



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:08 AM UTC

PDB ID : 3SLD / pdb_00003sld
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to A trisaccharide
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.
Deposited on : 2011-06-24
Resolution : 2.68 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

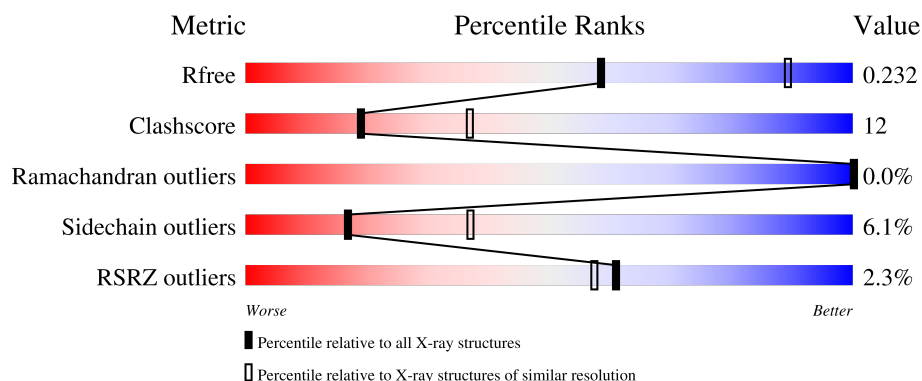
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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% 77% 19% ..
1	B	311	2% 77% 19% ..
1	C	311	0% 82% 16% .
1	D	311	0% 75% 21% ..
1	E	311	0% 78% 18% ..

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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	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24607 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
			2380	1505	407	458	10			
1	H	293	Total	C	N	O	S	0	0	0
			2274	1445	386	434	9			
1	I	286	Total	C	N	O	S	0	0	0
			2189	1391	376	414	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:

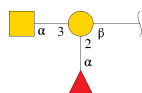
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	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)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	L	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	M	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	N	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	O	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	P	3	Total	C	N	O	0	0	0
			36	20	1	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	R	3	Total	C	N	O	0	0	0
			36	20	1	15			

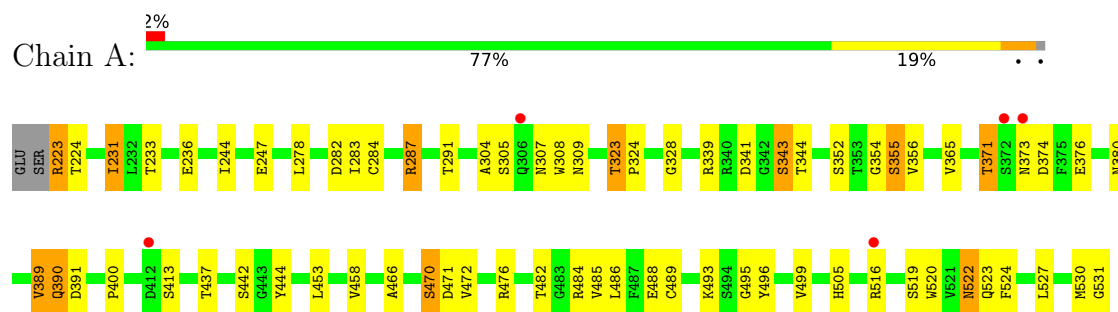
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	100	Total	O	0	0
			100	100		
3	C	93	Total	O	0	0
			93	93		
3	D	83	Total	O	0	0
			83	83		
3	E	80	Total	O	0	0
			80	80		
3	F	50	Total	O	0	0
			50	50		
3	G	50	Total	O	0	0
			50	50		
3	H	48	Total	O	0	0
			48	48		
3	I	30	Total	O	0	0
			30	30		
3	J	68	Total	O	0	0
			68	68		

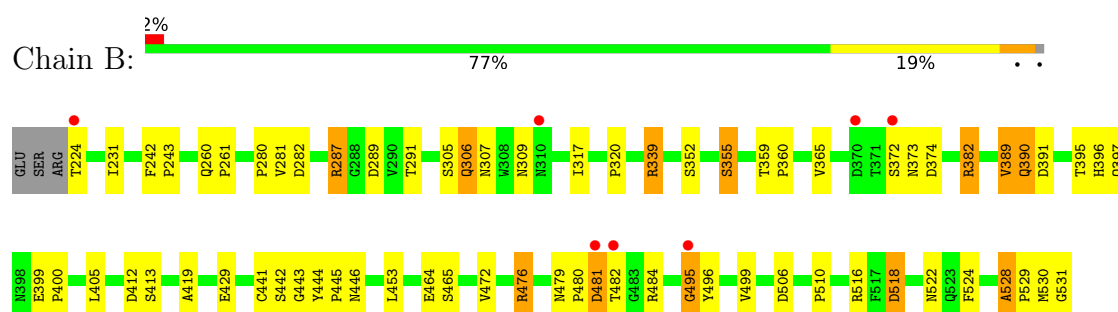
3 Residue-property plots

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.

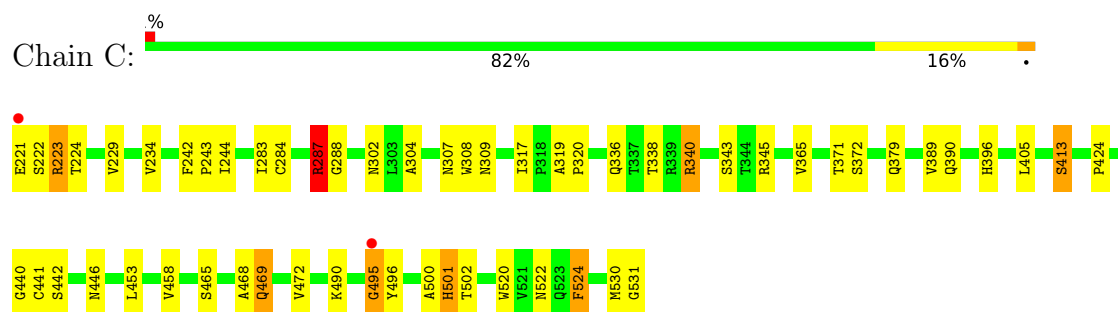
• Molecule 1: Capsid



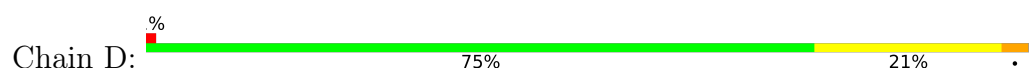
• Molecule 1: Capsid

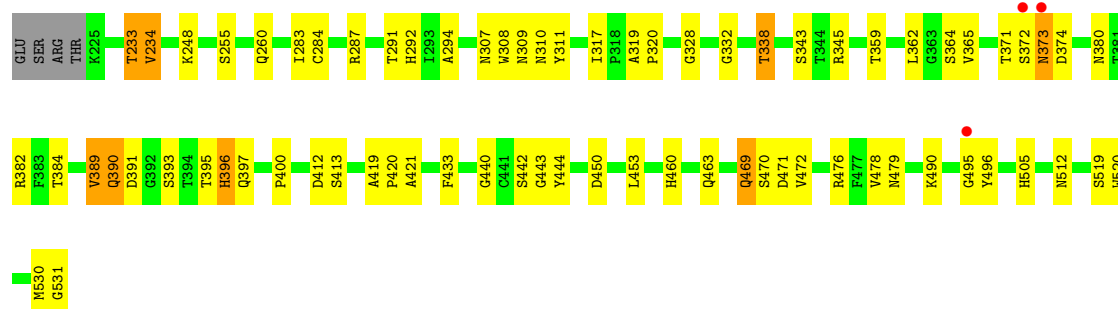


• Molecule 1: Capsid

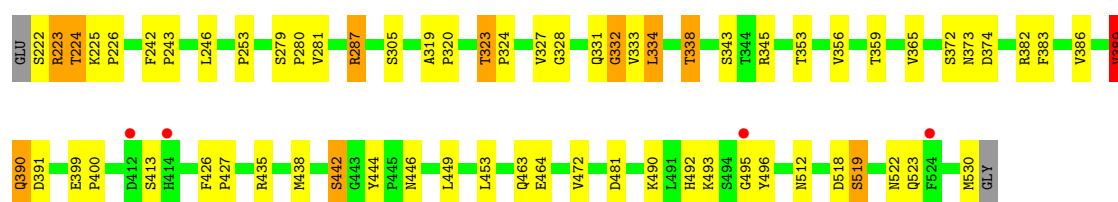
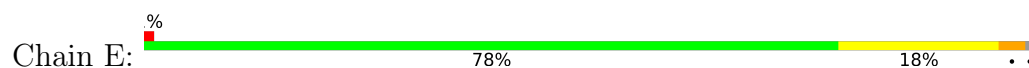


• Molecule 1: Capsid

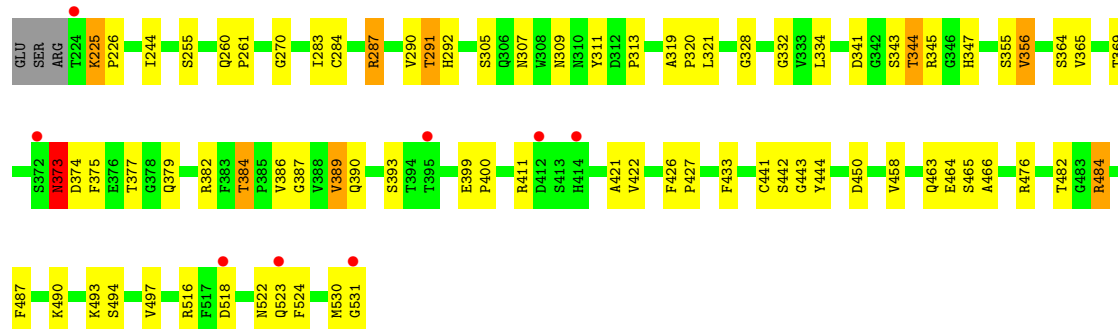
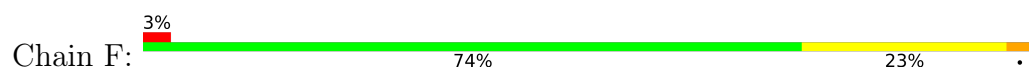




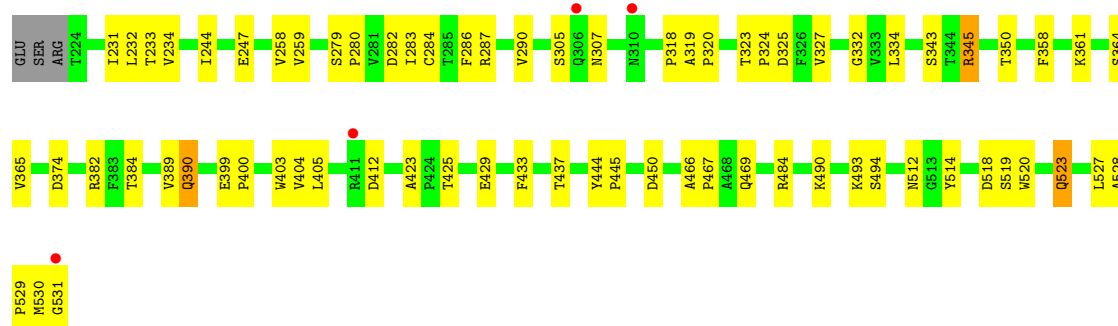
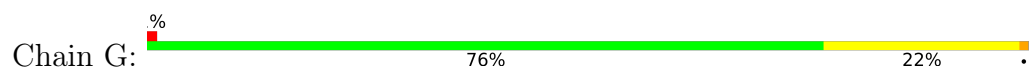
- Molecule 1: Capsid



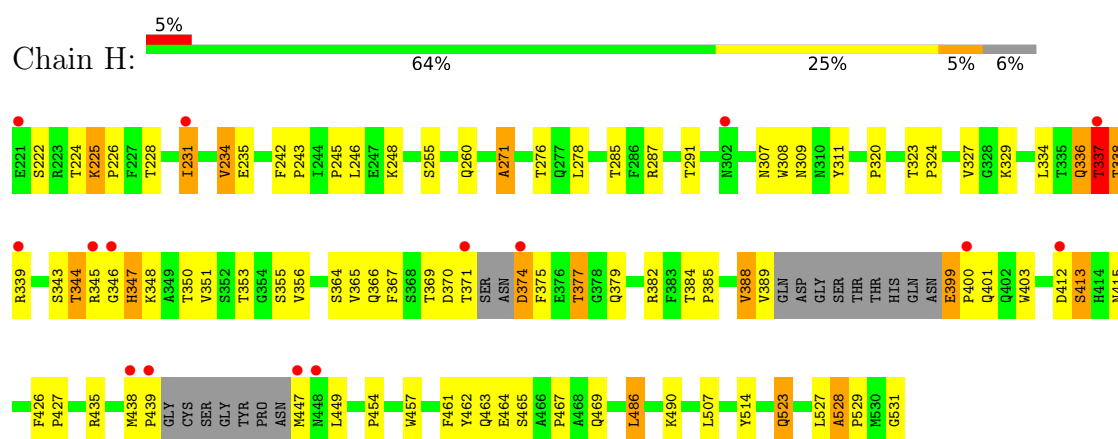
- Molecule 1: Capsid



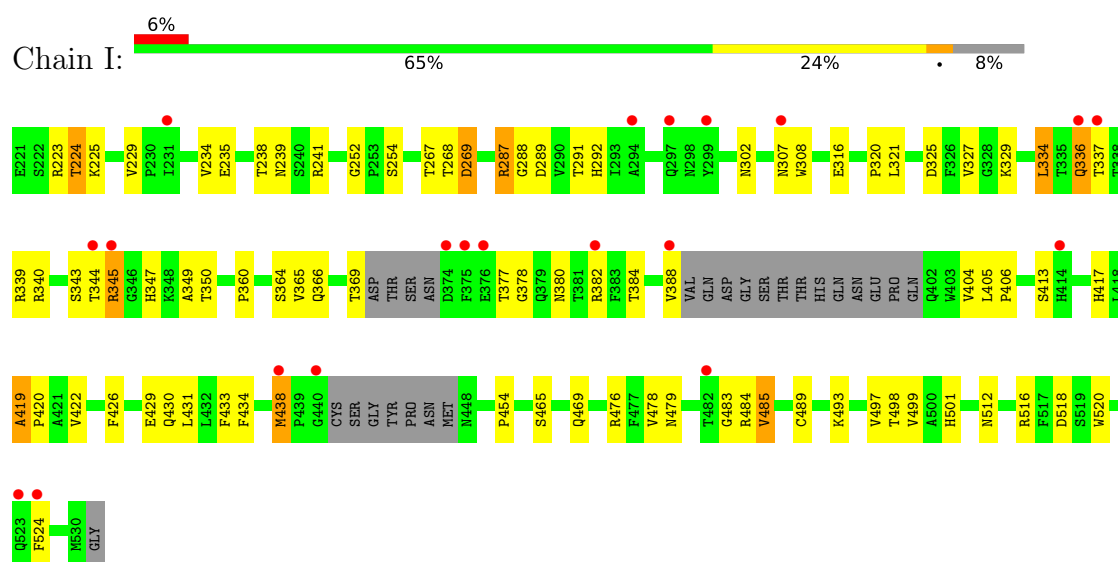
- Molecule 1: Capsid



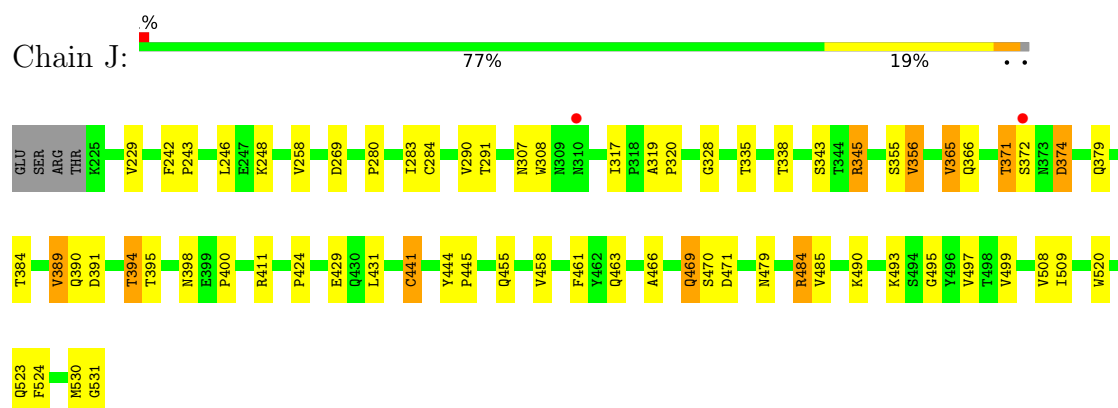
- Molecule 1: Capsid



- Molecule 1: Capsid



- Molecule 1: Capsid



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





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

Chain L:



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

Chain M:



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

Chain N:



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

Chain O:



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

Chain P:



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

Chain Q:



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

Chain R:

100%

GAL1
FUC2
A2G3

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	244.54Å 341.46Å 124.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.66 – 2.68 41.66 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (41.66-2.68) 98.1 (41.66-2.68)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.181 , 0.230 0.186 , 0.232	Depositor DCC
R_{free} test set	7203 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.6	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	24607	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: GAL, FUC, A2G

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	1.41	9/2474 (0.4%)	1.31	14/3385 (0.4%)
1	B	1.33	4/2462 (0.2%)	1.30	14/3369 (0.4%)
1	C	1.27	7/2472 (0.3%)	1.26	7/3384 (0.2%)
1	D	1.23	2/2455 (0.1%)	1.29	12/3360 (0.4%)
1	E	1.26	6/2476 (0.2%)	1.27	8/3388 (0.2%)
1	F	1.13	0/2463	1.29	17/3371 (0.5%)
1	G	1.16	1/2450 (0.0%)	1.23	13/3355 (0.4%)
1	H	1.21	3/2338 (0.1%)	1.31	17/3197 (0.5%)
1	I	1.11	1/2251 (0.0%)	1.21	15/3080 (0.5%)
1	J	1.22	4/2456 (0.2%)	1.30	13/3361 (0.4%)
All	All	1.24	37/24297 (0.2%)	1.28	130/33250 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
All	All	0	2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	GLU	C-N	12.49	1.50	1.33
1	C	524	PHE	CA-CB	8.12	1.65	1.53
1	E	333	VAL	C-O	-7.26	1.16	1.24
1	A	472	VAL	C-O	-7.20	1.16	1.24
1	B	287	ARG	C-O	-6.19	1.16	1.23
1	C	502	THR	C-O	-6.13	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	C-N	-6.13	1.24	1.33
1	E	332	GLY	C-O	-6.01	1.17	1.23
1	E	359	THR	CA-CB	5.96	1.60	1.53
1	I	366	GLN	CA-C	5.86	1.59	1.52
1	J	429	GLU	C-O	-5.73	1.17	1.23
1	J	485	VAL	C-O	-5.69	1.17	1.24
1	G	231	ILE	CA-CB	-5.68	1.46	1.54
1	C	500	ALA	CA-CB	-5.64	1.45	1.52
1	A	282	ASP	C-O	-5.50	1.17	1.24
1	B	320	PRO	C-O	5.43	1.30	1.23
1	A	522	ASN	C-O	-5.43	1.17	1.23
1	A	516	ARG	CD-NE	5.42	1.53	1.46
1	A	485	VAL	C-O	-5.38	1.18	1.24
1	H	234	VAL	CA-CB	5.38	1.61	1.54
1	E	331	GLN	C-O	-5.37	1.17	1.23
1	C	234	VAL	CA-CB	-5.32	1.48	1.54
1	H	271	ALA	CA-CB	5.31	1.60	1.53
1	A	519	SER	C-O	-5.31	1.17	1.23
1	C	501	HIS	C-O	-5.28	1.17	1.23
1	C	287	ARG	C-O	-5.26	1.17	1.23
1	E	389	VAL	C-O	-5.18	1.18	1.24
1	H	228	THR	CA-CB	5.18	1.62	1.53
1	E	442	SER	C-O	-5.18	1.17	1.23
1	B	518	ASP	CB-CG	5.13	1.64	1.52
1	D	476	ARG	CA-C	-5.09	1.46	1.52
1	D	234	VAL	C-O	-5.08	1.18	1.24
1	A	470	SER	C-O	-5.08	1.18	1.23
1	J	470	SER	C-O	-5.03	1.20	1.24
1	B	289	ASP	CA-C	-5.02	1.46	1.52
1	J	441	CYS	C-O	-5.01	1.17	1.24
1	C	229	VAL	C-O	-5.00	1.18	1.24

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	337	THR	O-C-N	14.95	141.20	122.81
1	J	374	ASP	N-CA-C	11.06	123.42	111.36
1	C	495	GLY	N-CA-C	10.52	129.78	114.95
1	A	374	ASP	N-CA-C	10.49	122.80	111.36
1	H	337	THR	N-CA-C	10.44	126.09	110.64
1	F	386	VAL	CB-CA-C	-9.76	101.35	110.91
1	E	374	ASP	N-CA-C	9.20	121.39	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	337	THR	CB-CA-C	-9.14	98.56	109.80
1	B	374	ASP	N-CA-C	8.62	120.76	111.36
1	A	231	ILE	CB-CA-C	-8.46	103.03	112.68
1	D	496	TYR	N-CA-C	8.42	122.07	109.95
1	H	338	THR	N-CA-C	8.21	121.84	110.35
1	A	339	ARG	N-CA-C	7.92	119.92	111.28
1	A	496	TYR	N-CA-CB	-7.86	98.80	111.22
1	E	496	TYR	N-CA-CB	-7.75	99.17	110.87
1	D	374	ASP	N-CA-C	7.74	119.71	111.28
1	H	345	ARG	CB-CA-C	-7.65	107.75	116.63
1	B	443	GLY	N-CA-C	7.58	124.70	111.50
1	I	484	ARG	N-CA-C	7.54	120.73	110.55
1	C	496	TYR	N-CA-CB	-7.45	99.60	110.70
1	D	496	TYR	N-CA-CB	-7.41	99.34	110.60
1	J	384	THR	CA-C-N	-7.24	113.21	120.31
1	J	384	THR	C-N-CA	-7.24	113.21	120.31
1	I	252	GLY	CA-C-N	-7.22	112.88	120.03
1	I	252	GLY	C-N-CA	-7.22	112.88	120.03
1	F	374	ASP	N-CA-C	7.20	118.91	111.14
1	H	336	GLN	CB-CA-C	-7.14	98.00	114.41
1	E	496	TYR	N-CA-C	6.87	119.58	109.69
1	G	412	ASP	N-CA-C	6.83	118.73	111.28
1	A	231	ILE	N-CA-CB	-6.82	105.45	112.06
1	H	413	SER	CA-C-N	-6.70	113.75	123.00
1	H	413	SER	C-N-CA	-6.70	113.75	123.00
1	I	366	GLN	N-CA-C	6.65	119.74	108.90
1	F	484	ARG	N-CA-C	6.59	121.04	109.96
1	C	458	VAL	CB-CA-C	-6.47	103.68	111.97
1	I	344	THR	N-CA-C	-6.46	100.00	110.20
1	D	396	HIS	N-CA-C	6.37	119.01	110.35
1	B	419	ALA	CA-C-N	6.36	126.31	119.76
1	B	419	ALA	C-N-CA	6.36	126.31	119.76
1	B	528	ALA	CA-C-N	-6.36	113.42	119.90
1	B	528	ALA	C-N-CA	-6.36	113.42	119.90
1	D	373	ASN	N-CA-C	6.31	123.54	114.39
1	J	479	ASN	CA-C-N	-6.27	113.17	119.56
1	J	479	ASN	C-N-CA	-6.27	113.17	119.56
1	J	495	GLY	N-CA-C	6.26	128.03	113.18
1	A	371	THR	O-C-N	6.21	130.68	123.17
1	B	496	TYR	N-CA-CB	-6.12	101.63	110.87
1	G	405	LEU	CA-C-N	6.10	126.95	120.11
1	G	405	LEU	C-N-CA	6.10	126.95	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	344	THR	N-CA-C	6.08	119.12	109.81
1	A	466	ALA	CA-C-N	6.08	126.02	119.76
1	A	466	ALA	C-N-CA	6.08	126.02	119.76
1	G	484	ARG	N-CA-C	6.03	119.64	109.76
1	B	495	GLY	N-CA-C	6.02	127.45	113.18
1	B	317	ILE	N-CA-C	-5.98	102.25	109.01
1	J	461	PHE	N-CA-C	-5.98	104.84	111.36
1	F	387	GLY	N-CA-C	5.90	120.63	111.08
1	A	458	VAL	CB-CA-C	-5.87	104.37	111.88
1	G	233	THR	N-CA-C	-5.86	102.97	110.53
1	A	323	THR	CA-C-N	-5.86	113.72	119.76
1	A	323	THR	C-N-CA	-5.86	113.72	119.76
1	F	225	LYS	N-CA-C	5.84	119.80	109.58
1	D	460	HIS	N-CA-C	-5.72	104.65	111.69
1	F	384	THR	CA-C-N	-5.71	113.31	120.51
1	F	384	THR	C-N-CA	-5.71	113.31	120.51
1	A	304	ALA	N-CA-C	-5.70	101.09	109.81
1	E	438	MET	CA-C-N	-5.69	113.90	119.76
1	E	438	MET	C-N-CA	-5.69	113.90	119.76
1	H	336	GLN	N-CA-C	-5.68	100.23	108.07
1	B	496	TYR	N-CA-C	5.64	117.82	109.69
1	H	435	ARG	N-CA-C	5.62	118.64	109.59
1	D	234	VAL	N-CA-CB	5.56	117.05	110.55
1	F	466	ALA	CA-C-N	-5.56	114.20	119.76
1	F	466	ALA	C-N-CA	-5.56	114.20	119.76
1	D	391	ASP	CA-C-N	5.51	126.22	119.99
1	D	391	ASP	C-N-CA	5.51	126.22	119.99
1	H	486	LEU	N-CA-C	5.45	117.03	111.14
1	I	419	ALA	CA-C-N	5.45	125.75	119.92
1	I	419	ALA	C-N-CA	5.45	125.75	119.92
1	J	258	VAL	CB-CA-C	-5.45	104.37	110.96
1	J	524	PHE	N-CA-C	5.38	118.96	112.93
1	H	507	LEU	CA-C-N	-5.37	116.53	123.19
1	H	507	LEU	C-N-CA	-5.37	116.53	123.19
1	B	465	SER	N-CA-C	5.37	118.84	111.54
1	I	347	HIS	N-CA-C	5.37	117.27	108.52
1	C	424	PRO	CA-C-N	-5.36	114.15	122.67
1	C	424	PRO	C-N-CA	-5.36	114.15	122.67
1	H	403	TRP	CA-C-N	-5.33	115.86	123.11
1	H	403	TRP	C-N-CA	-5.33	115.86	123.11
1	A	354	GLY	N-CA-C	-5.33	106.34	115.61
1	I	268	THR	CA-C-N	5.33	129.61	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	268	THR	C-N-CA	5.33	129.61	120.72
1	F	458	VAL	CB-CA-C	-5.32	105.16	111.97
1	F	369	THR	N-CA-C	5.31	115.30	108.34
1	G	247	GLU	N-CA-C	-5.29	106.14	113.18
1	F	270	GLY	CA-C-N	-5.28	115.98	122.84
1	F	270	GLY	C-N-CA	-5.28	115.98	122.84
1	H	344	THR	N-CA-C	5.27	117.11	111.36
1	D	505	HIS	N-CA-C	5.27	117.19	108.13
1	I	316	GLU	N-CA-C	5.24	117.97	110.68
1	J	523	GLN	N-CA-C	5.24	118.78	112.38
1	H	528	ALA	CA-C-N	-5.23	114.33	119.93
1	H	528	ALA	C-N-CA	-5.23	114.33	119.93
1	G	374	ASP	CA-C-N	-5.21	113.97	121.42
1	G	374	ASP	C-N-CA	-5.21	113.97	121.42
1	G	437	THR	N-CA-C	5.21	117.10	108.20
1	A	471	ASP	N-CA-C	5.19	116.93	111.28
1	F	393	SER	N-CA-C	-5.15	106.50	112.89
1	J	291	THR	CB-CA-C	-5.13	102.76	110.24
1	J	229	VAL	CA-C-N	5.12	125.11	119.89
1	J	229	VAL	C-N-CA	5.12	125.11	119.89
1	D	233	THR	CA-C-N	-5.12	114.11	120.56
1	D	233	THR	C-N-CA	-5.12	114.11	120.56
1	I	497	VAL	N-CA-C	5.08	115.22	108.11
1	C	223	ARG	N-CA-C	5.05	117.31	108.52
1	I	479	ASN	CA-C-N	5.05	124.71	119.56
1	I	479	ASN	C-N-CA	5.05	124.71	119.56
1	C	413	SER	N-CA-C	-5.05	100.05	110.80
1	E	435	ARG	N-CA-C	5.05	117.80	109.72
1	G	350	THR	CA-C-N	-5.04	116.60	123.10
1	G	350	THR	C-N-CA	-5.04	116.60	123.10
1	E	323	THR	N-CA-C	5.03	115.38	109.60
1	F	244	ILE	CB-CA-C	-5.02	102.23	111.36
1	E	519	SER	N-CA-C	5.02	116.05	108.07
1	F	373	ASN	N-CA-C	5.01	121.66	114.39
1	G	358	PHE	CA-C-N	-5.01	117.17	122.28
1	G	358	PHE	C-N-CA	-5.01	117.17	122.28
1	B	405	LEU	CA-C-N	5.01	125.28	119.92
1	B	405	LEU	C-N-CA	5.01	125.28	119.92
1	B	464	GLU	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	223	ARG	Sidechain
1	I	223	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	2404	0	2295	55	0
1	B	2392	0	2278	61	0
1	C	2403	0	2282	45	0
1	D	2385	0	2272	46	0
1	E	2406	0	2297	55	1
1	F	2393	0	2282	64	0
1	G	2380	0	2263	51	0
1	H	2274	0	2173	81	0
1	I	2189	0	2066	62	1
1	J	2386	0	2275	53	0
2	K	36	0	32	2	0
2	L	36	0	32	0	0
2	M	36	0	32	1	0
2	N	36	0	32	1	0
2	O	36	0	32	2	0
2	P	36	0	32	0	0
2	Q	36	0	32	2	0
2	R	36	0	32	3	0
3	A	105	0	0	6	0
3	B	100	0	0	6	0
3	C	93	0	0	10	0
3	D	83	0	0	6	0
3	E	80	0	0	8	0
3	F	50	0	0	10	0
3	G	50	0	0	8	0
3	H	48	0	0	22	0
3	I	30	0	0	25	0
3	J	68	0	0	5	0
All	All	24607	0	22739	552	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 12.

All (552) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:LEU:HD21	1:C:495:GLY:O	1.33	1.27
1:D:310:ASN:HB3	3:D:555:HOH:O	1.48	1.14
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.01	1.10
1:A:223:ARG:HG2	1:A:224:THR:H	0.94	1.10
1:H:531:GLY:HA3	3:H:586:HOH:O	1.50	1.08
1:H:337:THR:HG23	1:H:337:THR:O	1.52	1.05
1:H:400:PRO:CG	1:H:438:MET:HE1	1.87	1.03
1:I:476:ARG:HD3	1:I:518:ASP:OD2	1.58	1.03
1:C:340:ARG:HG3	3:C:114:HOH:O	1.59	1.02
1:A:344:THR:CG2	1:C:440:GLY:C	2.33	1.01
1:J:484:ARG:HG3	1:J:484:ARG:HH11	1.25	1.01
1:I:478:VAL:HG22	3:I:690:HOH:O	1.61	1.00
1:J:394:THR:CG2	1:J:398:ASN:HD21	1.73	1.00
1:A:223:ARG:HG2	1:A:224:THR:N	1.72	0.99
1:H:438:MET:HE3	1:H:447:MET:N	1.78	0.99
1:D:530:MET:O	1:D:531:GLY:C	2.03	0.97
1:B:339:ARG:HG3	1:B:339:ARG:NH1	1.74	0.94
1:F:307:ASN:HD21	1:F:309:ASN:HD22	1.06	0.94
1:H:337:THR:O	1:H:337:THR:CG2	2.17	0.93
1:B:390:GLN:HG2	1:B:444:TYR:C	1.93	0.92
1:J:390:GLN:HG2	1:J:444:TYR:C	1.93	0.92
1:H:438:MET:HG2	1:H:447:MET:O	1.68	0.92
1:A:223:ARG:CG	1:A:224:THR:H	1.82	0.92
1:G:287:ARG:HG3	1:G:287:ARG:HH11	1.35	0.91
1:I:378:GLY:HA2	3:I:776:HOH:O	1.68	0.91
1:H:400:PRO:HG2	1:H:438:MET:HE1	1.53	0.91
1:B:481:ASP:O	1:B:482:THR:HG23	1.71	0.90
1:D:307:ASN:OD1	1:D:309:ASN:HB2	1.73	0.89
1:F:390:GLN:HE21	1:F:444:TYR:H	1.18	0.89
1:C:453:LEU:CD2	1:C:495:GLY:O	2.20	0.89
1:G:382:ARG:HD2	3:G:675:HOH:O	1.73	0.89
1:F:311:TYR:O	1:F:313:PRO:HD3	1.73	0.88
1:B:522:ASN:HD22	1:B:524:PHE:HB2	1.39	0.88
1:A:344:THR:HG21	1:C:440:GLY:C	1.96	0.88
1:F:307:ASN:HD21	1:F:309:ASN:ND2	1.71	0.88
1:B:412:ASP:OD2	1:J:394:THR:HG23	1.73	0.88
1:A:344:THR:HG23	1:C:440:GLY:O	1.73	0.88
1:A:530:MET:O	1:A:531:GLY:C	2.17	0.88
1:H:438:MET:CE	1:H:447:MET:N	2.36	0.87
1:B:476:ARG:HD3	1:B:518:ASP:OD2	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:THR:CG2	1:E:345:ARG:HH22	1.87	0.86
1:I:307:ASN:O	1:I:308:TRP:HB2	1.75	0.85
1:H:347:HIS:N	1:H:347:HIS:CD2	2.44	0.85
1:F:476:ARG:HD3	1:F:518:ASP:OD2	1.76	0.85
1:E:338:THR:HG23	1:E:343:SER:OG	1.76	0.85
1:F:307:ASN:ND2	1:F:309:ASN:HD22	1.74	0.84
1:J:394:THR:CG2	1:J:398:ASN:ND2	2.40	0.84
1:J:338:THR:HG23	1:J:379:GLN:NE2	1.93	0.84
1:B:481:ASP:C	1:B:482:THR:HG23	2.03	0.83
1:F:530:MET:O	1:F:531:GLY:C	2.19	0.83
1:G:382:ARG:HD2	3:G:541:HOH:O	1.78	0.83
1:F:287:ARG:HD3	3:F:821:HOH:O	1.80	0.82
1:H:388:VAL:HG21	1:H:400:PRO:HG3	1.61	0.82
1:B:390:GLN:CG	1:B:444:TYR:H	1.92	0.82
1:I:340:ARG:HD2	1:J:317:ILE:HG22	1.61	0.82
1:J:508:VAL:HA	3:J:538:HOH:O	1.78	0.82
1:B:390:GLN:HG3	1:B:444:TYR:H	1.45	0.81
1:C:396:HIS:HD2	3:C:552:HOH:O	1.61	0.81
1:F:390:GLN:HE21	1:F:444:TYR:N	1.77	0.81
1:H:399:GLU:HA	1:H:400:PRO:O	1.79	0.81
1:H:399:GLU:HA	1:H:400:PRO:C	2.05	0.81
1:F:389:VAL:HG22	1:F:442:SER:HB3	1.63	0.81
1:A:505:HIS:HD2	3:A:574:HOH:O	1.64	0.80
1:I:417:HIS:CE1	3:I:532:HOH:O	2.34	0.80
3:C:760:HOH:O	2:K:1:GAL:H61	1.81	0.79
1:I:485:VAL:HG12	3:I:663:HOH:O	1.80	0.79
1:J:394:THR:HG21	1:J:398:ASN:HD21	1.47	0.79
1:J:394:THR:HG22	1:J:398:ASN:ND2	1.95	0.79
1:C:396:HIS:CD2	3:C:552:HOH:O	2.36	0.78
1:J:484:ARG:HG3	1:J:484:ARG:NH1	1.97	0.78
1:A:287:ARG:HD2	3:A:820:HOH:O	1.83	0.78
1:C:340:ARG:CG	3:C:114:HOH:O	2.24	0.78
1:H:231:ILE:HG22	1:H:231:ILE:O	1.83	0.78
1:D:469:GLN:HG3	1:D:520:TRP:CD1	2.18	0.78
1:I:235:GLU:HG2	3:I:571:HOH:O	1.84	0.77
1:I:485:VAL:C	3:I:663:HOH:O	2.27	0.77
1:J:394:THR:HG22	1:J:398:ASN:HD21	1.47	0.77
1:H:514:TYR:HB2	3:H:796:HOH:O	1.85	0.76
1:I:289:ASP:HB2	3:I:776:HOH:O	1.85	0.76
1:I:404:VAL:HA	3:I:569:HOH:O	1.85	0.76
1:D:283:ILE:O	1:D:284:CYS:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:374:ASP:OD1	1:H:374:ASP:C	2.30	0.75
1:E:389:VAL:HG22	1:E:442:SER:HB3	1.66	0.74
1:F:307:ASN:ND2	1:F:309:ASN:ND2	2.33	0.74
1:B:522:ASN:ND2	1:B:524:PHE:HB2	2.01	0.74
1:G:530:MET:O	1:G:531:GLY:C	2.30	0.74
1:G:287:ARG:HG3	1:G:287:ARG:NH1	2.02	0.74
1:D:413:SER:HA	3:D:688:HOH:O	1.87	0.73
1:B:453:LEU:HD21	1:B:495:GLY:O	1.88	0.73
1:E:343:SER:HB2	2:O:2:FUC:H63	1.70	0.73
1:F:319:ALA:HB1	1:F:320:PRO:HD2	1.69	0.73
1:G:469:GLN:HG3	1:G:520:TRP:CD1	2.23	0.73
1:B:339:ARG:HH11	1:B:339:ARG:CG	1.90	0.73
1:D:472:VAL:HG11	1:D:490:LYS:HG2	1.71	0.72
1:F:390:GLN:NE2	1:F:444:TYR:H	1.87	0.72
1:H:400:PRO:CG	1:H:438:MET:CE	2.66	0.72
1:J:530:MET:O	1:J:531:GLY:C	2.29	0.72
1:I:485:VAL:HA	3:I:690:HOH:O	1.89	0.72
1:B:481:ASP:O	1:B:482:THR:CG2	2.36	0.72
1:F:464:GLU:O	1:F:465:SER:HB2	1.89	0.72
1:C:530:MET:O	1:C:531:GLY:C	2.31	0.72
1:G:319:ALA:HB1	1:G:320:PRO:HD2	1.72	0.72
1:F:530:MET:HA	3:F:589:HOH:O	1.89	0.71
1:H:400:PRO:HG2	1:H:438:MET:CE	2.21	0.71
1:A:391:ASP:C	1:A:391:ASP:OD1	2.33	0.70
1:A:522:ASN:HD22	1:A:524:PHE:H	1.38	0.70
1:E:463:GLN:HG2	3:E:541:HOH:O	1.91	0.70
1:B:382:ARG:HG3	3:B:552:HOH:O	1.91	0.70
1:H:399:GLU:HB3	1:H:401:GLN:HG3	1.73	0.69
1:A:505:HIS:CD2	3:A:574:HOH:O	2.43	0.69
1:C:469:GLN:HG3	1:C:520:TRP:CD1	2.26	0.69
1:G:390:GLN:HG2	1:G:444:TYR:C	2.17	0.69
1:J:319:ALA:HB1	1:J:320:PRO:HD2	1.75	0.69
1:I:336:GLN:HB3	1:I:345:ARG:NH1	2.08	0.69
1:I:291:THR:HG22	1:I:292:HIS:O	1.92	0.69
1:F:356:VAL:HG12	1:F:411:ARG:HG2	1.75	0.68
1:H:347:HIS:CD2	1:H:347:HIS:H	2.11	0.68
1:E:319:ALA:HB1	1:E:320:PRO:HD2	1.75	0.68
1:D:307:ASN:HD21	1:D:309:ASN:ND2	1.92	0.67
1:H:523:GLN:HB2	3:H:194:HOH:O	1.93	0.67
1:J:343:SER:HB2	2:R:2:FUC:C6	2.24	0.67
1:I:289:ASP:CB	3:I:776:HOH:O	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ILE:O	1:C:284:CYS:HB2	1.94	0.67
1:B:390:GLN:HG3	1:B:444:TYR:N	2.09	0.67
1:B:481:ASP:O	1:B:482:THR:CB	2.43	0.67
1:F:494:SER:HB2	3:F:599:HOH:O	1.94	0.67
1:A:344:THR:HG23	1:C:440:GLY:C	2.10	0.66
1:A:476:ARG:NH2	1:A:488:GLU:OE2	2.27	0.66
1:J:471:ASP:HA	1:J:493:LYS:HD3	1.76	0.66
1:D:471:ASP:HB2	3:D:575:HOH:O	1.94	0.66
1:B:481:ASP:O	1:B:482:THR:OG1	2.13	0.66
1:A:390:GLN:HG2	1:A:444:TYR:C	2.20	0.66
1:J:371:THR:OG1	1:J:374:ASP:HB2	1.95	0.66
1:E:530:MET:C	3:E:550:HOH:O	2.39	0.66
1:A:344:THR:HG21	1:C:440:GLY:CA	2.26	0.65
1:F:341:ASP:HB3	1:F:343:SER:H	1.60	0.65
1:F:373:ASN:OD1	1:F:373:ASN:N	2.30	0.65
1:H:384:THR:HG23	3:H:542:HOH:O	1.95	0.65
1:B:390:GLN:CG	1:B:444:TYR:N	2.59	0.65
1:B:282:ASP:OD2	1:B:306:GLN:HG2	1.97	0.64
1:E:338:THR:HG22	1:E:345:ARG:HH12	1.62	0.64
1:H:400:PRO:HG3	1:H:438:MET:HE1	1.78	0.64
1:H:531:GLY:CA	3:H:586:HOH:O	2.23	0.64
1:H:336:GLN:HE21	1:H:375:PHE:HD1	1.46	0.64
1:A:231:ILE:HG22	1:A:231:ILE:O	1.96	0.64
1:D:373:ASN:OD1	1:D:373:ASN:N	2.31	0.64
1:C:522:ASN:HB2	3:C:207:HOH:O	1.98	0.64
1:I:336:GLN:HB3	1:I:345:ARG:HH11	1.62	0.64
1:F:390:GLN:HG2	1:F:444:TYR:C	2.23	0.64
1:J:469:GLN:HG3	1:J:520:TRP:CD1	2.33	0.64
1:A:344:THR:CG2	1:C:440:GLY:O	2.38	0.63
1:J:371:THR:HA	3:J:705:HOH:O	1.98	0.63
1:F:390:GLN:O	1:F:443:GLY:HA3	1.97	0.63
1:H:222:SER:HB3	1:H:469:GLN:HE22	1.64	0.63
1:J:343:SER:HB2	2:R:2:FUC:H63	1.79	0.63
1:B:476:ARG:NH1	1:B:518:ASP:OD2	2.25	0.63
1:G:390:GLN:HG3	1:G:444:TYR:H	1.63	0.63
1:J:338:THR:HG23	1:J:379:GLN:HE21	1.64	0.62
1:I:334:LEU:CD2	1:I:349:ALA:CB	2.78	0.62
1:A:344:THR:HG22	1:C:442:SER:N	2.14	0.62
1:E:518:ASP:O	1:E:519:SER:HB3	1.99	0.62
1:G:382:ARG:CD	3:G:675:HOH:O	2.37	0.62
1:J:390:GLN:CG	1:J:444:TYR:H	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:SER:OG	1:A:309:ASN:HB2	2.00	0.61
1:G:382:ARG:NE	3:G:675:HOH:O	2.32	0.61
1:I:430:GLN:HG3	1:I:501:HIS:O	2.00	0.61
1:A:307:ASN:OD1	1:A:307:ASN:C	2.44	0.60
1:D:319:ALA:HB1	1:D:320:PRO:HD2	1.82	0.60
3:B:544:HOH:O	1:E:279:SER:HB2	2.02	0.60
1:C:287:ARG:HD3	3:C:541:HOH:O	2.00	0.60
1:B:373:ASN:OD1	1:B:373:ASN:N	2.31	0.60
1:F:319:ALA:HB1	1:F:320:PRO:CD	2.31	0.60
1:G:423:ALA:O	1:G:425:THR:HG23	2.02	0.60
1:H:377:THR:O	1:H:379:GLN:HG2	2.01	0.60
1:H:438:MET:HG2	1:H:447:MET:C	2.26	0.60
1:I:469:GLN:HB2	1:I:520:TRP:CD1	2.36	0.60
1:H:346:GLY:HA2	1:H:347:HIS:CD2	2.37	0.59
1:F:390:GLN:NE2	1:F:444:TYR:HB2	2.17	0.59
1:I:307:ASN:O	1:I:308:TRP:CB	2.49	0.59
1:H:231:ILE:O	1:H:231:ILE:CG2	2.49	0.59
1:E:319:ALA:HB1	1:E:320:PRO:CD	2.33	0.58
1:I:485:VAL:CA	3:I:690:HOH:O	2.50	0.58
1:J:391:ASP:O	1:J:394:THR:HB	2.02	0.58
1:H:384:THR:CB	3:H:542:HOH:O	2.50	0.58
1:C:319:ALA:HB1	1:C:320:PRO:HD2	1.85	0.58
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.86	0.58
1:F:390:GLN:HG3	1:F:444:TYR:H	1.69	0.58
1:B:481:ASP:C	1:B:482:THR:CG2	2.74	0.57
1:I:417:HIS:HE1	3:I:532:HOH:O	1.80	0.57
1:B:530:MET:O	1:B:531:GLY:C	2.47	0.57
1:E:338:THR:HG22	1:E:345:ARG:HH22	1.65	0.57
1:G:283:ILE:O	1:G:284:CYS:HB2	2.03	0.57
1:B:522:ASN:HD22	1:B:524:PHE:H	1.51	0.57
1:H:438:MET:HE2	1:H:447:MET:N	2.18	0.57
1:D:260:GLN:HG3	1:D:421:ALA:HA	1.87	0.57
1:I:349:ALA:HB2	1:I:369:THR:HG22	1.87	0.57
1:C:223:ARG:NH2	1:H:276:THR:O	2.34	0.57
1:H:454:PRO:HG2	1:H:457:TRP:CD1	2.40	0.57
1:H:248:LYS:HB2	3:H:658:HOH:O	2.05	0.56
1:D:453:LEU:HD21	1:D:495:GLY:O	2.04	0.56
1:I:422:VAL:HA	3:I:735:HOH:O	2.05	0.56
1:E:328:GLY:HA3	1:E:400:PRO:HB3	1.87	0.56
1:G:323:THR:CG2	1:G:324:PRO:HD2	2.36	0.56
1:H:454:PRO:HG2	1:H:457:TRP:CG	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:241:ARG:HB3	3:I:533:HOH:O	2.05	0.56
1:J:390:GLN:HG2	1:J:445:PRO:N	2.20	0.56
1:F:487:PHE:CB	3:F:589:HOH:O	2.54	0.56
1:J:319:ALA:HB1	1:J:320:PRO:CD	2.34	0.56
1:J:283:ILE:O	1:J:284:CYS:HB2	2.04	0.56
1:B:479:ASN:C	1:B:479:ASN:OD1	2.49	0.56
1:A:484:ARG:NH1	1:A:484:ARG:HG3	2.20	0.56
1:I:369:THR:C	3:I:812:HOH:O	2.49	0.56
1:I:405:LEU:N	3:I:569:HOH:O	2.38	0.56
1:J:242:PHE:CD2	1:J:243:PRO:HD2	2.41	0.56
1:A:453:LEU:HD21	1:A:495:GLY:O	2.06	0.55
1:G:469:GLN:HB2	1:G:520:TRP:CG	2.41	0.55
1:B:453:LEU:CD2	1:B:495:GLY:O	2.53	0.55
1:E:356:VAL:HG13	3:E:755:HOH:O	2.05	0.55
1:F:328:GLY:HA3	1:F:400:PRO:HB3	1.88	0.55
1:B:522:ASN:ND2	1:B:524:PHE:H	2.05	0.55
1:E:472:VAL:HG11	1:E:490:LYS:HD3	1.88	0.55
1:A:522:ASN:ND2	1:A:524:PHE:H	2.05	0.55
1:B:287:ARG:HG3	1:B:287:ARG:HH11	1.72	0.55
1:A:389:VAL:HG22	1:A:442:SER:HB3	1.89	0.55
1:C:307:ASN:O	1:C:308:TRP:HB2	2.06	0.55
1:E:332:GLY:HA2	1:E:386:VAL:HG23	1.88	0.55
1:E:343:SER:HB2	2:O:2:FUC:C6	2.36	0.55
1:F:482:THR:OG1	1:F:484:ARG:HB2	2.07	0.55
1:H:307:ASN:OD1	1:H:309:ASN:HB2	2.07	0.55
1:I:235:GLU:CG	3:I:571:HOH:O	2.50	0.55
1:D:389:VAL:HG22	1:D:442:SER:HB3	1.88	0.54
1:H:400:PRO:HG3	1:H:438:MET:CE	2.36	0.54
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.43	0.54
1:A:390:GLN:HG3	1:A:444:TYR:H	1.73	0.54
1:F:476:ARG:HD3	1:F:518:ASP:CG	2.32	0.54
1:H:400:PRO:CB	1:H:438:MET:HE1	2.37	0.54
1:G:332:GLY:HA3	1:G:384:THR:O	2.08	0.54
1:E:225:LYS:NZ	1:E:464:GLU:O	2.34	0.54
1:E:327:VAL:HA	1:E:353:THR:OG1	2.07	0.54
1:H:307:ASN:O	1:H:308:TRP:HB2	2.08	0.54
1:I:287:ARG:HH11	1:I:287:ARG:HB2	1.73	0.54
1:J:390:GLN:HG3	1:J:444:TYR:H	1.73	0.53
1:D:260:GLN:HG3	1:D:421:ALA:CA	2.37	0.53
1:F:260:GLN:HG3	1:F:421:ALA:N	2.24	0.53
1:C:287:ARG:CD	3:C:541:HOH:O	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:399:GLU:CA	1:H:400:PRO:C	2.77	0.53
1:B:453:LEU:HD11	1:B:495:GLY:O	2.09	0.53
1:B:382:ARG:CD	3:B:552:HOH:O	2.57	0.53
1:F:433:PHE:HB3	1:F:450:ASP:HB3	1.90	0.53
1:A:344:THR:HG21	1:C:440:GLY:HA3	1.89	0.52
1:A:470:SER:OG	1:A:520:TRP:HB3	2.07	0.52
1:J:390:GLN:HE21	1:J:444:TYR:H	1.57	0.52
1:J:490:LYS:O	1:J:497:VAL:HA	2.09	0.52
1:E:391:ASP:OD1	1:E:391:ASP:C	2.53	0.52
1:B:528:ALA:O	1:B:529:PRO:C	2.52	0.52
1:G:258:VAL:HB	3:G:92:HOH:O	2.08	0.52
1:H:464:GLU:CD	3:H:822:HOH:O	2.52	0.52
1:I:334:LEU:HD23	1:I:349:ALA:HB2	1.92	0.52
1:E:390:GLN:HG3	1:E:444:TYR:H	1.74	0.52
1:D:319:ALA:HB1	1:D:320:PRO:CD	2.40	0.52
1:D:371:THR:O	1:D:371:THR:HG23	2.07	0.52
1:G:444:TYR:CE1	1:J:343:SER:HB3	2.45	0.52
1:J:390:GLN:CG	1:J:444:TYR:N	2.74	0.52
1:D:512:ASN:OD1	1:D:512:ASN:N	2.32	0.51
1:G:390:GLN:CG	1:G:444:TYR:H	2.23	0.51
1:A:390:GLN:HB2	3:A:564:HOH:O	2.10	0.51
1:B:307:ASN:OD1	1:B:309:ASN:HB2	2.11	0.51
1:G:323:THR:CG2	1:G:324:PRO:CD	2.89	0.51
1:G:433:PHE:HB3	1:G:450:ASP:HB3	1.91	0.51
1:C:472:VAL:CG1	1:C:490:LYS:HG2	2.41	0.51
1:A:482:THR:OG1	1:A:484:ARG:HB2	2.11	0.51
1:A:352:SER:O	1:A:355:SER:HB3	2.11	0.51
1:H:384:THR:HA	3:H:542:HOH:O	2.09	0.51
1:I:334:LEU:HD23	1:I:349:ALA:CB	2.40	0.51
1:C:304:ALA:HB1	1:C:309:ASN:O	2.11	0.51
1:E:224:THR:CG2	3:E:595:HOH:O	2.57	0.51
1:J:365:VAL:CG1	1:J:366:GLN:N	2.73	0.51
1:C:472:VAL:HG11	1:C:490:LYS:HG2	1.91	0.51
1:H:438:MET:CG	1:H:447:MET:O	2.51	0.51
1:D:343:SER:HB3	1:F:444:TYR:CE1	2.46	0.51
1:G:523:GLN:HB2	3:G:741:HOH:O	2.11	0.51
1:H:384:THR:CG2	3:H:542:HOH:O	2.57	0.50
1:D:292:HIS:CE1	1:D:294:ALA:HA	2.45	0.50
1:D:390:GLN:O	1:D:443:GLY:HA3	2.12	0.50
1:I:224:THR:HG23	1:I:225:LYS:N	2.26	0.50
1:B:506:ASP:HB3	3:B:668:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:ASP:CG	1:E:512:ASN:HD21	2.20	0.50
1:I:485:VAL:CB	3:I:663:HOH:O	2.58	0.50
1:J:269:ASP:HB3	1:J:466:ALA:O	2.11	0.50
1:D:248:LYS:HD2	3:D:124:HOH:O	2.12	0.50
1:G:528:ALA:O	1:G:529:PRO:C	2.53	0.50
1:H:287:ARG:HB2	1:H:287:ARG:NH1	2.26	0.50
1:F:390:GLN:CG	1:F:444:TYR:C	2.85	0.50
1:F:522:ASN:OD1	1:F:524:PHE:N	2.44	0.50
1:I:339:ARG:HG3	1:I:343:SER:O	2.12	0.50
1:G:514:TYR:CD1	1:G:514:TYR:C	2.90	0.50
1:B:390:GLN:HG2	1:B:445:PRO:N	2.27	0.49
1:F:341:ASP:CB	1:F:343:SER:H	2.24	0.49
1:I:378:GLY:CA	3:I:776:HOH:O	2.43	0.49
1:D:390:GLN:CG	1:D:444:TYR:C	2.86	0.49
1:G:232:LEU:HD21	1:J:463:GLN:NE2	2.27	0.49
1:D:371:THR:O	1:D:371:THR:CG2	2.57	0.49
1:J:343:SER:HB2	2:R:2:FUC:H62	1.93	0.49
1:D:317:ILE:HD12	1:D:319:ALA:O	2.12	0.49
1:F:307:ASN:OD1	1:F:307:ASN:C	2.55	0.49
1:F:320:PRO:HA	3:F:191:HOH:O	2.12	0.49
1:E:242:PHE:CD2	1:E:243:PRO:HD2	2.47	0.49
1:E:287:ARG:HH11	1:E:287:ARG:HB2	1.77	0.49
1:F:516:ARG:HA	3:F:93:HOH:O	2.11	0.49
1:F:321:LEU:N	3:F:191:HOH:O	2.41	0.49
1:B:287:ARG:HG3	1:B:287:ARG:NH1	2.28	0.49
1:F:487:PHE:HB2	3:F:589:HOH:O	2.10	0.49
1:H:374:ASP:OD1	1:H:374:ASP:O	2.30	0.49
1:C:338:THR:HG23	1:C:379:GLN:NE2	2.27	0.49
1:E:334:LEU:CD1	1:E:383:PHE:HB2	2.42	0.49
1:I:229:VAL:HG23	3:I:742:HOH:O	2.12	0.49
1:A:488:GLU:HG3	1:A:527:LEU:HD22	1.94	0.49
1:G:518:ASP:O	1:G:519:SER:HB3	2.12	0.49
1:B:476:ARG:HD3	1:B:518:ASP:CG	2.36	0.48
1:F:341:ASP:HB3	1:F:343:SER:N	2.26	0.48
1:F:389:VAL:HG23	1:F:441:CYS:HB2	1.95	0.48
1:H:235:GLU:HB2	3:H:533:HOH:O	2.14	0.48
1:C:287:ARG:NE	3:C:541:HOH:O	2.45	0.48
1:I:478:VAL:HG21	1:I:516:ARG:NH1	2.28	0.48
1:C:501:HIS:ND1	1:C:530:MET:HE2	2.29	0.48
1:I:404:VAL:HG13	3:I:569:HOH:O	2.14	0.48
1:B:382:ARG:CG	3:B:552:HOH:O	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:THR:CG2	1:E:345:ARG:NH2	2.67	0.48
1:F:390:GLN:HG3	1:F:444:TYR:N	2.28	0.48
1:J:248:LYS:HD2	3:J:21:HOH:O	2.13	0.48
1:D:343:SER:HB2	2:N:2:FUC:H63	1.95	0.48
1:D:359:THR:HB	1:D:362:LEU:HD12	1.94	0.48
1:D:472:VAL:CG1	1:D:490:LYS:HG2	2.40	0.48
1:H:369:THR:OG1	1:H:370:ASP:N	2.44	0.48
1:J:484:ARG:NH1	1:J:484:ARG:CG	2.72	0.48
1:H:347:HIS:H	1:H:347:HIS:HD2	1.59	0.48
1:F:291:THR:HG22	1:F:292:HIS:O	2.14	0.48
1:C:441:CYS:O	1:C:442:SER:HB2	2.14	0.47
1:D:308:TRP:CH2	1:D:380:ASN:HB3	2.48	0.47
1:D:390:GLN:HG2	1:D:444:TYR:C	2.38	0.47
1:E:334:LEU:HD13	1:E:383:PHE:HB2	1.95	0.47
1:E:338:THR:HG22	1:E:345:ARG:NH1	2.28	0.47
1:B:396:HIS:O	1:B:397:GLN:HB2	2.13	0.47
1:C:336:GLN:OE1	1:C:345:ARG:HD2	2.14	0.47
1:G:323:THR:HG22	1:G:324:PRO:HD2	1.96	0.47
1:B:453:LEU:CG	1:B:495:GLY:O	2.62	0.47
1:F:399:GLU:HB2	1:F:400:PRO:HA	1.97	0.47
1:G:490:LYS:HG3	1:G:527:LEU:HD11	1.96	0.47
1:H:438:MET:HG3	1:H:447:MET:HA	1.96	0.47
1:H:490:LYS:HG3	1:H:527:LEU:HD21	1.96	0.47
1:B:231:ILE:O	1:B:231:ILE:HG22	2.14	0.47
1:E:338:THR:HG22	1:E:345:ARG:NH2	2.30	0.47
1:B:242:PHE:CD2	1:B:243:PRO:HD2	2.50	0.47
1:C:224:THR:HG22	1:H:271:ALA:HA	1.95	0.47
1:I:404:VAL:CA	3:I:569:HOH:O	2.51	0.47
1:J:394:THR:O	1:J:395:THR:C	2.56	0.47
1:C:317:ILE:HD12	1:C:319:ALA:O	2.15	0.47
1:I:382:ARG:HG2	1:I:382:ARG:HH11	1.80	0.47
1:F:426:PHE:O	1:F:427:PRO:C	2.58	0.47
1:B:280:PRO:HG2	1:E:280:PRO:HG2	1.97	0.47
1:A:380:ASN:HA	3:A:766:HOH:O	2.13	0.46
1:E:399:GLU:HB2	1:E:400:PRO:HA	1.97	0.46
1:G:399:GLU:HA	1:G:400:PRO:C	2.39	0.46
1:H:242:PHE:HB2	1:H:449:LEU:HD21	1.96	0.46
1:H:323:THR:HG23	1:H:324:PRO:HD2	1.98	0.46
1:I:254:SER:HB3	3:I:42:HOH:O	2.15	0.46
1:C:524:PHE:CB	3:C:777:HOH:O	2.64	0.46
1:D:470:SER:OG	1:D:520:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:PRO:HB3	3:H:102:HOH:O	2.14	0.46
1:D:310:ASN:OD1	1:D:311:TYR:N	2.46	0.46
1:C:446:ASN:OD1	1:C:446:ASN:C	2.57	0.46
1:G:232:LEU:HD21	1:J:463:GLN:HE21	1.81	0.46
1:G:343:SER:HB2	2:Q:2:FUC:H63	1.98	0.46
1:G:390:GLN:HG3	1:G:444:TYR:N	2.29	0.46
1:G:469:GLN:CG	1:G:520:TRP:CD1	2.96	0.46
1:B:352:SER:O	1:B:355:SER:HB3	2.16	0.46
1:I:434:PHE:CD1	1:I:454:PRO:HG3	2.50	0.46
1:J:328:GLY:HA3	1:J:400:PRO:HB3	1.98	0.46
1:E:512:ASN:OD1	1:E:512:ASN:N	2.47	0.46
1:G:512:ASN:OD1	1:G:512:ASN:N	2.44	0.46
1:H:323:THR:HG22	1:H:324:PRO:N	2.31	0.46
1:H:327:VAL:HA	1:H:353:THR:OG1	2.15	0.46
1:E:323:THR:HG23	1:E:324:PRO:HD2	1.98	0.46
1:A:390:GLN:HG3	1:A:444:TYR:N	2.31	0.45
1:C:222:SER:HB3	1:C:469:GLN:OE1	2.16	0.45
1:D:396:HIS:O	1:D:397:GLN:C	2.58	0.45
1:E:446:ASN:OD1	1:E:446:ASN:C	2.59	0.45
1:F:260:GLN:N	1:F:261:PRO:CD	2.79	0.45
1:G:323:THR:HG23	1:G:324:PRO:HD2	1.97	0.45
1:G:390:GLN:HG2	1:G:445:PRO:N	2.31	0.45
1:H:235:GLU:HB2	3:H:549:HOH:O	2.16	0.45
1:A:328:GLY:HA3	1:A:400:PRO:HB3	1.98	0.45
1:A:233:THR:OG1	1:A:236:GLU:HG3	2.16	0.45
1:B:359:THR:N	1:B:360:PRO:CD	2.79	0.45
1:H:242:PHE:CD2	1:H:243:PRO:HD2	2.51	0.45
1:I:382:ARG:HH11	1:I:382:ARG:CG	2.29	0.45
1:I:426:PHE:CZ	1:I:524:PHE:O	2.69	0.45
1:C:242:PHE:CD2	1:C:243:PRO:HD2	2.51	0.45
1:C:468:ALA:HA	1:C:520:TRP:CZ2	2.52	0.45
1:D:338:THR:HG1	1:D:345:ARG:HH12	1.62	0.45
1:I:512:ASN:OD1	1:I:512:ASN:N	2.50	0.45
1:B:382:ARG:HD2	3:B:552:HOH:O	2.17	0.45
1:H:278:LEU:HD11	1:H:462:TYR:CD2	2.52	0.44
1:H:351:VAL:HB	1:H:367:PHE:CE1	2.52	0.44
1:F:347:HIS:HD2	1:F:375:PHE:CE2	2.35	0.44
1:F:490:LYS:O	1:F:497:VAL:HA	2.16	0.44
1:G:325:ASP:OD2	1:G:325:ASP:C	2.59	0.44
1:I:485:VAL:CG1	3:I:663:HOH:O	2.48	0.44
1:A:231:ILE:CD1	3:H:822:HOH:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:476:ARG:HG2	1:I:485:VAL:HG11	2.00	0.44
1:B:399:GLU:HA	1:B:400:PRO:C	2.43	0.44
1:J:390:GLN:HG3	1:J:444:TYR:N	2.32	0.44
1:D:469:GLN:HG3	1:D:520:TRP:NE1	2.31	0.44
1:E:453:LEU:CG	1:E:495:GLY:O	2.66	0.44
1:G:286:PHE:HE1	3:G:610:HOH:O	2.00	0.44
1:H:415:ASN:HA	3:H:536:HOH:O	2.17	0.44
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.82	0.44
1:B:390:GLN:HG2	1:B:444:TYR:CA	2.48	0.44
1:E:338:THR:CG2	1:E:343:SER:OG	2.58	0.44
1:E:426:PHE:CD2	1:E:427:PRO:HD2	2.52	0.44
1:B:446:ASN:OD1	1:B:446:ASN:C	2.60	0.44
1:E:453:LEU:HG	1:E:495:GLY:O	2.18	0.44
1:F:463:GLN:HG2	3:F:713:HOH:O	2.18	0.44
1:H:339:ARG:HB2	1:H:343:SER:O	2.18	0.44
1:I:419:ALA:HA	1:I:420:PRO:HD3	1.79	0.44
1:F:377:THR:O	1:F:379:GLN:HG2	2.18	0.44
1:I:288:GLY:HA3	1:I:302:ASN:O	2.18	0.44
1:E:246:LEU:HD23	1:E:246:LEU:HA	1.84	0.43
1:E:390:GLN:HG3	1:E:444:TYR:N	2.32	0.43
1:G:323:THR:HG22	1:G:324:PRO:CD	2.48	0.43
1:A:283:ILE:O	1:A:284:CYS:HB2	2.17	0.43
1:A:341:ASP:OD2	1:A:343:SER:OG	2.36	0.43
1:D:233:THR:HG21	1:D:512:ASN:HA	1.99	0.43
1:D:440:GLY:HA3	1:F:344:THR:HG21	2.00	0.43
1:E:373:ASN:OD1	1:E:373:ASN:C	2.60	0.43
1:J:509:ILE:N	3:J:538:HOH:O	2.32	0.43
1:E:253:PRO:HD2	3:E:696:HOH:O	2.18	0.43
1:H:366:GLN:OE1	3:H:548:HOH:O	2.21	0.43
1:F:225:LYS:HA	1:F:226:PRO:HD3	1.92	0.43
1:J:307:ASN:O	1:J:308:TRP:HB2	2.18	0.43
1:B:339:ARG:NH1	1:B:339:ARG:CG	2.56	0.43
1:F:390:GLN:HE21	1:F:444:TYR:HB2	1.83	0.43
1:A:341:ASP:CG	1:A:343:SER:OG	2.60	0.43
1:B:281:VAL:HG12	1:E:281:VAL:HG12	2.01	0.43
1:E:287:ARG:HB2	1:E:287:ARG:NH1	2.34	0.43
1:E:382:ARG:HG2	1:E:382:ARG:HH11	1.84	0.43
1:H:260:GLN:OE1	3:H:616:HOH:O	2.21	0.43
1:I:325:ASP:C	1:I:325:ASP:OD2	2.62	0.43
1:G:429:GLU:OE2	1:G:490:LYS:NZ	2.44	0.43
1:J:389:VAL:HG23	1:J:441:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HD11	3:H:822:HOH:O	2.19	0.43
1:H:336:GLN:NE2	1:H:375:PHE:HD1	2.12	0.43
1:A:389:VAL:HG21	3:A:611:HOH:O	2.18	0.43
1:E:530:MET:HA	3:E:550:HOH:O	2.17	0.43
1:G:327:VAL:HG23	1:G:404:VAL:O	2.19	0.43
1:B:516:ARG:HE	1:B:516:ARG:HB3	1.62	0.43
1:E:226:PRO:HD2	3:E:700:HOH:O	2.19	0.43
1:B:389:VAL:HG23	1:B:441:CYS:HB2	2.00	0.42
1:G:319:ALA:HB1	1:G:320:PRO:CD	2.47	0.42
1:H:438:MET:HA	1:H:439:PRO:HD3	1.88	0.42
1:I:238:THR:HG22	1:I:239:ASN:O	2.19	0.42
1:I:405:LEU:HA	1:I:406:PRO:HD3	1.86	0.42
1:A:390:GLN:CG	1:A:444:TYR:H	2.31	0.42
1:H:242:PHE:CZ	1:H:385:PRO:HB2	2.55	0.42
1:A:307:ASN:O	1:A:308:TRP:HB2	2.20	0.42
1:B:390:GLN:HG2	1:B:444:TYR:N	2.34	0.42
1:B:479:ASN:CG	1:B:510:PRO:HG3	2.44	0.42
1:F:287:ARG:CD	3:F:821:HOH:O	2.50	0.42
1:G:279:SER:HB2	3:J:186:HOH:O	2.19	0.42
1:A:484:ARG:HH11	1:A:484:ARG:CG	2.32	0.42
1:E:242:PHE:HB2	1:E:449:LEU:CD2	2.50	0.42
1:E:389:VAL:HG22	1:E:442:SER:CB	2.44	0.42
1:G:259:VAL:HG13	1:G:403:TRP:CZ3	2.55	0.42
1:H:224:THR:HG21	1:H:467:PRO:HG2	2.01	0.42
1:I:426:PHE:HB3	1:I:429:GLU:CD	2.45	0.42
1:I:489:CYS:HB3	1:I:499:VAL:HG12	2.02	0.42
1:E:481:ASP:OD2	1:E:512:ASN:ND2	2.48	0.42
1:G:345:ARG:HG3	2:Q:2:FUC:O3	2.19	0.42
1:I:320:PRO:HD2	1:I:360:PRO:HB2	2.02	0.42
1:A:484:ARG:HG3	1:A:484:ARG:HH11	1.83	0.42
1:C:288:GLY:HA3	1:C:302:ASN:O	2.20	0.42
1:C:340:ARG:HG3	1:C:340:ARG:H	1.66	0.42
1:D:310:ASN:CG	1:D:311:TYR:N	2.78	0.42
1:D:478:VAL:HG12	1:D:479:ASN:N	2.35	0.42
1:F:493:LYS:HG3	1:F:494:SER:N	2.34	0.42
1:H:426:PHE:CD2	1:H:427:PRO:HD2	2.54	0.42
1:B:479:ASN:OD1	1:B:480:PRO:HD2	2.20	0.42
1:H:531:GLY:HA3	3:H:541:HOH:O	2.20	0.42
1:I:334:LEU:HD22	1:I:349:ALA:HB3	2.01	0.42
1:A:223:ARG:CG	1:A:224:THR:N	2.52	0.42
1:E:253:PRO:CD	3:E:696:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:ASN:CG	1:F:309:ASN:HD22	2.27	0.41
1:F:319:ALA:O	1:F:320:PRO:C	2.62	0.41
1:F:332:GLY:HA3	1:F:384:THR:O	2.20	0.41
1:F:484:ARG:HG3	1:F:484:ARG:HH11	1.84	0.41
1:G:287:ARG:NH1	1:G:287:ARG:CG	2.68	0.41
1:B:391:ASP:OD1	1:B:391:ASP:C	2.63	0.41
1:C:343:SER:HB2	2:M:2:FUC:H63	2.02	0.41
1:H:225:LYS:HA	1:H:226:PRO:HD3	1.83	0.41
1:A:344:THR:CG2	1:C:440:GLY:CA	2.92	0.41
1:G:466:ALA:HA	1:G:467:PRO:HD3	1.92	0.41
1:A:323:THR:O	1:A:324:PRO:C	2.62	0.41
1:B:260:GLN:N	1:B:261:PRO:CD	2.83	0.41
1:D:419:ALA:HA	1:D:420:PRO:HD3	1.88	0.41
1:F:283:ILE:O	1:F:284:CYS:HB2	2.18	0.41
1:H:222:SER:HB3	1:H:469:GLN:NE2	2.32	0.41
1:J:242:PHE:CG	1:J:243:PRO:HD2	2.54	0.41
1:J:391:ASP:OD2	1:J:391:ASP:C	2.63	0.41
1:A:489:CYS:HB3	1:A:499:VAL:HG12	2.03	0.41
1:B:429:GLU:HA	1:B:499:VAL:O	2.20	0.41
1:F:347:HIS:HD2	1:F:375:PHE:CZ	2.39	0.41
1:G:318:PRO:O	1:G:361:LYS:HD3	2.21	0.41
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.89	0.41
1:I:388:VAL:HG13	1:I:438:MET:SD	2.61	0.41
1:J:424:PRO:HD3	1:J:431:LEU:HG	2.02	0.41
1:E:522:ASN:OD1	1:E:522:ASN:C	2.63	0.41
1:G:280:PRO:HG2	1:J:280:PRO:HG2	2.02	0.41
1:H:382:ARG:NH2	3:H:195:HOH:O	2.53	0.41
1:J:356:VAL:HG23	1:J:411:ARG:CG	2.50	0.41
1:A:247:GLU:CD	1:A:437:THR:H	2.27	0.41
1:A:344:THR:CG2	1:C:441:CYS:N	2.81	0.41
1:B:260:GLN:N	1:B:261:PRO:HD3	2.36	0.41
1:E:492:HIS:O	1:E:493:LYS:C	2.64	0.41
1:F:441:CYS:O	1:F:442:SER:HB2	2.20	0.41
1:H:246:LEU:HD11	1:H:454:PRO:HB3	2.02	0.41
1:H:285:THR:HG22	1:H:385:PRO:HD3	2.02	0.41
1:H:366:GLN:HB2	3:H:548:HOH:O	2.21	0.41
1:H:461:PHE:O	1:H:462:TYR:C	2.60	0.41
1:H:528:ALA:O	1:H:529:PRO:C	2.60	0.41
1:I:489:CYS:HB2	1:I:498:THR:O	2.20	0.41
1:D:310:ASN:C	3:D:555:HOH:O	2.64	0.41
1:D:328:GLY:HA3	1:D:400:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:ARG:NH1	1:F:518:ASP:OD2	2.43	0.41
1:I:267:THR:C	1:I:269:ASP:N	2.76	0.41
1:I:485:VAL:HB	3:I:663:HOH:O	2.21	0.41
1:D:283:ILE:O	1:D:284:CYS:CB	2.58	0.40
1:D:332:GLY:HA3	1:D:384:THR:O	2.21	0.40
1:H:248:LYS:CD	3:H:658:HOH:O	2.69	0.40
1:H:311:TYR:CE1	1:H:320:PRO:HG3	2.56	0.40
1:I:431:LEU:HD12	1:I:433:PHE:CZ	2.56	0.40
1:J:455:GLN:O	1:J:458:VAL:HB	2.22	0.40
1:A:341:ASP:OD1	1:A:343:SER:OG	2.38	0.40
1:E:279:SER:HA	1:E:280:PRO:HD3	1.88	0.40
1:I:336:GLN:NE2	1:I:380:ASN:O	2.53	0.40
1:G:494:SER:HB2	3:G:657:HOH:O	2.21	0.40
1:F:390:GLN:CG	1:F:444:TYR:H	2.31	0.40
1:G:305:SER:C	1:G:307:ASN:N	2.79	0.40
1:J:246:LEU:HD23	1:J:246:LEU:HA	1.89	0.40
1:A:344:THR:O	2:K:2:FUC:H2	2.21	0.40
1:C:319:ALA:HB1	1:C:320:PRO:CD	2.49	0.40
1:D:463:GLN:HG2	3:D:559:HOH:O	2.22	0.40
1:J:335:THR:HA	1:J:345:ARG:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ARG:NH1	1:I:321:LEU:CD2[4_555]	2.11	0.09

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%)	299 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	306/311 (98%)	296 (97%)	10 (3%)	0	100	100
1	C	309/311 (99%)	301 (97%)	8 (3%)	0	100	100
1	D	305/311 (98%)	294 (96%)	11 (4%)	0	100	100
1	E	307/311 (99%)	296 (96%)	11 (4%)	0	100	100
1	F	306/311 (98%)	290 (95%)	16 (5%)	0	100	100
1	G	306/311 (98%)	293 (96%)	13 (4%)	0	100	100
1	H	285/311 (92%)	264 (93%)	21 (7%)	0	100	100
1	I	278/311 (89%)	266 (96%)	11 (4%)	1 (0%)	30	51
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3014/3110 (97%)	2894 (96%)	119 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	483	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/272 (99%)	254 (94%)	16 (6%)	18	38
1	B	269/272 (99%)	251 (93%)	18 (7%)	15	32
1	C	269/272 (99%)	257 (96%)	12 (4%)	24	49
1	D	267/272 (98%)	251 (94%)	16 (6%)	17	38
1	E	271/272 (100%)	259 (96%)	12 (4%)	25	50
1	F	269/272 (99%)	253 (94%)	16 (6%)	18	38
1	G	266/272 (98%)	254 (96%)	12 (4%)	24	49
1	H	254/272 (93%)	225 (89%)	29 (11%)	5	12
1	I	238/272 (88%)	219 (92%)	19 (8%)	11	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	268/272 (98%)	256 (96%)	12 (4%)	24	49
All	All	2641/2720 (97%)	2479 (94%)	162 (6%)	17	37

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ARG
1	A	244	ILE
1	A	287	ARG
1	A	291	THR
1	A	343	SER
1	A	355	SER
1	A	356	VAL
1	A	365	VAL
1	A	371	THR
1	A	373	ASN
1	A	389	VAL
1	A	390	GLN
1	A	413	SER
1	A	486	LEU
1	A	493	LYS
1	A	523	GLN
1	B	224	THR
1	B	291	THR
1	B	305	SER
1	B	306	GLN
1	B	339	ARG
1	B	355	SER
1	B	365	VAL
1	B	372	SER
1	B	382	ARG
1	B	389	VAL
1	B	390	GLN
1	B	395	THR
1	B	413	SER
1	B	442	SER
1	B	472	VAL
1	B	476	ARG
1	B	481	ASP
1	B	484	ARG
1	C	221	GLU
1	C	244	ILE

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Mol	Chain	Res	Type
1	C	287	ARG
1	C	340	ARG
1	C	365	VAL
1	C	371	THR
1	C	372	SER
1	C	389	VAL
1	C	390	GLN
1	C	413	SER
1	C	465	SER
1	C	469	GLN
1	D	234	VAL
1	D	255	SER
1	D	287	ARG
1	D	291	THR
1	D	338	THR
1	D	364	SER
1	D	365	VAL
1	D	372	SER
1	D	382	ARG
1	D	389	VAL
1	D	390	GLN
1	D	393	SER
1	D	395	THR
1	D	412	ASP
1	D	469	GLN
1	D	519	SER
1	E	222	SER
1	E	224	THR
1	E	287	ARG
1	E	305	SER
1	E	334	LEU
1	E	338	THR
1	E	365	VAL
1	E	372	SER
1	E	389	VAL
1	E	390	GLN
1	E	413	SER
1	E	523	GLN
1	F	255	SER
1	F	287	ARG
1	F	290	VAL
1	F	291	THR

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Mol	Chain	Res	Type
1	F	305	SER
1	F	334	LEU
1	F	345	ARG
1	F	355	SER
1	F	356	VAL
1	F	364	SER
1	F	365	VAL
1	F	373	ASN
1	F	382	ARG
1	F	389	VAL
1	F	422	VAL
1	F	523	GLN
1	G	234	VAL
1	G	244	ILE
1	G	282	ASP
1	G	290	VAL
1	G	334	LEU
1	G	345	ARG
1	G	364	SER
1	G	365	VAL
1	G	389	VAL
1	G	390	GLN
1	G	493	LYS
1	G	523	GLN
1	H	225	LYS
1	H	231	ILE
1	H	234	VAL
1	H	255	SER
1	H	291	THR
1	H	329	LYS
1	H	334	LEU
1	H	337	THR
1	H	338	THR
1	H	344	THR
1	H	347	HIS
1	H	348	LYS
1	H	350	THR
1	H	355	SER
1	H	356	VAL
1	H	364	SER
1	H	365	VAL
1	H	371	THR

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Mol	Chain	Res	Type
1	H	374	ASP
1	H	377	THR
1	H	388	VAL
1	H	389	VAL
1	H	399	GLU
1	H	412	ASP
1	H	413	SER
1	H	463	GLN
1	H	465	SER
1	H	486	LEU
1	H	523	GLN
1	I	224	THR
1	I	234	VAL
1	I	269	ASP
1	I	287	ARG
1	I	327	VAL
1	I	329	LYS
1	I	334	LEU
1	I	336	GLN
1	I	345	ARG
1	I	350	THR
1	I	364	SER
1	I	365	VAL
1	I	377	THR
1	I	384	THR
1	I	413	SER
1	I	438	MET
1	I	465	SER
1	I	485	VAL
1	I	493	LYS
1	J	290	VAL
1	J	345	ARG
1	J	355	SER
1	J	356	VAL
1	J	365	VAL
1	J	371	THR
1	J	372	SER
1	J	389	VAL
1	J	394	THR
1	J	469	GLN
1	J	484	ARG
1	J	499	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	309	ASN
1	A	357	HIS
1	A	396	HIS
1	A	417	HIS
1	A	469	GLN
1	A	522	ASN
1	A	523	GLN
1	B	417	HIS
1	B	522	ASN
1	C	292	HIS
1	C	306	GLN
1	C	309	ASN
1	C	366	GLN
1	C	396	HIS
1	C	417	HIS
1	C	448	ASN
1	D	263	ASN
1	D	309	ASN
1	E	309	ASN
1	E	366	GLN
1	E	396	HIS
1	E	397	GLN
1	E	523	GLN
1	F	309	ASN
1	F	347	HIS
1	F	390	GLN
1	F	523	GLN
1	G	298	ASN
1	G	396	HIS
1	G	523	GLN
1	H	297	GLN
1	H	331	GLN
1	H	336	GLN
1	H	347	HIS
1	H	357	HIS
1	H	366	GLN
1	H	401	GLN
1	H	414	HIS
1	H	492	HIS
1	I	263	ASN

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Mol	Chain	Res	Type
1	I	347	HIS
1	I	357	HIS
1	I	417	HIS
1	J	292	HIS
1	J	309	ASN
1	J	331	GLN
1	J	366	GLN
1	J	398	ASN
1	J	417	HIS
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 ⓘ

24 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	GAL	K	1	2	12,12,12	0.47	0	17,17,17	0.78	1 (5%)
2	FUC	K	2	2	10,10,11	0.43	0	14,14,16	0.81	0
2	A2G	K	3	2	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	GAL	L	1	2	12,12,12	0.47	0	17,17,17	0.78	1 (5%)
2	FUC	L	2	2	10,10,11	0.42	0	14,14,16	0.81	0
2	A2G	L	3	2	14,14,15	0.55	0	17,19,21	0.85	0
2	GAL	M	1	2	12,12,12	0.47	0	17,17,17	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	M	2	2	10,10,11	0.42	0	14,14,16	0.82	0
2	A2G	M	3	2	14,14,15	0.55	0	17,19,21	0.85	1 (5%)
2	GAL	N	1	2	12,12,12	0.47	0	17,17,17	0.78	1 (5%)
2	FUC	N	2	2	10,10,11	0.43	0	14,14,16	0.80	0
2	A2G	N	3	2	14,14,15	0.55	0	17,19,21	0.85	0
2	GAL	O	1	2	12,12,12	0.48	0	17,17,17	0.78	1 (5%)
2	FUC	O	2	2	10,10,11	0.42	0	14,14,16	0.81	0
2	A2G	O	3	2	14,14,15	0.54	0	17,19,21	0.85	0
2	GAL	P	1	2	12,12,12	0.46	0	17,17,17	0.78	1 (5%)
2	FUC	P	2	2	10,10,11	0.41	0	14,14,16	0.80	0
2	A2G	P	3	2	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	GAL	Q	1	2	12,12,12	0.47	0	17,17,17	0.78	1 (5%)
2	FUC	Q	2	2	10,10,11	0.41	0	14,14,16	0.81	0
2	A2G	Q	3	2	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	GAL	R	1	2	12,12,12	0.47	0	17,17,17	0.78	1 (5%)
2	FUC	R	2	2	10,10,11	0.42	0	14,14,16	0.82	0
2	A2G	R	3	2	14,14,15	0.54	0	17,19,21	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	K	1	2	-	2/2/22/22	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	A2G	K	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	1	2	-	2/2/22/22	0/1/1/1
2	FUC	L	2	2	-	-	0/1/1/1
2	A2G	L	3	2	-	1/6/23/26	0/1/1/1
2	GAL	M	1	2	-	2/2/22/22	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
2	A2G	M	3	2	-	2/6/23/26	0/1/1/1
2	GAL	N	1	2	-	2/2/22/22	0/1/1/1
2	FUC	N	2	2	-	-	0/1/1/1
2	A2G	N	3	2	-	1/6/23/26	0/1/1/1
2	GAL	O	1	2	-	2/2/22/22	0/1/1/1
2	FUC	O	2	2	-	-	0/1/1/1
2	A2G	O	3	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	P	1	2	-	1/2/22/22	0/1/1/1
2	FUC	P	2	2	-	-	0/1/1/1
2	A2G	P	3	2	-	2/6/23/26	0/1/1/1
2	GAL	Q	1	2	-	2/2/22/22	0/1/1/1
2	FUC	Q	2	2	-	-	0/1/1/1
2	A2G	Q	3	2	-	2/6/23/26	0/1/1/1
2	GAL	R	1	2	-	2/2/22/22	0/1/1/1
2	FUC	R	2	2	-	-	0/1/1/1
2	A2G	R	3	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GAL	C1-O5-C5	-2.18	109.43	113.65
2	O	1	GAL	C1-O5-C5	-2.17	109.46	113.65
2	L	1	GAL	C1-O5-C5	-2.17	109.46	113.65
2	M	1	GAL	C1-O5-C5	-2.16	109.48	113.65
2	N	1	GAL	C1-O5-C5	-2.14	109.51	113.65
2	P	1	GAL	C1-O5-C5	-2.13	109.53	113.65
2	R	1	GAL	C1-O5-C5	-2.12	109.54	113.65
2	Q	1	GAL	C1-O5-C5	-2.12	109.55	113.65
2	Q	3	A2G	C1-O5-C5	-2.04	109.45	112.19
2	R	3	A2G	C1-O5-C5	-2.04	109.46	112.19
2	P	3	A2G	C1-O5-C5	-2.02	109.48	112.19
2	M	3	A2G	C1-O5-C5	-2.01	109.49	112.19
2	K	3	A2G	C1-O5-C5	-2.00	109.50	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	GAL	O5-C5-C6-O6
2	M	1	GAL	O5-C5-C6-O6
2	P	3	A2G	O5-C5-C6-O6
2	O	1	GAL	O5-C5-C6-O6
2	M	1	GAL	C4-C5-C6-O6
2	P	3	A2G	C4-C5-C6-O6
2	K	3	A2G	O5-C5-C6-O6
2	L	1	GAL	C4-C5-C6-O6

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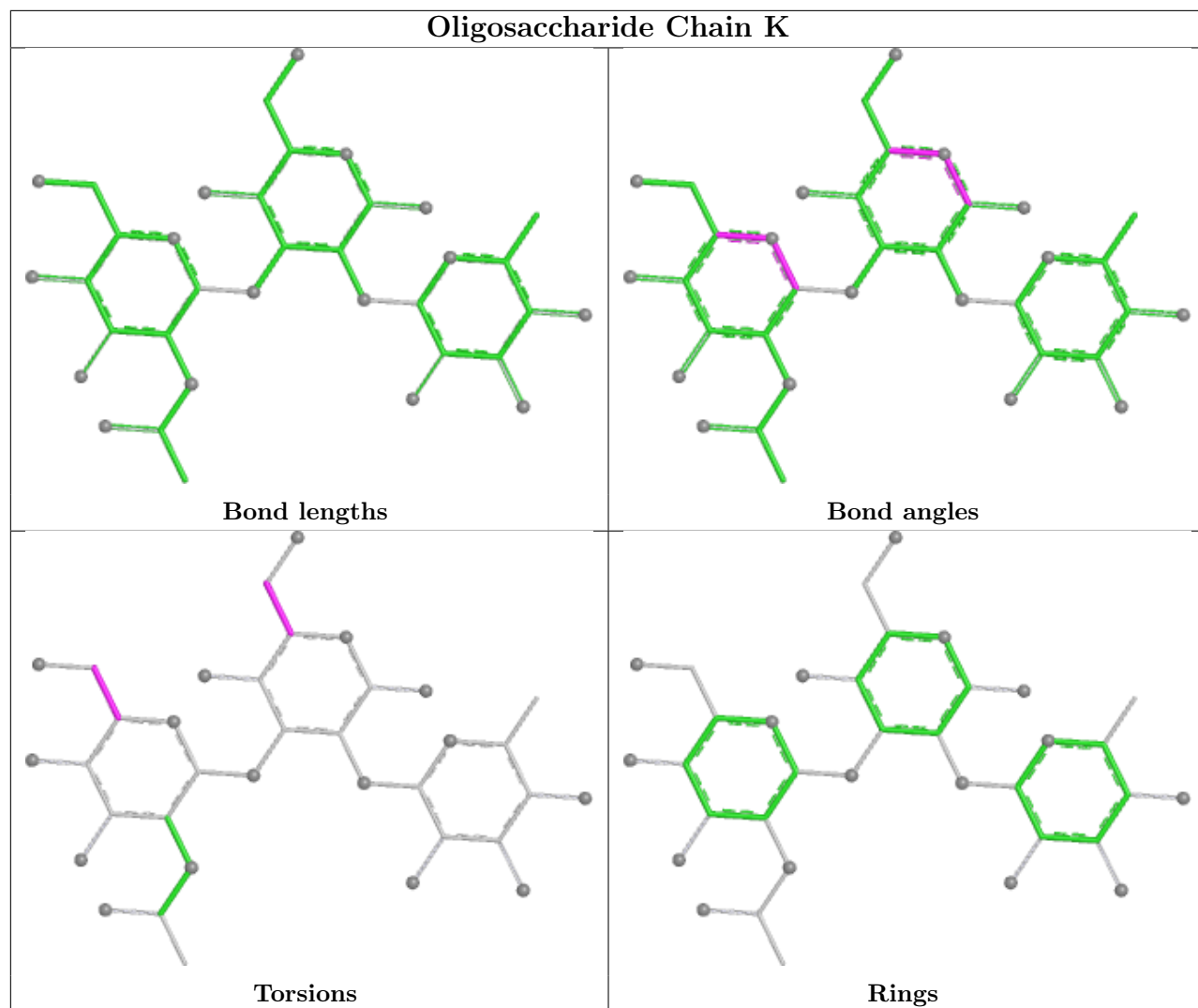
Mol	Chain	Res	Type	Atoms
2	R	1	GAL	O5-C5-C6-O6
2	K	1	GAL	O5-C5-C6-O6
2	Q	3	A2G	O5-C5-C6-O6
2	R	1	GAL	C4-C5-C6-O6
2	K	1	GAL	C4-C5-C6-O6
2	Q	1	GAL	C4-C5-C6-O6
2	Q	3	A2G	C4-C5-C6-O6
2	M	3	A2G	O5-C5-C6-O6
2	Q	1	GAL	O5-C5-C6-O6
2	O	1	GAL	C4-C5-C6-O6
2	O	3	A2G	O5-C5-C6-O6
2	P	1	GAL	O5-C5-C6-O6
2	K	3	A2G	C4-C5-C6-O6
2	N	3	A2G	O5-C5-C6-O6
2	L	3	A2G	O5-C5-C6-O6
2	R	3	A2G	O5-C5-C6-O6
2	N	1	GAL	C4-C5-C6-O6
2	M	3	A2G	C4-C5-C6-O6
2	N	1	GAL	O5-C5-C6-O6

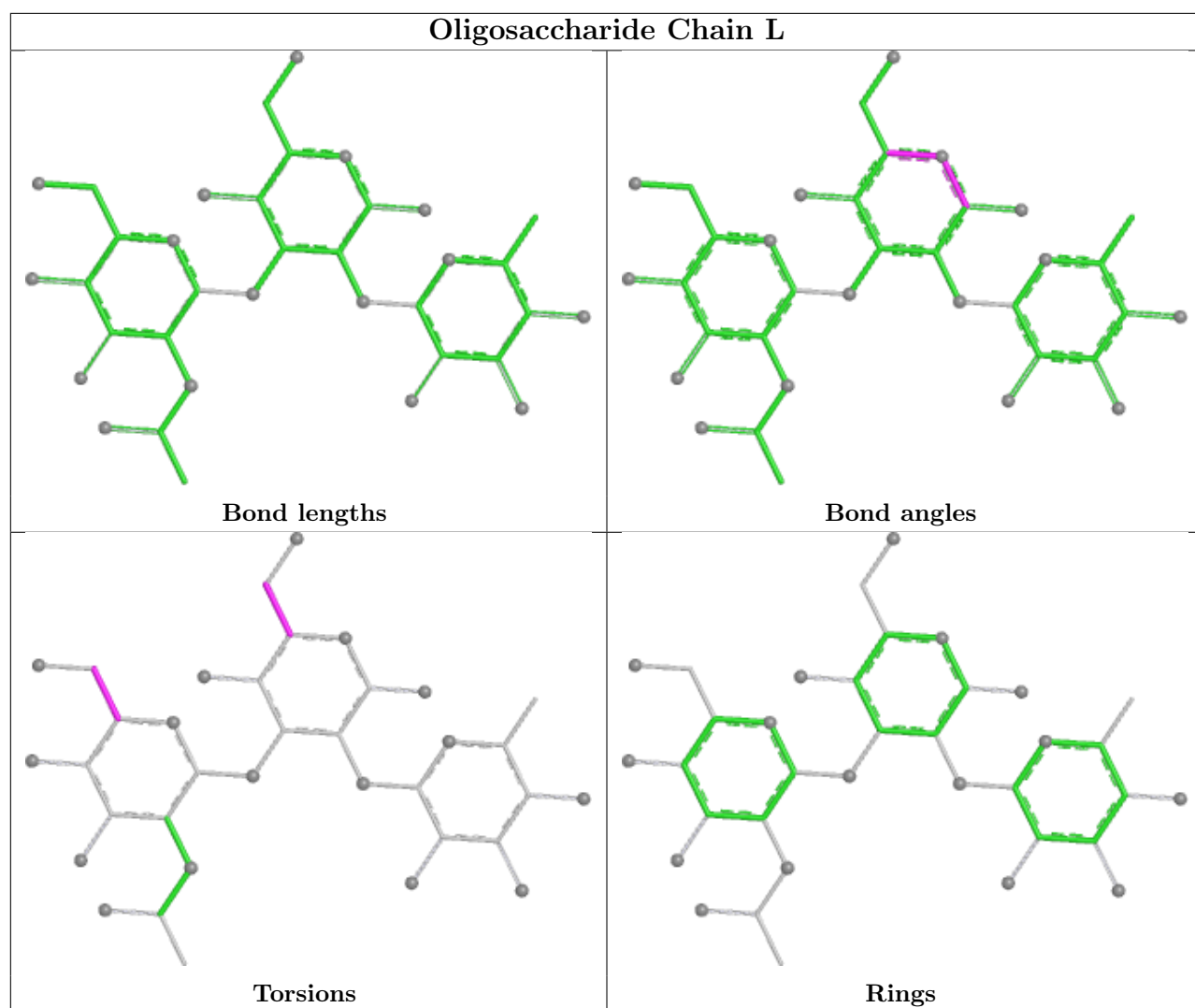
There are no ring outliers.

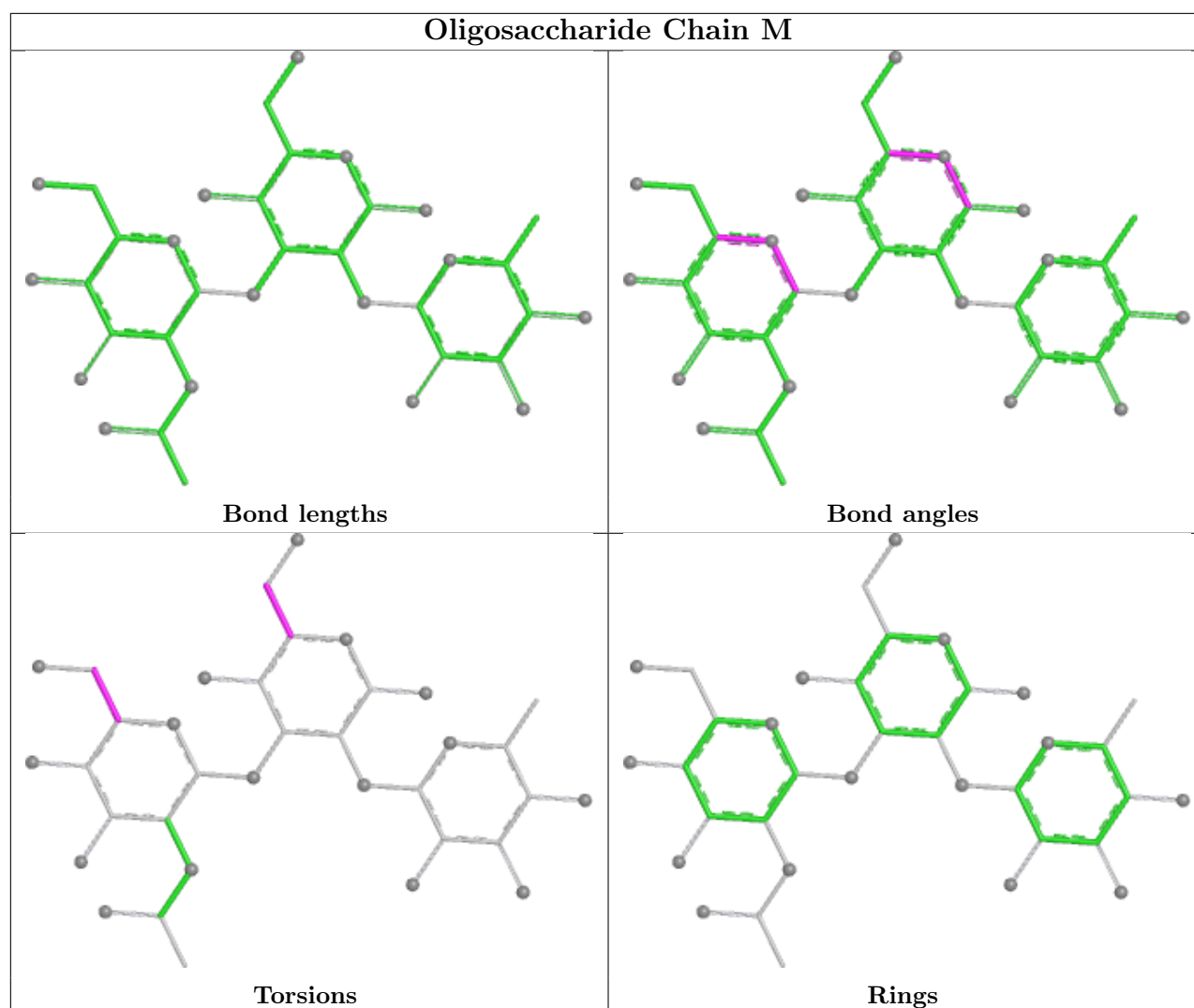
7 monomers are involved in 11 short contacts:

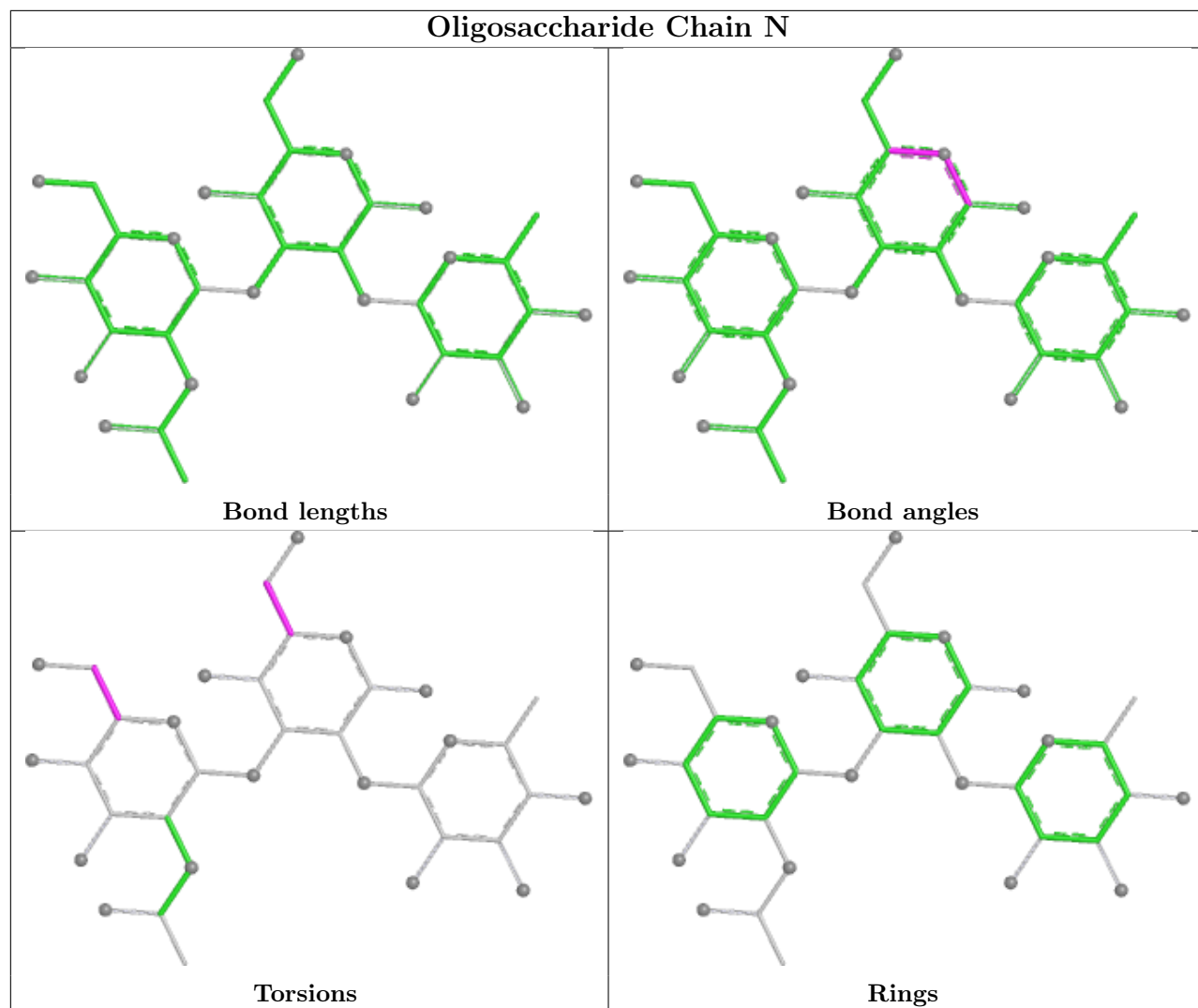
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	2	FUC	1	0
2	K	1	GAL	1	0
2	M	2	FUC	1	0
2	O	2	FUC	2	0
2	R	2	FUC	3	0
2	Q	2	FUC	2	0
2	K	2	FUC	1	0

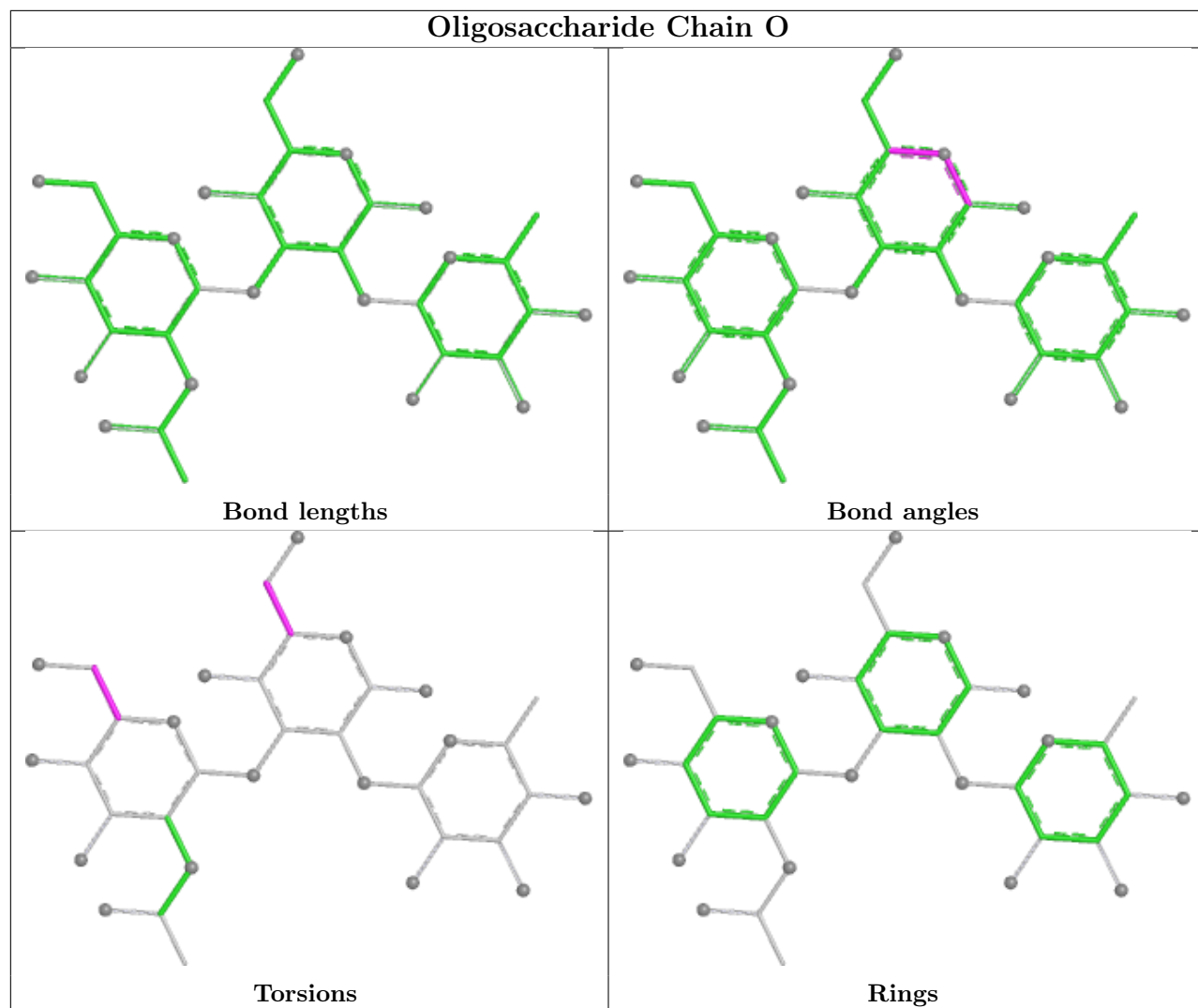
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

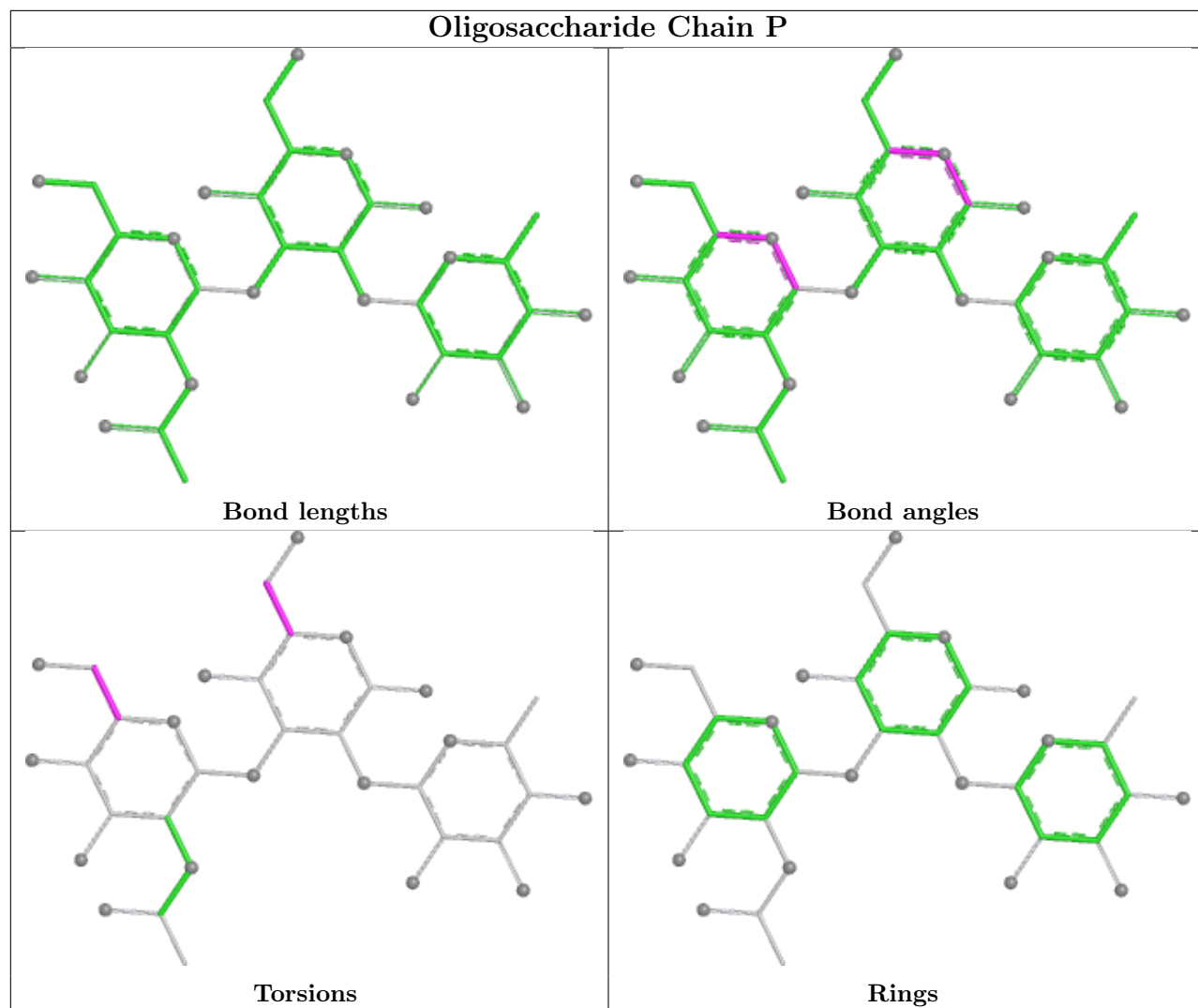


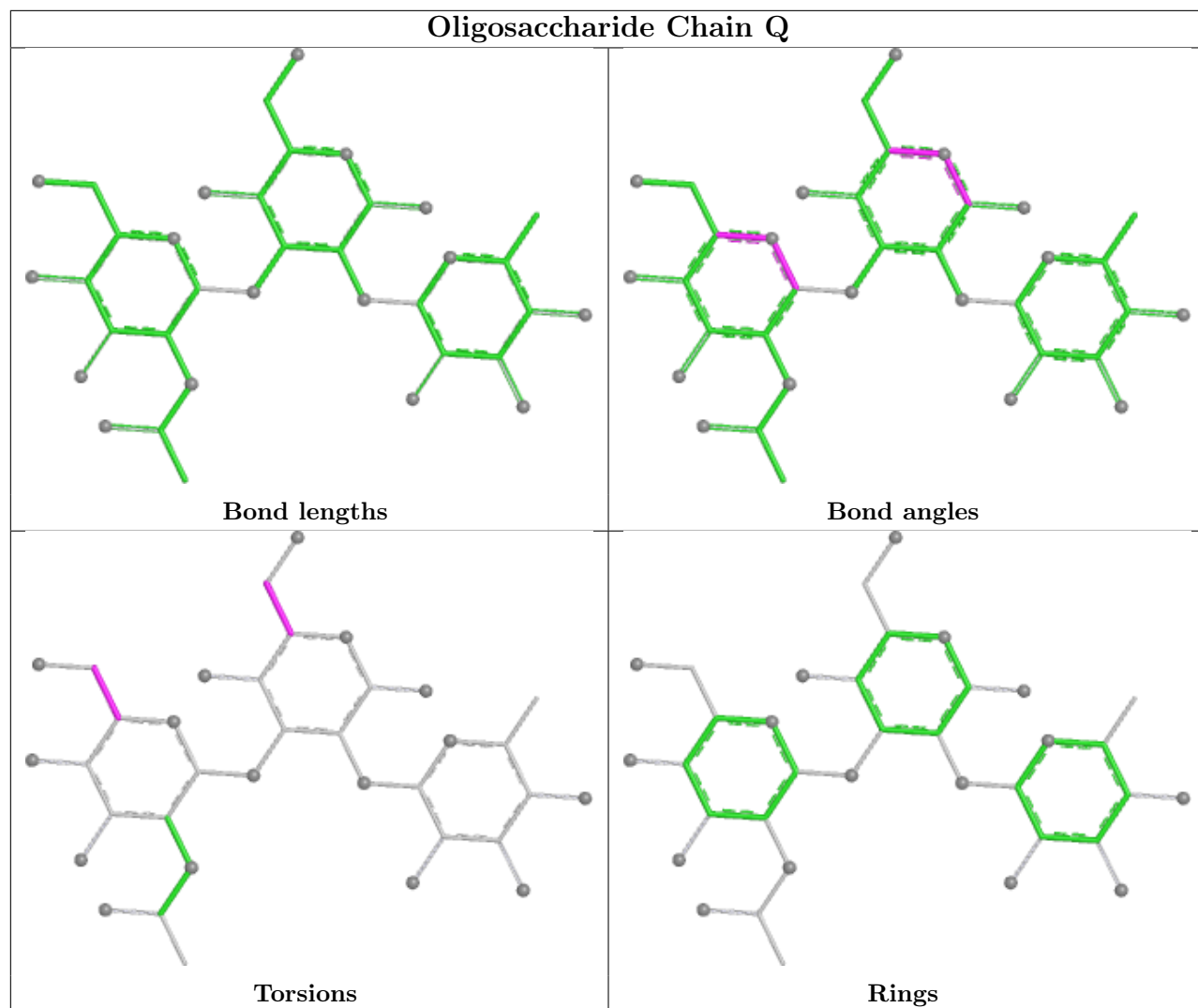


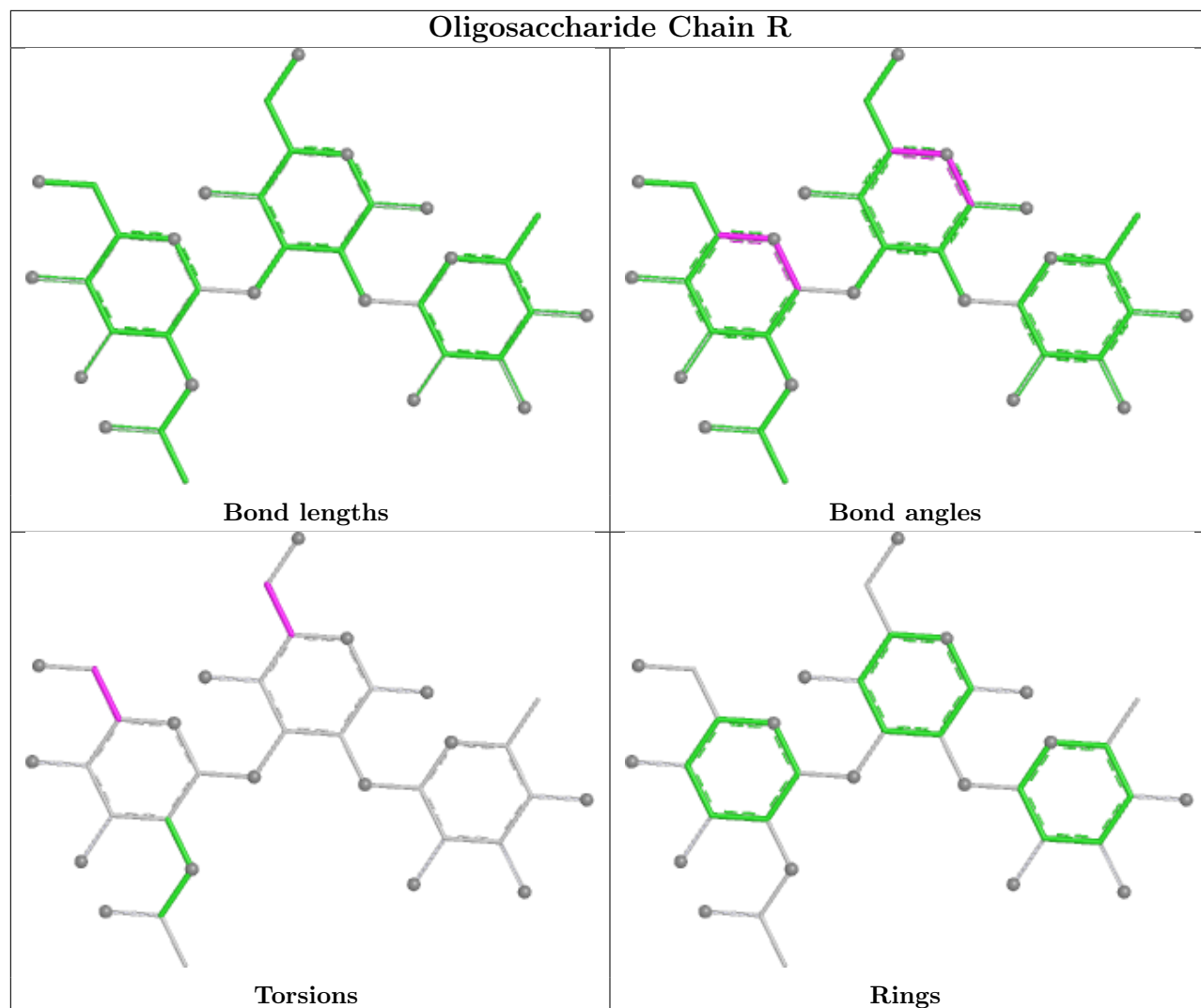












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/311 (99%)	-0.59	5 (1%) 70 68	16, 26, 50, 69	0
1	B	308/311 (99%)	-0.59	7 (2%) 61 57	16, 28, 51, 74	0
1	C	311/311 (100%)	-0.58	2 (0%) 85 84	16, 30, 53, 79	0
1	D	307/311 (98%)	-0.57	3 (0%) 79 77	16, 29, 56, 75	0
1	E	309/311 (99%)	-0.59	4 (1%) 75 73	18, 29, 53, 72	0
1	F	308/311 (99%)	-0.35	8 (2%) 57 53	20, 37, 64, 86	0
1	G	308/311 (99%)	-0.43	4 (1%) 75 73	22, 35, 58, 85	0
1	H	293/311 (94%)	-0.10	15 (5%) 33 29	22, 41, 70, 81	0
1	I	286/311 (91%)	0.43	20 (6%) 22 19	34, 57, 81, 106	0
1	J	307/311 (98%)	-0.62	2 (0%) 84 82	17, 29, 54, 69	0
All	All	3046/3110 (97%)	-0.41	70 (2%) 61 57	16, 33, 66, 106	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	374	ASP	6.9
1	H	374	ASP	6.4
1	I	336	GLN	6.1
1	H	337	THR	5.0
1	I	345	ARG	4.7
1	I	376	GLU	4.3
1	H	447	MET	4.1
1	H	371	THR	4.1
1	I	440	GLY	3.9
1	H	438	MET	3.9
1	I	388	VAL	3.8
1	I	307	ASN	3.7
1	I	337	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	481	ASP	3.6
1	H	221	GLU	3.5
1	I	524	PHE	3.5
1	C	495	GLY	3.5
1	H	439	PRO	3.4
1	H	400	PRO	3.3
1	I	375	PHE	3.1
1	I	231	ILE	3.1
1	F	395	THR	3.0
1	E	495	GLY	2.9
1	F	518	ASP	2.9
1	E	414	HIS	2.9
1	I	523	GLN	2.9
1	A	373	ASN	2.8
1	G	411	ARG	2.7
1	G	306	GLN	2.7
1	H	345	ARG	2.7
1	H	231	ILE	2.7
1	B	495	GLY	2.7
1	B	482	THR	2.7
1	H	412	ASP	2.7
1	F	412	ASP	2.6
1	B	310	ASN	2.6
1	I	382	ARG	2.6
1	D	373	ASN	2.6
1	I	299	TYR	2.5
1	F	523	GLN	2.5
1	G	310	ASN	2.5
1	I	344	THR	2.5
1	E	412	ASP	2.4
1	F	414	HIS	2.4
1	D	495	GLY	2.4
1	I	438	MET	2.4
1	I	414	HIS	2.4
1	A	516	ARG	2.4
1	A	306	GLN	2.4
1	B	370	ASP	2.3
1	H	339	ARG	2.3
1	B	224	THR	2.3
1	A	412	ASP	2.3
1	D	372	SER	2.3
1	F	372	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	224	THR	2.3
1	F	531	GLY	2.2
1	G	531	GLY	2.2
1	I	297	GLN	2.2
1	B	372	SER	2.2
1	H	448	ASN	2.1
1	J	310	ASN	2.1
1	A	372	SER	2.1
1	E	524	PHE	2.1
1	J	372	SER	2.1
1	C	221	GLU	2.1
1	H	346	GLY	2.1
1	I	294	ALA	2.0
1	I	482	THR	2.0
1	H	302	ASN	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.

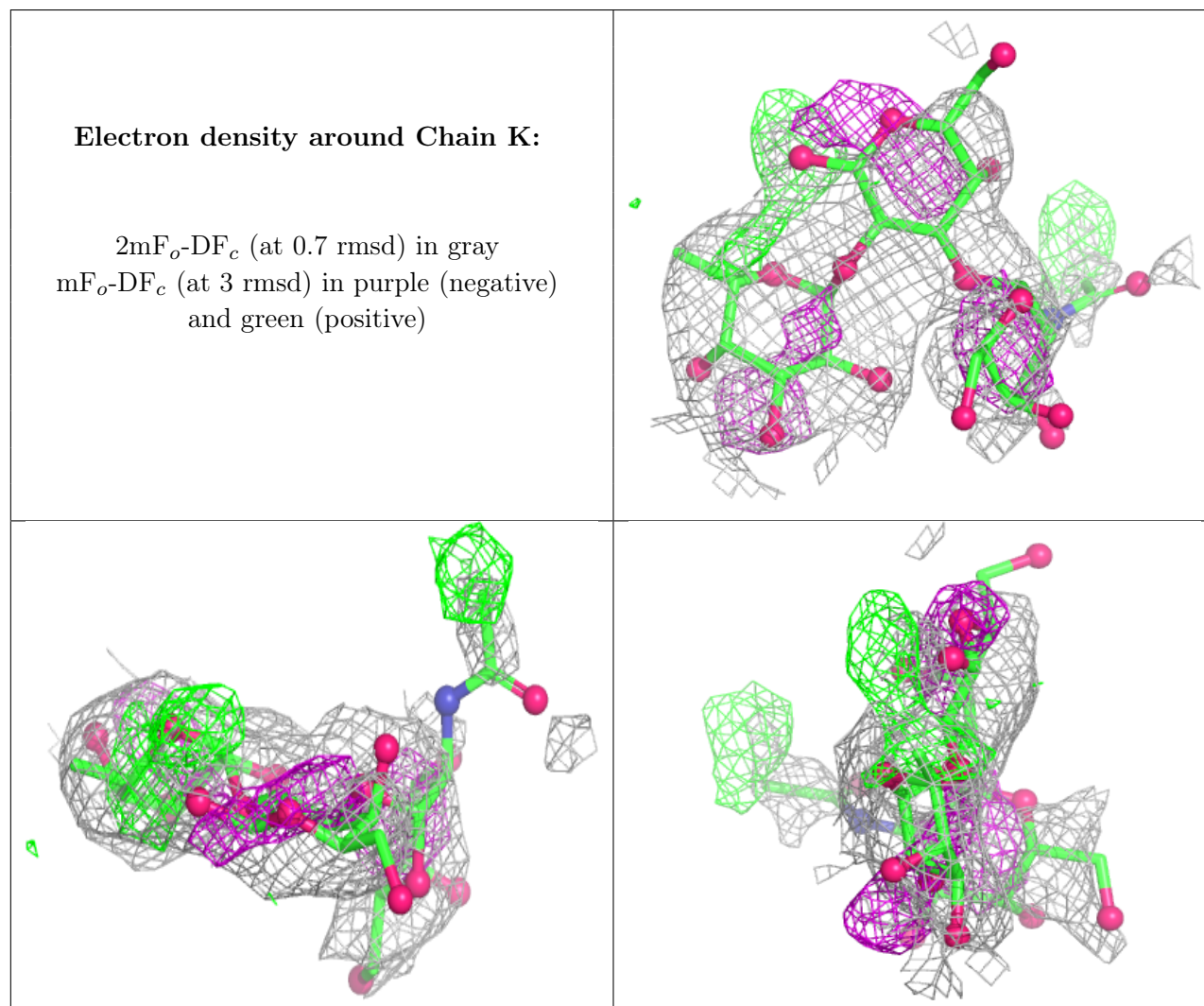
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	K	1	12/12	0.38	0.23	83,93,95,99	0
2	A2G	P	3	14/15	0.42	0.28	108,115,120,121	0
2	A2G	R	3	14/15	0.42	0.30	91,97,100,101	0
2	A2G	N	3	14/15	0.43	0.27	112,114,118,118	0
2	A2G	Q	3	14/15	0.47	0.26	114,116,117,117	0
2	A2G	O	3	14/15	0.49	0.28	110,111,112,112	0
2	A2G	K	3	14/15	0.50	0.29	102,104,105,105	0
2	GAL	O	1	12/12	0.50	0.22	89,101,102,105	0
2	GAL	M	1	12/12	0.50	0.21	87,98,98,102	0
2	A2G	M	3	14/15	0.51	0.28	105,109,110,110	0
2	GAL	Q	1	12/12	0.51	0.21	102,109,110,114	0
2	A2G	L	3	14/15	0.55	0.25	93,95,96,96	0
2	GAL	P	1	12/12	0.60	0.20	100,108,110,113	0

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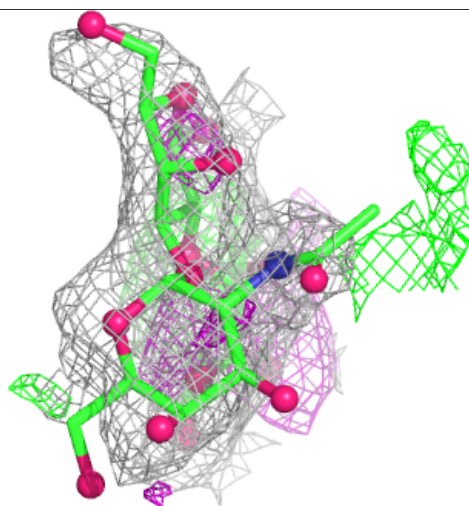
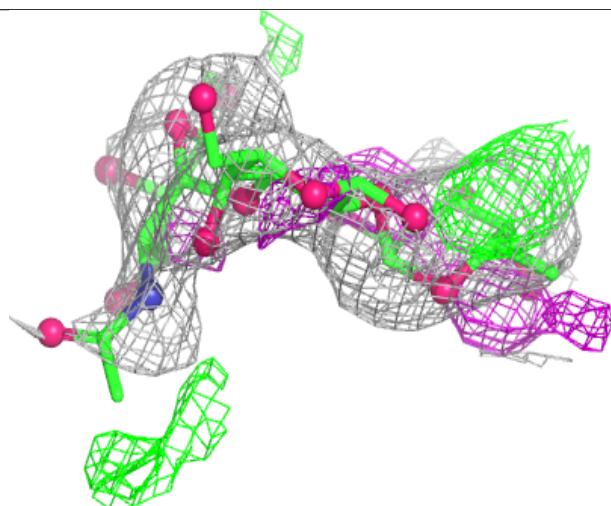
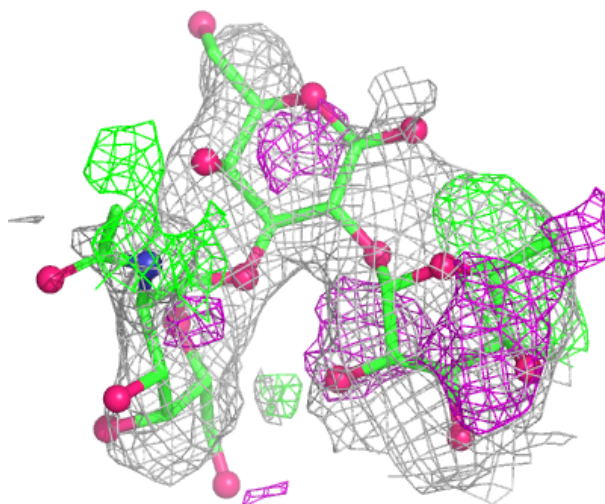
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	R	1	12/12	0.61	0.22	81,91,92,93	0
2	GAL	N	1	12/12	0.66	0.18	93,103,105,110	0
2	GAL	L	1	12/12	0.69	0.18	75,87,89,90	0
2	FUC	L	2	10/11	0.71	0.23	50,54,60,64	0
2	FUC	R	2	10/11	0.78	0.19	65,69,72,74	0
2	FUC	M	2	10/11	0.78	0.22	67,71,76,79	0
2	FUC	O	2	10/11	0.80	0.22	65,73,77,81	0
2	FUC	N	2	10/11	0.81	0.22	76,79,82,85	0
2	FUC	K	2	10/11	0.83	0.20	62,67,70,74	0
2	FUC	Q	2	10/11	0.83	0.25	86,91,93,96	0
2	FUC	P	2	10/11	0.84	0.21	83,89,91,93	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.



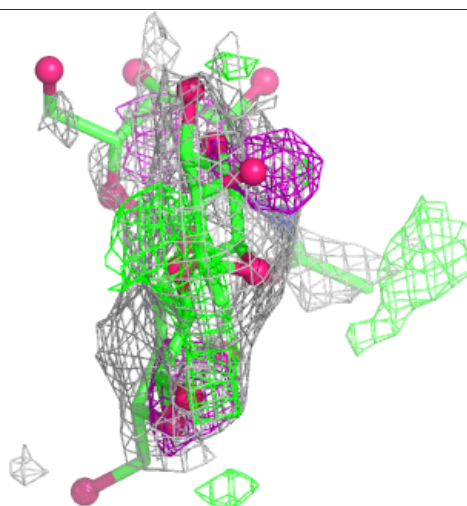
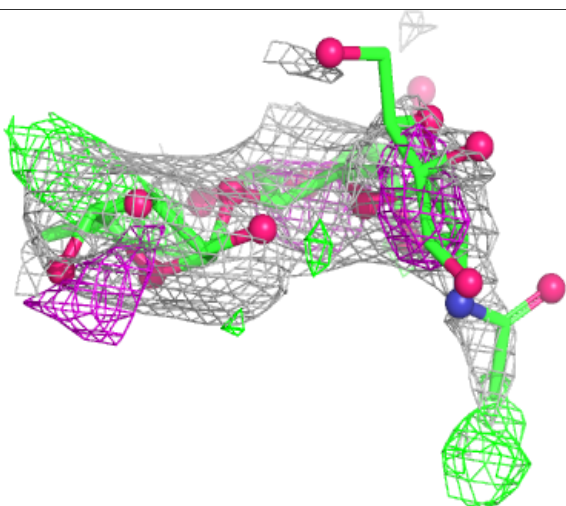
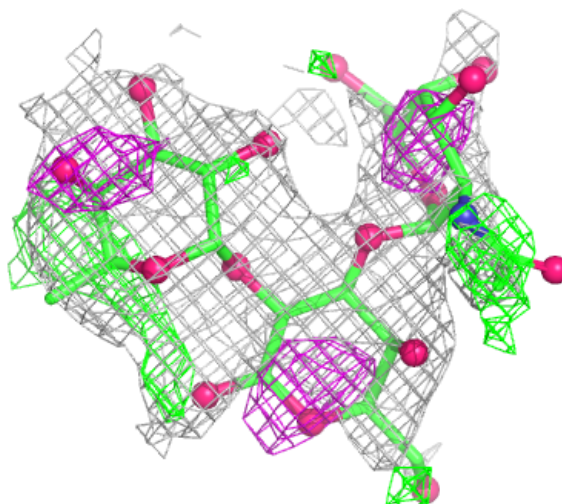
Electron density around Chain L:

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



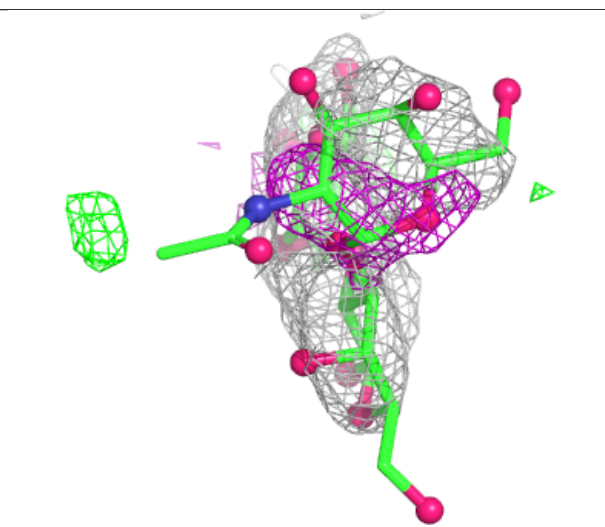
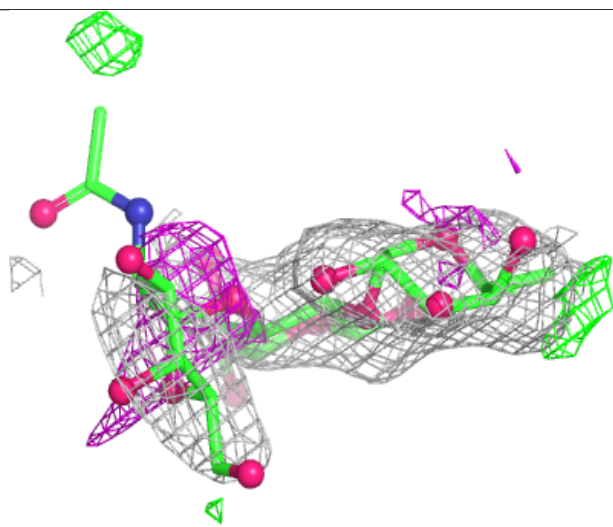
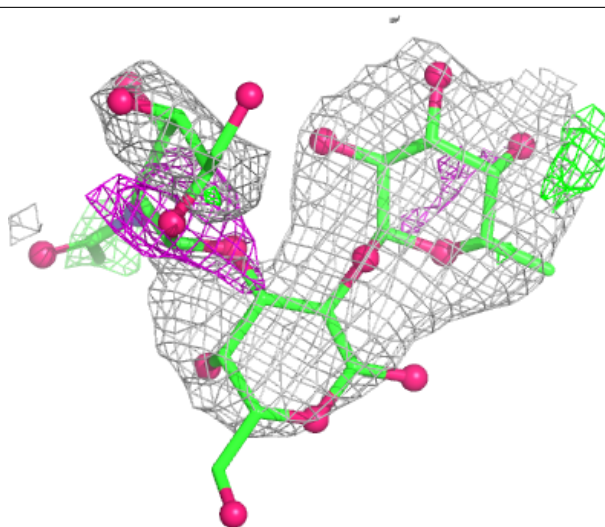
Electron density around Chain M:

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



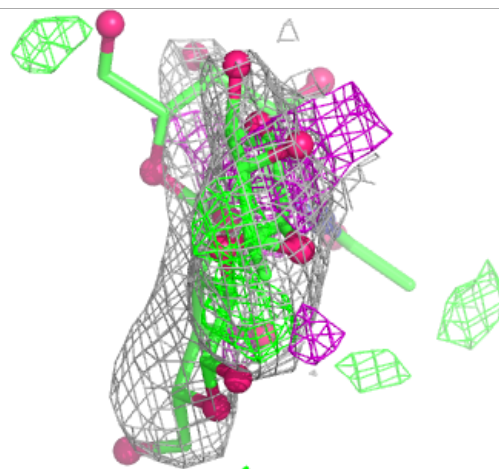
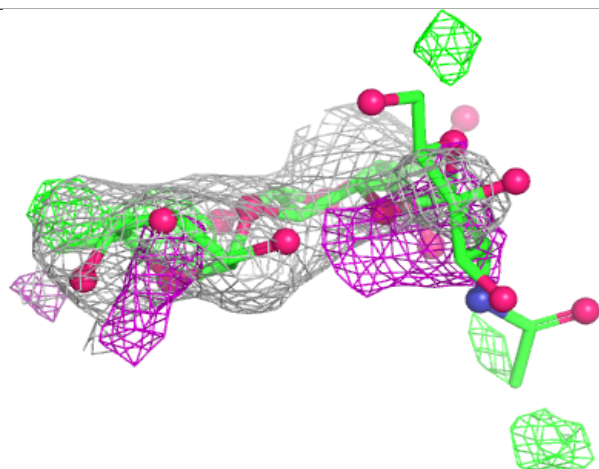
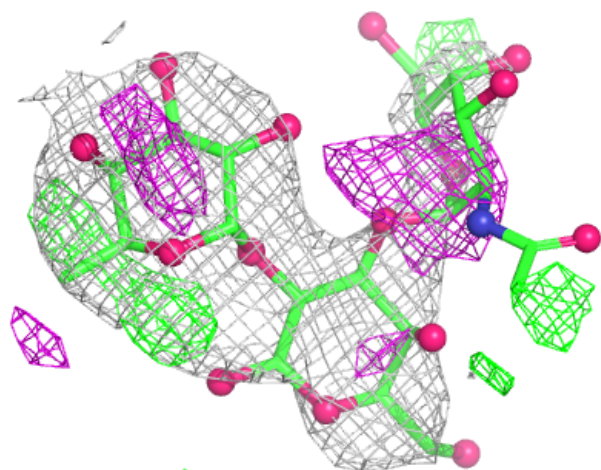
Electron density around Chain N:

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



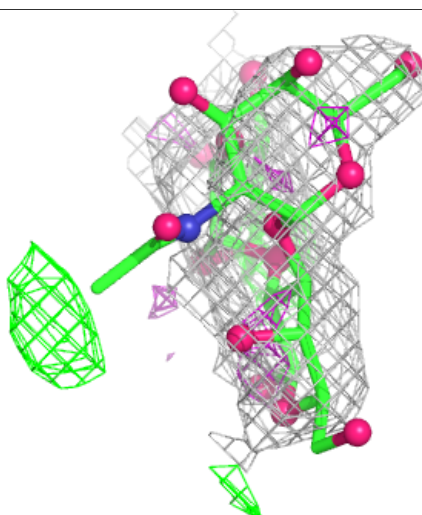
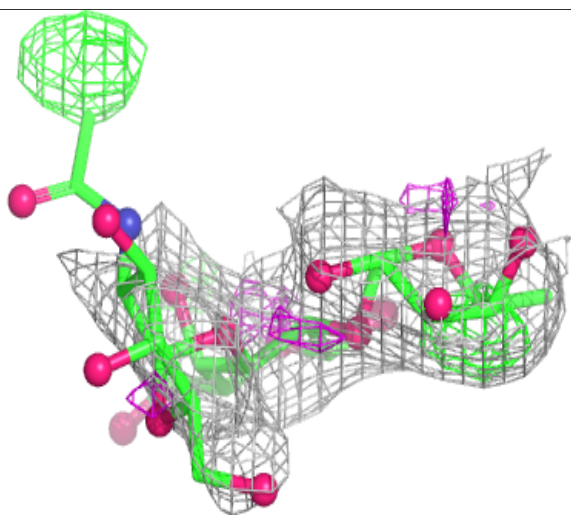
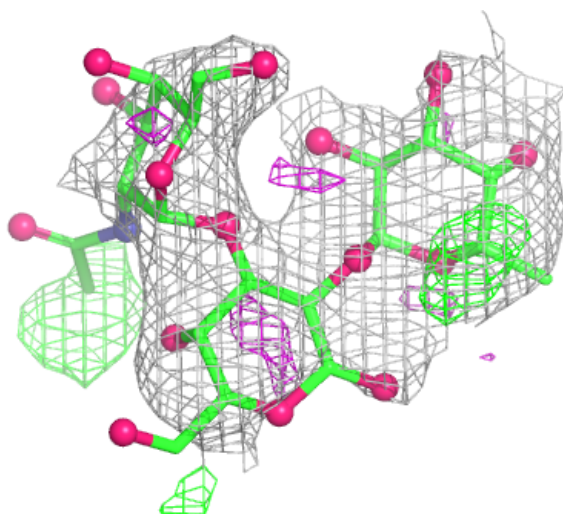
Electron density around Chain O:

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



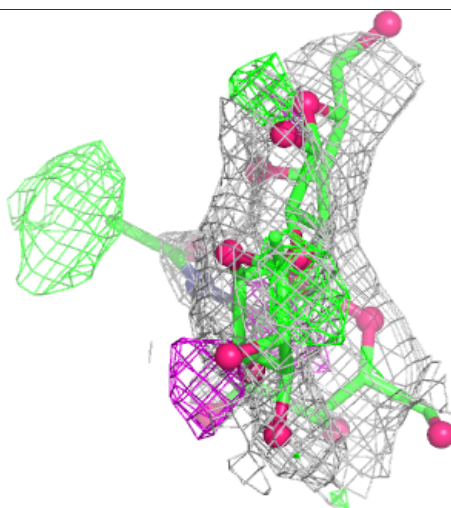
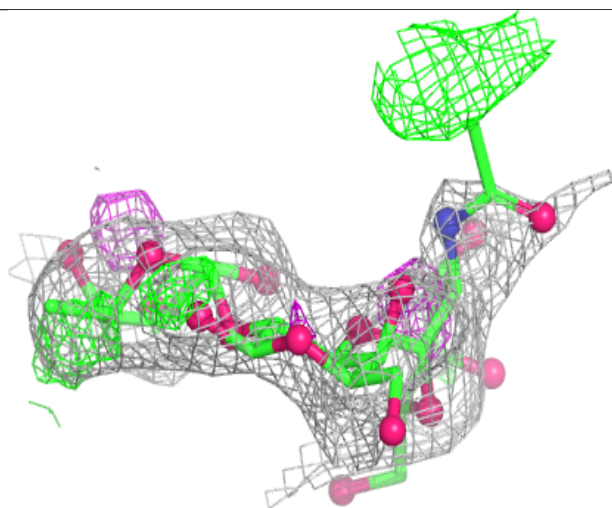
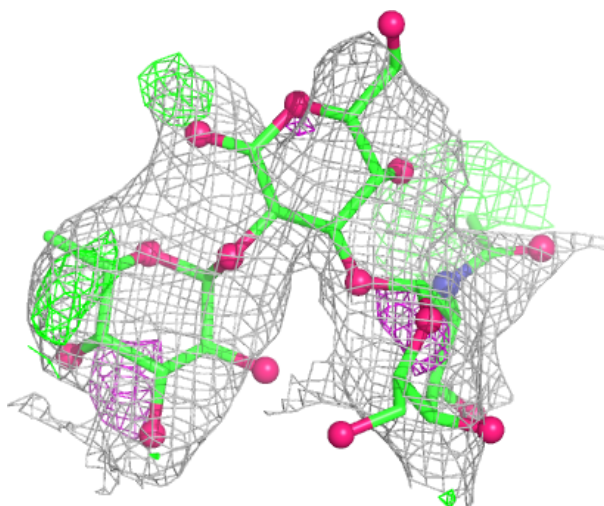
Electron density around Chain P:

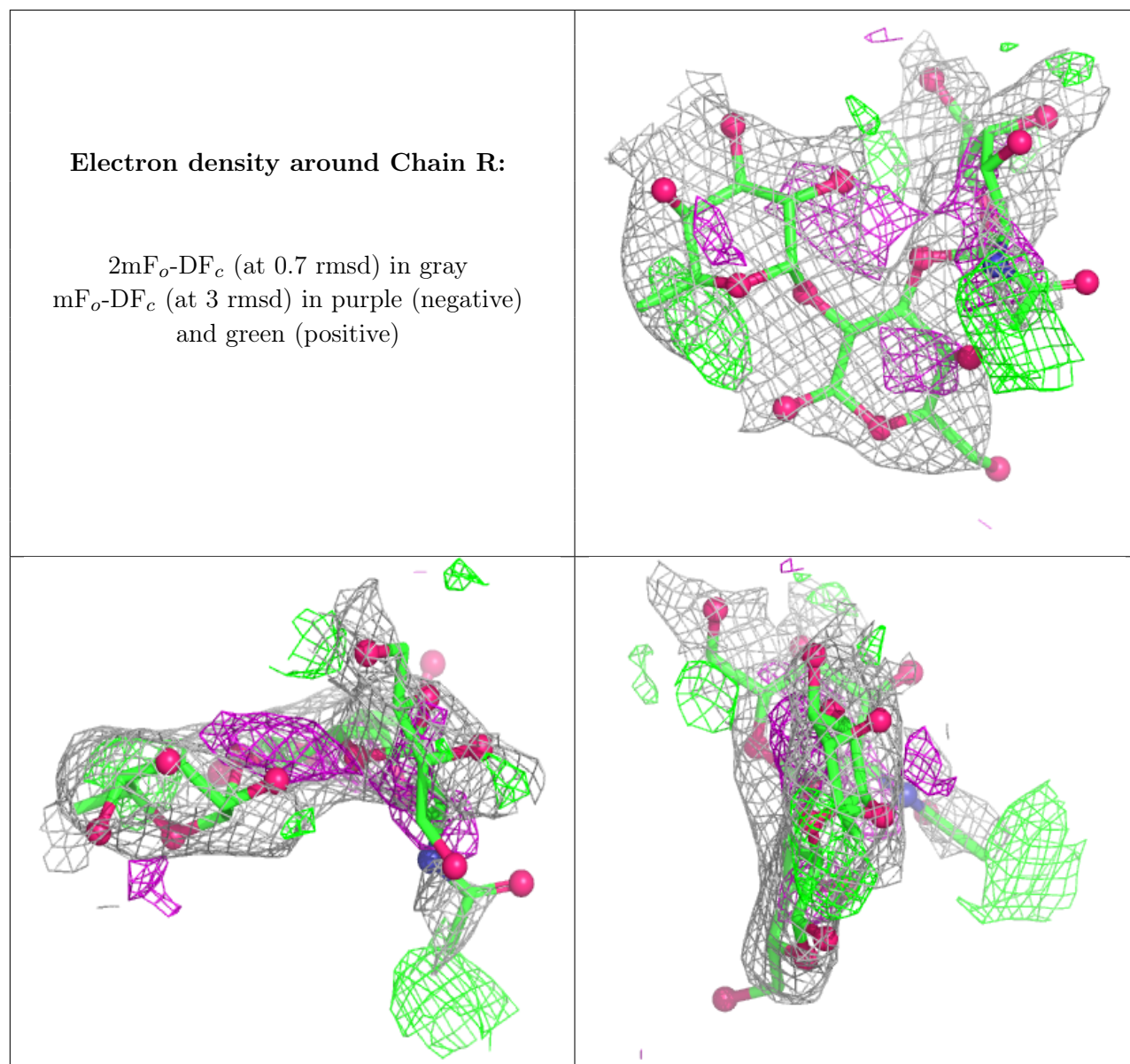
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.