



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:17 AM UTC

PDB ID : 4FFI / pdb_00004ffi
Title : Crystal Structure of Levan Fructotransferase D54N mutant from *Arthrobacter ureafaciens* in complex with levanbiose
Authors : Park, J.; Rhee, S.
Deposited on : 2012-06-01
Resolution : 2.30 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

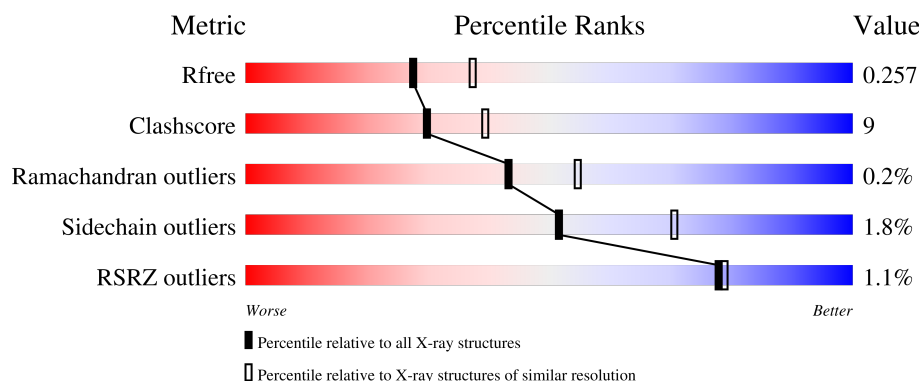
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



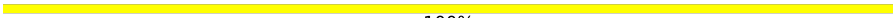
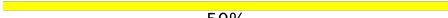
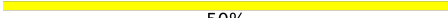
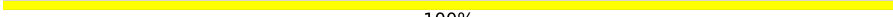
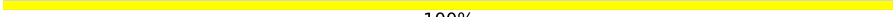
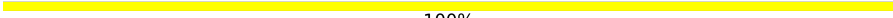
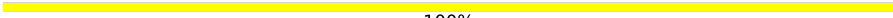
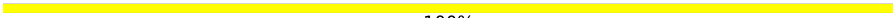
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	492	% 80% 16% ..
1	B	492	2% 77% 17% ..
1	C	492	% 81% 14% ..
1	D	492	% 78% 17% ..
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 50%  50%
2	I	2	 50%  50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
3	H	3	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16025 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 Levan fructotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2375	646	710	8			
1	B	480	Total	C	N	O	S	0	0	0
			3739	2375	646	710	8			
1	C	479	Total	C	N	O	S	0	0	0
			3734	2372	645	709	8			
1	D	478	Total	C	N	O	S	0	0	0
			3725	2367	643	707	8			

There are 52 discrepancies between the modelled and reference sequences:

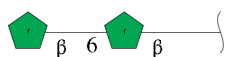
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q9KJD0
A	54	ASN	ASP	engineered mutation	UNP Q9KJD0
A	115	ASP	GLY	conflict	UNP Q9KJD0
A	522	LEU	-	expression tag	UNP Q9KJD0
A	523	GLU	-	expression tag	UNP Q9KJD0
A	524	HIS	-	expression tag	UNP Q9KJD0
A	525	HIS	-	expression tag	UNP Q9KJD0
A	526	HIS	-	expression tag	UNP Q9KJD0
A	527	HIS	-	expression tag	UNP Q9KJD0
A	528	HIS	-	expression tag	UNP Q9KJD0
A	529	HIS	-	expression tag	UNP Q9KJD0
A	530	HIS	-	expression tag	UNP Q9KJD0
A	531	HIS	-	expression tag	UNP Q9KJD0
B	40	MET	-	expression tag	UNP Q9KJD0
B	54	ASN	ASP	engineered mutation	UNP Q9KJD0
B	115	ASP	GLY	conflict	UNP Q9KJD0
B	522	LEU	-	expression tag	UNP Q9KJD0
B	523	GLU	-	expression tag	UNP Q9KJD0
B	524	HIS	-	expression tag	UNP Q9KJD0
B	525	HIS	-	expression tag	UNP Q9KJD0
B	526	HIS	-	expression tag	UNP Q9KJD0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	527	HIS	-	expression tag	UNP Q9KJD0
B	528	HIS	-	expression tag	UNP Q9KJD0
B	529	HIS	-	expression tag	UNP Q9KJD0
B	530	HIS	-	expression tag	UNP Q9KJD0
B	531	HIS	-	expression tag	UNP Q9KJD0
C	40	MET	-	expression tag	UNP Q9KJD0
C	54	ASN	ASP	engineered mutation	UNP Q9KJD0
C	115	ASP	GLY	conflict	UNP Q9KJD0
C	522	LEU	-	expression tag	UNP Q9KJD0
C	523	GLU	-	expression tag	UNP Q9KJD0
C	524	HIS	-	expression tag	UNP Q9KJD0
C	525	HIS	-	expression tag	UNP Q9KJD0
C	526	HIS	-	expression tag	UNP Q9KJD0
C	527	HIS	-	expression tag	UNP Q9KJD0
C	528	HIS	-	expression tag	UNP Q9KJD0
C	529	HIS	-	expression tag	UNP Q9KJD0
C	530	HIS	-	expression tag	UNP Q9KJD0
C	531	HIS	-	expression tag	UNP Q9KJD0
D	40	MET	-	expression tag	UNP Q9KJD0
D	54	ASN	ASP	engineered mutation	UNP Q9KJD0
D	115	ASP	GLY	conflict	UNP Q9KJD0
D	522	LEU	-	expression tag	UNP Q9KJD0
D	523	GLU	-	expression tag	UNP Q9KJD0
D	524	HIS	-	expression tag	UNP Q9KJD0
D	525	HIS	-	expression tag	UNP Q9KJD0
D	526	HIS	-	expression tag	UNP Q9KJD0
D	527	HIS	-	expression tag	UNP Q9KJD0
D	528	HIS	-	expression tag	UNP Q9KJD0
D	529	HIS	-	expression tag	UNP Q9KJD0
D	530	HIS	-	expression tag	UNP Q9KJD0
D	531	HIS	-	expression tag	UNP Q9KJD0

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



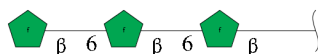
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	3	Total	C	O	0	0	0
			34	18	16			

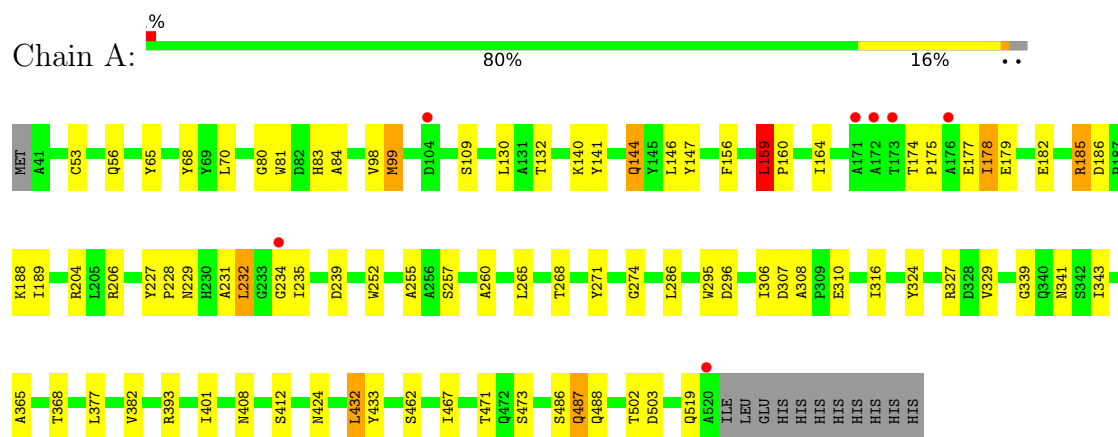
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	192	Total	O	0	0
			192	192		
4	C	227	Total	O	0	0
			227	227		
4	D	235	Total	O	0	0
			235	235		

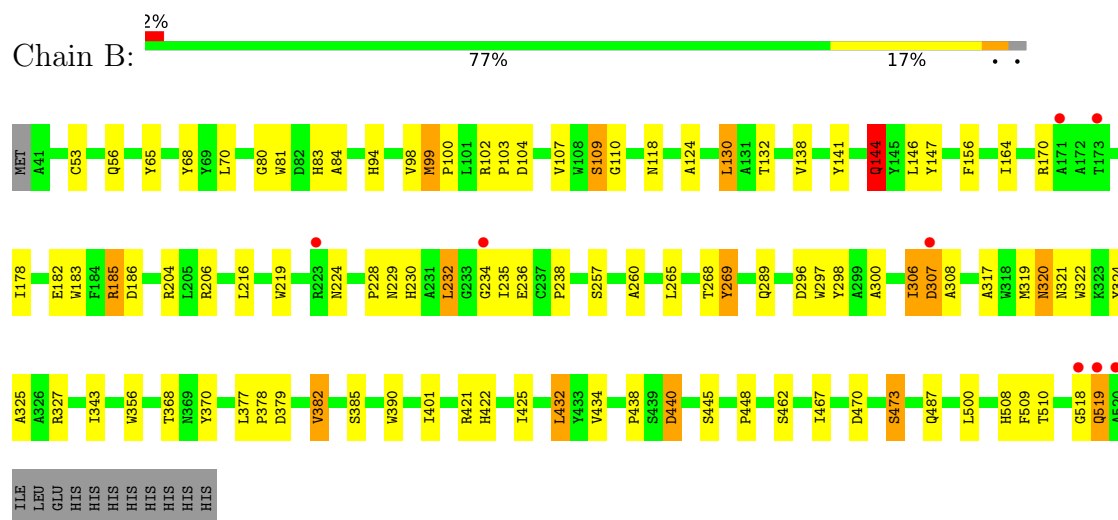
3 Residue-property plots

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.

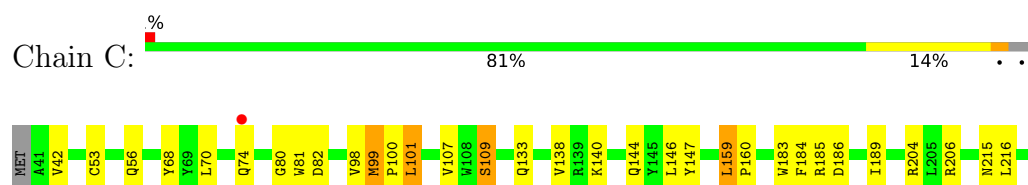
• Molecule 1: Levan fructotransferase

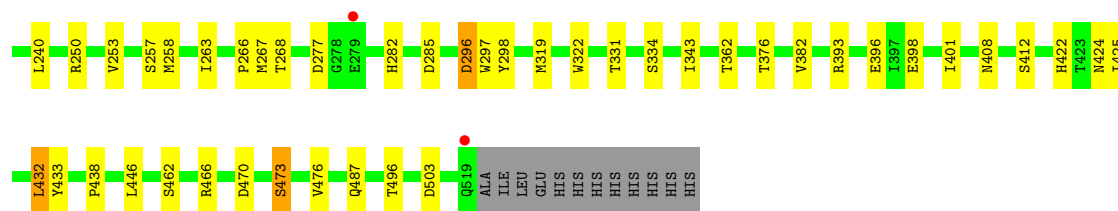


• Molecule 1: Levan fructotransferase

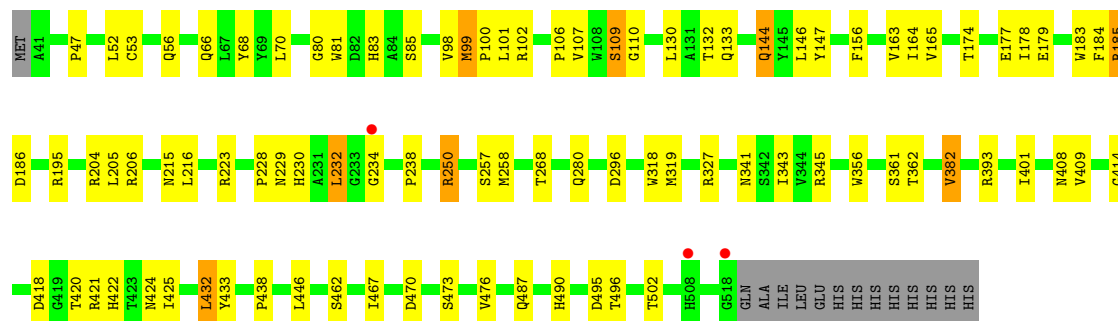
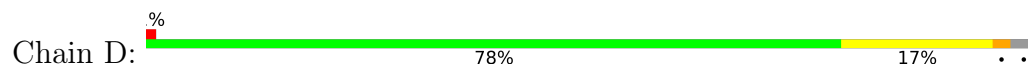


• Molecule 1: Levan fructotransferase





- Molecule 1: Levan fructotransferase



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain J:  100%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain K:  100%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain L:  100%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain M:  100%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain N:  100%

FRU1
FRU2

- Molecule 3: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain H:  100%

FRU1
FRU2
FRU3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.51Å 168.12Å 263.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.30) 93.0 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.00 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.251 0.221 , 0.257	Depositor DCC
R_{free} test set	15335 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16025	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: FRU

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	0.42	0/3863	0.92	17/5312 (0.3%)
1	B	0.42	0/3863	0.92	14/5312 (0.3%)
1	C	0.42	0/3858	0.93	21/5305 (0.4%)
1	D	0.43	0/3849	0.93	14/5293 (0.3%)
All	All	0.42	0/15433	0.93	66/21222 (0.3%)

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

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

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	MET	CA-C-N	7.38	127.39	119.78
1	B	99	MET	C-N-CA	7.38	127.39	119.78
1	D	99	MET	CA-C-N	7.38	127.38	119.78
1	D	99	MET	C-N-CA	7.38	127.38	119.78
1	C	99	MET	CA-C-N	6.51	126.49	119.78
1	C	99	MET	C-N-CA	6.51	126.49	119.78
1	C	432	LEU	N-CA-C	-6.49	94.65	107.69
1	B	185	ARG	N-CA-C	6.42	117.04	108.38
1	B	343	ILE	N-CA-C	-6.35	103.04	110.21
1	D	343	ILE	N-CA-C	-6.34	103.05	110.21
1	A	339	GLY	N-CA-C	6.34	120.02	111.72
1	B	432	LEU	N-CA-C	-6.32	95.17	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	432	LEU	N-CA-C	-6.29	95.06	107.69
1	D	467	ILE	N-CA-C	6.28	116.91	107.75
1	A	432	LEU	N-CA-C	-6.26	95.29	107.62
1	D	185	ARG	N-CA-C	6.24	117.36	108.74
1	A	227	TYR	CA-C-N	6.23	125.45	118.97
1	A	227	TYR	C-N-CA	6.23	125.45	118.97
1	C	144	GLN	N-CA-C	6.19	118.80	108.96
1	D	100	PRO	N-CA-C	6.14	120.97	111.21
1	A	144	GLN	N-CA-C	6.10	118.23	108.41
1	C	267	MET	N-CA-C	-6.02	103.17	110.88
1	D	144	GLN	N-CA-C	6.01	118.44	109.25
1	A	308	ALA	CA-C-N	5.98	126.41	119.47
1	A	308	ALA	C-N-CA	5.98	126.41	119.47
1	A	185	ARG	N-CA-C	5.96	118.02	109.14
1	A	343	ILE	N-CA-C	-5.94	103.50	110.21
1	B	473	SER	N-CA-C	5.89	117.49	108.42
1	C	343	ILE	N-CA-C	-5.89	101.97	109.80
1	A	467	ILE	N-CA-C	5.88	116.34	107.75
1	D	228	PRO	N-CA-C	5.86	121.25	113.40
1	D	109	SER	N-CA-C	5.80	118.19	110.53
1	B	307	ASP	N-CA-C	5.78	118.53	111.82
1	C	42	VAL	N-CA-C	5.77	116.55	110.72
1	A	433	TYR	N-CA-C	5.77	119.36	110.42
1	A	473	SER	N-CA-C	5.72	117.55	108.79
1	A	307	ASP	N-CA-C	5.65	118.38	111.82
1	A	99	MET	CA-C-N	5.64	125.55	119.85
1	A	99	MET	C-N-CA	5.64	125.55	119.85
1	D	433	TYR	N-CA-C	5.64	119.16	110.42
1	C	476	VAL	N-CA-C	5.63	115.96	107.80
1	D	476	VAL	N-CA-C	5.62	115.95	107.80
1	D	165	VAL	N-CA-C	5.59	117.36	108.87
1	C	109	SER	N-CA-C	5.57	117.73	110.43
1	B	296	ASP	N-CA-C	5.55	119.49	107.49
1	B	100	PRO	N-CA-C	5.53	120.01	111.21
1	C	473	SER	N-CA-C	5.49	116.87	108.42
1	C	185	ARG	N-CA-C	5.48	116.31	108.74
1	C	227	TYR	CA-C-N	5.47	125.12	119.05
1	C	227	TYR	C-N-CA	5.47	125.12	119.05
1	B	308	ALA	CA-C-N	5.47	125.29	119.28
1	B	308	ALA	C-N-CA	5.47	125.29	119.28
1	A	159	LEU	N-CA-C	-5.46	100.74	109.04
1	B	144	GLN	N-CA-C	5.43	117.60	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	ILE	N-CA-C	5.40	116.08	108.36
1	C	100	PRO	N-CA-C	5.39	119.78	111.21
1	B	467	ILE	N-CA-C	5.26	115.54	108.17
1	C	101	LEU	N-CA-C	-5.24	103.11	110.50
1	C	296	ASP	N-CA-C	5.18	118.67	107.49
1	C	159	LEU	CA-C-N	5.17	126.30	119.84
1	C	159	LEU	C-N-CA	5.17	126.30	119.84
1	B	109	SER	N-CA-C	5.11	117.27	110.53
1	C	433	TYR	N-CA-C	5.07	117.99	110.14
1	A	471	THR	N-CA-C	5.05	118.91	112.34
1	C	266	PRO	N-CA-C	5.05	118.55	111.33
1	D	296	ASP	N-CA-C	5.02	118.97	107.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	269	TYR	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	3739	0	3491	63	0
1	B	3739	0	3491	66	0
1	C	3734	0	3486	50	0
1	D	3725	0	3478	68	0
2	E	23	0	22	1	0
2	F	23	0	22	0	0
2	G	23	0	22	2	0
2	I	23	0	22	1	0
2	J	23	0	22	0	0
2	K	23	0	22	0	0
2	L	23	0	22	0	0
2	M	23	0	21	3	0
2	N	23	0	22	0	0
3	H	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	193	0	0	3	0
4	B	192	0	0	8	0
4	C	227	0	0	7	0
4	D	235	0	0	3	0
All	All	16025	0	14173	250	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 (250) 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:B:102:ARG:HD3	4:B:784:HOH:O	1.80	0.80
1:A:81:TRP:HB2	1:A:99:MET:HB2	1.66	0.78
1:D:250:ARG:HG2	1:D:250:ARG:HH11	1.52	0.75
1:D:53:CYS:HB3	1:D:70:LEU:HB2	1.68	0.74
1:B:206:ARG:HH11	1:B:234:GLY:HA3	1.52	0.74
1:C:53:CYS:HB3	1:C:70:LEU:HB2	1.72	0.71
1:C:393:ARG:HD3	1:C:496:THR:HG22	1.74	0.70
1:A:175:PRO:HA	1:A:178:ILE:HD12	1.75	0.69
2:M:1:FRU:H62	2:M:2:FRU:H61	1.76	0.68
2:E:1:FRU:H62	2:E:2:FRU:H61	1.76	0.67
1:A:206:ARG:HH11	1:A:234:GLY:HA3	1.59	0.67
1:D:327:ARG:HH22	1:D:490:HIS:HE1	1.43	0.67
1:A:206:ARG:NH1	1:A:234:GLY:HA3	2.10	0.66
1:D:81:TRP:HB2	1:D:99:MET:HB2	1.76	0.66
1:D:206:ARG:HH11	1:D:234:GLY:CA	2.10	0.65
1:B:206:ARG:NH1	1:B:234:GLY:HA3	2.12	0.64
1:B:401:ILE:O	1:B:462:SER:HA	1.96	0.64
1:A:53:CYS:HB3	1:A:70:LEU:HB2	1.80	0.63
1:A:140:LYS:HG3	1:A:141:TYR:CD1	2.33	0.63
1:D:146:LEU:HD23	1:D:146:LEU:C	2.25	0.62
1:B:53:CYS:HB3	1:B:70:LEU:HB2	1.82	0.62
1:D:206:ARG:NH1	1:D:234:GLY:H	1.98	0.61
1:B:229:ASN:O	1:B:232:LEU:HB2	2.01	0.61
1:D:422:HIS:CD2	1:D:424:ASN:HD21	2.18	0.61
1:D:66:GLN:NE2	1:D:85:SER:HB3	2.15	0.61
1:D:418:ASP:OD1	1:D:420:THR:HG22	2.00	0.61
1:D:206:ARG:NH1	1:D:234:GLY:N	2.48	0.61
1:A:146:LEU:HD23	1:A:147:TYR:N	2.16	0.60
1:C:80:GLY:HA2	1:C:107:VAL:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ARG:HG2	1:D:250:ARG:NH1	2.17	0.60
1:D:327:ARG:HH22	1:D:490:HIS:CE1	2.19	0.60
1:D:345:ARG:HD3	1:D:361:SER:HB3	1.84	0.60
1:D:66:GLN:HE22	1:D:85:SER:HB3	1.66	0.60
1:C:277:ASP:OD1	1:C:282:HIS:HE1	1.85	0.59
1:D:133:GLN:NE2	1:D:147:TYR:OH	2.35	0.59
1:D:102:ARG:HD3	4:D:830:HOH:O	2.01	0.59
1:C:446:LEU:HD23	4:C:718:HOH:O	2.01	0.59
1:C:206:ARG:NH1	1:C:234:GLY:N	2.50	0.58
1:A:159:LEU:HD23	1:A:160:PRO:HD2	1.84	0.58
1:A:324:TYR:O	1:A:327:ARG:HG2	2.03	0.58
1:B:98:VAL:HG22	1:B:156:PHE:HD1	1.67	0.58
1:C:206:ARG:HH11	1:C:234:GLY:CA	2.17	0.58
1:A:98:VAL:HG22	1:A:156:PHE:HD1	1.69	0.57
1:C:81:TRP:HB2	1:C:99:MET:HB2	1.86	0.57
1:B:300:ALA:HB2	1:B:317:ALA:HB2	1.84	0.57
1:A:368:THR:HG23	4:A:773:HOH:O	2.05	0.57
1:A:401:ILE:O	1:A:462:SER:HA	2.03	0.57
1:C:206:ARG:NH1	1:C:234:GLY:H	2.02	0.57
1:C:206:ARG:HD3	1:C:234:GLY:HA2	1.87	0.57
1:D:422:HIS:HD2	1:D:424:ASN:HD21	1.51	0.56
1:B:146:LEU:HD23	1:B:147:TYR:N	2.21	0.56
1:C:74:GLN:HG2	4:C:877:HOH:O	2.06	0.56
1:B:306:ILE:HD13	1:B:306:ILE:C	2.30	0.56
1:B:94:HIS:HB3	4:B:802:HOH:O	2.04	0.56
1:B:183:TRP:O	1:B:204:ARG:HD3	2.05	0.56
1:C:319:MET:HE1	1:C:473:SER:HB2	1.88	0.56
1:B:440:ASP:OD2	1:B:445:SER:HB2	2.06	0.56
1:A:486:SER:O	1:A:487:GLN:HG3	2.06	0.55
1:B:141:TYR:CE1	1:B:170:ARG:HD3	2.40	0.55
1:B:422:HIS:O	1:B:438:PRO:HB2	2.07	0.55
1:B:518:GLY:C	1:B:519:GLN:OE1	2.49	0.55
1:A:204:ARG:O	1:A:234:GLY:O	2.24	0.54
1:A:56:GLN:HB2	1:A:68:TYR:HB2	1.90	0.54
1:B:80:GLY:HA2	1:B:107:VAL:HB	1.89	0.54
1:A:146:LEU:HD23	1:A:146:LEU:C	2.33	0.54
1:A:140:LYS:HG3	1:A:141:TYR:HD1	1.72	0.54
1:A:206:ARG:HD3	1:A:234:GLY:HA2	1.89	0.54
1:C:470:ASP:HB3	4:C:712:HOH:O	2.07	0.54
1:D:183:TRP:O	1:D:204:ARG:HD2	2.08	0.53
1:D:362:THR:HG22	4:D:746:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:TYR:O	1:B:327:ARG:HG2	2.08	0.53
1:D:257:SER:HA	1:D:268:THR:O	2.09	0.53
1:A:178:ILE:HD13	1:A:179:GLU:N	2.23	0.53
1:B:508:HIS:HB3	4:B:702:HOH:O	2.09	0.53
1:C:376:THR:HG23	4:C:825:HOH:O	2.09	0.53
1:C:160:PRO:HG2	4:C:871:HOH:O	2.09	0.53
1:A:174:THR:O	1:A:178:ILE:HG23	2.09	0.53
1:C:215:ASN:O	1:C:216:LEU:HB2	2.07	0.53
1:C:257:SER:HA	1:C:268:THR:O	2.09	0.53
1:B:204:ARG:O	1:B:234:GLY:O	2.27	0.52
1:C:393:ARG:CD	1:C:496:THR:HG22	2.39	0.52
1:A:178:ILE:HD13	1:A:179:GLU:H	1.75	0.52
1:B:228:PRO:HG2	4:B:820:HOH:O	2.10	0.52
1:C:109:SER:HB2	1:C:186:ASP:OD1	2.09	0.52
1:A:98:VAL:HG13	1:A:99:MET:HE3	1.91	0.52
1:D:109:SER:HB2	1:D:186:ASP:OD1	2.09	0.52
1:D:99:MET:HE3	1:D:147:TYR:CD2	2.45	0.52
1:A:174:THR:HG23	1:A:177:GLU:OE2	2.10	0.51
1:B:146:LEU:HD23	1:B:146:LEU:C	2.36	0.51
1:B:98:VAL:CG2	1:B:156:PHE:HD1	2.24	0.51
1:D:144:GLN:HG2	1:D:164:ILE:HB	1.93	0.51
1:A:408:ASN:HB3	1:A:503:ASP:HB3	1.91	0.51
1:B:83:HIS:CD2	1:B:84:ALA:N	2.79	0.51
1:C:412:SER:OG	1:C:424:ASN:ND2	2.43	0.51
1:B:224:ASN:OD1	2:G:1:FRU:H11	2.11	0.51
1:A:229:ASN:O	1:A:232:LEU:HB2	2.10	0.50
1:C:232:LEU:HD12	1:C:263:ILE:HD11	1.92	0.50
1:D:401:ILE:O	1:D:462:SER:HA	2.12	0.50
1:D:393:ARG:CD	1:D:496:THR:HG22	2.41	0.50
1:A:178:ILE:O	1:A:182:GLU:HG3	2.12	0.50
1:B:110:GLY:HA3	1:B:130:LEU:O	2.12	0.50
1:D:132:THR:HG21	1:D:185:ARG:HB3	1.92	0.50
1:B:425:ILE:N	1:B:425:ILE:HD12	2.27	0.50
1:D:56:GLN:HB2	1:D:68:TYR:HB2	1.93	0.50
1:B:206:ARG:HD3	1:B:234:GLY:HA2	1.94	0.49
1:B:385:SER:HA	1:B:500:LEU:O	2.11	0.49
1:C:146:LEU:C	1:C:146:LEU:HD23	2.37	0.49
1:B:56:GLN:HB2	1:B:68:TYR:HB2	1.95	0.49
1:D:422:HIS:HD2	1:D:424:ASN:ND2	2.09	0.49
1:C:184:PHE:HA	1:C:204:ARG:HD3	1.94	0.49
1:D:319:MET:HE1	1:D:473:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:SER:HB3	1:B:298:TYR:CE2	2.48	0.49
1:D:98:VAL:HG22	1:D:156:PHE:HD1	1.78	0.49
1:D:425:ILE:N	1:D:425:ILE:HD12	2.28	0.49
1:A:140:LYS:HE3	1:A:141:TYR:HE1	1.78	0.48
1:C:183:TRP:O	1:C:204:ARG:HD2	2.12	0.48
1:B:118:ASN:HB2	1:B:124:ALA:HA	1.95	0.48
1:D:206:ARG:HH11	1:D:234:GLY:HA3	1.78	0.48
1:B:257:SER:HA	1:B:268:THR:O	2.14	0.48
1:B:138:VAL:HB	1:B:141:TYR:CD2	2.48	0.48
1:D:229:ASN:O	1:D:232:LEU:HB2	2.14	0.48
1:B:216:LEU:HA	1:B:219:TRP:CZ2	2.49	0.48
1:D:144:GLN:N	1:D:144:GLN:CD	2.70	0.48
1:D:232:LEU:O	1:D:258:MET:HB3	2.14	0.48
1:D:414:GLY:O	1:D:495:ASP:HB3	2.13	0.48
1:A:188:LYS:HG2	1:A:239:ASP:HA	1.95	0.47
1:A:486:SER:C	1:A:487:GLN:HG3	2.39	0.47
1:C:184:PHE:HD1	1:C:204:ARG:HD3	1.79	0.47
1:A:206:ARG:HH11	1:A:234:GLY:CA	2.24	0.47
1:D:146:LEU:HD23	1:D:147:TYR:N	2.29	0.47
1:D:179:GLU:HG2	1:D:205:LEU:HD22	1.95	0.47
1:D:206:ARG:HH11	1:D:234:GLY:N	2.12	0.47
1:D:393:ARG:HD2	1:D:496:THR:HG22	1.96	0.47
1:A:140:LYS:HG3	1:A:141:TYR:CE1	2.49	0.47
1:C:206:ARG:HD3	1:C:234:GLY:CA	2.45	0.47
1:D:186:ASP:HB2	1:D:238:PRO:HD2	1.96	0.47
1:D:215:ASN:O	1:D:216:LEU:HB2	2.15	0.47
1:A:109:SER:HB2	1:A:186:ASP:OD1	2.15	0.47
1:A:365:ALA:HB3	4:A:738:HOH:O	2.15	0.47
1:B:144:GLN:HG2	1:B:164:ILE:HB	1.97	0.47
1:D:206:ARG:HD3	1:D:234:GLY:HA2	1.97	0.47
1:A:377:LEU:N	1:A:377:LEU:HD12	2.29	0.46
1:C:401:ILE:O	1:C:462:SER:HA	2.14	0.46
1:D:422:HIS:O	1:D:438:PRO:HB2	2.15	0.46
1:A:329:VAL:HG11	4:A:823:HOH:O	2.15	0.46
1:B:109:SER:HB2	1:B:186:ASP:OD1	2.15	0.46
1:B:132:THR:HG21	1:B:185:ARG:HB3	1.98	0.46
2:M:1:FRU:H62	2:M:2:FRU:C6	2.43	0.46
1:B:224:ASN:HD21	2:G:1:FRU:H11	1.80	0.46
1:B:432:LEU:HD22	1:B:432:LEU:HA	1.83	0.46
1:A:519:GLN:HA	1:A:519:GLN:NE2	2.30	0.46
1:B:236:GLU:OE1	1:B:298:TYR:OH	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:PHE:HD1	1:D:204:ARG:HD3	1.80	0.46
1:A:132:THR:HG21	1:A:185:ARG:HB3	1.98	0.45
1:C:159:LEU:HD12	1:C:160:PRO:HD2	1.98	0.45
1:D:66:GLN:NE2	1:D:83:HIS:NE2	2.60	0.45
1:C:206:ARG:HH11	1:C:234:GLY:N	2.15	0.45
1:A:229:ASN:HD21	1:A:231:ALA:HB3	1.82	0.45
1:C:398:GLU:HG2	1:C:466:ARG:HG3	1.97	0.45
1:D:223:ARG:HB2	1:D:280:GLN:HB3	1.99	0.45
1:C:257:SER:HB3	1:C:298:TYR:CE2	2.52	0.45
1:B:206:ARG:HA	1:B:234:GLY:HA2	1.99	0.45
1:A:296:ASP:OD2	1:A:488:GLN:HG2	2.16	0.45
1:A:260:ALA:HB1	1:A:265:LEU:HB2	1.99	0.45
1:A:130:LEU:HD13	1:A:189:ILE:HD11	1.98	0.45
1:A:393:ARG:HG3	1:A:393:ARG:HH11	1.83	0.45
1:C:232:LEU:O	1:C:258:MET:HB3	2.17	0.45
1:A:144:GLN:HG2	1:A:164:ILE:HB	1.99	0.44
1:C:99:MET:HG2	1:C:147:TYR:CD1	2.52	0.44
1:C:232:LEU:HB3	1:C:258:MET:HE3	1.99	0.44
1:B:81:TRP:HB2	1:B:99:MET:HB2	1.99	0.44
1:B:186:ASP:HB2	1:B:238:PRO:HD2	2.00	0.44
1:D:230:HIS:C	1:D:232:LEU:H	2.25	0.44
1:A:70:LEU:HA	1:A:80:GLY:O	2.18	0.44
1:B:289:GLN:NE2	1:B:356:TRP:HZ3	2.15	0.44
1:C:138:VAL:HG12	1:C:140:LYS:HG2	2.00	0.44
1:A:83:HIS:CD2	1:A:84:ALA:N	2.86	0.44
1:C:432:LEU:HD22	1:C:432:LEU:HA	1.88	0.44
1:A:432:LEU:HD13	1:A:432:LEU:C	2.43	0.43
1:C:206:ARG:HH11	1:C:234:GLY:HA3	1.83	0.43
1:D:174:THR:O	1:D:178:ILE:HG13	2.18	0.43
1:A:432:LEU:HD22	1:A:432:LEU:HA	1.73	0.43
1:B:319:MET:HE1	1:B:473:SER:HB2	2.00	0.43
1:D:80:GLY:HA2	1:D:107:VAL:HB	2.00	0.43
1:B:98:VAL:HG22	1:B:156:PHE:CD1	2.51	0.43
1:B:368:THR:HG23	4:B:875:HOH:O	2.17	0.43
1:A:98:VAL:HG22	1:A:156:PHE:CD1	2.51	0.43
1:B:300:ALA:CB	1:B:317:ALA:HB2	2.49	0.43
1:D:204:ARG:HH21	2:M:1:FRU:H3	1.83	0.43
1:D:420:THR:HG23	1:D:421:ARG:HG3	1.99	0.43
1:B:379:ASP:HB3	1:B:510:THR:HG22	2.01	0.43
1:B:382:VAL:HG13	1:B:509:PHE:CD2	2.54	0.43
1:D:47:PRO:HD3	1:D:52:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:O	1:B:422:HIS:HB3	2.19	0.43
1:A:255:ALA:HB2	1:A:271:TYR:HB3	2.00	0.43
1:B:230:HIS:C	1:B:232:LEU:H	2.26	0.43
1:A:65:TYR:OH	1:A:306:ILE:HG22	2.18	0.43
1:A:228:PRO:HD3	1:A:286:LEU:HD13	2.01	0.43
1:A:252:TRP:HB2	1:A:274:GLY:O	2.18	0.43
1:C:408:ASN:HB3	1:C:503:ASP:HB3	2.01	0.42
1:B:65:TYR:OH	1:B:306:ILE:HG22	2.19	0.42
1:D:382:VAL:HG22	1:D:502:THR:HG23	2.01	0.42
1:B:434:VAL:HG11	1:B:487:GLN:CD	2.44	0.42
1:C:68:TYR:HA	1:C:82:ASP:O	2.19	0.42
1:B:320:ASN:HD22	1:B:321:ASN:H	1.67	0.42
1:A:295:TRP:H	1:A:487:GLN:HG3	1.85	0.42
1:C:331:THR:HA	1:C:334:SER:OG	2.20	0.42
1:D:195:ARG:HG3	1:D:195:ARG:HH11	1.84	0.42
1:A:316:ILE:HD11	1:A:341:ASN:HB3	2.00	0.42
1:B:434:VAL:HG11	1:B:487:GLN:NE2	2.35	0.42
1:D:110:GLY:HA3	1:D:130:LEU:O	2.20	0.42
1:C:362:THR:HG22	4:C:766:HOH:O	2.20	0.42
1:C:425:ILE:HD12	1:C:425:ILE:N	2.35	0.42
1:C:56:GLN:HB2	1:C:68:TYR:HB2	2.02	0.41
1:A:206:ARG:NH1	1:A:234:GLY:CA	2.81	0.41
1:B:370:TYR:HD2	1:B:519:GLN:HA	1.85	0.41
1:D:356:TRP:H	1:D:356:TRP:CD1	2.38	0.41
1:C:322:TRP:CZ2	2:I:1:FRU:H5	2.55	0.41
1:D:408:ASN:HD22	1:D:409:VAL:N	2.18	0.41
1:B:260:ALA:CB	1:B:265:LEU:HB2	2.51	0.41
1:B:470:ASP:HB3	4:B:746:HOH:O	2.21	0.41
1:C:285:ASP:HB3	4:C:851:HOH:O	2.20	0.41
1:D:174:THR:OG1	1:D:177:GLU:HG3	2.20	0.41
1:D:206:ARG:NH1	1:D:234:GLY:CA	2.81	0.41
1:B:269:TYR:HB2	4:B:724:HOH:O	2.19	0.41
1:B:178:ILE:O	1:B:182:GLU:HG3	2.21	0.41
1:B:322:TRP:CE3	1:B:325:ALA:HB3	2.56	0.41
1:B:390:TRP:HA	4:B:759:HOH:O	2.20	0.41
1:C:422:HIS:O	1:C:438:PRO:HB2	2.21	0.41
1:D:163:VAL:HG23	1:D:164:ILE:HG13	2.02	0.41
1:A:382:VAL:HG23	1:A:502:THR:HG23	2.03	0.41
1:B:118:ASN:HB2	1:B:124:ALA:CA	2.50	0.41
1:C:240:LEU:HA	1:C:253:VAL:O	2.21	0.41
1:C:296:ASP:HB3	1:C:319:MET:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASN:C	1:D:229:ASN:HD22	2.29	0.41
1:A:206:ARG:HA	1:A:234:GLY:HA2	2.03	0.40
1:A:229:ASN:C	1:A:229:ASN:HD22	2.29	0.40
1:A:310:GLU:OE2	1:A:310:GLU:HA	2.22	0.40
1:C:396:GLU:CD	1:C:466:ARG:HE	2.28	0.40
1:D:432:LEU:HD22	1:D:432:LEU:HA	1.91	0.40
1:A:519:GLN:HA	1:A:519:GLN:HE21	1.86	0.40
1:B:377:LEU:HA	1:B:378:PRO:HD3	1.95	0.40
1:C:133:GLN:NE2	1:C:147:TYR:OH	2.53	0.40
1:D:318:TRP:HA	1:D:341:ASN:HD22	1.86	0.40
1:D:183:TRP:CE3	1:D:205:LEU:HD13	2.56	0.40
1:A:257:SER:HA	1:A:268:THR:O	2.21	0.40
1:A:412:SER:OG	1:A:424:ASN:ND2	2.54	0.40
1:A:519:GLN:HE21	1:A:519:GLN:CA	2.35	0.40
1:D:101:LEU:HD12	1:D:106:PRO:HA	2.02	0.40
1:D:470:ASP:HB3	4:D:752:HOH:O	2.21	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	478/492 (97%)	448 (94%)	29 (6%)	1 (0%)	43	55
1	B	478/492 (97%)	446 (93%)	30 (6%)	2 (0%)	30	38
1	C	477/492 (97%)	452 (95%)	25 (5%)	0	100	100
1	D	476/492 (97%)	443 (93%)	33 (7%)	0	100	100
All	All	1909/1968 (97%)	1789 (94%)	117 (6%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	B	235	ILE
1	B	103	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/393 (97%)	377 (99%)	4 (1%)	68	82
1	B	381/393 (97%)	369 (97%)	12 (3%)	35	52
1	C	381/393 (97%)	374 (98%)	7 (2%)	51	70
1	D	380/393 (97%)	375 (99%)	5 (1%)	61	77
All	All	1523/1572 (97%)	1495 (98%)	28 (2%)	51	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	178	ILE
1	A	232	LEU
1	A	487	GLN
1	B	104	ASP
1	B	130	LEU
1	B	144	GLN
1	B	232	LEU
1	B	297	TRP
1	B	306	ILE
1	B	307	ASP
1	B	320	ASN
1	B	382	VAL
1	B	440	ASP
1	B	448	PRO
1	B	519	GLN
1	C	98	VAL
1	C	101	LEU
1	C	232	LEU

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Mol	Chain	Res	Type
1	C	250	ARG
1	C	297	TRP
1	C	382	VAL
1	C	487	GLN
1	D	232	LEU
1	D	250	ARG
1	D	382	VAL
1	D	446	LEU
1	D	487	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	75	ASN
1	A	133	GLN
1	A	229	ASN
1	A	340	GLN
1	A	391	ASN
1	A	424	ASN
1	A	479	ASN
1	A	519	GLN
1	B	62	HIS
1	B	94	HIS
1	B	133	GLN
1	B	144	GLN
1	B	229	ASN
1	B	289	GLN
1	B	320	ASN
1	B	341	ASN
1	B	408	ASN
1	B	488	GLN
1	C	75	ASN
1	C	133	GLN
1	C	144	GLN
1	C	224	ASN
1	C	282	HIS
1	C	341	ASN
1	C	391	ASN
1	C	408	ASN
1	C	422	HIS
1	C	424	ASN

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Mol	Chain	Res	Type
1	C	487	GLN
1	C	519	GLN
1	D	66	GLN
1	D	74	GLN
1	D	75	ASN
1	D	133	GLN
1	D	229	ASN
1	D	341	ASN
1	D	408	ASN
1	D	422	HIS
1	D	424	ASN
1	D	487	GLN
1	D	488	GLN
1	D	490	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 ⓘ

21 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	FRU	E	1	2	11,12,12	1.45	2 (18%)	10,18,18	1.21	1 (10%)
2	FRU	E	2	2	11,11,12	1.58	2 (18%)	15,15,18	1.29	3 (20%)
2	FRU	F	1	2	11,12,12	1.34	1 (9%)	10,18,18	0.87	0
2	FRU	F	2	2	11,11,12	1.45	1 (9%)	15,15,18	1.14	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRU	G	1	2	11,12,12	1.49	2 (18%)	10,18,18	1.12	1 (10%)
2	FRU	G	2	2	11,11,12	1.54	1 (9%)	15,15,18	1.40	3 (20%)
3	FRU	H	1	3	11,12,12	1.77	3 (27%)	10,18,18	1.18	0
3	FRU	H	2	3	11,11,12	1.41	2 (18%)	15,15,18	1.14	1 (6%)
3	FRU	H	3	3	11,11,12	1.36	1 (9%)	15,15,18	1.28	3 (20%)
2	FRU	I	1	2	11,12,12	1.18	2 (18%)	10,18,18	1.39	2 (20%)
2	FRU	I	2	2	11,11,12	1.56	2 (18%)	15,15,18	1.33	2 (13%)
2	FRU	J	1	2	11,12,12	1.58	3 (27%)	10,18,18	1.39	1 (10%)
2	FRU	J	2	2	11,11,12	1.44	1 (9%)	15,15,18	1.15	1 (6%)
2	FRU	K	1	2	11,12,12	1.58	4 (36%)	10,18,18	1.06	1 (10%)
2	FRU	K	2	2	11,11,12	1.62	1 (9%)	15,15,18	1.32	3 (20%)
2	FRU	L	1	2	11,12,12	1.19	1 (9%)	10,18,18	1.48	2 (20%)
2	FRU	L	2	2	11,11,12	1.62	2 (18%)	15,15,18	1.45	2 (13%)
2	FRU	M	1	2	11,12,12	1.66	2 (18%)	10,18,18	1.50	1 (10%)
2	FRU	M	2	2	11,11,12	1.55	1 (9%)	15,15,18	1.12	1 (6%)
2	FRU	N	1	2	11,12,12	1.51	2 (18%)	10,18,18	1.36	2 (20%)
2	FRU	N	2	2	11,11,12	1.46	1 (9%)	15,15,18	1.29	3 (20%)

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	FRU	E	1	2	-	2/5/24/24	0/1/1/1
2	FRU	E	2	2	-	0/4/20/24	0/1/1/1
2	FRU	F	1	2	-	2/5/24/24	0/1/1/1
2	FRU	F	2	2	-	2/4/20/24	0/1/1/1
2	FRU	G	1	2	-	5/5/24/24	0/1/1/1
2	FRU	G	2	2	-	2/4/20/24	0/1/1/1
3	FRU	H	1	3	-	2/5/24/24	0/1/1/1
3	FRU	H	2	3	-	2/4/20/24	0/1/1/1
3	FRU	H	3	3	-	2/4/20/24	0/1/1/1
2	FRU	I	1	2	-	0/5/24/24	0/1/1/1
2	FRU	I	2	2	-	0/4/20/24	0/1/1/1
2	FRU	J	1	2	-	1/5/24/24	0/1/1/1
2	FRU	J	2	2	-	1/4/20/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	K	1	2	-	2/5/24/24	0/1/1/1
2	FRU	K	2	2	-	2/4/20/24	0/1/1/1
2	FRU	L	1	2	-	0/5/24/24	0/1/1/1
2	FRU	L	2	2	-	2/4/20/24	0/1/1/1
2	FRU	M	1	2	-	1/5/24/24	0/1/1/1
2	FRU	M	2	2	-	1/4/20/24	0/1/1/1
2	FRU	N	1	2	-	2/5/24/24	0/1/1/1
2	FRU	N	2	2	-	4/4/20/24	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	FRU	C4-C3	-3.76	1.43	1.53
2	L	2	FRU	C4-C3	-3.58	1.43	1.53
2	M	2	FRU	C4-C3	-3.54	1.43	1.53
2	G	2	FRU	C4-C3	-3.52	1.43	1.53
2	E	2	FRU	C4-C3	-3.50	1.43	1.53
2	F	2	FRU	C4-C3	-3.40	1.44	1.53
2	I	2	FRU	C4-C3	-3.40	1.44	1.53
3	H	3	FRU	C4-C3	-3.28	1.44	1.53
2	N	2	FRU	C4-C3	-3.23	1.44	1.53
2	J	2	FRU	C4-C3	-3.22	1.44	1.53
2	M	1	FRU	O3-C3	-3.15	1.36	1.42
3	H	1	FRU	O4-C4	-3.12	1.35	1.43
3	H	1	FRU	O5-C2	-3.04	1.38	1.43
3	H	2	FRU	O4-C4	-2.97	1.35	1.43
3	H	1	FRU	C4-C3	-2.81	1.41	1.53
2	J	1	FRU	O3-C3	-2.74	1.37	1.42
2	N	1	FRU	O3-C3	-2.54	1.37	1.42
2	K	1	FRU	O3-C3	-2.49	1.37	1.42
2	G	1	FRU	O3-C3	-2.44	1.37	1.42
2	E	1	FRU	O3-C3	-2.44	1.37	1.42
2	N	1	FRU	C4-C3	-2.33	1.43	1.53
2	M	1	FRU	C4-C3	-2.32	1.43	1.53
2	K	1	FRU	C4-C3	-2.31	1.43	1.53
2	J	1	FRU	C4-C3	-2.18	1.44	1.53
3	H	2	FRU	C4-C3	-2.15	1.47	1.53
2	L	2	FRU	O3-C3	-2.12	1.37	1.43
2	I	1	FRU	C4-C3	-2.07	1.44	1.53
2	L	1	FRU	O3-C3	-2.07	1.38	1.42
2	E	1	FRU	C4-C3	-2.06	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	FRU	O2-C2	-2.06	1.37	1.40
2	I	2	FRU	O3-C3	-2.05	1.37	1.43
2	J	1	FRU	O2-C2	-2.04	1.37	1.40
2	G	1	FRU	C4-C5	-2.04	1.47	1.53
2	I	1	FRU	O3-C3	-2.03	1.38	1.42
2	K	1	FRU	O4-C4	-2.01	1.38	1.43
2	F	1	FRU	O3-C3	-2.00	1.38	1.42
2	E	2	FRU	O3-C3	-2.00	1.38	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	FRU	O1-C1-C2	3.48	119.38	111.67
2	L	2	FRU	O5-C5-C6	3.31	116.22	109.22
2	J	1	FRU	O1-C1-C2	3.23	118.82	111.67
2	L	1	FRU	O1-C1-C2	3.09	118.51	111.67
2	I	1	FRU	O1-C1-C2	3.08	118.48	111.67
2	I	2	FRU	O5-C5-C6	2.97	115.50	109.22
2	G	2	FRU	O6-C6-C5	2.79	120.82	111.33
3	H	3	FRU	O6-C6-C5	2.72	120.60	111.33
2	G	2	FRU	O5-C5-C6	2.67	114.86	109.22
2	J	2	FRU	O6-C6-C5	2.60	120.18	111.33
2	G	1	FRU	O1-C1-C2	2.59	117.41	111.67
2	K	2	FRU	O6-C6-C5	2.50	119.84	111.33
2	F	2	FRU	O1-C1-C2	2.49	119.83	111.33
2	K	2	FRU	O5-C5-C6	2.48	114.46	109.22
2	M	2	FRU	O6-C6-C5	2.47	119.75	111.33
2	K	2	FRU	C1-C2-C3	-2.37	109.50	115.10
2	N	1	FRU	O4-C4-C3	-2.33	105.17	112.16
2	N	2	FRU	C1-C2-C3	-2.33	109.61	115.10
2	N	2	FRU	O1-C1-C2	2.29	119.12	111.33
2	L	1	FRU	O4-C4-C3	-2.28	105.32	112.16
2	N	1	FRU	O6-C6-C5	2.28	119.08	111.33
2	G	2	FRU	O1-C1-C2	2.27	119.06	111.33
2	N	2	FRU	O6-C6-C5	2.25	118.98	111.33
2	F	2	FRU	O6-C6-C5	2.20	118.82	111.33
2	I	1	FRU	O4-C4-C3	-2.15	105.70	112.16
2	L	2	FRU	O1-C1-C2	2.14	118.62	111.33
2	K	1	FRU	O1-C1-C2	2.14	116.40	111.67
3	H	3	FRU	C3-C4-C5	2.12	106.71	102.61
3	H	2	FRU	O5-C2-C1	-2.12	104.73	109.22
2	E	1	FRU	O1-C1-C2	2.09	116.29	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	FRU	O6-C6-C5	2.05	118.30	111.33
3	H	3	FRU	O1-C1-C2	2.05	118.30	111.33
2	E	2	FRU	O1-C1-C2	2.04	118.28	111.33
2	E	2	FRU	O6-C6-C5	2.02	118.20	111.33
2	E	2	FRU	C1-C2-C3	-2.02	110.34	115.10

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	FRU	O1-C1-C2-C3
2	N	2	FRU	O5-C5-C6-O6
2	K	2	FRU	O1-C1-C2-O5
2	L	2	FRU	O1-C1-C2-O5
2	F	1	FRU	C4-C5-C6-O6
2	K	1	FRU	C4-C5-C6-O6
2	L	2	FRU	O1-C1-C2-C3
2	N	2	FRU	C4-C5-C6-O6
2	K	1	FRU	O5-C5-C6-O6
2	N	2	FRU	O1-C1-C2-O5
3	H	3	FRU	O5-C5-C6-O6
2	G	2	FRU	C4-C5-C6-O6
3	H	1	FRU	C4-C5-C6-O6
2	F	1	FRU	O5-C5-C6-O6
2	F	2	FRU	O1-C1-C2-O5
2	G	2	FRU	O5-C5-C6-O6
2	N	2	FRU	O1-C1-C2-C3
3	H	1	FRU	O5-C5-C6-O6
2	F	2	FRU	O1-C1-C2-C3
2	E	1	FRU	O5-C5-C6-O6
2	N	1	FRU	O5-C5-C6-O6
3	H	2	FRU	O5-C5-C6-O6
3	H	2	FRU	C4-C5-C6-O6
2	E	1	FRU	C4-C5-C6-O6
2	N	1	FRU	C4-C5-C6-O6
2	G	1	FRU	O5-C5-C6-O6
2	J	2	FRU	O1-C1-C2-O5
2	M	2	FRU	O1-C1-C2-O5
2	G	1	FRU	O1-C1-C2-O5
2	G	1	FRU	C4-C5-C6-O6
3	H	3	FRU	C4-C5-C6-O6
2	J	1	FRU	O5-C5-C6-O6

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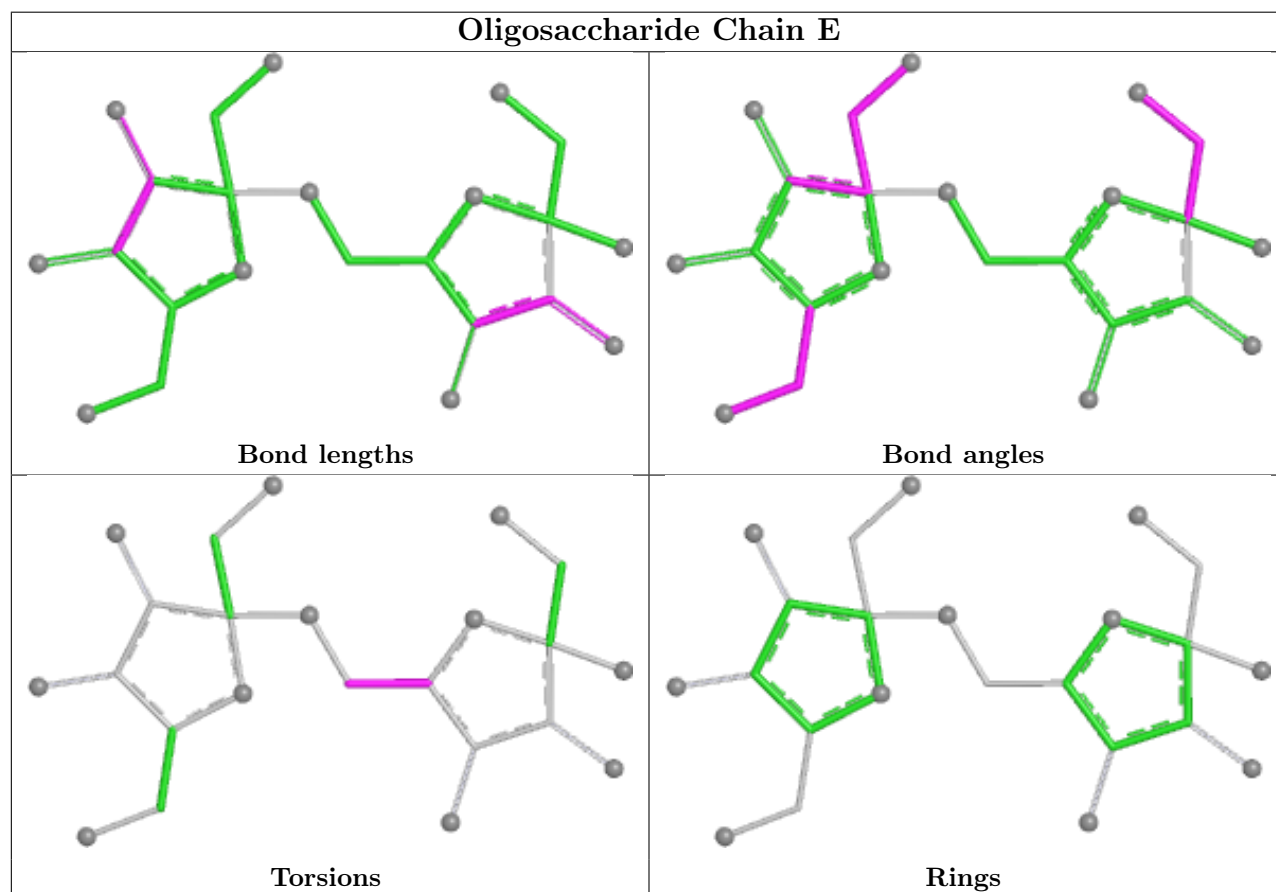
Mol	Chain	Res	Type	Atoms
2	M	1	FRU	O5-C5-C6-O6
2	G	1	FRU	O1-C1-C2-O2
2	G	1	FRU	O1-C1-C2-C3

There are no ring outliers.

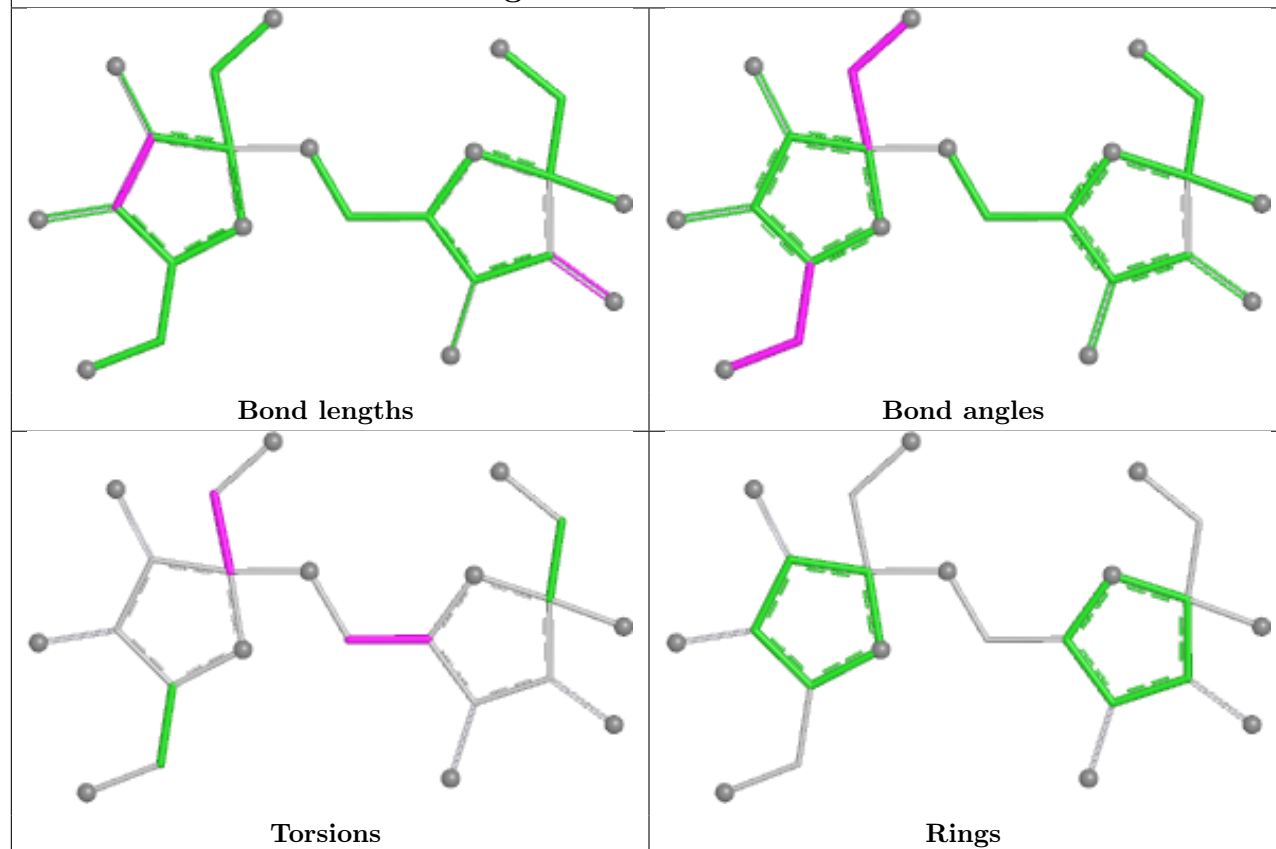
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	FRU	3	0
2	M	2	FRU	2	0
2	E	1	FRU	1	0
2	I	1	FRU	1	0
2	G	1	FRU	2	0
2	E	2	FRU	1	0

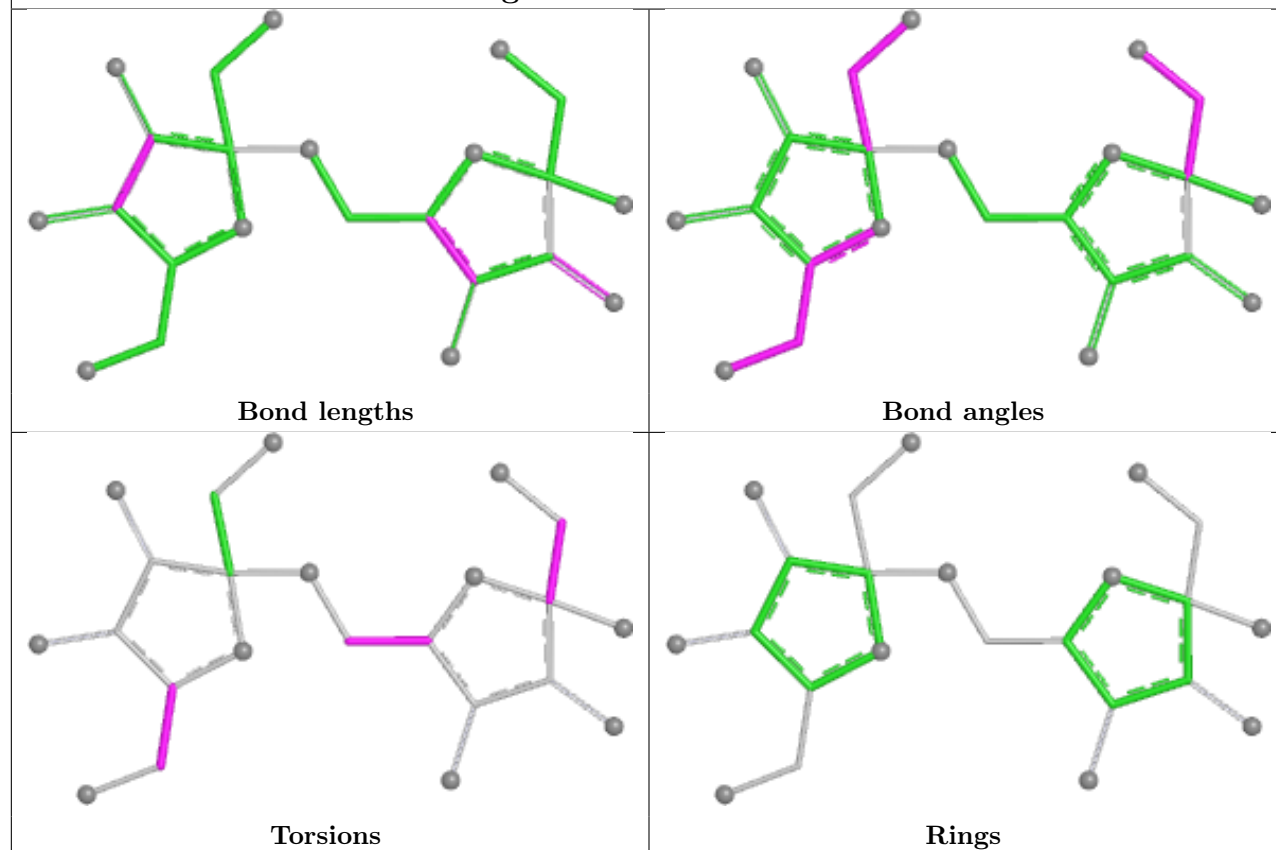
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

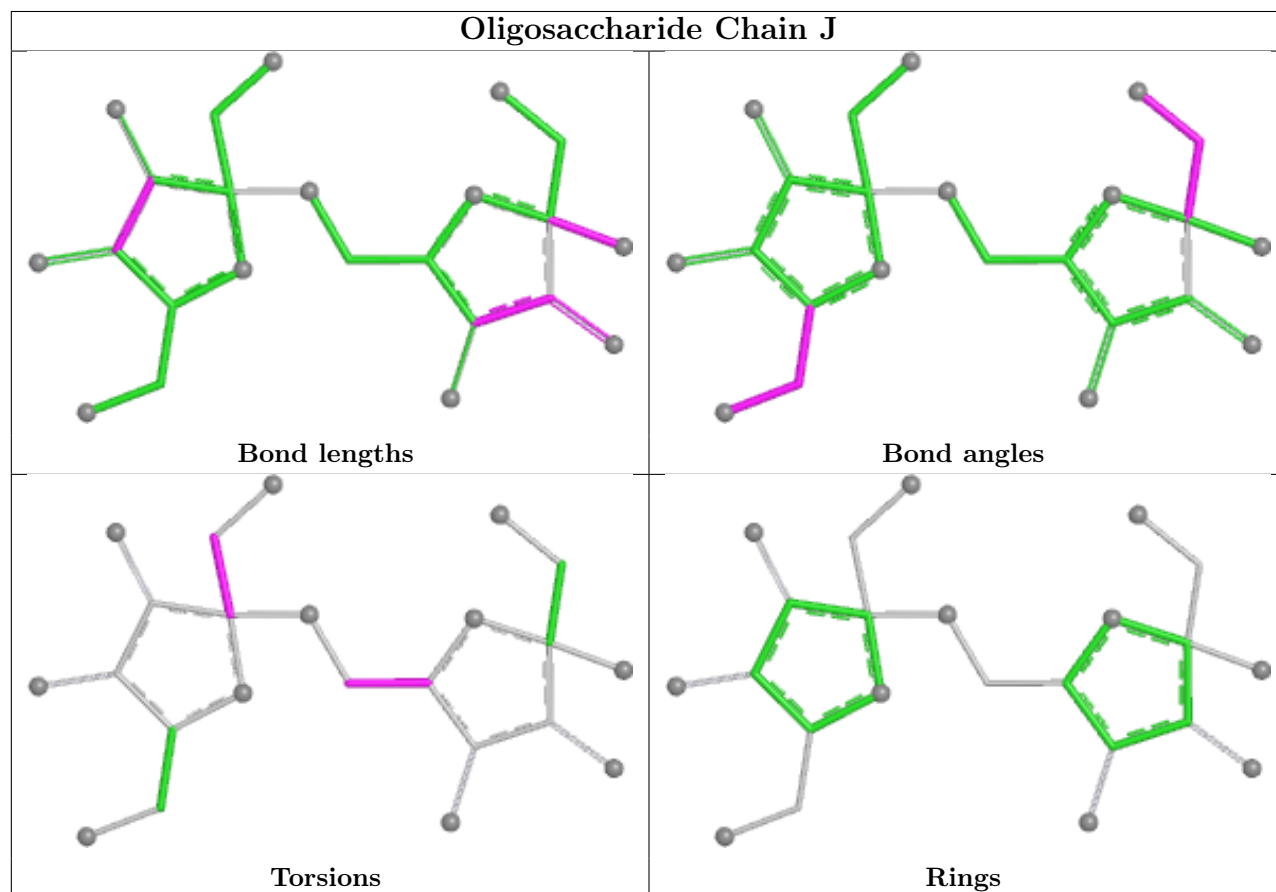
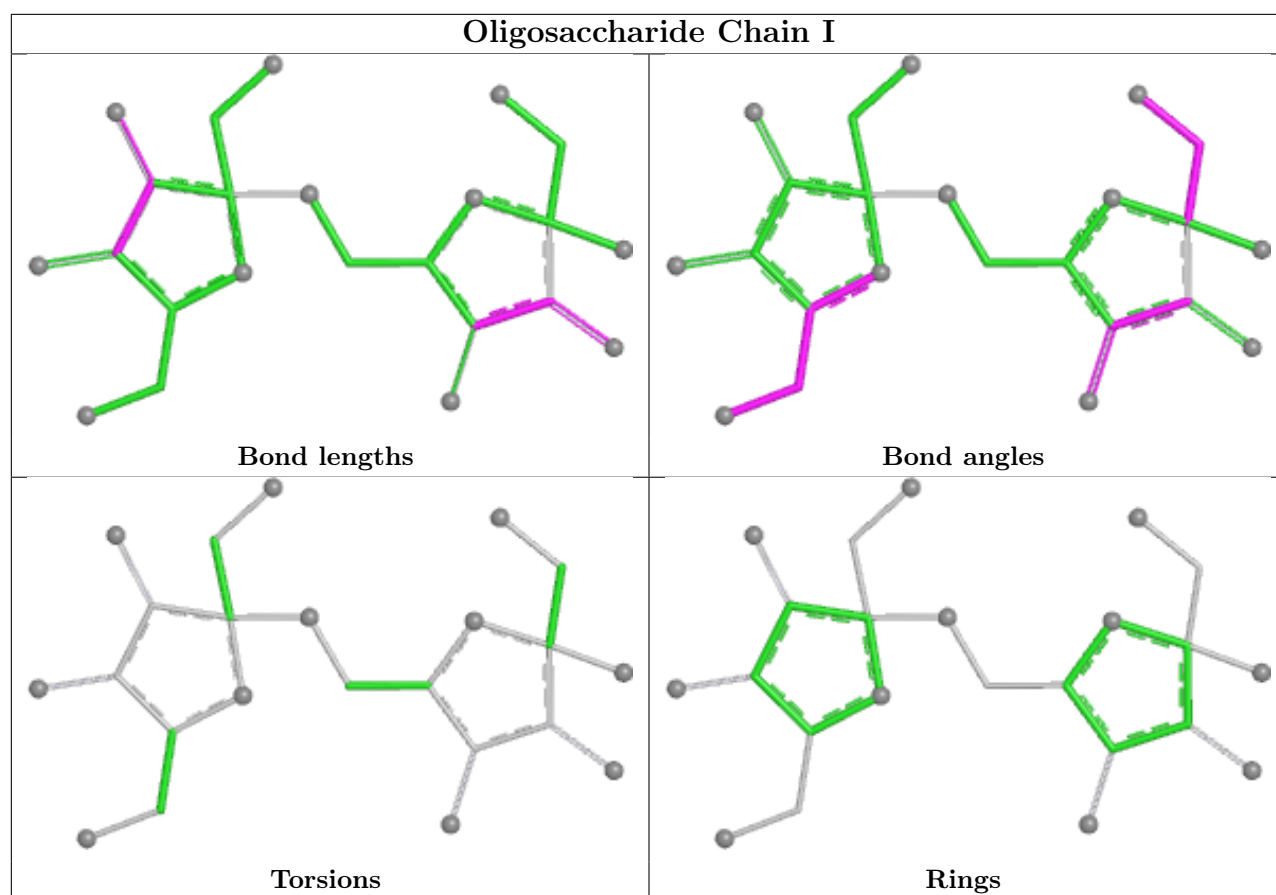


Oligosaccharide Chain F

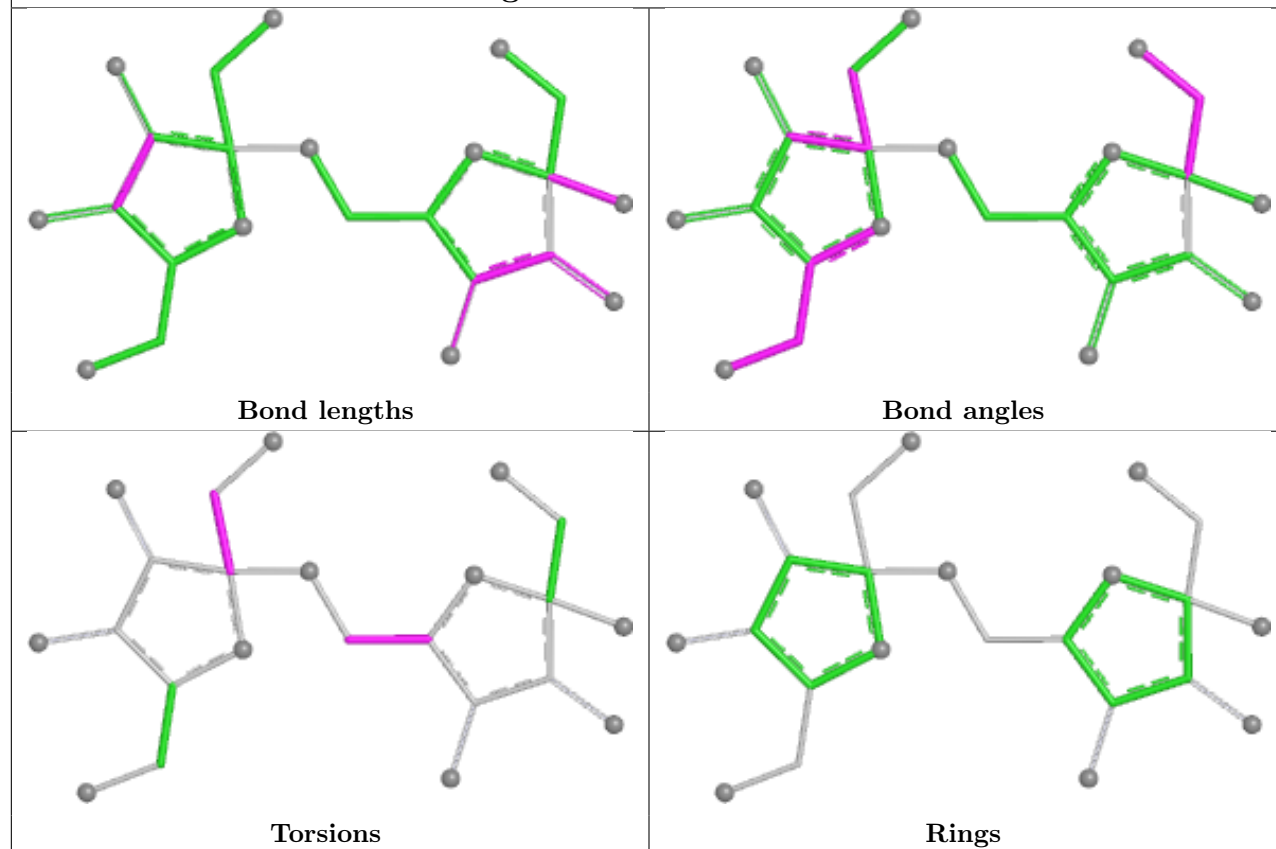


Oligosaccharide Chain G

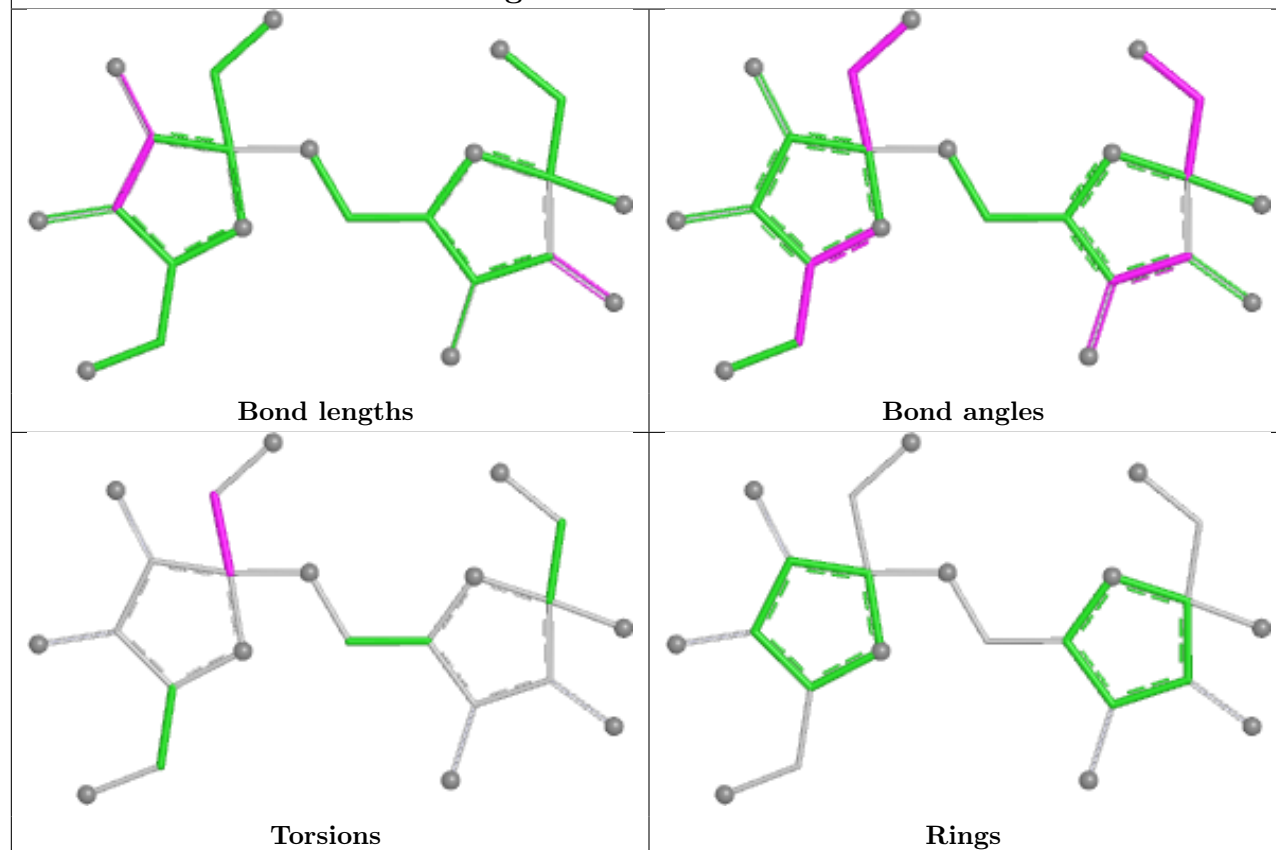




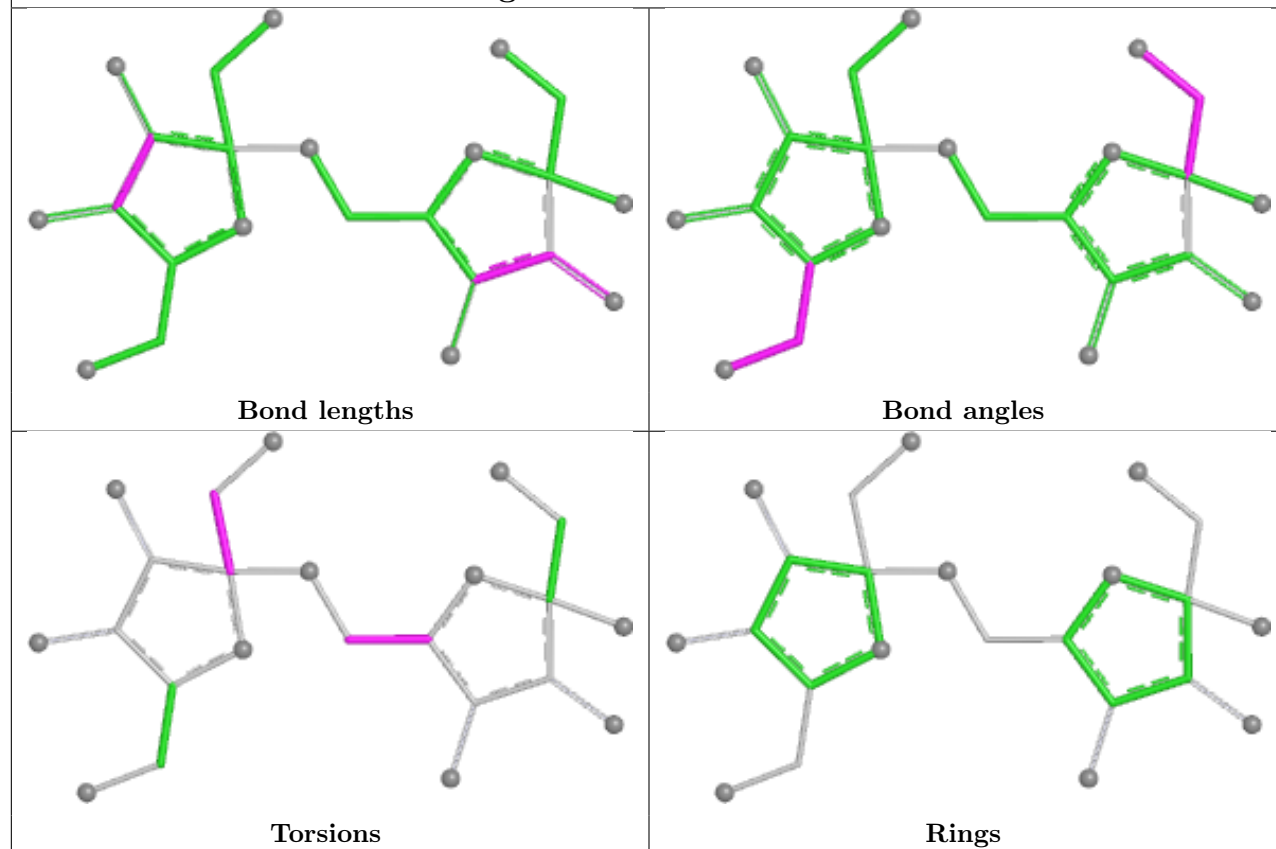
Oligosaccharide Chain K



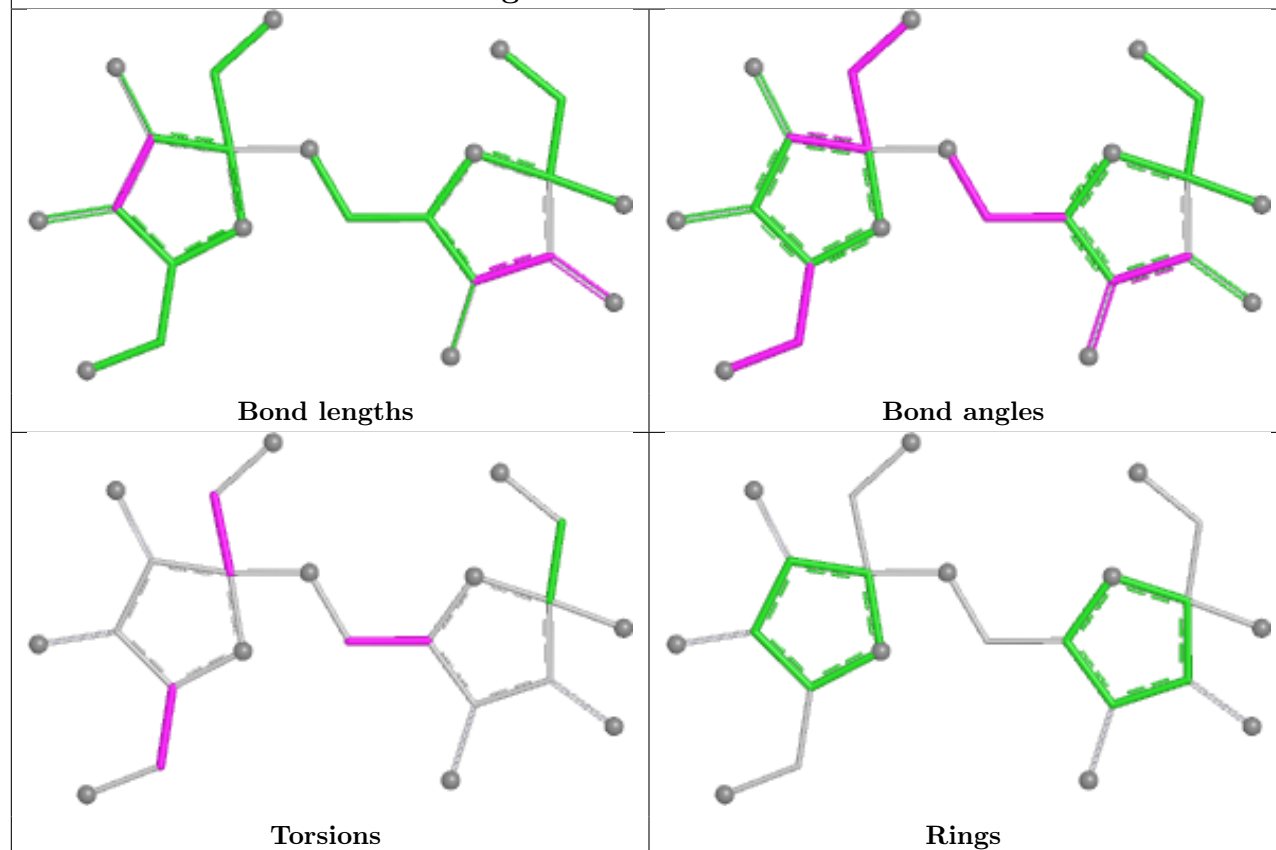
Oligosaccharide Chain L

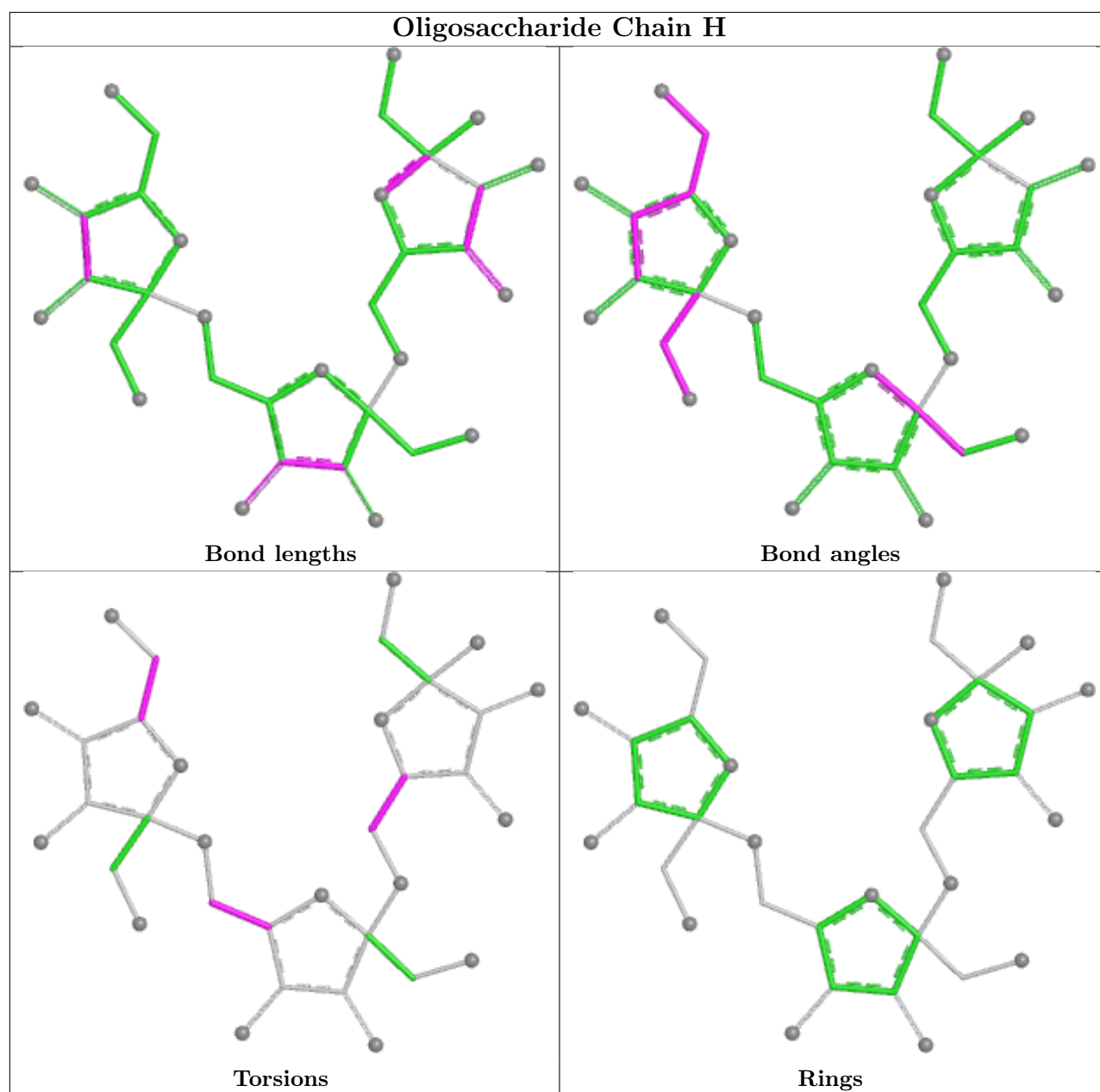


Oligosaccharide Chain M



Oligosaccharide Chain N





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 ⓘ

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	480/492 (97%)	-0.06	7 (1%) 72 73	11, 23, 37, 55	0
1	B	480/492 (97%)	-0.13	8 (1%) 69 70	12, 22, 36, 58	0
1	C	479/492 (97%)	-0.21	4 (0%) 82 83	9, 20, 29, 48	0
1	D	478/492 (97%)	-0.15	3 (0%) 85 86	8, 21, 33, 42	0
All	All	1917/1968 (97%)	-0.14	22 (1%) 78 79	8, 21, 34, 58	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	GLY	6.9
1	B	520	ALA	5.1
1	D	234	GLY	5.1
1	A	520	ALA	5.0
1	A	234	GLY	4.3
1	B	234	GLY	4.1
1	B	519	GLN	4.0
1	C	519	GLN	3.4
1	A	172	ALA	3.1
1	A	171	ALA	3.0
1	D	518	GLY	2.6
1	B	173	THR	2.6
1	B	171	ALA	2.5
1	B	307	ASP	2.4
1	C	279	GLU	2.4
1	B	518	GLY	2.4
1	B	223	ARG	2.4
1	A	104	ASP	2.3
1	A	173	THR	2.3
1	A	176	ALA	2.3
1	D	508	HIS	2.1
1	C	74	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

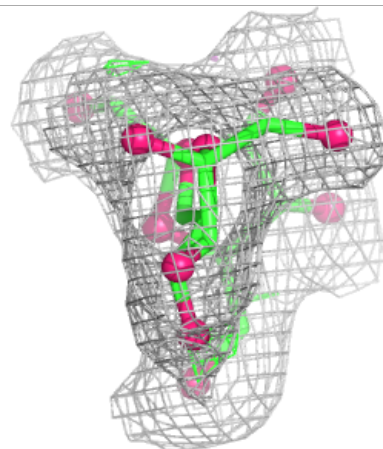
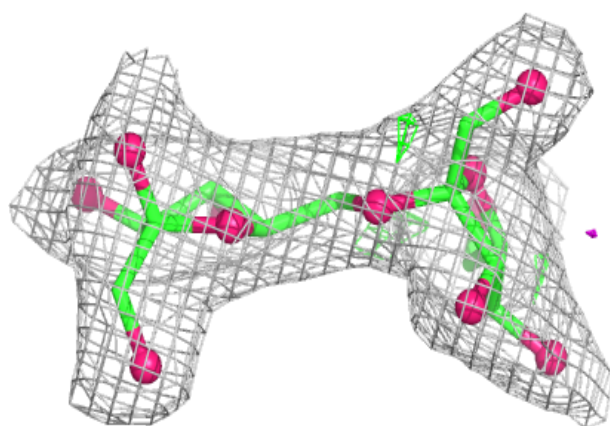
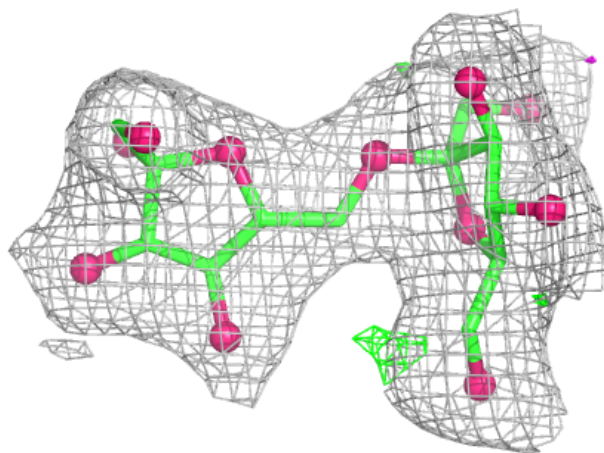
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	L	1	12/12	0.74	0.25	59,62,63,64	0
2	FRU	K	2	11/12	0.81	0.17	42,43,44,45	0
2	FRU	F	2	11/12	0.82	0.15	37,39,41,43	0
2	FRU	I	1	12/12	0.84	0.17	46,49,49,50	0
2	FRU	L	2	11/12	0.84	0.19	54,58,60,60	0
2	FRU	E	2	11/12	0.90	0.10	34,34,36,37	0
2	FRU	G	2	11/12	0.90	0.11	33,35,35,40	0
2	FRU	F	1	12/12	0.90	0.11	23,28,32,37	0
2	FRU	N	2	11/12	0.90	0.10	30,31,33,35	0
3	FRU	H	2	11/12	0.90	0.10	33,34,35,36	0
2	FRU	G	1	12/12	0.91	0.09	34,35,36,38	0
3	FRU	H	3	11/12	0.91	0.11	33,38,41,43	0
2	FRU	M	2	11/12	0.92	0.09	26,30,34,35	0
2	FRU	I	2	11/12	0.92	0.12	45,48,49,49	0
2	FRU	J	2	11/12	0.93	0.08	28,30,31,34	0
2	FRU	E	1	12/12	0.94	0.08	24,30,32,32	0
2	FRU	M	1	12/12	0.94	0.09	21,23,25,27	0
2	FRU	J	1	12/12	0.95	0.08	21,23,26,28	0
3	FRU	H	1	12/12	0.95	0.08	18,21,26,30	0
2	FRU	K	1	12/12	0.96	0.08	25,29,34,39	0
2	FRU	N	1	12/12	0.96	0.06	19,22,24,27	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.

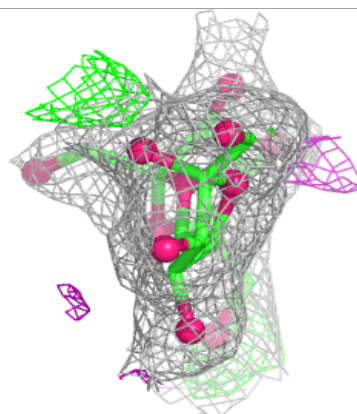
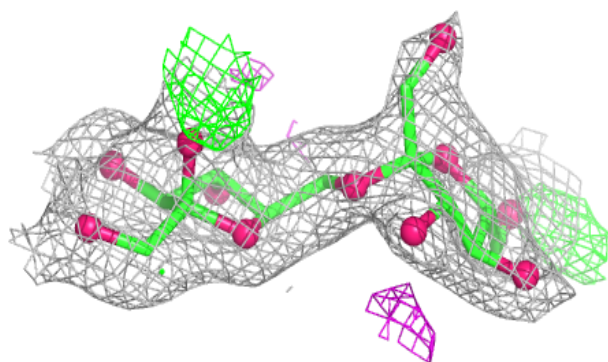
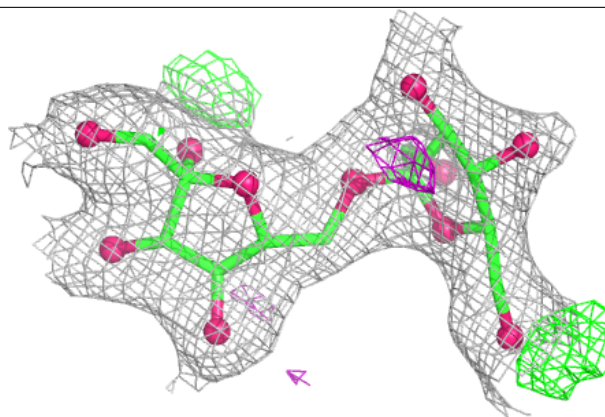
Electron density around Chain E:

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



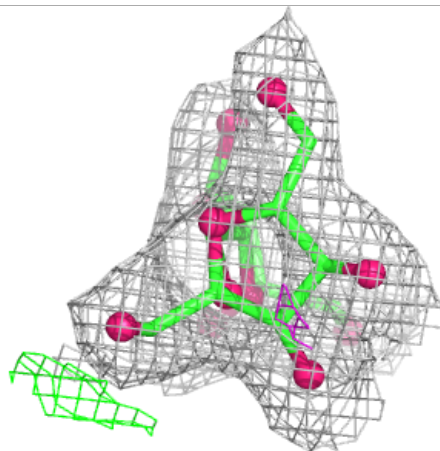
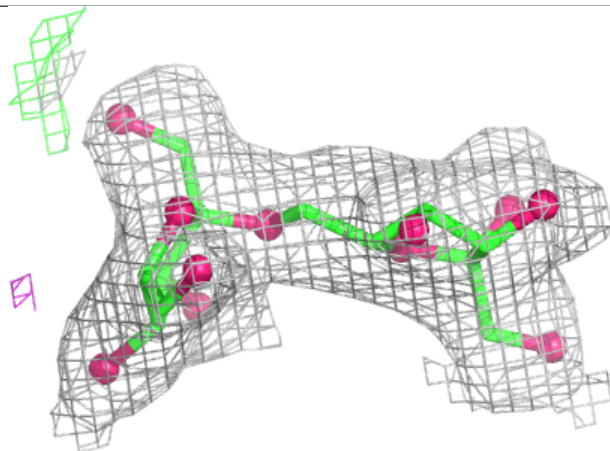
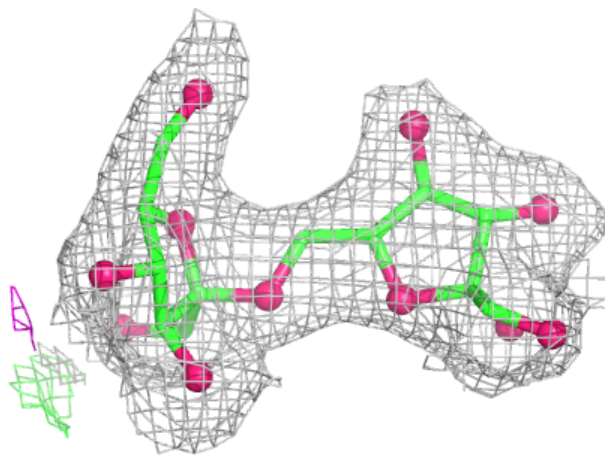
Electron density around Chain F:

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



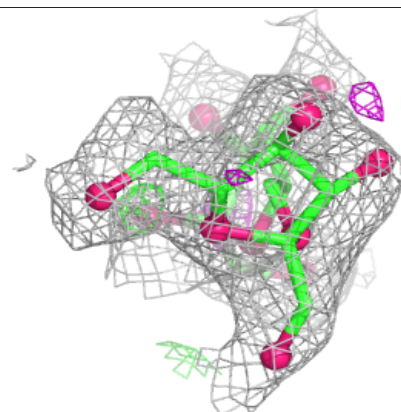
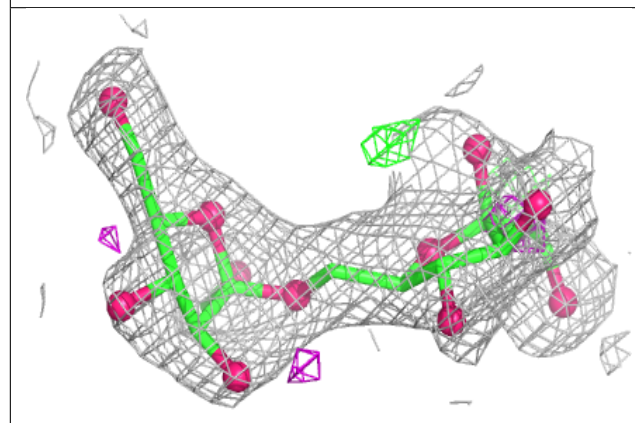
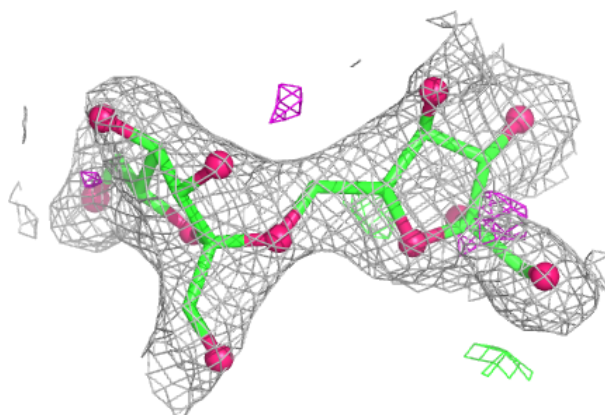
Electron density around Chain G:

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



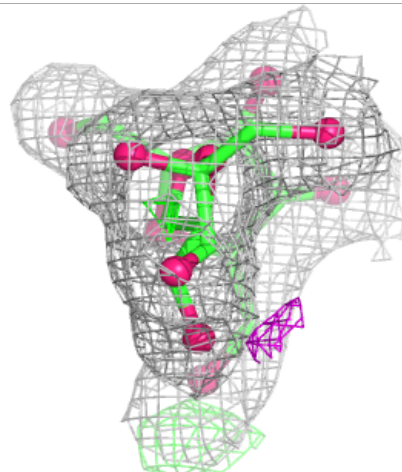
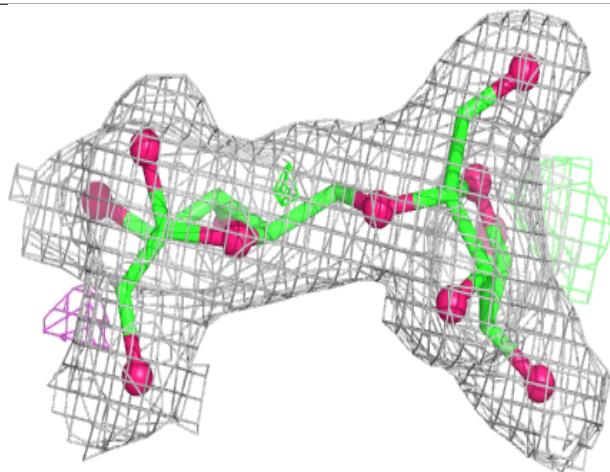
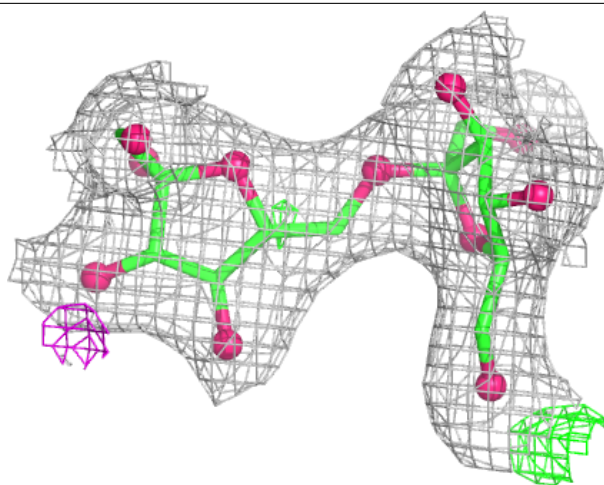
Electron density around Chain I:

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



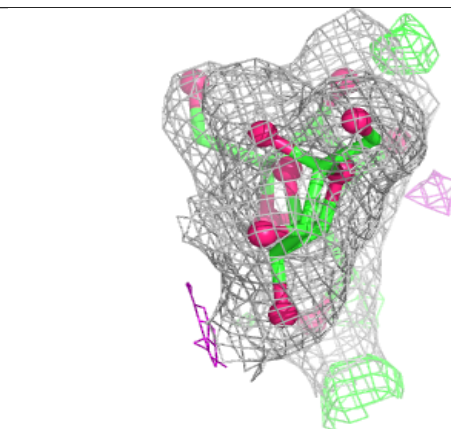
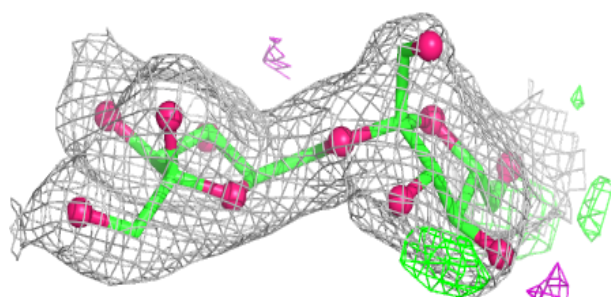
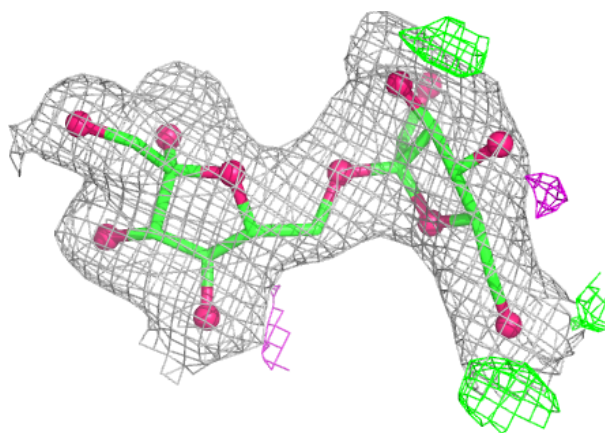
Electron density around Chain J:

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

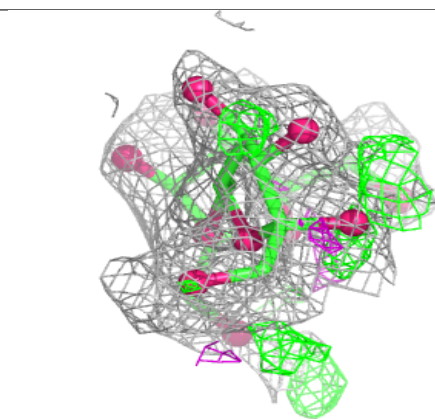
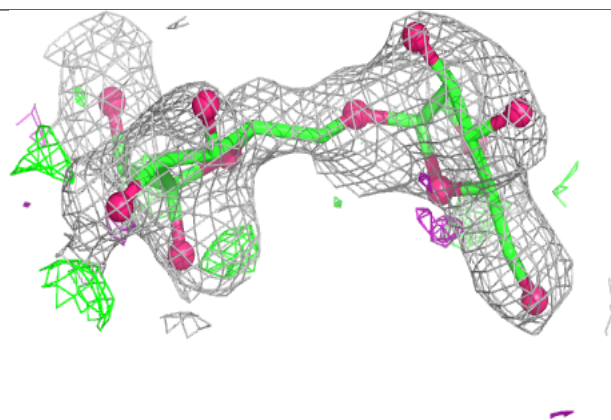
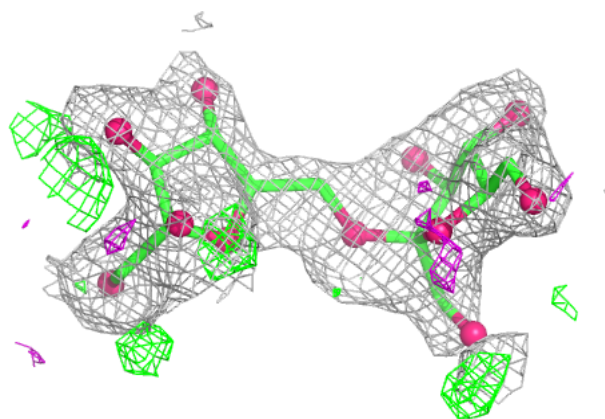


Electron density around Chain K:

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

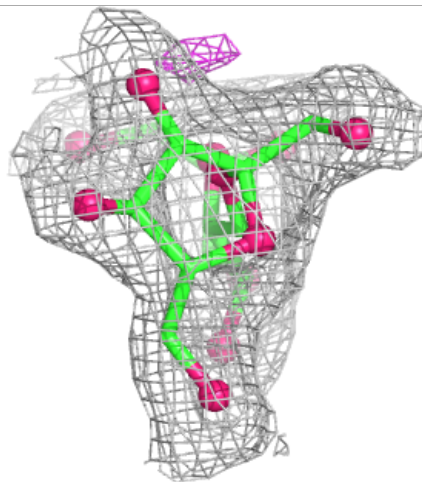
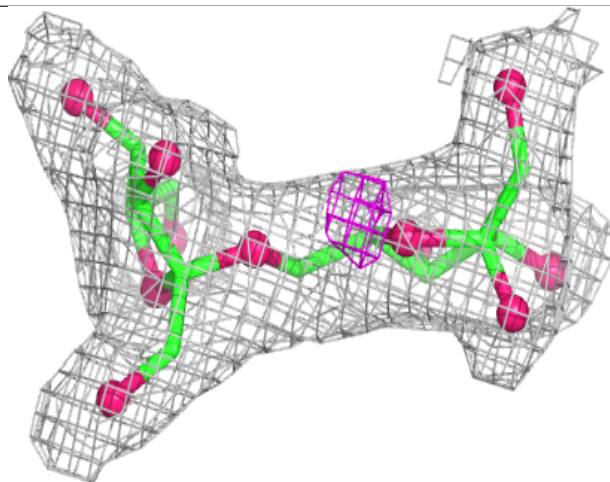
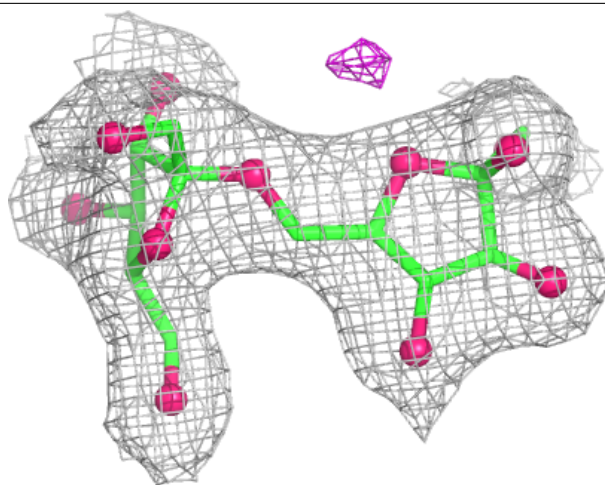
**Electron density around Chain L:**

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



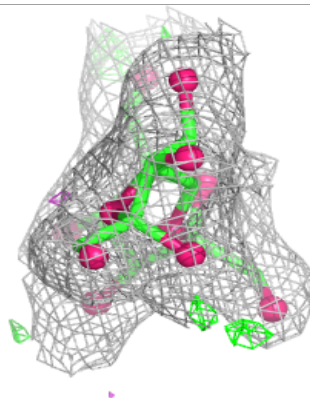
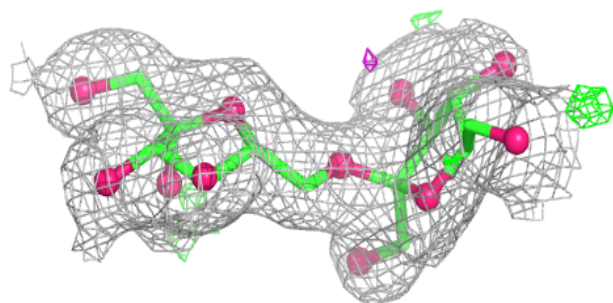
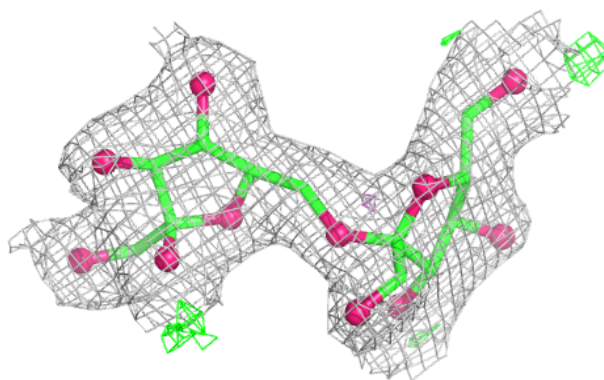
Electron density around Chain M:

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

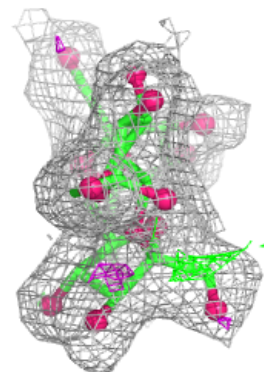
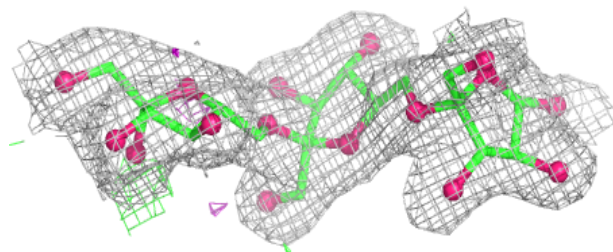
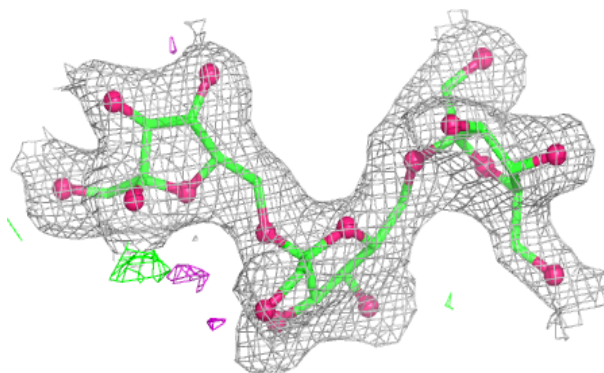


Electron density around Chain N:

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

**Electron density around Chain H:**

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.