGC	1	0
2	P	4	GAL	3	0
2	K	4	GAL	1	0
2	M	3	NAG	3	0
2	N	3	NAG	4	0
2	R	5	FUC	5	0
2	N	4	GAL	4	0
2	P	6	FUC	4	0
2	L	6	FUC	4	0
2	O	1	BGC	4	0
2	Q	1	BGC	2	0
2	Q	2	GAL	4	0
2	N	5	FUC	8	0
2	P	1	BGC	1	0
2	Q	3	NAG	2	0
2	L	1	BGC	2	0
2	L	5	FUC	2	0
2	Q	4	GAL	3	0
2	L	3	NAG	4	0
2	M	2	GAL	2	0
2	R	2	GAL	6	0
2	M	5	FUC	8	0
2	O	2	GAL	1	0
2	M	6	FUC	8	0
2	Q	6	FUC	5	0
2	R	1	BGC	6	0
2	O	6	FUC	2	0
2	R	4	GAL	3	0
2	R	3	NAG	2	0
2	L	2	GAL	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/311 (99%)	-0.82	2 (0%) 85 69	10, 22, 54, 90	0
1	B	307/311 (98%)	-0.80	0 100 100	15, 26, 51, 65	0
1	C	311/311 (100%)	-0.82	1 (0%) 90 79	13, 27, 49, 64	0
1	D	307/311 (98%)	-0.75	2 (0%) 84 66	11, 27, 59, 82	0
1	E	309/311 (99%)	-0.77	1 (0%) 90 79	15, 28, 60, 74	0
1	F	308/311 (99%)	-0.57	1 (0%) 90 79	20, 39, 68, 83	0
1	G	308/311 (99%)	-0.55	7 (2%) 61 37	22, 38, 63, 104	0
1	H	300/311 (96%)	-0.33	9 (3%) 52 29	17, 41, 79, 109	0
1	I	284/311 (91%)	0.93	39 (13%) 6 4	51, 81, 110, 140	0
1	J	307/311 (98%)	-0.63	2 (0%) 84 66	17, 33, 62, 79	0
All	All	3050/3110 (98%)	-0.52	64 (2%) 63 39	10, 33, 83, 140	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	413	SER	5.6
1	H	391	ASP	4.6
1	I	388	VAL	4.5
1	G	412	ASP	4.4
1	H	442	SER	4.3
1	H	390	GLN	3.9
1	I	528	ALA	3.6
1	G	414	HIS	3.5
1	H	374	ASP	3.5
1	I	523	GLN	3.5
1	I	375	PHE	3.4
1	I	300	THR	3.4
1	G	495	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	373	ASN	3.3
1	I	486	LEU	3.2
1	A	394	THR	3.2
1	H	370	ASP	3.1
1	G	415	ASN	3.1
1	I	257	PHE	3.1
1	I	329	LYS	3.0
1	I	524	PHE	3.0
1	I	440	GLY	2.9
1	I	376	GLU	2.8
1	J	394	THR	2.8
1	I	527	LEU	2.7
1	H	336	GLN	2.7
1	D	393	SER	2.6
1	F	412	ASP	2.6
1	I	506	ASP	2.6
1	I	369	THR	2.6
1	H	447	MET	2.5
1	I	519	SER	2.5
1	I	530	MET	2.5
1	E	524	PHE	2.5
1	I	338	THR	2.4
1	I	305	SER	2.4
1	I	379	GLN	2.4
1	J	495	GLY	2.3
1	I	386	VAL	2.3
1	I	317	ILE	2.3
1	I	482	THR	2.3
1	I	347	HIS	2.3
1	I	411	ARG	2.3
1	I	344	THR	2.2
1	G	411	ARG	2.2
1	H	372	SER	2.2
1	I	423	ALA	2.2
1	I	511	PRO	2.2
1	I	526	THR	2.2
1	I	290	VAL	2.2
1	D	442	SER	2.2
1	I	432	LEU	2.1
1	I	415	ASN	2.1
1	I	439	PRO	2.1
1	I	291	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	438	MET	2.1
1	I	513	GLY	2.1
1	I	258	VAL	2.1
1	I	522	ASN	2.1
1	C	221	GLU	2.1
1	I	427	PRO	2.1
1	G	310	ASN	2.0
1	A	306	GLN	2.0
1	I	336	GLN	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	K	1	12/12	0.13	0.18	126,130,130,131	0
2	BGC	M	1	12/12	0.19	0.17	122,125,126,126	0
2	GAL	M	2	11/12	0.30	0.20	108,115,118,118	0
2	BGC	L	1	12/12	0.34	0.19	124,130,130,130	0
2	BGC	N	1	12/12	0.39	0.16	123,126,126,127	0
2	BGC	R	1	12/12	0.41	0.16	129,133,133,133	0
2	GAL	N	2	11/12	0.45	0.18	111,115,119,120	0
2	GAL	K	2	11/12	0.47	0.17	113,119,122,123	0
2	GAL	P	2	11/12	0.51	0.16	126,130,131,132	0
2	GAL	R	2	11/12	0.53	0.16	119,122,125,126	0
2	BGC	O	1	12/12	0.61	0.21	105,109,109,109	0
2	BGC	P	1	12/12	0.62	0.16	134,136,136,136	0
2	GAL	O	2	11/12	0.63	0.19	93,97,101,101	0
2	NAG	Q	3	14/15	0.64	0.22	97,103,106,106	0
2	FUC	L	6	10/11	0.65	0.22	92,96,97,98	0
2	NAG	K	3	14/15	0.65	0.20	98,104,107,108	0
2	GAL	L	2	11/12	0.66	0.16	111,116,119,120	0
2	FUC	M	6	10/11	0.69	0.20	91,93,94,95	0
2	GAL	L	4	11/12	0.69	0.15	85,91,93,93	0

Continued on next page...

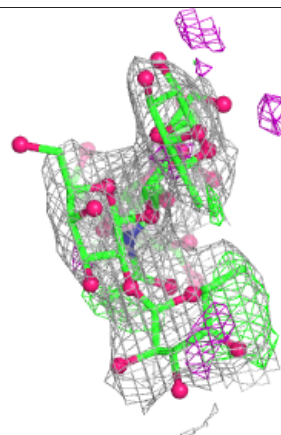
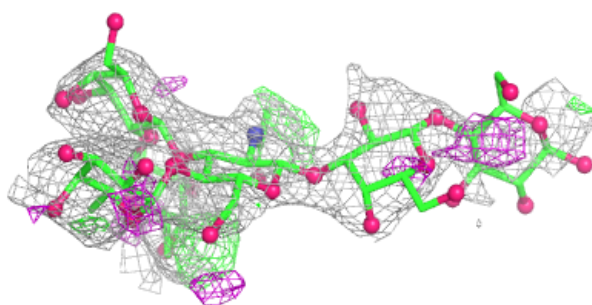
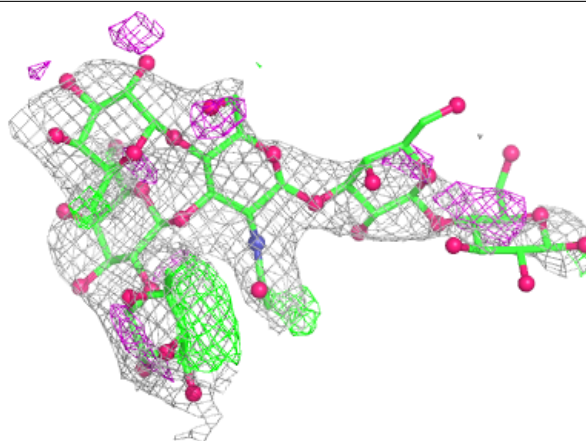
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	M	4	11/12	0.70	0.15	83,88,89,90	0
2	GAL	Q	4	11/12	0.70	0.15	85,96,97,97	0
2	FUC	K	6	10/11	0.70	0.19	99,100,101,101	0
2	GAL	Q	2	11/12	0.70	0.18	110,113,114,114	0
2	FUC	Q	5	10/11	0.71	0.19	70,74,76,79	0
2	FUC	N	6	10/11	0.72	0.18	97,99,99,99	0
2	NAG	O	3	14/15	0.73	0.18	79,83,86,88	0
2	NAG	L	3	14/15	0.73	0.20	98,102,104,106	0
2	FUC	K	5	10/11	0.73	0.20	74,77,78,80	0
2	FUC	R	6	10/11	0.73	0.17	107,108,109,109	0
2	GAL	N	4	11/12	0.74	0.14	92,94,96,96	0
2	GAL	R	4	11/12	0.74	0.13	92,96,99,99	0
2	NAG	M	3	14/15	0.74	0.17	93,97,101,103	0
2	NAG	R	3	14/15	0.75	0.16	104,111,112,114	0
2	GAL	P	4	11/12	0.75	0.16	108,112,113,114	0
2	BGC	Q	1	12/12	0.75	0.23	113,116,117,117	0
2	FUC	R	5	10/11	0.77	0.17	83,84,86,88	0
2	NAG	P	3	14/15	0.77	0.17	117,121,123,124	0
2	FUC	N	5	10/11	0.78	0.20	84,87,88,89	0
2	FUC	Q	6	10/11	0.78	0.16	100,101,102,102	0
2	FUC	O	6	10/11	0.79	0.16	73,75,76,77	0
2	FUC	P	6	10/11	0.80	0.17	119,120,121,121	0
2	FUC	M	5	10/11	0.81	0.18	73,74,77,79	0
2	FUC	L	5	10/11	0.81	0.18	71,72,75,78	0
2	NAG	N	3	14/15	0.81	0.16	97,102,105,106	0
2	FUC	O	5	10/11	0.82	0.17	57,61,62,63	0
2	GAL	O	4	11/12	0.83	0.12	68,72,74,75	0
2	GAL	K	4	11/12	0.86	0.10	84,91,92,92	0
2	FUC	P	5	10/11	0.89	0.15	100,101,102,104	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.

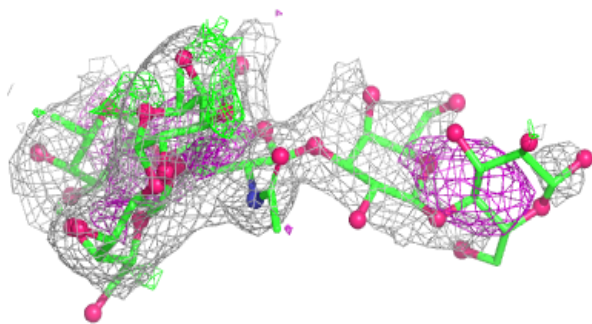
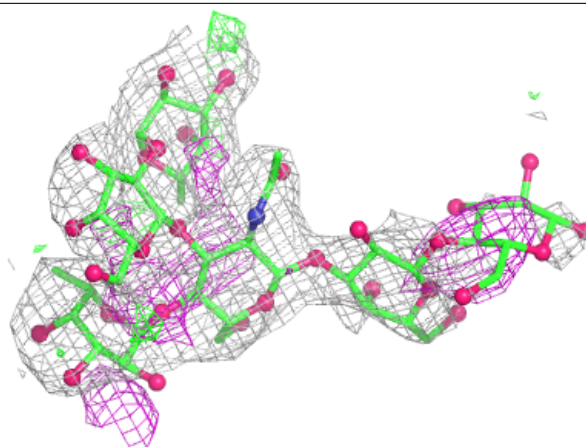
Electron density around Chain K:

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



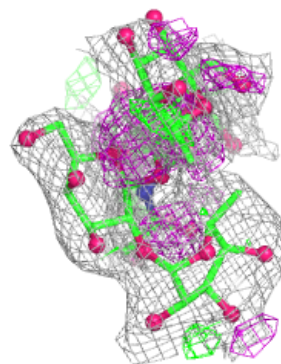
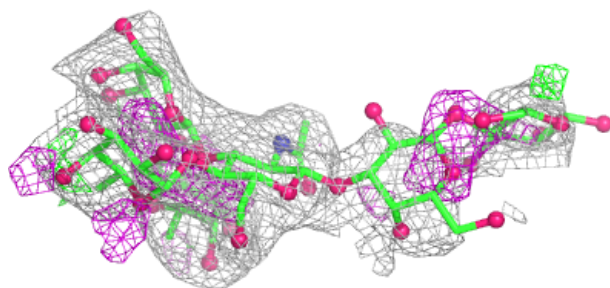
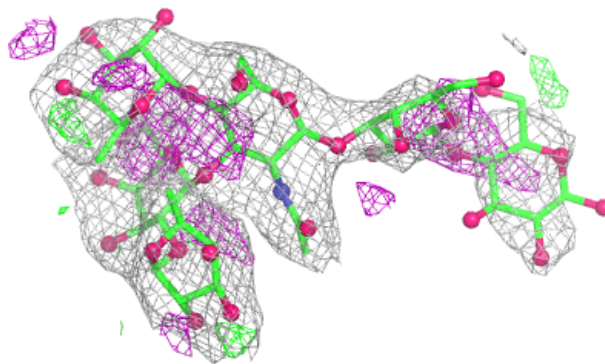
Electron density around Chain L:

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



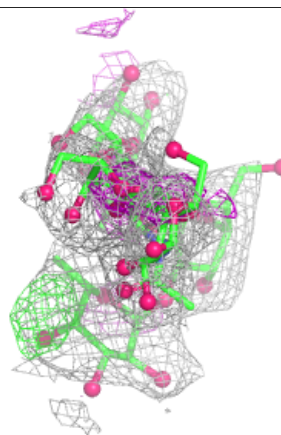
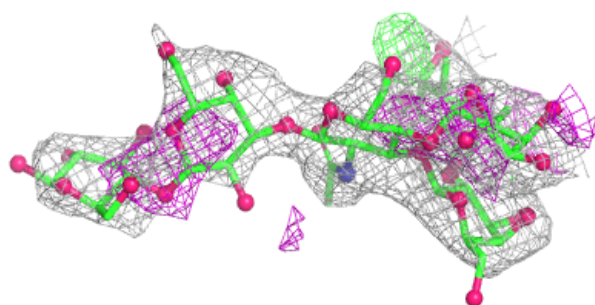
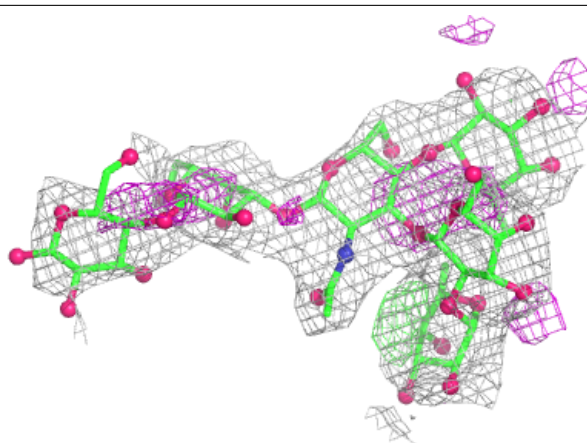
Electron density around Chain M:

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



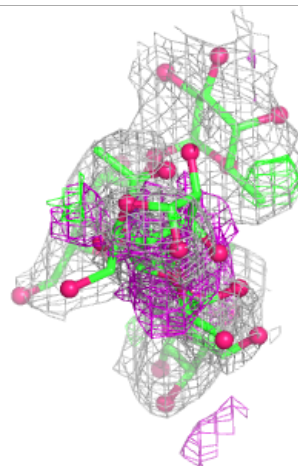
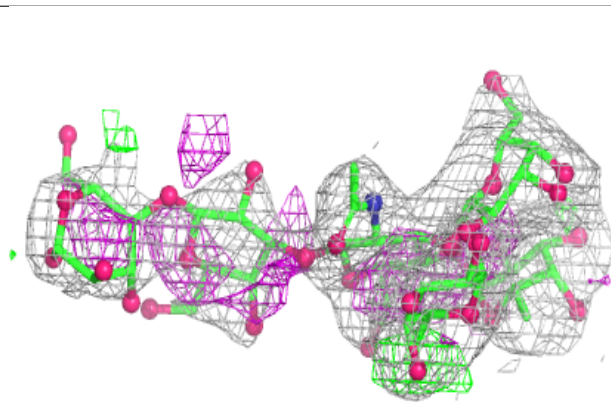
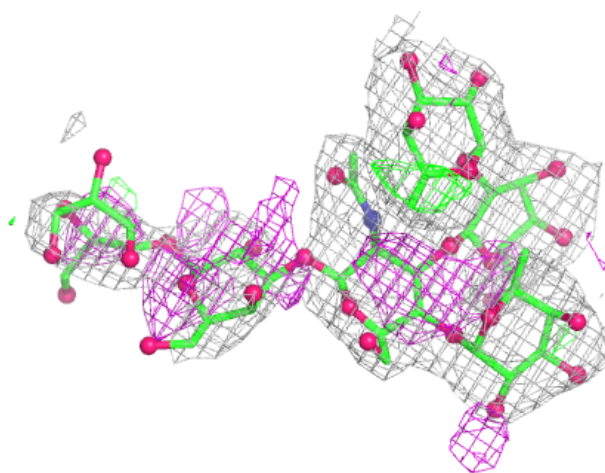
Electron density around Chain N:

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



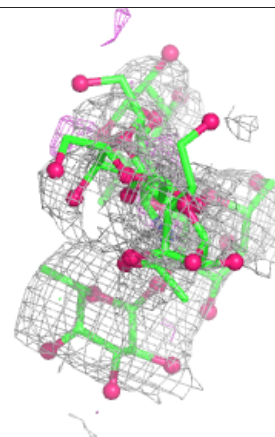
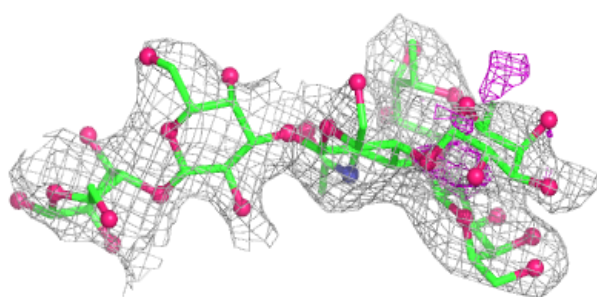
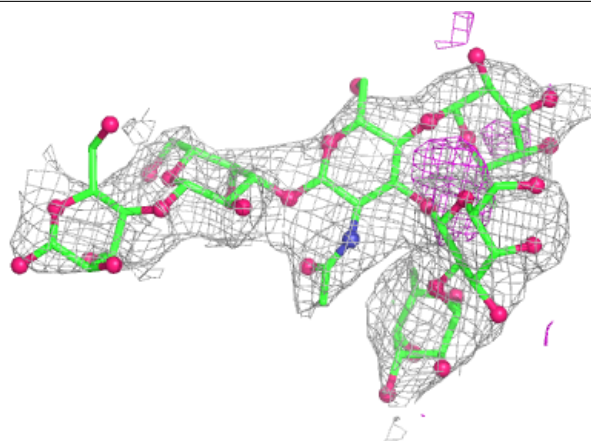
Electron density around Chain O:

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



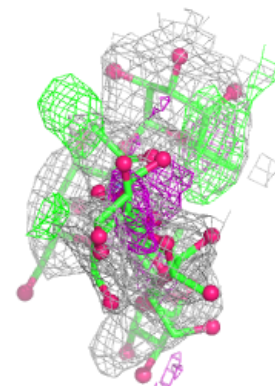
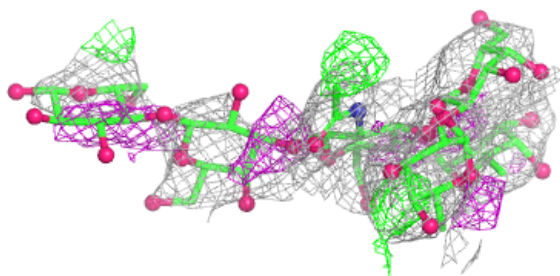
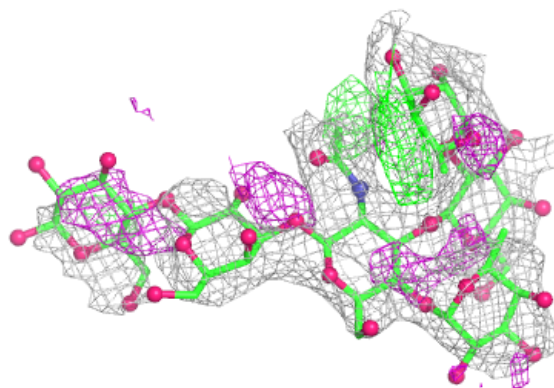
Electron density around Chain P:

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

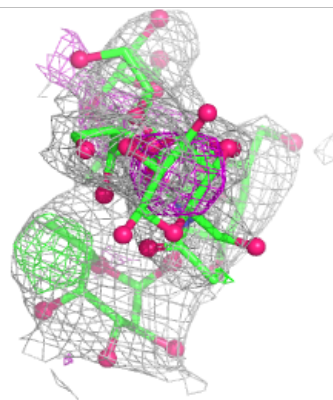
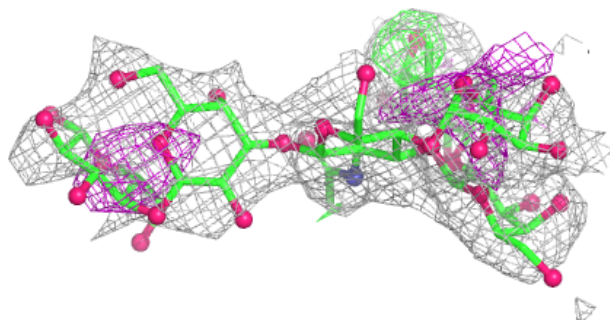
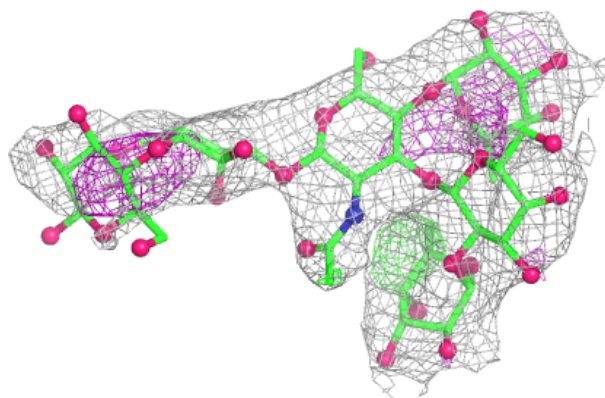


Electron density around Chain Q:

$2mF_o-DF_c$ (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.