



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:45 PM UTC

PDB ID : 7BJC / pdb_00007bjc
Title : Inulosucrase from Halalkalicoccus jeotgali in complex with sucrose
Authors : Ghauri, K.; Pijning, T.; Munawar, N.; Ali, H.; Ghauri, M.A.; Anwar, M.A.; Wallis, R.
Deposited on : 2021-01-14
Resolution : 3.11 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

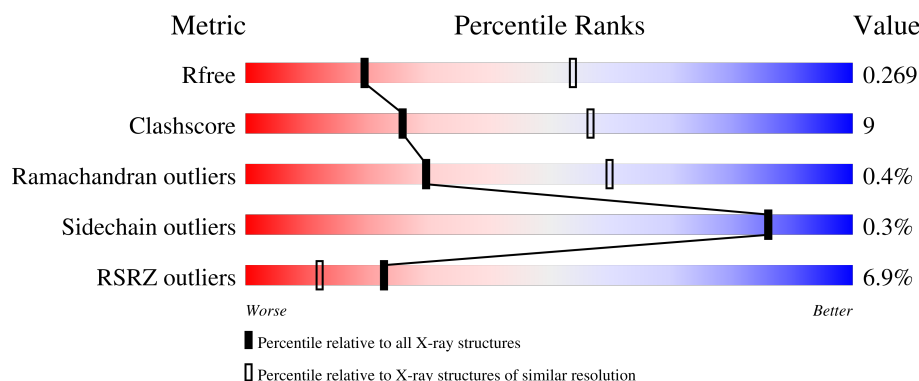
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	428	4% 80% 14% 5%
1	B	428	5% 79% 16% 5%
1	C	428	4% 79% 15% 5%
1	D	428	3% 76% 18% • 5%
1	E	428	5% 79% 16% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	
1	I	428	
1	J	428	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	

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	FRU	M	2	-	-	X	-

2 Entry composition [i](#)

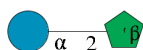
There are 2 unique types of molecules in this entry. The entry contains 31988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Levansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3173	2008	545	616	4			
1	B	405	Total	C	N	O	S	0	0	0
			3173	2008	545	616	4			
1	C	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	D	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	E	405	Total	C	N	O	S	0	0	0
			3173	2008	545	616	4			
1	F	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	G	405	Total	C	N	O	S	0	0	0
			3173	2008	545	616	4			
1	H	405	Total	C	N	O	S	0	0	0
			3173	2008	545	616	4			
1	I	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	J	405	Total	C	N	O	S	0	0	0
			3173	2008	545	616	4			

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

Continued on next page...

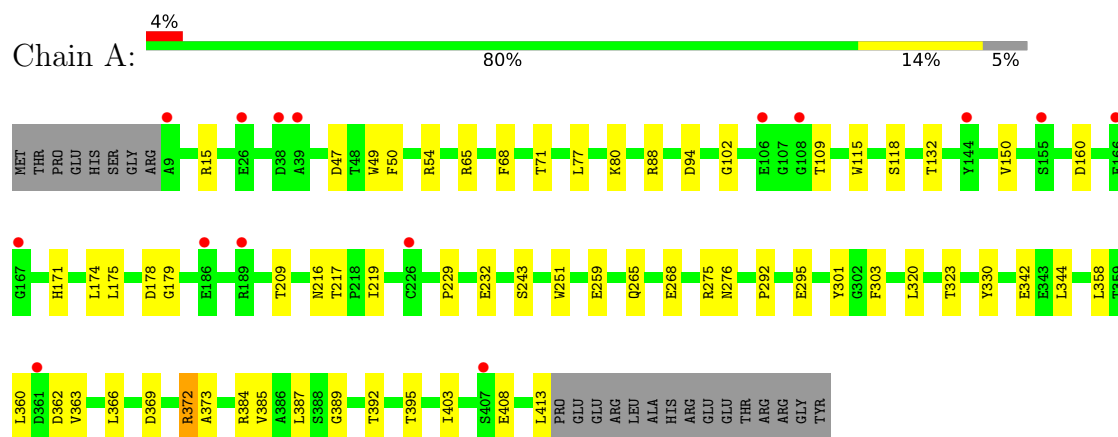
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C	O	0	0	0
			23	12	11			
2	T	2	Total	C	O	0	0	0
			23	12	11			

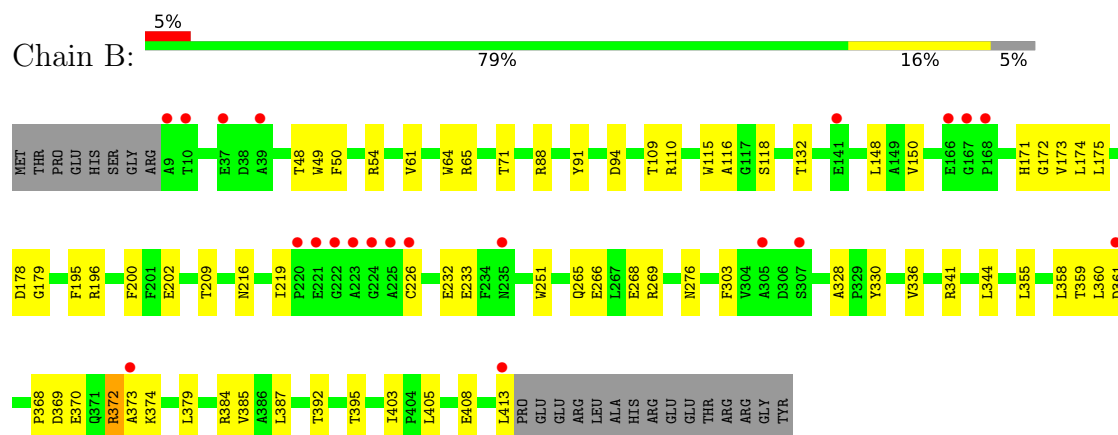
3 Residue-property plots [i](#)

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

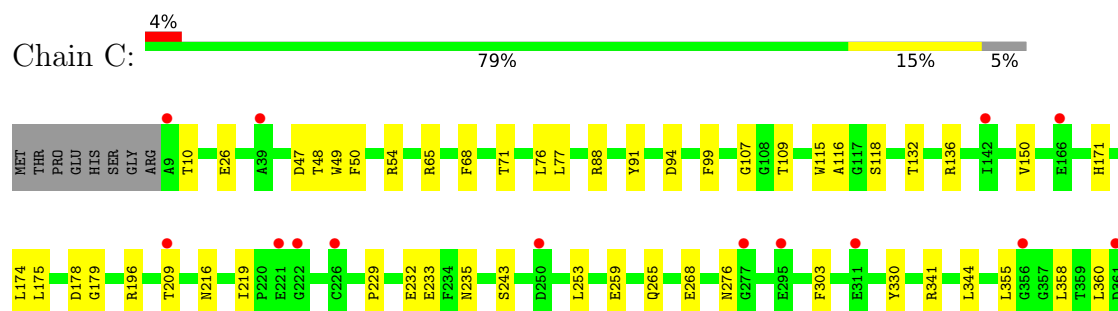
• Molecule 1: Levansucrase



• Molecule 1: Levansucrase

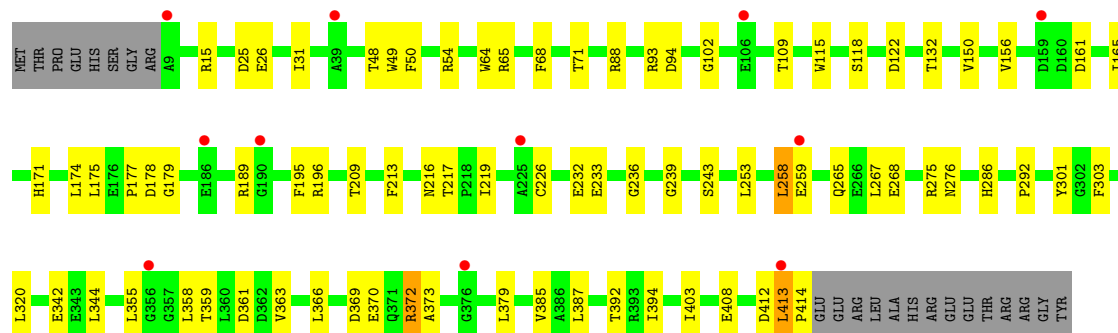
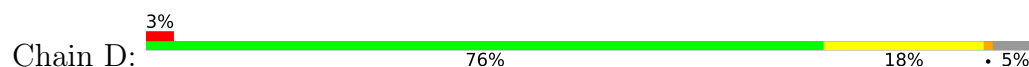


• Molecule 1: Levansucrase

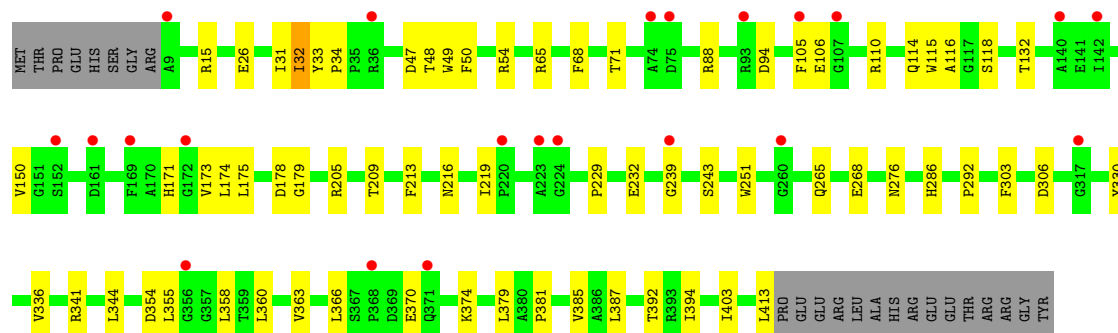
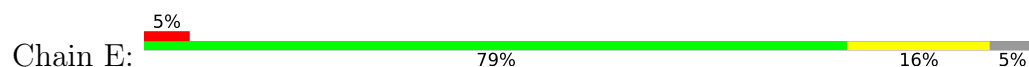




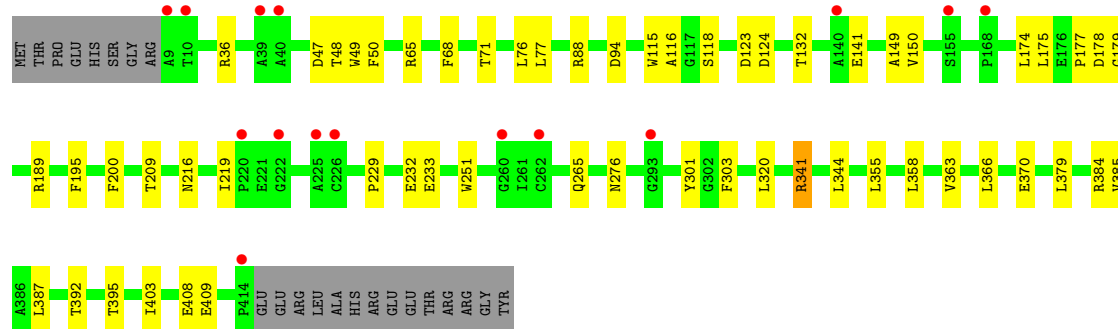
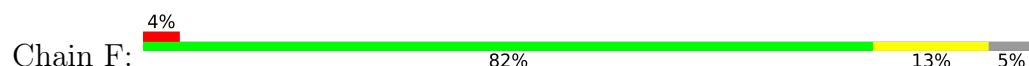
• Molecule 1: Levansucrase



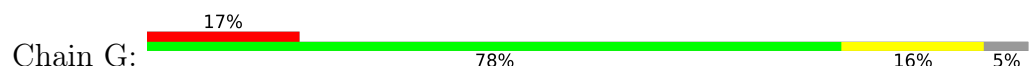
• Molecule 1: Levansucrase

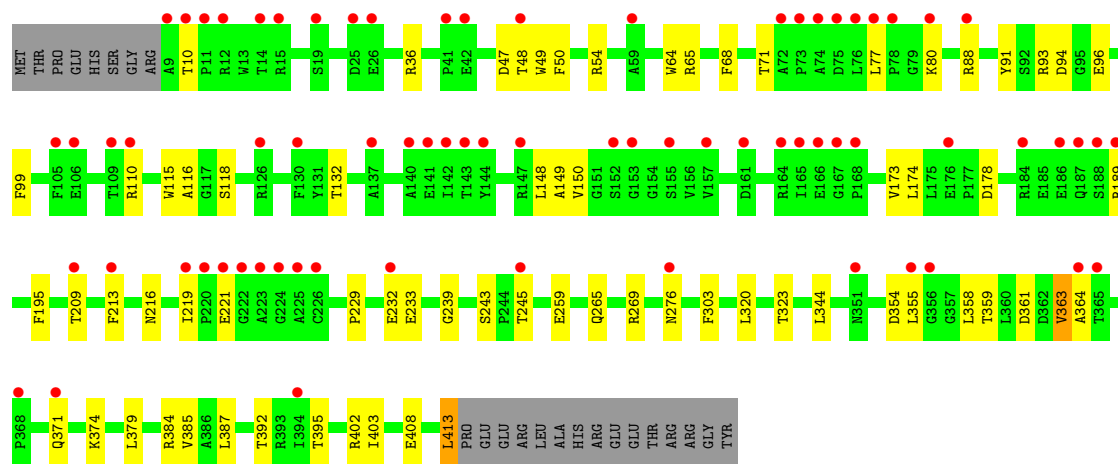


• Molecule 1: Levansucrase

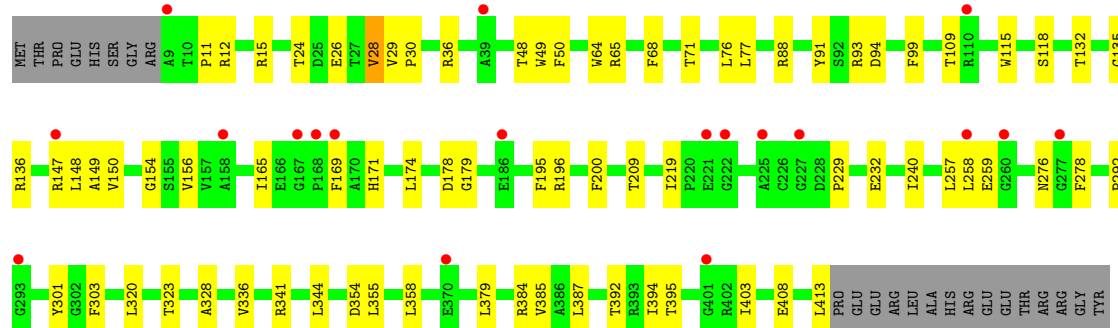
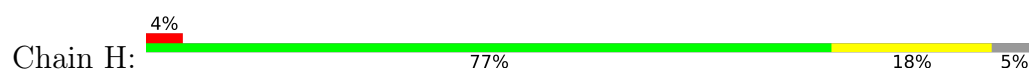


• Molecule 1: Levansucrase

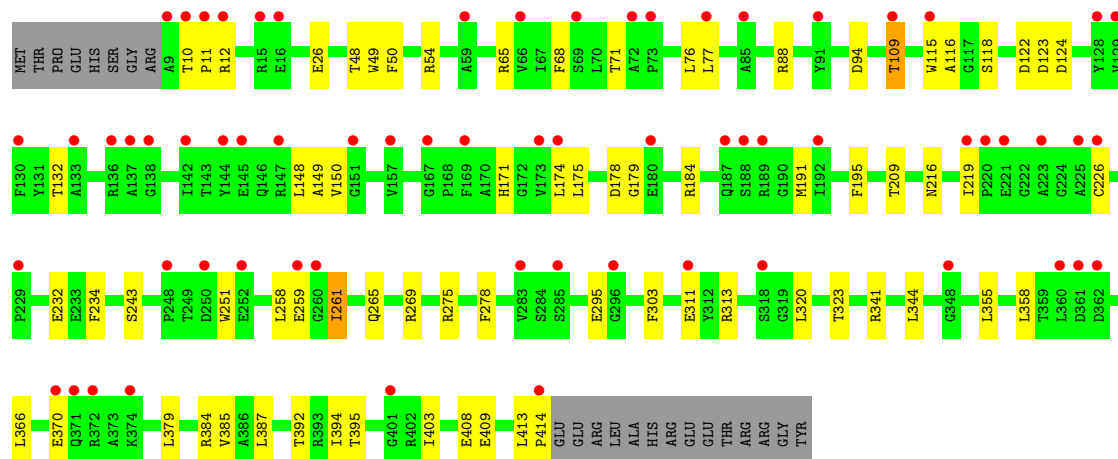
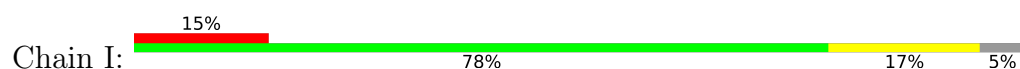




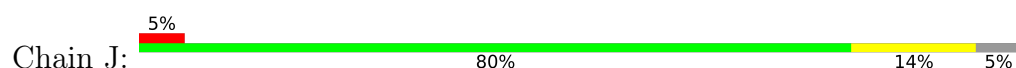
• Molecule 1: Levansucrase

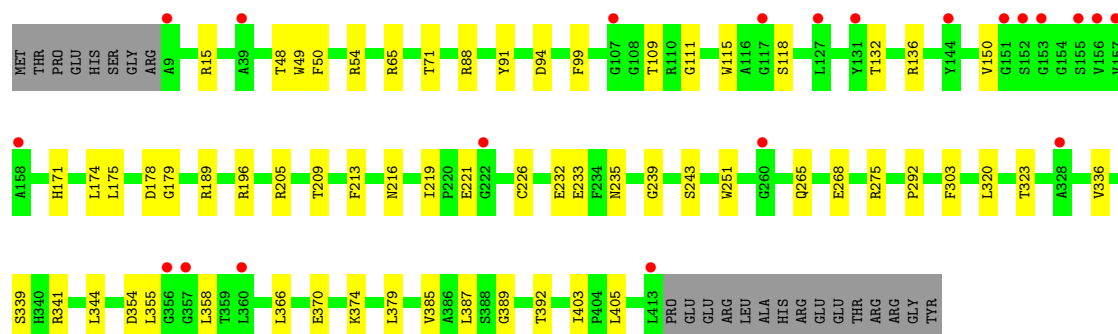


• Molecule 1: Levansucrase



• Molecule 1: Levansucrase





- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain K: 50% 50%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L: 50% 50%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M: 50% 50%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N: 100%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O: 100%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P: 50% 50%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q:  50% 50%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain R:  50% 50%

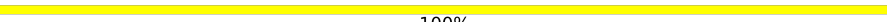


- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S:  50% 50%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.75Å 141.80Å 169.32Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	60.60 – 3.11 60.60 – 3.11	Depositor EDS
% Data completeness (in resolution range)	77.1 (60.60-3.11) 77.4 (60.60-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.13Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.243 , 0.266 0.245 , 0.269	Depositor DCC
R_{free} test set	3769 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtrriage
Anisotropy	0.107	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	31988	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1146e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FRU, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.95	0/3266	1.22	2/4454 (0.0%)
1	B	0.96	0/3266	1.24	1/4454 (0.0%)
1	C	0.96	0/3274	1.21	1/4466 (0.0%)
1	D	0.96	0/3274	1.21	2/4466 (0.0%)
1	E	1.00	2/3266 (0.1%)	1.26	3/4454 (0.1%)
1	F	0.95	0/3274	1.22	0/4466
1	G	0.97	0/3266	1.23	4/4454 (0.1%)
1	H	0.98	1/3266 (0.0%)	1.22	0/4454
1	I	0.97	0/3274	1.23	2/4466 (0.0%)
1	J	0.96	0/3266	1.21	0/4454
All	All	0.97	3/32692 (0.0%)	1.23	15/44588 (0.0%)

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	B	0	1
1	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	34	PRO	C-N	13.33	1.50	1.33
1	H	30	PRO	C-O	-6.72	1.15	1.23
1	E	32	ILE	C-O	-5.36	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	PRO	CA-C-N	12.65	133.46	119.92
1	E	34	PRO	C-N-CA	12.65	133.46	119.92
1	E	34	PRO	CB-CA-C	-9.84	98.91	110.92
1	G	245	THR	CA-C-O	-8.67	111.97	121.94
1	G	363	VAL	N-CA-C	-7.42	101.83	110.21
1	I	94	ASP	CA-C-O	-6.58	111.09	120.51
1	G	363	VAL	CA-C-O	-6.22	115.23	122.13
1	A	372	ARG	N-CA-C	-5.93	102.14	110.50
1	D	372	ARG	N-CA-C	-5.78	102.34	110.50
1	G	413	LEU	CA-C-O	5.59	130.31	120.80
1	D	372	ARG	CA-C-O	-5.58	115.47	121.56
1	A	372	ARG	CA-C-O	-5.49	115.57	121.56
1	B	61	VAL	CA-C-O	-5.37	114.07	120.78
1	C	107	GLY	CA-C-O	-5.27	116.66	121.72
1	I	109	THR	CA-CB-OG1	5.02	117.13	109.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	ALA	Peptide
1	E	114	GLN	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	3173	0	2970	53	0
1	B	3173	0	2970	61	0
1	C	3180	0	2977	48	0
1	D	3180	0	2977	77	0
1	E	3173	0	2970	60	0
1	F	3180	0	2977	47	0
1	G	3173	0	2970	58	0
1	H	3173	0	2970	72	0
1	I	3180	0	2977	78	0
1	J	3173	0	2970	52	0
2	K	23	0	21	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	23	0	21	6	0
2	M	23	0	21	6	0
2	N	23	0	21	3	0
2	O	23	0	21	6	0
2	P	23	0	21	4	0
2	Q	23	0	21	4	0
2	R	23	0	21	2	0
2	S	23	0	21	3	0
2	T	23	0	21	4	0
All	All	31988	0	29938	587	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 9.

All (587) 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:D:413:LEU:CG	1:D:414:PRO:HD3	1.67	1.23
1:I:261:ILE:HD12	1:I:261:ILE:O	1.40	1.19
1:D:413:LEU:HG	1:D:414:PRO:HD3	1.16	1.13
1:E:105:PHE:CE1	1:E:171:HIS:NE2	2.14	1.12
1:E:105:PHE:HD1	1:E:171:HIS:CE1	1.68	1.11
1:I:12:ARG:HH21	1:I:261:ILE:HD11	0.97	1.08
1:E:105:PHE:CD1	1:E:171:HIS:NE2	2.22	1.06
1:B:65:ARG:NH2	1:B:408:GLU:OE2	1.89	1.05
1:I:12:ARG:NH2	1:I:261:ILE:HD11	1.72	1.04
1:E:105:PHE:CD1	1:E:171:HIS:CE1	2.46	1.03
1:H:11:PRO:O	1:H:258:LEU:HD12	1.56	1.02
1:J:65:ARG:NH1	1:J:94:ASP:O	1.95	0.99
1:G:65:ARG:NH2	1:G:94:ASP:O	1.97	0.98
1:F:65:ARG:NH2	1:F:94:ASP:O	1.97	0.97
1:C:65:ARG:NH2	1:C:94:ASP:O	1.97	0.97
1:D:65:ARG:NH2	1:D:94:ASP:O	1.97	0.97
1:A:65:ARG:NH2	1:A:94:ASP:O	1.97	0.96
1:H:65:ARG:NH2	1:H:94:ASP:O	1.97	0.96
1:E:65:ARG:NH2	1:E:94:ASP:O	1.98	0.96
1:I:12:ARG:HH21	1:I:261:ILE:CD1	1.78	0.95
1:D:413:LEU:HG	1:D:414:PRO:CD	1.97	0.95
1:H:24:THR:O	1:H:28:VAL:HG23	1.66	0.94
1:B:65:ARG:NH1	1:B:405:LEU:HG	1.85	0.92
1:B:110:ARG:NH1	1:B:173:VAL:HG23	1.86	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:GLU:O	1:B:374:LYS:HD2	1.71	0.90
1:B:110:ARG:HH12	1:B:173:VAL:HG23	1.35	0.87
1:C:413:LEU:HB3	1:C:414:PRO:HD2	1.55	0.86
1:G:150:VAL:HG12	1:G:174:LEU:HD11	1.59	0.84
1:H:150:VAL:HG12	1:H:174:LEU:HD11	1.60	0.83
1:F:150:VAL:HG12	1:F:174:LEU:HD11	1.59	0.83
1:I:150:VAL:HG12	1:I:174:LEU:HD11	1.60	0.82
1:B:65:ARG:HH22	1:B:408:GLU:CD	1.87	0.81
1:D:413:LEU:CG	1:D:414:PRO:CD	2.54	0.81
1:I:261:ILE:HD12	1:I:261:ILE:C	2.04	0.81
1:E:229:PRO:O	1:E:232:GLU:HG2	1.82	0.80
1:E:105:PHE:HD1	1:E:171:HIS:HE1	1.27	0.80
1:F:229:PRO:O	1:F:232:GLU:HG2	1.81	0.80
1:D:413:LEU:CB	1:D:414:PRO:CD	2.60	0.80
1:G:354:ASP:O	1:G:374:LYS:NZ	2.15	0.79
1:B:268:GLU:OE1	2:L:2:FRU:H12	1.81	0.79
1:H:229:PRO:O	1:H:232:GLU:HG2	1.82	0.79
1:G:189:ARG:NH2	1:G:221:GLU:HG2	1.96	0.79
1:A:229:PRO:O	1:A:232:GLU:HG2	1.82	0.79
1:C:229:PRO:O	1:C:232:GLU:HG2	1.82	0.79
1:G:229:PRO:O	1:G:232:GLU:HG2	1.83	0.78
1:E:32:ILE:HD13	1:E:381:PRO:HD2	1.65	0.78
1:H:64:TRP:CE2	1:H:93:ARG:HD3	2.20	0.77
1:E:354:ASP:O	1:E:374:LYS:NZ	2.17	0.77
1:H:29:VAL:HG23	1:H:323:THR:O	1.85	0.76
1:D:413:LEU:CD2	1:D:414:PRO:HD3	2.14	0.76
1:C:413:LEU:CB	1:C:414:PRO:HD2	2.16	0.76
1:E:105:PHE:HE1	1:E:171:HIS:NE2	1.79	0.76
1:D:161:ASP:OD2	1:J:111:GLY:N	2.18	0.74
1:D:413:LEU:CB	1:D:414:PRO:HD3	2.17	0.73
1:J:354:ASP:O	1:J:374:LYS:NZ	2.18	0.73
1:H:136:ARG:HD3	1:H:147:ARG:NH1	2.03	0.73
1:E:354:ASP:C	1:E:374:LYS:NZ	2.47	0.73
1:H:11:PRO:C	1:H:258:LEU:HD12	2.13	0.73
1:A:389:GLY:HA2	1:H:278:PHE:CE2	2.24	0.73
1:I:261:ILE:O	1:I:261:ILE:CD1	2.30	0.73
1:D:268:GLU:OE1	2:N:2:FRU:H12	1.90	0.72
1:C:216:ASN:ND2	1:C:265:GLN:OE1	2.24	0.70
1:D:413:LEU:HB3	1:D:414:PRO:CD	2.21	0.70
1:E:355:LEU:HD23	1:E:374:LYS:HZ1	1.56	0.70
1:B:216:ASN:ND2	1:B:265:GLN:OE1	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:ASN:ND2	1:F:265:GLN:OE1	2.25	0.69
1:J:216:ASN:ND2	1:J:265:GLN:OE1	2.25	0.69
1:A:217:THR:HG21	1:A:259:GLU:OE2	1.92	0.69
1:D:216:ASN:ND2	1:D:265:GLN:OE1	2.25	0.69
1:G:216:ASN:ND2	1:G:265:GLN:OE1	2.24	0.69
1:I:261:ILE:CD1	1:I:261:ILE:C	2.66	0.69
1:J:268:GLU:OE1	2:T:2:FRU:H12	1.94	0.68
1:J:15:ARG:NH2	1:J:292:PRO:O	2.27	0.68
1:H:15:ARG:NH2	1:H:292:PRO:O	2.27	0.67
1:A:15:ARG:NH2	1:A:292:PRO:O	2.27	0.67
1:E:344:LEU:HB3	1:E:385:VAL:HG23	1.77	0.67
1:D:217:THR:HG21	1:D:259:GLU:CD	2.20	0.67
1:B:64:TRP:CZ3	1:B:91:TYR:HD2	2.13	0.66
1:E:15:ARG:NH2	1:E:292:PRO:O	2.28	0.66
1:B:54:ARG:HG2	1:B:202:GLU:OE1	1.94	0.66
1:H:344:LEU:HB3	1:H:385:VAL:HG23	1.78	0.66
1:D:54:ARG:HD2	1:D:122:ASP:OD1	1.96	0.66
1:H:24:THR:O	1:H:28:VAL:CG2	2.43	0.66
1:A:344:LEU:HB3	1:A:385:VAL:HG23	1.78	0.66
1:D:15:ARG:NH2	1:D:292:PRO:O	2.27	0.65
1:G:344:LEU:HB3	1:G:385:VAL:HG23	1.77	0.65
1:B:116:ALA:HB3	2:L:2:FRU:O4	1.96	0.65
1:B:344:LEU:HB3	1:B:385:VAL:HG23	1.77	0.65
1:E:48:THR:HG21	1:E:379:LEU:HD21	1.79	0.65
1:C:344:LEU:HB3	1:C:385:VAL:HG23	1.78	0.65
1:D:258:LEU:C	1:D:258:LEU:HD23	2.22	0.65
1:D:275:ARG:NH2	1:D:342:GLU:C	2.55	0.65
1:J:344:LEU:HB3	1:J:385:VAL:HG23	1.77	0.65
1:F:344:LEU:HB3	1:F:385:VAL:HG23	1.78	0.65
1:I:54:ARG:HD2	1:I:122:ASP:OD1	1.96	0.65
1:B:65:ARG:HH12	1:B:405:LEU:H	1.45	0.64
1:I:344:LEU:HB3	1:I:385:VAL:HG23	1.78	0.64
1:D:344:LEU:HB3	1:D:385:VAL:HG23	1.78	0.64
1:F:48:THR:HG21	1:F:379:LEU:HD21	1.79	0.64
1:H:115:TRP:CG	2:R:2:FRU:H62	2.32	0.64
1:E:116:ALA:HB3	2:O:2:FRU:O4	1.97	0.64
1:H:11:PRO:C	1:H:258:LEU:CD1	2.71	0.64
1:D:156:VAL:HG23	1:D:156:VAL:O	1.98	0.64
1:I:48:THR:HG21	1:I:379:LEU:HD21	1.80	0.64
1:G:110:ARG:HH11	1:G:173:VAL:HG23	1.63	0.63
1:H:156:VAL:O	1:H:156:VAL:HG23	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:TRP:CE3	1:B:91:TYR:HD2	2.15	0.63
1:I:116:ALA:HB3	2:S:2:FRU:O4	1.98	0.63
1:C:48:THR:HG21	1:C:379:LEU:HD21	1.81	0.63
1:I:341:ARG:NH2	1:I:409:GLU:HA	2.14	0.63
1:D:217:THR:HG21	1:D:259:GLU:OE2	1.98	0.63
1:F:141:GLU:CD	1:H:93:ARG:HH21	2.07	0.63
1:H:48:THR:HG21	1:H:379:LEU:HD21	1.80	0.62
1:E:330:TYR:CZ	1:E:360:LEU:HD21	2.34	0.62
1:G:48:THR:HG21	1:G:379:LEU:HD21	1.81	0.62
1:A:389:GLY:HA2	1:H:278:PHE:HE2	1.61	0.62
1:C:76:LEU:HD23	1:C:77:LEU:O	1.99	0.62
1:D:48:THR:HG21	1:D:379:LEU:HD21	1.80	0.62
1:G:116:ALA:HB3	2:Q:2:FRU:O4	1.99	0.62
1:A:88:ARG:NH1	1:A:102:GLY:HA2	2.13	0.62
1:J:355:LEU:HD23	1:J:374:LYS:HE3	1.82	0.62
1:B:64:TRP:CZ3	1:B:91:TYR:CD2	2.87	0.62
1:I:76:LEU:HD23	1:I:77:LEU:O	1.99	0.62
1:D:88:ARG:NH1	1:D:102:GLY:HA2	2.14	0.62
1:H:64:TRP:CD2	1:H:93:ARG:HD3	2.34	0.62
1:D:413:LEU:HB3	1:D:414:PRO:HD2	1.80	0.62
1:E:32:ILE:CD1	1:E:381:PRO:HD2	2.30	0.62
1:A:109:THR:HA	1:A:171:HIS:ND1	2.15	0.61
1:H:240:ILE:HG21	1:H:257:LEU:HD21	1.82	0.61
1:F:76:LEU:HD23	1:F:77:LEU:O	2.00	0.61
1:J:387:LEU:CD2	1:J:392:THR:HG22	2.30	0.61
1:A:216:ASN:HD21	1:A:265:GLN:NE2	1.98	0.61
1:I:10:THR:HG21	1:I:259:GLU:HG3	1.82	0.61
1:E:216:ASN:HD21	1:E:265:GLN:NE2	1.98	0.61
1:B:48:THR:HG21	1:B:379:LEU:HD21	1.82	0.61
1:I:109:THR:HA	1:I:171:HIS:ND1	2.15	0.61
1:I:413:LEU:HB3	1:I:414:PRO:HD2	1.82	0.61
1:D:387:LEU:CD2	1:D:392:THR:HG22	2.31	0.61
1:C:115:TRP:CG	2:M:2:FRU:H62	2.36	0.61
1:F:387:LEU:CD2	1:F:392:THR:HG22	2.31	0.61
1:A:275:ARG:NH2	1:A:342:GLU:HA	2.15	0.61
1:H:387:LEU:CD2	1:H:392:THR:HG22	2.31	0.61
1:J:109:THR:HA	1:J:171:HIS:ND1	2.16	0.61
1:J:48:THR:HG21	1:J:379:LEU:HD21	1.81	0.61
1:C:109:THR:HA	1:C:171:HIS:ND1	2.15	0.60
1:B:109:THR:HA	1:B:171:HIS:ND1	2.16	0.60
1:B:387:LEU:CD2	1:B:392:THR:HG22	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:ASN:HD21	1:I:265:GLN:NE2	1.99	0.60
1:C:116:ALA:HB3	2:M:2:FRU:O4	2.01	0.60
1:H:109:THR:HA	1:H:171:HIS:ND1	2.15	0.60
1:C:91:TYR:CE1	1:C:99:PHE:HB2	2.37	0.60
1:D:286:HIS:NE2	2:N:1:GLC:O2	2.34	0.60
1:H:76:LEU:HD23	1:H:77:LEU:O	2.01	0.60
1:I:387:LEU:CD2	1:I:392:THR:HG22	2.32	0.60
1:D:109:THR:HA	1:D:171:HIS:ND1	2.15	0.60
1:C:387:LEU:CD2	1:C:392:THR:HG22	2.31	0.60
1:E:387:LEU:CD2	1:E:392:THR:HG22	2.31	0.60
1:G:363:VAL:O	1:G:364:ALA:HB3	2.01	0.60
1:B:219:ILE:HG21	1:B:232:GLU:HB3	1.84	0.59
1:B:368:PRO:HG3	1:J:221:GLU:HB3	1.84	0.59
1:D:275:ARG:NH2	1:D:342:GLU:O	2.35	0.59
1:A:387:LEU:CD2	1:A:392:THR:HG22	2.32	0.59
1:H:12:ARG:HG2	1:H:259:GLU:HG3	1.83	0.59
1:D:189:ARG:HG2	1:D:233:GLU:HG2	1.84	0.59
1:G:387:LEU:CD2	1:G:392:THR:HG22	2.32	0.59
1:H:135:GLY:O	1:H:136:ARG:HD2	2.01	0.59
1:I:313:ARG:CZ	1:J:205:ARG:NH1	2.65	0.59
1:J:233:GLU:O	1:J:265:GLN:NE2	2.36	0.58
1:I:116:ALA:CB	2:S:2:FRU:O4	2.52	0.58
1:I:313:ARG:NH2	1:J:205:ARG:NH1	2.51	0.58
1:J:91:TYR:CE1	1:J:99:PHE:HB2	2.39	0.58
1:A:358:LEU:HD22	1:A:362:ASP:HB3	1.84	0.58
1:D:233:GLU:O	1:D:265:GLN:NE2	2.37	0.58
1:E:355:LEU:HD23	1:E:374:LYS:NZ	2.18	0.58
1:C:10:THR:HG21	1:C:259:GLU:HG3	1.84	0.58
1:G:189:ARG:CZ	1:G:221:GLU:HG2	2.33	0.58
1:F:115:TRP:HB2	1:F:132:THR:HB	1.86	0.58
1:D:372:ARG:O	1:D:373:ALA:HB3	2.03	0.57
1:E:355:LEU:HD23	1:E:374:LYS:HE3	1.86	0.57
1:F:233:GLU:O	1:F:265:GLN:NE2	2.37	0.57
1:F:189:ARG:HG2	1:F:233:GLU:HG2	1.86	0.57
1:H:156:VAL:HG12	1:H:165:ILE:HD12	1.84	0.57
1:C:233:GLU:O	1:C:265:GLN:NE2	2.37	0.57
1:H:115:TRP:HB2	1:H:132:THR:HB	1.86	0.57
1:B:115:TRP:CG	2:L:2:FRU:H62	2.39	0.57
1:G:10:THR:HG21	1:G:259:GLU:HG3	1.86	0.57
1:I:115:TRP:HB2	1:I:132:THR:HB	1.86	0.57
1:B:196:ARG:NE	2:L:2:FRU:O3	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:TRP:HB2	1:G:132:THR:HB	1.87	0.57
1:B:233:GLU:O	1:B:265:GLN:NE2	2.37	0.57
1:F:116:ALA:HB3	2:P:2:FRU:O4	2.05	0.57
1:J:189:ARG:HG2	1:J:233:GLU:HG2	1.87	0.57
1:B:115:TRP:HB2	1:B:132:THR:HB	1.87	0.56
1:I:12:ARG:CZ	1:I:261:ILE:HD11	2.33	0.56
1:D:115:TRP:HB2	1:D:132:THR:HB	1.88	0.56
1:A:77:LEU:HB2	1:A:80:LYS:HE2	1.87	0.56
1:G:64:TRP:CE2	1:G:93:ARG:HD3	2.41	0.56
1:A:115:TRP:CG	2:K:2:FRU:H62	2.40	0.56
1:H:136:ARG:CD	1:H:147:ARG:NH1	2.68	0.56
1:E:355:LEU:HD23	1:E:374:LYS:CE	2.35	0.56
1:G:233:GLU:O	1:G:265:GLN:NE2	2.37	0.56
1:C:115:TRP:HB2	1:C:132:THR:HB	1.87	0.56
1:E:115:TRP:HB2	1:E:132:THR:HB	1.86	0.56
1:G:91:TYR:CE1	1:G:99:PHE:HB2	2.40	0.56
1:A:115:TRP:HB2	1:A:132:THR:HB	1.87	0.56
1:D:196:ARG:NE	2:N:2:FRU:O3	2.38	0.56
1:A:47:ASP:OD2	2:K:2:FRU:H11	2.05	0.55
1:G:96:GLU:OE2	1:G:402:ARG:NH1	2.40	0.55
1:J:115:TRP:HB2	1:J:132:THR:HB	1.88	0.55
1:C:413:LEU:N	1:C:413:LEU:HD12	2.22	0.55
1:E:32:ILE:HD13	1:E:381:PRO:CD	2.35	0.55
1:H:91:TYR:CE1	1:H:99:PHE:HB2	2.41	0.55
1:G:115:TRP:CG	2:Q:2:FRU:H62	2.42	0.55
1:D:156:VAL:HG12	1:D:165:ILE:HD12	1.87	0.55
1:I:226:CYS:HB2	1:I:232:GLU:HG2	1.88	0.55
1:A:372:ARG:O	1:A:373:ALA:HB3	2.05	0.55
1:G:77:LEU:HB2	1:G:80:LYS:HE2	1.88	0.54
1:F:219:ILE:HG21	1:F:232:GLU:HB2	1.90	0.54
1:H:219:ILE:HG21	1:H:232:GLU:HB2	1.89	0.54
1:E:413:LEU:N	1:E:413:LEU:HD22	2.22	0.54
1:C:413:LEU:HB3	1:C:414:PRO:CD	2.35	0.54
1:G:413:LEU:N	1:G:413:LEU:HD22	2.23	0.54
1:B:359:THR:OG1	1:B:361:ASP:OD1	2.14	0.54
1:A:160:ASP:O	1:C:136:ARG:NH1	2.40	0.53
1:C:413:LEU:CB	1:C:414:PRO:CD	2.85	0.53
1:A:219:ILE:HG21	1:A:232:GLU:HB2	1.90	0.53
1:B:413:LEU:N	1:B:413:LEU:HD22	2.24	0.53
1:C:71:THR:HG21	1:C:88:ARG:HD2	1.91	0.53
1:H:148:LEU:N	1:H:148:LEU:HD12	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:LEU:HD12	1:I:148:LEU:N	2.23	0.53
1:G:64:TRP:CZ3	1:G:93:ARG:HG2	2.44	0.53
1:B:65:ARG:HH12	1:B:405:LEU:N	2.06	0.53
1:E:205:ARG:NH2	1:E:306:ASP:O	2.43	0.52
1:G:110:ARG:NH1	1:G:173:VAL:HG23	2.24	0.52
1:J:226:CYS:HB2	1:J:232:GLU:HG2	1.90	0.52
1:C:54:ARG:HH12	1:C:209:THR:HG21	1.74	0.52
1:C:219:ILE:HG21	1:C:232:GLU:HB2	1.91	0.52
1:I:275:ARG:HD3	1:I:387:LEU:HD12	1.91	0.52
1:D:226:CYS:HB2	1:D:232:GLU:HG2	1.90	0.52
1:G:148:LEU:N	1:G:148:LEU:HD12	2.24	0.52
1:G:355:LEU:HD23	1:G:374:LYS:HE3	1.91	0.52
1:E:219:ILE:HG21	1:E:232:GLU:HB2	1.91	0.52
1:J:54:ARG:HH12	1:J:209:THR:HG21	1.75	0.52
1:D:161:ASP:O	1:J:136:ARG:HD3	2.10	0.52
1:A:54:ARG:HH12	1:A:209:THR:HG21	1.75	0.51
1:A:413:LEU:HD22	1:A:413:LEU:N	2.25	0.51
1:A:268:GLU:OE1	2:K:2:FRU:H12	2.10	0.51
1:A:275:ARG:HH21	1:A:342:GLU:HA	1.76	0.51
1:H:136:ARG:CD	1:H:147:ARG:HH12	2.23	0.51
1:E:110:ARG:NH1	1:E:173:VAL:HG23	2.26	0.51
1:G:384:ARG:O	1:G:395:THR:HG22	2.11	0.51
1:A:384:ARG:O	1:A:395:THR:HG22	2.11	0.51
1:D:413:LEU:HD23	1:D:414:PRO:HD3	1.89	0.51
1:J:196:ARG:NE	2:T:2:FRU:O3	2.42	0.51
1:C:196:ARG:NE	2:M:2:FRU:O3	2.44	0.51
1:E:354:ASP:C	1:E:374:LYS:HZ1	2.19	0.51
1:D:54:ARG:NH2	1:D:209:THR:HG21	2.27	0.51
1:E:54:ARG:HH12	1:E:209:THR:HG21	1.74	0.51
1:I:384:ARG:O	1:I:395:THR:HG22	2.11	0.51
1:I:384:ARG:CZ	1:I:413:LEU:HD21	2.40	0.51
1:J:219:ILE:HG21	1:J:232:GLU:HB3	1.93	0.51
1:I:219:ILE:HG21	1:I:232:GLU:HB3	1.93	0.50
1:C:268:GLU:OE1	2:M:2:FRU:H12	2.11	0.50
1:C:384:ARG:O	1:C:395:THR:HG22	2.11	0.50
1:B:148:LEU:N	1:B:148:LEU:HD12	2.25	0.50
1:A:217:THR:CB	1:A:259:GLU:OE2	2.59	0.50
1:H:384:ARG:O	1:H:395:THR:HG22	2.11	0.50
1:B:384:ARG:O	1:B:395:THR:HG22	2.11	0.50
1:H:36:ARG:O	1:H:36:ARG:NH1	2.42	0.50
1:H:136:ARG:HD3	1:H:147:ARG:HH12	1.72	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ILE:HG21	1:D:232:GLU:HB3	1.94	0.50
1:J:387:LEU:HD23	1:J:392:THR:HG22	1.94	0.50
1:G:36:ARG:O	1:G:36:ARG:NH1	2.45	0.50
1:H:64:TRP:CZ3	1:H:93:ARG:HG2	2.46	0.49
1:B:369:ASP:O	1:B:372:ARG:O	2.29	0.49
1:F:384:ARG:O	1:F:395:THR:HG22	2.11	0.49
1:B:226:CYS:HB2	1:B:232:GLU:HG2	1.94	0.49
1:E:71:THR:HG21	1:E:88:ARG:HD3	1.94	0.49
1:D:387:LEU:HD23	1:D:392:THR:HG22	1.94	0.49
1:F:149:ALA:HA	1:F:174:LEU:HD13	1.94	0.49
1:G:209:THR:OG1	1:G:243:SER:HB3	2.12	0.49
1:I:54:ARG:NH2	1:I:209:THR:HG21	2.27	0.49
1:H:71:THR:HG21	1:H:88:ARG:HD3	1.95	0.49
1:C:219:ILE:CD1	1:C:235:ASN:HB3	2.43	0.49
1:F:384:ARG:C	1:F:395:THR:HG22	2.38	0.49
1:I:384:ARG:C	1:I:395:THR:HG22	2.38	0.49
1:A:387:LEU:HD23	1:A:392:THR:HG22	1.95	0.49
1:D:64:TRP:CZ3	1:D:93:ARG:HG3	2.48	0.49
1:G:71:THR:HG21	1:G:88:ARG:HD3	1.95	0.49
1:G:364:ALA:HA	1:G:371:GLN:NE2	2.28	0.49
1:I:116:ALA:HB3	2:S:2:FRU:HO4	1.76	0.49
1:I:149:ALA:HA	1:I:174:LEU:HD13	1.93	0.49
1:C:209:THR:OG1	1:C:243:SER:HB3	2.13	0.48
1:C:330:TYR:CZ	1:C:360:LEU:HD21	2.48	0.48
1:D:275:ARG:HH22	1:D:342:GLU:C	2.18	0.48
1:E:209:THR:OG1	1:E:243:SER:HB3	2.12	0.48
1:F:387:LEU:HD23	1:F:392:THR:HG22	1.95	0.48
1:J:209:THR:OG1	1:J:243:SER:HB3	2.13	0.48
1:B:330:TYR:CZ	1:B:360:LEU:HD21	2.47	0.48
1:C:384:ARG:C	1:C:395:THR:HG22	2.37	0.48
1:G:149:ALA:HA	1:G:174:LEU:HD13	1.94	0.48
1:J:71:THR:HG21	1:J:88:ARG:HD3	1.95	0.48
1:B:387:LEU:HD23	1:B:392:THR:HG22	1.95	0.48
1:H:154:GLY:HA3	1:H:169:PHE:CZ	2.48	0.48
1:A:384:ARG:C	1:A:395:THR:HG22	2.38	0.48
1:H:11:PRO:HB2	1:H:258:LEU:HD13	1.94	0.48
1:F:71:THR:HG21	1:F:88:ARG:HD3	1.95	0.48
1:H:384:ARG:C	1:H:395:THR:HG22	2.38	0.48
1:B:384:ARG:C	1:B:395:THR:HG22	2.39	0.48
1:H:156:VAL:HG12	1:H:165:ILE:CD1	2.44	0.48
1:I:209:THR:OG1	1:I:243:SER:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:ARG:NH2	1:G:221:GLU:CG	2.73	0.48
1:A:217:THR:CG2	1:A:259:GLU:OE2	2.61	0.48
1:B:71:THR:HG21	1:B:88:ARG:HD3	1.95	0.48
1:D:209:THR:OG1	1:D:243:SER:HB3	2.13	0.48
1:F:189:ARG:HH12	1:F:232:GLU:CG	2.27	0.48
1:I:71:THR:HG21	1:I:88:ARG:HD3	1.95	0.48
1:F:123:ASP:O	1:I:124:ASP:HA	2.14	0.48
1:G:54:ARG:HH12	1:G:209:THR:HG21	1.78	0.48
1:G:219:ILE:HG21	1:G:232:GLU:HB2	1.95	0.48
1:G:384:ARG:C	1:G:395:THR:HG22	2.38	0.48
1:H:387:LEU:HD23	1:H:392:THR:HG22	1.95	0.47
1:A:209:THR:OG1	1:A:243:SER:HB3	2.13	0.47
1:E:33:TYR:CD2	1:H:354:ASP:HB2	2.48	0.47
1:E:216:ASN:ND2	1:E:265:GLN:NE2	2.61	0.47
1:I:226:CYS:HB2	1:I:232:GLU:CG	2.45	0.47
1:D:275:ARG:NH2	1:D:342:GLU:HA	2.29	0.47
1:G:359:THR:OG1	1:G:361:ASP:OD1	2.22	0.47
1:I:311:GLU:OE1	1:I:313:ARG:NE	2.48	0.47
1:A:216:ASN:ND2	1:A:265:GLN:NE2	2.61	0.47
1:B:65:ARG:NH2	1:B:94:ASP:O	2.48	0.47
1:I:341:ARG:HH22	1:I:409:GLU:HA	1.78	0.47
1:D:71:THR:HG21	1:D:88:ARG:HD2	1.97	0.47
1:H:149:ALA:HA	1:H:174:LEU:HD13	1.95	0.47
1:A:369:ASP:O	1:A:372:ARG:O	2.33	0.47
1:G:387:LEU:HD23	1:G:392:THR:HG22	1.96	0.47
1:A:330:TYR:CZ	1:A:360:LEU:HD21	2.49	0.47
1:I:216:ASN:ND2	1:I:265:GLN:NE2	2.62	0.47
1:E:355:LEU:CD2	1:E:374:LYS:HE3	2.45	0.47
1:E:387:LEU:HD23	1:E:392:THR:HG22	1.95	0.46
1:I:148:LEU:HD13	1:I:195:PHE:CD2	2.50	0.46
1:F:175:LEU:HD11	1:F:251:TRP:HB2	1.98	0.46
1:C:402:ARG:HH12	1:C:410:LEU:CD2	2.29	0.46
1:E:213:PHE:CE1	1:E:239:GLY:HA3	2.50	0.46
1:G:148:LEU:HD13	1:G:195:PHE:CD2	2.51	0.46
1:G:174:LEU:HD12	1:G:174:LEU:N	2.31	0.46
1:B:116:ALA:CB	2:L:2:FRU:O4	2.64	0.46
1:J:213:PHE:CE1	1:J:239:GLY:HA3	2.51	0.46
1:C:47:ASP:OD2	2:M:2:FRU:H11	2.16	0.46
1:H:174:LEU:N	1:H:174:LEU:HD12	2.30	0.46
1:J:268:GLU:OE2	2:T:1:GLC:H3	2.16	0.46
1:B:148:LEU:HD13	1:B:195:PHE:CD2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:LEU:N	1:I:174:LEU:HD12	2.31	0.46
1:I:65:ARG:NH2	1:I:408:GLU:OE2	2.49	0.46
1:J:275:ARG:NH1	1:J:339:SER:OG	2.49	0.46
1:A:295:GLU:O	1:A:295:GLU:HG3	2.16	0.45
1:C:387:LEU:HD22	1:C:392:THR:HG22	1.97	0.45
1:E:31:ILE:HD12	1:H:328:ALA:HB2	1.97	0.45
1:F:174:LEU:N	1:F:174:LEU:HD12	2.31	0.45
1:I:295:GLU:HG3	1:I:295:GLU:O	2.16	0.45
1:C:47:ASP:OD2	2:M:2:FRU:C1	2.65	0.45
1:I:109:THR:HA	1:I:171:HIS:CE1	2.51	0.45
1:E:268:GLU:OE1	2:O:2:FRU:H12	2.16	0.45
1:H:109:THR:HA	1:H:171:HIS:CE1	2.51	0.45
1:E:330:TYR:CE1	1:E:360:LEU:HD21	2.52	0.45
1:H:148:LEU:HD13	1:H:195:PHE:CD2	2.50	0.45
1:I:148:LEU:N	1:I:148:LEU:CD1	2.80	0.45
1:I:387:LEU:HD23	1:I:392:THR:HG22	1.98	0.45
1:G:213:PHE:CE1	1:G:239:GLY:HA3	2.50	0.45
1:A:71:THR:HG21	1:A:88:ARG:HD2	1.98	0.45
1:B:226:CYS:HB2	1:B:232:GLU:CG	2.46	0.45
1:D:213:PHE:CE1	1:D:239:GLY:HA3	2.51	0.45
1:D:226:CYS:HB2	1:D:232:GLU:CG	2.46	0.45
1:D:369:ASP:O	1:D:372:ARG:O	2.35	0.45
1:I:11:PRO:O	1:I:258:LEU:HD12	2.17	0.45
1:I:387:LEU:HD22	1:I:392:THR:HG22	1.97	0.45
1:J:226:CYS:HB2	1:J:232:GLU:CG	2.47	0.45
1:G:116:ALA:CB	2:Q:2:FRU:O4	2.64	0.45
1:H:148:LEU:N	1:H:148:LEU:CD1	2.80	0.45
1:I:341:ARG:HH22	1:I:409:GLU:CB	2.29	0.45
1:J:226:CYS:HB3	1:J:232:GLU:HG3	1.99	0.45
1:C:50:PHE:CE1	1:C:403:ILE:HG12	2.52	0.45
1:D:156:VAL:HG12	1:D:165:ILE:CD1	2.47	0.45
1:H:154:GLY:CA	1:H:169:PHE:CZ	3.00	0.45
1:I:54:ARG:HH21	1:I:209:THR:HG21	1.81	0.45
1:G:47:ASP:OD2	2:Q:2:FRU:H11	2.18	0.45
1:D:109:THR:HA	1:D:171:HIS:CE1	2.52	0.44
1:I:341:ARG:HH22	1:I:409:GLU:CA	2.30	0.44
1:J:366:LEU:HD22	1:J:370:GLU:OE1	2.18	0.44
1:F:36:ARG:O	1:F:36:ARG:NH1	2.44	0.44
1:G:387:LEU:HD22	1:G:392:THR:HG22	1.99	0.44
1:D:54:ARG:HH21	1:D:209:THR:HG21	1.82	0.44
1:D:275:ARG:HH22	1:D:342:GLU:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:PHE:CE1	1:E:403:ILE:HG12	2.53	0.44
1:G:64:TRP:CZ2	1:G:93:ARG:HD3	2.53	0.44
1:H:136:ARG:NE	1:H:147:ARG:NH2	2.65	0.44
1:I:413:LEU:N	1:I:413:LEU:HD22	2.32	0.44
1:C:387:LEU:HD23	1:C:392:THR:HG22	1.97	0.44
1:E:47:ASP:OD2	2:O:2:FRU:H11	2.17	0.44
1:G:148:LEU:N	1:G:148:LEU:CD1	2.80	0.44
1:H:50:PHE:CE1	1:H:403:ILE:HG12	2.53	0.44
1:A:330:TYR:CE1	1:A:360:LEU:HD21	2.52	0.44
1:B:109:THR:HA	1:B:171:HIS:CE1	2.52	0.44
1:D:275:ARG:HH22	1:D:342:GLU:CA	2.31	0.44
1:H:65:ARG:NH2	1:H:408:GLU:OE2	2.49	0.44
1:I:191:MET:HE1	1:I:234:PHE:CE2	2.52	0.44
1:J:50:PHE:CE1	1:J:403:ILE:HG12	2.53	0.44
1:J:268:GLU:OE1	2:T:2:FRU:O2	2.36	0.44
1:I:50:PHE:CE1	1:I:403:ILE:HG12	2.53	0.44
1:B:64:TRP:CE3	1:B:91:TYR:CD2	3.00	0.44
1:F:47:ASP:OD2	2:P:2:FRU:H11	2.17	0.44
1:F:355:LEU:O	1:F:358:LEU:HD13	2.18	0.44
1:C:109:THR:HA	1:C:171:HIS:CE1	2.52	0.44
1:E:175:LEU:HD11	1:E:251:TRP:HB2	2.00	0.44
1:G:50:PHE:CE1	1:G:403:ILE:HG12	2.53	0.44
1:H:355:LEU:O	1:H:358:LEU:HD13	2.18	0.44
1:F:178:ASP:OD1	1:F:179:GLY:N	2.51	0.43
1:F:200:PHE:CZ	1:F:209:THR:HG23	2.53	0.43
1:J:109:THR:HA	1:J:171:HIS:CE1	2.53	0.43
1:A:50:PHE:CE1	1:A:403:ILE:HG12	2.53	0.43
1:B:50:PHE:CE1	1:B:403:ILE:HG12	2.53	0.43
1:C:363:VAL:HA	1:C:366:LEU:HD13	2.00	0.43
1:D:156:VAL:O	1:D:156:VAL:CG2	2.64	0.43
1:H:148:LEU:HD13	1:H:195:PHE:CE2	2.54	0.43
1:B:65:ARG:HH12	1:B:405:LEU:HG	1.77	0.43
1:E:355:LEU:O	1:E:358:LEU:HD13	2.18	0.43
1:B:148:LEU:N	1:B:148:LEU:CD1	2.81	0.43
1:E:355:LEU:N	1:E:374:LYS:HZ1	2.17	0.43
1:F:366:LEU:HB3	1:F:370:GLU:HB3	2.01	0.43
1:A:109:THR:HA	1:A:171:HIS:CE1	2.53	0.43
1:C:178:ASP:OD1	1:C:179:GLY:N	2.51	0.43
1:E:116:ALA:CB	2:O:2:FRU:O4	2.64	0.43
1:F:124:ASP:HB2	1:I:123:ASP:HB3	2.00	0.43
1:F:341:ARG:HH22	1:F:409:GLU:HG2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:LEU:HD11	1:I:251:TRP:HB2	2.00	0.43
1:I:278:PHE:HE2	1:J:389:GLY:HA2	1.84	0.43
1:A:150:VAL:HB	1:A:174:LEU:HD11	2.01	0.43
1:B:110:ARG:NH2	1:B:172:GLY:HA2	2.34	0.43
1:F:387:LEU:HD22	1:F:392:THR:HG22	2.01	0.43
1:I:148:LEU:HD13	1:I:195:PHE:CE2	2.53	0.43
1:A:275:ARG:NH2	1:A:342:GLU:CA	2.81	0.43
1:D:161:ASP:CG	1:J:111:GLY:H	2.21	0.43
1:F:189:ARG:HH12	1:F:232:GLU:HG3	1.83	0.43
1:H:178:ASP:OD1	1:H:179:GLY:N	2.52	0.43
1:I:355:LEU:O	1:I:358:LEU:HD13	2.19	0.43
1:D:175:LEU:HD22	1:D:253:LEU:HD11	2.01	0.43
1:D:366:LEU:HB3	1:D:370:GLU:HB3	2.00	0.43
1:D:387:LEU:HD22	1:D:392:THR:HG22	2.01	0.43
1:A:49:TRP:CD1	1:A:118:SER:HA	2.54	0.43
1:B:178:ASP:OD1	1:B:179:GLY:N	2.51	0.43
1:B:226:CYS:HB3	1:B:232:GLU:HG3	2.00	0.43
1:C:49:TRP:CD1	1:C:118:SER:HA	2.54	0.43
1:D:49:TRP:CD1	1:D:118:SER:HA	2.54	0.43
1:D:178:ASP:OD1	1:D:179:GLY:N	2.52	0.43
1:E:387:LEU:HD22	1:E:392:THR:HG22	2.01	0.43
1:H:64:TRP:CZ2	1:H:93:ARG:HD3	2.54	0.43
1:A:387:LEU:HD22	1:A:392:THR:HG22	2.01	0.43
1:B:266:GLU:OE1	2:L:1:GLC:O3	2.36	0.43
1:J:49:TRP:CD1	1:J:118:SER:HA	2.54	0.43
1:J:355:LEU:O	1:J:358:LEU:HD13	2.19	0.43
1:A:65:ARG:NH2	1:A:408:GLU:OE2	2.49	0.42
1:B:148:LEU:HD13	1:B:195:PHE:CE2	2.54	0.42
1:B:303:PHE:CD1	1:B:303:PHE:N	2.87	0.42
1:D:50:PHE:CE1	1:D:403:ILE:HG12	2.53	0.42
1:D:150:VAL:HB	1:D:174:LEU:HD11	2.01	0.42
1:J:178:ASP:OD1	1:J:179:GLY:N	2.52	0.42
1:C:150:VAL:HB	1:C:174:LEU:HD11	2.01	0.42
1:E:286:HIS:NE2	2:O:1:GLC:O2	2.42	0.42
1:F:303:PHE:CD1	1:F:303:PHE:N	2.87	0.42
1:I:178:ASP:OD1	1:I:179:GLY:N	2.52	0.42
1:A:175:LEU:HD11	1:A:251:TRP:HB2	2.01	0.42
1:D:355:LEU:O	1:D:358:LEU:HD13	2.19	0.42
1:E:344:LEU:HB3	1:E:385:VAL:CG2	2.48	0.42
1:F:50:PHE:CE1	1:F:403:ILE:HG12	2.53	0.42
1:I:313:ARG:CZ	1:J:205:ARG:CZ	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LEU:HD22	1:B:392:THR:HG22	2.00	0.42
1:F:49:TRP:CD1	1:F:118:SER:HA	2.55	0.42
1:F:65:ARG:NH2	1:F:408:GLU:OE2	2.48	0.42
1:G:49:TRP:CD1	1:G:118:SER:HA	2.54	0.42
1:H:303:PHE:CD1	1:H:303:PHE:N	2.87	0.42
1:I:49:TRP:CD1	1:I:118:SER:HA	2.54	0.42
1:J:303:PHE:CD1	1:J:303:PHE:N	2.88	0.42
1:A:178:ASP:OD1	1:A:179:GLY:N	2.51	0.42
1:A:303:PHE:CD1	1:A:303:PHE:N	2.88	0.42
1:B:200:PHE:CE1	1:B:209:THR:HG23	2.54	0.42
1:E:178:ASP:OD1	1:E:179:GLY:N	2.52	0.42
1:G:148:LEU:HD13	1:G:195:PHE:CE2	2.55	0.42
1:J:150:VAL:HB	1:J:174:LEU:HD11	2.01	0.42
1:D:226:CYS:HB3	1:D:232:GLU:HG3	2.01	0.42
1:E:49:TRP:CD1	1:E:118:SER:HA	2.55	0.42
1:E:150:VAL:HB	1:E:174:LEU:HD11	2.01	0.42
1:F:116:ALA:CB	2:P:2:FRU:O4	2.67	0.42
1:B:226:CYS:CB	1:B:232:GLU:HG3	2.49	0.42
1:D:359:THR:OG1	1:D:361:ASP:OD1	2.20	0.42
1:E:303:PHE:CD1	1:E:303:PHE:N	2.87	0.42
1:G:355:LEU:O	1:G:358:LEU:HD13	2.19	0.42
1:H:156:VAL:O	1:H:156:VAL:CG2	2.67	0.42
1:I:341:ARG:NH2	1:I:409:GLU:CA	2.81	0.42
1:B:49:TRP:CD1	1:B:118:SER:HA	2.55	0.42
1:F:115:TRP:CG	2:P:2:FRU:H62	2.55	0.42
1:H:395:THR:OG1	1:H:413:LEU:HD22	2.20	0.42
1:I:178:ASP:O	1:I:184:ARG:CZ	2.68	0.42
1:I:313:ARG:NH2	1:J:205:ARG:HH11	2.16	0.42
1:I:366:LEU:HB3	1:I:370:GLU:HB3	2.00	0.42
1:D:88:ARG:HH12	1:D:102:GLY:HA2	1.82	0.42
1:I:226:CYS:HB3	1:I:232:GLU:HG3	2.02	0.42
1:D:303:PHE:CD1	1:D:303:PHE:N	2.87	0.42
1:H:49:TRP:CD1	1:H:118:SER:HA	2.55	0.42
1:C:65:ARG:NH2	1:C:408:GLU:OE2	2.49	0.41
1:E:366:LEU:HB3	1:E:370:GLU:HB3	2.02	0.41
1:F:301:TYR:CD1	1:F:320:LEU:HA	2.55	0.41
1:G:303:PHE:CD1	1:G:303:PHE:N	2.87	0.41
1:H:301:TYR:CD1	1:H:320:LEU:HA	2.55	0.41
1:F:189:ARG:NH1	1:F:232:GLU:HG3	2.35	0.41
1:I:150:VAL:CG1	1:I:174:LEU:HD11	2.41	0.41
1:I:269:ARG:HG2	1:I:269:ARG:HH11	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD22	1:A:362:ASP:CB	2.49	0.41
1:B:355:LEU:O	1:B:358:LEU:HD13	2.19	0.41
1:A:301:TYR:CD1	1:A:320:LEU:HA	2.56	0.41
1:C:303:PHE:CD1	1:C:303:PHE:N	2.88	0.41
1:D:161:ASP:HA	1:J:136:ARG:HH11	1.86	0.41
1:D:301:TYR:CD1	1:D:320:LEU:HA	2.55	0.41
1:I:303:PHE:CD1	1:I:303:PHE:N	2.87	0.41
1:J:336:VAL:HG23	1:J:336:VAL:O	2.21	0.41
1:C:49:TRP:CE2	1:C:68:PHE:HB2	2.56	0.41
1:J:235:ASN:OD1	1:J:235:ASN:N	2.54	0.41
1:G:174:LEU:N	1:G:174:LEU:CD1	2.84	0.41
1:H:200:PHE:CE1	1:H:209:THR:HG23	2.56	0.41
1:I:26:GLU:O	1:I:394:ILE:HG12	2.21	0.41
1:A:363:VAL:HA	1:A:366:LEU:HD13	2.02	0.41
1:B:336:VAL:O	1:B:336:VAL:HG23	2.21	0.41
1:D:236:GLY:HA3	1:D:267:LEU:HD13	2.03	0.41
1:D:363:VAL:HA	1:D:366:LEU:HD13	2.03	0.41
1:E:115:TRP:CG	2:O:2:FRU:H62	2.56	0.41
1:F:174:LEU:N	1:F:174:LEU:CD1	2.84	0.41
1:H:26:GLU:O	1:H:394:ILE:HG12	2.21	0.41
1:H:320:LEU:HD11	1:H:323:THR:HB	2.03	0.41
1:B:150:VAL:HB	1:B:174:LEU:HD11	2.02	0.41
1:B:328:ALA:HB2	1:D:31:ILE:HD12	2.02	0.41
1:H:174:LEU:N	1:H:174:LEU:CD1	2.84	0.41
1:J:175:LEU:HD11	1:J:251:TRP:HB2	2.02	0.41
1:B:175:LEU:HD11	1:B:251:TRP:HB2	2.03	0.41
1:C:26:GLU:O	1:C:394:ILE:HG12	2.21	0.41
1:D:49:TRP:CE2	1:D:68:PHE:HB2	2.56	0.41
1:D:226:CYS:CB	1:D:232:GLU:HG3	2.51	0.41
1:E:49:TRP:CE2	1:E:68:PHE:HB2	2.56	0.41
1:F:49:TRP:CE2	1:F:68:PHE:HB2	2.56	0.41
1:F:344:LEU:HB3	1:F:385:VAL:CG2	2.49	0.41
1:G:49:TRP:CE2	1:G:68:PHE:HB2	2.56	0.41
1:G:320:LEU:HD11	1:G:323:THR:HB	2.03	0.41
1:G:364:ALA:HA	1:G:371:GLN:CD	2.46	0.41
1:H:196:ARG:NE	2:R:2:FRU:O3	2.54	0.41
1:J:65:ARG:NH2	1:J:405:LEU:HG	2.36	0.41
1:J:387:LEU:HD22	1:J:392:THR:HG22	2.01	0.41
1:C:355:LEU:O	1:C:358:LEU:HD13	2.20	0.41
1:E:336:VAL:O	1:E:336:VAL:HG23	2.21	0.41
1:F:150:VAL:CG1	1:F:174:LEU:HD11	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:VAL:HA	1:F:366:LEU:HD13	2.03	0.41
1:G:65:ARG:NH2	1:G:408:GLU:OE2	2.49	0.41
1:G:269:ARG:HG2	1:G:269:ARG:HH11	1.86	0.41
1:I:49:TRP:CE2	1:I:68:PHE:HB2	2.56	0.41
1:C:235:ASN:OD1	1:C:235:ASN:N	2.54	0.40
1:E:26:GLU:O	1:E:394:ILE:HG12	2.21	0.40
1:F:177:PRO:HB3	1:F:195:PHE:CD2	2.57	0.40
1:H:136:ARG:CD	1:H:147:ARG:CZ	2.99	0.40
1:I:178:ASP:O	1:I:184:ARG:NH2	2.54	0.40
1:A:49:TRP:CE2	1:A:68:PHE:HB2	2.56	0.40
1:B:200:PHE:CE1	1:B:209:THR:CG2	3.04	0.40
1:D:177:PRO:HB3	1:D:195:PHE:CD2	2.57	0.40
1:D:372:ARG:O	1:D:373:ALA:CB	2.70	0.40
1:I:174:LEU:N	1:I:174:LEU:CD1	2.84	0.40
1:A:320:LEU:HD11	1:A:323:THR:HB	2.03	0.40
1:B:269:ARG:HG2	1:B:269:ARG:HH11	1.86	0.40
1:D:26:GLU:O	1:D:394:ILE:HG12	2.21	0.40
1:H:336:VAL:O	1:H:336:VAL:HG23	2.20	0.40
1:J:226:CYS:CB	1:J:232:GLU:HG3	2.51	0.40
1:A:275:ARG:NH2	1:A:342:GLU:C	2.79	0.40
1:E:363:VAL:HA	1:E:366:LEU:HD13	2.04	0.40
1:G:344:LEU:HB3	1:G:385:VAL:CG2	2.49	0.40
1:I:384:ARG:NH2	1:I:413:LEU:HD21	2.37	0.40
1:J:320:LEU:HD11	1:J:323:THR:HB	2.04	0.40
1:A:88:ARG:HH12	1:A:102:GLY:HA2	1.83	0.40
1:C:175:LEU:HD22	1:C:253:LEU:HD11	2.03	0.40
1:D:65:ARG:NH2	1:D:408:GLU:OE2	2.49	0.40
1:H:49:TRP:CE2	1:H:68:PHE:HB2	2.56	0.40
1:H:200:PHE:CE1	1:H:209:THR:CG2	3.05	0.40
1:I:320:LEU:HD11	1:I:323:THR:HB	2.03	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	403/428 (94%)	382 (95%)	20 (5%)	1 (0%)	43	71
1	B	403/428 (94%)	380 (94%)	21 (5%)	2 (0%)	24	55
1	C	404/428 (94%)	381 (94%)	21 (5%)	2 (0%)	24	55
1	D	404/428 (94%)	382 (95%)	20 (5%)	2 (0%)	24	55
1	E	403/428 (94%)	381 (94%)	20 (5%)	2 (0%)	24	55
1	F	404/428 (94%)	383 (95%)	19 (5%)	2 (0%)	24	55
1	G	403/428 (94%)	381 (94%)	20 (5%)	2 (0%)	24	55
1	H	403/428 (94%)	382 (95%)	19 (5%)	2 (0%)	24	55
1	I	404/428 (94%)	384 (95%)	20 (5%)	0	100	100
1	J	403/428 (94%)	384 (95%)	18 (4%)	1 (0%)	43	71
All	All	4034/4280 (94%)	3820 (95%)	198 (5%)	16 (0%)	30	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	413	LEU
1	A	276	ASN
1	B	276	ASN
1	C	276	ASN
1	D	276	ASN
1	E	276	ASN
1	H	276	ASN
1	B	341	ARG
1	C	341	ARG
1	E	341	ARG
1	F	276	ASN
1	F	341	ARG
1	G	276	ASN
1	J	341	ARG
1	G	178	ASP
1	H	341	ARG

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	328/348 (94%)	328 (100%)	0	100	100
1	B	328/348 (94%)	327 (100%)	1 (0%)	86	86
1	C	329/348 (94%)	327 (99%)	2 (1%)	78	81
1	D	329/348 (94%)	326 (99%)	3 (1%)	70	78
1	E	328/348 (94%)	327 (100%)	1 (0%)	86	86
1	F	329/348 (94%)	329 (100%)	0	100	100
1	G	328/348 (94%)	328 (100%)	0	100	100
1	H	328/348 (94%)	327 (100%)	1 (0%)	86	86
1	I	329/348 (94%)	328 (100%)	1 (0%)	86	86
1	J	328/348 (94%)	328 (100%)	0	100	100
All	All	3284/3480 (94%)	3275 (100%)	9 (0%)	86	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	372	ARG
1	C	412	ASP
1	C	413	LEU
1	D	25	ASP
1	D	258	LEU
1	D	412	ASP
1	E	106	GLU
1	H	28	VAL
1	I	261	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	265	GLN
1	A	288	HIS
1	B	114	GLN
1	B	288	HIS
1	B	351	ASN
1	C	114	GLN
1	C	288	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	GLN
1	D	288	HIS
1	E	265	GLN
1	E	288	HIS
1	F	114	GLN
1	F	171	HIS
1	F	276	ASN
1	F	288	HIS
1	G	114	GLN
1	G	171	HIS
1	G	351	ASN
1	H	288	HIS
1	I	114	GLN
1	I	265	GLN
1	J	114	GLN
1	J	276	ASN
1	J	288	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 ⓘ

20 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	GLC	K	1	2	11,11,12	0.32	0	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRU	K	2	2	11,12,12	0.88	1 (9%)	10,18,18	0.76	0
2	GLC	L	1	2	11,11,12	0.35	0	15,15,17	0.86	0
2	FRU	L	2	2	11,12,12	0.80	1 (9%)	10,18,18	0.77	0
2	GLC	M	1	2	11,11,12	0.47	0	15,15,17	0.97	1 (6%)
2	FRU	M	2	2	11,12,12	0.82	1 (9%)	10,18,18	0.95	0
2	GLC	N	1	2	11,11,12	0.43	0	15,15,17	0.88	1 (6%)
2	FRU	N	2	2	11,12,12	0.99	1 (9%)	10,18,18	0.93	0
2	GLC	O	1	2	11,11,12	0.43	0	15,15,17	1.12	3 (20%)
2	FRU	O	2	2	11,12,12	1.05	1 (9%)	10,18,18	0.93	0
2	GLC	P	1	2	11,11,12	0.40	0	15,15,17	0.74	0
2	FRU	P	2	2	11,12,12	0.78	1 (9%)	10,18,18	0.99	0
2	GLC	Q	1	2	11,11,12	0.24	0	15,15,17	0.74	0
2	FRU	Q	2	2	11,12,12	0.66	0	10,18,18	0.87	0
2	GLC	R	1	2	11,11,12	0.42	0	15,15,17	0.60	0
2	FRU	R	2	2	11,12,12	0.79	1 (9%)	10,18,18	1.08	1 (10%)
2	GLC	S	1	2	11,11,12	0.25	0	15,15,17	0.76	0
2	FRU	S	2	2	11,12,12	0.52	0	10,18,18	1.01	0
2	GLC	T	1	2	11,11,12	0.34	0	15,15,17	0.82	0
2	FRU	T	2	2	11,12,12	0.68	0	10,18,18	0.90	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	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	FRU	K	2	2	-	1/5/24/24	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	FRU	L	2	2	-	3/5/24/24	0/1/1/1
2	GLC	M	1	2	-	0/2/19/22	0/1/1/1
2	FRU	M	2	2	-	3/5/24/24	0/1/1/1
2	GLC	N	1	2	-	0/2/19/22	0/1/1/1
2	FRU	N	2	2	-	3/5/24/24	0/1/1/1
2	GLC	O	1	2	-	2/2/19/22	0/1/1/1
2	FRU	O	2	2	-	3/5/24/24	0/1/1/1
2	GLC	P	1	2	-	0/2/19/22	0/1/1/1
2	FRU	P	2	2	-	3/5/24/24	0/1/1/1
2	GLC	Q	1	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	Q	2	2	-	3/5/24/24	0/1/1/1
2	GLC	R	1	2	-	0/2/19/22	0/1/1/1
2	FRU	R	2	2	-	3/5/24/24	0/1/1/1
2	GLC	S	1	2	-	0/2/19/22	0/1/1/1
2	FRU	S	2	2	-	3/5/24/24	0/1/1/1
2	GLC	T	1	2	-	2/2/19/22	0/1/1/1
2	FRU	T	2	2	-	3/5/24/24	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	FRU	O2-C2	3.22	1.46	1.40
2	N	2	FRU	O2-C2	2.93	1.45	1.40
2	K	2	FRU	O2-C2	2.61	1.45	1.40
2	L	2	FRU	O2-C2	2.35	1.44	1.40
2	M	2	FRU	O2-C2	2.27	1.44	1.40
2	R	2	FRU	O2-C2	2.19	1.44	1.40
2	P	2	FRU	O2-C2	2.14	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	GLC	C1-C2-C3	2.26	112.93	109.64
2	R	2	FRU	O4-C4-C3	-2.25	105.40	112.16
2	O	1	GLC	O3-C3-C2	-2.17	105.62	110.05
2	N	1	GLC	C1-C2-C3	2.17	112.81	109.64
2	O	1	GLC	C1-C2-C3	2.05	112.62	109.64
2	O	1	GLC	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2	FRU	O1-C1-C2-O2
2	M	2	FRU	O1-C1-C2-C3
2	M	2	FRU	O1-C1-C2-O2
2	N	2	FRU	O1-C1-C2-C3
2	N	2	FRU	O1-C1-C2-O2
2	O	2	FRU	O1-C1-C2-C3
2	O	2	FRU	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	P	2	FRU	O1-C1-C2-C3
2	P	2	FRU	O1-C1-C2-O2
2	Q	2	FRU	O1-C1-C2-C3
2	Q	2	FRU	O1-C1-C2-O2
2	R	2	FRU	O1-C1-C2-O2
2	S	2	FRU	O1-C1-C2-C3
2	S	2	FRU	O1-C1-C2-O2
2	S	2	FRU	O1-C1-C2-O5
2	T	2	FRU	O1-C1-C2-O2
2	T	1	GLC	O5-C5-C6-O6
2	M	2	FRU	O1-C1-C2-O5
2	Q	2	FRU	O1-C1-C2-O5
2	L	2	FRU	O1-C1-C2-C3
2	N	2	FRU	O1-C1-C2-O5
2	P	2	FRU	O1-C1-C2-O5
2	T	1	GLC	C4-C5-C6-O6
2	L	2	FRU	O1-C1-C2-O5
2	O	1	GLC	C4-C5-C6-O6
2	K	2	FRU	O1-C1-C2-C3
2	R	2	FRU	O1-C1-C2-C3
2	T	2	FRU	O1-C1-C2-C3
2	O	2	FRU	O1-C1-C2-O5
2	O	1	GLC	O5-C5-C6-O6
2	R	2	FRU	O1-C1-C2-O5
2	T	2	FRU	O1-C1-C2-O5

There are no ring outliers.

14 monomers are involved in 41 short contacts:

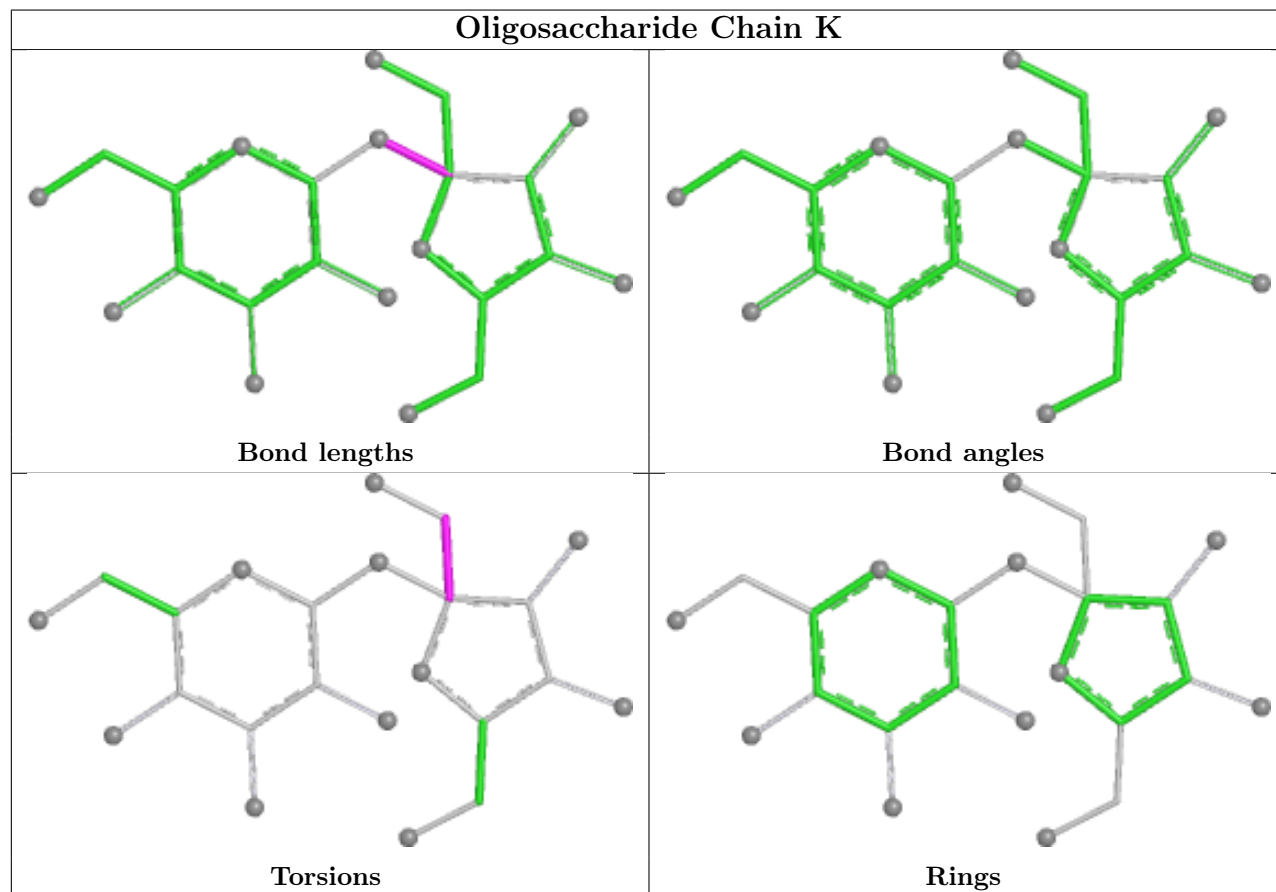
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	FRU	6	0
2	O	1	GLC	1	0
2	P	2	FRU	4	0
2	L	2	FRU	5	0
2	K	2	FRU	3	0
2	N	2	FRU	2	0
2	T	2	FRU	3	0
2	N	1	GLC	1	0
2	T	1	GLC	1	0
2	R	2	FRU	2	0
2	S	2	FRU	3	0
2	O	2	FRU	5	0

Continued on next page...

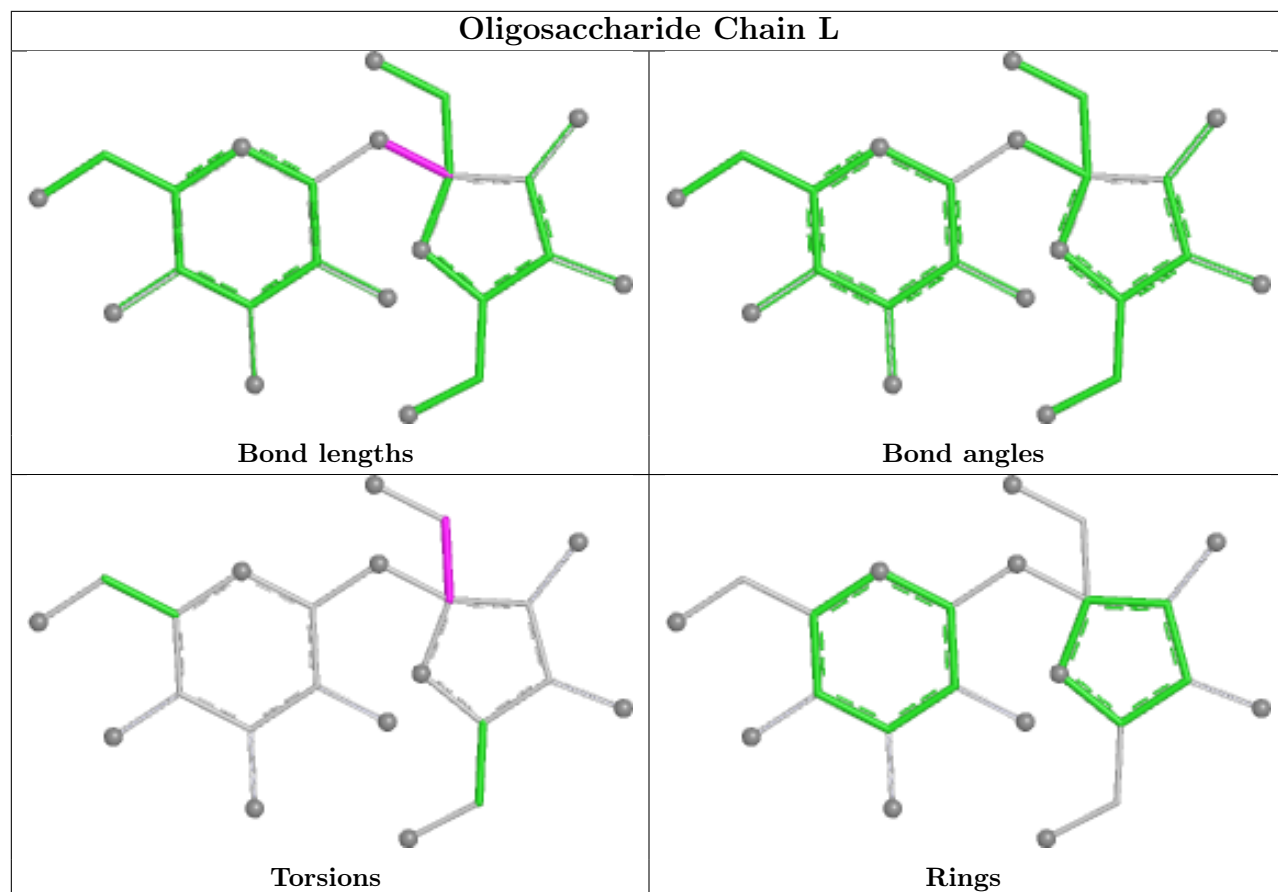
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	2	FRU	4	0
2	L	1	GLC	1	0

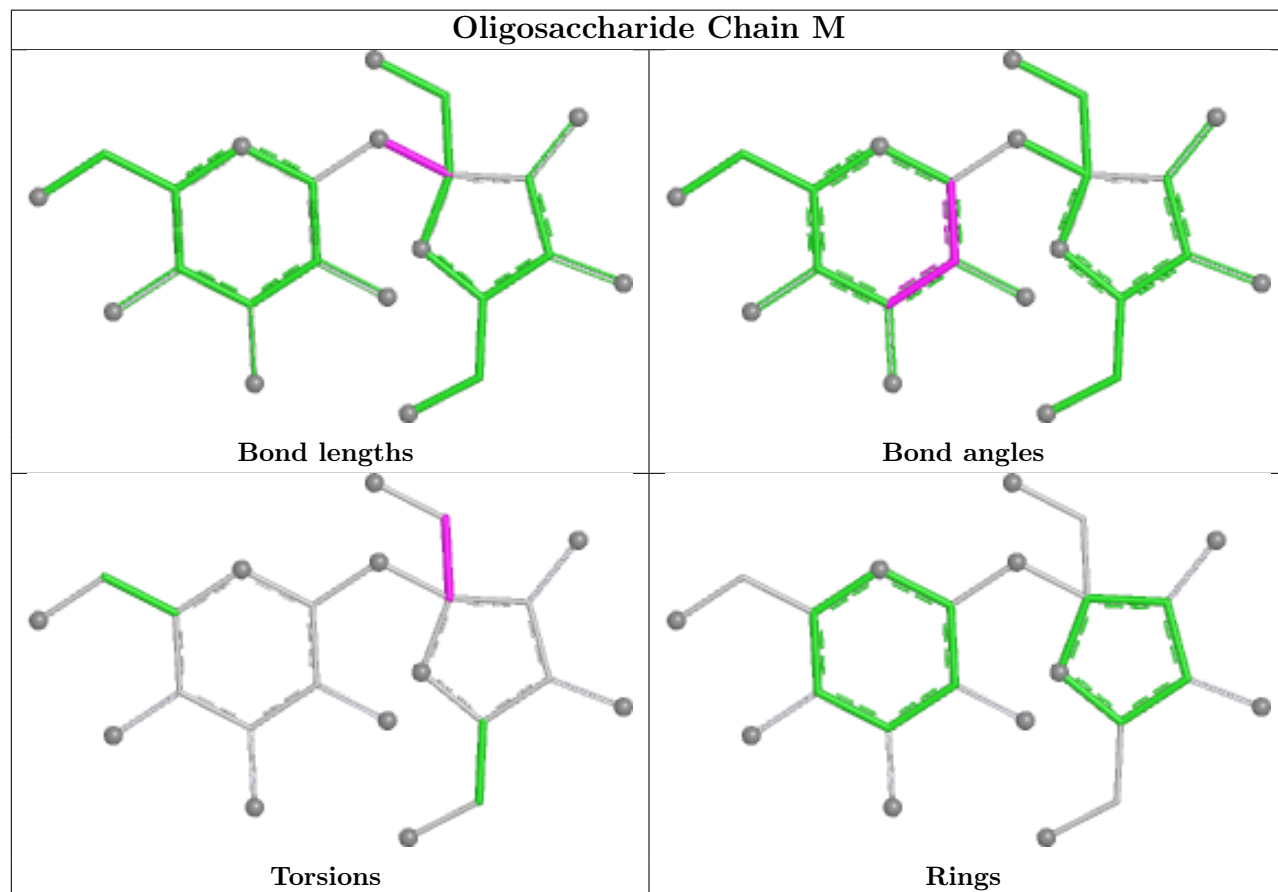
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

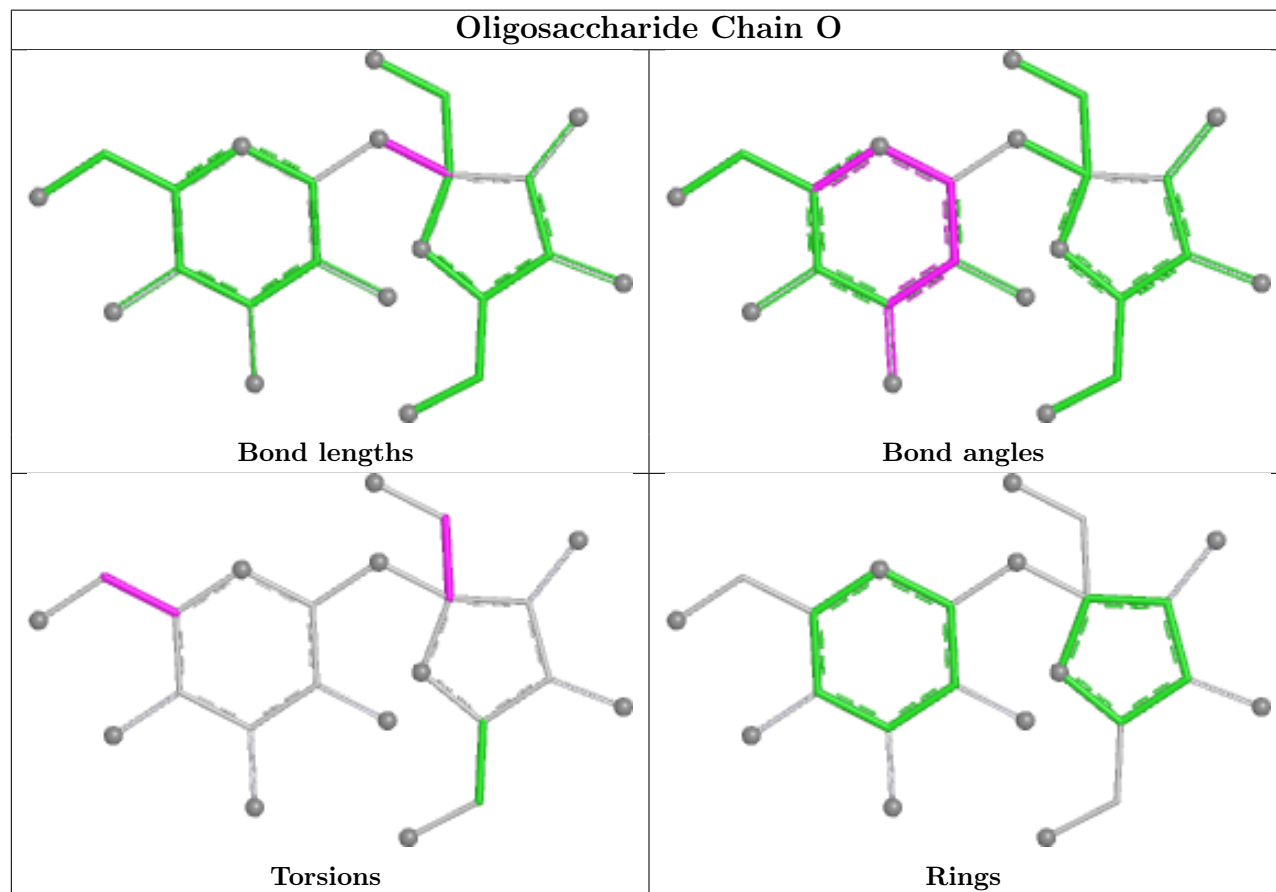
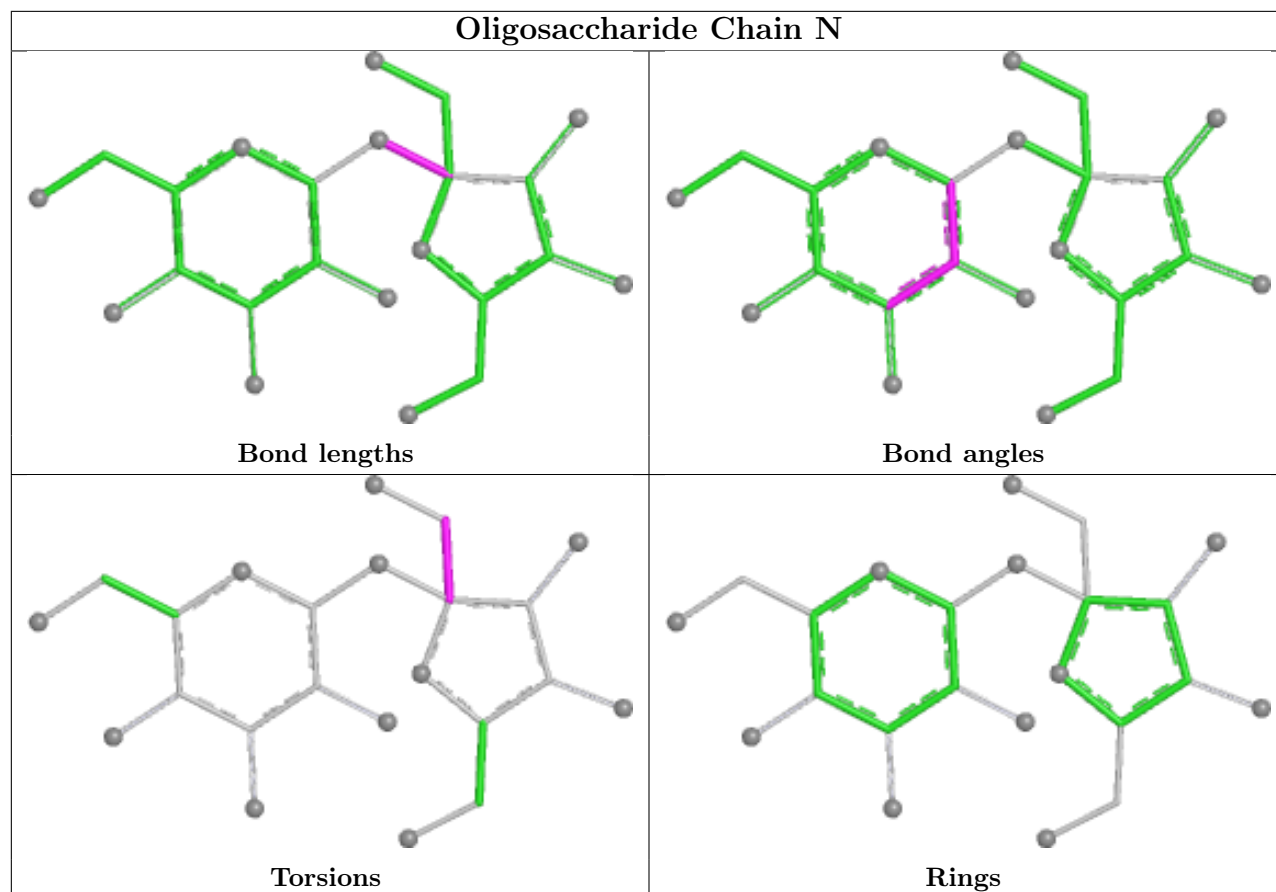


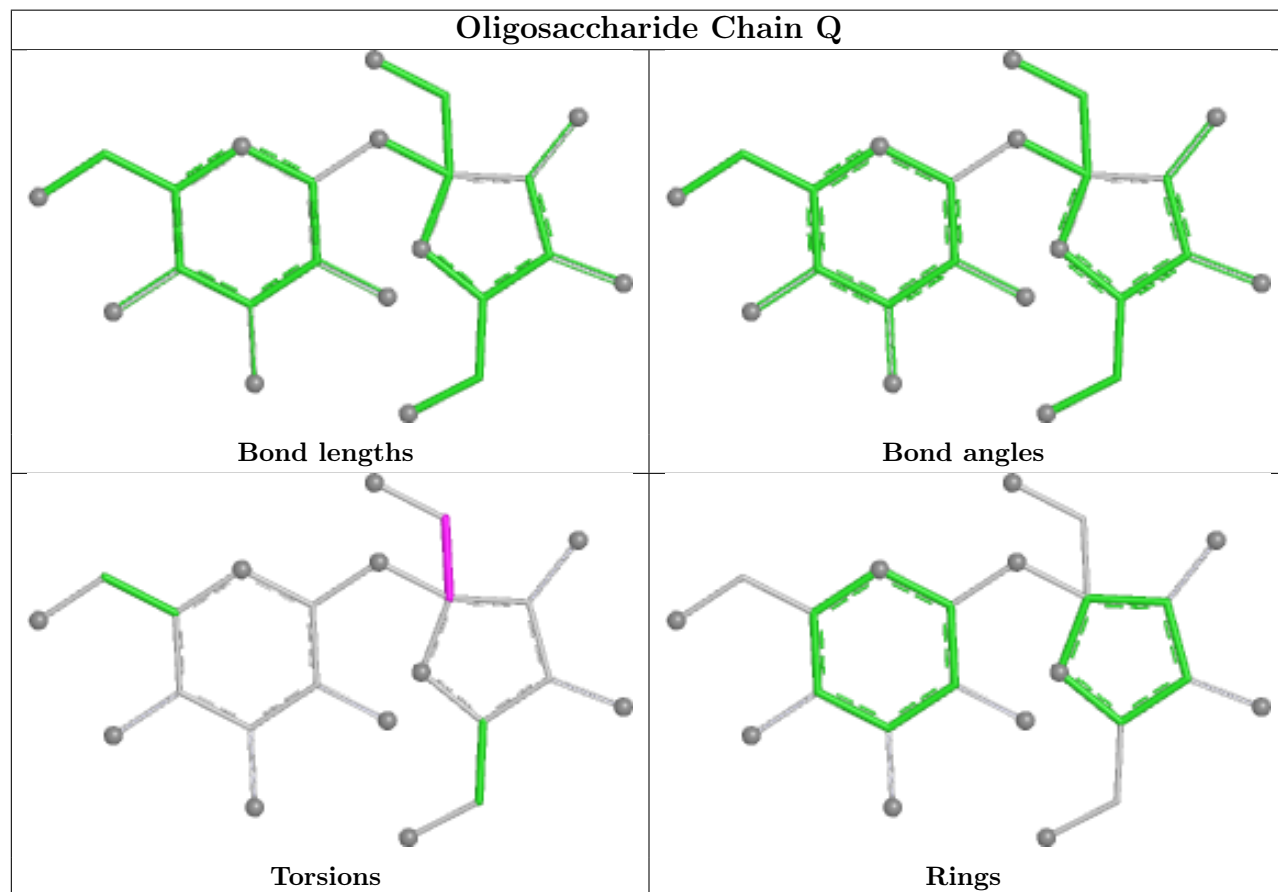
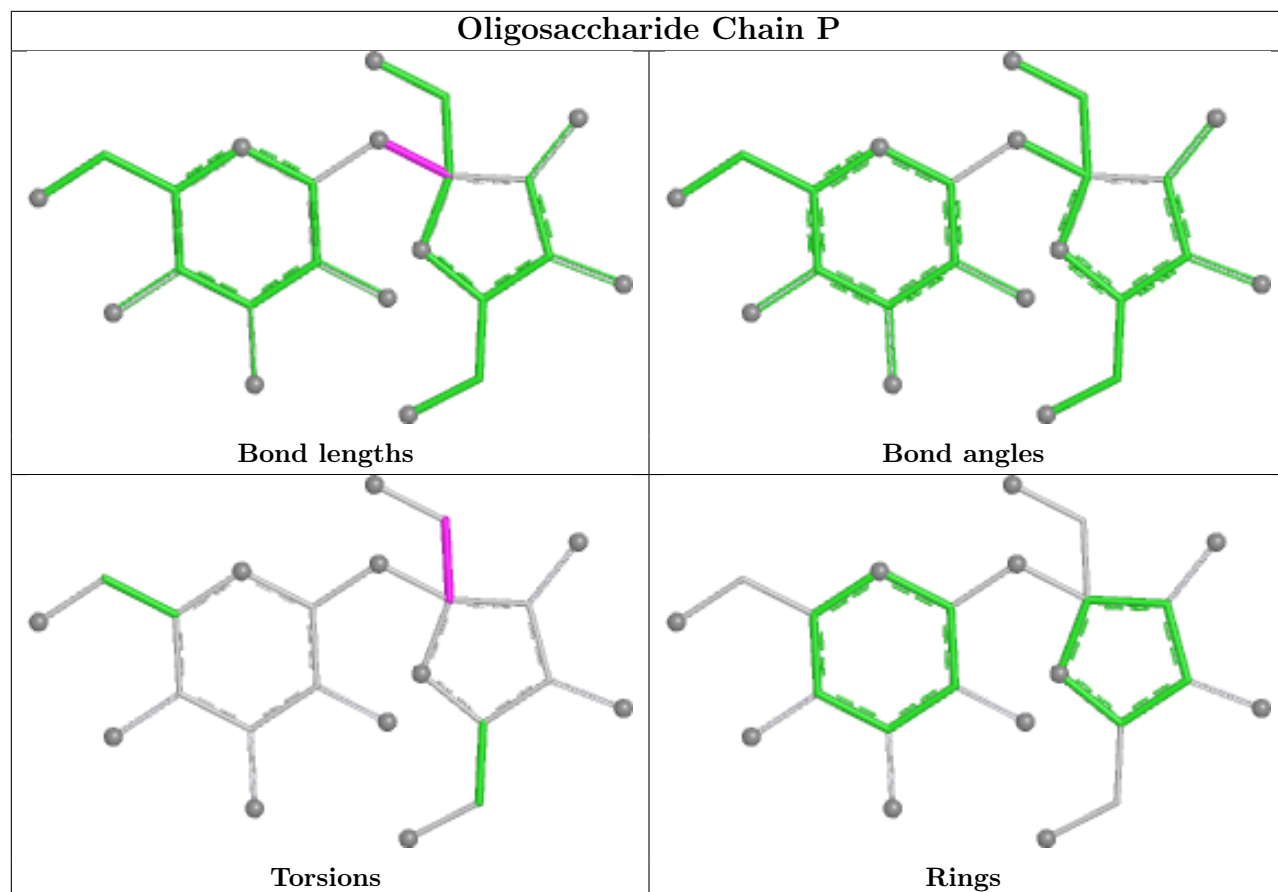
Oligosaccharide Chain L



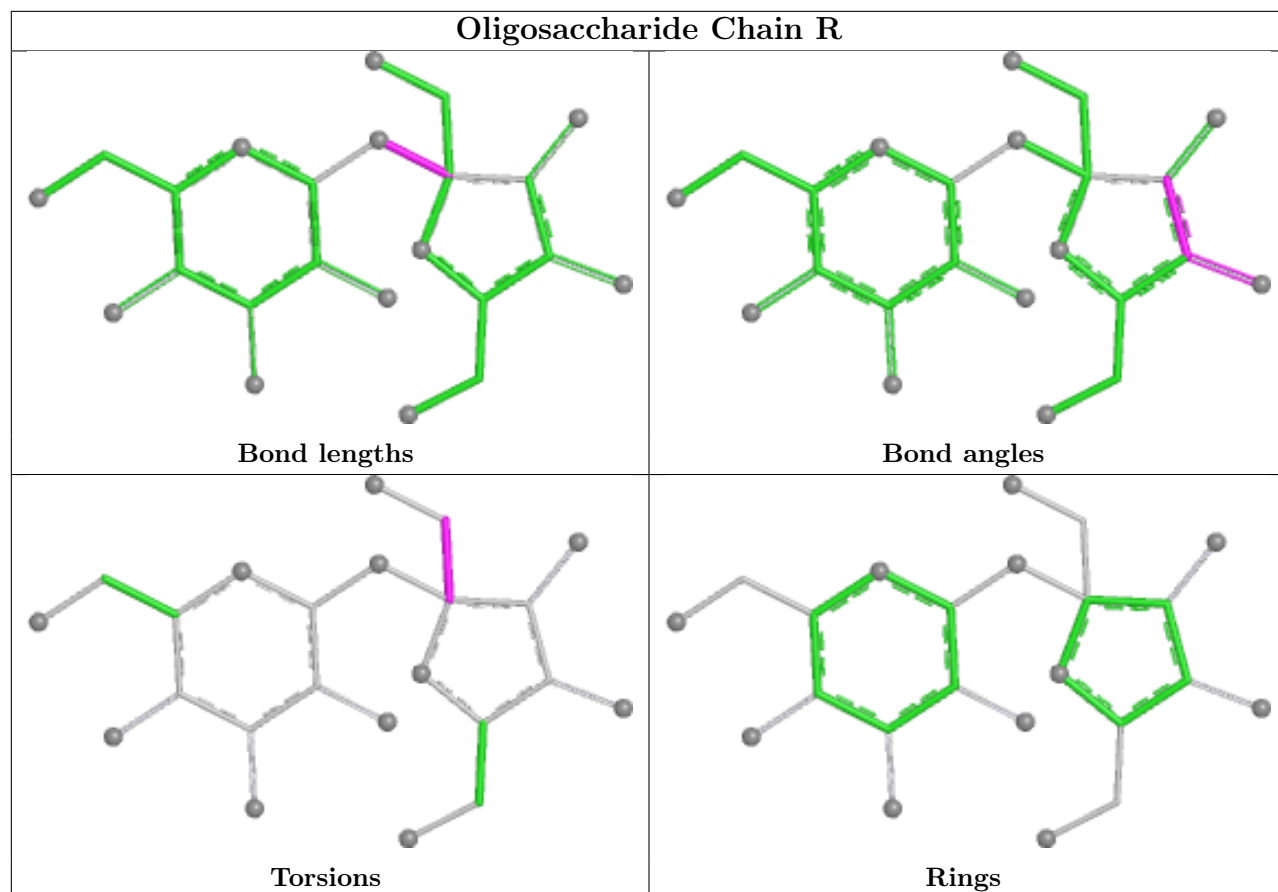
Oligosaccharide Chain M



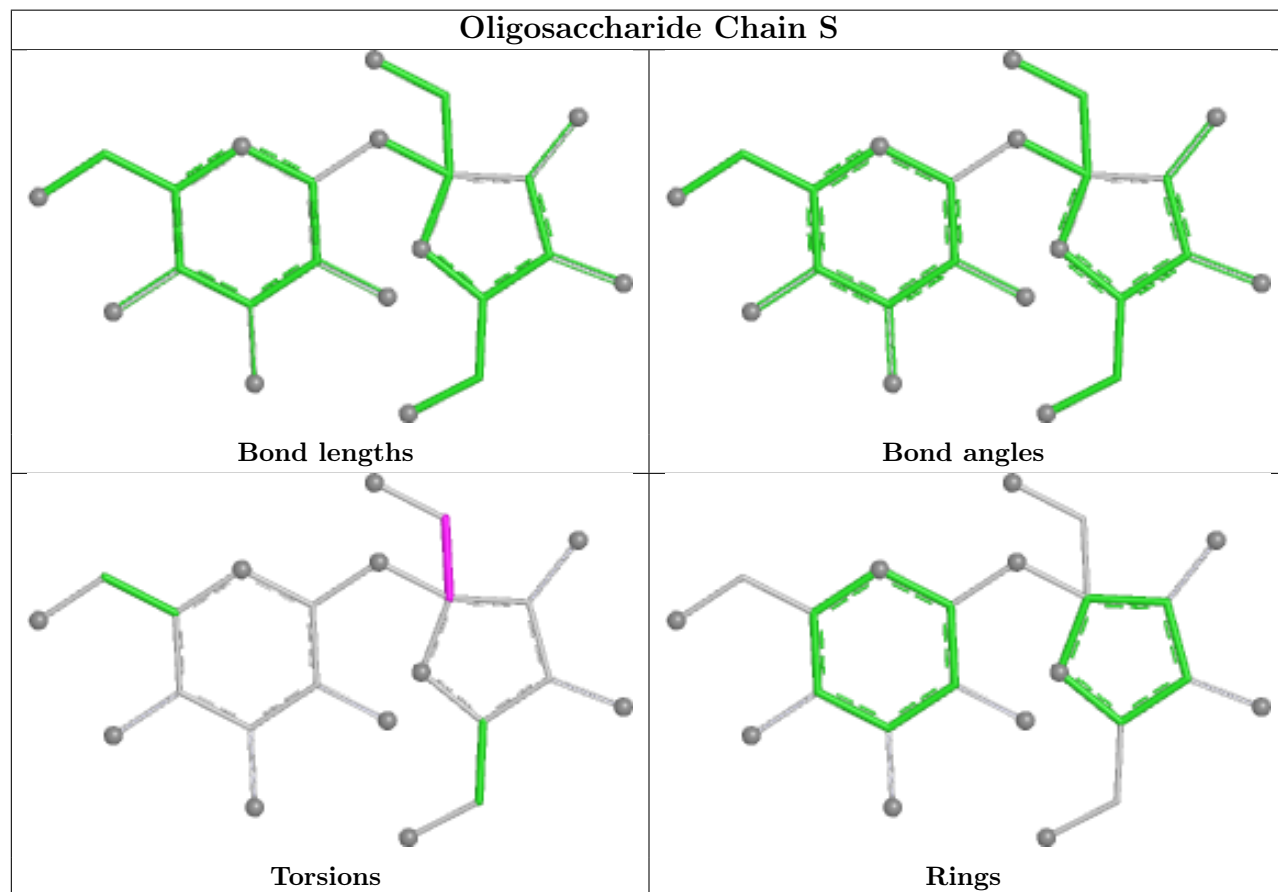


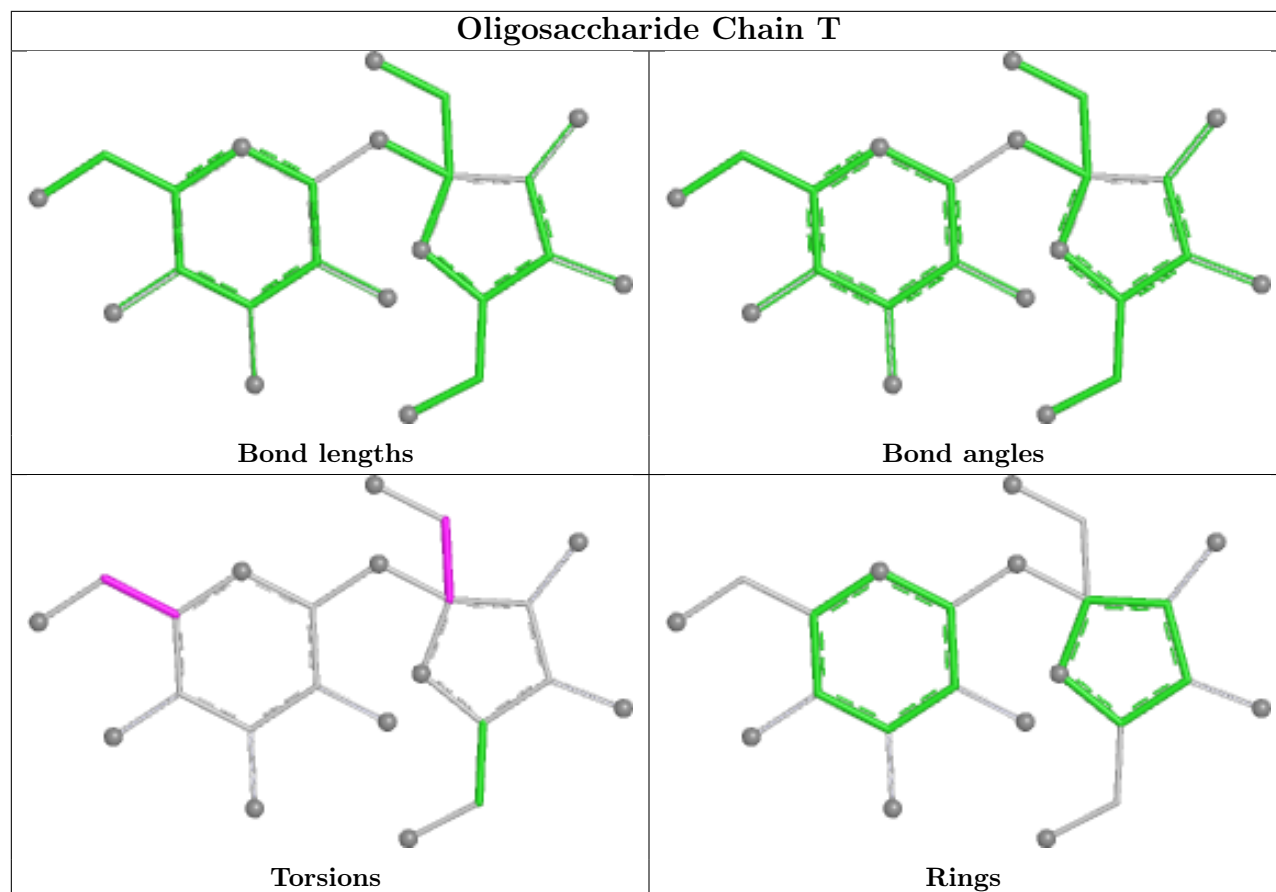


Oligosaccharide Chain R



Oligosaccharide Chain S





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	405/428 (94%)	0.59	15 (3%)	45	25	23, 44, 75, 89	0
1	B	405/428 (94%)	0.63	21 (5%)	33	17	20, 51, 90, 111	0
1	C	406/428 (94%)	0.50	17 (4%)	40	22	17, 43, 72, 91	0
1	D	406/428 (94%)	0.43	11 (2%)	56	35	19, 40, 66, 89	0
1	E	405/428 (94%)	0.64	22 (5%)	31	17	19, 46, 87, 112	0
1	F	406/428 (94%)	0.64	15 (3%)	45	25	18, 47, 79, 109	0
1	G	405/428 (94%)	1.22	72 (17%)	4	2	32, 74, 125, 153	0
1	H	405/428 (94%)	0.67	19 (4%)	36	19	16, 54, 101, 124	0
1	I	406/428 (94%)	1.17	65 (16%)	5	2	38, 77, 124, 172	0
1	J	405/428 (94%)	0.77	21 (5%)	33	17	30, 54, 83, 109	0
All	All	4054/4280 (94%)	0.72	278 (6%)	23	12	16, 51, 101, 172	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	9	ALA	6.1
1	F	39	ALA	4.9
1	H	39	ALA	4.7
1	G	9	ALA	4.6
1	G	140	ALA	4.5
1	I	260	GLY	4.3
1	J	260	GLY	4.3
1	I	220	PRO	4.3
1	G	225	ALA	4.2
1	H	260	GLY	4.0
1	G	220	PRO	3.9
1	F	168	PRO	3.8
1	J	39	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	361	ASP	3.8
1	I	137	ALA	3.8
1	I	115	TRP	3.7
1	J	356	GLY	3.7
1	F	293	GLY	3.6
1	D	9	ALA	3.6
1	H	221	GLU	3.5
1	G	144	TYR	3.5
1	J	152	SER	3.5
1	I	10	THR	3.4
1	I	225	ALA	3.4
1	B	220	PRO	3.4
1	I	180	GLU	3.4
1	A	189	ARG	3.4
1	E	220	PRO	3.4
1	I	311	GLU	3.4
1	E	9	ALA	3.4
1	I	348	GLY	3.4
1	C	166	GLU	3.4
1	B	39	ALA	3.3
1	B	166	GLU	3.3
1	I	59	ALA	3.3
1	G	168	PRO	3.3
1	I	147	ARG	3.3
1	F	9	ALA	3.3
1	H	168	PRO	3.2
1	J	157	VAL	3.2
1	G	10	THR	3.2
1	G	186	GLU	3.2
1	H	186	GLU	3.2
1	B	167	GLY	3.2
1	G	153	GLY	3.1
1	B	221	GLU	3.1
1	G	76	LEU	3.1
1	D	190	GLY	3.1
1	B	225	ALA	3.0
1	J	9	ALA	3.0
1	E	161	ASP	3.0
1	G	223	ALA	3.0
1	G	226	CYS	3.0
1	I	360	LEU	3.0
1	C	365	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	142	ILE	3.0
1	I	15	ARG	3.0
1	I	219	ILE	3.0
1	A	39	ALA	3.0
1	A	407	SER	3.0
1	G	59	ALA	3.0
1	I	142	ILE	3.0
1	H	370	GLU	2.9
1	I	221	GLU	2.9
1	G	356	GLY	2.9
1	G	15	ARG	2.9
1	G	78	PRO	2.9
1	I	252	GLU	2.9
1	G	165	ILE	2.9
1	G	109	THR	2.9
1	C	9	ALA	2.9
1	I	11	PRO	2.9
1	G	184	ARG	2.9
1	J	360	LEU	2.9
1	F	414	PRO	2.9
1	I	372	ARG	2.9
1	I	285	SER	2.8
1	G	75	ASP	2.8
1	I	12	ARG	2.8
1	J	131	TYR	2.8
1	G	41	PRO	2.8
1	G	42	GLU	2.8
1	H	9	ALA	2.8
1	I	66	VAL	2.8
1	I	169	PHE	2.8
1	E	74	ALA	2.8
1	F	225	ALA	2.8
1	G	73	PRO	2.8
1	J	155	SER	2.8
1	D	259	GLU	2.8
1	I	130	PHE	2.7
1	G	222	GLY	2.7
1	E	371	GLN	2.7
1	J	151	GLY	2.7
1	G	219	ILE	2.7
1	C	277	GLY	2.7
1	E	224	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	166	GLU	2.7
1	I	370	GLU	2.7
1	I	133	ALA	2.7
1	J	158	ALA	2.7
1	J	328	ALA	2.7
1	G	106	GLU	2.6
1	C	250	ASP	2.6
1	H	169	PHE	2.6
1	G	221	GLU	2.6
1	B	361	ASP	2.6
1	G	77	LEU	2.6
1	G	364	ALA	2.6
1	J	156	VAL	2.6
1	G	164	ARG	2.6
1	G	11	PRO	2.6
1	B	373	ALA	2.6
1	F	226	CYS	2.6
1	E	152	SER	2.6
1	E	169	PHE	2.6
1	F	155	SER	2.6
1	D	356	GLY	2.6
1	D	106	GLU	2.6
1	B	10	THR	2.6
1	C	226	CYS	2.5
1	F	262	CYS	2.5
1	I	144	TYR	2.5
1	B	222	GLY	2.5
1	B	141	GLU	2.5
1	I	296	GLY	2.5
1	I	401	GLY	2.5
1	J	127	LEU	2.5
1	C	364	ALA	2.5
1	I	259	GLU	2.5
1	G	189	ARG	2.5
1	F	140	ALA	2.5
1	H	158	ALA	2.5
1	B	37	GLU	2.5
1	C	209	THR	2.5
1	I	128	TYR	2.5
1	G	167	GLY	2.5
1	H	222	GLY	2.5
1	G	161	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	14	THR	2.5
1	G	80	LYS	2.5
1	B	223	ALA	2.4
1	E	223	ALA	2.4
1	A	155	SER	2.4
1	C	356	GLY	2.4
1	I	129	VAL	2.4
1	E	140	ALA	2.4
1	E	93	ARG	2.4
1	I	374	LYS	2.4
1	E	75	ASP	2.4
1	G	157	VAL	2.4
1	H	167	GLY	2.4
1	I	167	GLY	2.4
1	I	283	VAL	2.4
1	I	371	GLN	2.4
1	A	106	GLU	2.4
1	G	143	THR	2.4
1	G	25	ASP	2.4
1	E	260	GLY	2.4
1	J	144	TYR	2.4
1	G	130	PHE	2.4
1	I	138	GLY	2.4
1	J	357	GLY	2.4
1	C	311	GLU	2.4
1	G	26	GLU	2.4
1	E	368	PRO	2.4
1	I	229	PRO	2.4
1	G	72	ALA	2.3
1	G	232	GLU	2.3
1	G	152	SER	2.3
1	I	248	PRO	2.3
1	C	142	ILE	2.3
1	G	48	THR	2.3
1	J	222	GLY	2.3
1	G	137	ALA	2.3
1	H	225	ALA	2.3
1	D	159	ASP	2.3
1	G	166	GLU	2.3
1	C	414	PRO	2.3
1	E	356	GLY	2.3
1	E	105	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	213	PHE	2.3
1	D	186	GLU	2.3
1	G	141	GLU	2.3
1	E	317	GLY	2.3
1	F	260	GLY	2.3
1	A	9	ALA	2.3
1	G	74	ALA	2.3
1	I	109	THR	2.3
1	I	188	SER	2.3
1	D	413	LEU	2.3
1	A	226	CYS	2.3
1	I	362	ASP	2.3
1	G	176	GLU	2.3
1	I	414	PRO	2.3
1	G	224	GLY	2.3
1	I	72	ALA	2.3
1	B	307	SER	2.3
1	G	187	GLN	2.3
1	I	136	ARG	2.3
1	J	153	GLY	2.2
1	B	413	LEU	2.2
1	H	258	LEU	2.2
1	G	365	THR	2.2
1	A	186	GLU	2.2
1	I	192	ILE	2.2
1	B	168	PRO	2.2
1	D	376	GLY	2.2
1	E	239	GLY	2.2
1	H	227	GLY	2.2
1	H	277	GLY	2.2
1	I	73	PRO	2.2
1	J	107	GLY	2.2
1	G	12	ARG	2.2
1	G	188	SER	2.2
1	C	361	ASP	2.2
1	G	355	LEU	2.2
1	G	368	PRO	2.2
1	G	88	ARG	2.2
1	I	318	SER	2.2
1	G	394	ILE	2.2
1	B	305	ALA	2.2
1	D	225	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	85	ALA	2.2
1	G	110	ARG	2.2
1	G	126	ARG	2.2
1	I	173	VAL	2.2
1	I	187	GLN	2.2
1	I	77	LEU	2.2
1	B	235	ASN	2.2
1	F	220	PRO	2.2
1	H	401	GLY	2.2
1	E	36	ARG	2.2
1	A	38	ASP	2.2
1	G	209	THR	2.1
1	I	174	LEU	2.1
1	B	9	ALA	2.1
1	I	145	GLU	2.1
1	A	108	GLY	2.1
1	J	117	GLY	2.1
1	A	144	TYR	2.1
1	G	371	GLN	2.1
1	C	221	GLU	2.1
1	G	19	SER	2.1
1	H	293	GLY	2.1
1	I	16	GLU	2.1
1	E	142	ILE	2.1
1	G	245	THR	2.1
1	I	189	ARG	2.1
1	C	222	GLY	2.1
1	I	151	GLY	2.1
1	I	69	SER	2.1
1	B	226	CYS	2.1
1	I	226	CYS	2.1
1	I	250	ASP	2.1
1	I	361	ASP	2.1
1	D	39	ALA	2.1
1	E	172	GLY	2.1
1	C	295	GLU	2.1
1	G	155	SER	2.1
1	I	157	VAL	2.1
1	F	222	GLY	2.1
1	G	276	ASN	2.0
1	G	351	ASN	2.0
1	J	413	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	224	GLY	2.0
1	E	107	GLY	2.0
1	G	105	PHE	2.0
1	G	147	ARG	2.0
1	H	110	ARG	2.0
1	C	39	ALA	2.0
1	F	10	THR	2.0
1	F	40	ALA	2.0
1	I	223	ALA	2.0
1	I	91	TYR	2.0
1	A	167	GLY	2.0
1	A	26	GLU	2.0
1	H	147	ARG	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.

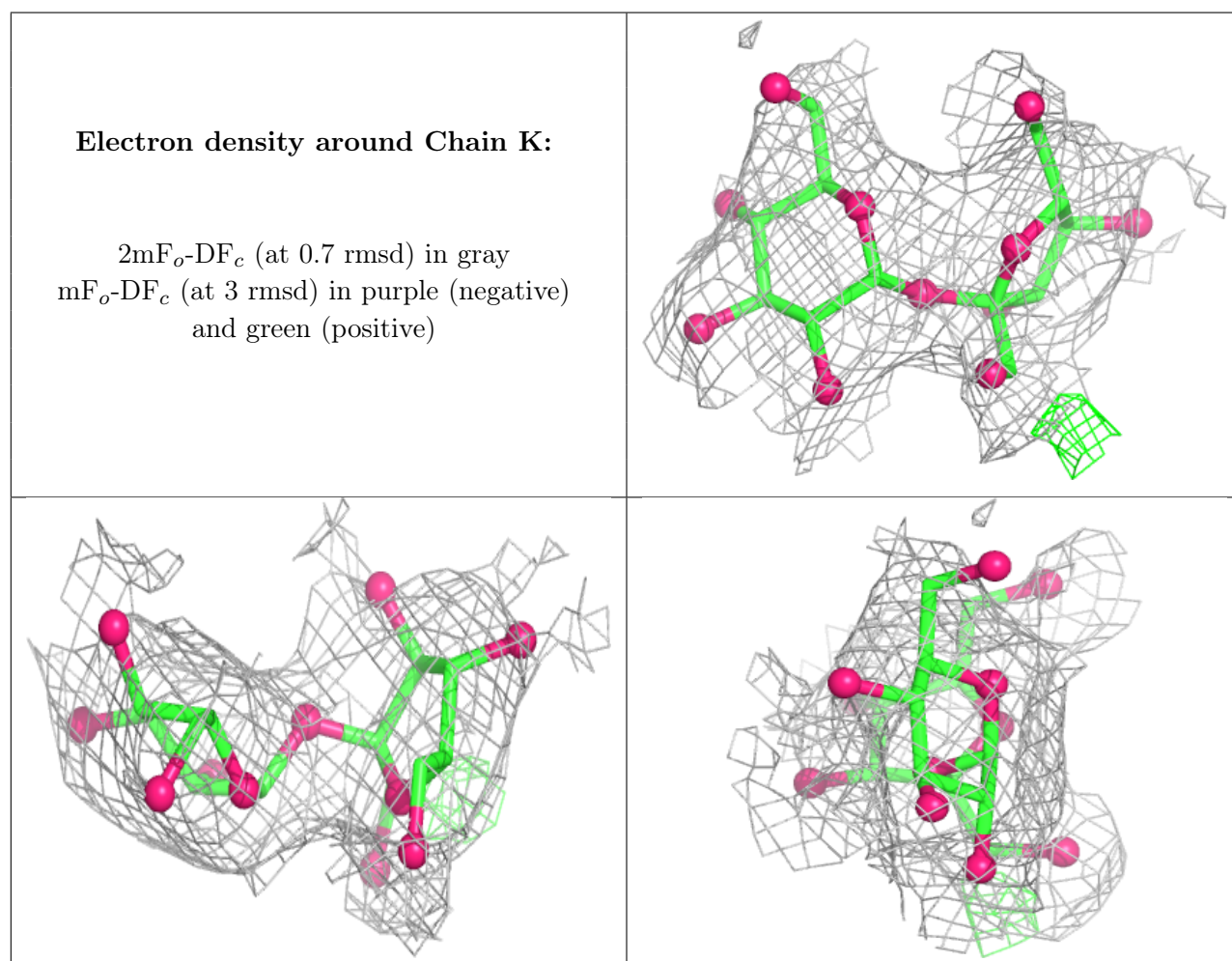
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	Q	2	12/12	0.74	0.15	75,80,84,85	0
2	FRU	S	2	12/12	0.74	0.17	43,74,86,87	0
2	GLC	S	1	11/12	0.79	0.13	74,82,88,90	0
2	FRU	O	2	12/12	0.80	0.18	49,66,76,80	0
2	FRU	M	2	12/12	0.81	0.16	41,52,65,66	0
2	GLC	Q	1	11/12	0.83	0.12	35,68,73,82	0
2	GLC	R	1	11/12	0.85	0.14	26,44,56,62	0
2	FRU	R	2	12/12	0.85	0.18	40,59,80,86	0
2	FRU	K	2	12/12	0.86	0.12	30,41,52,55	0
2	FRU	P	2	12/12	0.86	0.13	38,57,71,76	0
2	GLC	P	1	11/12	0.87	0.11	33,46,65,69	0
2	FRU	N	2	12/12	0.88	0.15	30,51,74,78	0
2	GLC	T	1	11/12	0.88	0.12	30,49,60,67	0
2	FRU	L	2	12/12	0.89	0.15	54,66,88,95	0
2	GLC	M	1	11/12	0.89	0.10	27,41,55,56	0

Continued on next page...

Continued from previous page...

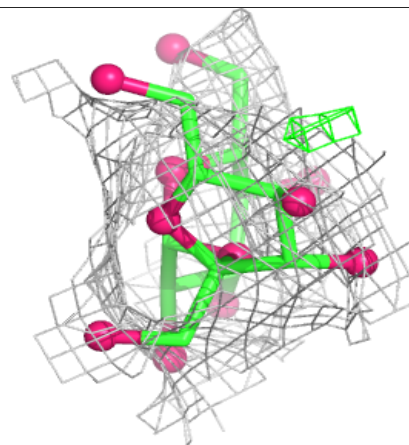
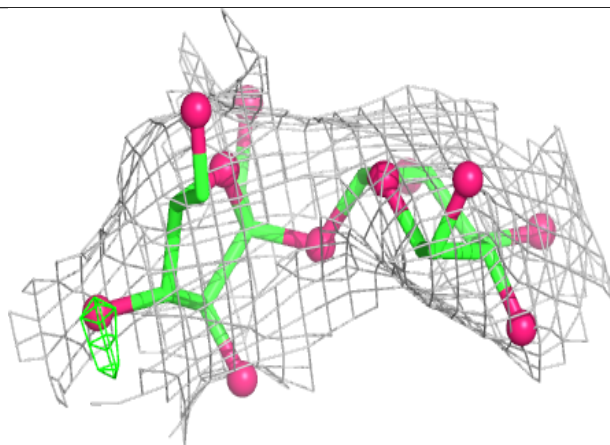
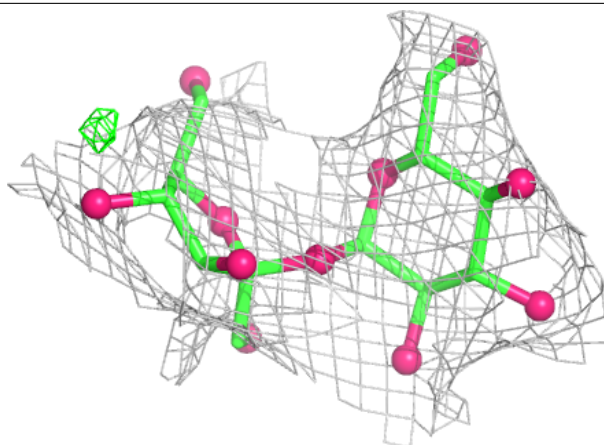
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRU	T	2	12/12	0.90	0.13	39,53,66,68	0
2	GLC	O	1	11/12	0.91	0.09	44,49,64,73	0
2	GLC	K	1	11/12	0.91	0.10	28,35,42,50	0
2	GLC	N	1	11/12	0.92	0.10	15,30,48,56	0
2	GLC	L	1	11/12	0.92	0.09	33,39,54,56	0

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.

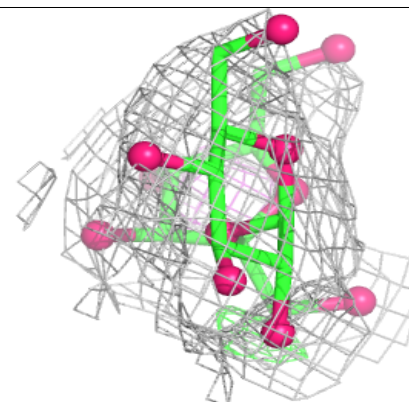
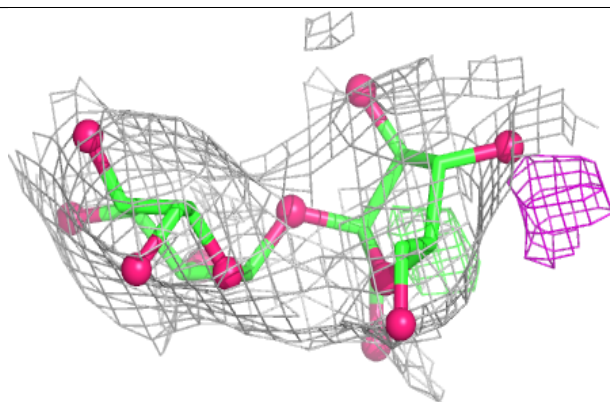
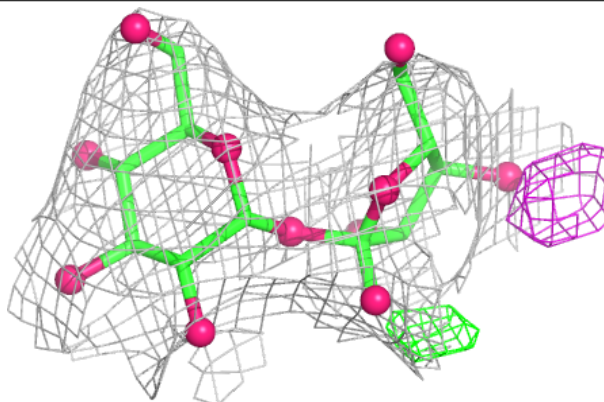


Electron density around Chain L:

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

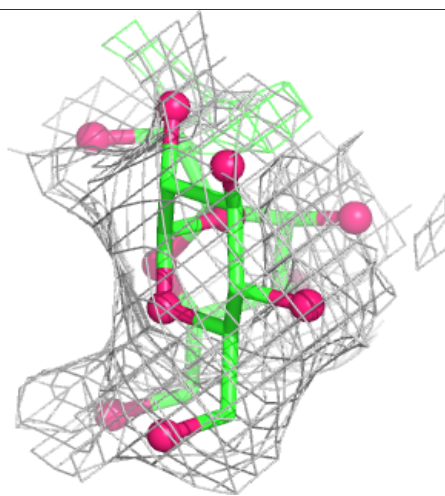
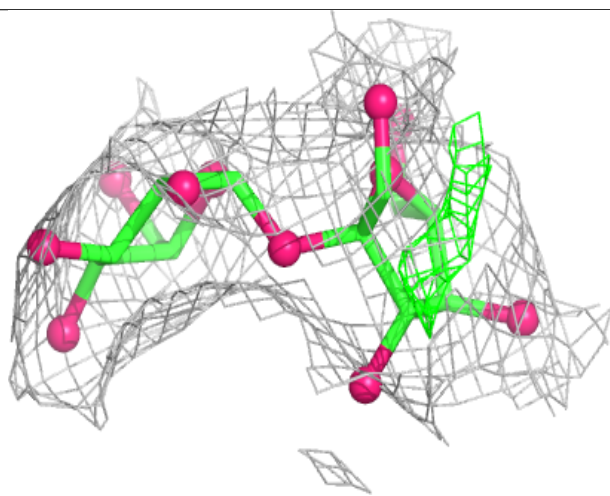
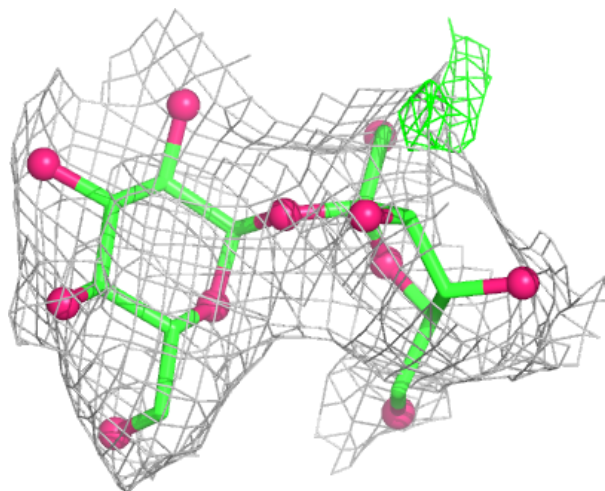
**Electron density around Chain M:**

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



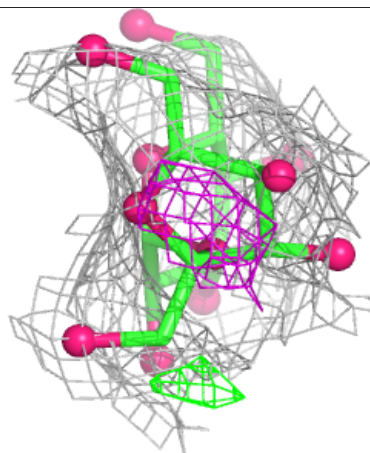
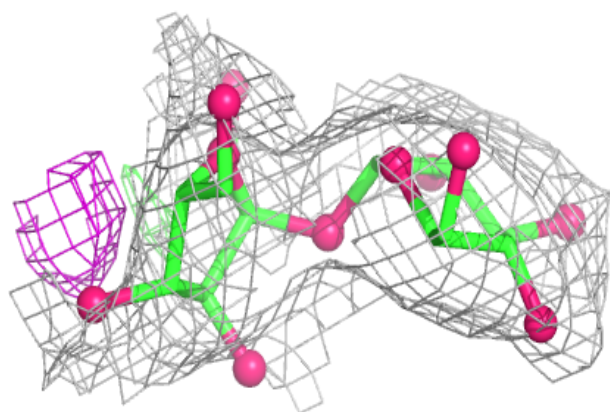
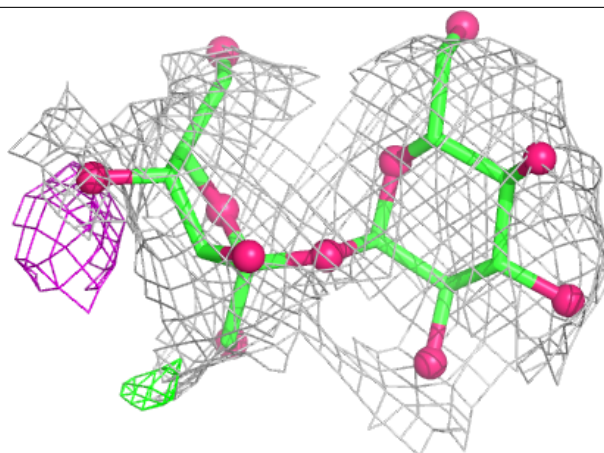
Electron density around Chain N:

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



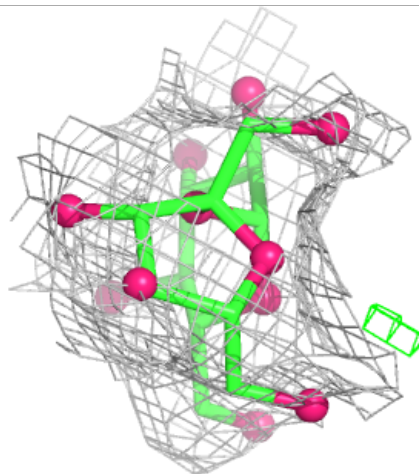
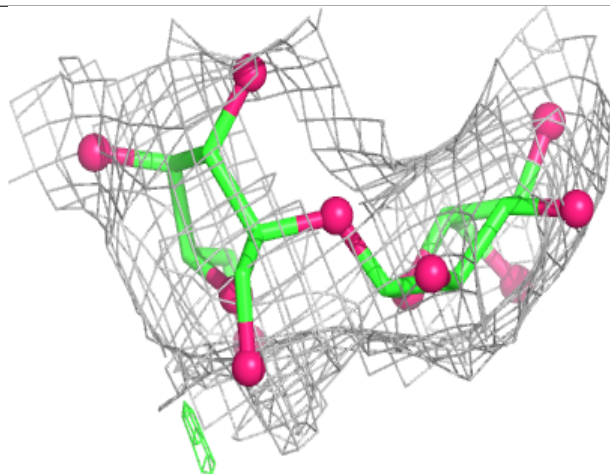
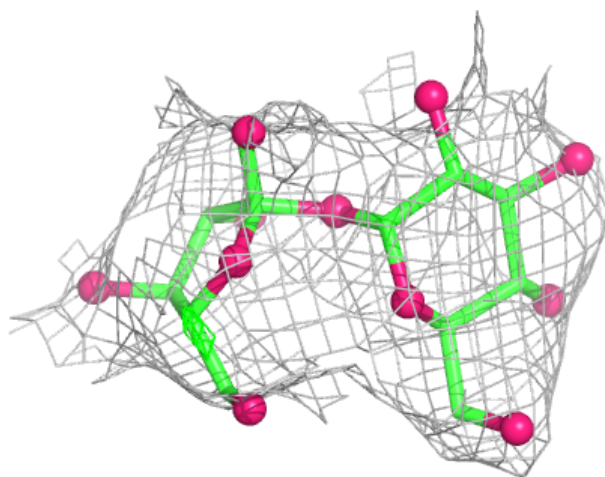
Electron density around Chain O:

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



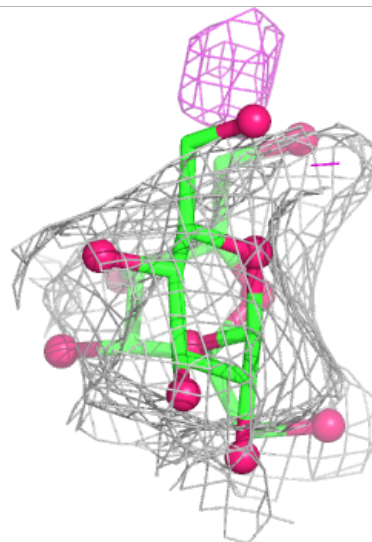
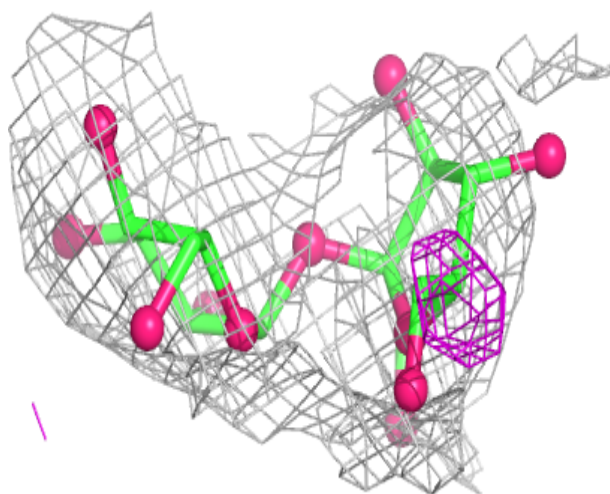
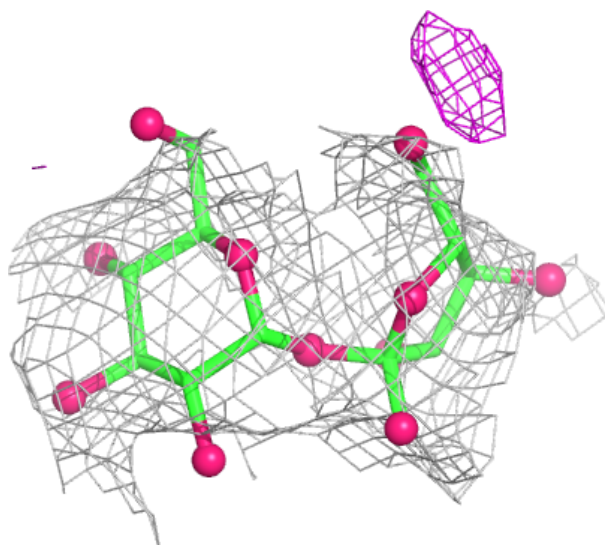
Electron density around Chain P:

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



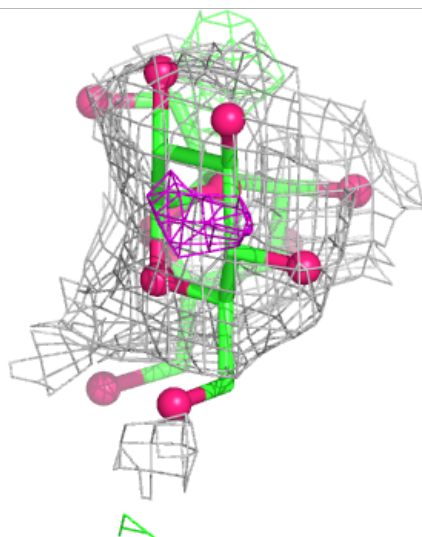
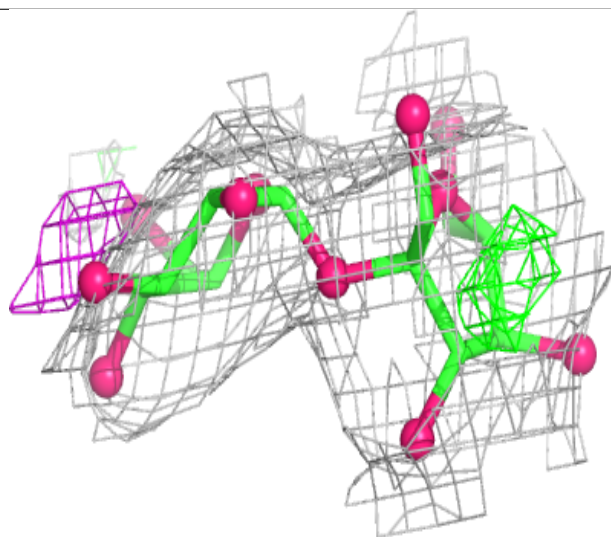
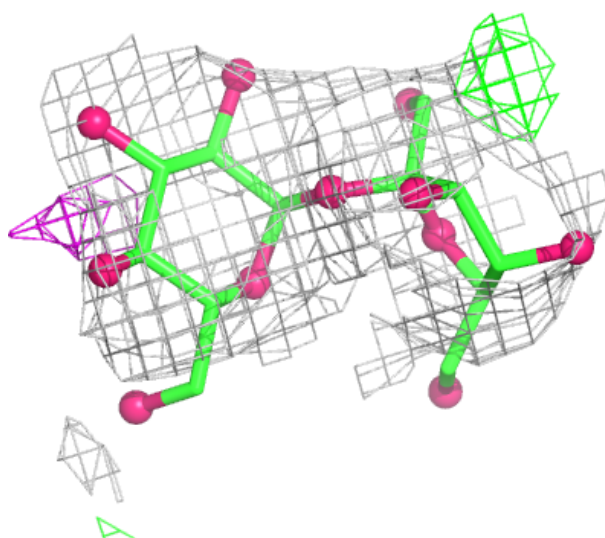
Electron density around Chain Q:

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



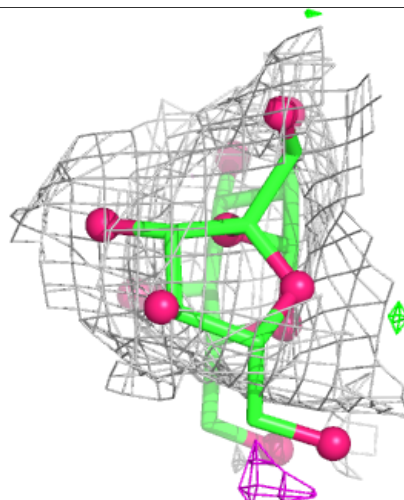
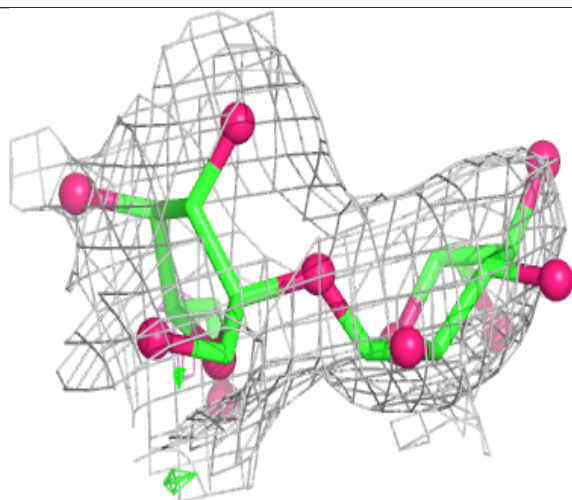
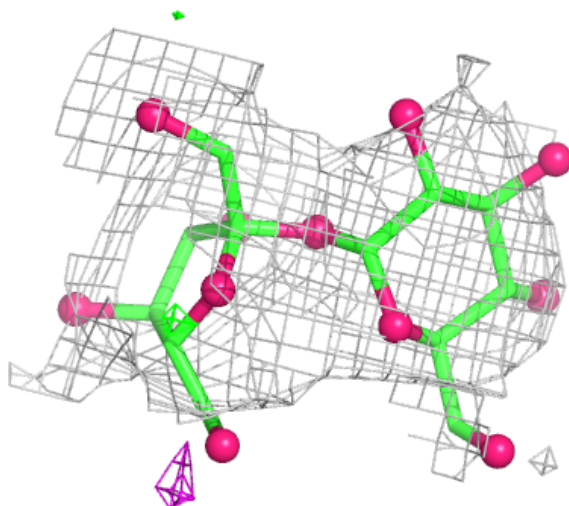
Electron density around Chain R:

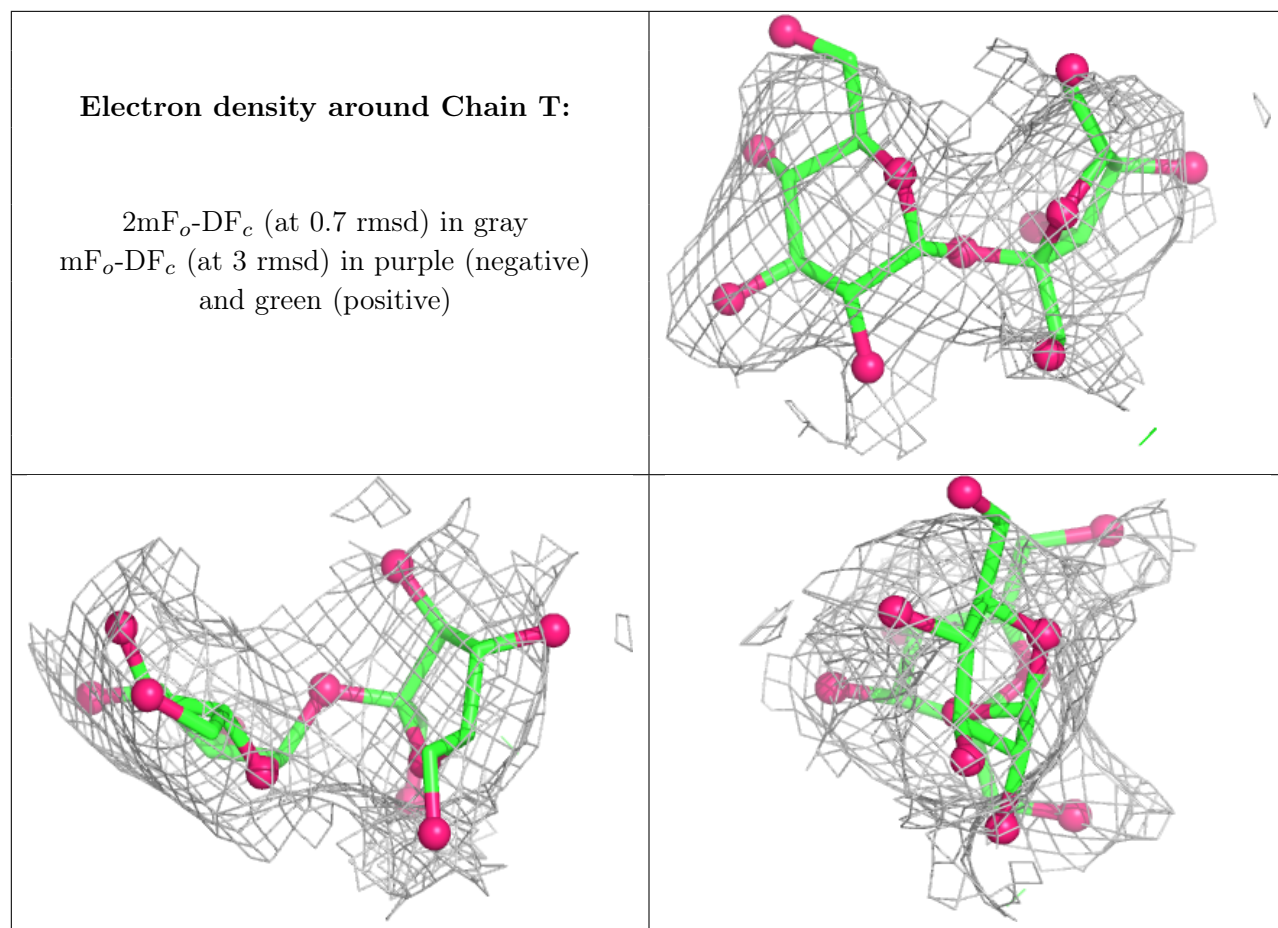
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain S:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.